



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 01:44 AM EST

PDB ID : 7KUX
EMDB ID : EMD-23040
Title : The Structure of the moss PSI-LHCI reveals the evolution of the LHCI antenna
Authors : Riddle, R.; Gorski, C.; Toporik, H.; Dobson, Z.; Da, Z.; Williams, D.; Mazor, Y.
Deposited on : 2020-11-25
Resolution : 2.80 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.dev113 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

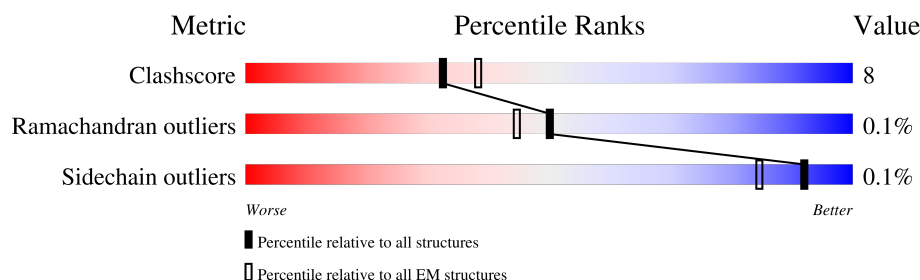
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 | A | 742 | |
| 2 | B | 732 | |
| 3 | 1 | 192 | |
| 4 | 2 | 203 | |
| 5 | 3 | 218 | |
| 6 | 4 | 203 | |
| 7 | C | 80 | |
| 8 | D | 142 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9 | E | 63 | |
| 10 | F | 160 | |
| 11 | G | 91 | |
| 12 | H | 87 | |
| 13 | I | 34 | |
| 14 | J | 41 | |
| 15 | K | 81 | |
| 16 | L | 160 | |
| 17 | M | 30 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 18 | CL0 | A | 1011 | X | - | - | - |
| 19 | CLA | 1 | 602 | X | - | - | - |
| 19 | CLA | 1 | 603 | X | - | - | - |
| 19 | CLA | 1 | 604 | X | - | - | - |
| 19 | CLA | 1 | 606 | X | - | - | - |
| 19 | CLA | 1 | 608 | X | - | - | - |
| 19 | CLA | 1 | 609 | X | - | - | - |
| 19 | CLA | 1 | 610 | X | - | - | - |
| 19 | CLA | 1 | 612 | X | - | - | - |
| 19 | CLA | 1 | 613 | X | - | - | - |
| 19 | CLA | 1 | 614 | X | - | - | - |
| 19 | CLA | 1 | 615 | X | - | - | - |
| 19 | CLA | 2 | 603 | X | - | - | - |
| 19 | CLA | 2 | 604 | X | - | - | - |
| 19 | CLA | 2 | 609 | X | - | - | - |
| 19 | CLA | 2 | 610 | X | - | - | - |
| 19 | CLA | 2 | 612 | X | - | - | - |
| 19 | CLA | 2 | 613 | X | - | - | - |
| 19 | CLA | 2 | 614 | X | - | - | - |
| 19 | CLA | 3 | 602 | X | - | - | - |
| 19 | CLA | 3 | 604 | X | - | - | - |
| 19 | CLA | 3 | 605 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 19 | CLA | 3 | 606 | X | - | - | - |
| 19 | CLA | 3 | 607 | X | - | - | - |
| 19 | CLA | 3 | 609 | X | - | - | - |
| 19 | CLA | 3 | 610 | X | - | - | - |
| 19 | CLA | 3 | 611 | X | - | - | - |
| 19 | CLA | 3 | 612 | X | - | - | - |
| 19 | CLA | 3 | 613 | X | - | - | - |
| 19 | CLA | 3 | 614 | X | - | - | - |
| 19 | CLA | 3 | 617 | X | - | - | - |
| 19 | CLA | 4 | 601 | X | - | - | - |
| 19 | CLA | 4 | 602 | X | - | - | - |
| 19 | CLA | 4 | 603 | X | - | - | - |
| 19 | CLA | 4 | 604 | X | - | - | - |
| 19 | CLA | 4 | 609 | X | - | - | - |
| 19 | CLA | 4 | 610 | X | - | - | - |
| 19 | CLA | 4 | 612 | X | - | - | - |
| 19 | CLA | 4 | 613 | X | - | - | - |
| 19 | CLA | 4 | 614 | X | - | - | - |
| 19 | CLA | A | 1022 | X | - | - | - |
| 19 | CLA | A | 1101 | X | - | - | - |
| 19 | CLA | A | 1103 | X | - | - | - |
| 19 | CLA | A | 1105 | X | - | - | - |
| 19 | CLA | A | 1106 | X | - | - | - |
| 19 | CLA | A | 1108 | X | - | - | - |
| 19 | CLA | A | 1109 | X | - | - | - |
| 19 | CLA | A | 1110 | X | - | - | - |
| 19 | CLA | A | 1114 | X | - | - | - |
| 19 | CLA | A | 1116 | X | - | - | - |
| 19 | CLA | A | 1117 | X | - | - | - |
| 19 | CLA | A | 1119 | X | - | - | - |
| 19 | CLA | A | 1121 | X | - | - | - |
| 19 | CLA | A | 1122 | X | - | - | - |
| 19 | CLA | A | 1125 | X | - | - | - |
| 19 | CLA | A | 1131 | X | - | - | - |
| 19 | CLA | A | 1132 | X | - | - | - |
| 19 | CLA | A | 1136 | X | - | - | - |
| 19 | CLA | A | 1137 | X | - | - | - |
| 19 | CLA | A | 1138 | X | - | - | - |
| 19 | CLA | A | 1139 | X | - | - | - |
| 19 | CLA | A | 1801 | X | - | - | - |
| 19 | CLA | B | 1012 | X | - | - | - |
| 19 | CLA | B | 1021 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 19 | CLA | B | 1201 | X | - | - | - |
| 19 | CLA | B | 1202 | X | - | - | - |
| 19 | CLA | B | 1203 | X | - | - | - |
| 19 | CLA | B | 1204 | X | - | - | - |
| 19 | CLA | B | 1205 | X | - | - | - |
| 19 | CLA | B | 1208 | X | - | - | - |
| 19 | CLA | B | 1210 | X | - | - | - |
| 19 | CLA | B | 1211 | X | - | - | - |
| 19 | CLA | B | 1215 | X | - | - | - |
| 19 | CLA | B | 1216 | X | - | - | - |
| 19 | CLA | B | 1220 | X | - | - | - |
| 19 | CLA | B | 1222 | X | - | - | - |
| 19 | CLA | B | 1223 | X | - | - | - |
| 19 | CLA | B | 1224 | X | - | - | - |
| 19 | CLA | B | 1226 | X | - | - | - |
| 19 | CLA | B | 1228 | X | - | - | - |
| 19 | CLA | B | 1229 | X | - | - | - |
| 19 | CLA | B | 1230 | X | - | - | - |
| 19 | CLA | B | 1232 | X | - | - | - |
| 19 | CLA | B | 1234 | X | - | - | - |
| 19 | CLA | B | 1235 | X | - | - | - |
| 19 | CLA | B | 1237 | X | - | - | - |
| 19 | CLA | B | 1238 | X | - | - | - |
| 19 | CLA | B | 1240 | X | - | - | - |
| 19 | CLA | F | 301 | X | - | - | - |
| 19 | CLA | F | 302 | X | - | - | - |
| 19 | CLA | F | 303 | X | - | - | - |
| 19 | CLA | G | 201 | X | - | - | - |
| 19 | CLA | G | 202 | X | - | - | - |
| 19 | CLA | H | 200 | X | - | - | - |
| 19 | CLA | J | 102 | X | - | - | - |
| 19 | CLA | K | 201 | X | - | - | - |
| 19 | CLA | K | 202 | X | - | - | - |
| 19 | CLA | K | 203 | X | - | - | - |
| 19 | CLA | K | 204 | X | - | - | - |
| 19 | CLA | L | 303 | X | - | - | - |
| 27 | CHL | 1 | 601 | X | - | - | - |
| 27 | CHL | 1 | 607 | X | - | - | - |
| 27 | CHL | 2 | 601 | X | - | - | - |
| 27 | CHL | 2 | 602 | X | - | - | - |
| 27 | CHL | 2 | 606 | X | - | - | - |
| 27 | CHL | 2 | 607 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 27 | CHL | 2 | 608 | X | - | - | - |
| 27 | CHL | 2 | 611 | X | - | - | - |
| 27 | CHL | 2 | 615 | X | - | - | - |
| 27 | CHL | 3 | 608 | X | - | - | - |
| 27 | CHL | 4 | 606 | X | - | - | - |
| 27 | CHL | 4 | 607 | X | - | - | - |
| 27 | CHL | 4 | 608 | X | - | - | - |
| 27 | CHL | 4 | 615 | X | - | - | - |
| 28 | LUT | 2 | 623 | X | - | - | - |
| 28 | LUT | 4 | 623 | X | - | - | - |

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 35803 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 742 | Total | C | N | O | S | 0 | 0 |
| | | | 5837 | 3827 | 993 | 998 | 19 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | B | 732 | Total | C | N | O | S | 0 | 0 |
| | | | 5845 | 3836 | 995 | 998 | 16 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | 1 | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1473 | 961 | 247 | 264 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | 2 | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1567 | 1021 | 262 | 280 | 4 | | |

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | 3 | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1678 | 1099 | 272 | 300 | 7 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | 4 | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1574 | 1024 | 264 | 281 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7 | C | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 596 | 365 | 103 | 117 | 11 | | |

- Molecule 8 is a protein called PsuD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | D | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1109 | 711 | 195 | 200 | 3 | | |

- Molecule 9 is a protein called PsuE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 9 | E | 63 | Total | C | N | O | 0 | 0 |
| | | | 500 | 317 | 89 | 94 | | |

- Molecule 10 is a protein called PSI-F.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | F | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1239 | 801 | 215 | 220 | 3 | | |

- Molecule 11 is a protein called PSI-G.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 11 | G | 91 | Total | C | N | O | 0 | 0 |
| | | | 689 | 444 | 119 | 126 | | |

- Molecule 12 is a protein called PsuH.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | H | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 659 | 418 | 114 | 126 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13 | I | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 266 | 181 | 35 | 48 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14 | J | 41 | Total | C | N | O | S | 0 | 0 |
| | | | 325 | 222 | 48 | 54 | 1 | | |

- Molecule 15 is a protein called PsaK.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 15 | K | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 561 | 352 | 97 | 108 | 4 | | |

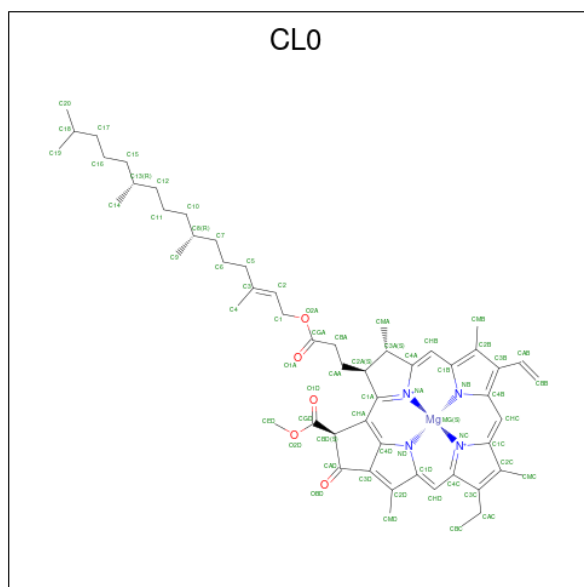
- Molecule 16 is a protein called PSI subunit V.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | L | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1171 | 771 | 188 | 210 | 2 | | |

- Molecule 17 is a protein called Photosystem I reaction center subunit XII.

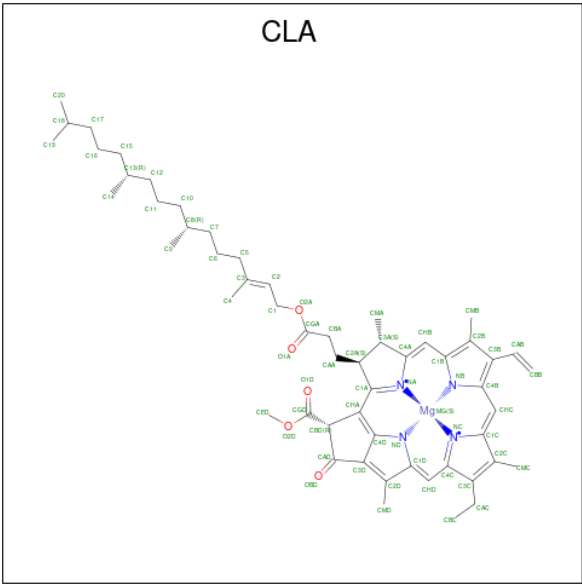
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 17 | M | 30 | Total | C | N | O | | 0 | 0 |
| | | | 223 | 146 | 36 | 41 | | | |

- Molecule 18 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 19 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 19 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 54 | C 44 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 54 | C 44 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 51 | C 41 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 57 | C 47 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 19 | A | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 51 | C 41 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 51 | C 41 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 19 | A | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 61 | C 51 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 61 | C 51 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 47 | C 37 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 59 | 49 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 49 | 39 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 19 | B | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 51 | C 41 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 47 | C 37 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 46 | C 36 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 46 | C 36 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 46 | C 36 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 1 | 1 | Total 46 | C 36 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 2 | 1 | Total 46 | C 36 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 19 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 19 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 19 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 19 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 19 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | | 0 |
| | | | 27 | 22 | 1 | 4 | | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 48 | 38 | 1 | 4 | 5 | |
| 19 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | |
| 19 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 19 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | |

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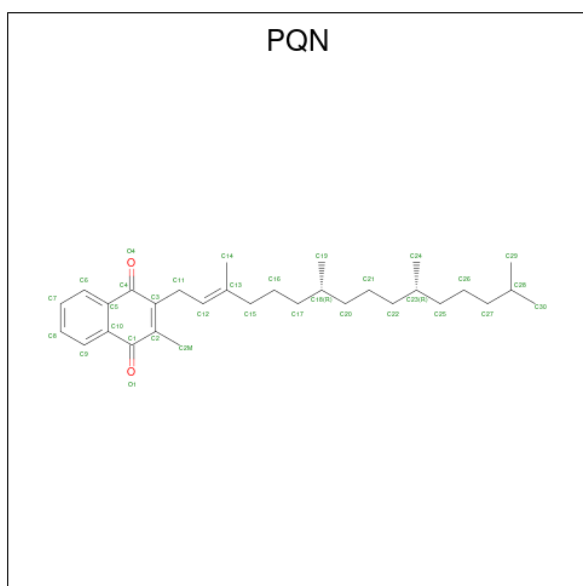
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 19 | 4 | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 4 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 4 | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 4 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 4 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 4 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 4 | 1 | Total 46 | C 36 | Mg 1 | N 4 | O 5 | 0 |
| 19 | 4 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | F | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | F | 1 | Total 46 | C 36 | Mg 1 | N 4 | O 5 | 0 |
| 19 | F | 1 | Total 27 | C 22 | Mg 1 | N 4 | | 0 |
| 19 | G | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | G | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 19 | G | 1 | Total 46 | C 36 | Mg 1 | N 4 | O 5 | 0 |
| 19 | H | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | I | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 19 | J | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 19 | K | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 19 | K | 1 | Total 46 | C 36 | Mg 1 | N 4 | O 5 | 0 |
| 19 | K | 1 | Total 27 | C 22 | Mg 1 | N 4 | | 0 |
| 19 | K | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |

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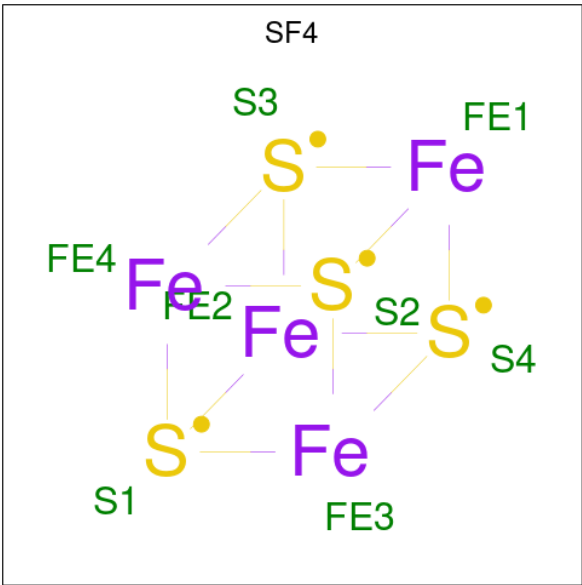
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 19 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 19 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



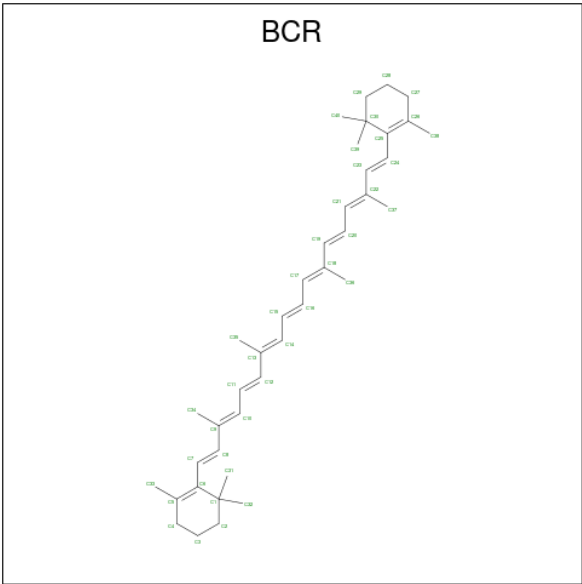
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 20 | A | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 20 | B | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 21 | A | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 21 | C | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 21 | C | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



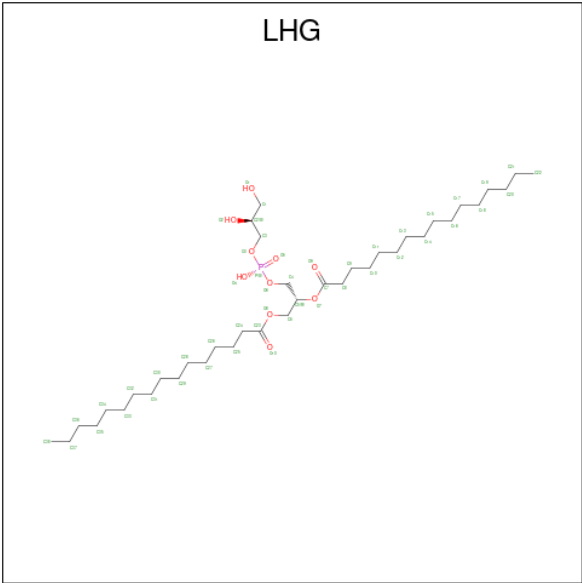
| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 22 | A | 1 | Total C 40 40 | 0 |
| 22 | A | 1 | Total C 40 40 | 0 |
| 22 | A | 1 | Total C 40 40 | 0 |
| 22 | A | 1 | Total C 40 40 | 0 |
| 22 | A | 1 | Total C 40 40 | 0 |
| 22 | A | 1 | Total C 40 40 | 0 |
| 22 | B | 1 | Total C 40 40 | 0 |
| 22 | B | 1 | Total C 40 40 | 0 |
| 22 | B | 1 | Total C 40 40 | 0 |
| 22 | B | 1 | Total C 40 40 | 0 |
| 22 | B | 1 | Total C 40 40 | 0 |
| 22 | B | 1 | Total C 40 40 | 0 |
| 22 | B | 1 | Total C 40 40 | 0 |
| 22 | B | 1 | Total C 40 40 | 0 |
| 22 | 1 | 1 | Total C 25 25 | 0 |
| 22 | 3 | 1 | Total C 40 40 | 0 |
| 22 | 3 | 1 | Total C 40 40 | 0 |
| 22 | F | 1 | Total C 40 40 | 0 |
| 22 | G | 1 | Total C 40 40 | 0 |
| 22 | I | 1 | Total C 40 40 | 0 |
| 22 | I | 1 | Total C 40 40 | 0 |
| 22 | J | 1 | Total C 40 40 | 0 |
| 22 | J | 1 | Total C 40 40 | 0 |

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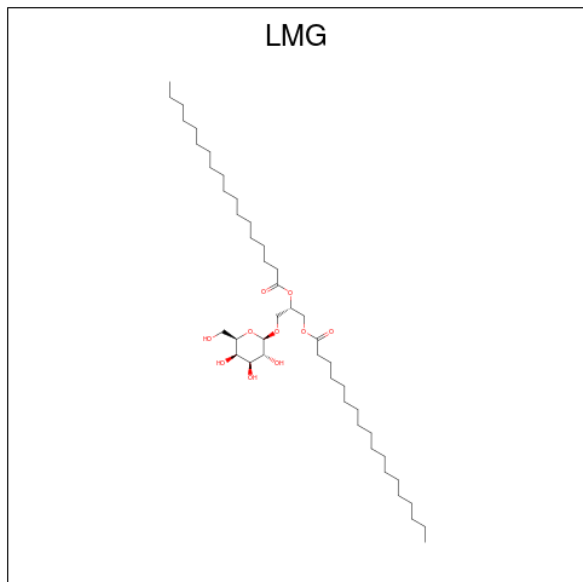
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 22 | K | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 22 | L | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 22 | L | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 22 | M | 1 | Total | C | 0 |
| | | | 40 | 40 | |

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 23 | A | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 23 | A | 1 | Total | C | O | P | 0 |
| | | | 31 | 20 | 10 | 1 | |
| 23 | B | 1 | Total | C | O | P | 0 |
| | | | 35 | 24 | 10 | 1 | |
| 23 | 1 | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |
| 23 | 2 | 1 | Total | C | O | P | 0 |
| | | | 32 | 21 | 10 | 1 | |
| 23 | 3 | 1 | Total | C | O | P | 0 |
| | | | 34 | 23 | 10 | 1 | |
| 23 | 4 | 1 | Total | C | O | P | 0 |
| | | | 38 | 27 | 10 | 1 | |

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).

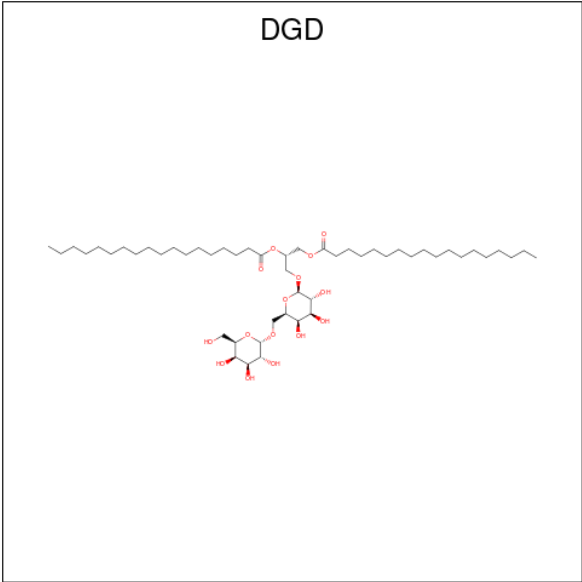


| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 24 | A | 1 | Total | C | O | 0 |
| | | | 34 | 24 | 10 | |
| 24 | 2 | 1 | Total | C | O | 0 |
| | | | 36 | 26 | 10 | |
| 24 | J | 1 | Total | C | O | 0 |
| | | | 49 | 39 | 10 | |
| 24 | J | 1 | Total | C | O | 0 |
| | | | 26 | 16 | 10 | |

- Molecule 25 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).

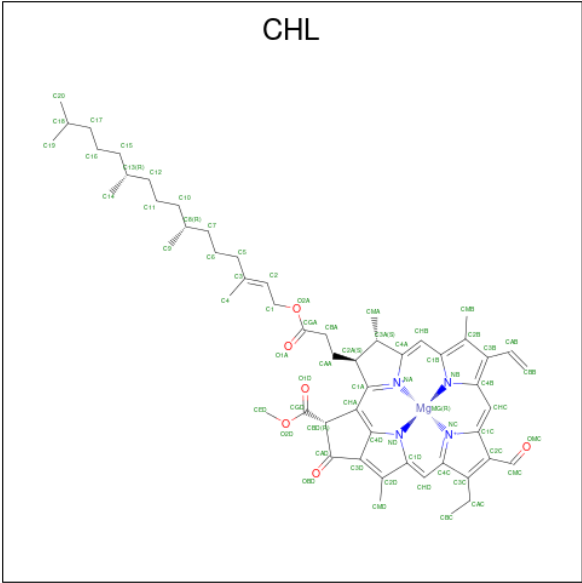


- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 26 | B | 1 | Total | C | O | 0 |
| | | | 61 | 46 | 15 | |

- Molecule 27 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



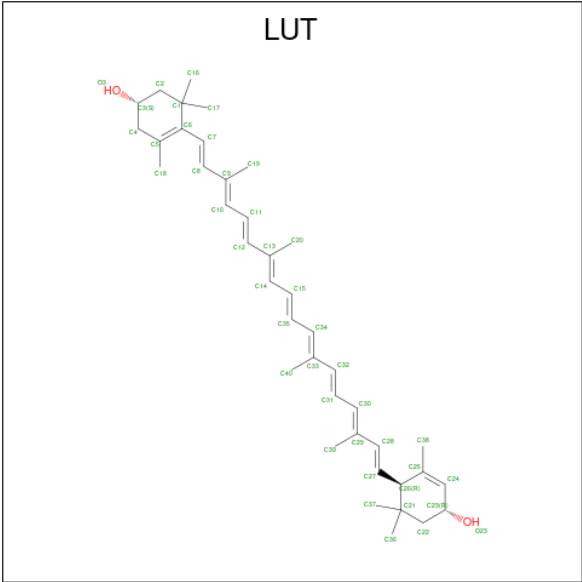
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 27 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 36 | 1 | 4 | 6 | |
| 27 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 45 | 1 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 27 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 45 | 1 | 4 | 6 | |
| 27 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 27 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 36 | 1 | 4 | 6 | |
| 27 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 48 | 37 | 1 | 4 | 6 | |
| 27 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 45 | 1 | 4 | 6 | |
| 27 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 36 | 1 | 4 | 6 | |
| 27 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 27 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 36 | 1 | 4 | 6 | |
| 27 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 36 | 1 | 4 | 6 | |
| 27 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 36 | 1 | 4 | 6 | |
| 27 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 40 | 1 | 4 | 6 | |
| 27 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 28 | 1 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 28 | 1 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 28 | 2 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 28 | 2 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 28 | 2 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 28 | 3 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 28 | 3 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 28 | 4 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 28 | 4 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 28 | 4 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |

- Molecule 29 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 29 | A | 15 | Total | O | 0 |
| | | | 15 | 15 | |
| 29 | B | 23 | Total | O | 0 |
| | | | 23 | 23 | |

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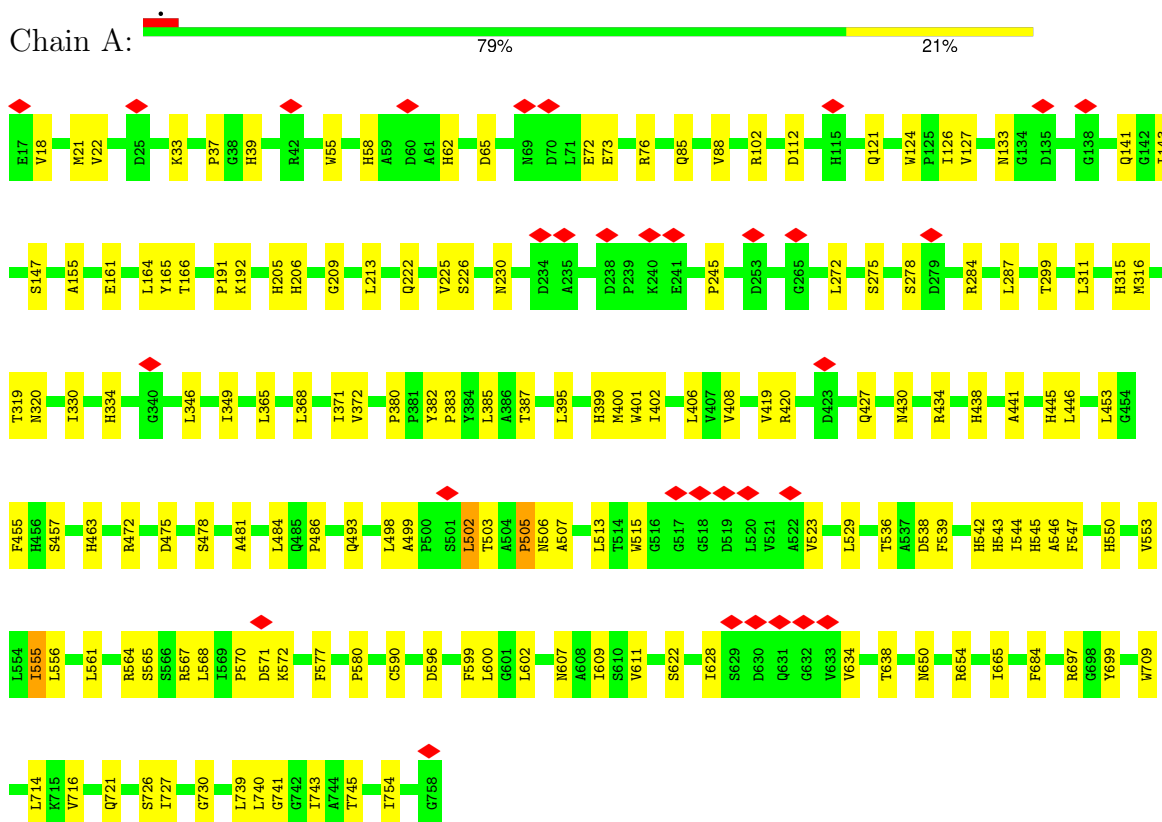
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|--------|---------|
| 29 | 3 | 1 | Total 1 | O 1 | 0 |
| 29 | 4 | 1 | Total 1 | O 1 | 0 |
| 29 | C | 2 | Total 2 | O 2 | 0 |
| 29 | D | 1 | Total 1 | O 1 | 0 |
| 29 | F | 1 | Total 1 | O 1 | 0 |
| 29 | G | 1 | Total 1 | O 1 | 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.

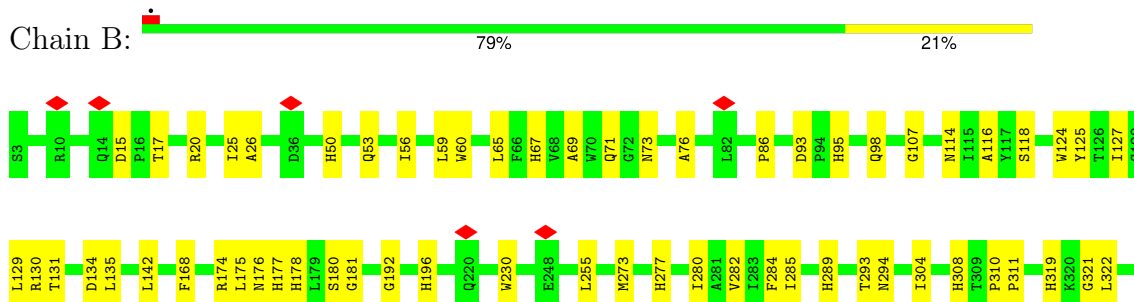
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

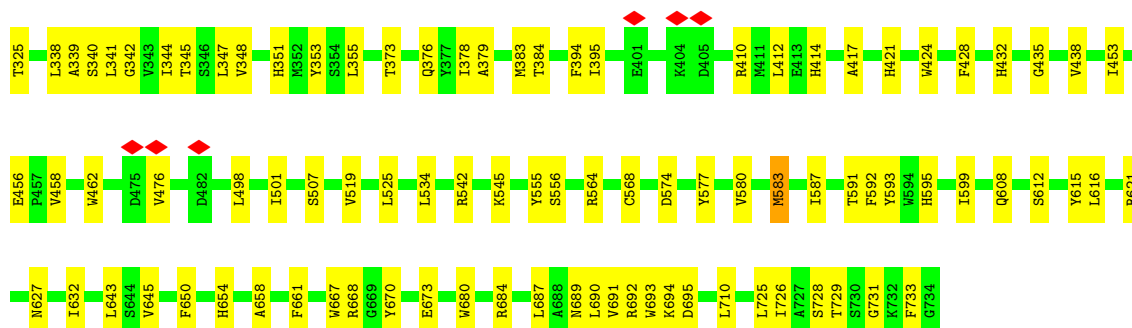
Chain A:



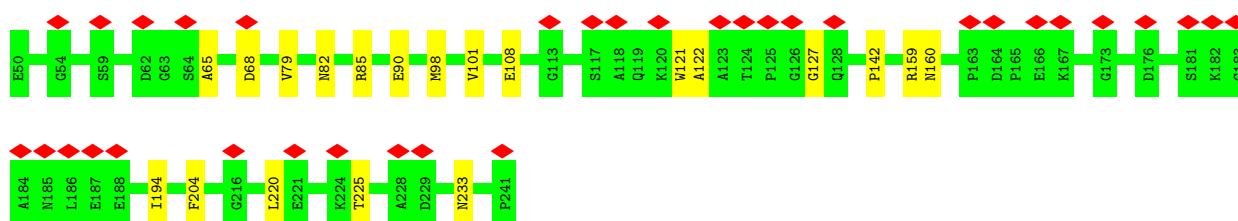
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

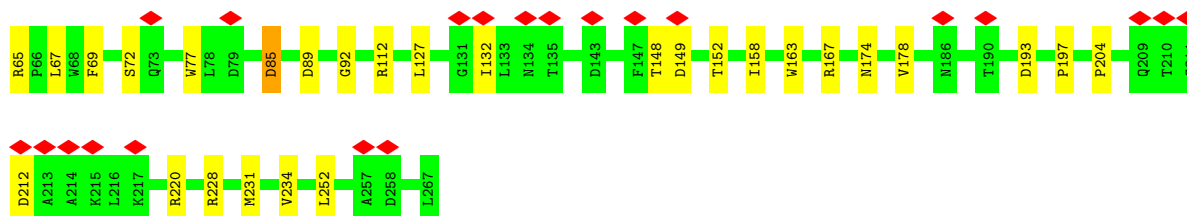
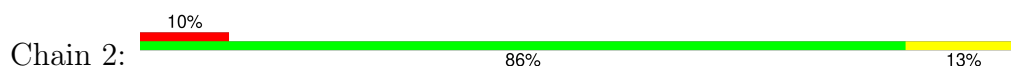




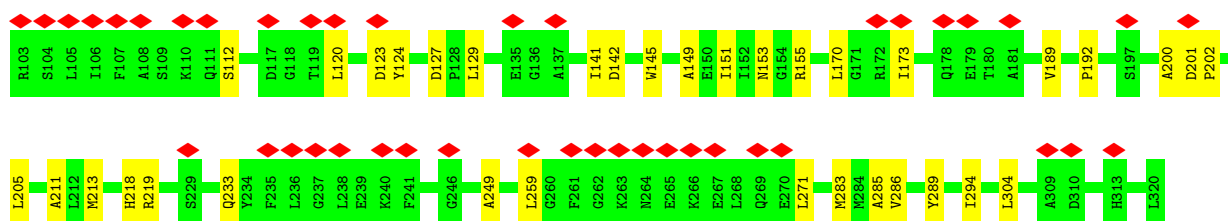
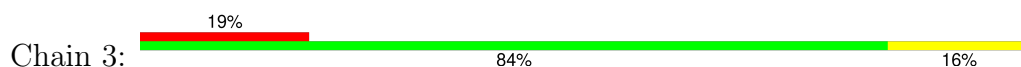
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



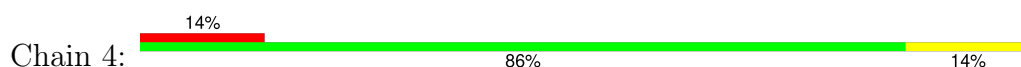
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

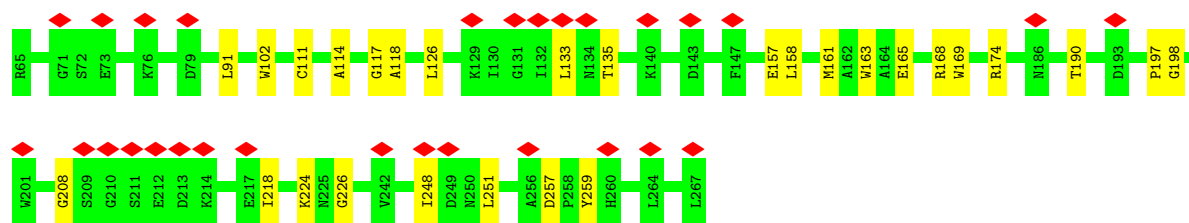


- Molecule 5: Chlorophyll a-b binding protein, chloroplastic

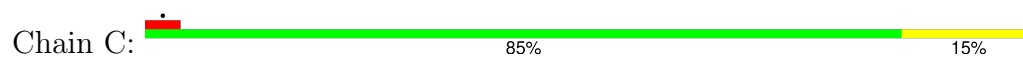


- Molecule 6: Chlorophyll a-b binding protein, chloroplastic

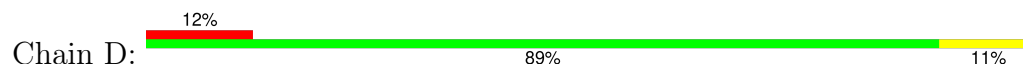




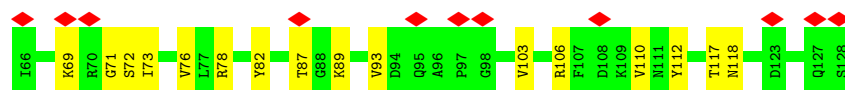
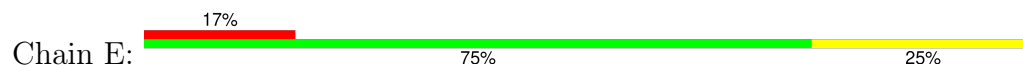
• Molecule 7: Photosystem I iron-sulfur center



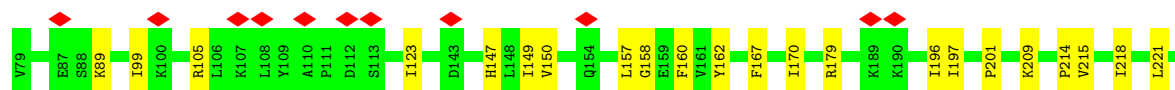
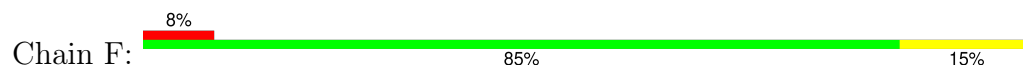
• Molecule 8: Psad



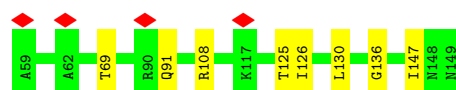
• Molecule 9: PsaE



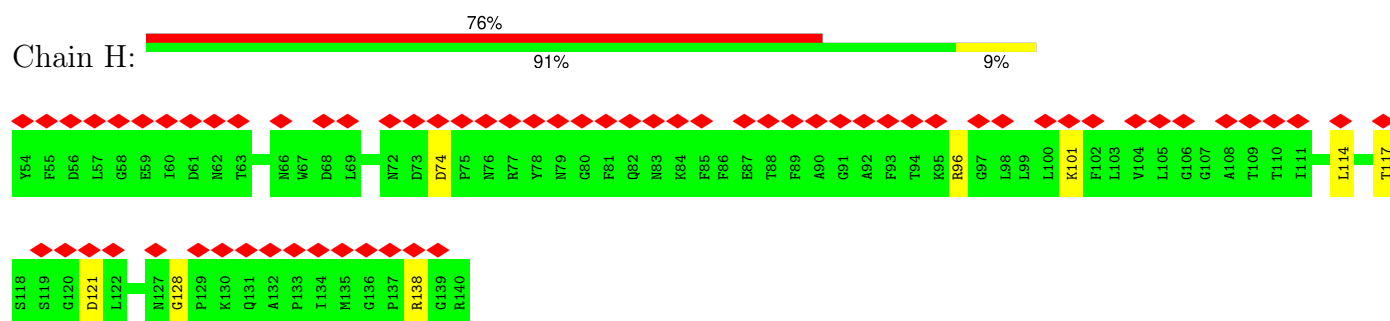
• Molecule 10: PSI-F



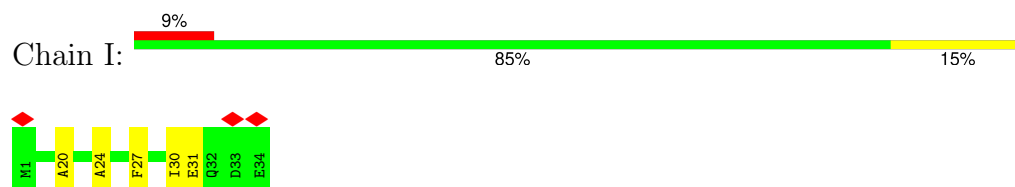
• Molecule 11: PSI-G



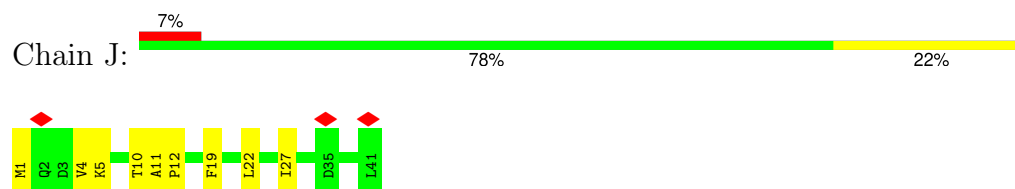
• Molecule 12: PsaH



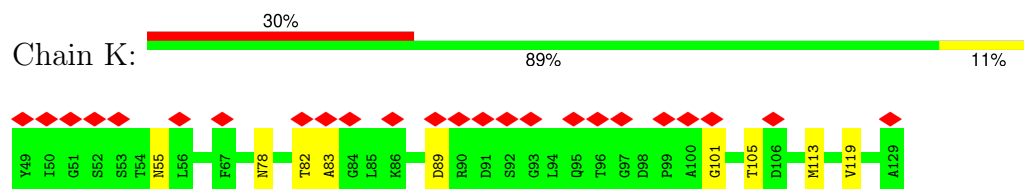
- Molecule 13: Photosystem I reaction center subunit VIII



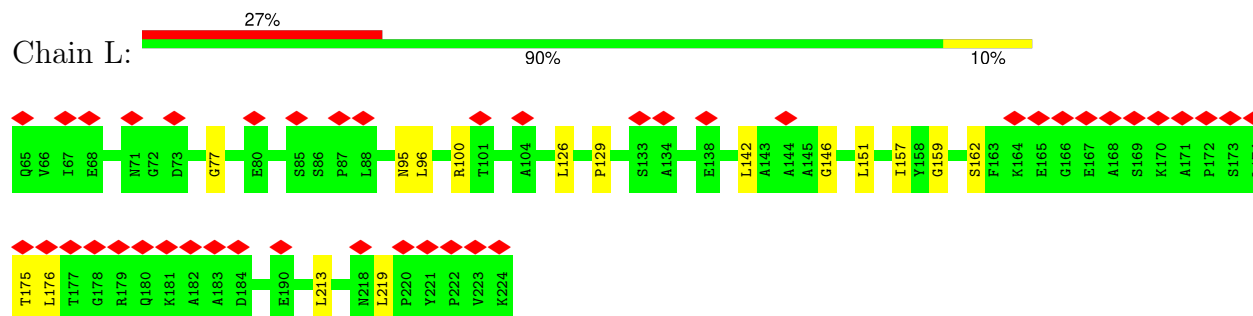
- Molecule 14: Photosystem I reaction center subunit IX



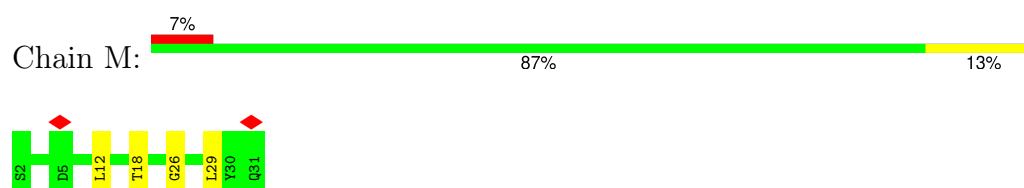
- Molecule 15: PsaK



- Molecule 16: PSI subunit V



- Molecule 17: Photosystem I reaction center subunit XII



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 114608 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1.6 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 4.882 | Depositor |
| Minimum map value | -3.405 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.144 | Depositor |
| Recommended contour level | 0.5 | Depositor |
| Map size (Å) | 291.2, 291.2, 291.2 | wwPDB |
| Map dimensions | 280, 280, 280 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.0400001, 1.0400001, 1.0400001 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, DGD, LHG, SF4, CLA, LMG, CL0, PQN, LUT, BCR, 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 | A | 0.35 | 1/6032 (0.0%) | 0.61 | 3/8227 (0.0%) |
| 2 | B | 0.35 | 0/6059 | 0.62 | 5/8267 (0.1%) |
| 3 | 1 | 0.31 | 0/1522 | 0.52 | 0/2081 |
| 4 | 2 | 0.27 | 0/1618 | 0.51 | 1/2218 (0.0%) |
| 5 | 3 | 0.29 | 0/1729 | 0.55 | 0/2349 |
| 6 | 4 | 0.30 | 0/1623 | 0.57 | 0/2219 |
| 7 | C | 0.30 | 0/606 | 0.56 | 0/821 |
| 8 | D | 0.28 | 0/1136 | 0.54 | 0/1538 |
| 9 | E | 0.30 | 0/511 | 0.46 | 0/694 |
| 10 | F | 0.32 | 0/1265 | 0.59 | 1/1710 (0.1%) |
| 11 | G | 0.27 | 0/704 | 0.44 | 0/960 |
| 12 | H | 0.29 | 0/673 | 0.58 | 1/909 (0.1%) |
| 13 | I | 0.30 | 0/273 | 0.69 | 0/373 |
| 14 | J | 0.28 | 0/334 | 0.50 | 0/457 |
| 15 | K | 0.25 | 0/567 | 0.48 | 0/768 |
| 16 | L | 0.30 | 0/1202 | 0.58 | 0/1645 |
| 17 | M | 0.24 | 0/224 | 0.41 | 0/302 |
| All | All | 0.32 | 1/26078 (0.0%) | 0.58 | 11/35538 (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 | B | 0 | 1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | A | 499 | ALA | C-N | 5.58 | 1.44 | 1.34 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | A | 498 | LEU | CA-CB-CG | 8.99 | 135.98 | 115.30 |
| 1 | A | 502 | LEU | CA-CB-CG | 8.33 | 134.46 | 115.30 |
| 10 | F | 157 | LEU | CA-CB-CG | 7.59 | 132.75 | 115.30 |
| 4 | 2 | 85 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 2 | B | 583 | MET | CG-SD-CE | 5.91 | 109.65 | 100.20 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | B | 667 | TRP | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 5837 | 0 | 5725 | 120 | 0 |
| 2 | B | 5845 | 0 | 5618 | 117 | 0 |
| 3 | 1 | 1473 | 0 | 1448 | 17 | 0 |
| 4 | 2 | 1567 | 0 | 1527 | 21 | 0 |
| 5 | 3 | 1678 | 0 | 1638 | 31 | 0 |
| 6 | 4 | 1574 | 0 | 1549 | 22 | 0 |
| 7 | C | 596 | 0 | 573 | 9 | 0 |
| 8 | D | 1109 | 0 | 1111 | 12 | 0 |
| 9 | E | 500 | 0 | 494 | 10 | 0 |
| 10 | F | 1239 | 0 | 1288 | 21 | 0 |
| 11 | G | 689 | 0 | 681 | 6 | 0 |
| 12 | H | 659 | 0 | 636 | 6 | 0 |
| 13 | I | 266 | 0 | 274 | 6 | 0 |
| 14 | J | 325 | 0 | 341 | 8 | 0 |
| 15 | K | 561 | 0 | 574 | 7 | 0 |
| 16 | L | 1171 | 0 | 1186 | 14 | 0 |
| 17 | M | 223 | 0 | 244 | 4 | 0 |
| 18 | A | 65 | 0 | 72 | 6 | 0 |
| 19 | 1 | 614 | 0 | 508 | 10 | 0 |
| 19 | 2 | 378 | 0 | 334 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | 3 | 648 | 0 | 530 | 16 | 0 |
| 19 | 4 | 527 | 0 | 448 | 9 | 0 |
| 19 | A | 2384 | 0 | 2226 | 103 | 0 |
| 19 | B | 2177 | 0 | 1998 | 106 | 0 |
| 19 | F | 118 | 0 | 69 | 4 | 0 |
| 19 | G | 151 | 0 | 121 | 1 | 0 |
| 19 | H | 45 | 0 | 33 | 2 | 0 |
| 19 | I | 65 | 0 | 72 | 7 | 0 |
| 19 | J | 45 | 0 | 33 | 0 | 0 |
| 19 | K | 173 | 0 | 118 | 3 | 0 |
| 19 | L | 155 | 0 | 131 | 9 | 0 |
| 20 | A | 33 | 0 | 46 | 2 | 0 |
| 20 | B | 33 | 0 | 46 | 5 | 0 |
| 21 | A | 8 | 0 | 0 | 0 | 0 |
| 21 | C | 16 | 0 | 0 | 0 | 0 |
| 22 | 1 | 25 | 0 | 33 | 0 | 0 |
| 22 | 3 | 80 | 0 | 112 | 5 | 0 |
| 22 | A | 240 | 0 | 336 | 8 | 0 |
| 22 | B | 280 | 0 | 392 | 28 | 0 |
| 22 | F | 40 | 0 | 56 | 2 | 0 |
| 22 | G | 40 | 0 | 56 | 4 | 0 |
| 22 | I | 80 | 0 | 112 | 5 | 0 |
| 22 | J | 80 | 0 | 112 | 4 | 0 |
| 22 | K | 40 | 0 | 56 | 1 | 0 |
| 22 | L | 80 | 0 | 112 | 7 | 0 |
| 22 | M | 40 | 0 | 56 | 5 | 0 |
| 23 | 1 | 37 | 0 | 44 | 1 | 0 |
| 23 | 2 | 32 | 0 | 34 | 2 | 0 |
| 23 | 3 | 34 | 0 | 38 | 1 | 0 |
| 23 | 4 | 38 | 0 | 46 | 2 | 0 |
| 23 | A | 80 | 0 | 106 | 4 | 0 |
| 23 | B | 35 | 0 | 40 | 0 | 0 |
| 24 | 2 | 36 | 0 | 42 | 0 | 0 |
| 24 | A | 34 | 0 | 38 | 2 | 0 |
| 24 | J | 75 | 0 | 90 | 4 | 0 |
| 25 | 1 | 35 | 0 | 46 | 2 | 0 |
| 25 | 4 | 35 | 0 | 45 | 3 | 0 |
| 25 | A | 33 | 0 | 39 | 1 | 0 |
| 25 | B | 31 | 0 | 35 | 0 | 0 |
| 25 | G | 66 | 0 | 80 | 3 | 0 |
| 26 | B | 61 | 0 | 83 | 5 | 0 |
| 27 | 1 | 103 | 0 | 78 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27 | 2 | 366 | 0 | 290 | 11 | 0 |
| 27 | 3 | 47 | 0 | 31 | 3 | 0 |
| 27 | 4 | 188 | 0 | 128 | 1 | 0 |
| 28 | 1 | 84 | 0 | 112 | 8 | 0 |
| 28 | 2 | 126 | 0 | 165 | 10 | 0 |
| 28 | 3 | 84 | 0 | 110 | 9 | 0 |
| 28 | 4 | 126 | 0 | 166 | 7 | 0 |
| 29 | 3 | 1 | 0 | 0 | 0 | 0 |
| 29 | 4 | 1 | 0 | 0 | 0 | 0 |
| 29 | A | 15 | 0 | 0 | 0 | 0 |
| 29 | B | 23 | 0 | 0 | 0 | 0 |
| 29 | C | 2 | 0 | 0 | 0 | 0 |
| 29 | D | 1 | 0 | 0 | 0 | 0 |
| 29 | F | 1 | 0 | 0 | 0 | 0 |
| 29 | G | 1 | 0 | 0 | 0 | 0 |
| All | All | 35803 | 0 | 35011 | 590 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 590 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:A:1134:CLA:H2A | 19:A:1134:CLA:HED3 | 1.63 | 0.80 |
| 19:4:601:CLA:HBB2 | 19:4:602:CLA:HHD | 1.64 | 0.79 |
| 19:3:610:CLA:HAB | 28:3:620:LUT:H32 | 1.67 | 0.75 |
| 19:4:610:CLA:HAB | 28:4:620:LUT:H32 | 1.69 | 0.75 |
| 1:A:209:GLY:HA3 | 19:A:1111:CLA:HBB1 | 1.71 | 0.72 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 740/742 (100%) | 699 (94%) | 38 (5%) | 3 (0%) | 30 | 61 |
| 2 | B | 730/732 (100%) | 708 (97%) | 22 (3%) | 0 | 100 | 100 |
| 3 | 1 | 190/192 (99%) | 182 (96%) | 8 (4%) | 0 | 100 | 100 |
| 4 | 2 | 201/203 (99%) | 198 (98%) | 3 (2%) | 0 | 100 | 100 |
| 5 | 3 | 216/218 (99%) | 206 (95%) | 10 (5%) | 0 | 100 | 100 |
| 6 | 4 | 201/203 (99%) | 197 (98%) | 4 (2%) | 0 | 100 | 100 |
| 7 | C | 78/80 (98%) | 74 (95%) | 4 (5%) | 0 | 100 | 100 |
| 8 | D | 140/142 (99%) | 136 (97%) | 4 (3%) | 0 | 100 | 100 |
| 9 | E | 61/63 (97%) | 56 (92%) | 5 (8%) | 0 | 100 | 100 |
| 10 | F | 158/160 (99%) | 153 (97%) | 5 (3%) | 0 | 100 | 100 |
| 11 | G | 89/91 (98%) | 88 (99%) | 1 (1%) | 0 | 100 | 100 |
| 12 | H | 85/87 (98%) | 82 (96%) | 3 (4%) | 0 | 100 | 100 |
| 13 | I | 32/34 (94%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 14 | J | 39/41 (95%) | 39 (100%) | 0 | 0 | 100 | 100 |
| 15 | K | 79/81 (98%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 16 | L | 158/160 (99%) | 149 (94%) | 9 (6%) | 0 | 100 | 100 |
| 17 | M | 28/30 (93%) | 28 (100%) | 0 | 0 | 100 | 100 |
| All | All | 3225/3259 (99%) | 3104 (96%) | 118 (4%) | 3 (0%) | 50 | 77 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 506 | ASN |
| 1 | A | 505 | PRO |
| 1 | A | 284 | ARG |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | A | 603/603 (100%) | 603 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 2 | B | 595/595 (100%) | 595 (100%) | 0 | 100 | 100 |
| 3 | 1 | 148/148 (100%) | 148 (100%) | 0 | 100 | 100 |
| 4 | 2 | 160/160 (100%) | 159 (99%) | 1 (1%) | 84 | 95 |
| 5 | 3 | 169/171 (99%) | 169 (100%) | 0 | 100 | 100 |
| 6 | 4 | 161/162 (99%) | 160 (99%) | 1 (1%) | 84 | 95 |
| 7 | C | 67/67 (100%) | 67 (100%) | 0 | 100 | 100 |
| 8 | D | 114/115 (99%) | 114 (100%) | 0 | 100 | 100 |
| 9 | E | 55/55 (100%) | 55 (100%) | 0 | 100 | 100 |
| 10 | F | 130/131 (99%) | 130 (100%) | 0 | 100 | 100 |
| 11 | G | 72/72 (100%) | 72 (100%) | 0 | 100 | 100 |
| 12 | H | 66/68 (97%) | 66 (100%) | 0 | 100 | 100 |
| 13 | I | 30/30 (100%) | 30 (100%) | 0 | 100 | 100 |
| 14 | J | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 15 | K | 57/58 (98%) | 57 (100%) | 0 | 100 | 100 |
| 16 | L | 116/118 (98%) | 116 (100%) | 0 | 100 | 100 |
| 17 | M | 25/25 (100%) | 25 (100%) | 0 | 100 | 100 |
| All | All | 2603/2613 (100%) | 2601 (100%) | 2 (0%) | 92 | 98 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2 | 174 | ASN |
| 6 | 4 | 174 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2 | 174 | ASN |
| 5 | 3 | 303 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

215 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 19 | CLA | 3 | 614 | - | 46,56,73 | 1.57 | 5 (10%) | 53,92,113 | 1.68 | 7 (13%) |
| 19 | CLA | B | 1234 | - | 49,59,73 | 1.48 | 6 (12%) | 56,96,113 | 1.67 | 8 (14%) |
| 22 | BCR | B | 4009 | - | 41,41,41 | 0.99 | 1 (2%) | 56,56,56 | 1.56 | 11 (19%) |
| 19 | CLA | A | 1126 | - | 58,68,73 | 1.36 | 7 (12%) | 68,107,113 | 1.94 | 15 (22%) |
| 24 | LMG | 2 | 631 | - | 36,36,55 | 0.94 | 0 | 44,44,63 | 1.21 | 5 (11%) |
| 22 | BCR | A | 4007 | - | 41,41,41 | 1.11 | 3 (7%) | 56,56,56 | 1.88 | 18 (32%) |
| 22 | BCR | M | 4021 | - | 41,41,41 | 0.99 | 2 (4%) | 56,56,56 | 1.31 | 9 (16%) |
| 19 | CLA | 1 | 604 | - | 48,58,73 | 1.53 | 5 (10%) | 56,95,113 | 1.69 | 8 (14%) |
| 22 | BCR | 1 | 623 | - | 25,25,41 | 1.04 | 2 (8%) | 33,33,56 | 1.29 | 5 (15%) |
| 19 | CLA | A | 1101 | - | 48,58,73 | 1.54 | 6 (12%) | 56,95,113 | 1.57 | 8 (14%) |
| 19 | CLA | B | 1021 | - | 63,73,73 | 1.34 | 7 (11%) | 74,113,113 | 1.41 | 10 (13%) |
| 19 | CLA | 4 | 613 | - | 53,63,73 | 1.48 | 6 (11%) | 62,101,113 | 1.49 | 6 (9%) |
| 23 | LHG | B | 5101 | - | 34,34,48 | 0.75 | 1 (2%) | 37,40,54 | 1.29 | 4 (10%) |
| 19 | CLA | 4 | 611 | - | 53,63,73 | 1.47 | 6 (11%) | 62,101,113 | 1.54 | 8 (12%) |
| 22 | BCR | B | 4010 | - | 41,41,41 | 1.08 | 1 (2%) | 56,56,56 | 1.70 | 13 (23%) |
| 19 | CLA | 3 | 604 | - | 48,58,73 | 1.54 | 5 (10%) | 56,95,113 | 1.63 | 9 (16%) |
| 19 | CLA | A | 8895 | - | 63,73,73 | 1.36 | 6 (9%) | 74,113,113 | 1.56 | 6 (8%) |
| 19 | CLA | B | 1220 | - | 43,53,73 | 1.60 | 6 (13%) | 50,89,113 | 1.59 | 7 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | LMG | J | 301 | - | 49,49,55 | 0.81 | 1 (2%) | 57,57,63 | 1.27 | 5 (8%) |
| 19 | CLA | K | 201 | - | 53,63,73 | 1.47 | 6 (11%) | 62,101,113 | 1.47 | 7 (11%) |
| 27 | CHL | 2 | 606 | - | 44,54,74 | 2.29 | 14 (31%) | 47,90,114 | 2.85 | 18 (38%) |
| 19 | CLA | 4 | 610 | - | 53,63,73 | 1.46 | 7 (13%) | 62,101,113 | 1.72 | 8 (12%) |
| 19 | CLA | A | 1117 | - | 63,73,73 | 1.33 | 6 (9%) | 74,113,113 | 1.66 | 13 (17%) |
| 19 | CLA | 4 | 602 | - | 58,68,73 | 1.39 | 5 (8%) | 68,107,113 | 1.55 | 8 (11%) |
| 19 | CLA | A | 1109 | - | 63,73,73 | 1.36 | 7 (11%) | 74,113,113 | 1.38 | 9 (12%) |
| 19 | CLA | 1 | 609 | - | 58,68,73 | 1.43 | 5 (8%) | 68,107,113 | 1.64 | 6 (8%) |
| 19 | CLA | L | 301 | - | 48,58,73 | 1.56 | 5 (10%) | 56,95,113 | 1.78 | 11 (19%) |
| 21 | SF4 | C | 1003 | 7 | 0,12,12 | - | - | - | - | - |
| 27 | CHL | 2 | 608 | - | 46,56,74 | 2.17 | 13 (28%) | 49,92,114 | 2.88 | 19 (38%) |
| 28 | LUT | 4 | 623 | - | 42,43,43 | 2.42 | 1 (2%) | 51,60,60 | 1.79 | 8 (15%) |
| 19 | CLA | B | 1203 | - | 63,73,73 | 1.34 | 6 (9%) | 74,113,113 | 1.46 | 10 (13%) |
| 19 | CLA | L | 302 | - | 58,68,73 | 1.37 | 5 (8%) | 68,107,113 | 1.37 | 8 (11%) |
| 19 | CLA | K | 204 | - | 43,53,73 | 1.64 | 6 (13%) | 50,89,113 | 1.64 | 11 (22%) |
| 19 | CLA | B | 1224 | - | 59,69,73 | 1.36 | 7 (11%) | 69,108,113 | 1.60 | 12 (17%) |
| 19 | CLA | 4 | 614 | - | 44,54,73 | 1.61 | 5 (11%) | 51,90,113 | 1.54 | 6 (11%) |
| 19 | CLA | B | 1238 | - | 63,73,73 | 1.30 | 5 (7%) | 74,113,113 | 1.40 | 8 (10%) |
| 19 | CLA | 3 | 602 | - | 58,68,73 | 1.39 | 6 (10%) | 68,107,113 | 1.67 | 9 (13%) |
| 28 | LUT | 4 | 621 | - | 42,43,43 | 2.53 | 4 (9%) | 51,60,60 | 3.06 | 14 (27%) |
| 19 | CLA | 1 | 603 | - | 53,63,73 | 1.46 | 5 (9%) | 62,101,113 | 1.45 | 9 (14%) |
| 19 | CLA | 2 | 604 | - | 48,58,73 | 1.53 | 5 (10%) | 56,95,113 | 1.53 | 7 (12%) |
| 19 | CLA | F | 302 | - | 44,54,73 | 1.60 | 5 (11%) | 51,90,113 | 1.52 | 7 (13%) |
| 27 | CHL | 4 | 607 | - | 45,55,74 | 2.27 | 14 (31%) | 48,91,114 | 2.82 | 19 (39%) |
| 19 | CLA | A | 1128 | - | 63,73,73 | 1.35 | 8 (12%) | 74,113,113 | 1.55 | 12 (16%) |
| 19 | CLA | B | 1201 | - | 48,58,73 | 1.51 | 5 (10%) | 56,95,113 | 1.57 | 10 (17%) |
| 19 | CLA | A | 1121 | - | 49,59,73 | 1.55 | 5 (10%) | 56,96,113 | 1.65 | 7 (12%) |
| 22 | BCR | A | 4008 | - | 41,41,41 | 1.01 | 1 (2%) | 56,56,56 | 1.86 | 15 (26%) |
| 19 | CLA | 4 | 604 | - | 48,58,73 | 1.50 | 5 (10%) | 56,95,113 | 1.58 | 8 (14%) |
| 22 | BCR | I | 118 | - | 41,41,41 | 1.03 | 2 (4%) | 56,56,56 | 1.30 | 8 (14%) |
| 19 | CLA | A | 1133 | - | 43,53,73 | 1.62 | 6 (13%) | 50,89,113 | 1.37 | 4 (8%) |
| 19 | CLA | A | 1801 | - | 48,58,73 | 1.52 | 6 (12%) | 56,95,113 | 1.66 | 6 (10%) |
| 19 | CLA | A | 1104 | - | 63,73,73 | 1.35 | 6 (9%) | 74,113,113 | 1.38 | 9 (12%) |
| 19 | CLA | 1 | 611 | - | 44,54,73 | 1.59 | 5 (11%) | 51,90,113 | 1.39 | 6 (11%) |
| 22 | BCR | K | 301 | - | 41,41,41 | 1.04 | 2 (4%) | 56,56,56 | 1.31 | 6 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 28 | LUT | 3 | 620 | - | 42,43,43 | 2.39 | 1 (2%) | 51,60,60 | 1.58 | 5 (9%) |
| 19 | CLA | 2 | 610 | - | 58,68,73 | 1.40 | 5 (8%) | 68,107,113 | 1.26 | 5 (7%) |
| 19 | CLA | B | 1205 | - | 63,73,73 | 1.36 | 6 (9%) | 74,113,113 | 1.53 | 9 (12%) |
| 19 | CLA | B | 1213 | - | 53,63,73 | 1.38 | 6 (11%) | 62,101,113 | 1.64 | 9 (14%) |
| 19 | CLA | 1 | 614 | - | 44,54,73 | 1.61 | 5 (11%) | 51,90,113 | 1.66 | 9 (17%) |
| 26 | DGD | B | 5002 | - | 62,62,67 | 0.97 | 4 (6%) | 76,76,81 | 1.26 | 8 (10%) |
| 19 | CLA | B | 1214 | - | 57,67,73 | 1.38 | 8 (14%) | 66,105,113 | 1.57 | 10 (15%) |
| 19 | CLA | 3 | 611 | - | 39,49,73 | 1.69 | 5 (12%) | 46,84,113 | 1.53 | 5 (10%) |
| 22 | BCR | 3 | 624 | - | 41,41,41 | 0.99 | 2 (4%) | 56,56,56 | 1.36 | 9 (16%) |
| 19 | CLA | 4 | 601 | - | 48,58,73 | 1.50 | 5 (10%) | 56,95,113 | 1.55 | 6 (10%) |
| 19 | CLA | 3 | 612 | - | 43,53,73 | 1.63 | 5 (11%) | 50,89,113 | 1.52 | 6 (12%) |
| 19 | CLA | A | 5005 | - | 48,58,73 | 1.50 | 5 (10%) | 56,95,113 | 1.54 | 10 (17%) |
| 22 | BCR | J | 212 | - | 41,41,41 | 1.09 | 2 (4%) | 56,56,56 | 1.29 | 7 (12%) |
| 19 | CLA | 3 | 613 | - | 53,63,73 | 1.48 | 5 (9%) | 62,101,113 | 1.43 | 5 (8%) |
| 23 | LHG | A | 5003 | - | 30,30,48 | 0.78 | 1 (3%) | 33,36,54 | 1.28 | 3 (9%) |
| 28 | LUT | 2 | 621 | - | 42,43,43 | 2.38 | 1 (2%) | 51,60,60 | 1.58 | 6 (11%) |
| 23 | LHG | 1 | 630 | - | 36,36,48 | 0.68 | 1 (2%) | 39,42,54 | 1.26 | 4 (10%) |
| 19 | CLA | J | 102 | - | 43,53,73 | 1.64 | 5 (11%) | 50,89,113 | 1.65 | 6 (12%) |
| 28 | LUT | 3 | 621 | - | 42,43,43 | 2.44 | 1 (2%) | 51,60,60 | 1.85 | 10 (19%) |
| 19 | CLA | B | 1209 | - | 43,53,73 | 1.63 | 5 (11%) | 50,89,113 | 1.67 | 6 (12%) |
| 19 | CLA | A | 1124 | - | 55,65,73 | 1.41 | 5 (9%) | 64,103,113 | 1.48 | 6 (9%) |
| 19 | CLA | A | 1120 | - | 43,53,73 | 1.61 | 5 (11%) | 50,89,113 | 1.59 | 5 (10%) |
| 19 | CLA | 1 | 610 | - | 53,63,73 | 1.44 | 6 (11%) | 62,101,113 | 1.84 | 10 (16%) |
| 19 | CLA | A | 1127 | - | 63,73,73 | 1.32 | 7 (11%) | 74,113,113 | 1.71 | 11 (14%) |
| 22 | BCR | L | 419 | - | 41,41,41 | 0.97 | 1 (2%) | 56,56,56 | 1.59 | 12 (21%) |
| 22 | BCR | A | 4011 | - | 41,41,41 | 1.03 | 2 (4%) | 56,56,56 | 1.23 | 6 (10%) |
| 28 | LUT | 1 | 620 | - | 42,43,43 | 2.72 | 2 (4%) | 51,60,60 | 2.30 | 14 (27%) |
| 19 | CLA | B | 1216 | - | 53,63,73 | 1.44 | 7 (13%) | 62,101,113 | 1.81 | 10 (16%) |
| 19 | CLA | A | 1132 | - | 63,73,73 | 1.29 | 6 (9%) | 74,113,113 | 1.77 | 13 (17%) |
| 22 | BCR | J | 213 | - | 41,41,41 | 1.03 | 2 (4%) | 56,56,56 | 1.37 | 7 (12%) |
| 27 | CHL | 4 | 606 | - | 45,55,74 | 2.25 | 14 (31%) | 48,91,114 | 2.83 | 19 (39%) |
| 19 | CLA | 1 | 608 | - | 48,58,73 | 1.52 | 5 (10%) | 56,95,113 | 1.60 | 8 (14%) |
| 19 | CLA | B | 1236 | - | 45,55,73 | 1.56 | 5 (11%) | 52,91,113 | 1.54 | 7 (13%) |
| 19 | CLA | B | 1206 | - | 45,55,73 | 1.55 | 6 (13%) | 52,91,113 | 1.69 | 7 (13%) |
| 19 | CLA | A | 1130 | - | 58,68,73 | 1.37 | 6 (10%) | 68,107,113 | 1.47 | 10 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 19 | CLA | I | 121 | - | 63,73,73 | 1.34 | 6 (9%) | 74,113,113 | 1.47 | 7 (9%) |
| 19 | CLA | B | 1204 | - | 59,69,73 | 1.37 | 5 (8%) | 69,108,113 | 1.31 | 7 (10%) |
| 19 | CLA | 3 | 610 | - | 53,63,73 | 1.42 | 5 (9%) | 62,101,113 | 1.41 | 7 (11%) |
| 19 | CLA | A | 1138 | - | 58,68,73 | 1.35 | 5 (8%) | 68,107,113 | 1.58 | 8 (11%) |
| 19 | CLA | A | 1118 | - | 53,63,73 | 1.42 | 5 (9%) | 62,101,113 | 1.36 | 6 (9%) |
| 19 | CLA | B | 1235 | - | 53,63,73 | 1.45 | 6 (11%) | 62,101,113 | 1.46 | 6 (9%) |
| 22 | BCR | I | 120 | - | 41,41,41 | 1.06 | 3 (7%) | 56,56,56 | 1.77 | 15 (26%) |
| 19 | CLA | B | 1023 | - | 59,69,73 | 1.43 | 7 (11%) | 69,108,113 | 1.63 | 14 (20%) |
| 19 | CLA | B | 1012 | - | 53,63,73 | 1.43 | 6 (11%) | 62,101,113 | 1.64 | 9 (14%) |
| 19 | CLA | A | 1119 | - | 63,73,73 | 1.30 | 6 (9%) | 74,113,113 | 1.56 | 9 (12%) |
| 19 | CLA | B | 1222 | - | 44,54,73 | 1.58 | 6 (13%) | 51,90,113 | 1.75 | 10 (19%) |
| 19 | CLA | 3 | 617 | - | 44,54,73 | 1.59 | 6 (13%) | 51,90,113 | 1.49 | 6 (11%) |
| 19 | CLA | A | 1135 | - | 49,59,73 | 1.51 | 6 (12%) | 56,96,113 | 1.53 | 8 (14%) |
| 22 | BCR | A | 4002 | - | 41,41,41 | 1.06 | 2 (4%) | 56,56,56 | 1.21 | 5 (8%) |
| 19 | CLA | A | 1113 | - | 43,53,73 | 1.61 | 6 (13%) | 50,89,113 | 1.73 | 10 (20%) |
| 19 | CLA | A | 1114 | - | 43,53,73 | 1.65 | 5 (11%) | 50,89,113 | 1.92 | 10 (20%) |
| 19 | CLA | B | 1211 | - | 54,64,73 | 1.45 | 5 (9%) | 63,102,113 | 1.63 | 7 (11%) |
| 19 | CLA | 3 | 605 | - | 28,35,73 | 2.27 | 8 (28%) | 28,60,113 | 1.72 | 6 (21%) |
| 27 | CHL | 2 | 602 | - | 54,64,74 | 2.09 | 16 (29%) | 59,102,114 | 2.61 | 22 (37%) |
| 19 | CLA | G | 218 | - | 53,63,73 | 1.45 | 5 (9%) | 62,101,113 | 1.41 | 6 (9%) |
| 22 | BCR | G | 311 | - | 41,41,41 | 0.99 | 2 (4%) | 56,56,56 | 1.36 | 9 (16%) |
| 19 | CLA | A | 1122 | - | 58,68,73 | 1.42 | 6 (10%) | 68,107,113 | 1.49 | 6 (8%) |
| 19 | CLA | 2 | 603 | - | 44,54,73 | 1.56 | 5 (11%) | 51,90,113 | 1.53 | 6 (11%) |
| 19 | CLA | B | 1231 | - | 43,53,73 | 1.63 | 5 (11%) | 50,89,113 | 1.61 | 8 (16%) |
| 19 | CLA | B | 1208 | - | 43,53,73 | 1.59 | 5 (11%) | 50,89,113 | 1.70 | 9 (18%) |
| 19 | CLA | H | 200 | - | 43,53,73 | 1.62 | 4 (9%) | 50,89,113 | 1.51 | 7 (14%) |
| 20 | PQN | A | 2001 | - | 34,34,34 | 0.41 | 0 | 43,45,45 | 1.04 | 1 (2%) |
| 27 | CHL | 3 | 608 | - | 45,55,74 | 2.21 | 13 (28%) | 48,91,114 | 2.83 | 20 (41%) |
| 27 | CHL | 2 | 601 | - | 64,74,74 | 1.88 | 13 (20%) | 71,114,114 | 2.51 | 26 (36%) |
| 19 | CLA | B | 1237 | - | 63,73,73 | 1.39 | 7 (11%) | 74,113,113 | 1.39 | 8 (10%) |
| 22 | BCR | B | 2004 | - | 41,41,41 | 1.05 | 2 (4%) | 56,56,56 | 1.29 | 5 (8%) |
| 19 | CLA | A | 1111 | - | 63,73,73 | 1.36 | 6 (9%) | 74,113,113 | 1.48 | 7 (9%) |
| 25 | LMT | B | 5001 | - | 32,32,36 | 1.24 | 6 (18%) | 43,43,47 | 0.96 | 0 |
| 27 | CHL | 4 | 615 | - | 41,51,74 | 2.29 | 13 (31%) | 42,86,114 | 2.93 | 18 (42%) |
| 19 | CLA | A | 1116 | - | 52,62,73 | 1.42 | 7 (13%) | 60,99,113 | 1.47 | 8 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 19 | CLA | 2 | 612 | - | 50,60,73 | 1.52 | 5 (10%) | 57,97,113 | 1.53 | 7 (12%) |
| 19 | CLA | 1 | 615 | - | 44,54,73 | 1.61 | 6 (13%) | 51,90,113 | 1.59 | 6 (11%) |
| 20 | PQN | B | 2002 | - | 34,34,34 | 0.42 | 0 | 43,45,45 | 1.07 | 1 (2%) |
| 22 | BCR | B | 4005 | - | 41,41,41 | 1.04 | 2 (4%) | 56,56,56 | 1.20 | 5 (8%) |
| 22 | BCR | B | 4014 | - | 41,41,41 | 1.03 | 2 (4%) | 56,56,56 | 1.41 | 9 (16%) |
| 25 | LMT | 1 | 631 | - | 36,36,36 | 1.15 | 4 (11%) | 47,47,47 | 0.97 | 2 (4%) |
| 23 | LHG | A | 5001 | - | 48,48,48 | 0.68 | 1 (2%) | 51,54,54 | 1.29 | 6 (11%) |
| 19 | CLA | B | 1225 | - | 63,73,73 | 1.32 | 6 (9%) | 74,113,113 | 1.51 | 8 (10%) |
| 19 | CLA | B | 1223 | - | 63,73,73 | 1.30 | 6 (9%) | 74,113,113 | 1.51 | 9 (12%) |
| 19 | CLA | B | 1226 | - | 53,63,73 | 1.48 | 6 (11%) | 62,101,113 | 1.92 | 10 (16%) |
| 19 | CLA | A | 1136 | - | 63,73,73 | 1.33 | 5 (7%) | 74,113,113 | 1.48 | 10 (13%) |
| 23 | LHG | 3 | 630 | - | 33,33,48 | 0.75 | 1 (3%) | 36,39,54 | 1.30 | 4 (11%) |
| 25 | LMT | G | 402 | - | 32,32,36 | 1.23 | 5 (15%) | 43,43,47 | 0.91 | 0 |
| 19 | CLA | 1 | 612 | - | 44,54,73 | 1.59 | 5 (11%) | 51,90,113 | 1.42 | 8 (15%) |
| 19 | CLA | B | 1230 | - | 43,53,73 | 1.63 | 6 (13%) | 50,89,113 | 1.52 | 7 (14%) |
| 19 | CLA | A | 1107 | - | 43,53,73 | 1.64 | 5 (11%) | 50,89,113 | 1.69 | 8 (16%) |
| 19 | CLA | 2 | 613 | - | 63,73,73 | 1.36 | 6 (9%) | 74,113,113 | 1.36 | 7 (9%) |
| 19 | CLA | B | 1240 | - | 63,73,73 | 1.35 | 6 (9%) | 74,113,113 | 1.48 | 10 (13%) |
| 19 | CLA | 1 | 613 | - | 53,63,73 | 1.49 | 6 (11%) | 62,101,113 | 1.41 | 8 (12%) |
| 19 | CLA | A | 1106 | - | 53,63,73 | 1.43 | 6 (11%) | 62,101,113 | 1.76 | 7 (11%) |
| 19 | CLA | B | 1221 | - | 52,62,73 | 1.51 | 8 (15%) | 60,99,113 | 1.78 | 9 (15%) |
| 21 | SF4 | C | 1002 | 7 | 0,12,12 | - | - | - | - | - |
| 19 | CLA | 4 | 609 | - | 53,63,73 | 1.49 | 5 (9%) | 62,101,113 | 1.83 | 9 (14%) |
| 19 | CLA | B | 1210 | - | 63,73,73 | 1.34 | 6 (9%) | 74,113,113 | 1.67 | 10 (13%) |
| 19 | CLA | L | 303 | - | 43,53,73 | 1.63 | 6 (13%) | 50,89,113 | 1.82 | 8 (16%) |
| 28 | LUT | 1 | 621 | - | 42,43,43 | 2.66 | 2 (4%) | 51,60,60 | 2.23 | 9 (17%) |
| 19 | CLA | K | 202 | - | 44,54,73 | 1.61 | 5 (11%) | 51,90,113 | 1.55 | 7 (13%) |
| 19 | CLA | A | 1022 | - | 63,73,73 | 1.38 | 6 (9%) | 74,113,113 | 1.34 | 7 (9%) |
| 19 | CLA | 1 | 606 | - | 43,53,73 | 1.64 | 6 (13%) | 50,89,113 | 1.76 | 9 (18%) |
| 22 | BCR | A | 4001 | - | 41,41,41 | 1.04 | 2 (4%) | 56,56,56 | 1.37 | 7 (12%) |
| 27 | CHL | 2 | 607 | - | 45,55,74 | 2.27 | 13 (28%) | 48,91,114 | 2.85 | 22 (45%) |
| 27 | CHL | 4 | 608 | - | 49,59,74 | 2.16 | 15 (30%) | 53,96,114 | 2.67 | 20 (37%) |
| 19 | CLA | 3 | 609 | - | 58,68,73 | 1.40 | 5 (8%) | 68,107,113 | 1.42 | 8 (11%) |
| 22 | BCR | B | 4006 | - | 41,41,41 | 1.06 | 2 (4%) | 56,56,56 | 1.22 | 5 (8%) |
| 19 | CLA | 4 | 603 | - | 53,63,73 | 1.45 | 6 (11%) | 62,101,113 | 1.45 | 8 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 19 | CLA | 4 | 612 | - | 44,54,73 | 1.60 | 5 (11%) | 51,90,113 | 1.44 | 6 (11%) |
| 19 | CLA | 3 | 606 | - | 44,54,73 | 1.61 | 6 (13%) | 51,90,113 | 1.46 | 5 (9%) |
| 24 | LMG | A | 5002 | - | 34,34,55 | 0.95 | 0 | 42,42,63 | 1.23 | 3 (7%) |
| 27 | CHL | 2 | 615 | - | 45,55,74 | 2.27 | 14 (31%) | 48,91,114 | 2.81 | 19 (39%) |
| 19 | CLA | A | 1013 | - | 54,64,73 | 1.35 | 7 (12%) | 63,102,113 | 1.91 | 13 (20%) |
| 19 | CLA | B | 1228 | - | 47,57,73 | 1.51 | 6 (12%) | 53,93,113 | 1.57 | 8 (15%) |
| 22 | BCR | B | 4017 | - | 41,41,41 | 1.11 | 3 (7%) | 56,56,56 | 1.26 | 5 (8%) |
| 19 | CLA | 3 | 603 | - | 53,63,73 | 1.49 | 6 (11%) | 62,101,113 | 1.49 | 7 (11%) |
| 18 | CL0 | A | 1011 | - | 63,73,73 | 1.36 | 7 (11%) | 74,113,113 | 1.42 | 8 (10%) |
| 19 | CLA | F | 303 | - | 28,35,73 | 2.27 | 8 (28%) | 28,60,113 | 1.69 | 5 (17%) |
| 19 | CLA | A | 1139 | - | 48,58,73 | 1.50 | 6 (12%) | 56,95,113 | 1.60 | 7 (12%) |
| 19 | CLA | B | 1202 | - | 63,73,73 | 1.30 | 6 (9%) | 74,113,113 | 1.62 | 7 (9%) |
| 25 | LMT | G | 401 | - | 36,36,36 | 1.15 | 5 (13%) | 47,47,47 | 1.04 | 1 (2%) |
| 28 | LUT | 4 | 620 | - | 42,43,43 | 2.51 | 2 (4%) | 51,60,60 | 2.04 | 12 (23%) |
| 19 | CLA | 2 | 609 | - | 53,63,73 | 1.47 | 5 (9%) | 62,101,113 | 1.78 | 7 (11%) |
| 23 | LHG | 4 | 630 | - | 37,37,48 | 0.83 | 2 (5%) | 40,43,54 | 1.26 | 3 (7%) |
| 27 | CHL | 1 | 607 | - | 45,55,74 | 2.29 | 14 (31%) | 48,91,114 | 2.92 | 22 (45%) |
| 25 | LMT | 4 | 631 | - | 36,36,36 | 1.18 | 5 (13%) | 47,47,47 | 0.95 | 1 (2%) |
| 19 | CLA | A | 1125 | - | 58,68,73 | 1.41 | 7 (12%) | 68,107,113 | 1.89 | 14 (20%) |
| 19 | CLA | 1 | 602 | - | 58,68,73 | 1.41 | 6 (10%) | 68,107,113 | 1.63 | 8 (11%) |
| 27 | CHL | 1 | 601 | - | 54,64,74 | 2.02 | 13 (24%) | 59,102,114 | 2.76 | 24 (40%) |
| 27 | CHL | 2 | 611 | - | 54,64,74 | 2.06 | 15 (27%) | 59,102,114 | 2.62 | 23 (38%) |
| 19 | CLA | A | 1137 | - | 43,53,73 | 1.60 | 5 (11%) | 50,89,113 | 1.52 | 4 (8%) |
| 19 | CLA | G | 202 | - | 44,54,73 | 1.59 | 5 (11%) | 51,90,113 | 1.51 | 5 (9%) |
| 19 | CLA | A | 1103 | - | 63,73,73 | 1.36 | 6 (9%) | 74,113,113 | 1.31 | 8 (10%) |
| 25 | LMT | A | 5004 | - | 34,34,36 | 1.20 | 4 (11%) | 45,45,47 | 1.05 | 1 (2%) |
| 19 | CLA | 2 | 614 | - | 48,58,73 | 1.52 | 5 (10%) | 56,95,113 | 1.63 | 8 (14%) |
| 19 | CLA | A | 1115 | - | 52,62,73 | 1.44 | 6 (11%) | 60,99,113 | 1.53 | 11 (18%) |
| 22 | BCR | A | 4003 | - | 41,41,41 | 1.01 | 2 (4%) | 56,56,56 | 1.35 | 8 (14%) |
| 19 | CLA | B | 1215 | - | 58,68,73 | 1.38 | 6 (10%) | 68,107,113 | 1.84 | 12 (17%) |
| 19 | CLA | A | 1131 | - | 63,73,73 | 1.35 | 5 (7%) | 74,113,113 | 1.34 | 8 (10%) |
| 22 | BCR | L | 420 | - | 41,41,41 | 0.99 | 1 (2%) | 56,56,56 | 1.50 | 10 (17%) |
| 19 | CLA | A | 1110 | - | 53,63,73 | 1.47 | 6 (11%) | 62,101,113 | 1.57 | 8 (12%) |
| 24 | LMG | J | 302 | - | 26,26,55 | 1.12 | 2 (7%) | 34,34,63 | 1.16 | 4 (11%) |
| 19 | CLA | A | 1102 | - | 43,53,73 | 1.56 | 6 (13%) | 50,89,113 | 1.56 | 7 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 19 | CLA | G | 201 | - | 48,58,73 | 1.54 | 5 (10%) | 56,95,113 | 1.50 | 7 (12%) |
| 21 | SF4 | A | 3001 | 2,1 | 0,12,12 | - | - | - | - | - |
| 19 | CLA | B | 1212 | - | 43,53,73 | 1.61 | 6 (13%) | 50,89,113 | 1.81 | 8 (16%) |
| 19 | CLA | B | 1232 | - | 43,53,73 | 1.66 | 5 (11%) | 50,89,113 | 1.96 | 9 (18%) |
| 23 | LHG | 2 | 630 | - | 31,31,48 | 0.79 | 2 (6%) | 34,37,54 | 1.24 | 3 (8%) |
| 19 | CLA | 3 | 607 | - | 58,68,73 | 1.40 | 5 (8%) | 68,107,113 | 1.38 | 6 (8%) |
| 19 | CLA | A | 1140 | - | 49,59,73 | 1.51 | 6 (12%) | 56,96,113 | 1.50 | 8 (14%) |
| 22 | BCR | 3 | 623 | - | 41,41,41 | 1.05 | 2 (4%) | 56,56,56 | 1.25 | 7 (12%) |
| 19 | CLA | B | 1229 | - | 53,63,73 | 1.45 | 6 (11%) | 62,101,113 | 1.45 | 8 (12%) |
| 19 | CLA | B | 1239 | - | 43,53,73 | 1.60 | 5 (11%) | 50,89,113 | 1.67 | 7 (14%) |
| 19 | CLA | F | 301 | - | 43,53,73 | 1.61 | 5 (11%) | 50,89,113 | 1.65 | 5 (10%) |
| 22 | BCR | F | 416 | - | 41,41,41 | 1.02 | 2 (4%) | 56,56,56 | 1.36 | 10 (17%) |
| 19 | CLA | A | 1112 | - | 43,53,73 | 1.59 | 6 (13%) | 50,89,113 | 1.48 | 9 (18%) |
| 19 | CLA | A | 1108 | - | 43,53,73 | 1.60 | 6 (13%) | 50,89,113 | 1.90 | 7 (14%) |
| 19 | CLA | B | 1217 | - | 43,53,73 | 1.58 | 5 (11%) | 50,89,113 | 1.54 | 7 (14%) |
| 19 | CLA | A | 1134 | - | 43,53,73 | 1.63 | 5 (11%) | 50,89,113 | 1.72 | 7 (14%) |
| 28 | LUT | 2 | 623 | - | 42,43,43 | 2.55 | 1 (2%) | 51,60,60 | 1.76 | 9 (17%) |
| 19 | CLA | B | 1227 | - | 43,53,73 | 1.63 | 7 (16%) | 50,89,113 | 1.83 | 12 (24%) |
| 19 | CLA | A | 1105 | - | 48,58,73 | 1.51 | 5 (10%) | 56,95,113 | 1.83 | 8 (14%) |
| 28 | LUT | 2 | 620 | - | 42,43,43 | 2.47 | 1 (2%) | 51,60,60 | 2.11 | 19 (37%) |
| 19 | CLA | B | 1219 | - | 43,53,73 | 1.65 | 6 (13%) | 50,89,113 | 1.86 | 10 (20%) |
| 19 | CLA | K | 203 | - | 28,35,73 | 2.27 | 8 (28%) | 28,60,113 | 1.67 | 5 (17%) |

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 |
|-----|------|-------|------|------|-----------|---------------|---------|
| 19 | CLA | 3 | 614 | - | 1/1/11/20 | 9/17/95/115 | - |
| 19 | CLA | B | 1234 | - | 1/1/12/20 | 6/21/99/115 | - |
| 22 | BCR | B | 4009 | - | - | 3/29/63/63 | 0/2/2/2 |
| 19 | CLA | A | 1126 | - | - | 11/31/109/115 | - |
| 24 | LMG | 2 | 631 | - | - | 6/31/51/70 | 0/1/1/1 |
| 22 | BCR | A | 4007 | - | - | 7/29/63/63 | 0/2/2/2 |
| 22 | BCR | M | 4021 | - | - | 5/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 19 | CLA | 1 | 604 | - | 1/1/12/20 | 4/19/97/115 | - |
| 22 | BCR | 1 | 623 | - | - | 5/18/35/63 | 0/1/1/2 |
| 19 | CLA | A | 1101 | - | 1/1/12/20 | 9/19/97/115 | - |
| 19 | CLA | B | 1021 | - | 1/1/15/20 | 16/37/115/115 | - |
| 19 | CLA | 4 | 613 | - | 1/1/13/20 | 7/25/103/115 | - |
| 23 | LHG | B | 5101 | - | - | 9/39/39/53 | - |
| 19 | CLA | 4 | 611 | - | - | 6/25/103/115 | - |
| 22 | BCR | B | 4010 | - | - | 6/29/63/63 | 0/2/2/2 |
| 19 | CLA | 3 | 604 | - | 1/1/12/20 | 5/19/97/115 | - |
| 19 | CLA | A | 8895 | - | - | 9/37/115/115 | - |
| 19 | CLA | B | 1220 | - | 1/1/11/20 | 4/13/91/115 | - |
| 24 | LMG | J | 301 | - | - | 15/44/64/70 | 0/1/1/1 |
| 19 | CLA | K | 201 | - | 1/1/13/20 | 7/25/103/115 | - |
| 27 | CHL | 2 | 606 | - | 3/3/16/26 | 7/15/113/137 | - |
| 19 | CLA | 4 | 610 | - | 1/1/13/20 | 6/25/103/115 | - |
| 19 | CLA | A | 1117 | - | 1/1/15/20 | 10/37/115/115 | - |
| 19 | CLA | 4 | 602 | - | 1/1/14/20 | 3/31/109/115 | - |
| 19 | CLA | A | 1109 | - | 1/1/15/20 | 8/37/115/115 | - |
| 19 | CLA | 1 | 609 | - | 1/1/14/20 | 6/31/109/115 | - |
| 27 | CHL | 2 | 608 | - | 3/3/16/26 | 9/18/116/137 | - |
| 28 | LUT | 4 | 623 | - | 1/1/12/27 | 12/29/67/67 | 0/2/2/2 |
| 19 | CLA | L | 301 | - | - | 7/19/97/115 | - |
| 21 | SF4 | C | 1003 | 7 | - | - | 0/6/5/5 |
| 19 | CLA | B | 1203 | - | 1/1/15/20 | 12/37/115/115 | - |
| 19 | CLA | L | 302 | - | - | 12/31/109/115 | - |
| 19 | CLA | K | 204 | - | 1/1/11/20 | 6/13/91/115 | - |
| 19 | CLA | B | 1224 | - | 1/1/14/20 | 11/33/111/115 | - |
| 19 | CLA | 4 | 614 | - | 1/1/11/20 | 7/15/93/115 | - |
| 19 | CLA | B | 1238 | - | 1/1/15/20 | 14/37/115/115 | - |
| 19 | CLA | 3 | 602 | - | 1/1/14/20 | 7/31/109/115 | - |
| 28 | LUT | 4 | 621 | - | - | 4/29/67/67 | 0/2/2/2 |
| 19 | CLA | 1 | 603 | - | 1/1/13/20 | 14/25/103/115 | - |
| 19 | CLA | 2 | 604 | - | 1/1/12/20 | 4/19/97/115 | - |
| 19 | CLA | F | 302 | - | 1/1/11/20 | 6/15/93/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 27 | CHL | 4 | 607 | - | 3/3/16/26 | 7/17/115/137 | - |
| 19 | CLA | A | 1128 | - | - | 12/37/115/115 | - |
| 19 | CLA | B | 1201 | - | 1/1/12/20 | 10/19/97/115 | - |
| 19 | CLA | A | 1121 | - | 1/1/12/20 | 7/21/99/115 | - |
| 22 | BCR | A | 4008 | - | - | 11/29/63/63 | 0/2/2/2 |
| 19 | CLA | 4 | 604 | - | 1/1/12/20 | 6/19/97/115 | - |
| 22 | BCR | I | 118 | - | - | 11/29/63/63 | 0/2/2/2 |
| 19 | CLA | A | 1133 | - | - | 7/13/91/115 | - |
| 19 | CLA | A | 1801 | - | 1/1/12/20 | 7/19/97/115 | - |
| 19 | CLA | A | 1104 | - | - | 17/37/115/115 | - |
| 19 | CLA | 1 | 611 | - | - | 4/15/93/115 | - |
| 22 | BCR | K | 301 | - | - | 14/29/63/63 | 0/2/2/2 |
| 28 | LUT | 3 | 620 | - | - | 2/29/67/67 | 0/2/2/2 |
| 19 | CLA | 2 | 610 | - | 1/1/14/20 | 9/31/109/115 | - |
| 19 | CLA | B | 1205 | - | 1/1/15/20 | 8/37/115/115 | - |
| 19 | CLA | B | 1213 | - | - | 6/25/103/115 | - |
| 19 | CLA | 1 | 614 | - | 1/1/11/20 | 6/15/93/115 | - |
| 26 | DGD | B | 5002 | - | - | 18/50/90/95 | 0/2/2/2 |
| 19 | CLA | 3 | 611 | - | 1/1/10/20 | 2/8/86/115 | - |
| 19 | CLA | B | 1214 | - | - | 8/30/108/115 | - |
| 22 | BCR | 3 | 624 | - | - | 16/29/63/63 | 0/2/2/2 |
| 19 | CLA | 4 | 601 | - | 1/1/12/20 | 8/19/97/115 | - |
| 19 | CLA | 3 | 612 | - | 1/1/11/20 | 4/13/91/115 | - |
| 19 | CLA | A | 5005 | - | - | 6/19/97/115 | - |
| 22 | BCR | J | 212 | - | - | 14/29/63/63 | 0/2/2/2 |
| 19 | CLA | 3 | 613 | - | 1/1/13/20 | 8/25/103/115 | - |
| 23 | LHG | A | 5003 | - | - | 11/35/35/53 | - |
| 28 | LUT | 2 | 621 | - | - | 2/29/67/67 | 0/2/2/2 |
| 23 | LHG | 1 | 630 | - | - | 14/41/41/53 | - |
| 19 | CLA | J | 102 | - | 1/1/11/20 | 8/13/91/115 | - |
| 28 | LUT | 3 | 621 | - | - | 8/29/67/67 | 0/2/2/2 |
| 19 | CLA | B | 1209 | - | - | 2/13/91/115 | - |
| 19 | CLA | A | 1124 | - | - | 11/28/106/115 | - |
| 19 | CLA | A | 1120 | - | - | 3/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 19 | CLA | 1 | 610 | - | 1/1/13/20 | 6/25/103/115 | - |
| 19 | CLA | A | 1127 | - | - | 18/37/115/115 | - |
| 22 | BCR | L | 419 | - | - | 4/29/63/63 | 0/2/2/2 |
| 22 | BCR | A | 4011 | - | - | 18/29/63/63 | 0/2/2/2 |
| 28 | LUT | 1 | 620 | - | - | 5/29/67/67 | 0/2/2/2 |
| 19 | CLA | B | 1216 | - | 1/1/13/20 | 7/25/103/115 | - |
| 19 | CLA | A | 1132 | - | 1/1/15/20 | 8/37/115/115 | - |
| 27 | CHL | 4 | 606 | - | 3/3/16/26 | 9/17/115/137 | - |
| 22 | BCR | J | 213 | - | - | 8/29/63/63 | 0/2/2/2 |
| 19 | CLA | 1 | 608 | - | 1/1/12/20 | 3/19/97/115 | - |
| 19 | CLA | B | 1236 | - | - | 4/16/94/115 | - |
| 19 | CLA | B | 1206 | - | - | 7/16/94/115 | - |
| 19 | CLA | A | 1130 | - | - | 6/31/109/115 | - |
| 19 | CLA | I | 121 | - | - | 12/37/115/115 | - |
| 19 | CLA | B | 1204 | - | 1/1/14/20 | 7/33/111/115 | - |
| 19 | CLA | 3 | 610 | - | 1/1/13/20 | 8/25/103/115 | - |
| 19 | CLA | A | 1138 | - | 1/1/14/20 | 7/31/109/115 | - |
| 19 | CLA | A | 1118 | - | - | 13/25/103/115 | - |
| 19 | CLA | B | 1235 | - | 1/1/13/20 | 8/25/103/115 | - |
| 22 | BCR | I | 120 | - | - | 14/29/63/63 | 0/2/2/2 |
| 19 | CLA | B | 1023 | - | - | 8/33/111/115 | - |
| 19 | CLA | B | 1012 | - | 1/1/13/20 | 13/25/103/115 | - |
| 19 | CLA | A | 1119 | - | 1/1/15/20 | 10/37/115/115 | - |
| 19 | CLA | B | 1222 | - | 1/1/11/20 | 6/15/93/115 | - |
| 19 | CLA | 3 | 617 | - | 1/1/11/20 | 6/15/93/115 | - |
| 19 | CLA | A | 1135 | - | - | 7/21/99/115 | - |
| 22 | BCR | A | 4002 | - | - | 9/29/63/63 | 0/2/2/2 |
| 19 | CLA | A | 1113 | - | - | 3/13/91/115 | - |
| 19 | CLA | A | 1114 | - | 1/1/11/20 | 6/13/91/115 | - |
| 19 | CLA | B | 1211 | - | 1/1/13/20 | 9/27/105/115 | - |
| 19 | CLA | 3 | 605 | - | 1/1/5/20 | - | - |
| 27 | CHL | 2 | 602 | - | 3/3/18/26 | 13/27/125/137 | - |
| 19 | CLA | G | 218 | - | - | 8/25/103/115 | - |
| 22 | BCR | G | 311 | - | - | 7/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 19 | CLA | A | 1122 | - | 1/1/14/20 | 12/31/109/115 | - |
| 19 | CLA | 2 | 603 | - | 1/1/11/20 | 6/15/93/115 | - |
| 19 | CLA | B | 1231 | - | - | 5/13/91/115 | - |
| 19 | CLA | B | 1208 | - | 1/1/11/20 | 3/13/91/115 | - |
| 19 | CLA | H | 200 | - | 1/1/11/20 | 4/13/91/115 | - |
| 20 | PQN | A | 2001 | - | - | 6/23/43/43 | 0/2/2/2 |
| 27 | CHL | 3 | 608 | - | 3/3/16/26 | 5/17/115/137 | - |
| 27 | CHL | 2 | 601 | - | 3/3/20/26 | 22/39/137/137 | - |
| 19 | CLA | B | 1237 | - | 1/1/15/20 | 11/37/115/115 | - |
| 22 | BCR | B | 2004 | - | - | 14/29/63/63 | 0/2/2/2 |
| 19 | CLA | A | 1111 | - | - | 14/37/115/115 | - |
| 27 | CHL | 4 | 615 | - | 3/3/15/26 | 2/12/110/137 | - |
| 25 | LMT | B | 5001 | - | - | 4/17/57/61 | 0/2/2/2 |
| 19 | CLA | A | 1116 | - | 1/1/12/20 | 7/24/102/115 | - |
| 19 | CLA | 2 | 612 | - | 1/1/12/20 | 5/22/100/115 | - |
| 19 | CLA | 1 | 615 | - | 1/1/11/20 | 8/15/93/115 | - |
| 20 | PQN | B | 2002 | - | - | 8/23/43/43 | 0/2/2/2 |
| 22 | BCR | B | 4005 | - | - | 8/29/63/63 | 0/2/2/2 |
| 22 | BCR | B | 4014 | - | - | 19/29/63/63 | 0/2/2/2 |
| 25 | LMT | 1 | 631 | - | - | 6/21/61/61 | 0/2/2/2 |
| 23 | LHG | A | 5001 | - | - | 20/53/53/53 | - |
| 19 | CLA | B | 1225 | - | - | 15/37/115/115 | - |
| 19 | CLA | B | 1223 | - | 1/1/15/20 | 6/37/115/115 | - |
| 19 | CLA | B | 1226 | - | 1/1/13/20 | 6/25/103/115 | - |
| 19 | CLA | A | 1136 | - | 1/1/15/20 | 10/37/115/115 | - |
| 23 | LHG | 3 | 630 | - | - | 12/38/38/53 | - |
| 25 | LMT | G | 402 | - | - | 6/17/57/61 | 0/2/2/2 |
| 19 | CLA | 1 | 612 | - | 1/1/11/20 | 6/15/93/115 | - |
| 19 | CLA | B | 1230 | - | 1/1/11/20 | 6/13/91/115 | - |
| 19 | CLA | A | 1107 | - | - | 8/13/91/115 | - |
| 19 | CLA | 2 | 613 | - | 1/1/15/20 | 11/37/115/115 | - |
| 19 | CLA | B | 1240 | - | 1/1/15/20 | 12/37/115/115 | - |
| 19 | CLA | 1 | 613 | - | 1/1/13/20 | 7/25/103/115 | - |
| 19 | CLA | A | 1106 | - | 1/1/13/20 | 7/25/103/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 19 | CLA | B | 1221 | - | - | 1/24/102/115 | - |
| 21 | SF4 | C | 1002 | 7 | - | - | 0/6/5/5 |
| 19 | CLA | 4 | 609 | - | 1/1/13/20 | 9/25/103/115 | - |
| 19 | CLA | B | 1210 | - | 1/1/15/20 | 22/37/115/115 | - |
| 19 | CLA | L | 303 | - | 1/1/11/20 | 7/13/91/115 | - |
| 28 | LUT | 1 | 621 | - | - | 5/29/67/67 | 0/2/2/2 |
| 19 | CLA | K | 202 | - | 1/1/11/20 | 8/15/93/115 | - |
| 19 | CLA | A | 1022 | - | 1/1/15/20 | 9/37/115/115 | - |
| 19 | CLA | 1 | 606 | - | 1/1/11/20 | 6/13/91/115 | - |
| 27 | CHL | 4 | 608 | - | 3/3/17/26 | 8/21/119/137 | - |
| 27 | CHL | 2 | 607 | - | 3/3/16/26 | 8/17/115/137 | - |
| 22 | BCR | A | 4001 | - | - | 15/29/63/63 | 0/2/2/2 |
| 19 | CLA | 3 | 609 | - | 1/1/14/20 | 10/31/109/115 | - |
| 22 | BCR | B | 4006 | - | - | 11/29/63/63 | 0/2/2/2 |
| 19 | CLA | 4 | 603 | - | 1/1/13/20 | 11/25/103/115 | - |
| 19 | CLA | 4 | 612 | - | 1/1/11/20 | 8/15/93/115 | - |
| 19 | CLA | 3 | 606 | - | 1/1/11/20 | 9/15/93/115 | - |
| 24 | LMG | A | 5002 | - | - | 13/29/49/70 | 0/1/1/1 |
| 27 | CHL | 2 | 615 | - | 3/3/16/26 | 11/17/115/137 | - |
| 19 | CLA | B | 1228 | - | 1/1/11/20 | 8/18/96/115 | - |
| 19 | CLA | A | 1013 | - | - | 3/27/105/115 | - |
| 22 | BCR | B | 4017 | - | - | 17/29/63/63 | 0/2/2/2 |
| 19 | CLA | 3 | 603 | - | - | 11/25/103/115 | - |
| 18 | CL0 | A | 1011 | - | 2/2/20/25 | 6/37/135/135 | - |
| 19 | CLA | F | 303 | - | 1/1/5/20 | - | - |
| 19 | CLA | A | 1139 | - | 1/1/12/20 | 4/19/97/115 | - |
| 19 | CLA | B | 1202 | - | 1/1/15/20 | 10/37/115/115 | - |
| 25 | LMT | G | 401 | - | - | 5/21/61/61 | 0/2/2/2 |
| 28 | LUT | 4 | 620 | - | - | 9/29/67/67 | 0/2/2/2 |
| 19 | CLA | 2 | 609 | - | 1/1/13/20 | 2/25/103/115 | - |
| 27 | CHL | 1 | 607 | - | 3/3/16/26 | 8/17/115/137 | - |
| 23 | LHG | 4 | 630 | - | - | 15/42/42/53 | - |
| 25 | LMT | 4 | 631 | - | - | 4/21/61/61 | 0/2/2/2 |
| 19 | CLA | A | 1125 | - | 1/1/14/20 | 13/31/109/115 | - |
| 19 | CLA | 1 | 602 | - | 1/1/14/20 | 2/31/109/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 27 | CHL | 1 | 601 | - | 3/3/18/26 | 10/27/125/137 | - |
| 27 | CHL | 2 | 611 | - | 3/3/18/26 | 6/27/125/137 | - |
| 19 | CLA | A | 1137 | - | 1/1/11/20 | 5/13/91/115 | - |
| 19 | CLA | G | 202 | - | 1/1/11/20 | 7/15/93/115 | - |
| 19 | CLA | A | 1103 | - | 1/1/15/20 | 15/37/115/115 | - |
| 25 | LMT | A | 5004 | - | - | 7/19/59/61 | 0/2/2/2 |
| 19 | CLA | 2 | 614 | - | 1/1/12/20 | 5/19/97/115 | - |
| 19 | CLA | A | 1115 | - | - | 6/24/102/115 | - |
| 22 | BCR | A | 4003 | - | - | 12/29/63/63 | 0/2/2/2 |
| 19 | CLA | B | 1215 | - | 1/1/14/20 | 11/31/109/115 | - |
| 19 | CLA | A | 1131 | - | 1/1/15/20 | 5/37/115/115 | - |
| 22 | BCR | L | 420 | - | - | 7/29/63/63 | 0/2/2/2 |
| 19 | CLA | A | 1110 | - | 1/1/13/20 | 6/25/103/115 | - |
| 24 | LMG | J | 302 | - | - | 6/21/41/70 | 0/1/1/1 |
| 19 | CLA | A | 1102 | - | - | 6/13/91/115 | - |
| 19 | CLA | G | 201 | - | 1/1/12/20 | 4/19/97/115 | - |
| 21 | SF4 | A | 3001 | 2,1 | - | - | 0/6/5/5 |
| 19 | CLA | B | 1212 | - | - | 3/13/91/115 | - |
| 19 | CLA | B | 1232 | - | 1/1/11/20 | 4/13/91/115 | - |
| 23 | LHG | 2 | 630 | - | - | 10/36/36/53 | - |
| 19 | CLA | 3 | 607 | - | 1/1/14/20 | 17/31/109/115 | - |
| 19 | CLA | A | 1140 | - | - | 6/21/99/115 | - |
| 22 | BCR | 3 | 623 | - | - | 14/29/63/63 | 0/2/2/2 |
| 19 | CLA | B | 1229 | - | 1/1/13/20 | 8/25/103/115 | - |
| 19 | CLA | B | 1239 | - | - | 5/13/91/115 | - |
| 19 | CLA | F | 301 | - | 1/1/11/20 | 2/13/91/115 | - |
| 22 | BCR | F | 416 | - | - | 17/29/63/63 | 0/2/2/2 |
| 19 | CLA | A | 1112 | - | - | 4/13/91/115 | - |
| 19 | CLA | A | 1108 | - | 1/1/11/20 | 5/13/91/115 | - |
| 19 | CLA | B | 1217 | - | - | 5/13/91/115 | - |
| 19 | CLA | A | 1134 | - | - | 6/13/91/115 | - |
| 28 | LUT | 2 | 623 | - | 1/1/12/27 | 9/29/67/67 | 0/2/2/2 |
| 19 | CLA | B | 1227 | - | - | 1/13/91/115 | - |
| 19 | CLA | A | 1105 | - | 1/1/12/20 | 0/19/97/115 | - |
| 28 | LUT | 2 | 620 | - | - | 6/29/67/67 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|----------|-------------|-------|
| 19 | CLA | B | 1219 | - | - | 3/13/91/115 | - |
| 19 | CLA | K | 203 | - | 1/1/5/20 | - | - |

The worst 5 of 1121 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28 | 1 | 620 | LUT | C24-C25 | 16.76 | 1.53 | 1.33 |
| 28 | 1 | 621 | LUT | C24-C25 | 16.27 | 1.52 | 1.33 |
| 28 | 2 | 623 | LUT | C24-C25 | 15.79 | 1.51 | 1.33 |
| 28 | 4 | 620 | LUT | C24-C25 | 15.47 | 1.51 | 1.33 |
| 28 | 2 | 620 | LUT | C24-C25 | 15.22 | 1.51 | 1.33 |

The worst 5 of 1822 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 28 | 4 | 621 | LUT | O23-C23-C22 | -11.92 | 88.94 | 110.06 |
| 19 | 2 | 609 | CLA | C4A-NA-C1A | 10.10 | 111.29 | 106.68 |
| 19 | 4 | 609 | CLA | C4A-NA-C1A | 9.85 | 111.17 | 106.68 |
| 19 | 1 | 609 | CLA | C4A-NA-C1A | 9.25 | 110.90 | 106.68 |
| 19 | A | 1106 | CLA | C4A-NA-C1A | 9.16 | 110.86 | 106.68 |

5 of 145 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 18 | A | 1011 | CL0 | NC |
| 18 | A | 1011 | CL0 | NA |
| 19 | A | 1022 | CLA | ND |
| 19 | A | 1101 | CLA | ND |
| 19 | A | 1103 | CLA | ND |

5 of 1710 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 19 | A | 1013 | CLA | CBD-CGD-O2D-CED |
| 19 | A | 1022 | CLA | C1A-C2A-CAA-CBA |
| 19 | A | 1022 | CLA | C3A-C2A-CAA-CBA |
| 19 | A | 1101 | CLA | CHA-CBD-CGD-O1D |
| 19 | A | 1101 | CLA | CHA-CBD-CGD-O2D |

There are no ring outliers.

167 monomers are involved in 365 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22 | B | 4009 | BCR | 2 | 0 |
| 19 | A | 1126 | CLA | 5 | 0 |
| 22 | A | 4007 | BCR | 2 | 0 |
| 22 | M | 4021 | BCR | 5 | 0 |
| 19 | A | 1101 | CLA | 2 | 0 |
| 19 | B | 1021 | CLA | 3 | 0 |
| 22 | B | 4010 | BCR | 5 | 0 |
| 19 | 3 | 604 | CLA | 1 | 0 |
| 19 | A | 8895 | CLA | 3 | 0 |
| 19 | B | 1220 | CLA | 2 | 0 |
| 24 | J | 301 | LMG | 3 | 0 |
| 19 | K | 201 | CLA | 1 | 0 |
| 19 | 4 | 610 | CLA | 3 | 0 |
| 19 | A | 1117 | CLA | 7 | 0 |
| 19 | 4 | 602 | CLA | 2 | 0 |
| 19 | A | 1109 | CLA | 2 | 0 |
| 19 | 1 | 609 | CLA | 3 | 0 |
| 19 | L | 301 | CLA | 1 | 0 |
| 27 | 2 | 608 | CHL | 3 | 0 |
| 28 | 4 | 623 | LUT | 1 | 0 |
| 19 | B | 1203 | CLA | 4 | 0 |
| 19 | L | 302 | CLA | 5 | 0 |
| 19 | K | 204 | CLA | 2 | 0 |
| 19 | B | 1224 | CLA | 4 | 0 |
| 19 | B | 1238 | CLA | 7 | 0 |
| 19 | 3 | 602 | CLA | 3 | 0 |
| 28 | 4 | 621 | LUT | 2 | 0 |
| 19 | 1 | 603 | CLA | 4 | 0 |
| 19 | 2 | 604 | CLA | 1 | 0 |
| 19 | A | 1128 | CLA | 5 | 0 |
| 19 | B | 1201 | CLA | 3 | 0 |
| 22 | A | 4008 | BCR | 2 | 0 |
| 22 | I | 118 | BCR | 1 | 0 |
| 19 | A | 1133 | CLA | 2 | 0 |
| 19 | A | 1801 | CLA | 1 | 0 |
| 19 | A | 1104 | CLA | 5 | 0 |
| 22 | K | 301 | BCR | 1 | 0 |
| 28 | 3 | 620 | LUT | 7 | 0 |
| 19 | 2 | 610 | CLA | 2 | 0 |
| 19 | B | 1205 | CLA | 4 | 0 |
| 19 | B | 1213 | CLA | 3 | 0 |
| 26 | B | 5002 | DGD | 5 | 0 |
| 19 | B | 1214 | CLA | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22 | 3 | 624 | BCR | 4 | 0 |
| 19 | 4 | 601 | CLA | 1 | 0 |
| 19 | 3 | 612 | CLA | 1 | 0 |
| 19 | A | 5005 | CLA | 4 | 0 |
| 22 | J | 212 | BCR | 1 | 0 |
| 19 | 3 | 613 | CLA | 2 | 0 |
| 23 | A | 5003 | LHG | 1 | 0 |
| 28 | 2 | 621 | LUT | 2 | 0 |
| 23 | 1 | 630 | LHG | 1 | 0 |
| 28 | 3 | 621 | LUT | 2 | 0 |
| 19 | B | 1209 | CLA | 2 | 0 |
| 19 | A | 1124 | CLA | 3 | 0 |
| 19 | A | 1120 | CLA | 1 | 0 |
| 19 | 1 | 610 | CLA | 1 | 0 |
| 19 | A | 1127 | CLA | 6 | 0 |
| 22 | L | 419 | BCR | 3 | 0 |
| 22 | A | 4011 | BCR | 1 | 0 |
| 28 | 1 | 620 | LUT | 3 | 0 |
| 19 | B | 1216 | CLA | 2 | 0 |
| 19 | A | 1132 | CLA | 4 | 0 |
| 22 | J | 213 | BCR | 3 | 0 |
| 19 | B | 1236 | CLA | 1 | 0 |
| 19 | B | 1206 | CLA | 4 | 0 |
| 19 | A | 1130 | CLA | 3 | 0 |
| 19 | I | 121 | CLA | 7 | 0 |
| 19 | B | 1204 | CLA | 5 | 0 |
| 19 | 3 | 610 | CLA | 4 | 0 |
| 19 | A | 1138 | CLA | 5 | 0 |
| 19 | A | 1118 | CLA | 4 | 0 |
| 19 | B | 1235 | CLA | 2 | 0 |
| 22 | I | 120 | BCR | 5 | 0 |
| 19 | B | 1023 | CLA | 5 | 0 |
| 19 | B | 1012 | CLA | 6 | 0 |
| 19 | A | 1119 | CLA | 2 | 0 |
| 19 | 3 | 617 | CLA | 1 | 0 |
| 19 | A | 1135 | CLA | 2 | 0 |
| 19 | A | 1113 | CLA | 1 | 0 |
| 19 | A | 1114 | CLA | 2 | 0 |
| 27 | 2 | 602 | CHL | 2 | 0 |
| 22 | G | 311 | BCR | 4 | 0 |
| 19 | A | 1122 | CLA | 4 | 0 |
| 19 | B | 1231 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 19 | B | 1208 | CLA | 4 | 0 |
| 19 | H | 200 | CLA | 2 | 0 |
| 20 | A | 2001 | PQN | 2 | 0 |
| 27 | 3 | 608 | CHL | 3 | 0 |
| 27 | 2 | 601 | CHL | 7 | 0 |
| 19 | B | 1237 | CLA | 8 | 0 |
| 22 | B | 2004 | BCR | 1 | 0 |
| 19 | A | 1111 | CLA | 6 | 0 |
| 19 | A | 1116 | CLA | 4 | 0 |
| 20 | B | 2002 | PQN | 5 | 0 |
| 22 | B | 4005 | BCR | 3 | 0 |
| 22 | B | 4014 | BCR | 7 | 0 |
| 25 | 1 | 631 | LMT | 2 | 0 |
| 23 | A | 5001 | LHG | 3 | 0 |
| 19 | B | 1225 | CLA | 6 | 0 |
| 19 | B | 1223 | CLA | 6 | 0 |
| 19 | B | 1226 | CLA | 3 | 0 |
| 19 | A | 1136 | CLA | 3 | 0 |
| 23 | 3 | 630 | LHG | 1 | 0 |
| 19 | B | 1230 | CLA | 3 | 0 |
| 19 | A | 1107 | CLA | 1 | 0 |
| 19 | 2 | 613 | CLA | 1 | 0 |
| 19 | B | 1240 | CLA | 2 | 0 |
| 19 | A | 1106 | CLA | 2 | 0 |
| 19 | B | 1221 | CLA | 5 | 0 |
| 19 | B | 1210 | CLA | 6 | 0 |
| 19 | L | 303 | CLA | 4 | 0 |
| 28 | 1 | 621 | LUT | 5 | 0 |
| 19 | A | 1022 | CLA | 8 | 0 |
| 19 | 1 | 606 | CLA | 1 | 0 |
| 22 | A | 4001 | BCR | 1 | 0 |
| 27 | 4 | 608 | CHL | 1 | 0 |
| 19 | 3 | 609 | CLA | 4 | 0 |
| 22 | B | 4006 | BCR | 4 | 0 |
| 19 | 4 | 603 | CLA | 4 | 0 |
| 19 | 3 | 606 | CLA | 1 | 0 |
| 24 | A | 5002 | LMG | 2 | 0 |
| 19 | A | 1013 | CLA | 2 | 0 |
| 19 | B | 1228 | CLA | 3 | 0 |
| 22 | B | 4017 | BCR | 6 | 0 |
| 18 | A | 1011 | CL0 | 6 | 0 |
| 19 | A | 1139 | CLA | 2 | 0 |

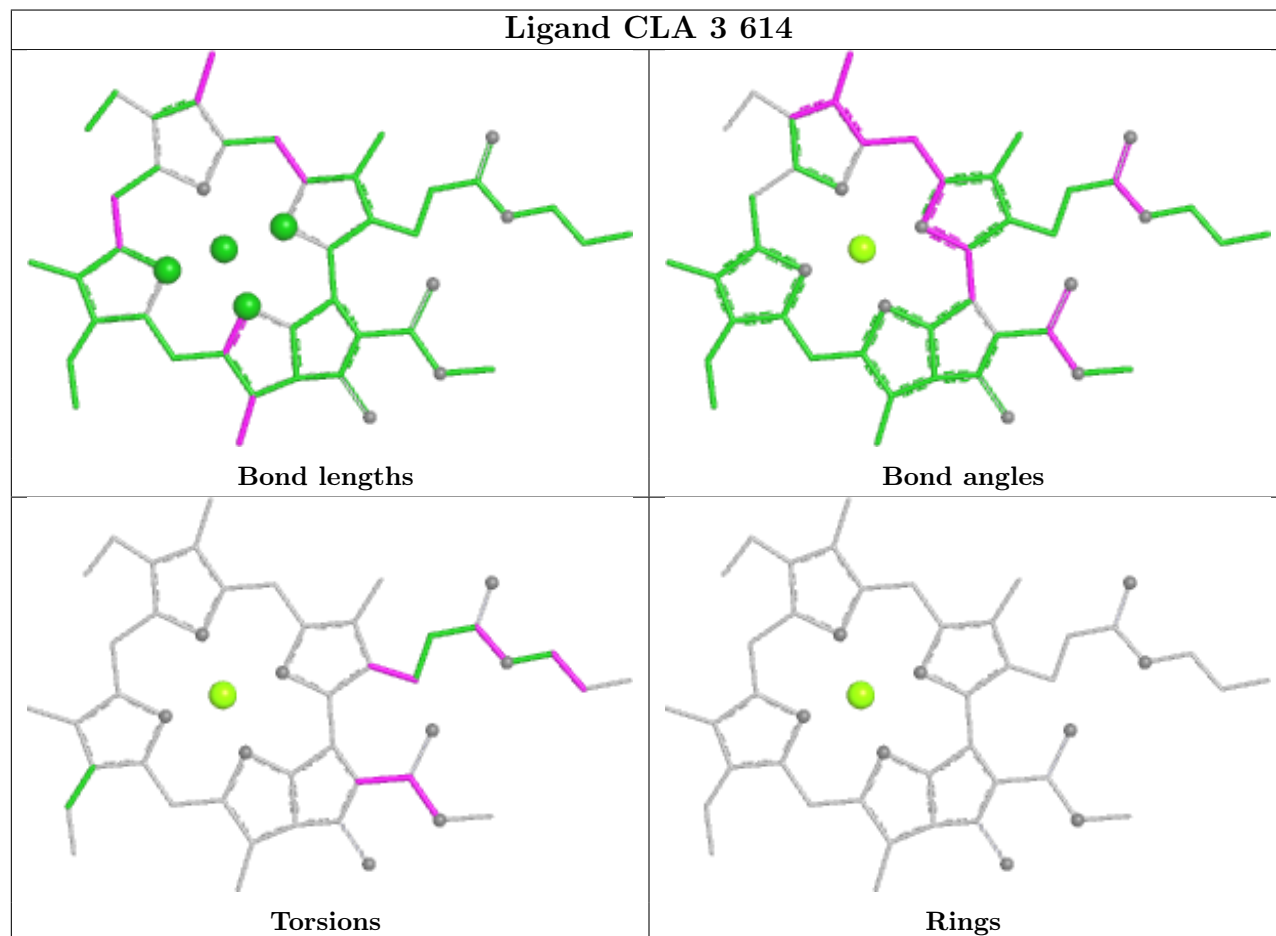
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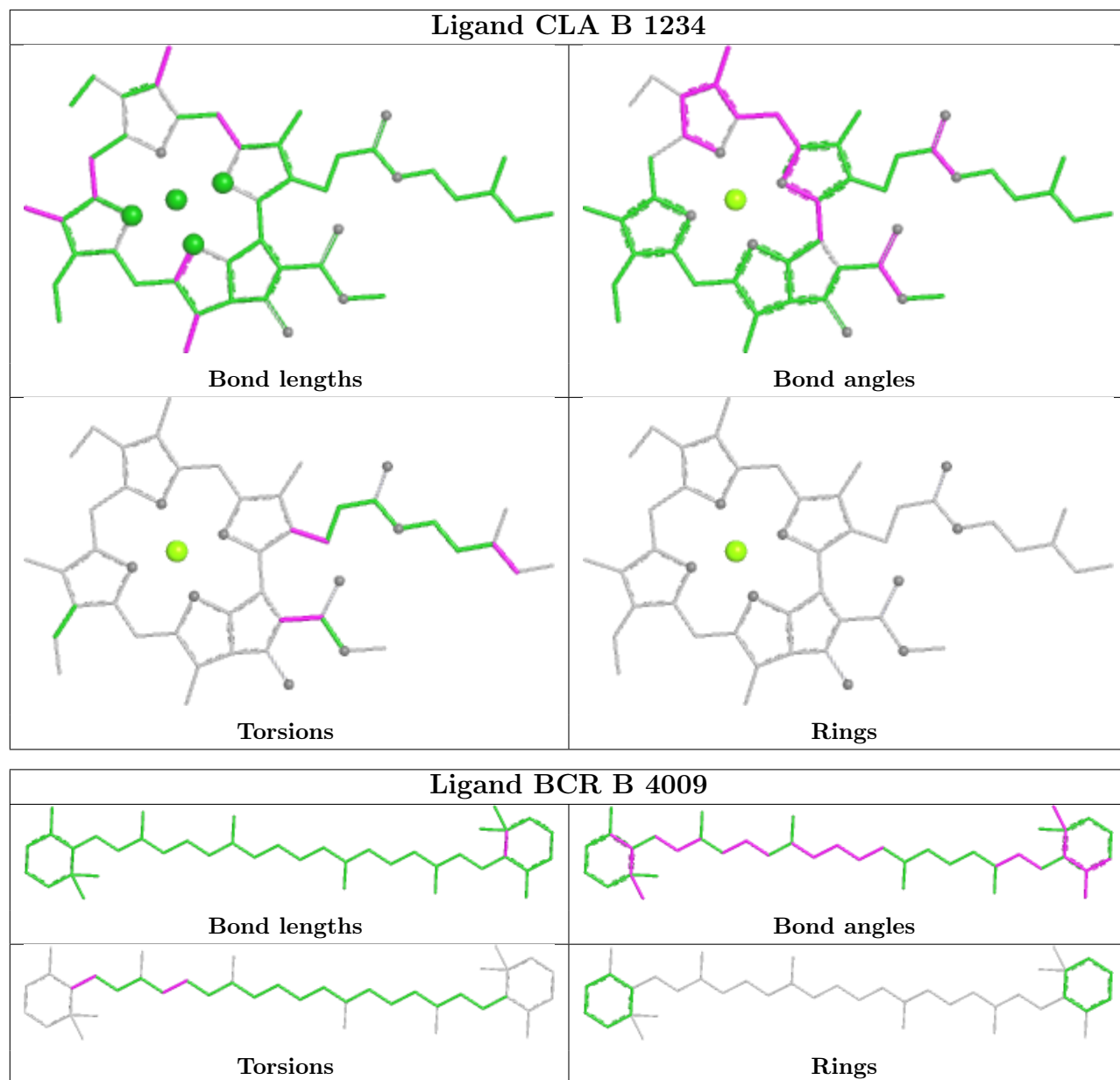
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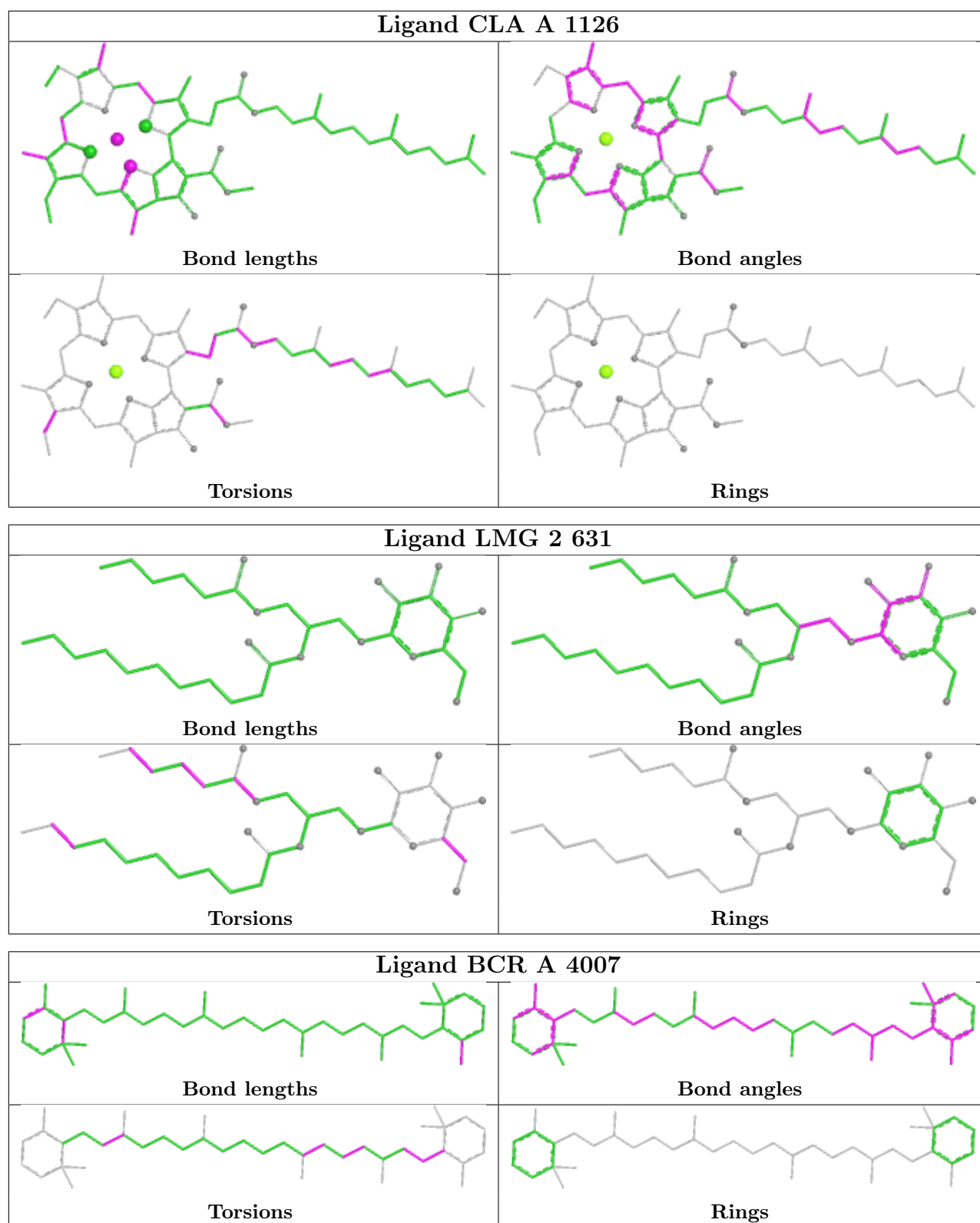
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 19 | B | 1202 | CLA | 6 | 0 |
| 25 | G | 401 | LMT | 3 | 0 |
| 28 | 4 | 620 | LUT | 4 | 0 |
| 19 | 2 | 609 | CLA | 1 | 0 |
| 23 | 4 | 630 | LHG | 2 | 0 |
| 27 | 1 | 607 | CHL | 2 | 0 |
| 25 | 4 | 631 | LMT | 3 | 0 |
| 19 | A | 1125 | CLA | 2 | 0 |
| 19 | 1 | 602 | CLA | 2 | 0 |
| 27 | 1 | 601 | CHL | 1 | 0 |
| 19 | A | 1137 | CLA | 3 | 0 |
| 19 | G | 202 | CLA | 1 | 0 |
| 19 | A | 1103 | CLA | 4 | 0 |
| 25 | A | 5004 | LMT | 1 | 0 |
| 19 | A | 1115 | CLA | 1 | 0 |
| 22 | A | 4003 | BCR | 2 | 0 |
| 19 | B | 1215 | CLA | 2 | 0 |
| 19 | A | 1131 | CLA | 2 | 0 |
| 22 | L | 420 | BCR | 4 | 0 |
| 19 | A | 1110 | CLA | 2 | 0 |
| 24 | J | 302 | LMG | 1 | 0 |
| 19 | A | 1102 | CLA | 4 | 0 |
| 19 | B | 1212 | CLA | 1 | 0 |
| 19 | B | 1232 | CLA | 1 | 0 |
| 23 | 2 | 630 | LHG | 2 | 0 |
| 19 | 3 | 607 | CLA | 1 | 0 |
| 19 | A | 1140 | CLA | 4 | 0 |
| 22 | 3 | 623 | BCR | 1 | 0 |
| 19 | B | 1229 | CLA | 1 | 0 |
| 19 | B | 1239 | CLA | 2 | 0 |
| 19 | F | 301 | CLA | 4 | 0 |
| 22 | F | 416 | BCR | 2 | 0 |
| 19 | A | 1108 | CLA | 3 | 0 |
| 19 | B | 1217 | CLA | 4 | 0 |
| 19 | A | 1134 | CLA | 1 | 0 |
| 28 | 2 | 623 | LUT | 2 | 0 |
| 19 | B | 1227 | CLA | 2 | 0 |
| 19 | A | 1105 | CLA | 1 | 0 |
| 28 | 2 | 620 | LUT | 6 | 0 |
| 19 | B | 1219 | CLA | 1 | 0 |

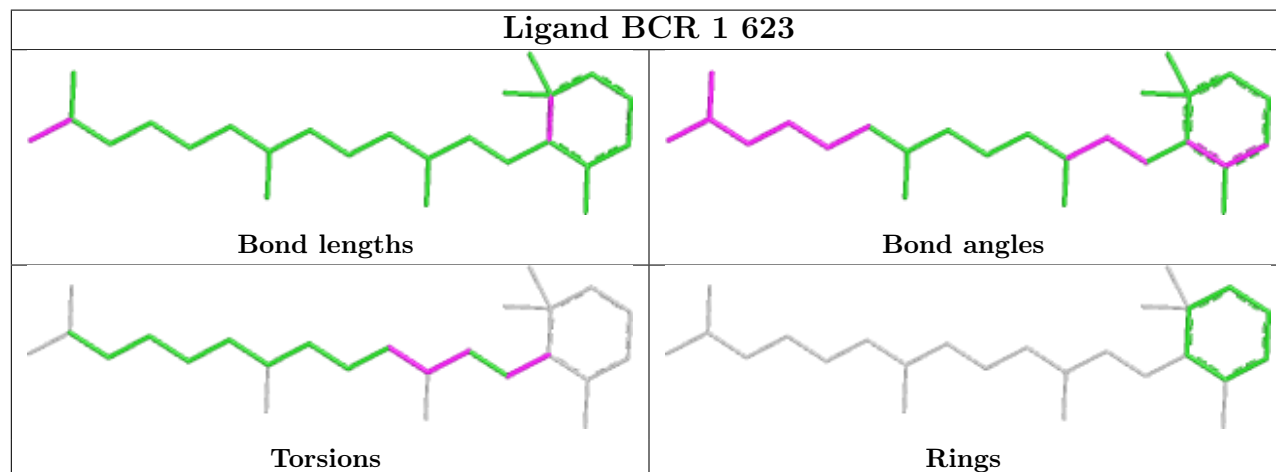
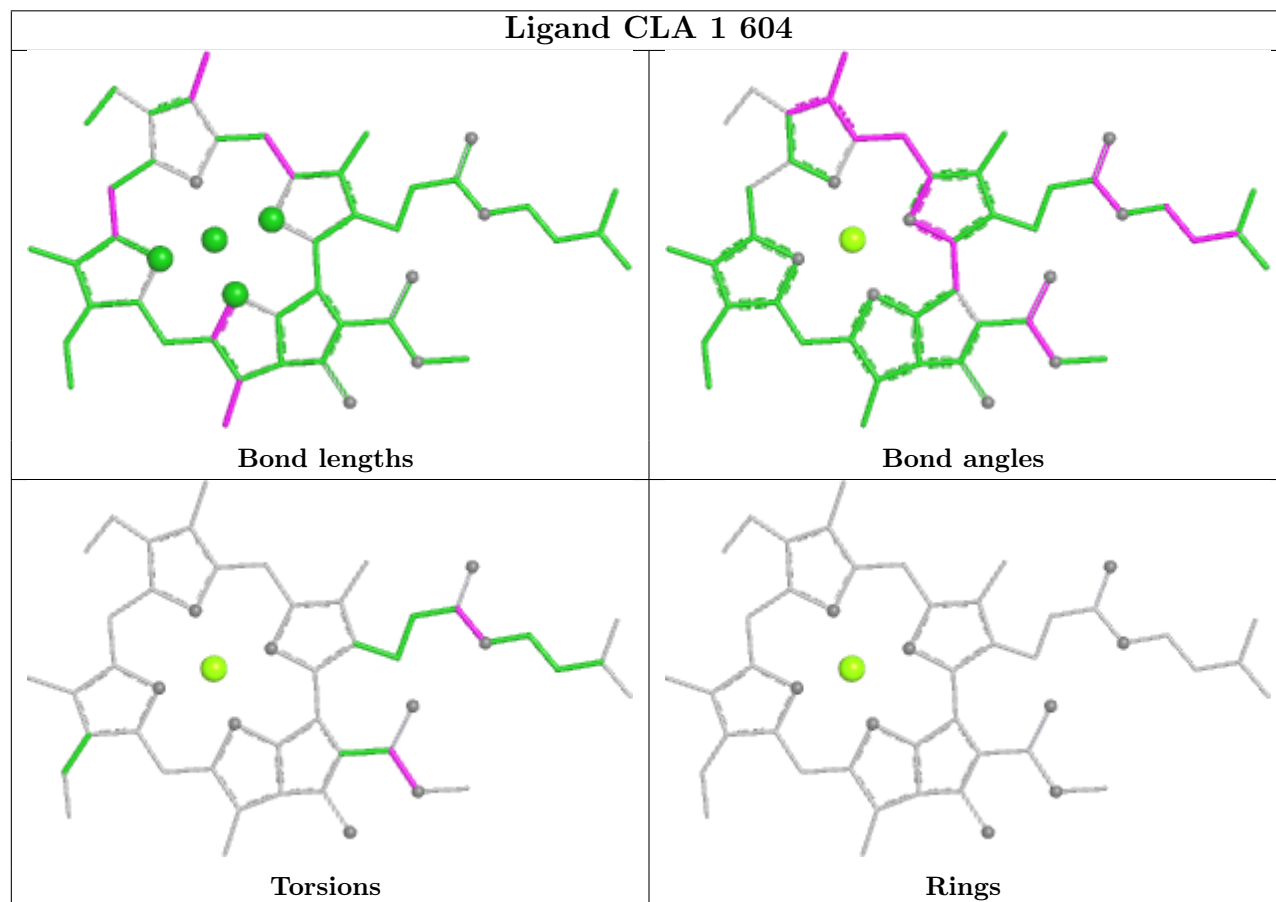
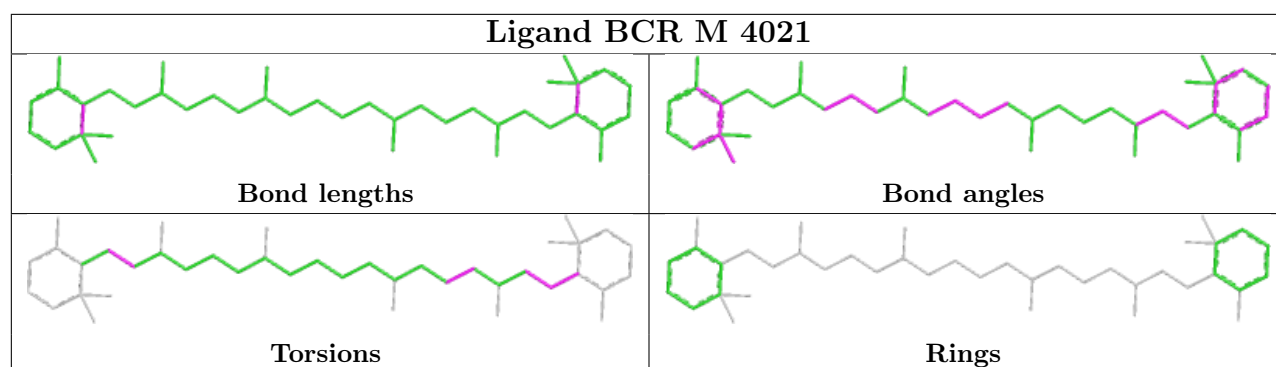
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

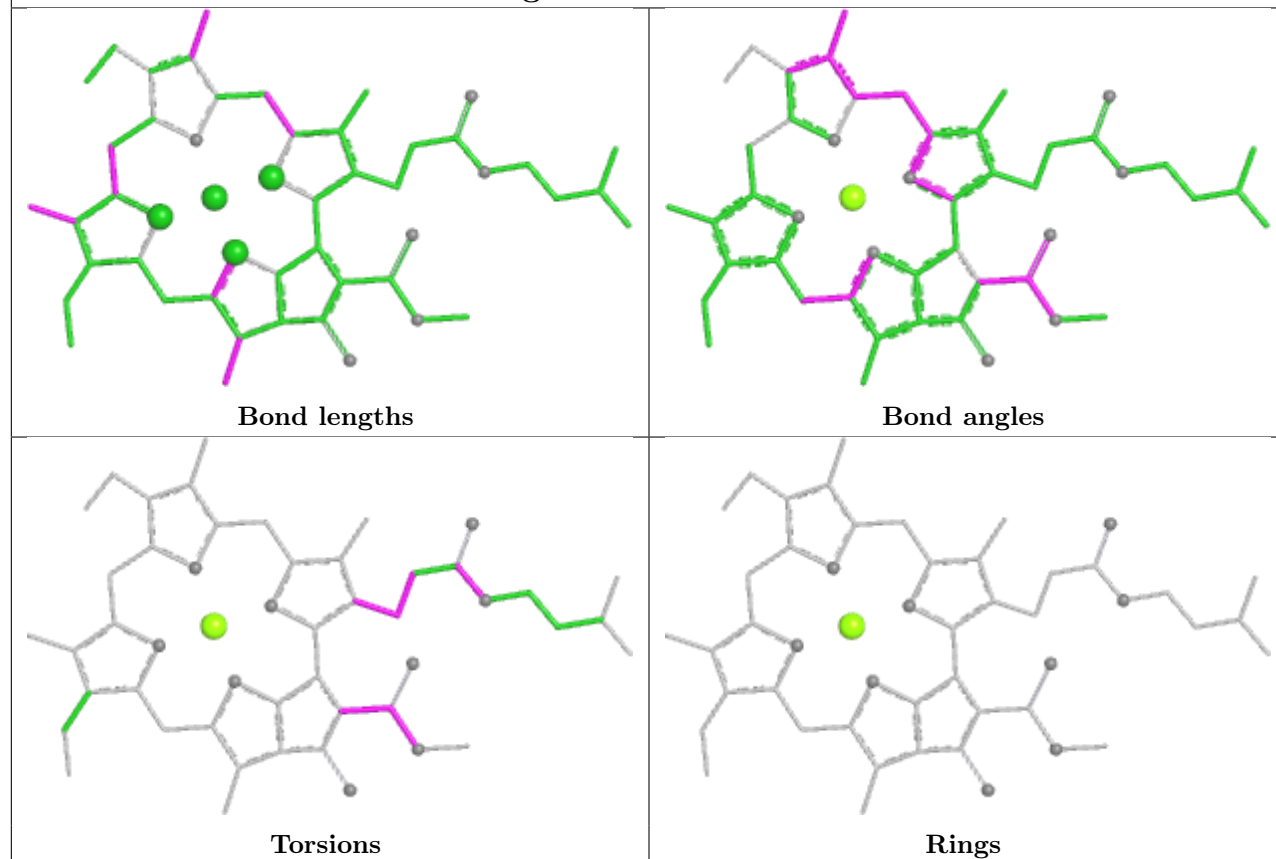




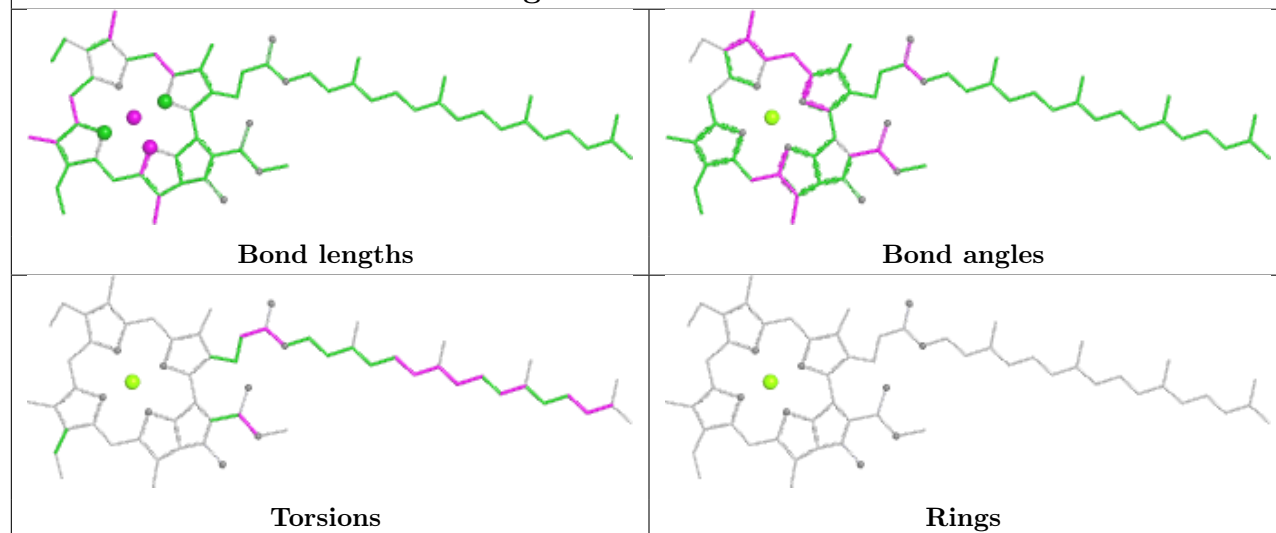


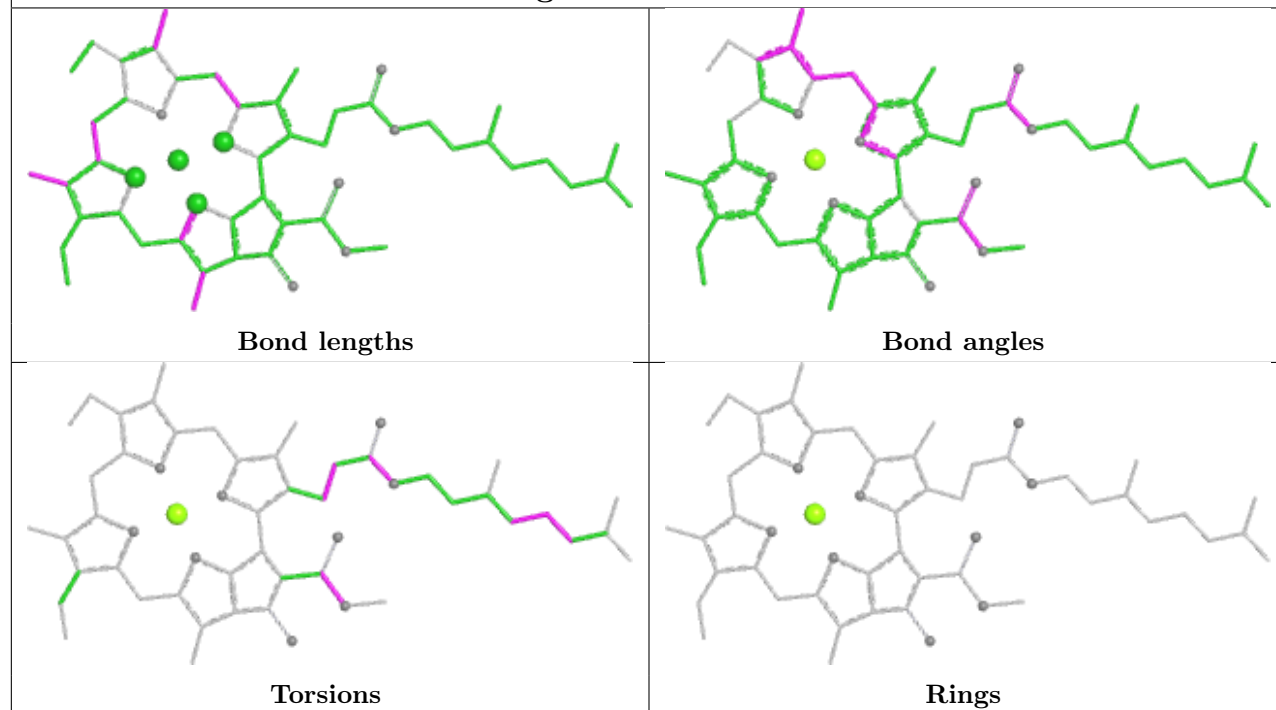
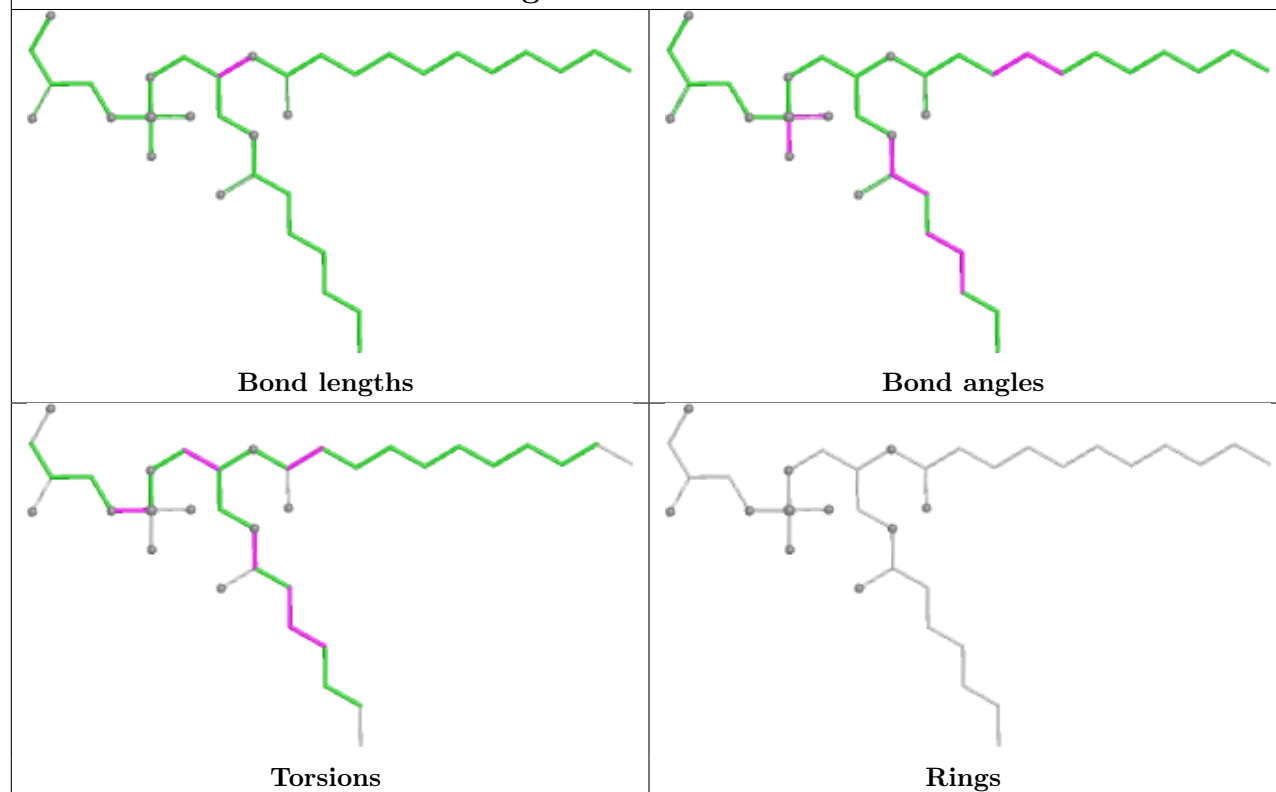


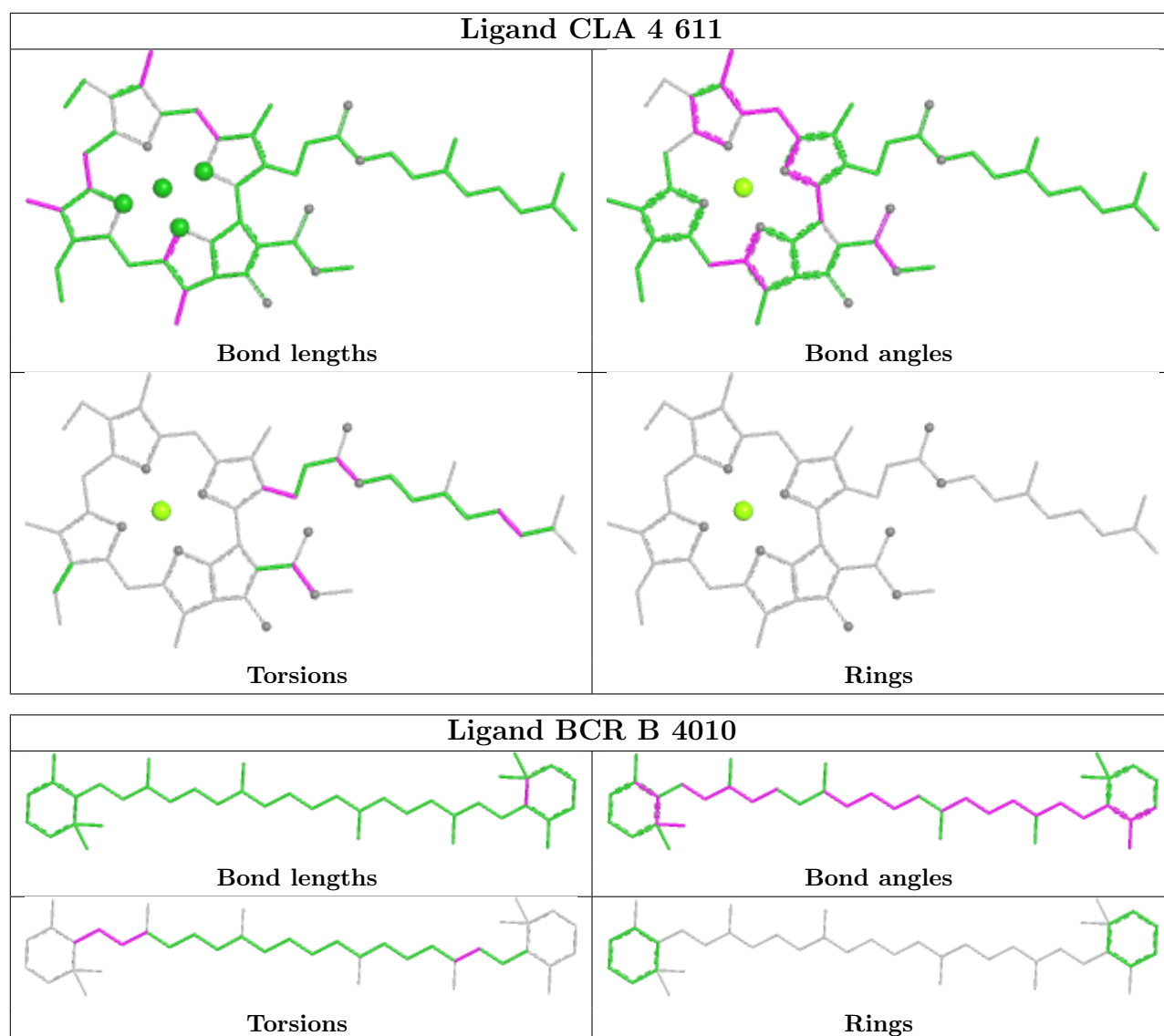
Ligand CLA A 1101



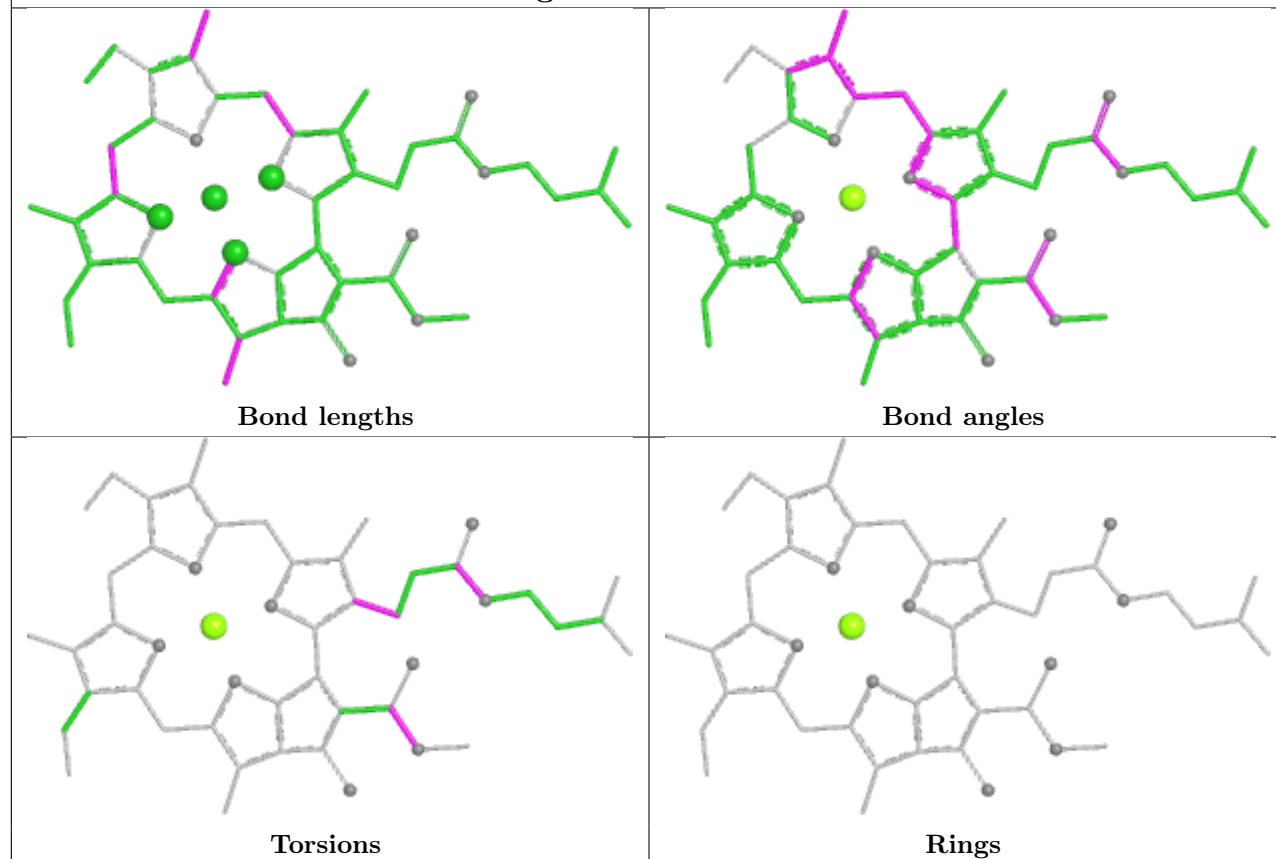
Ligand CLA B 1021



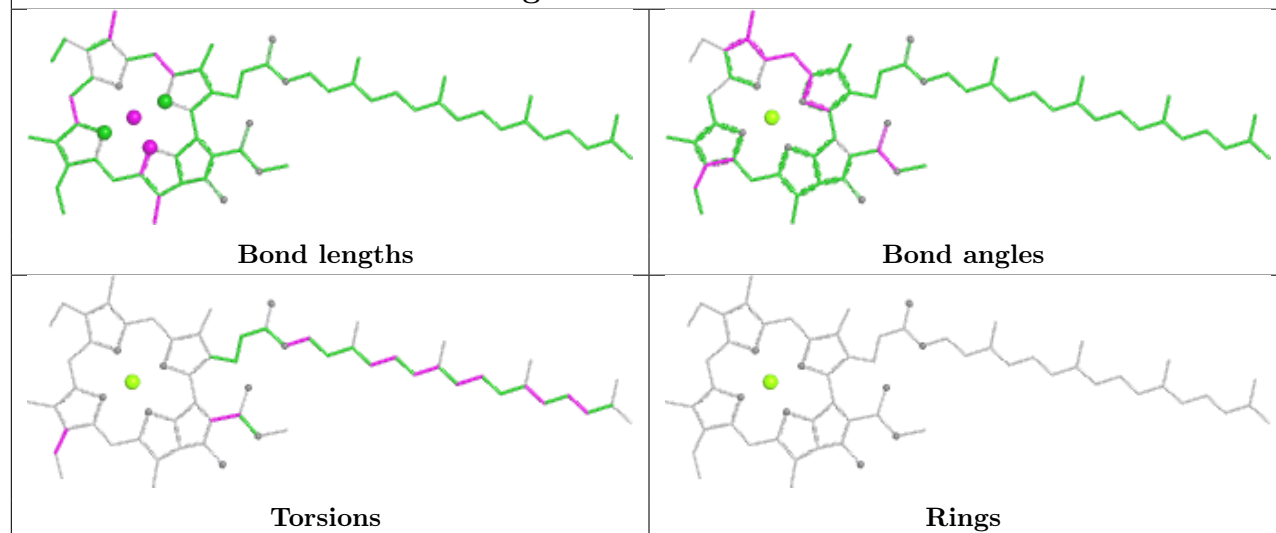
Ligand CLA 4 613**Ligand LHG B 5101**

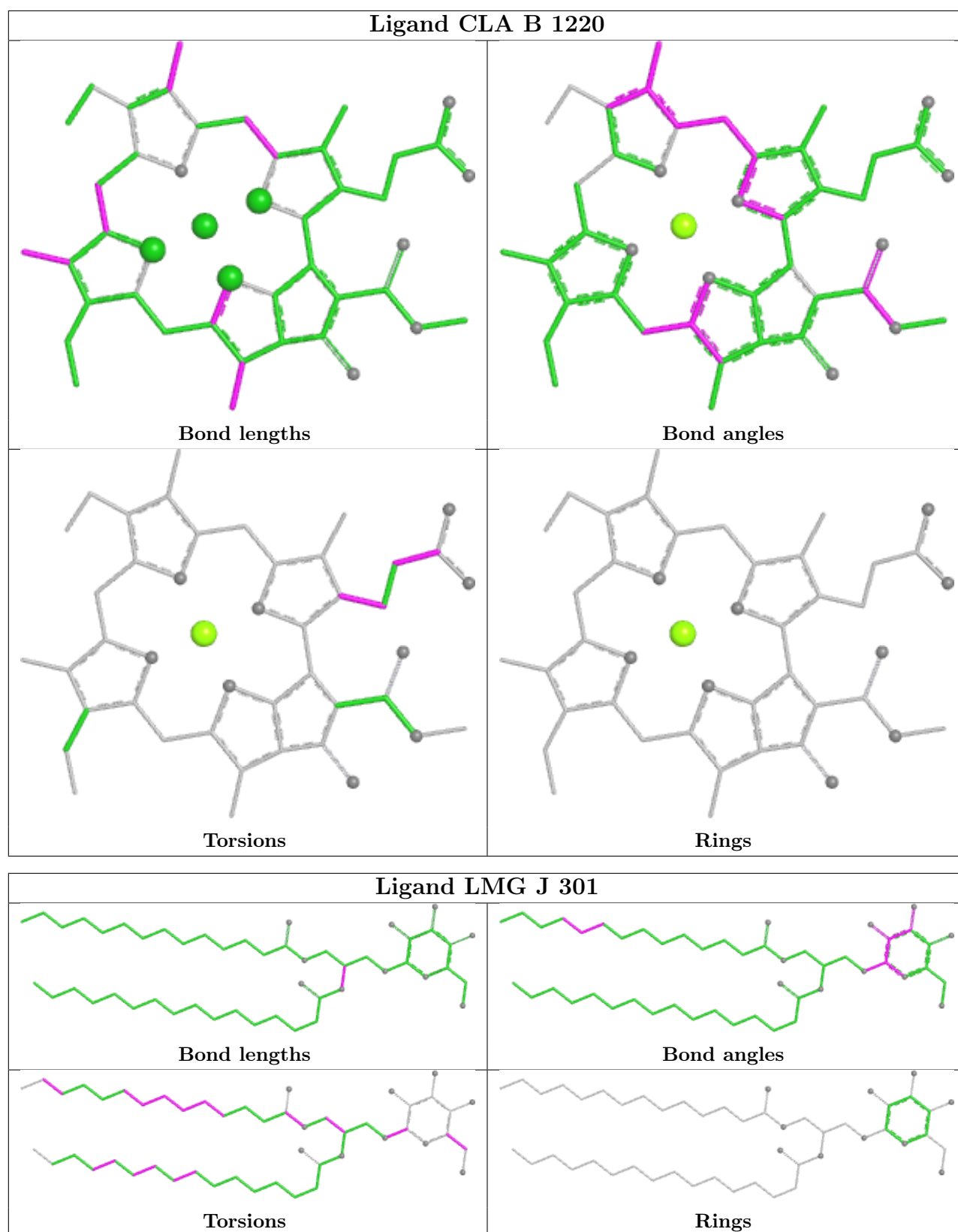


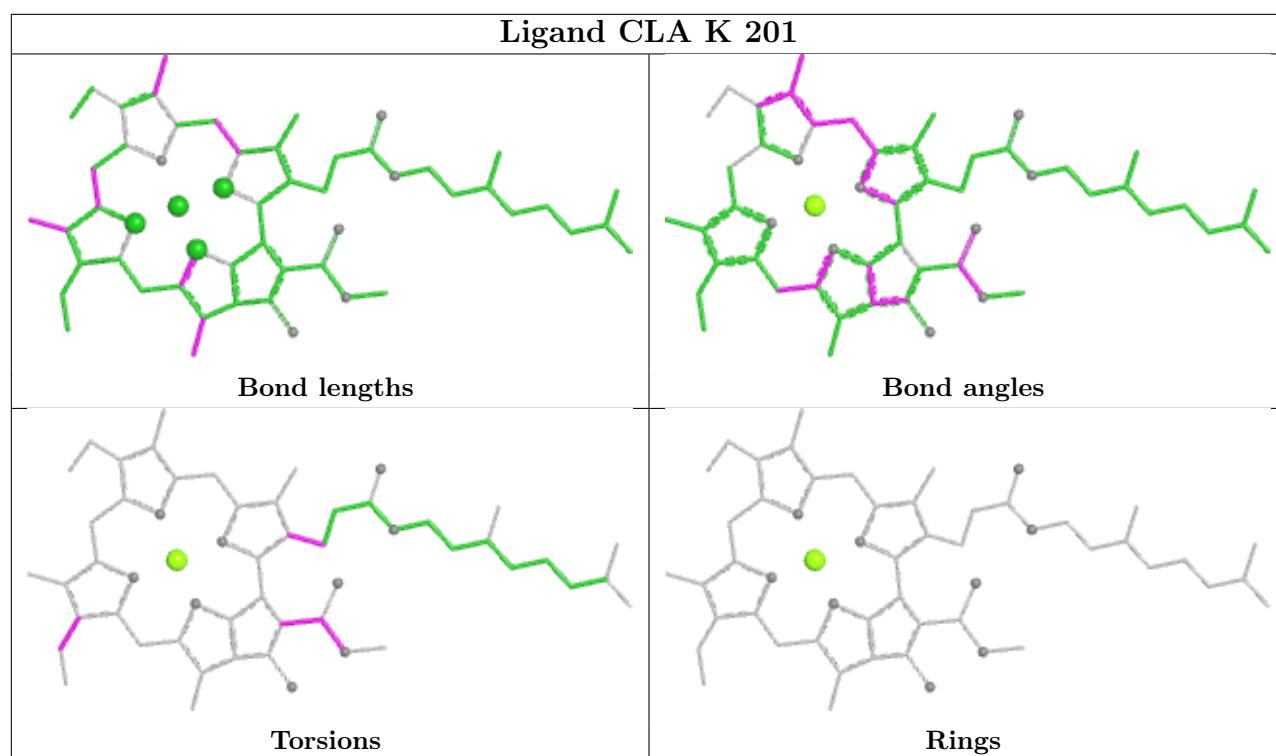
Ligand CLA 3 604



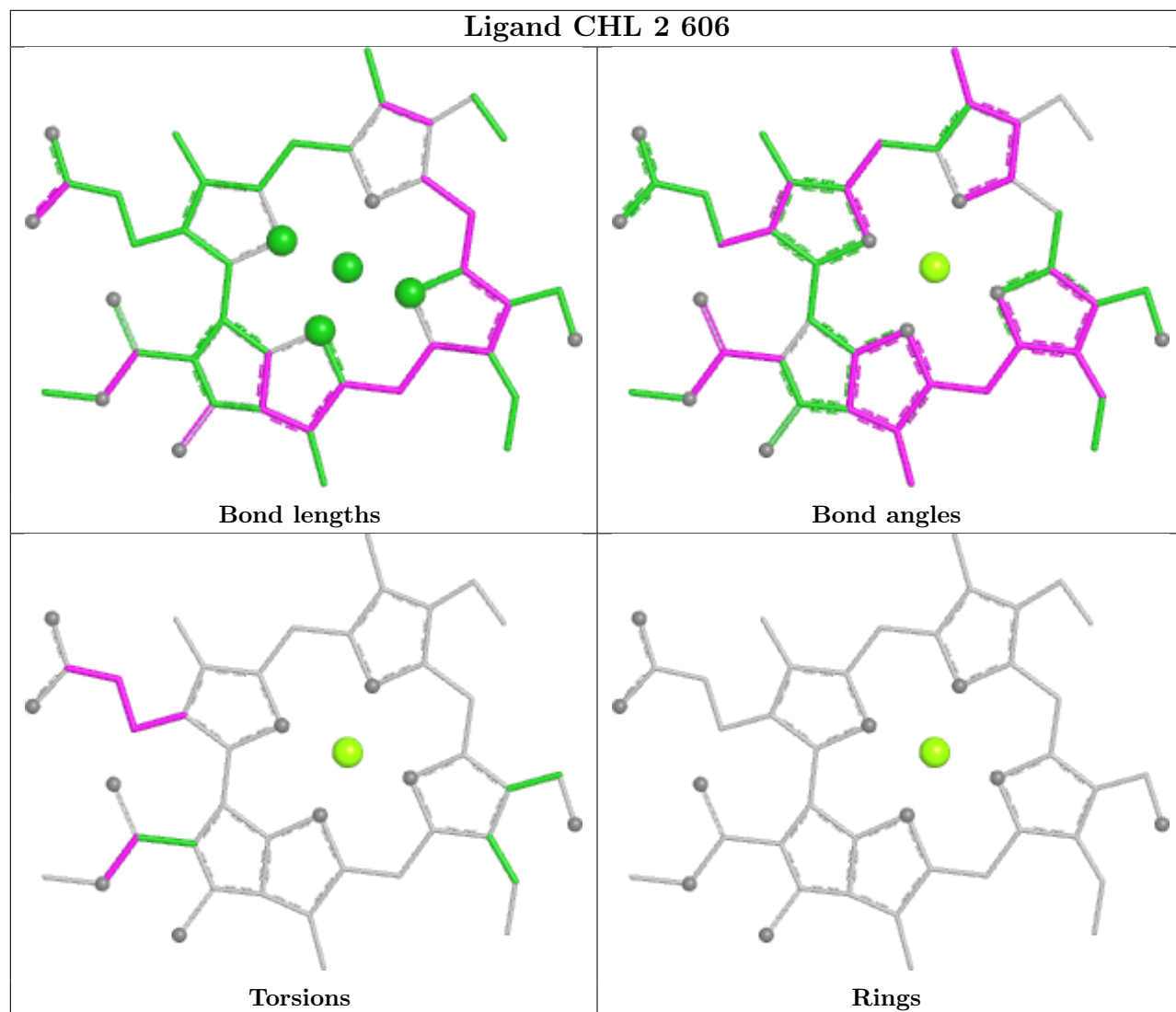
Ligand CLA A 8895



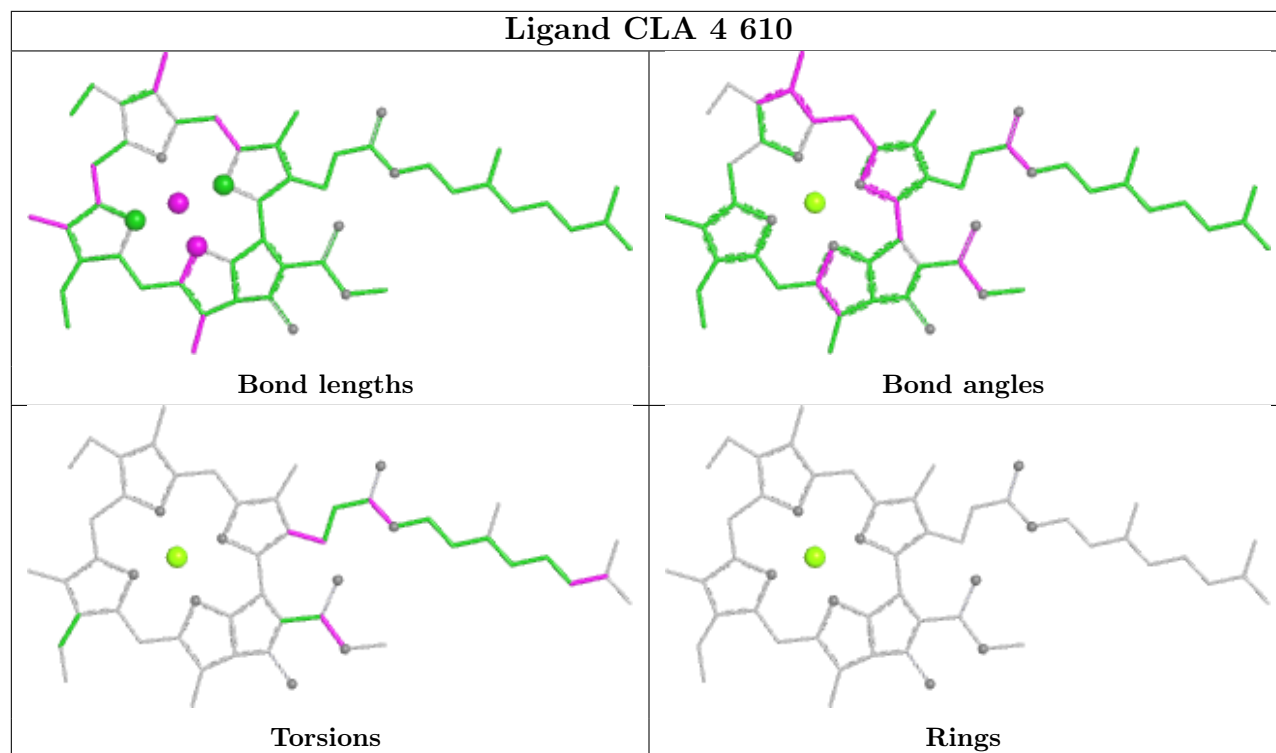




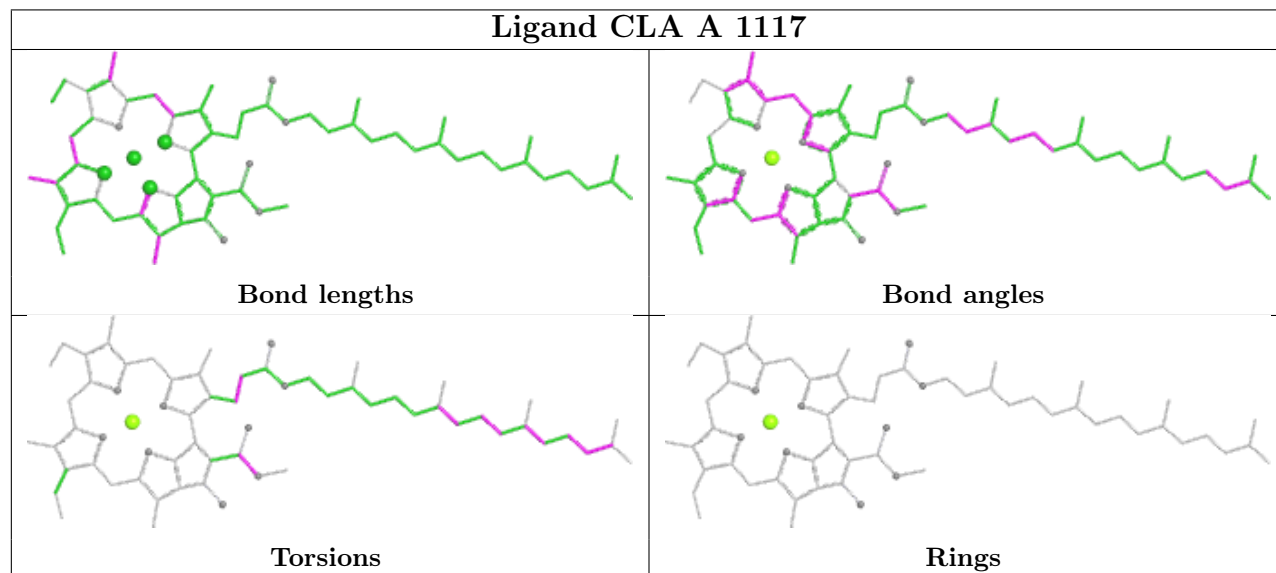
Ligand CHL 2 606

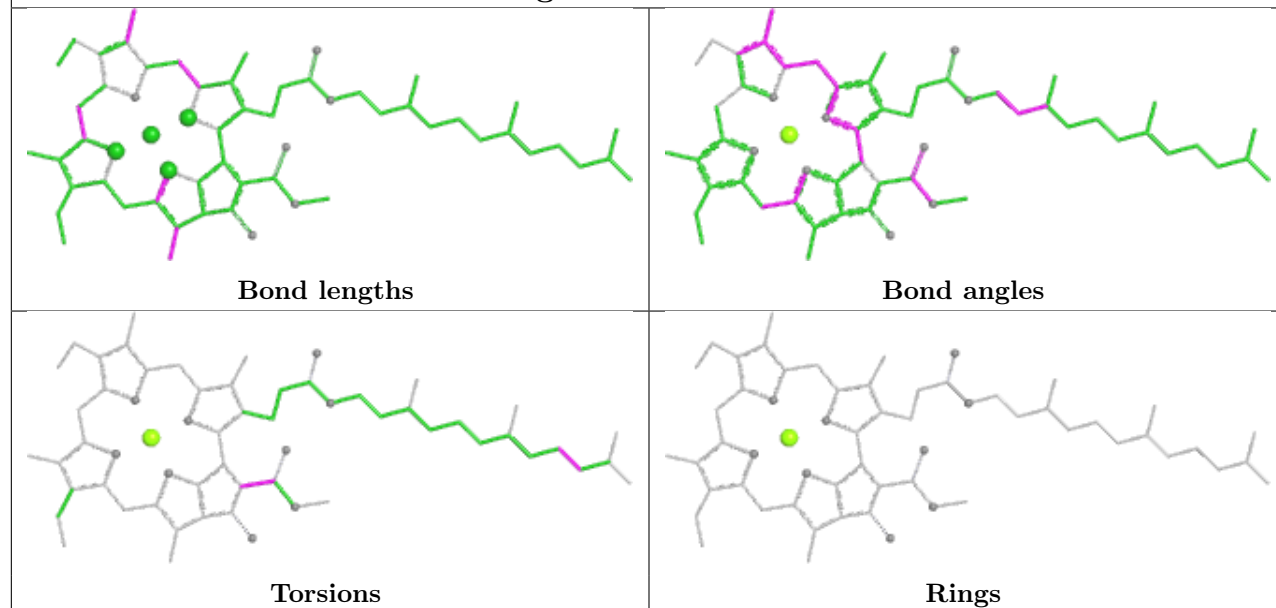
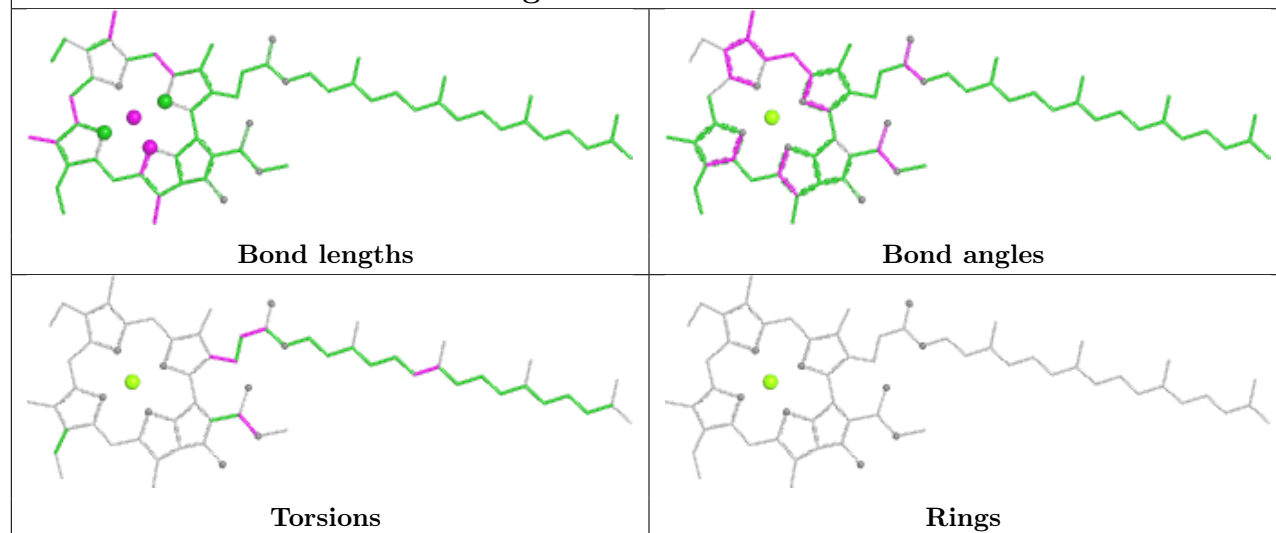


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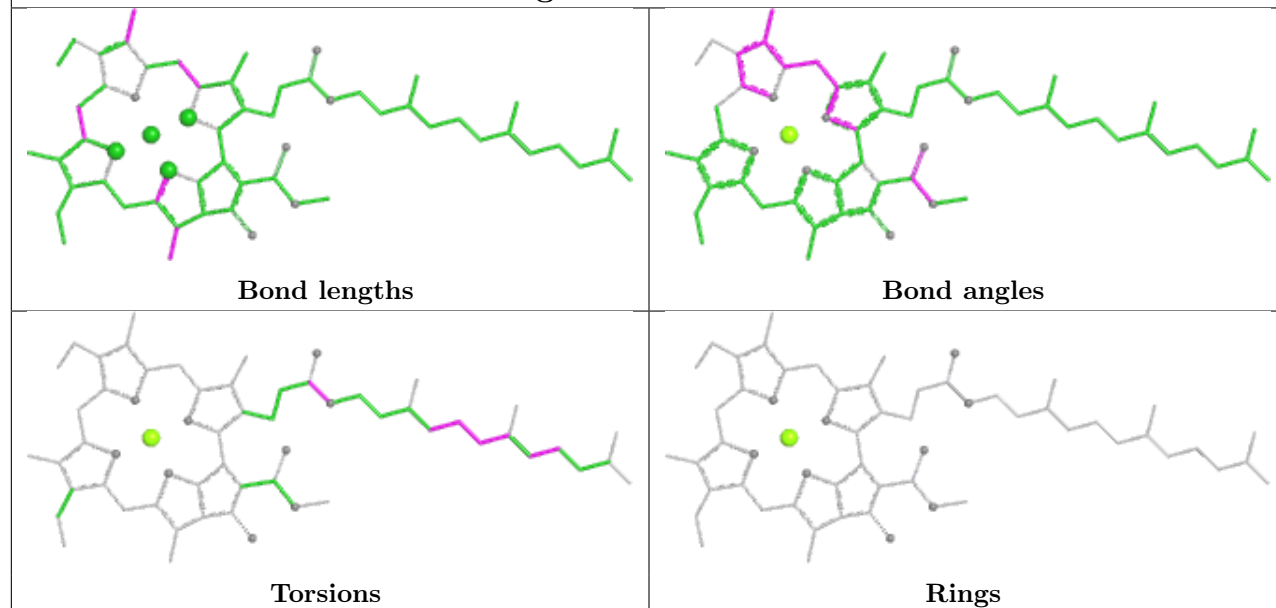


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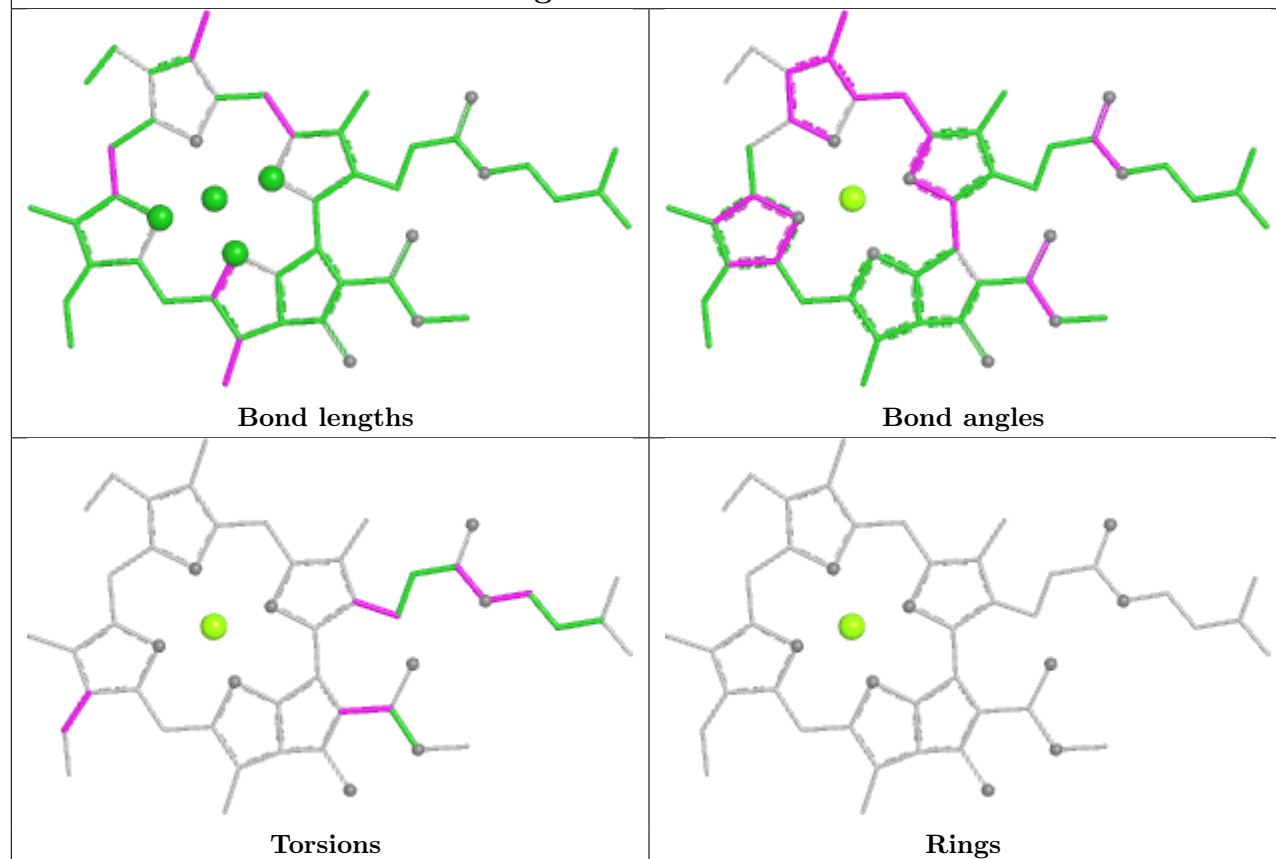


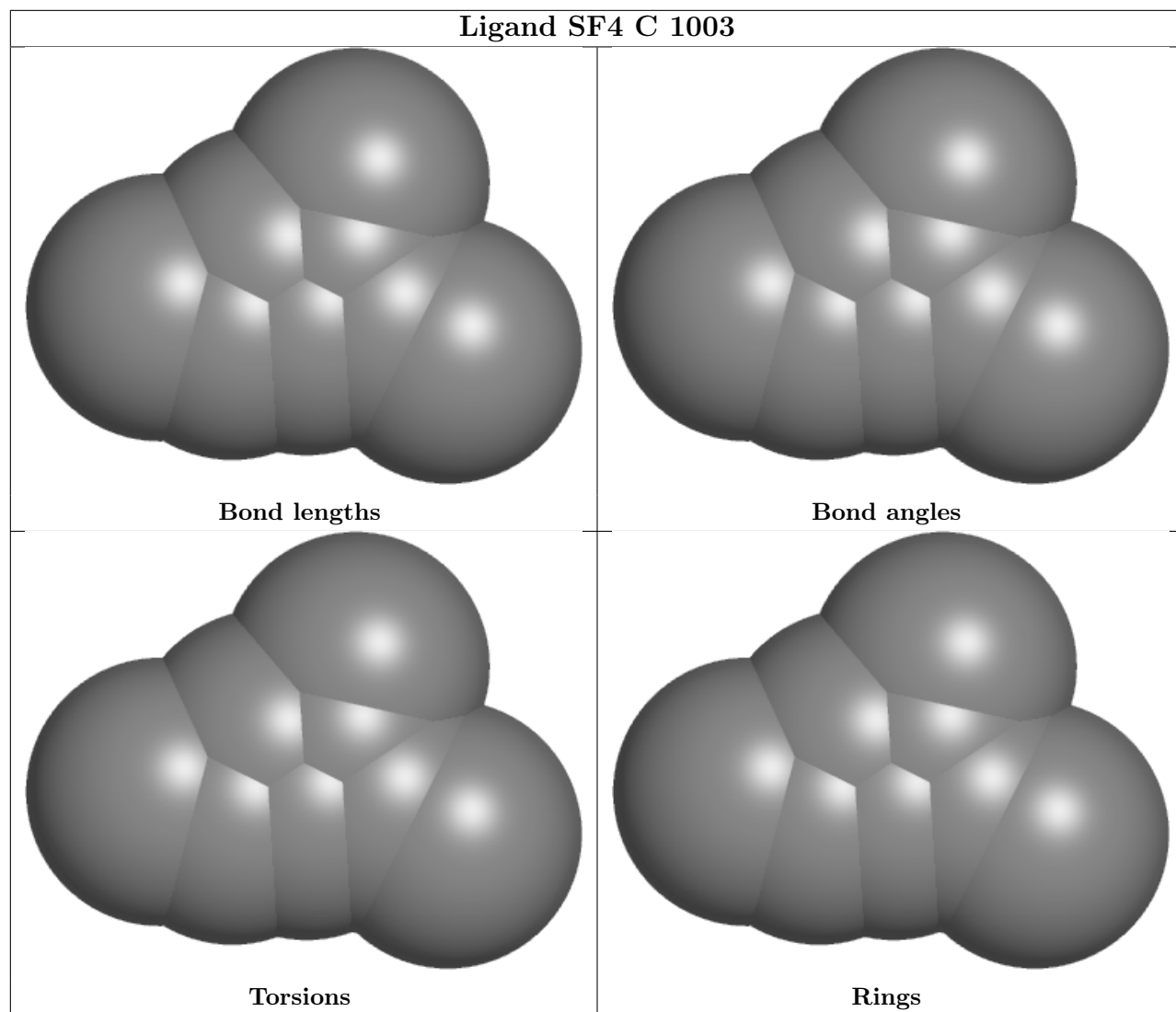
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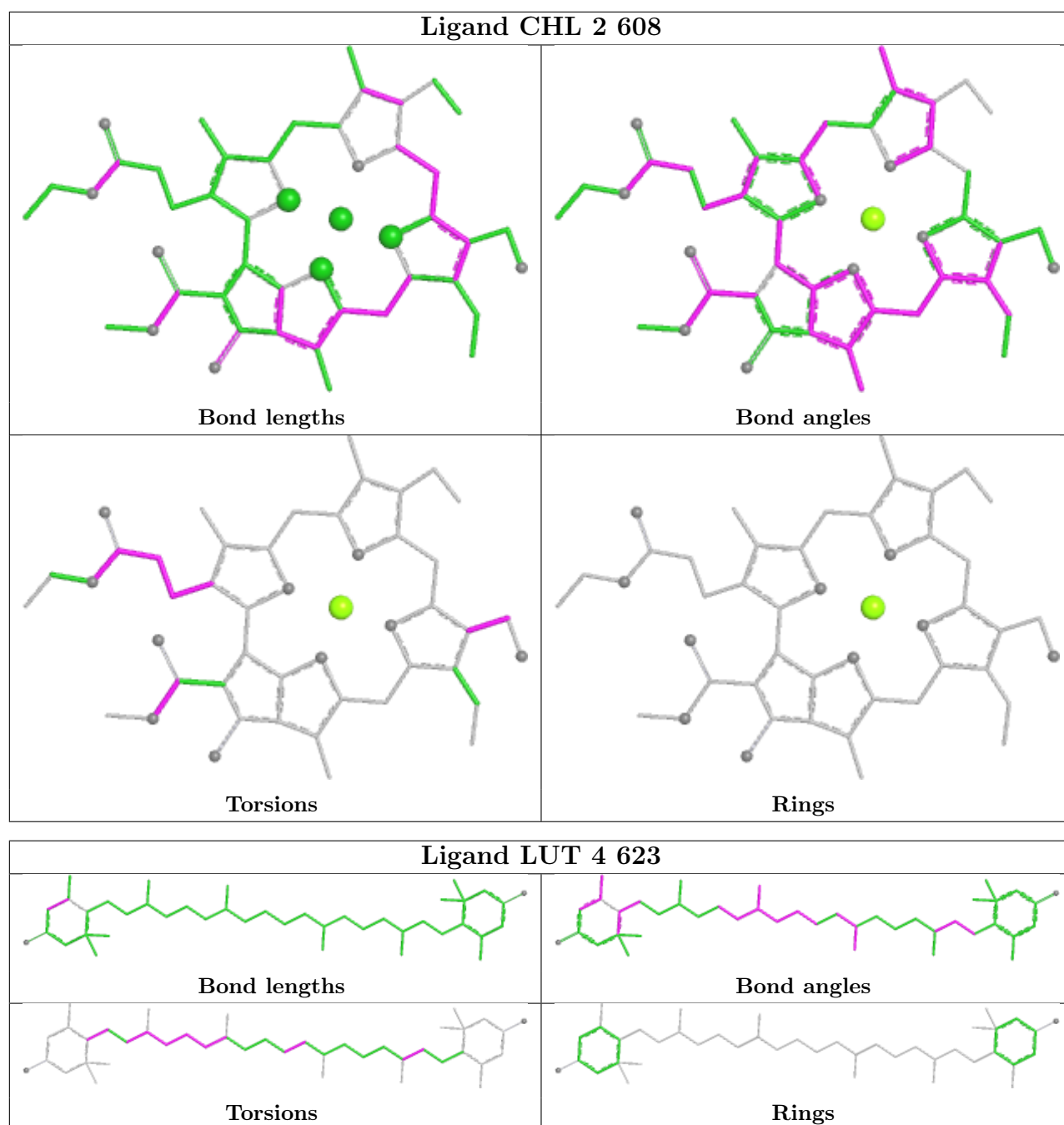
Ligand CLA 1 609

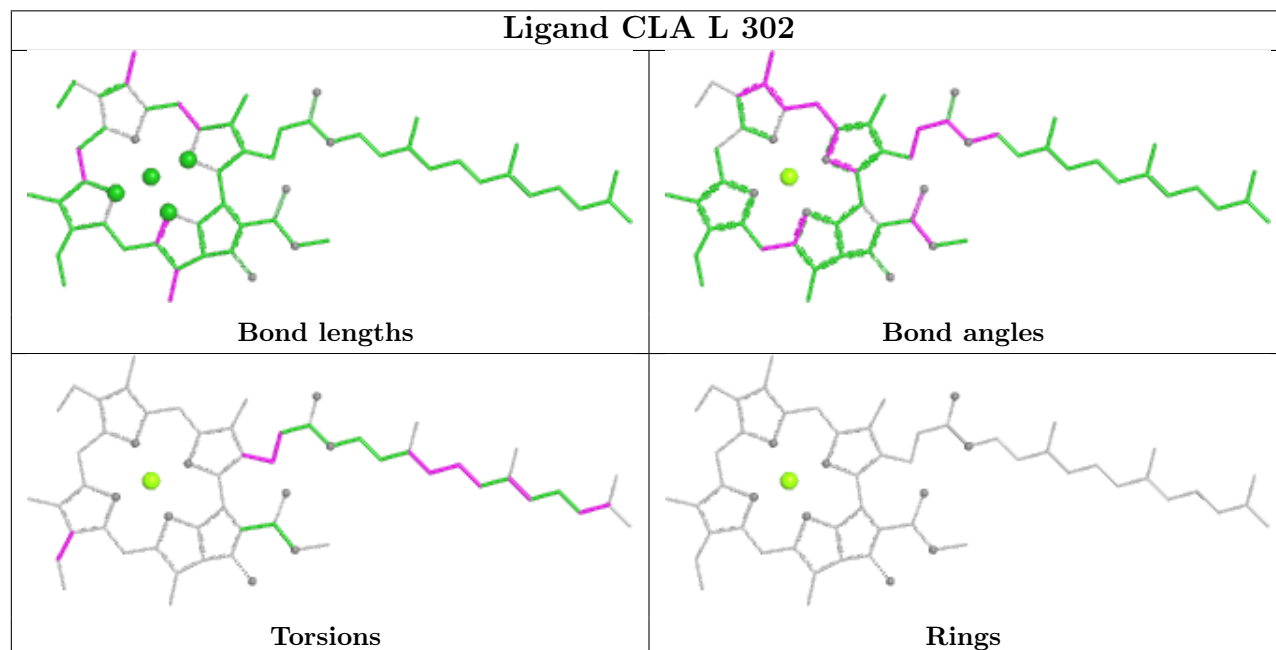
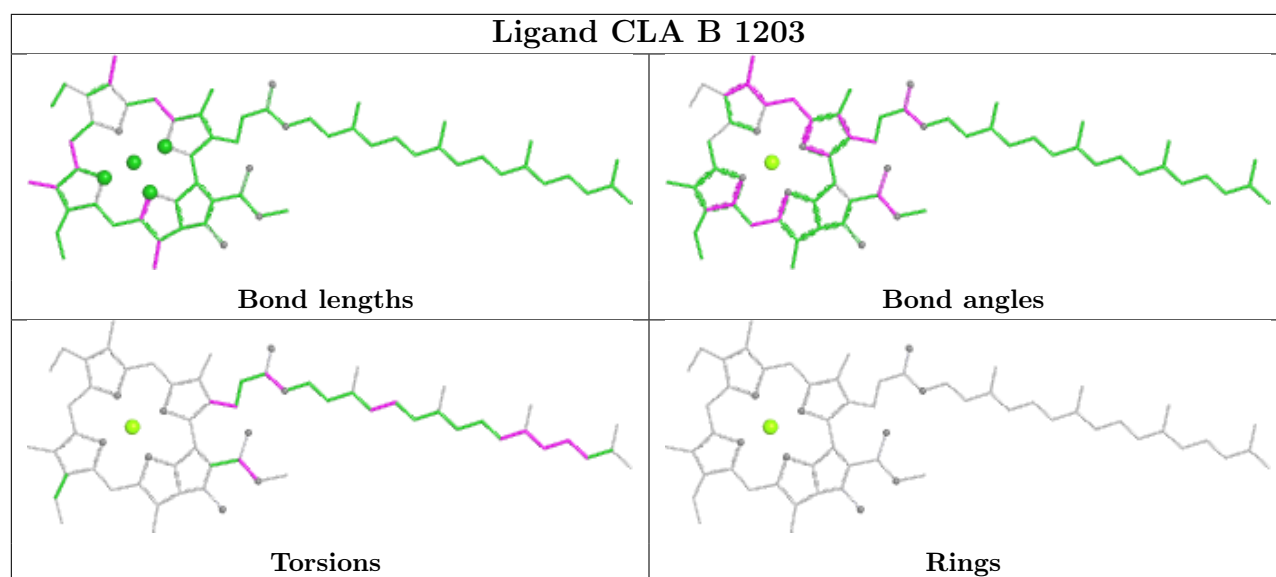


Ligand CLA L 301

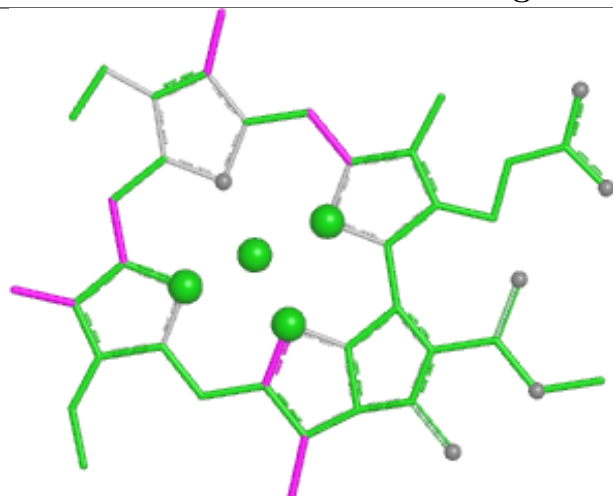




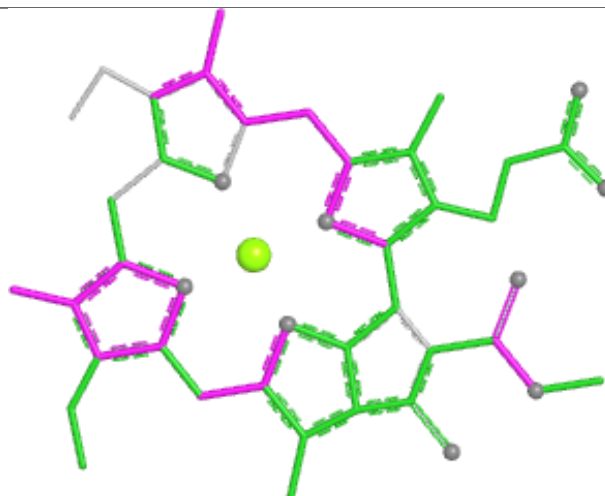




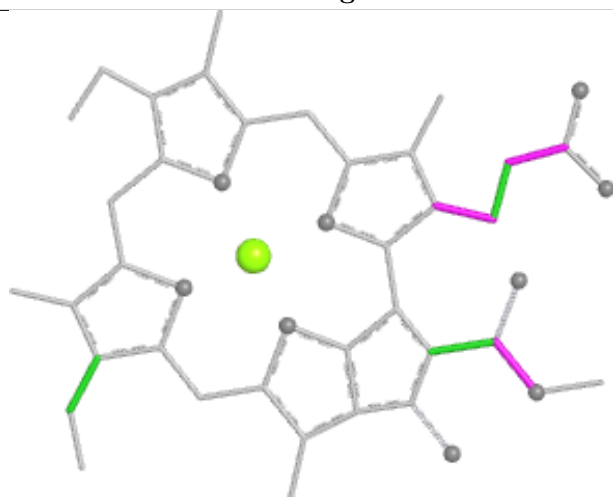
Ligand CLA K 204



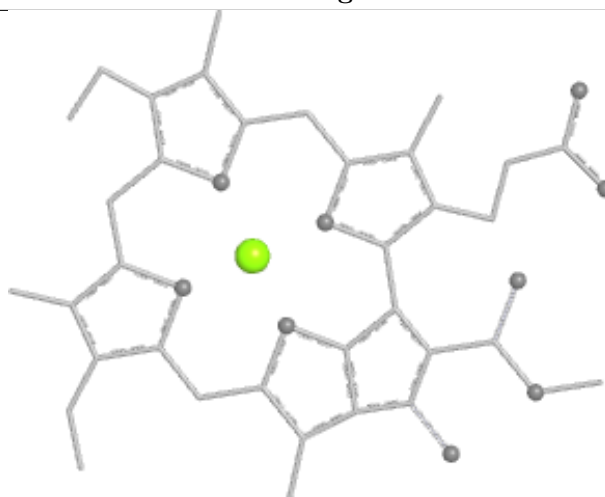
Bond lengths



Bond angles

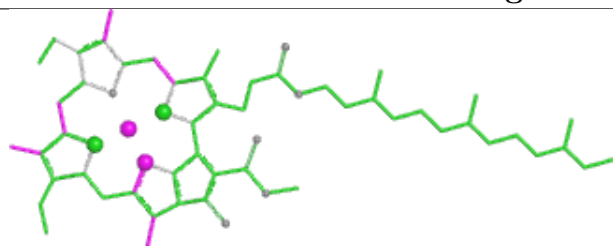


Torsions

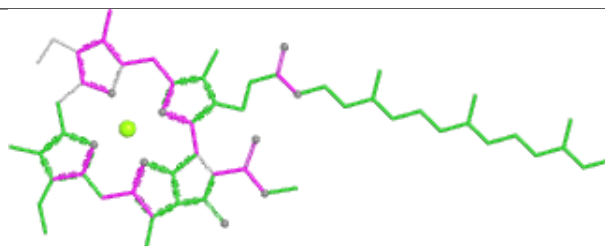


Rings

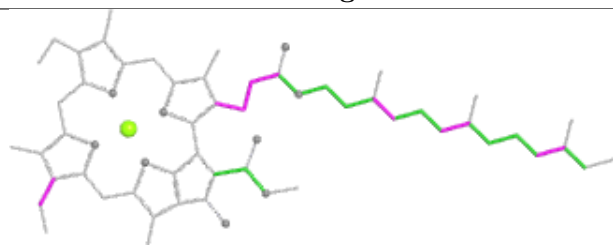
Ligand CLA B 1224



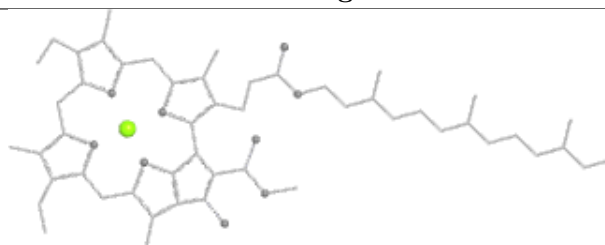
Bond lengths



Bond angles

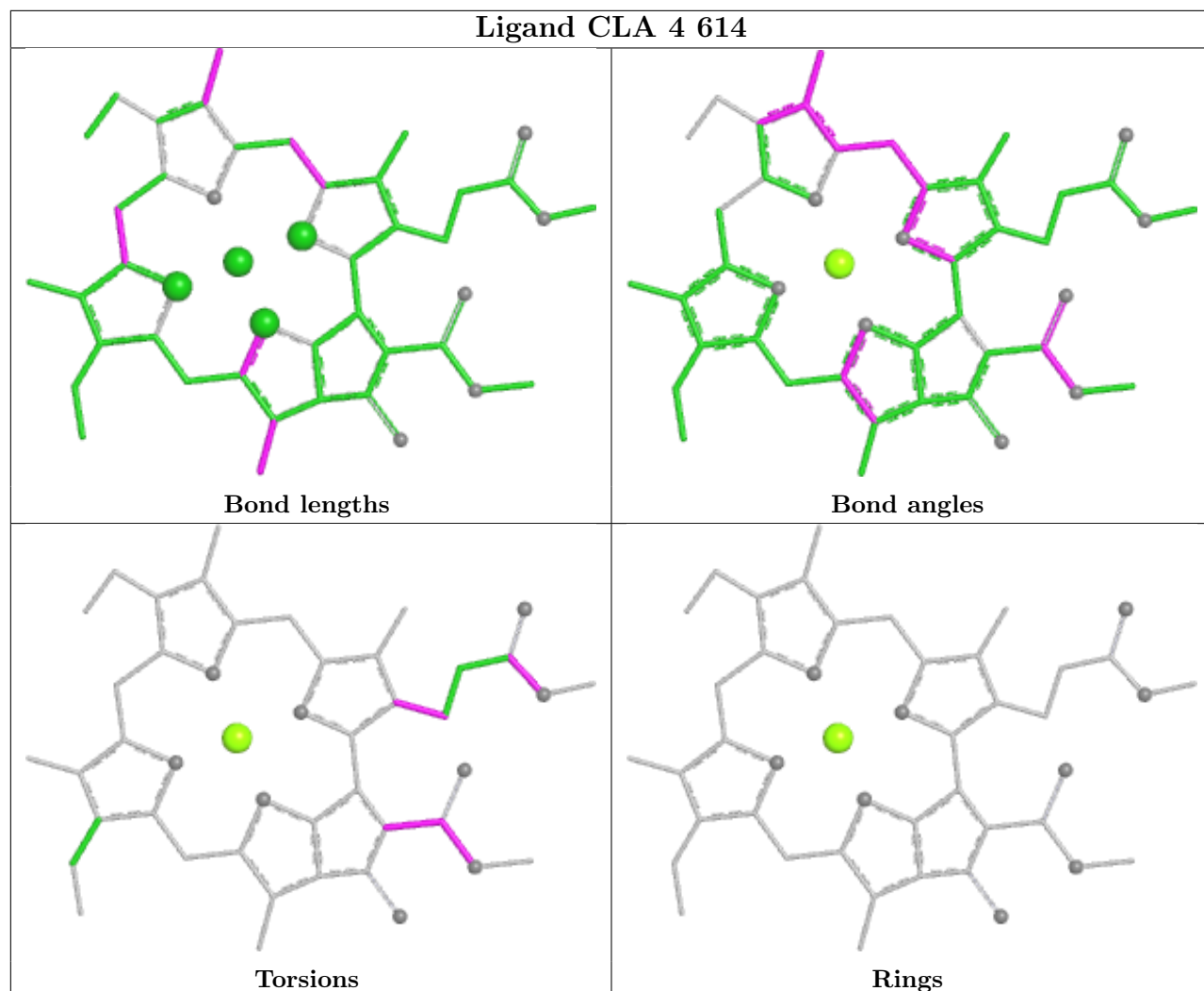


Torsions

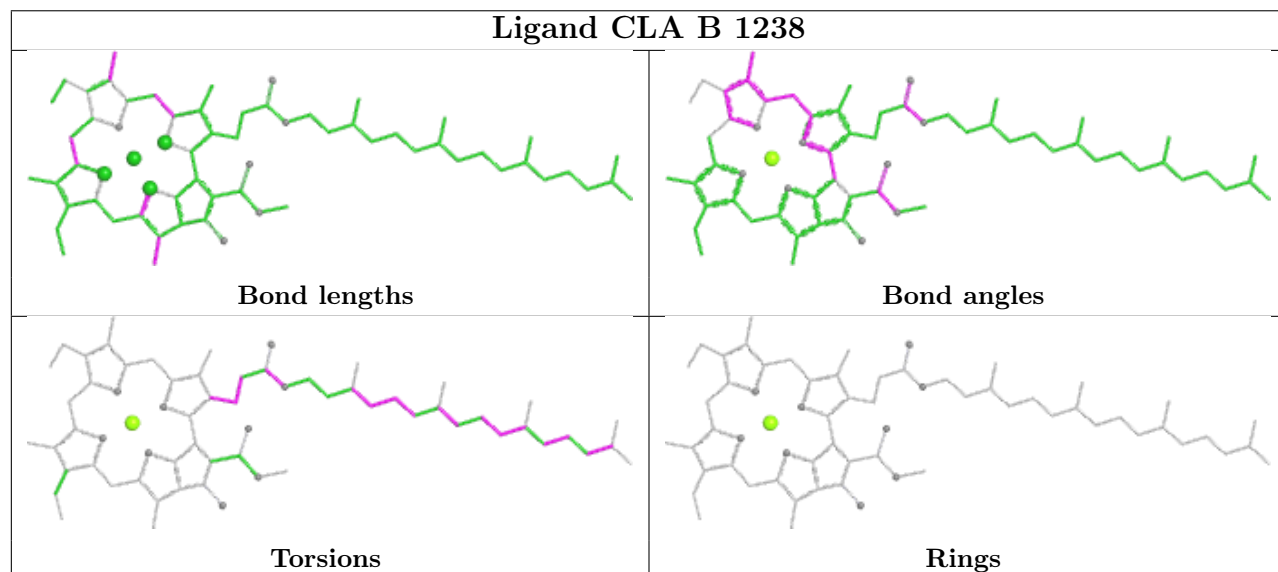


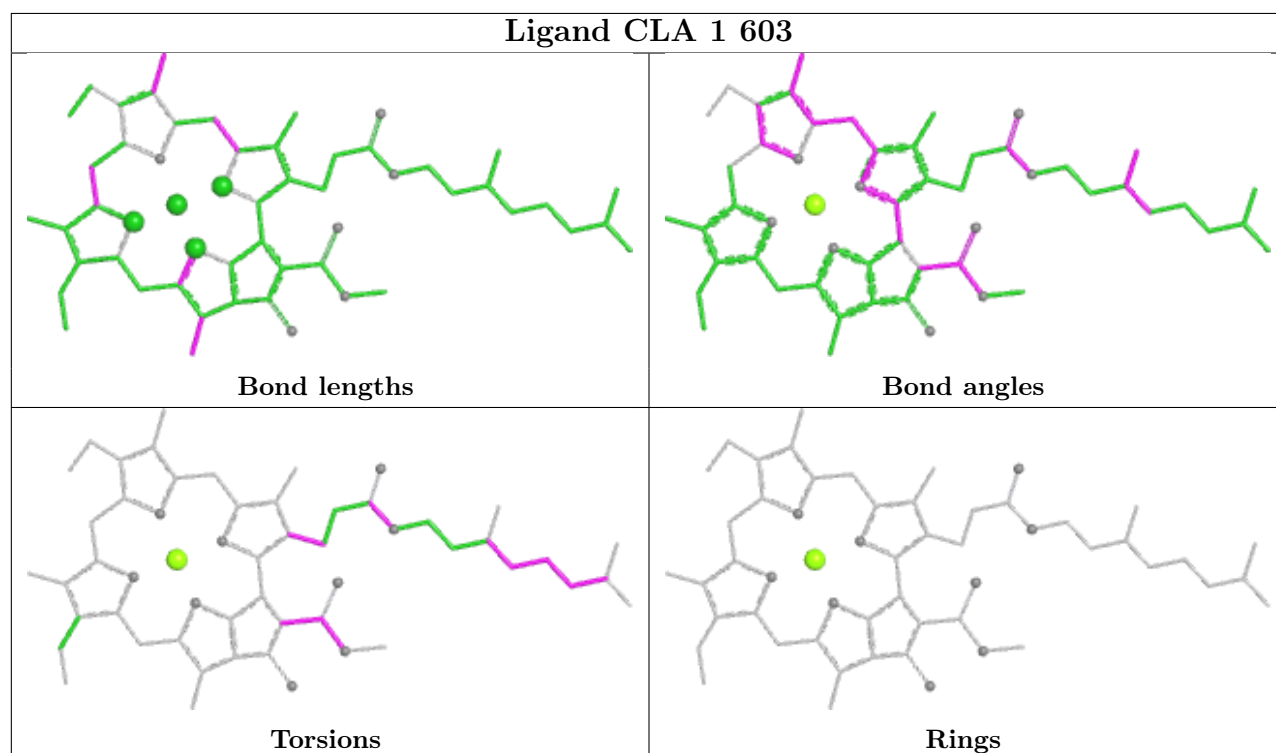
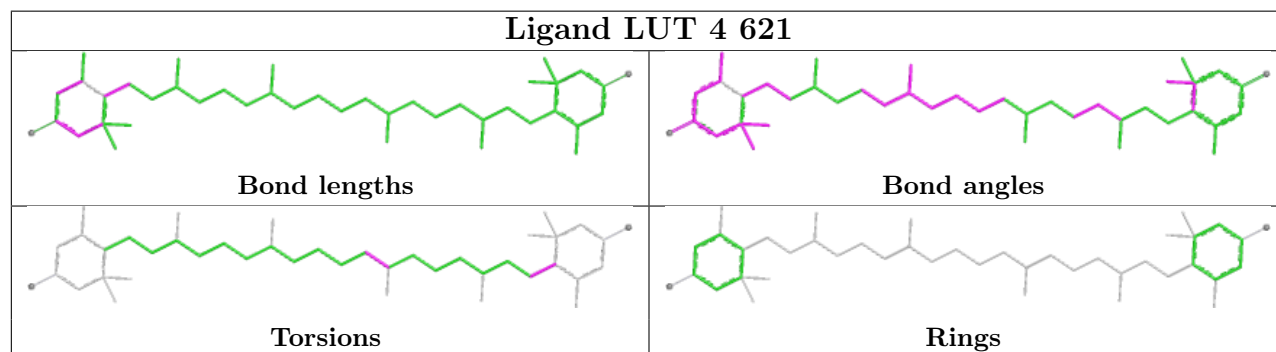
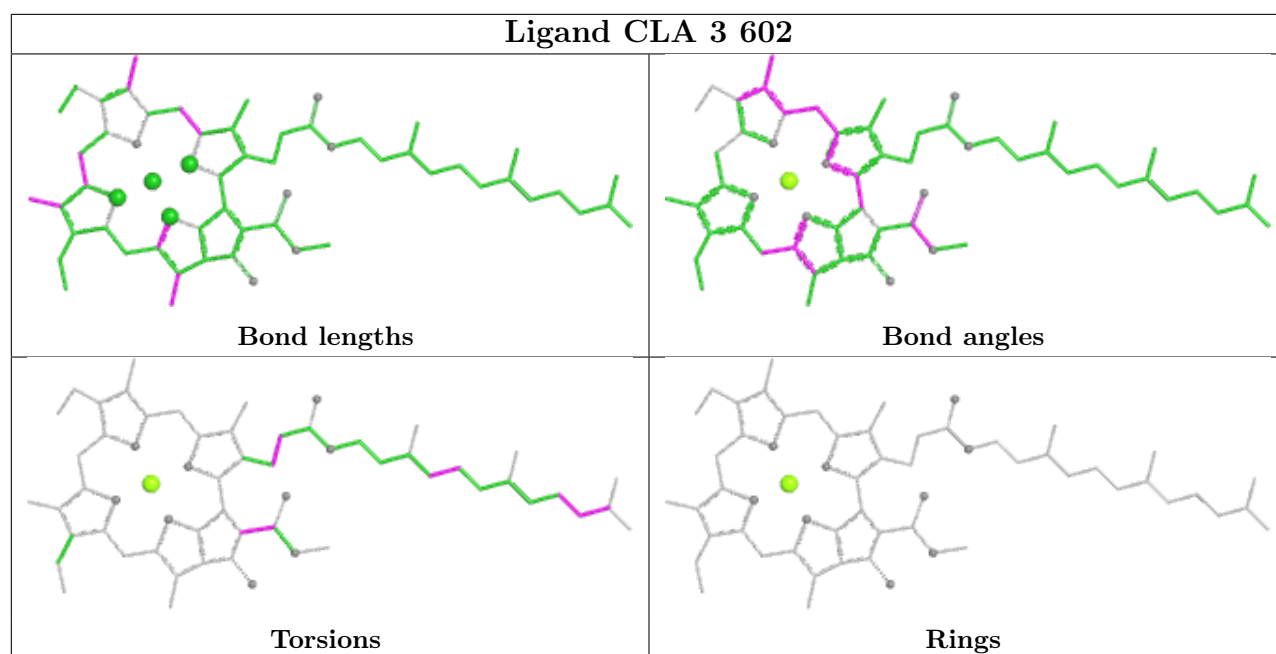
Rings

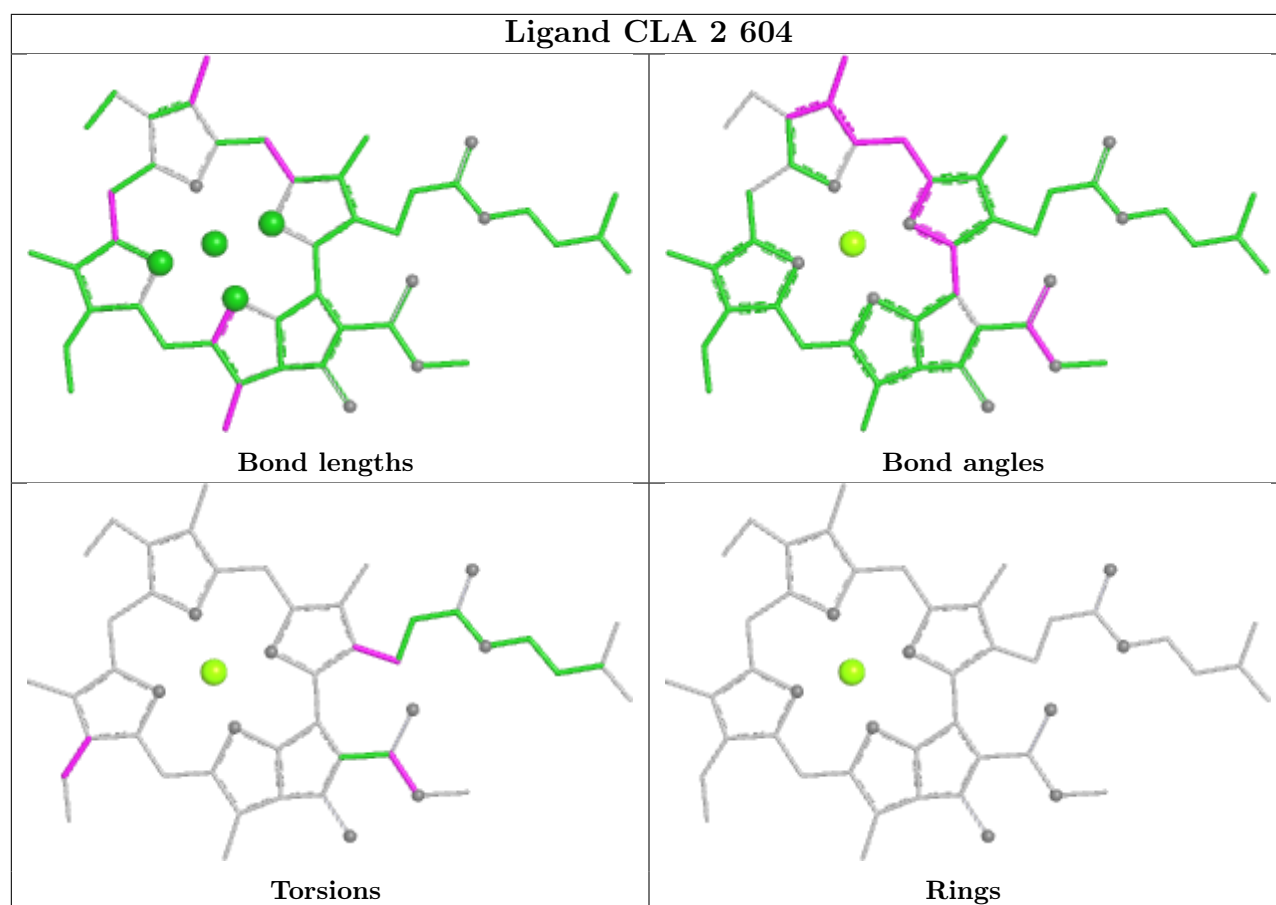
Ligand CLA 4 614



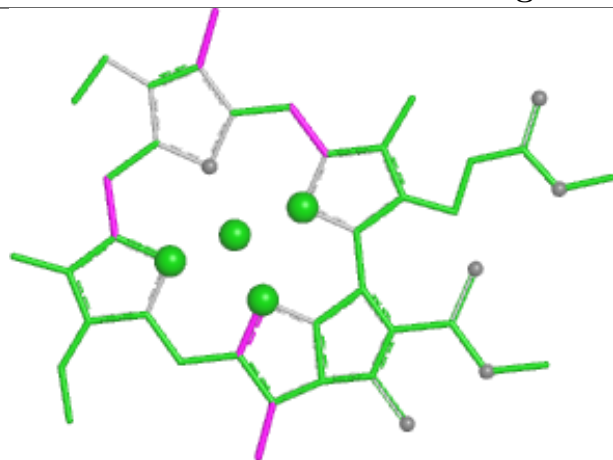
Ligand CLA B 1238



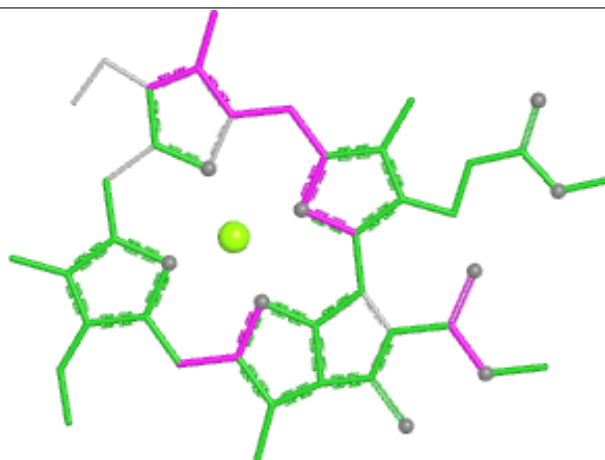




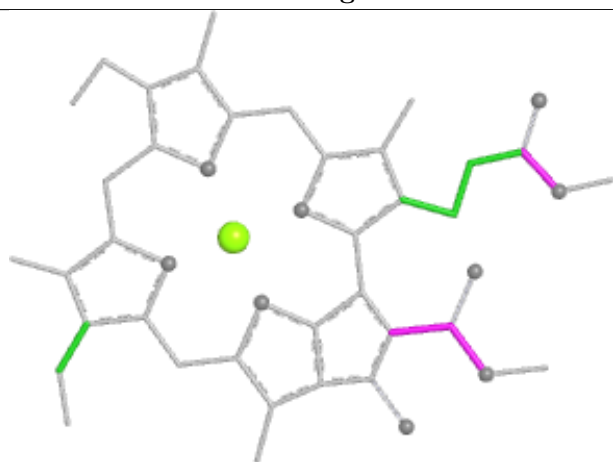
Ligand CLA F 302



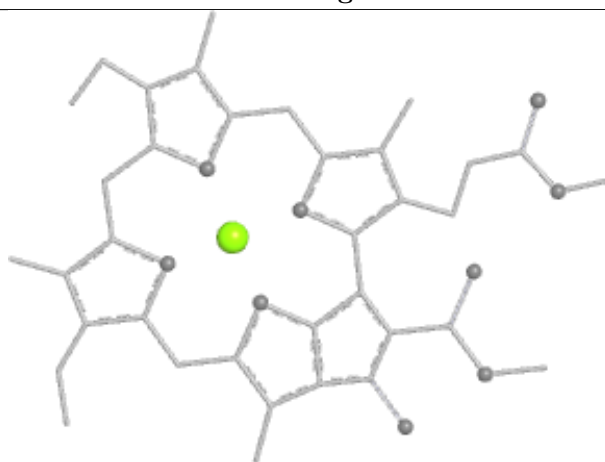
Bond lengths



Bond angles

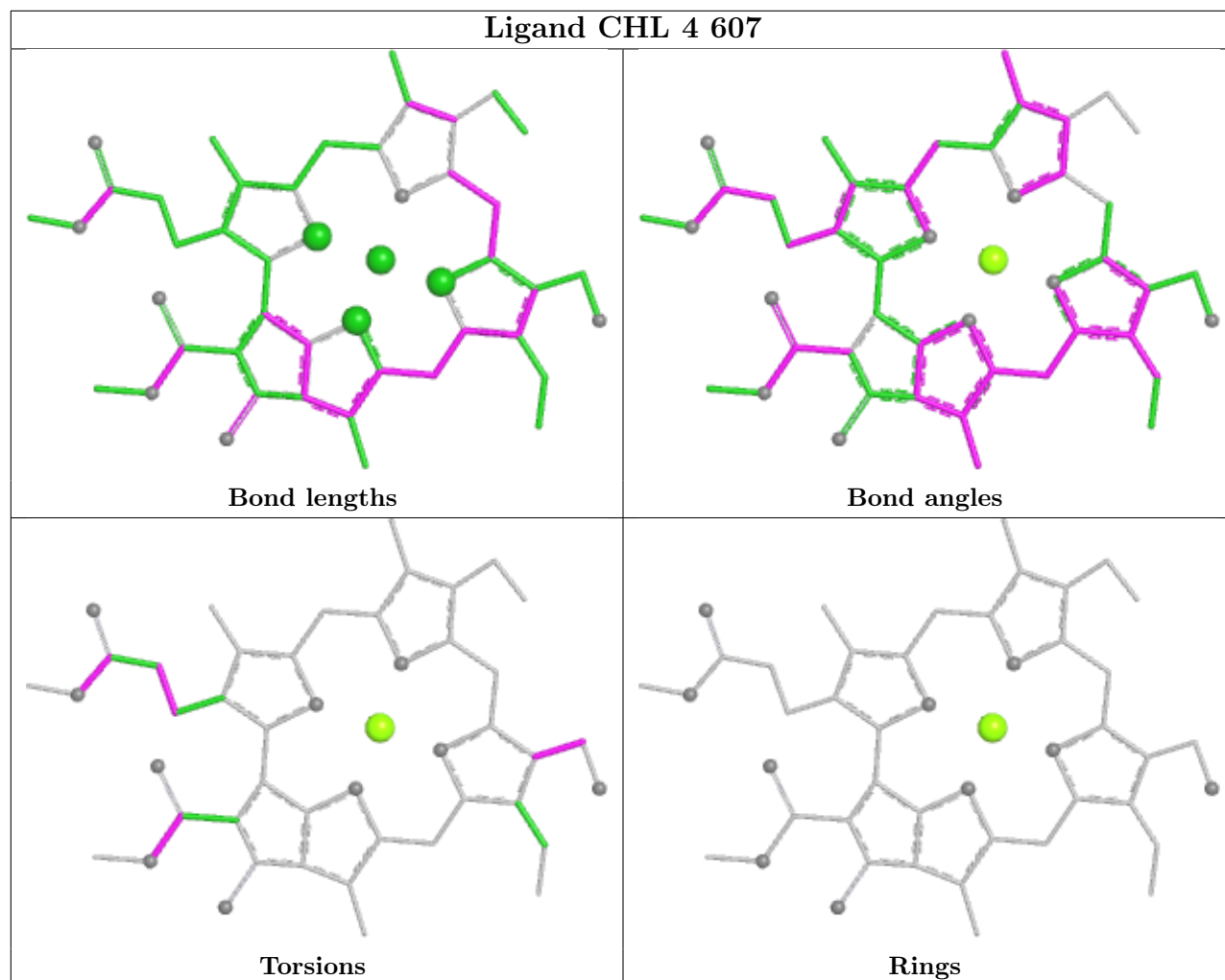


Torsions

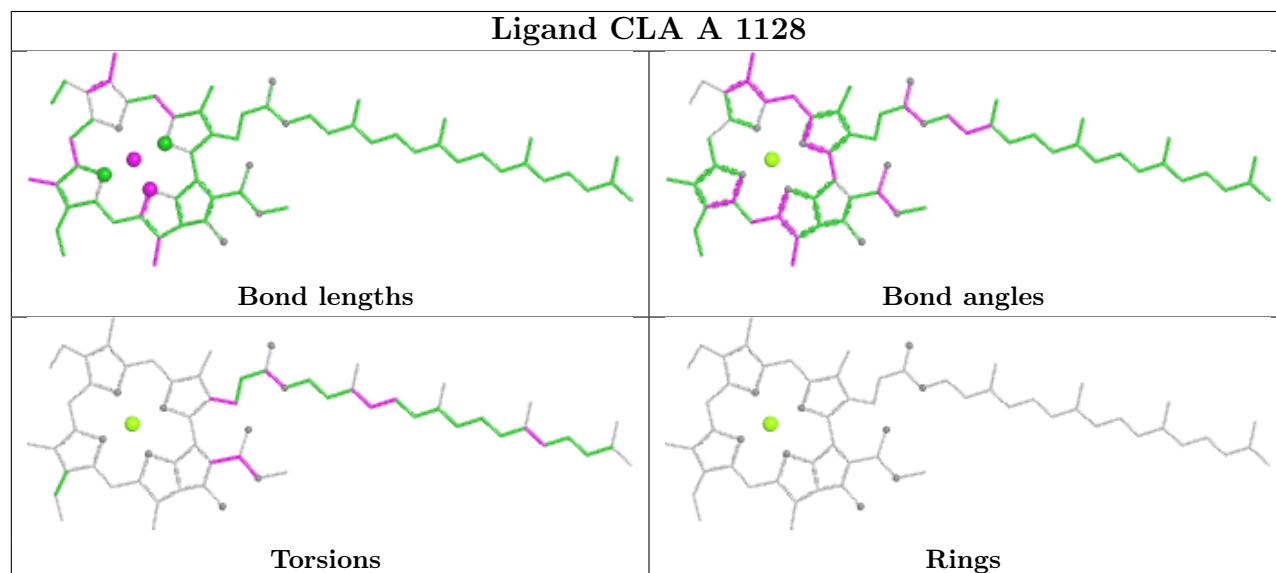


Rings

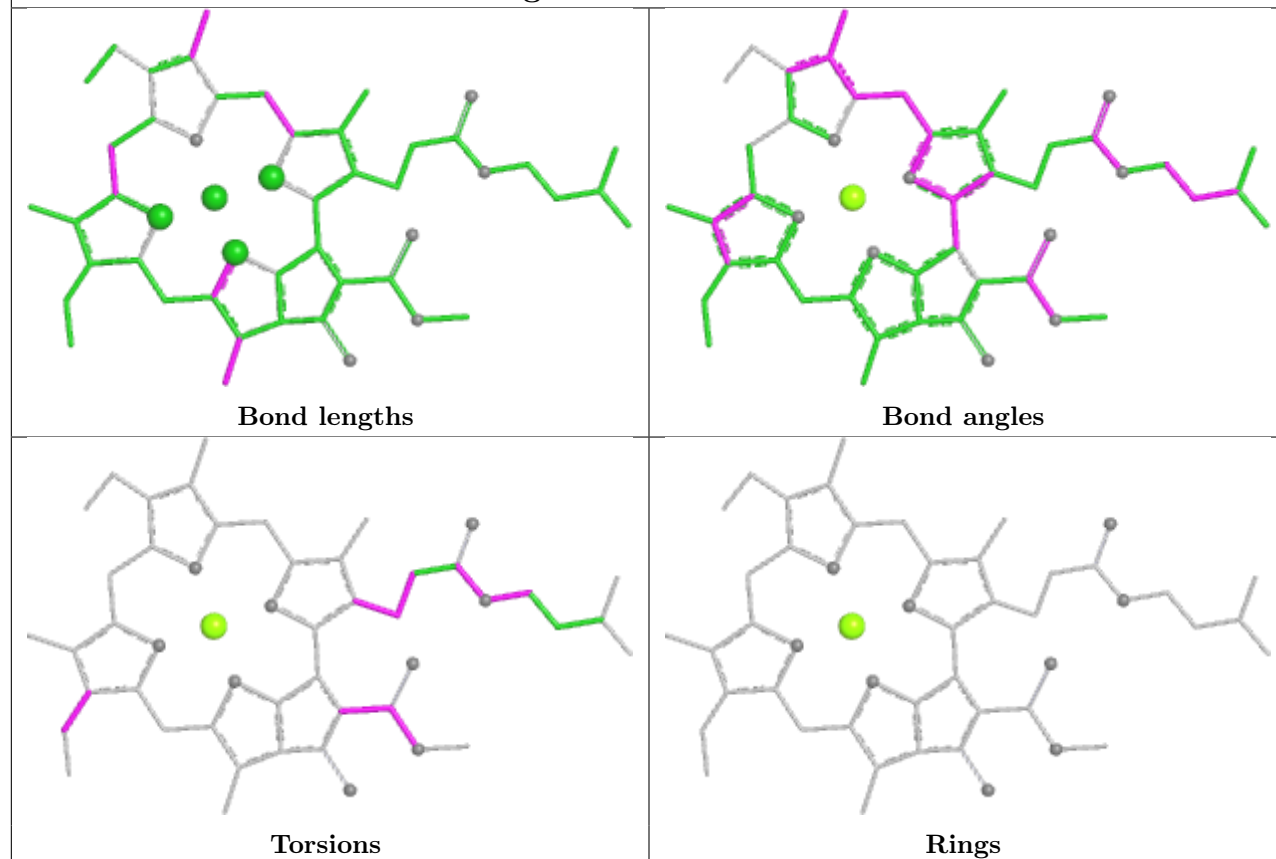
Ligand CHL 4 607



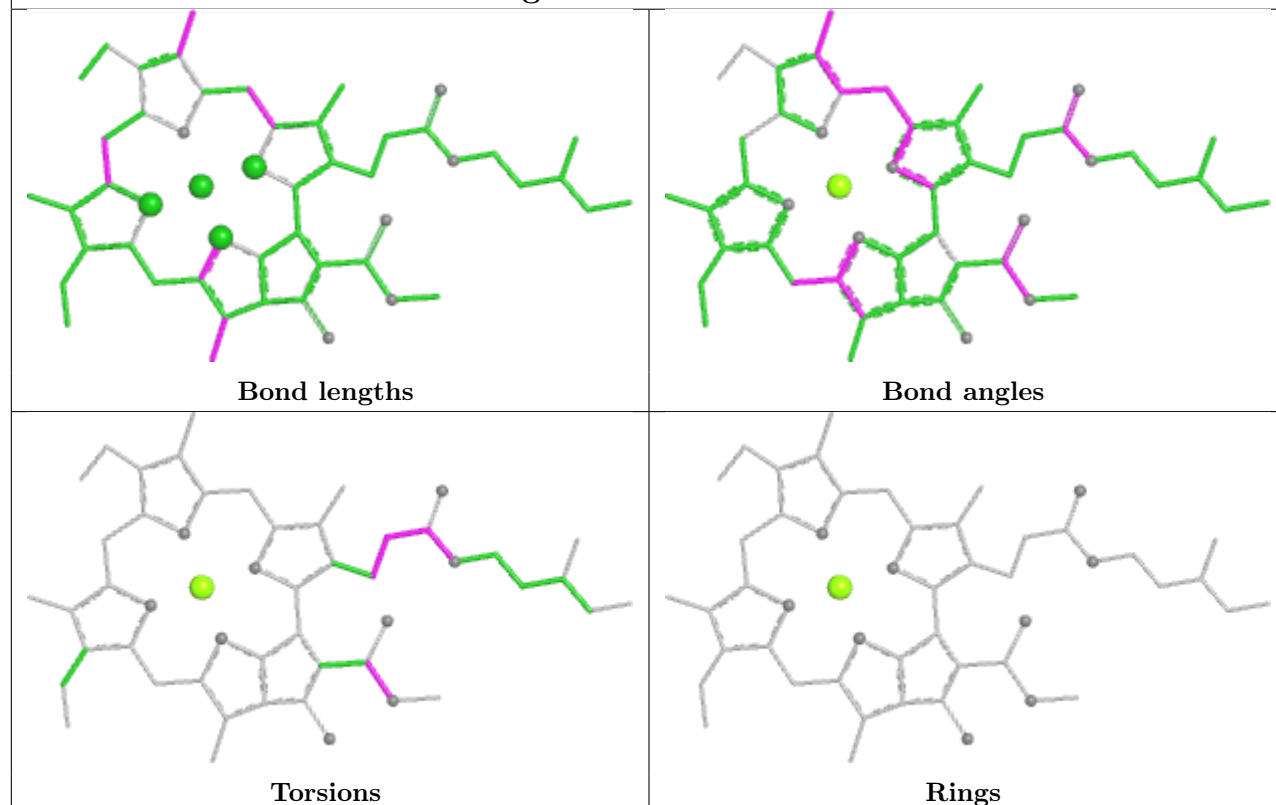
Ligand CLA A 1128

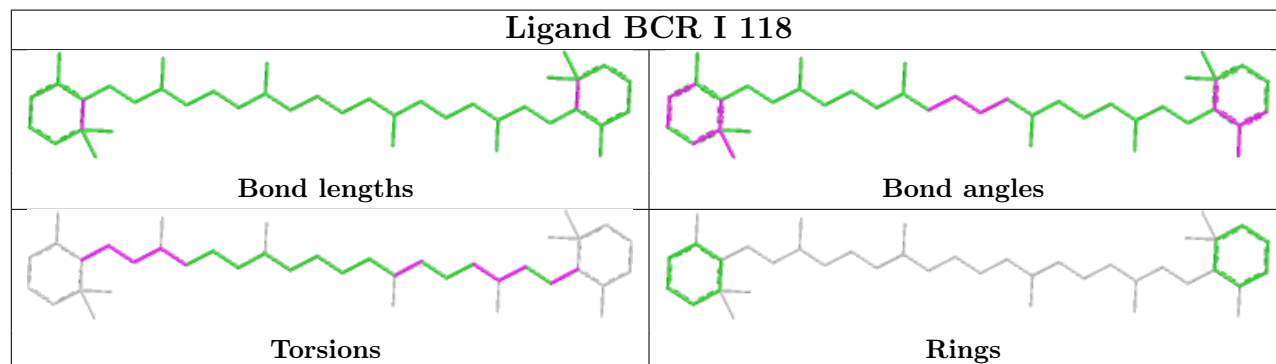
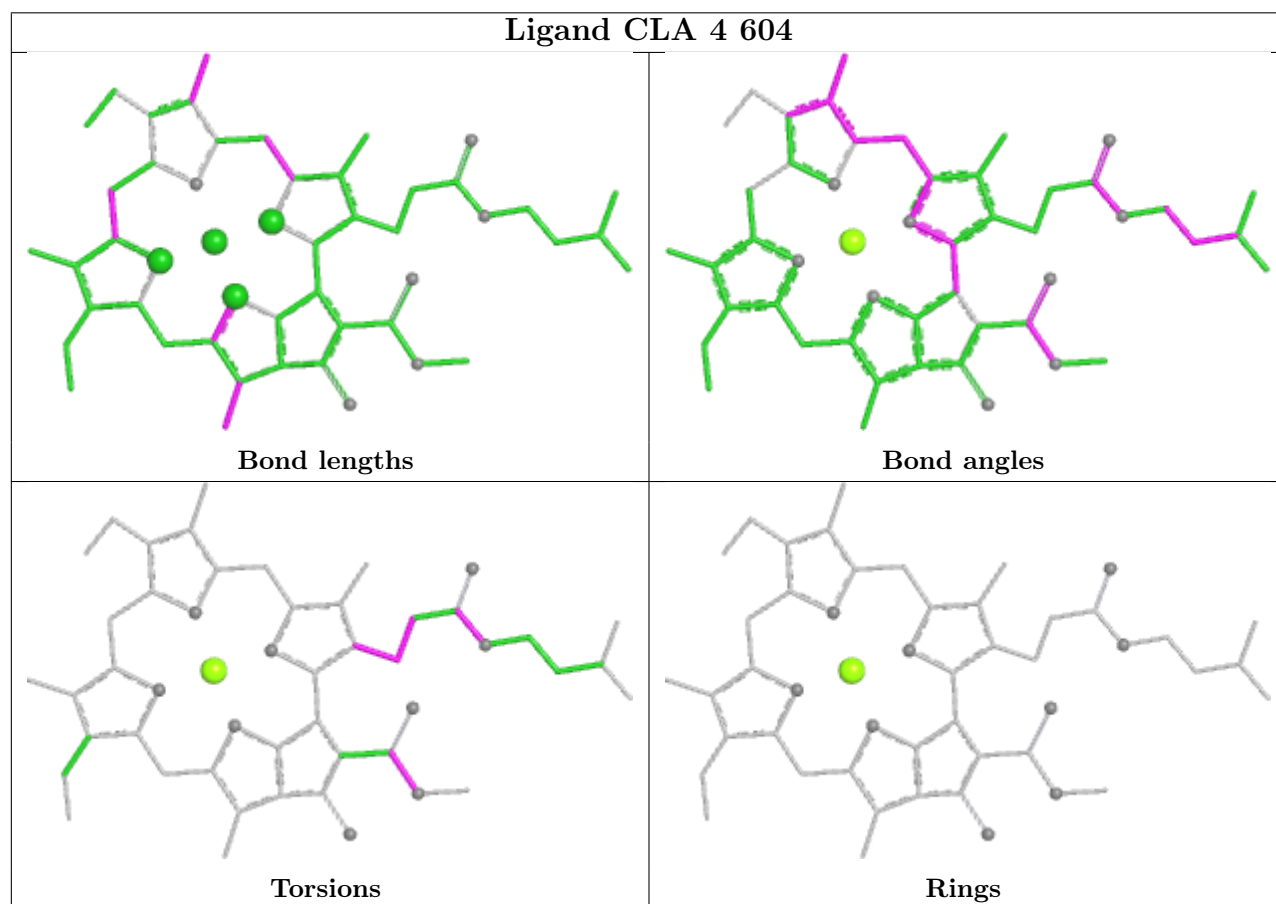
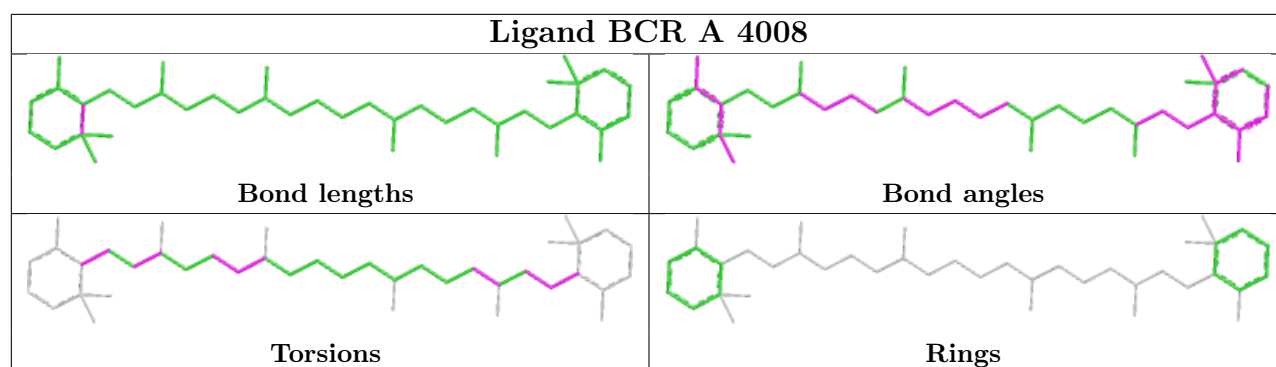


Ligand CLA B 1201

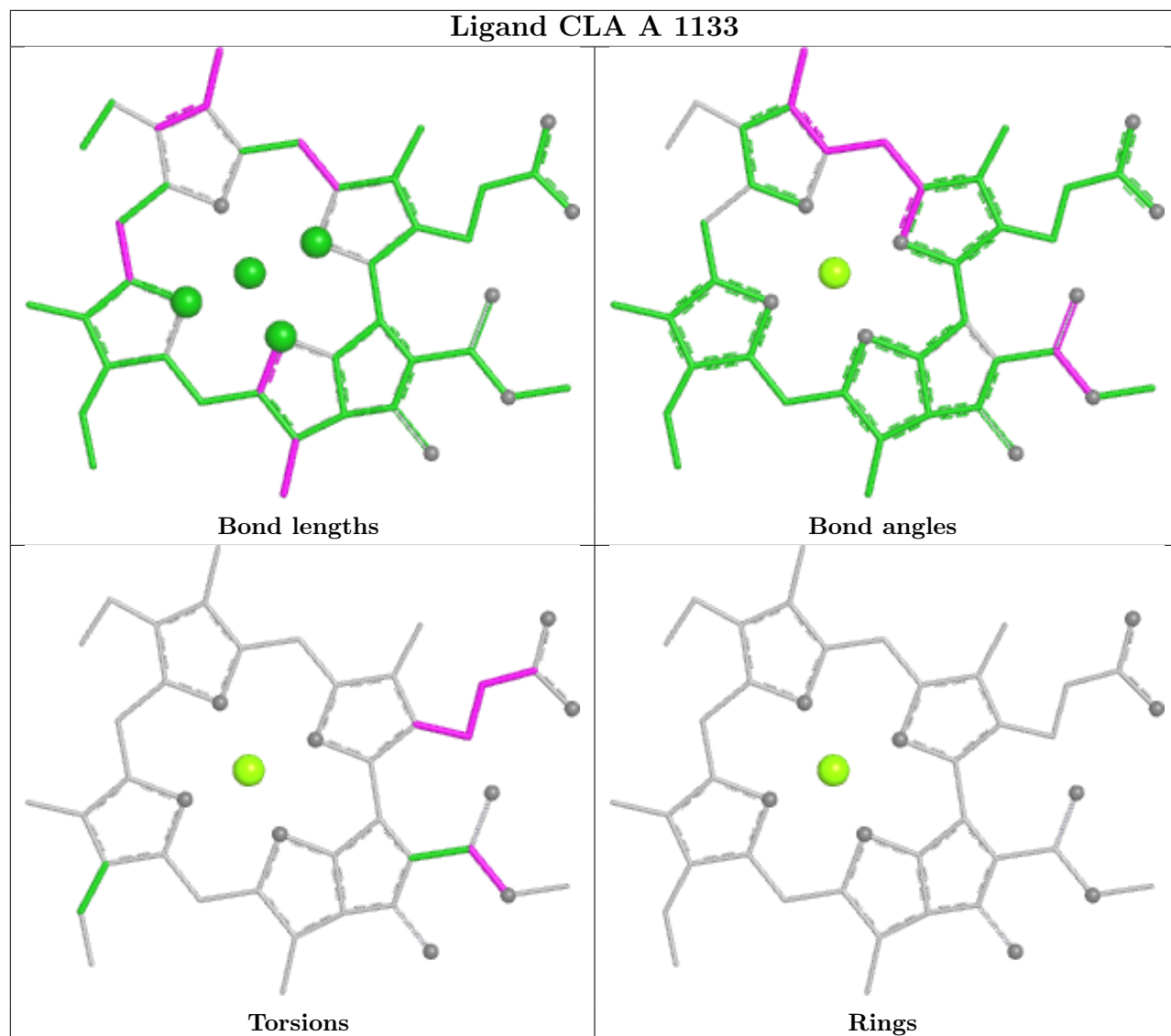


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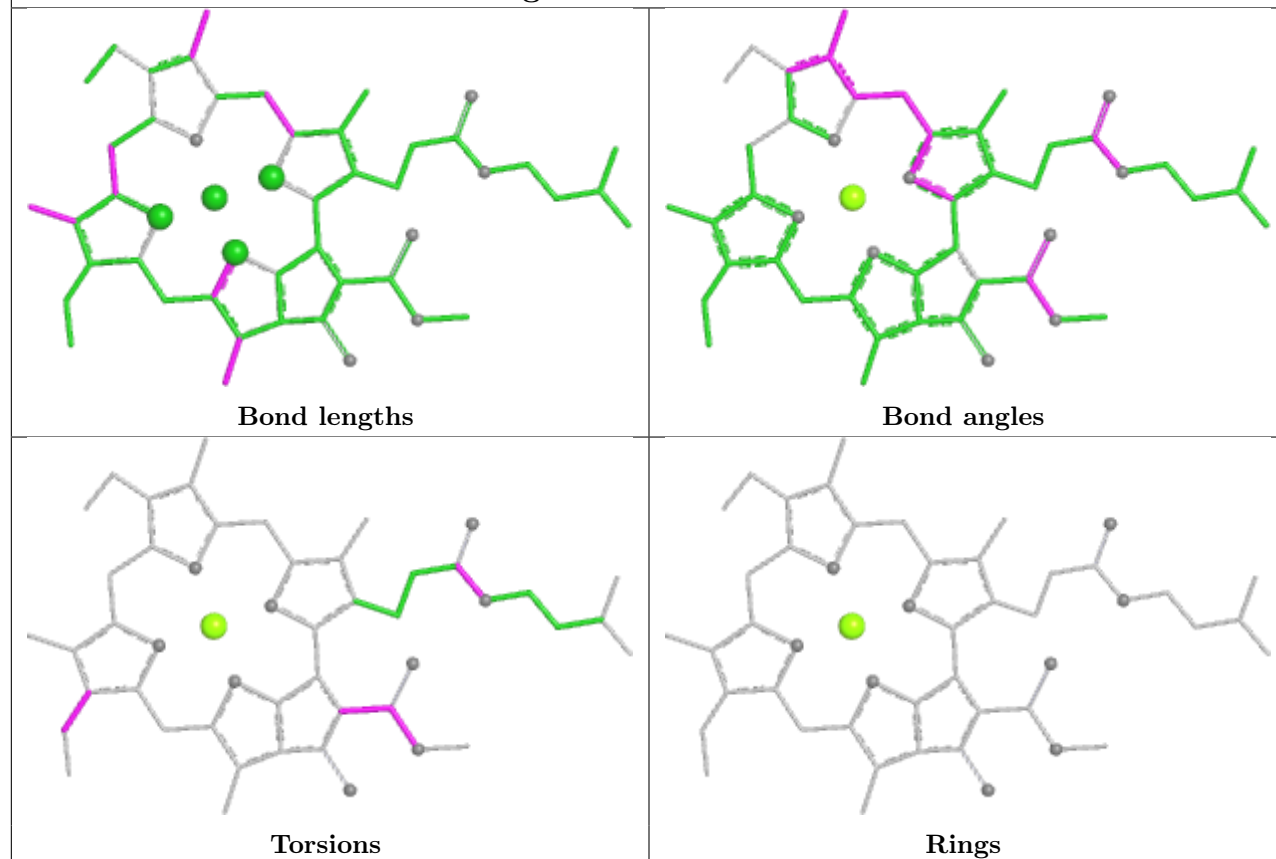




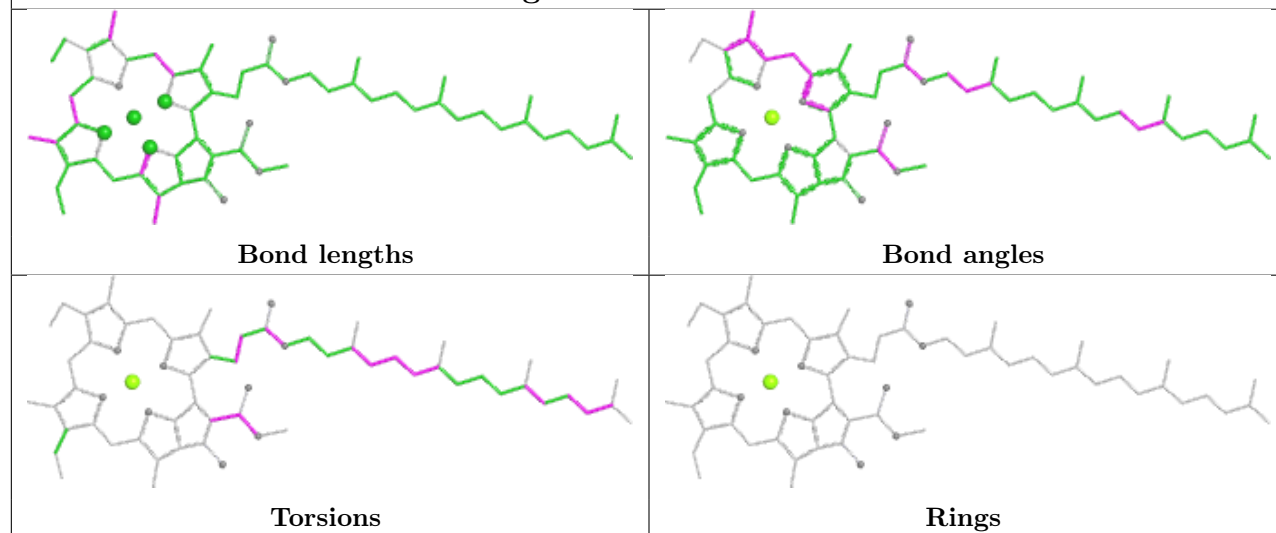
Ligand CLA A 1133



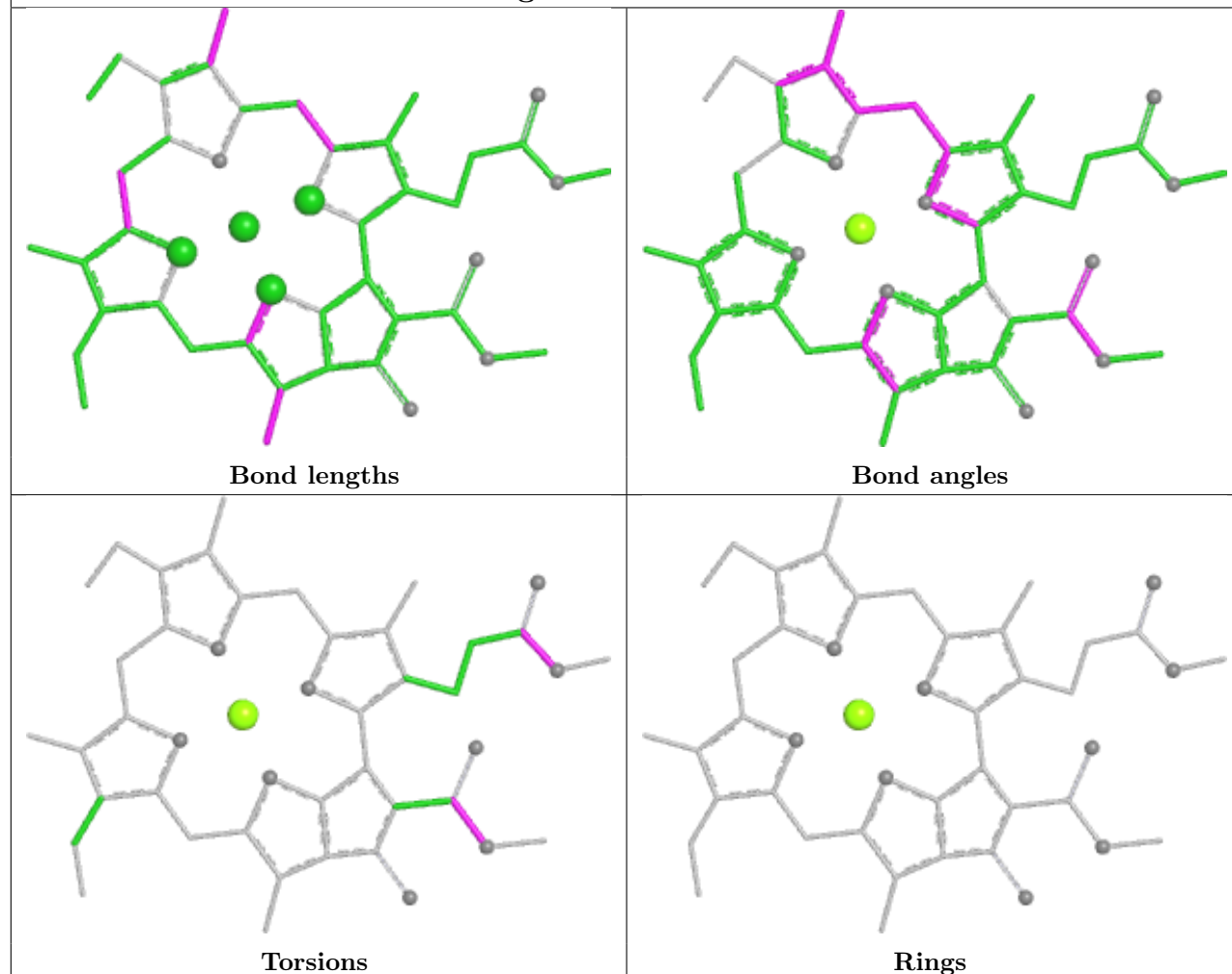
Ligand CLA A 1801



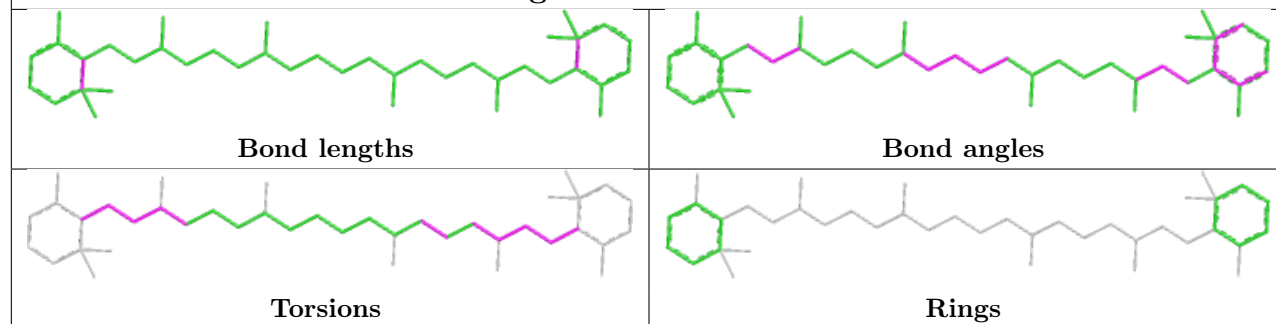
Ligand CLA A 1104



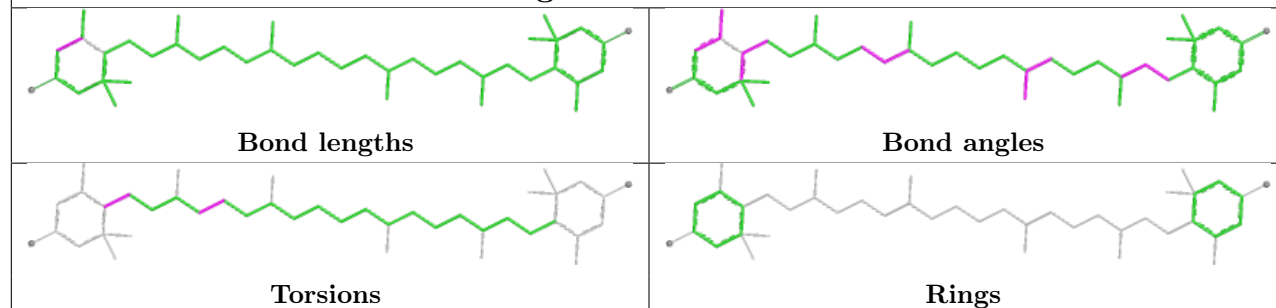
Ligand CLA 1 611

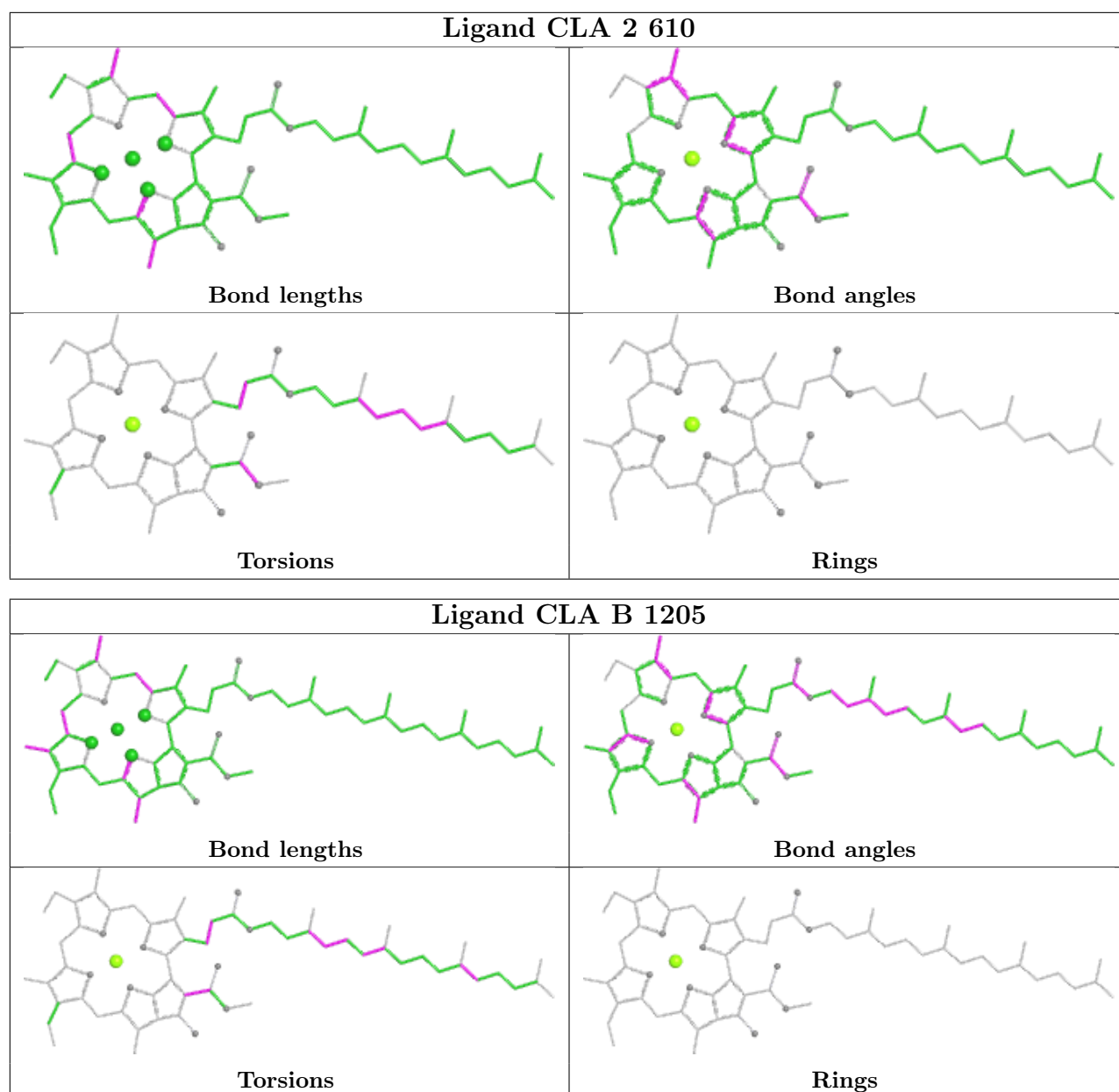


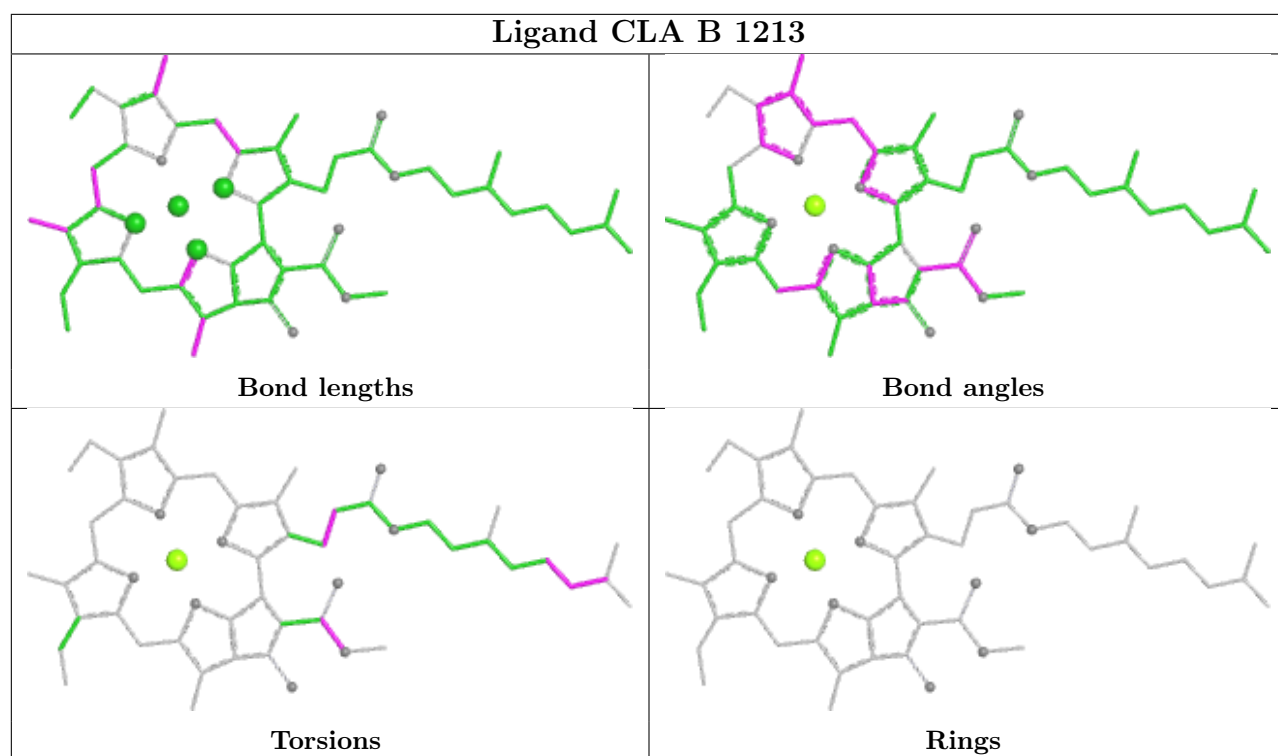
Ligand BCR K 301



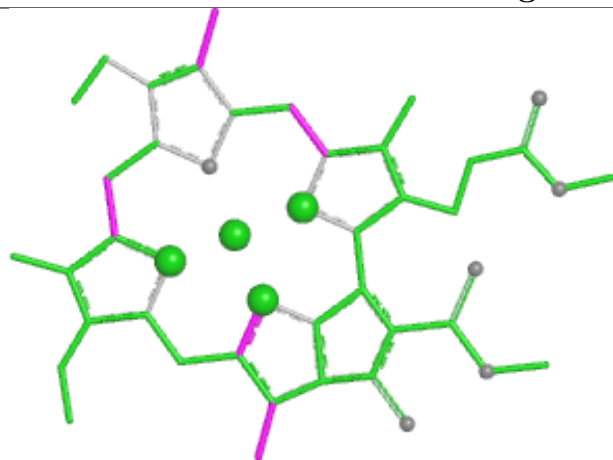
Ligand LUT 3 620



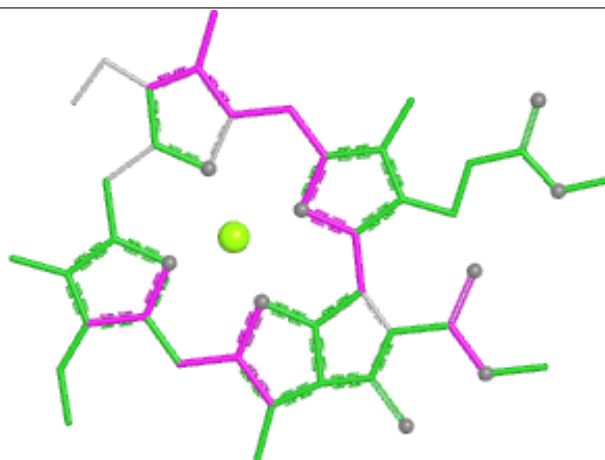




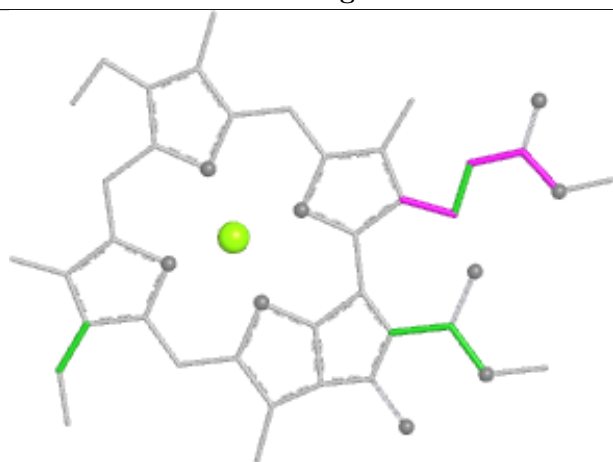
Ligand CLA 1 614



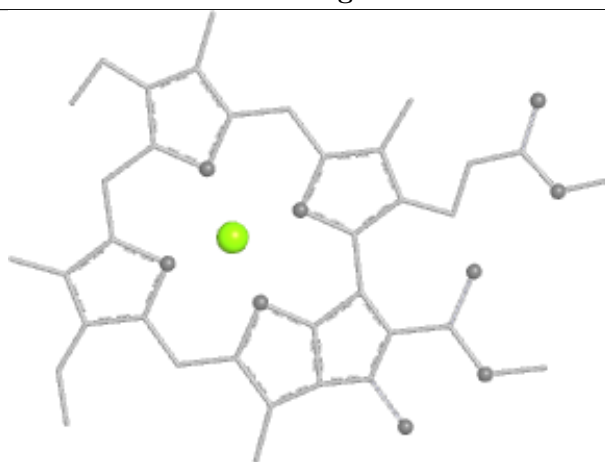
Bond lengths



Bond angles

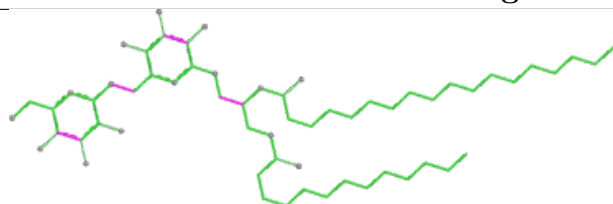


Torsions

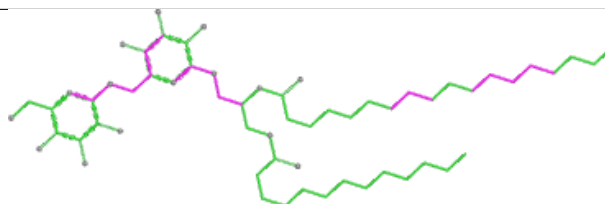


Rings

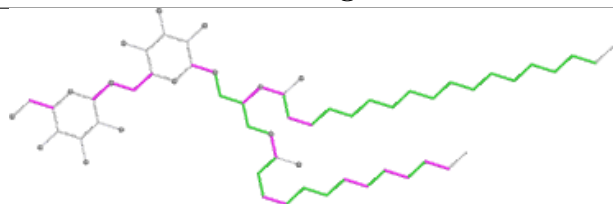
Ligand DGD B 5002



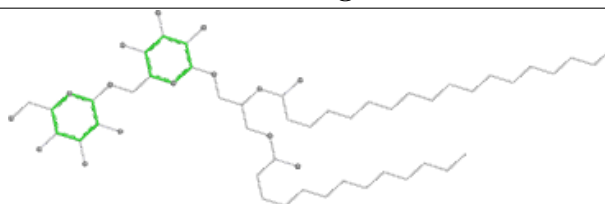
Bond lengths



Bond angles

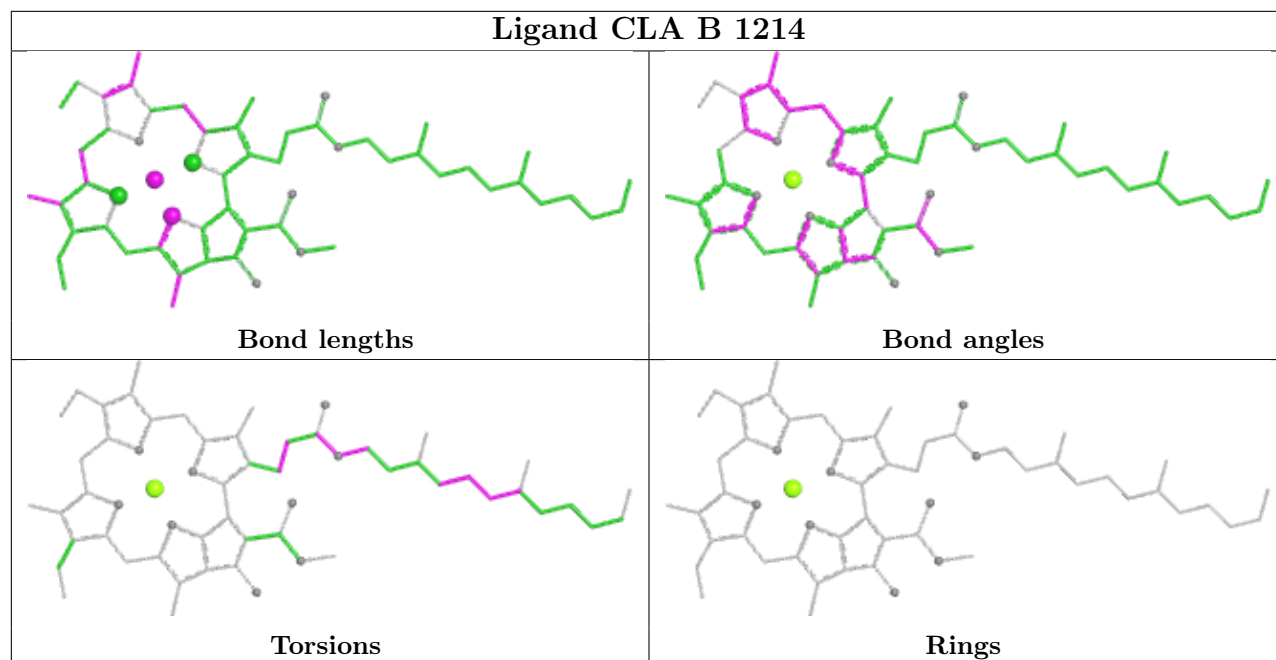


Torsions

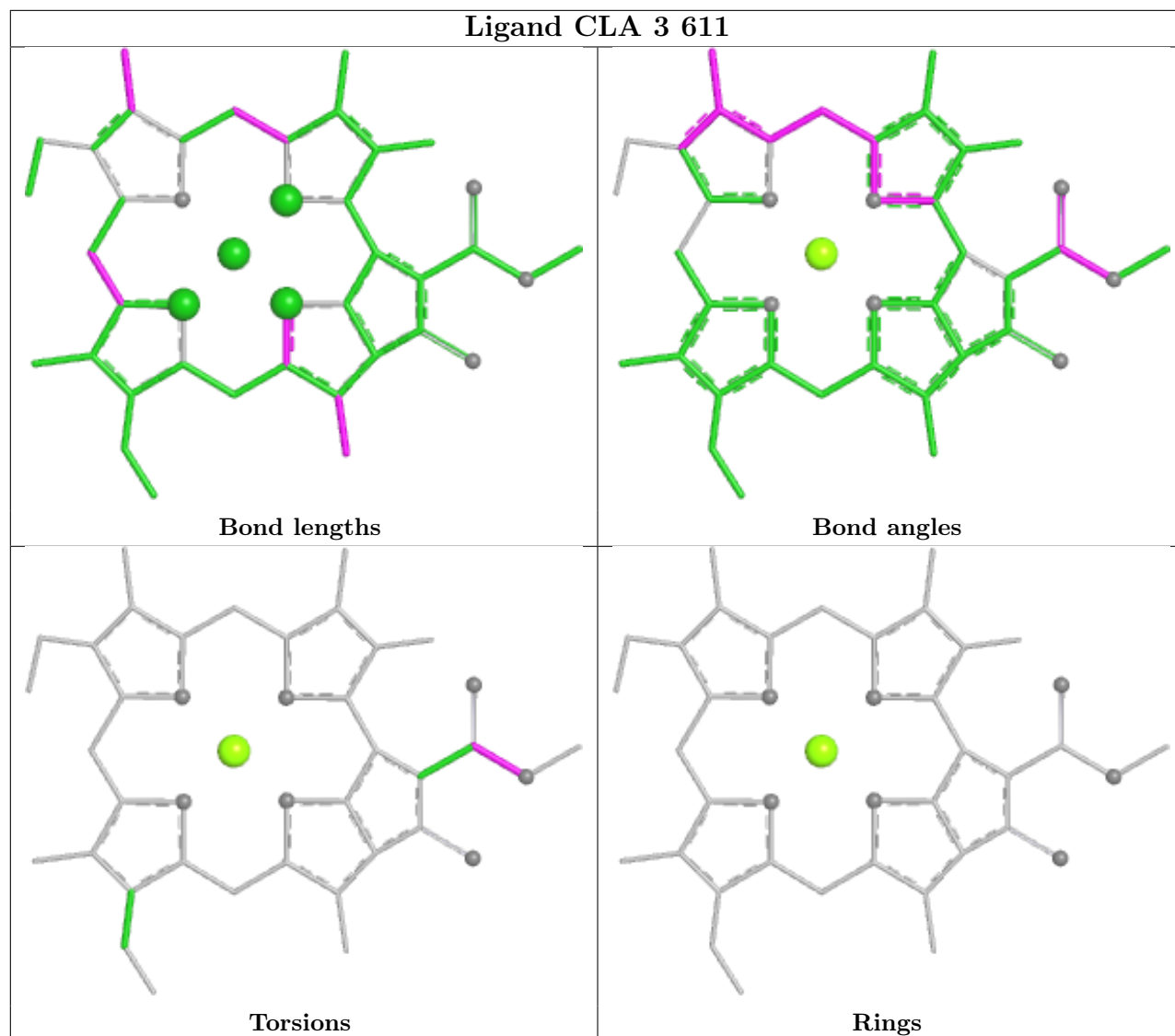


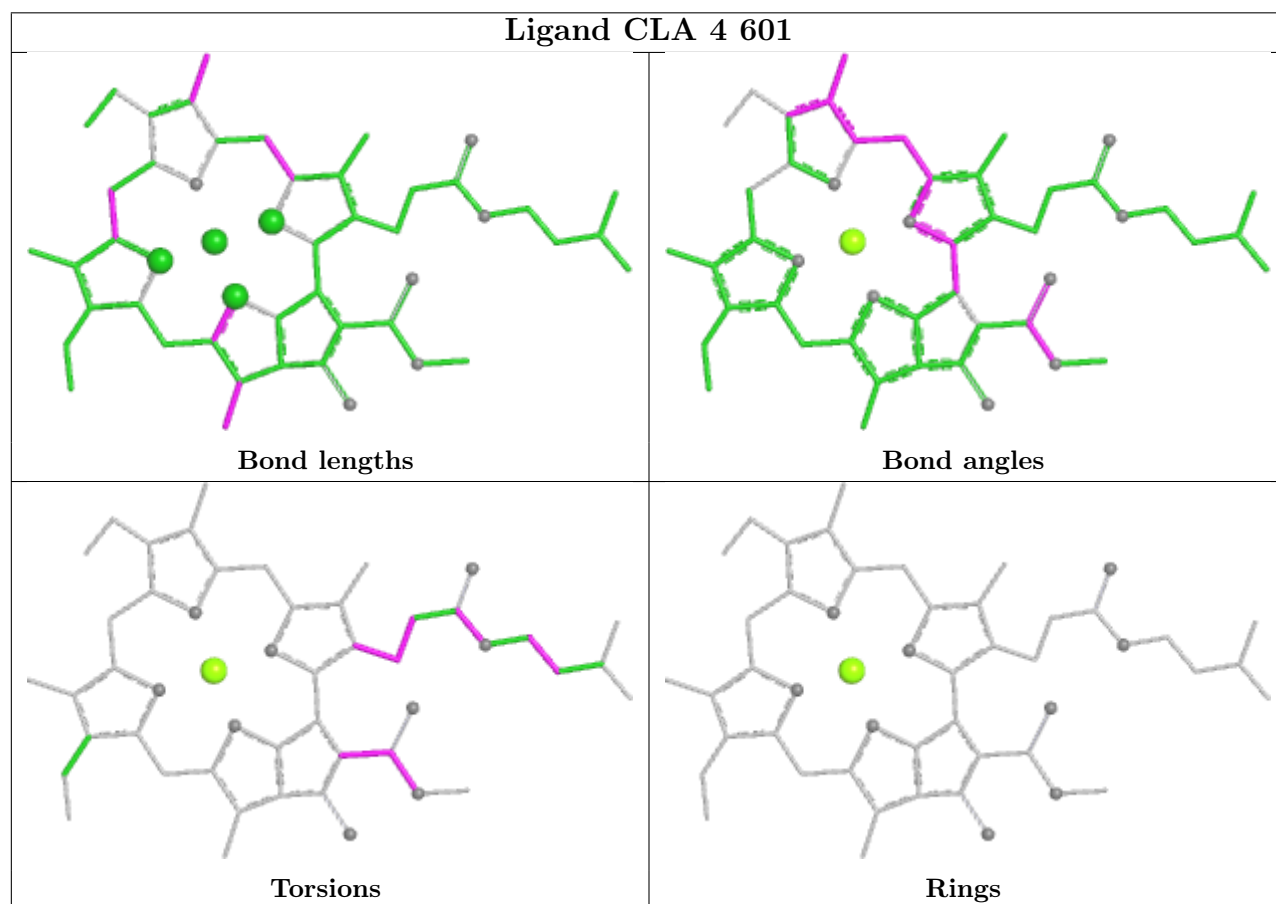
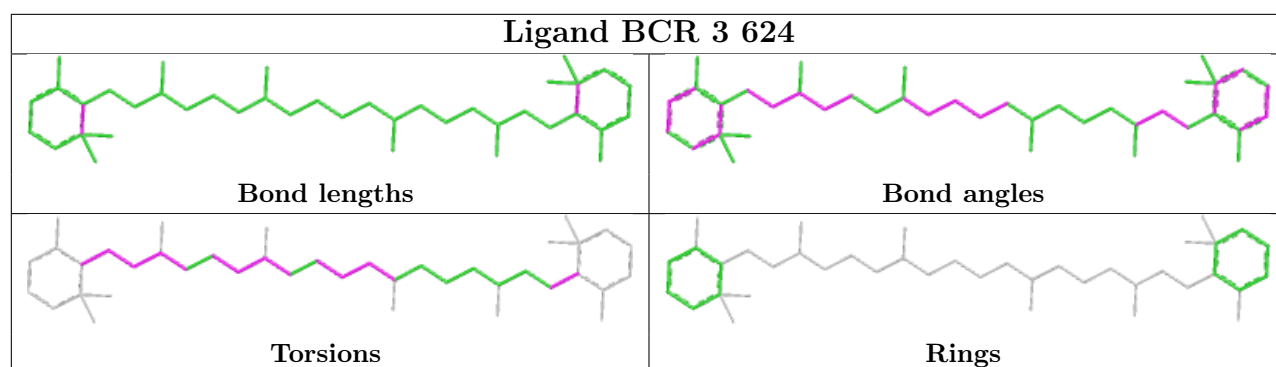
Rings

Ligand CLA B 1214

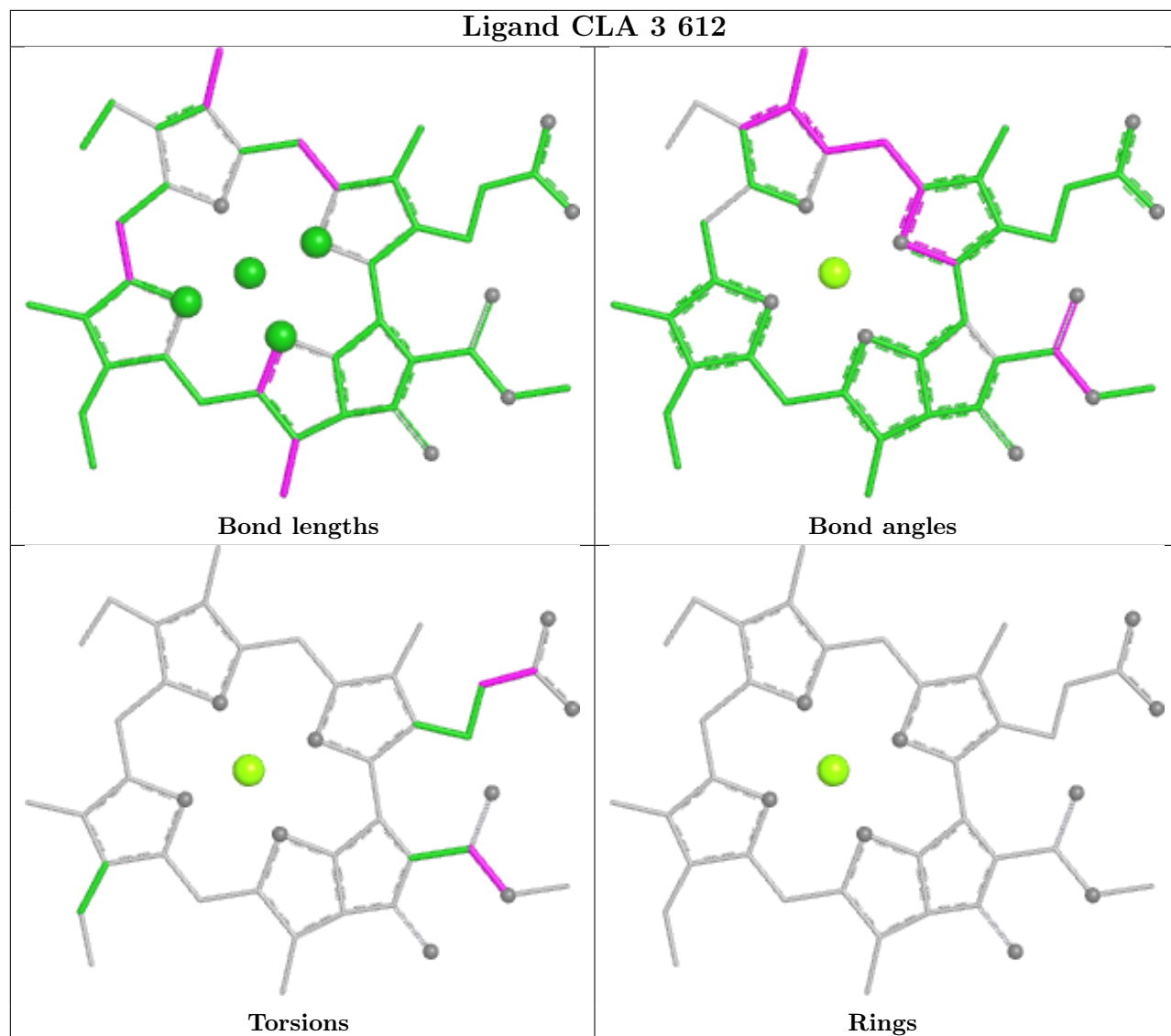


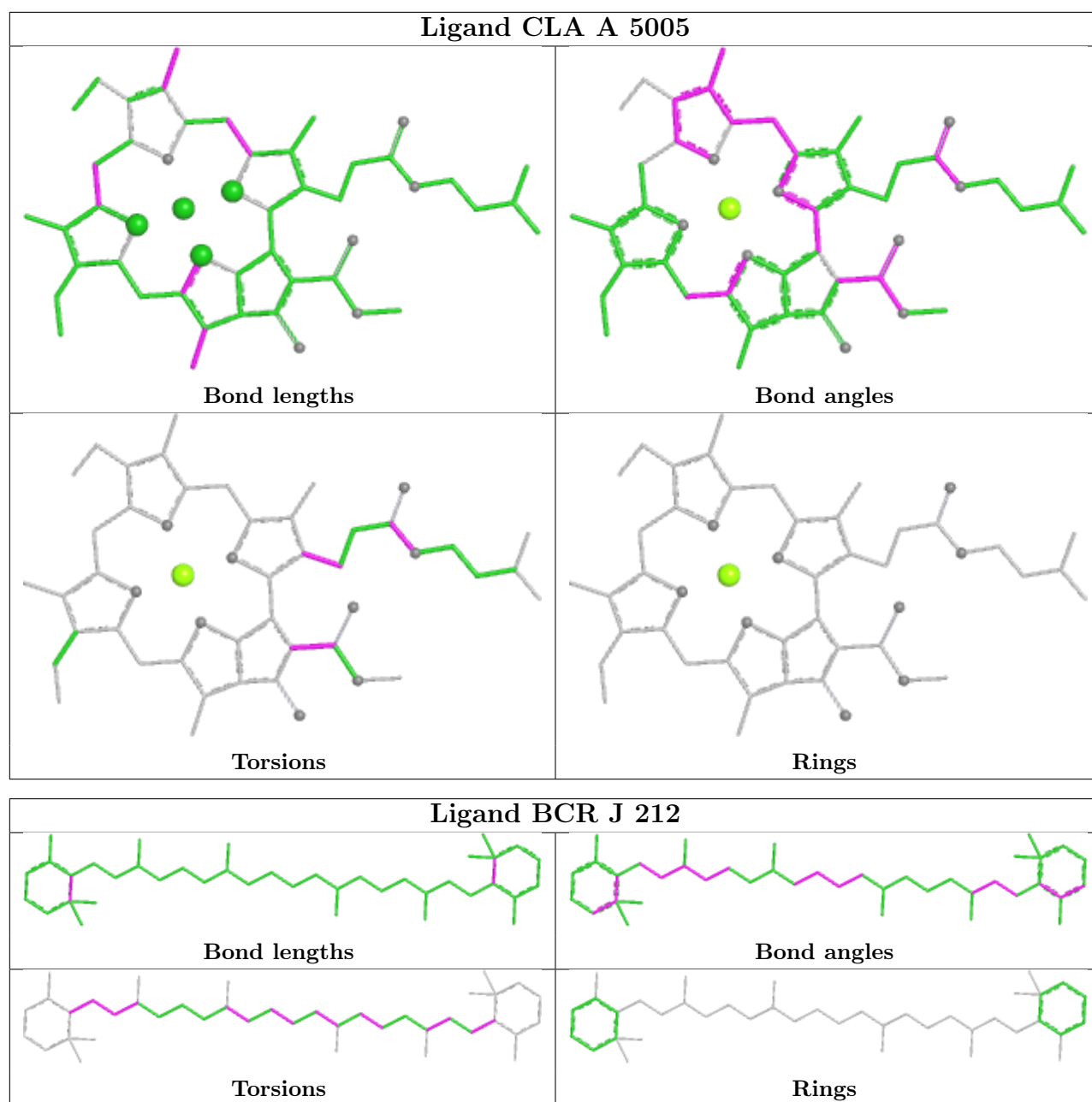
Ligand CLA 3 611

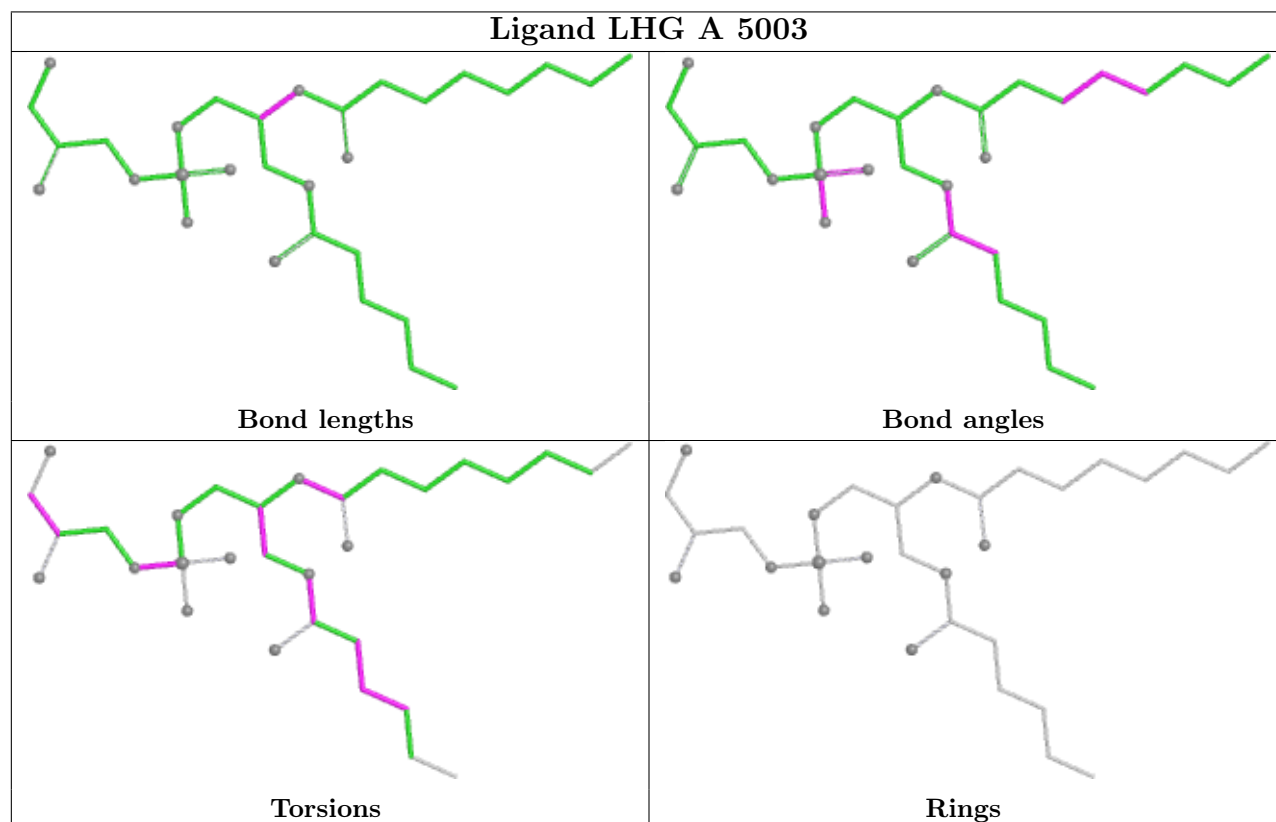
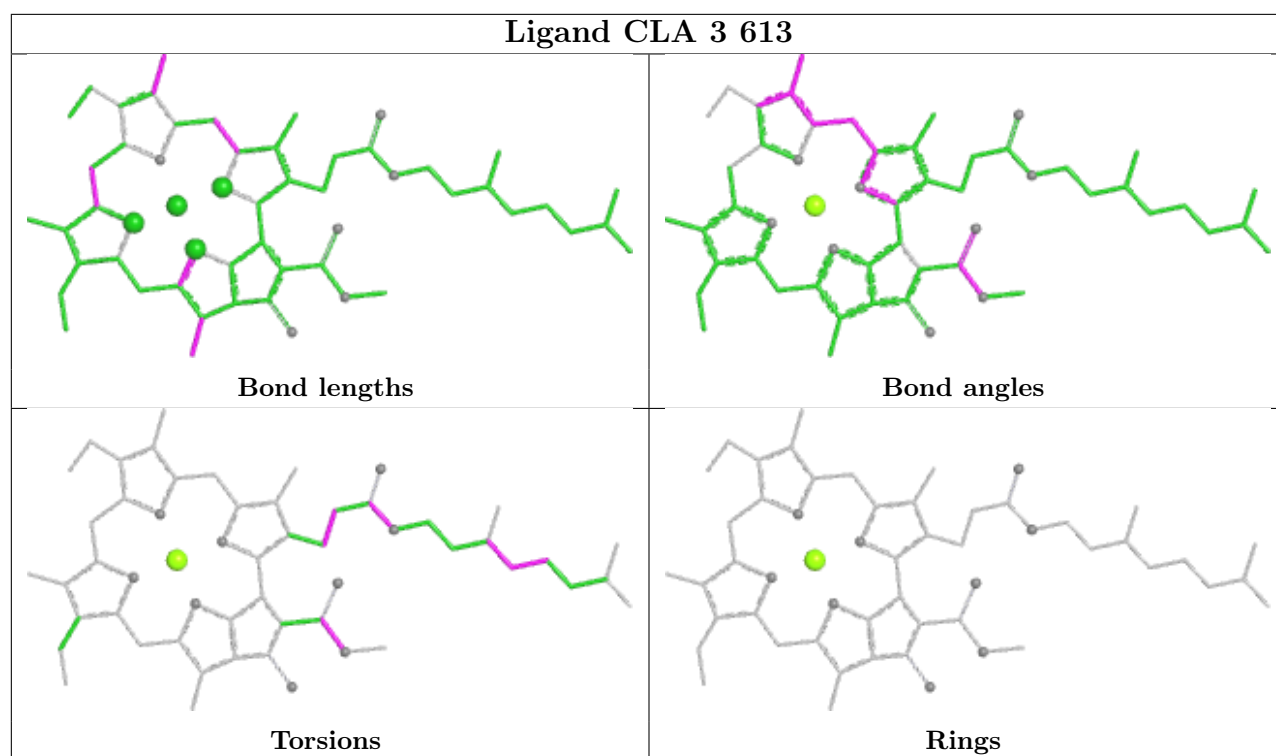


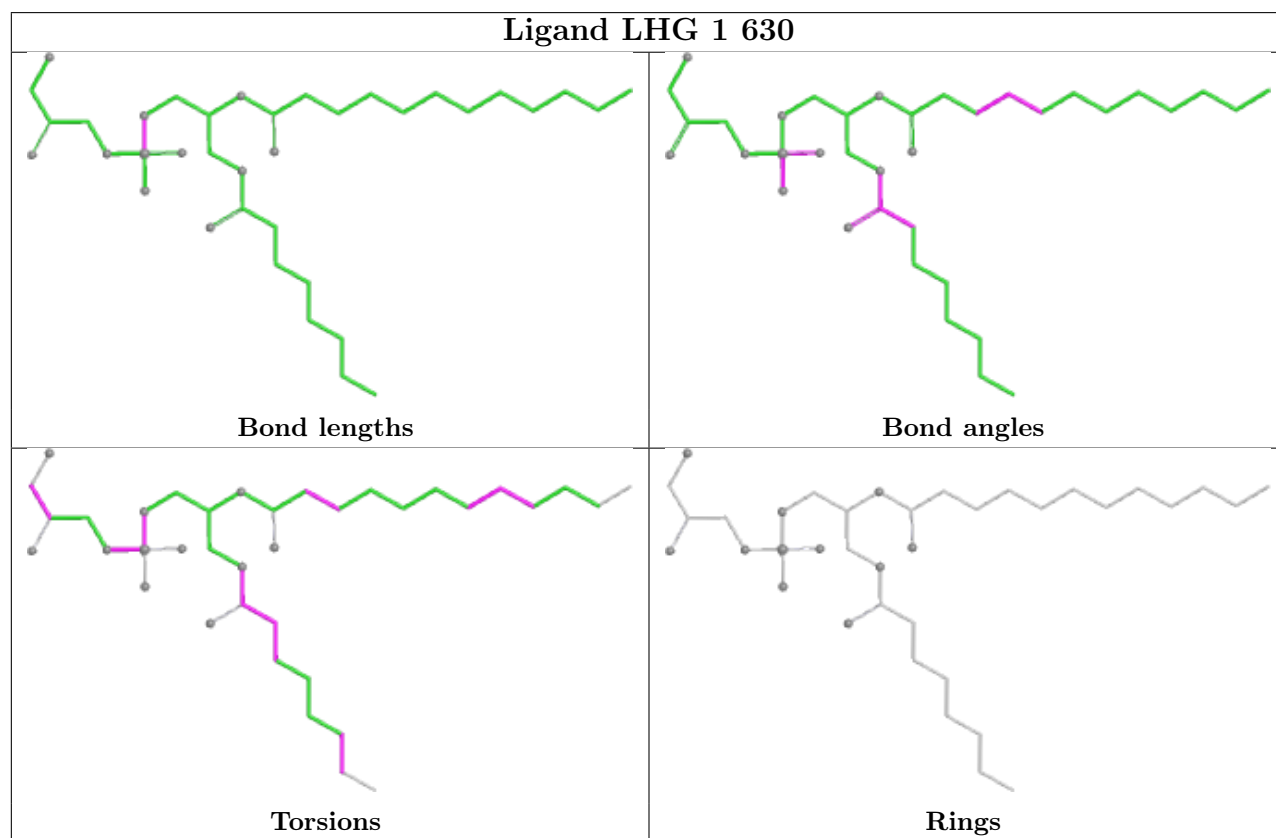
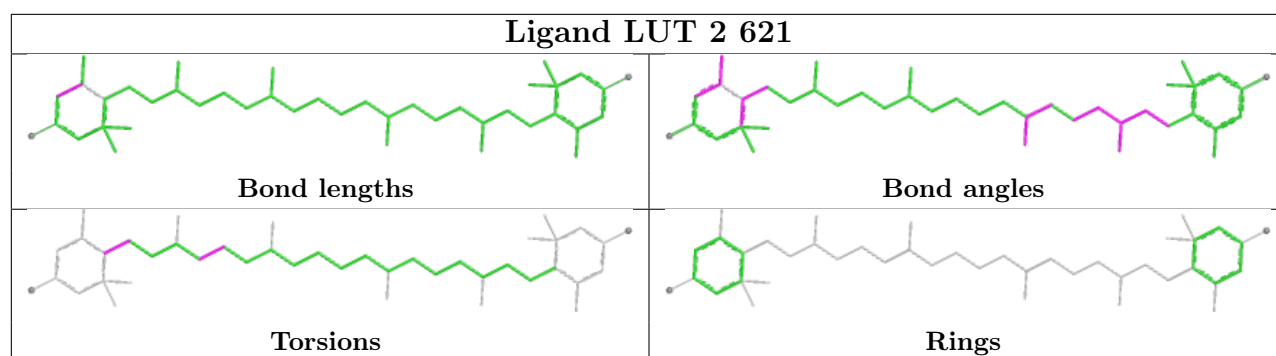


Ligand CLA 3 612

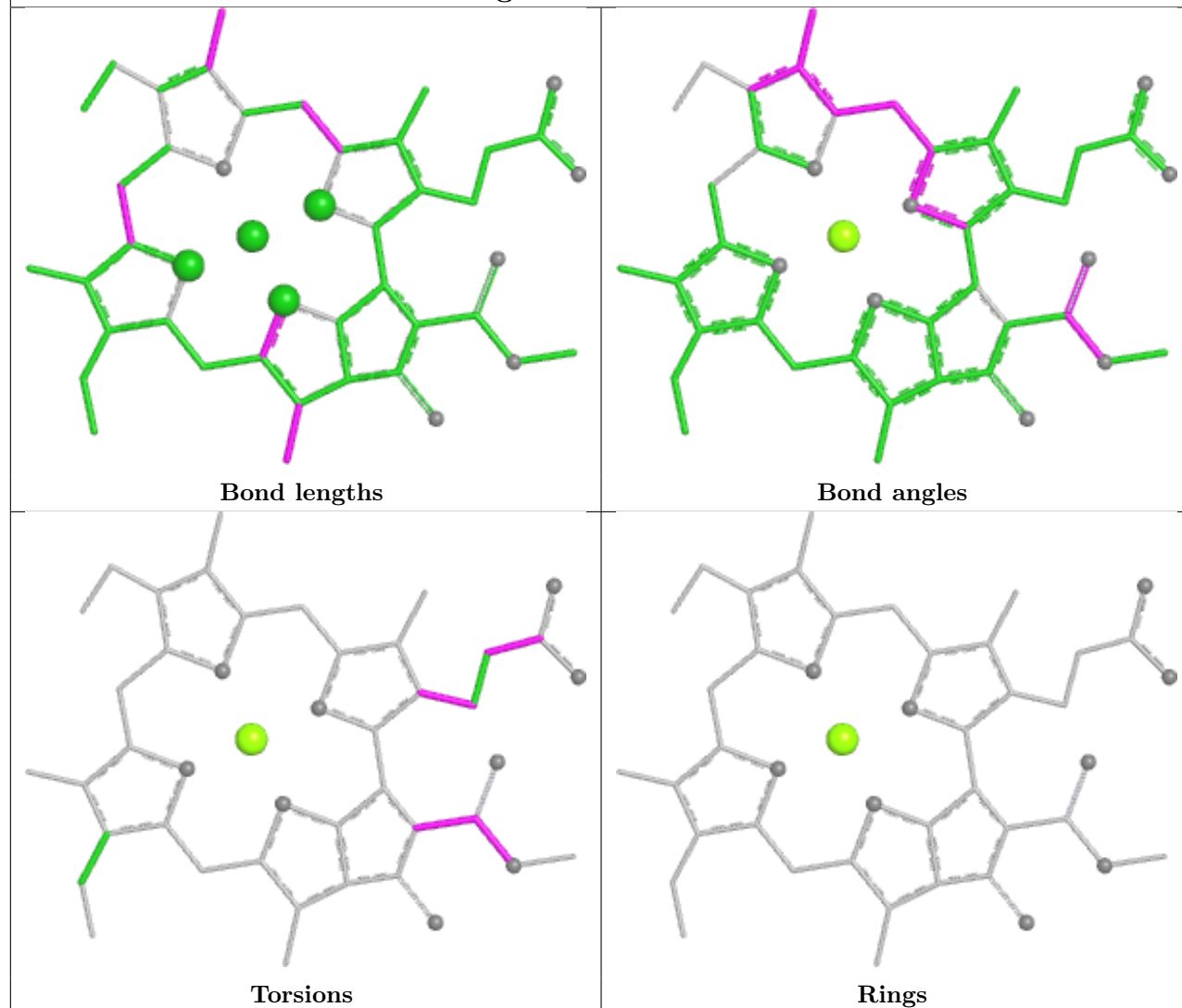




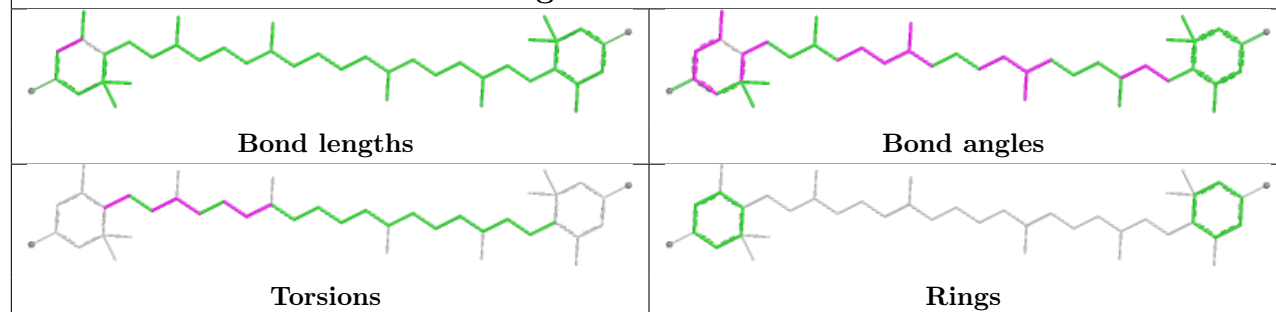




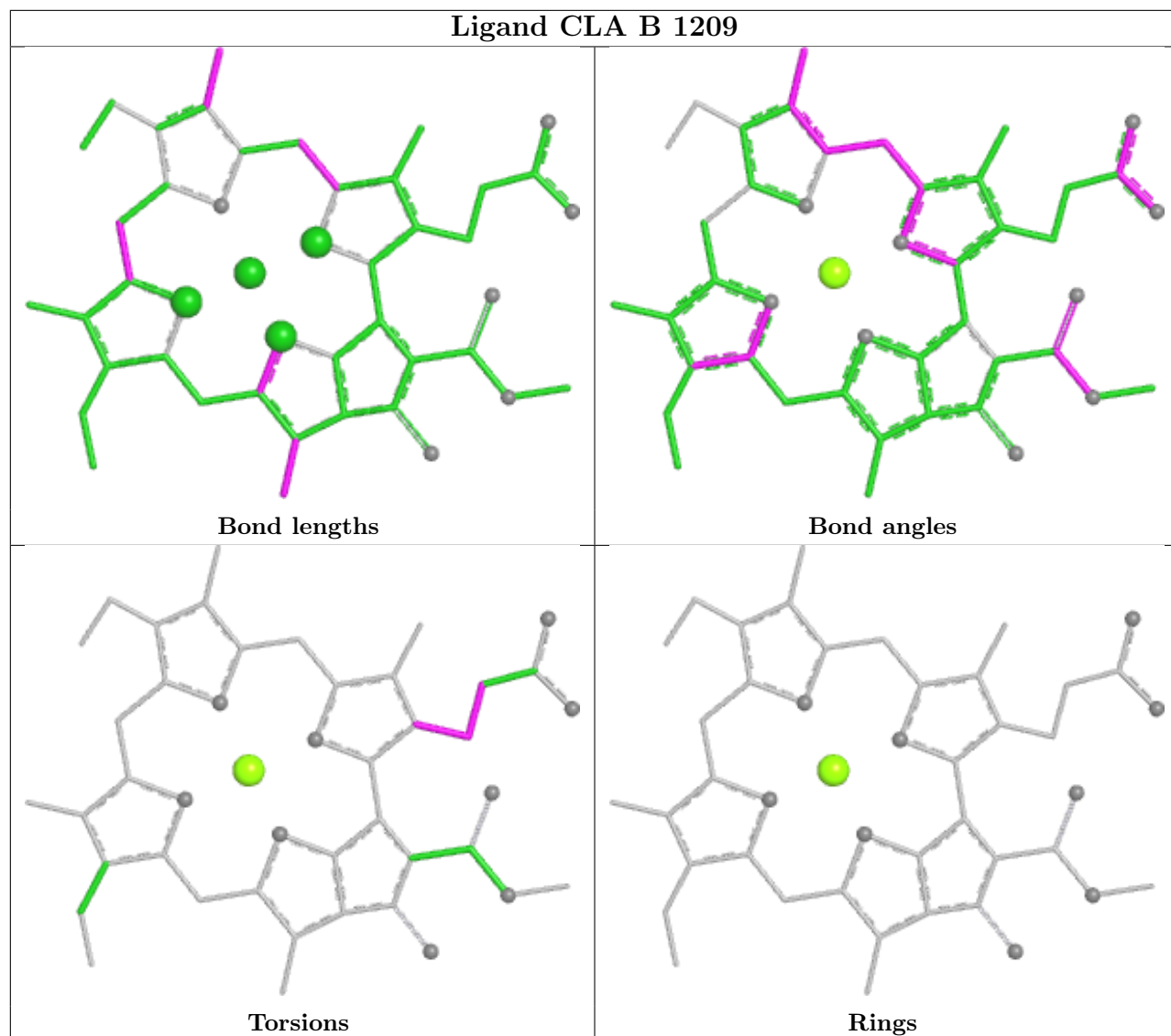
Ligand CLA J 102

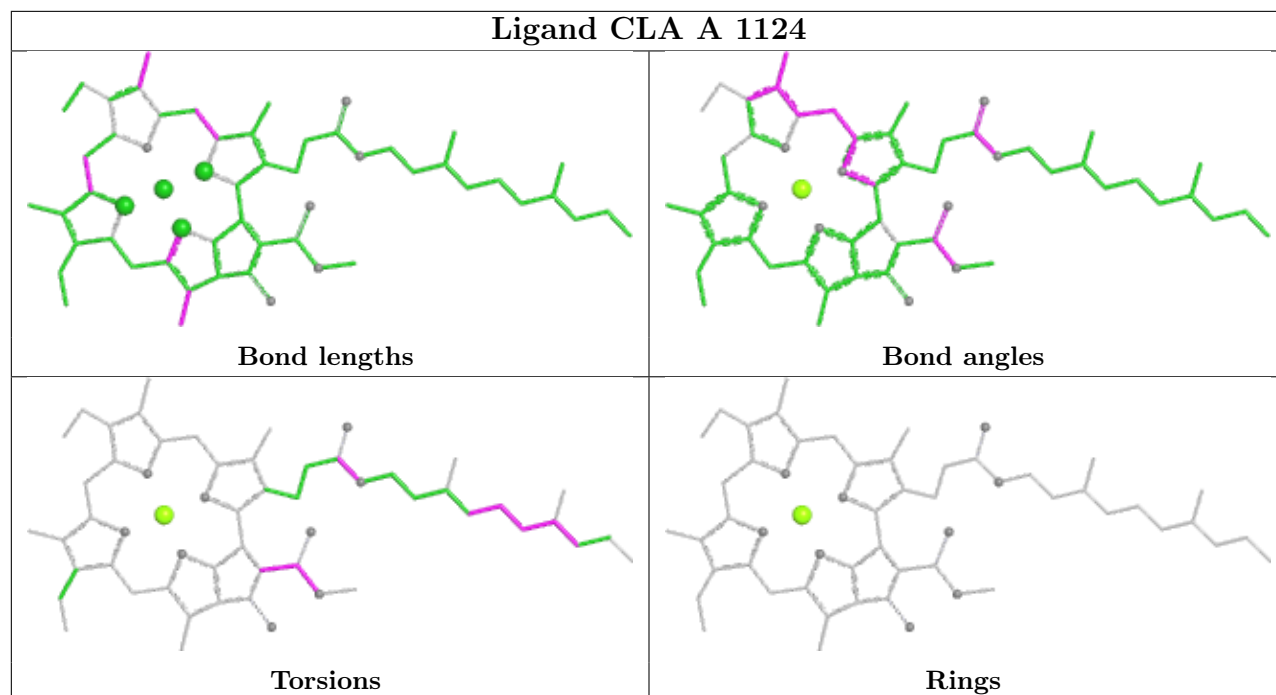


Ligand LUT 3 621

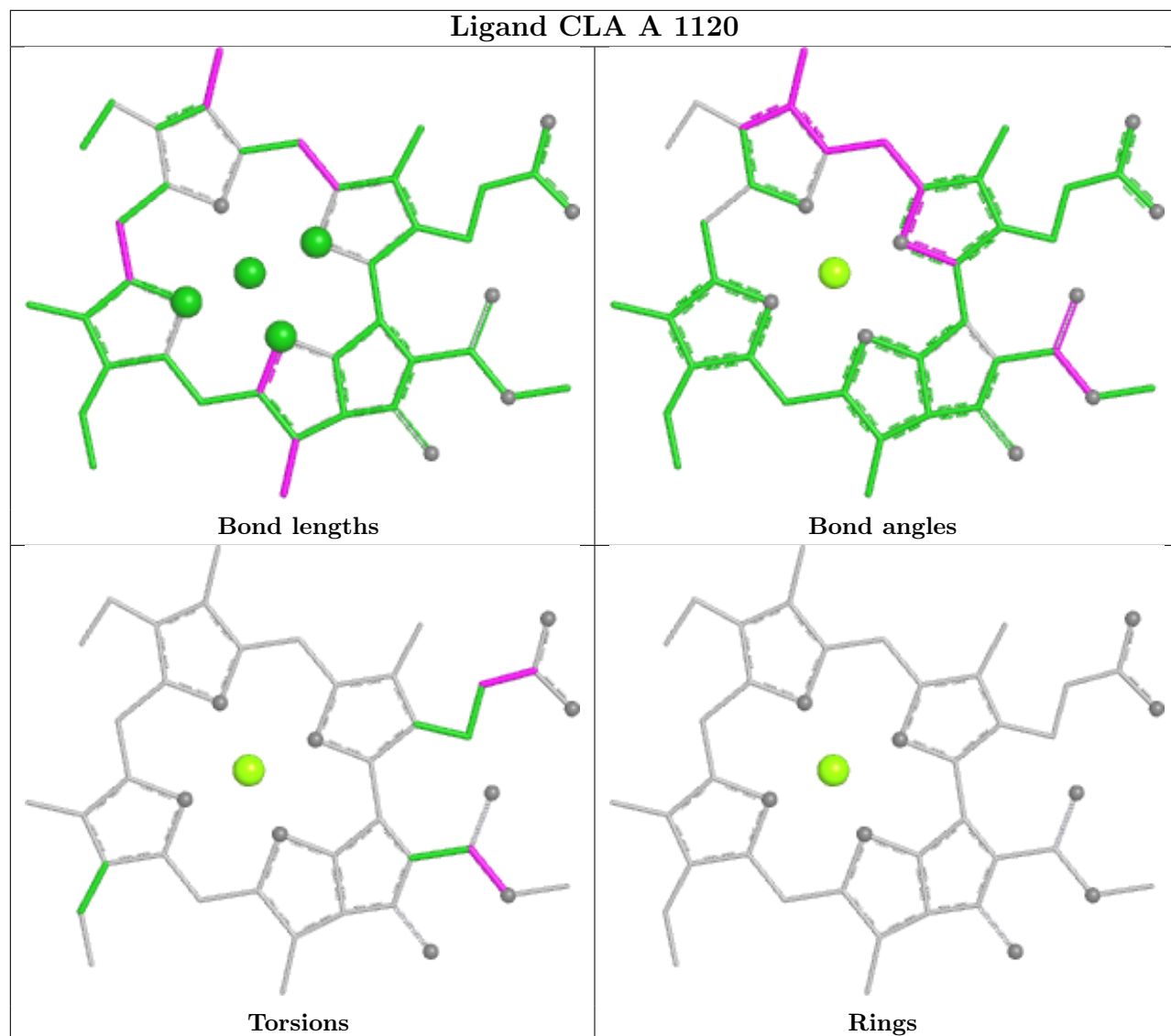


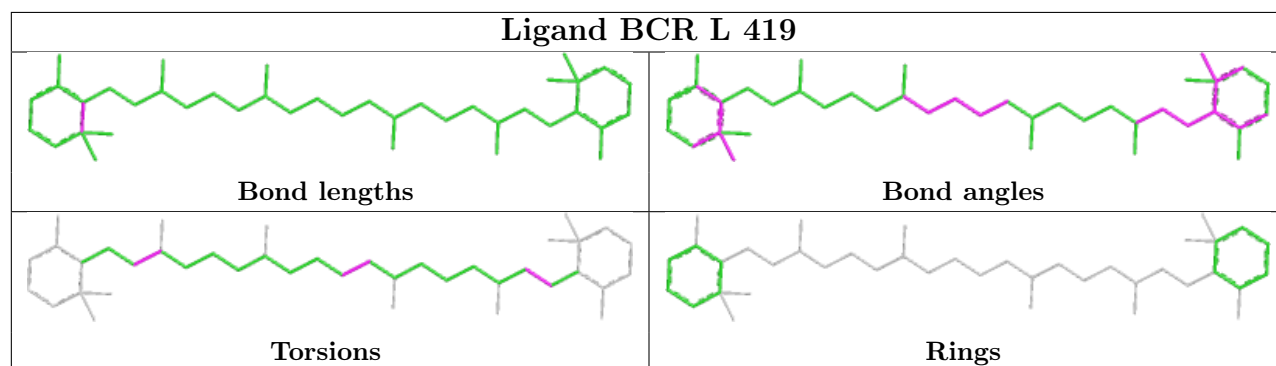
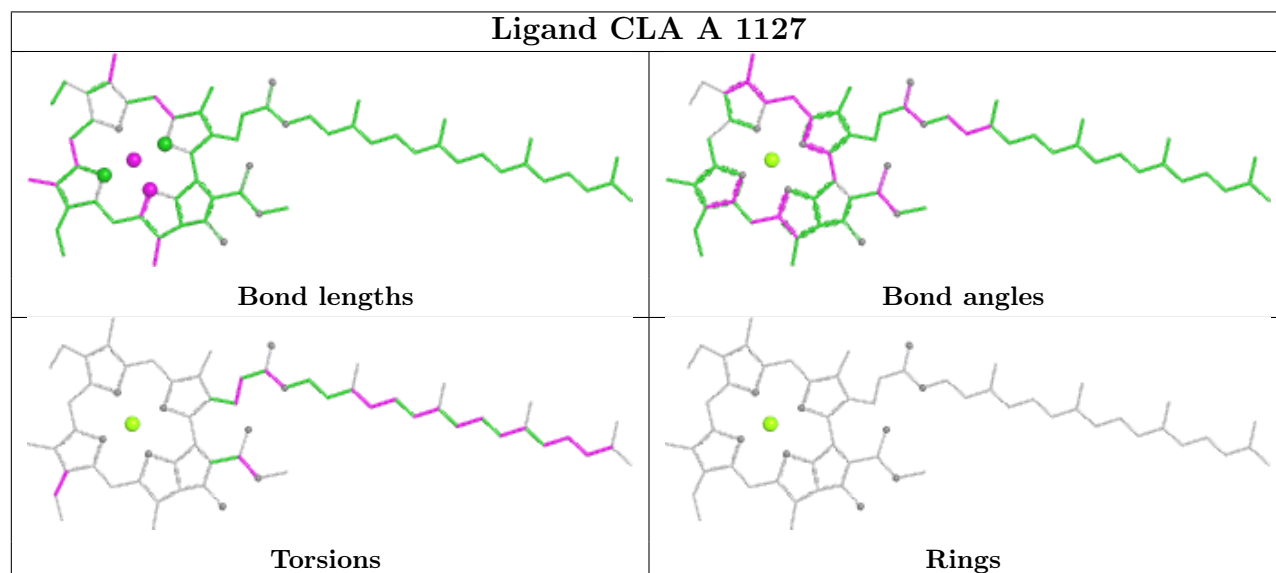
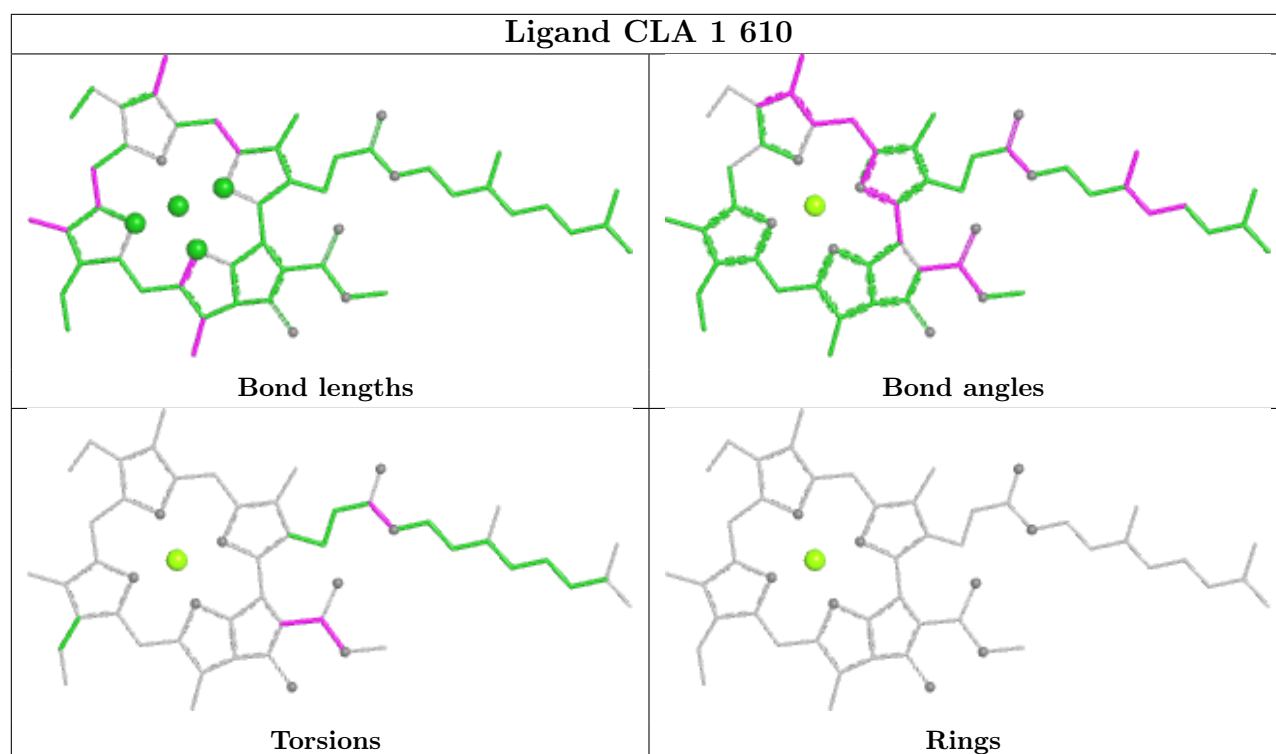
Ligand CLA B 1209

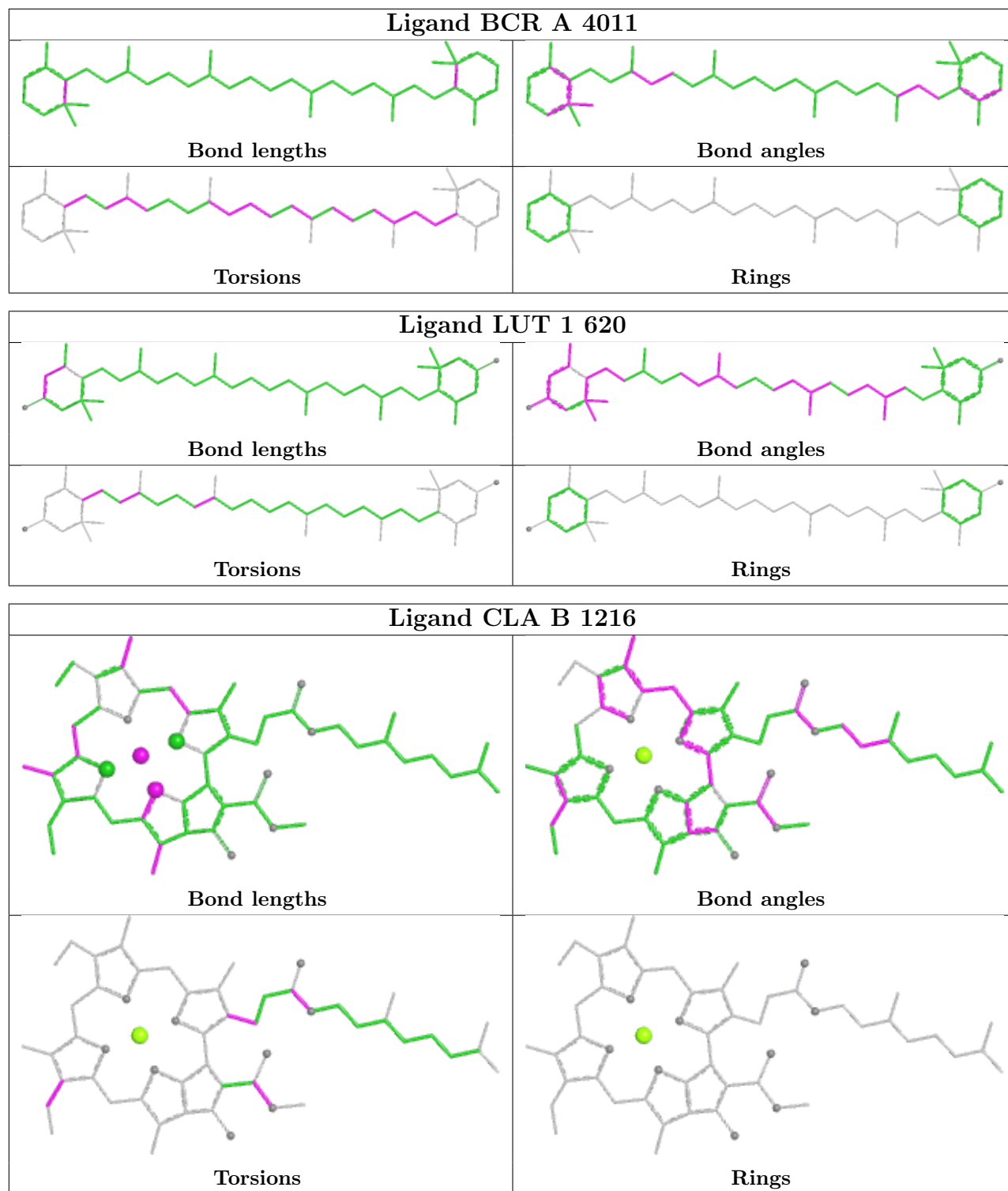


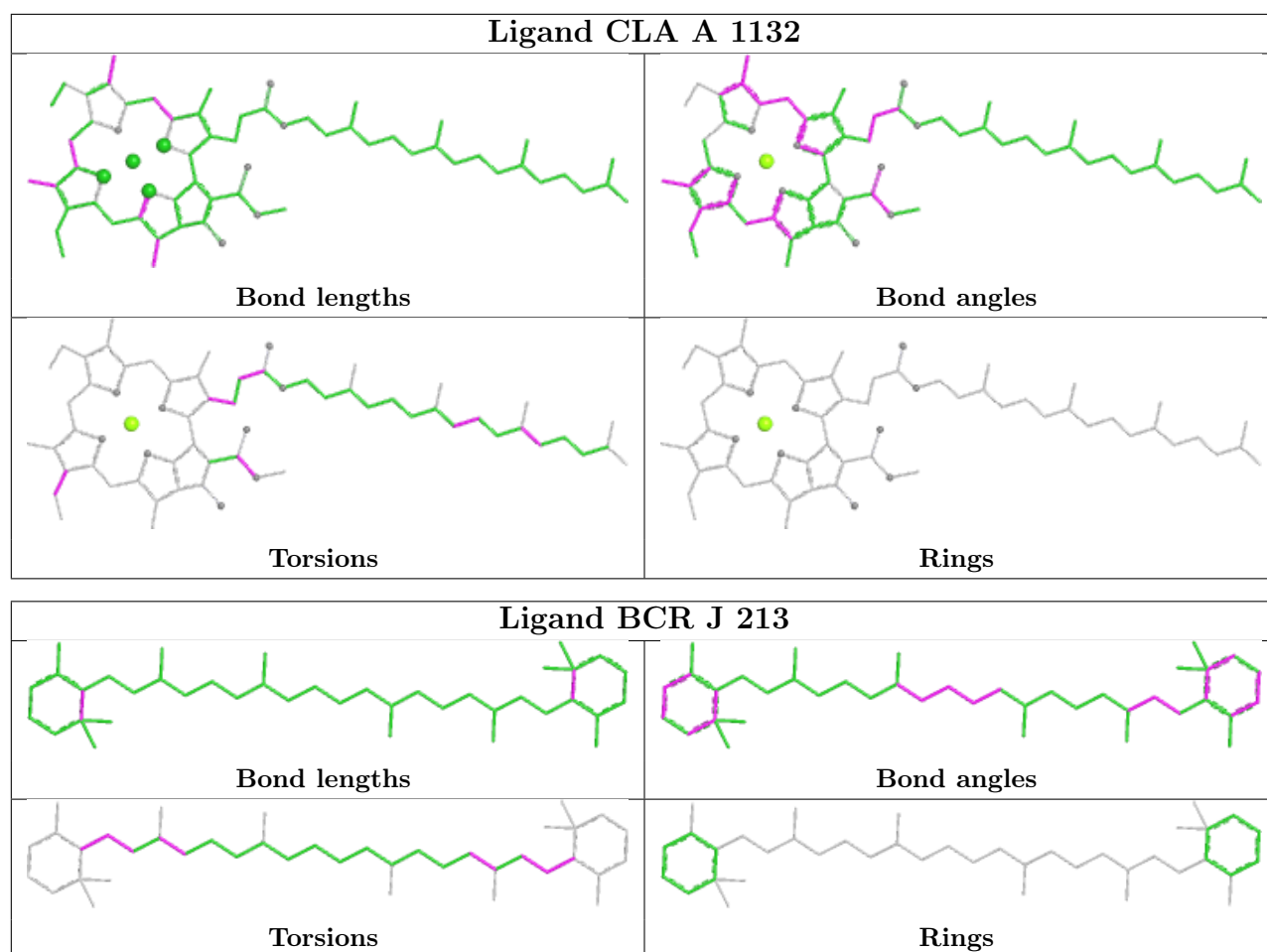


Ligand CLA A 1120

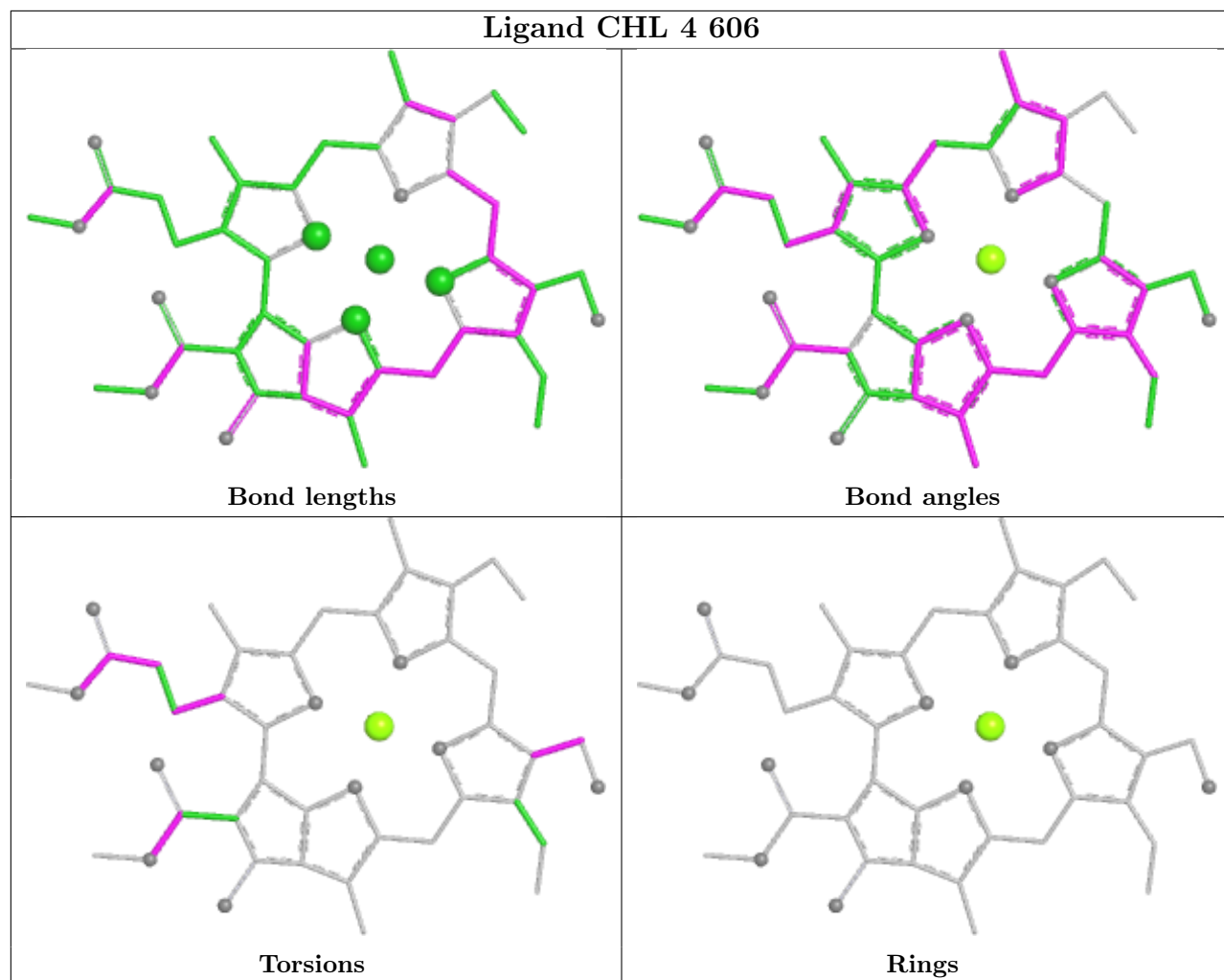




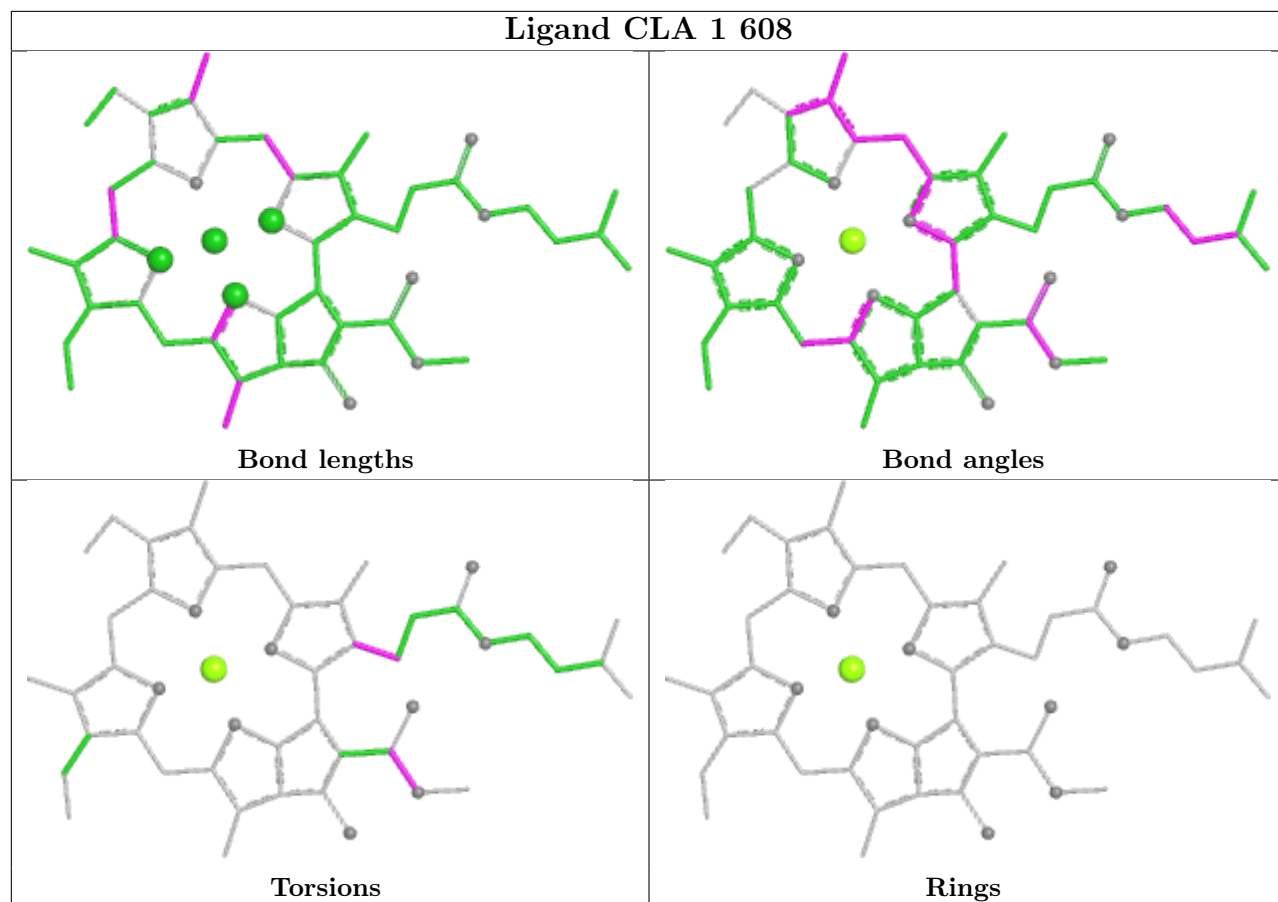


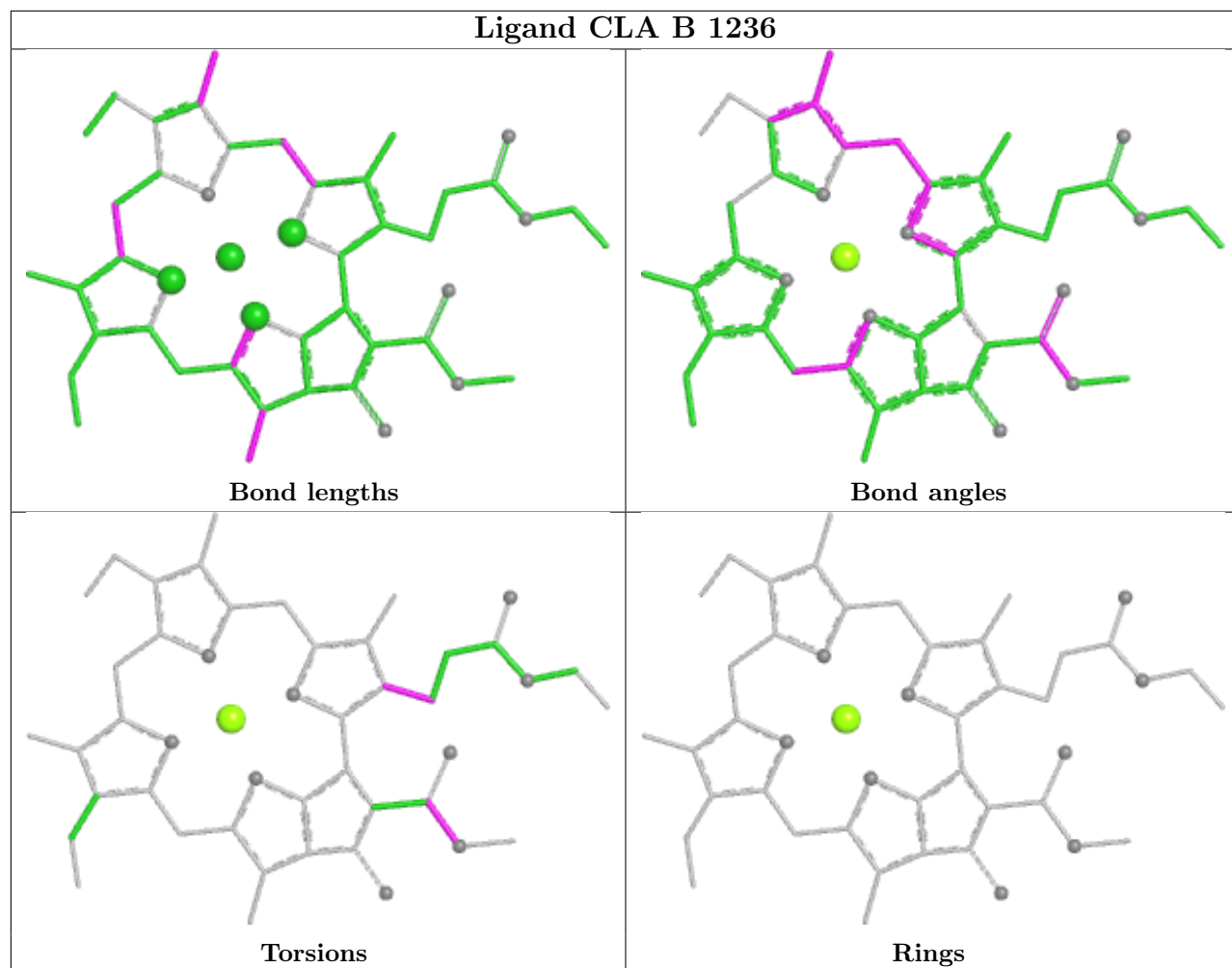


Ligand CHL 4 606

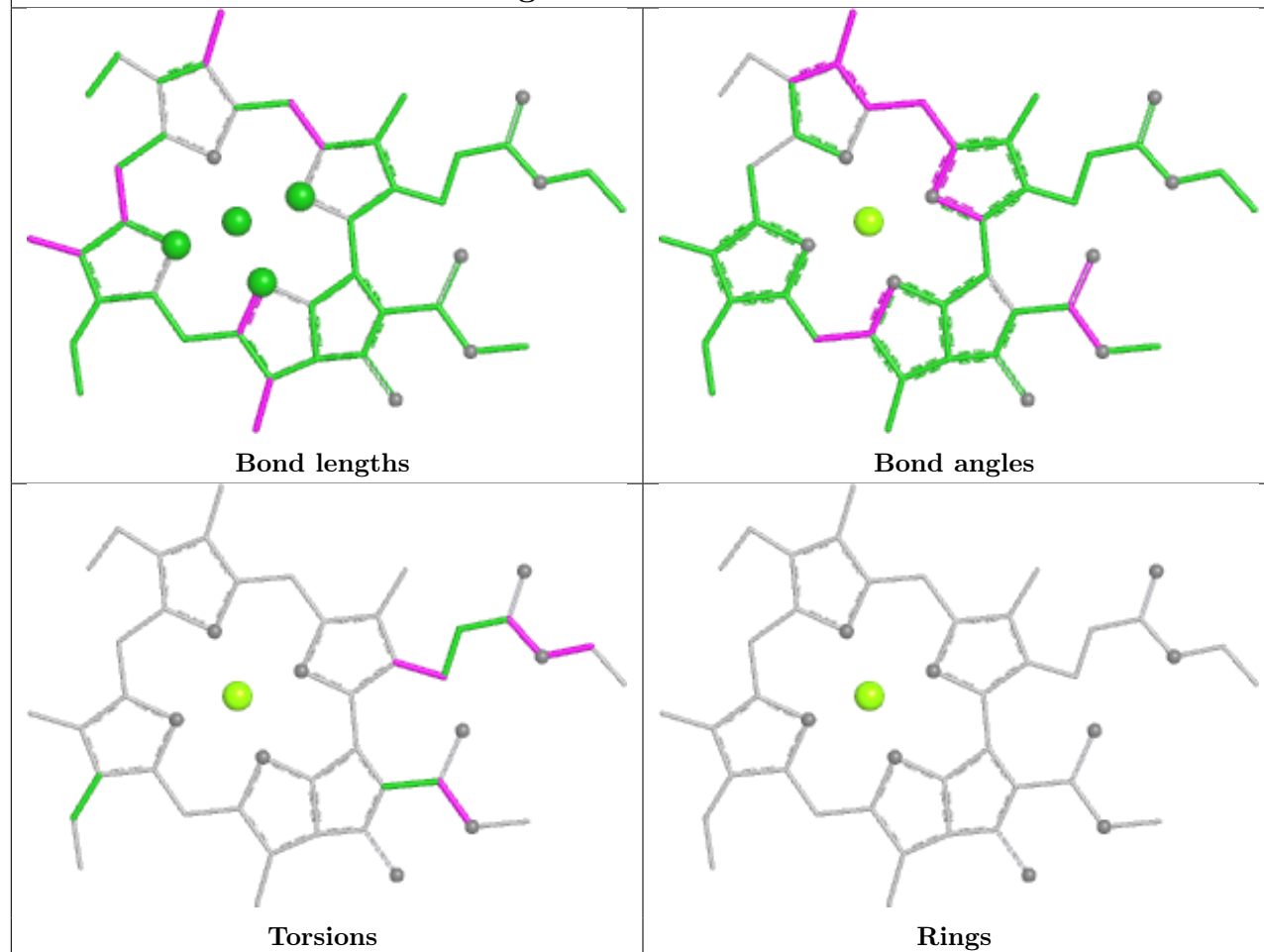


Ligand CLA 1 608

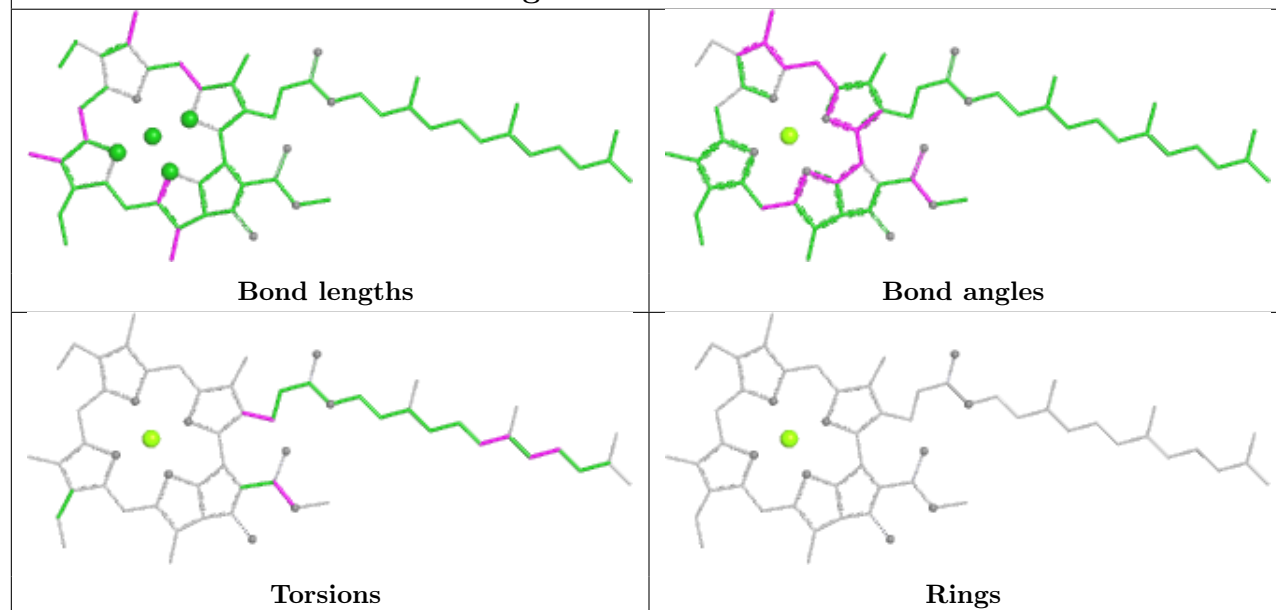


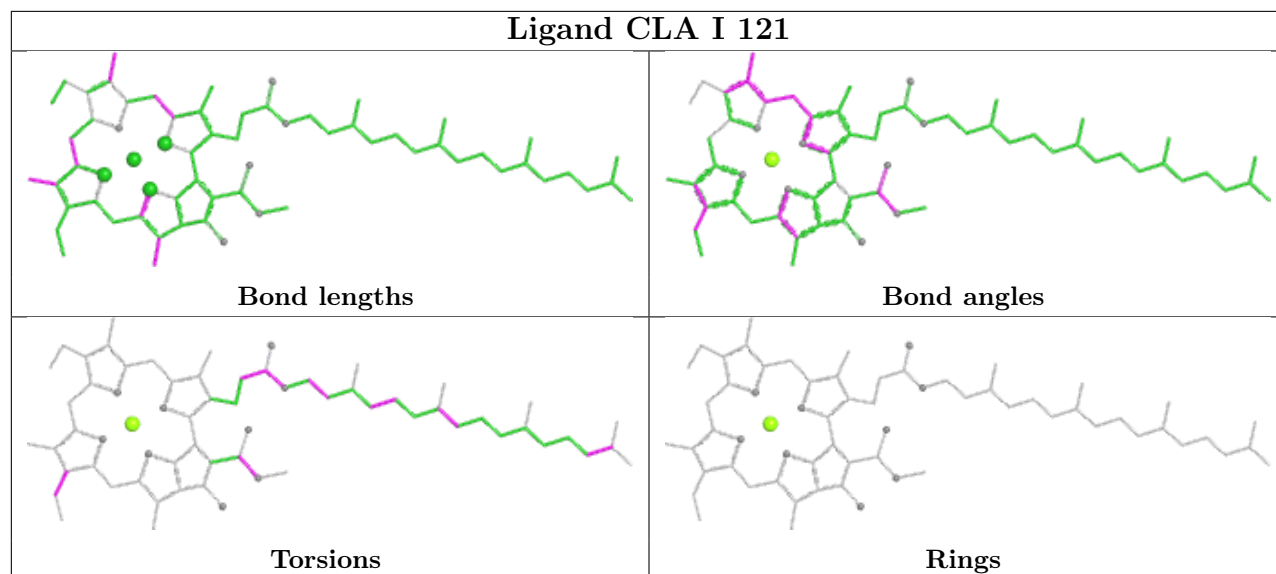
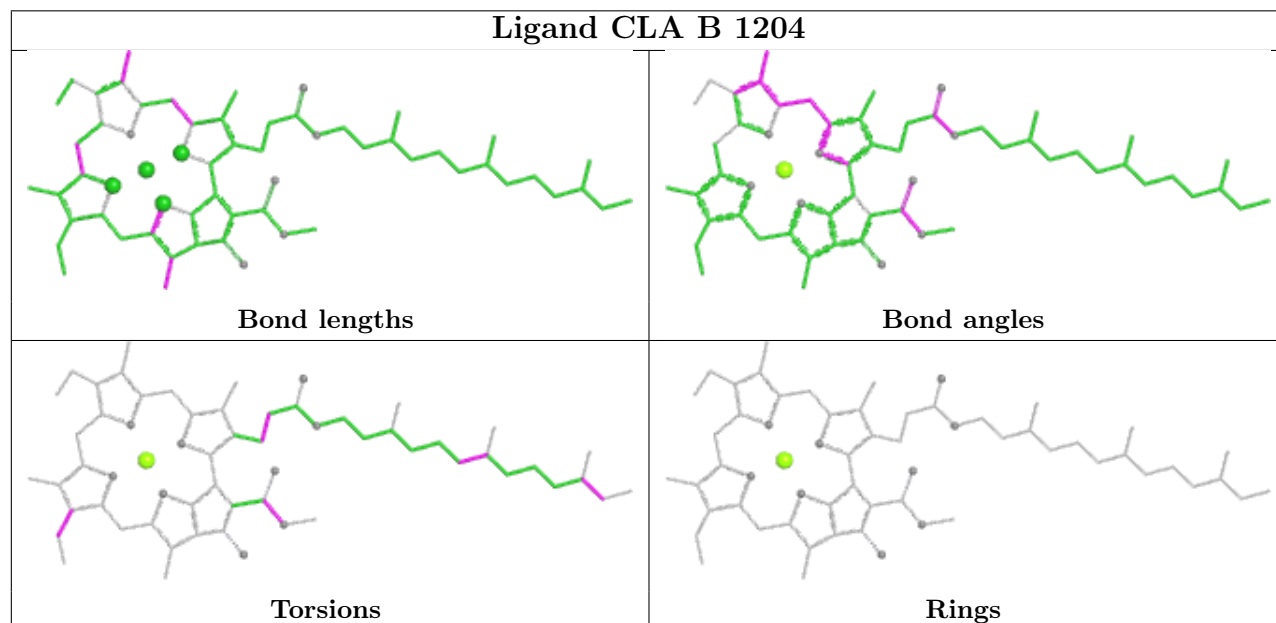


Ligand CLA B 1206

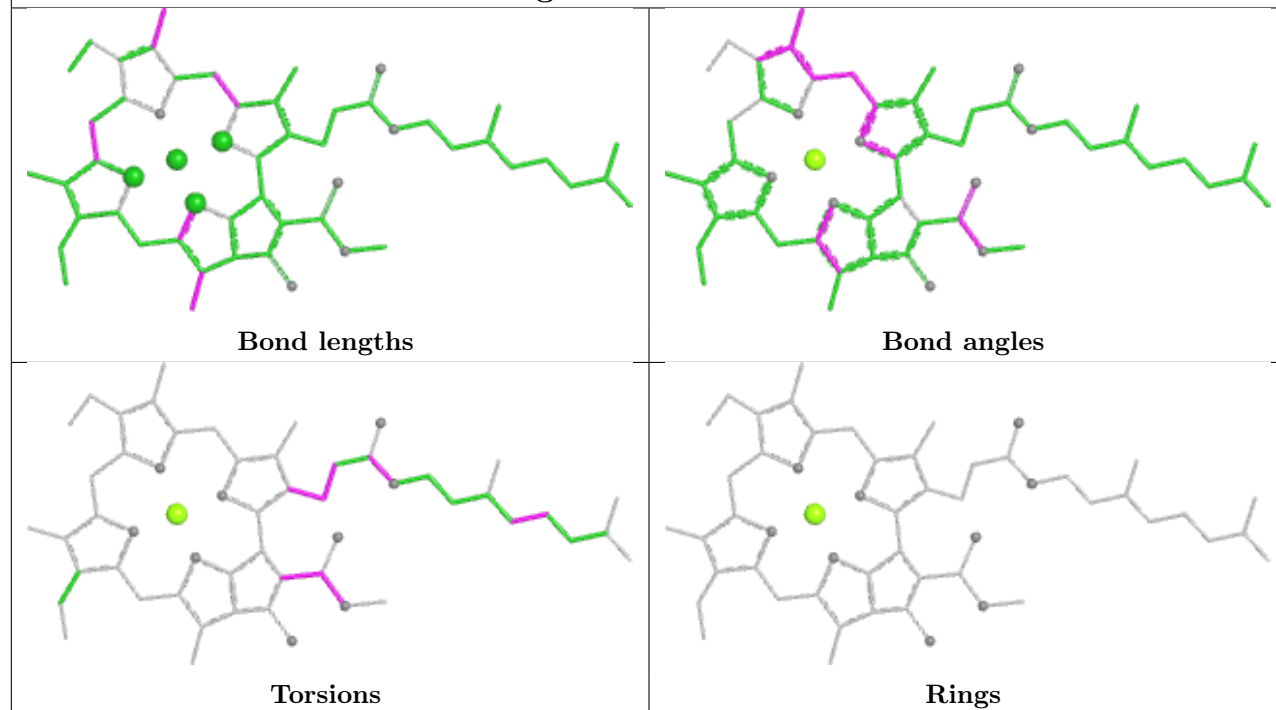


Ligand CLA A 1130

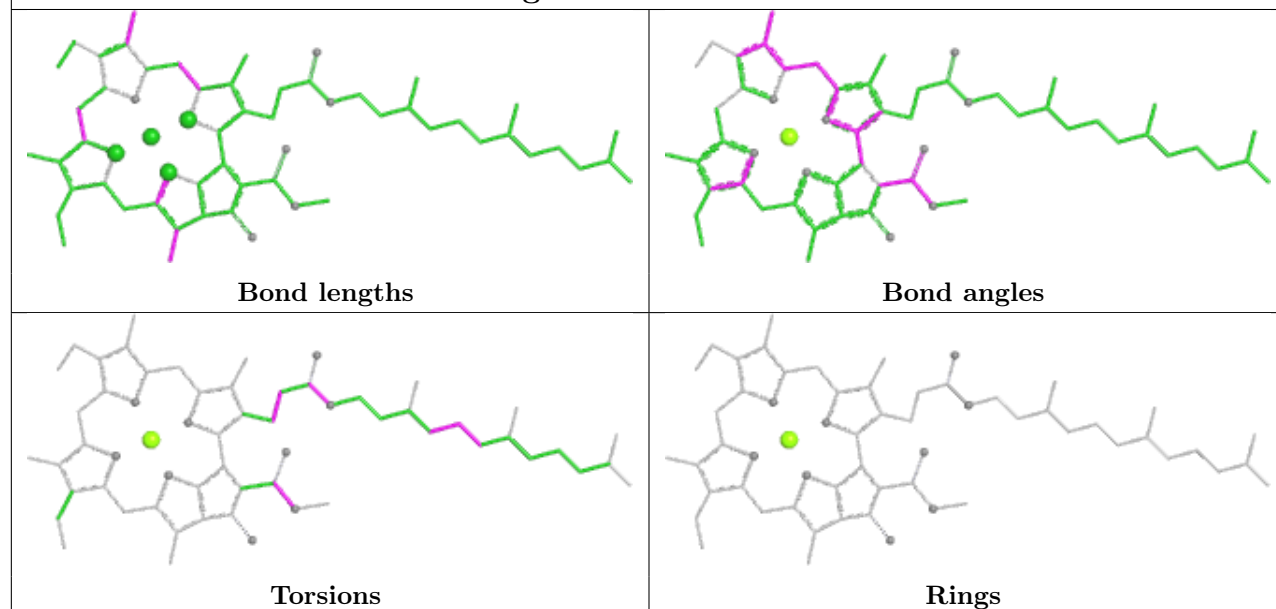


Ligand CLA I 121**Ligand CLA B 1204**

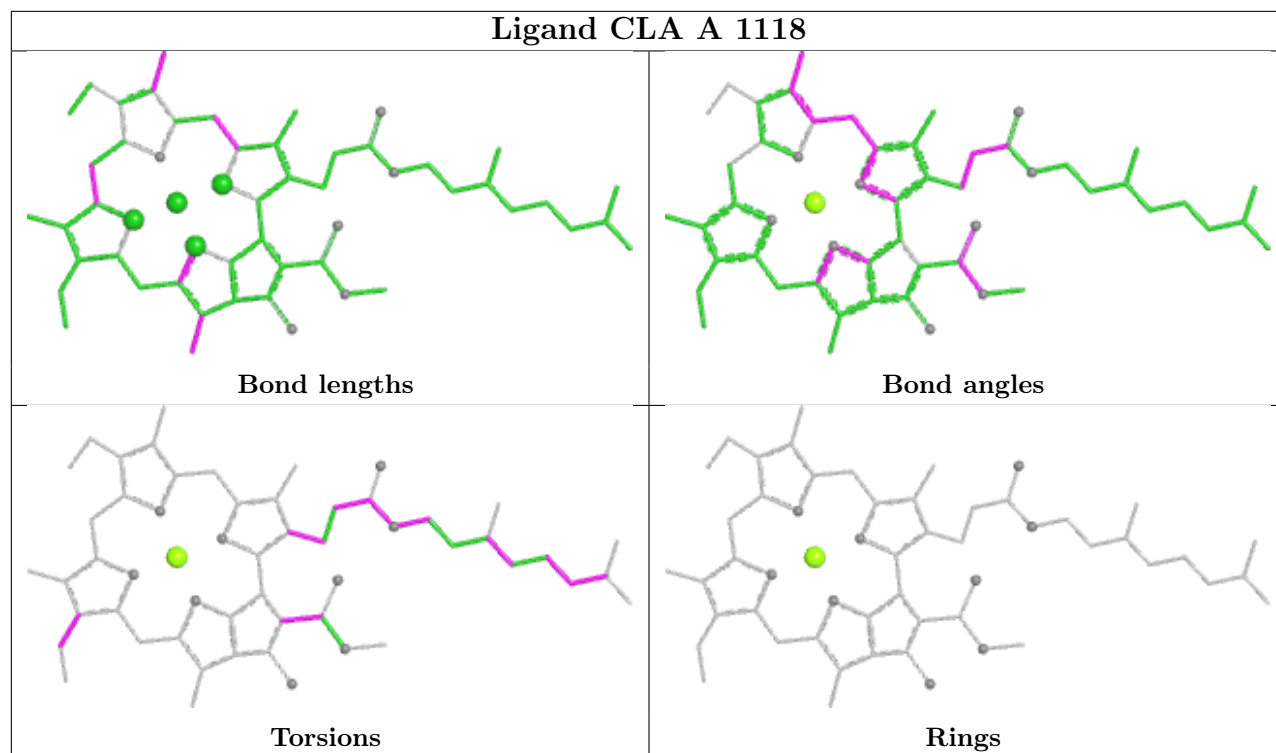
Ligand CLA 3 610



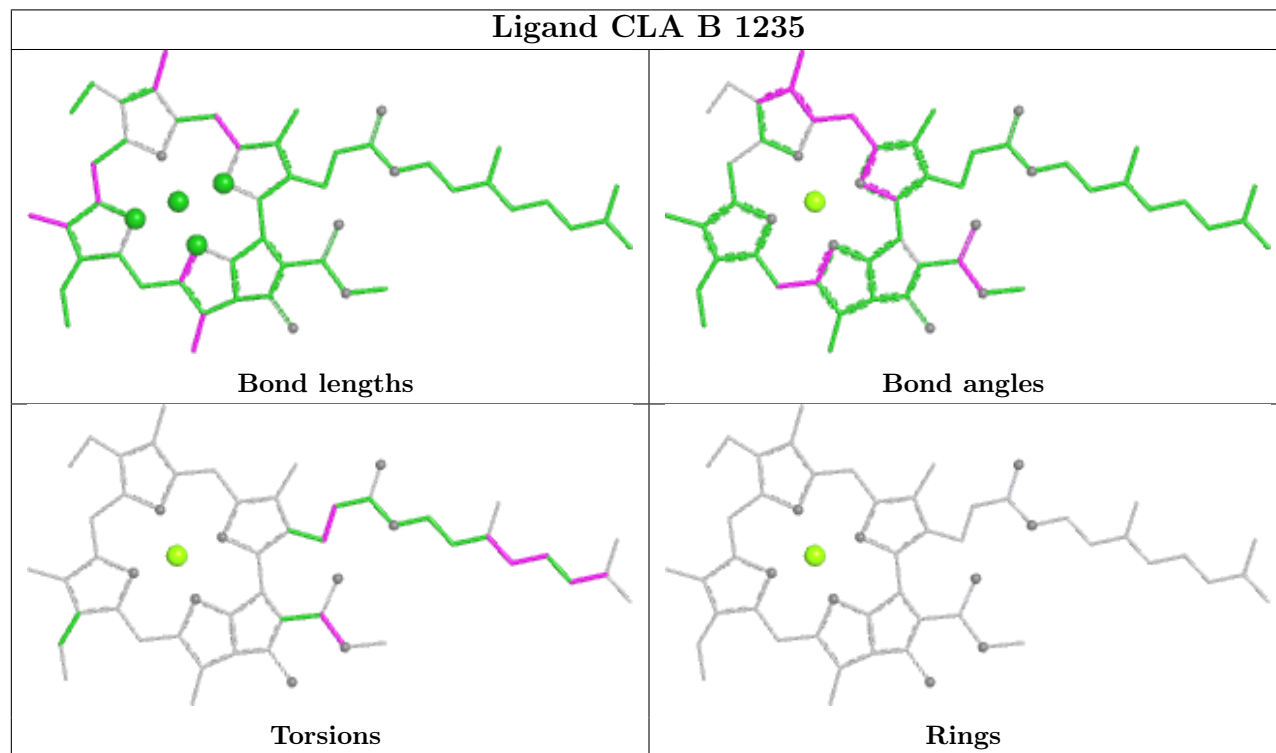
Ligand CLA A 1138

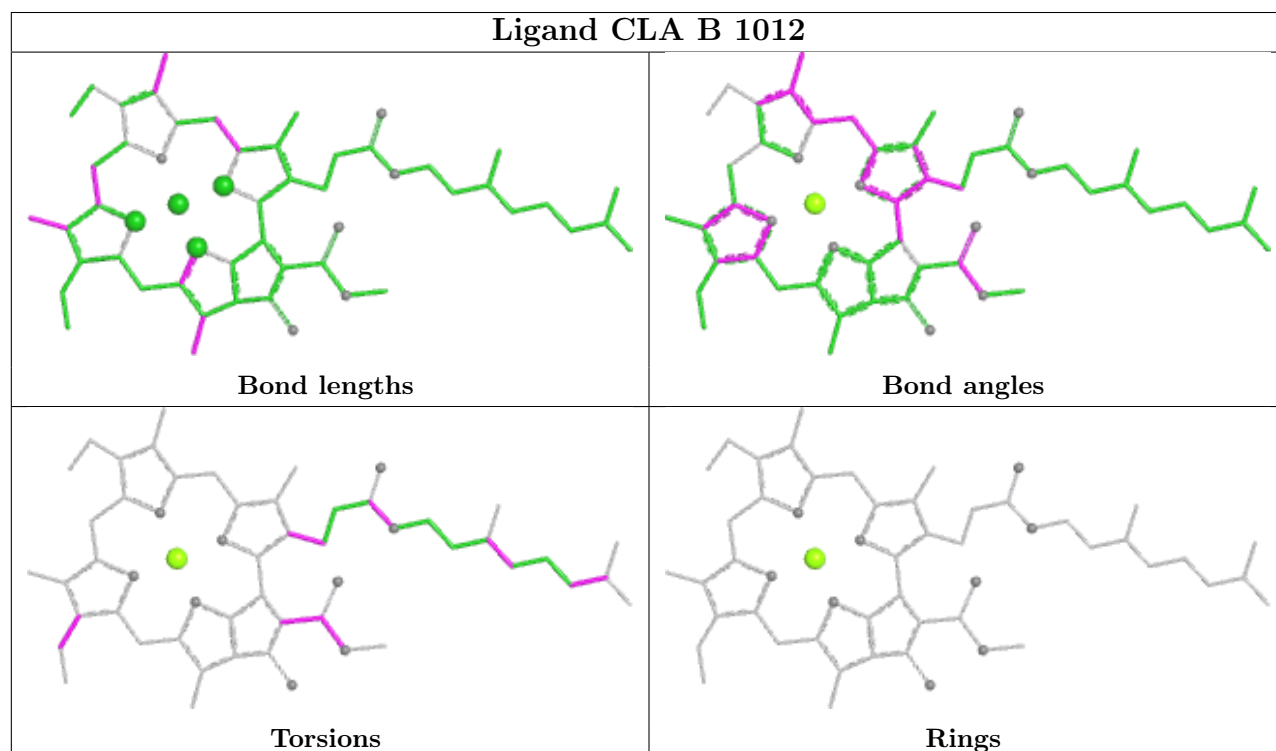
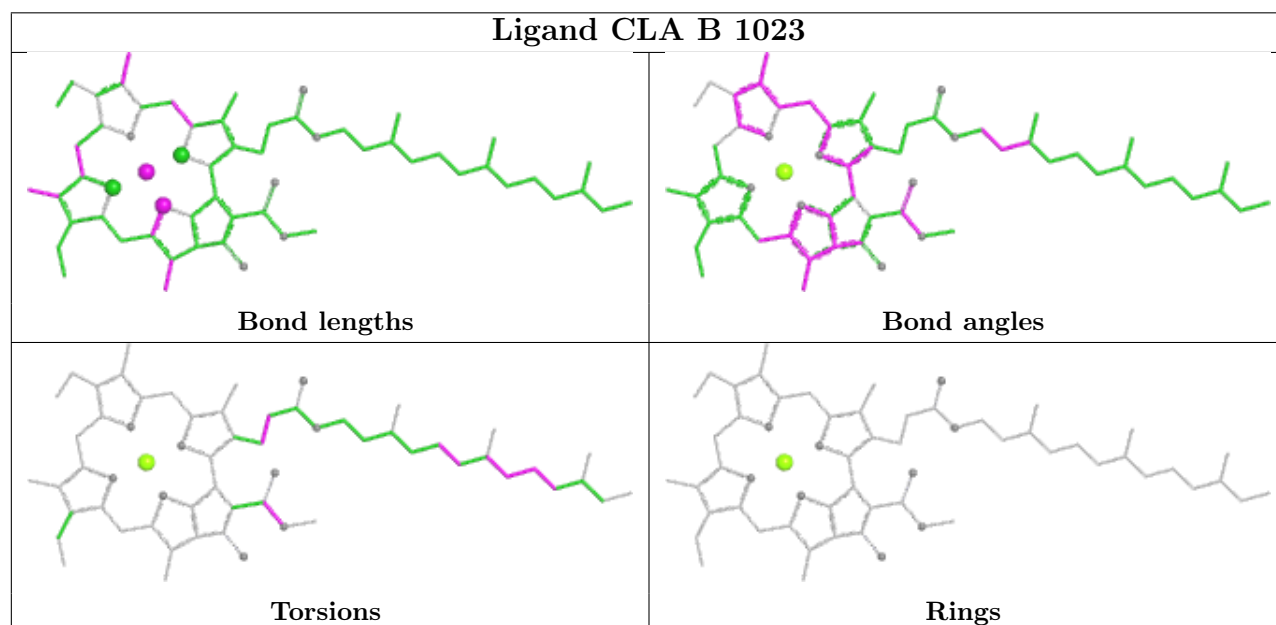
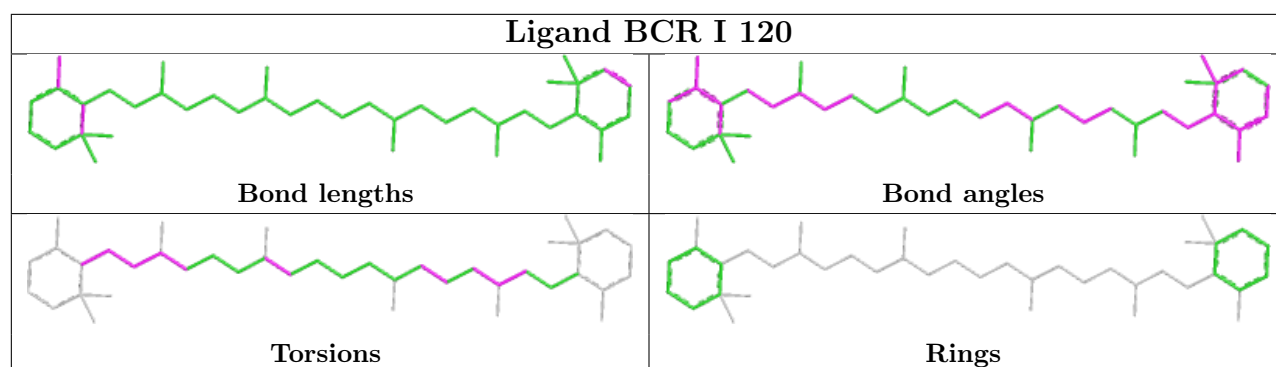


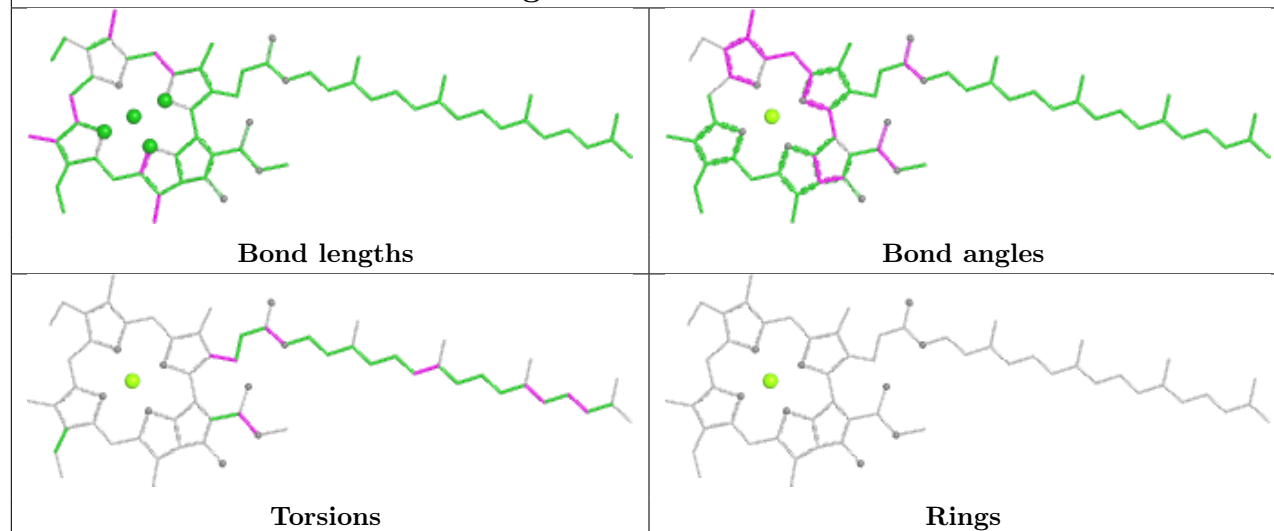
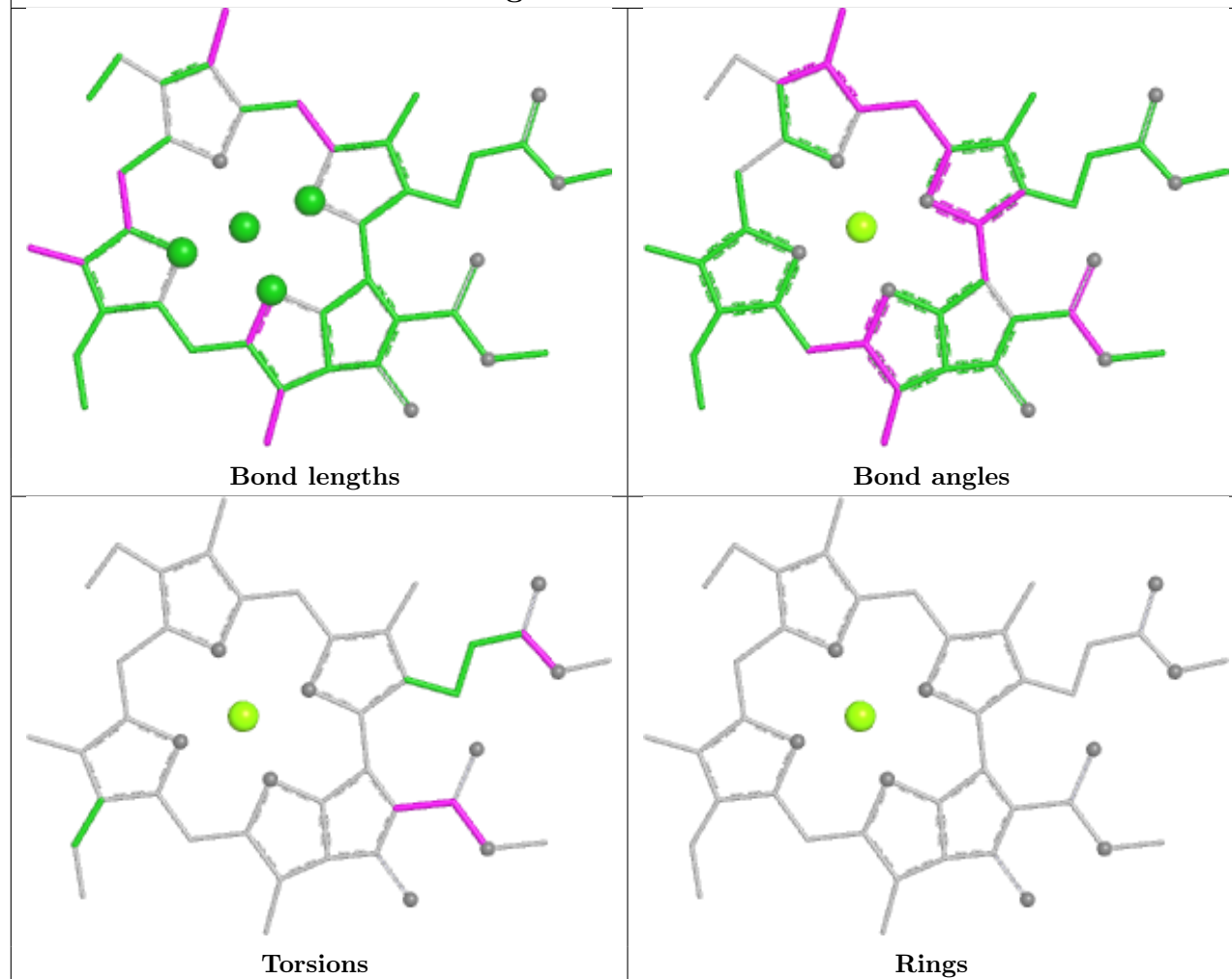
Ligand CLA A 1118



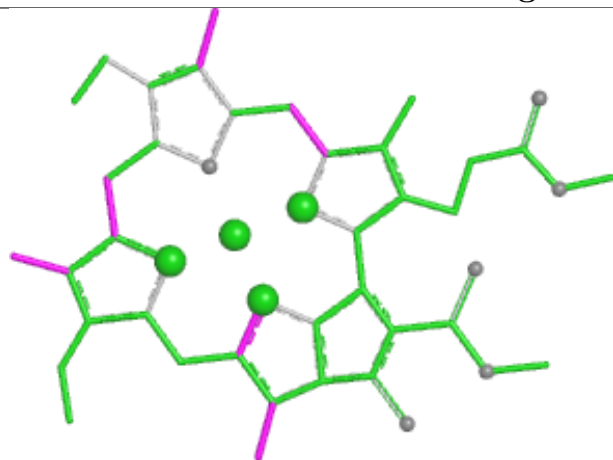
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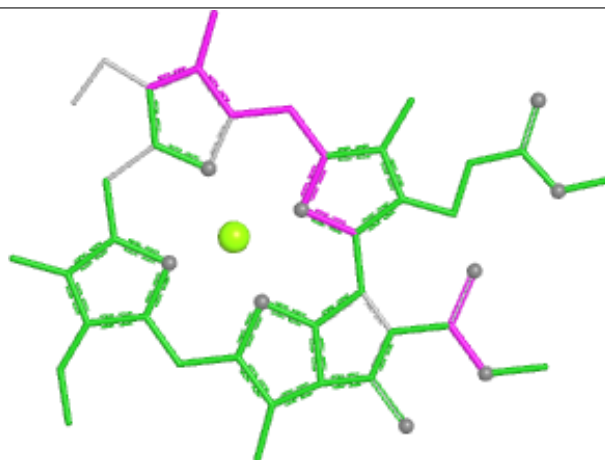


Ligand CLA A 1119**Ligand CLA B 1222**

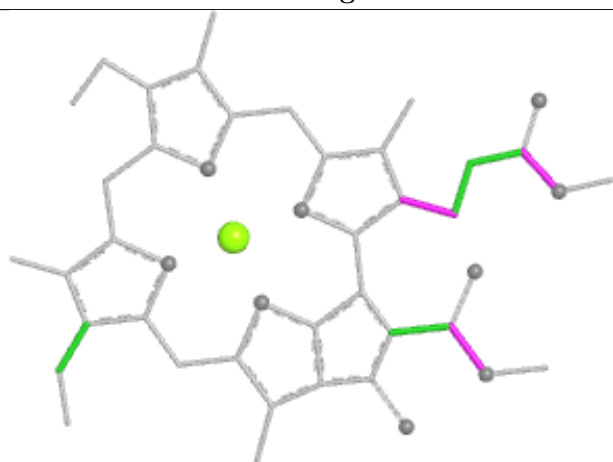
Ligand CLA 3 617



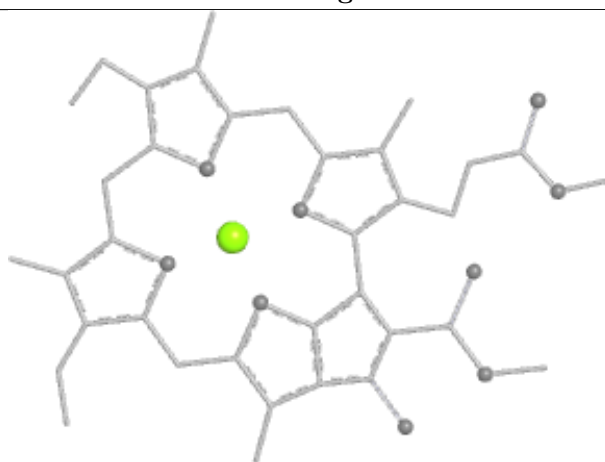
Bond lengths



Bond angles

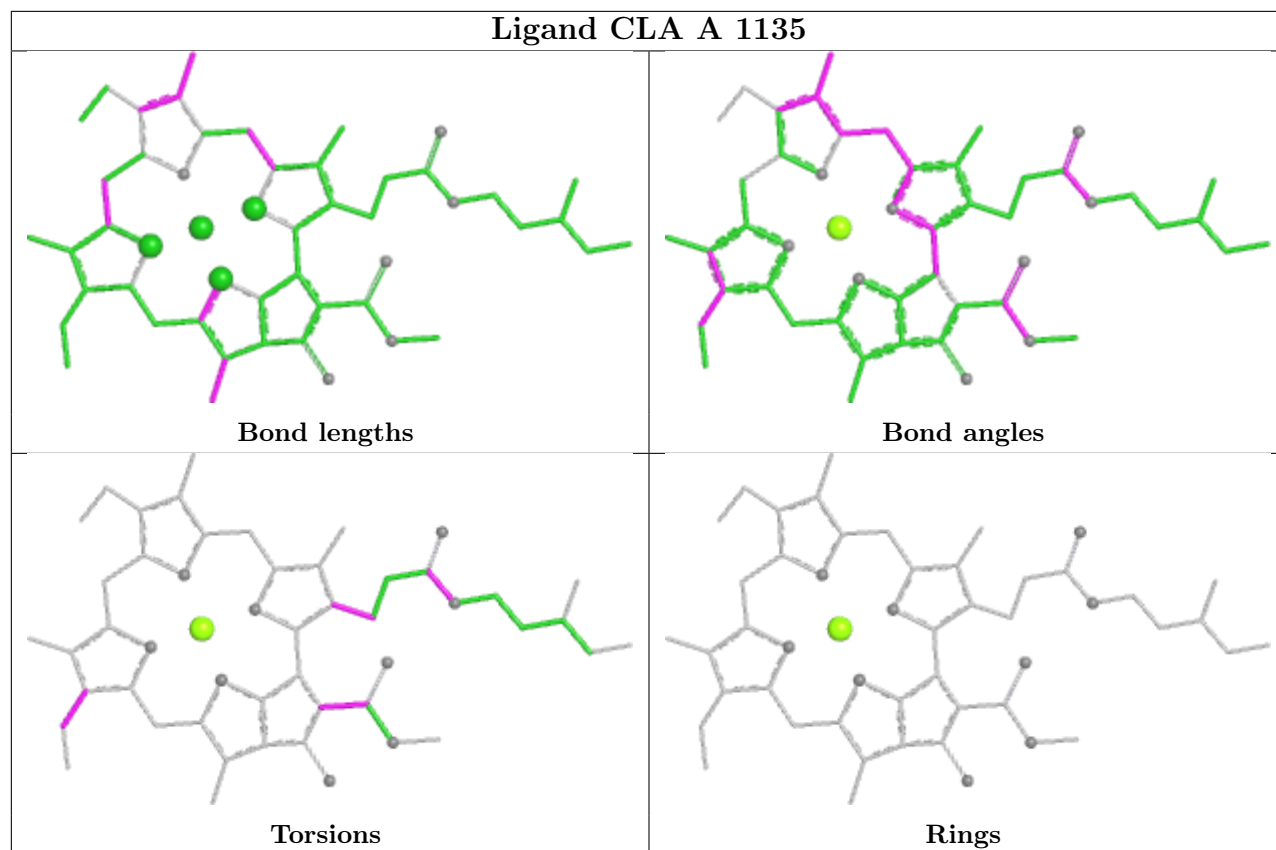


Torsions

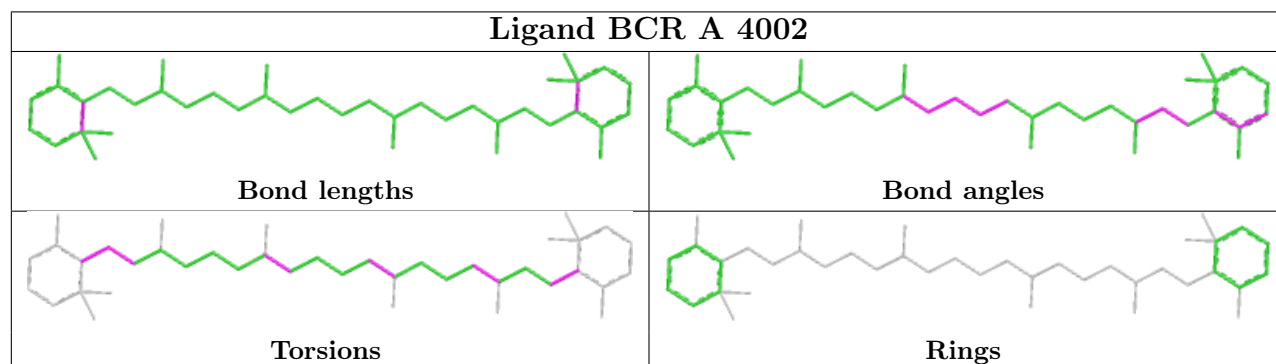


Rings

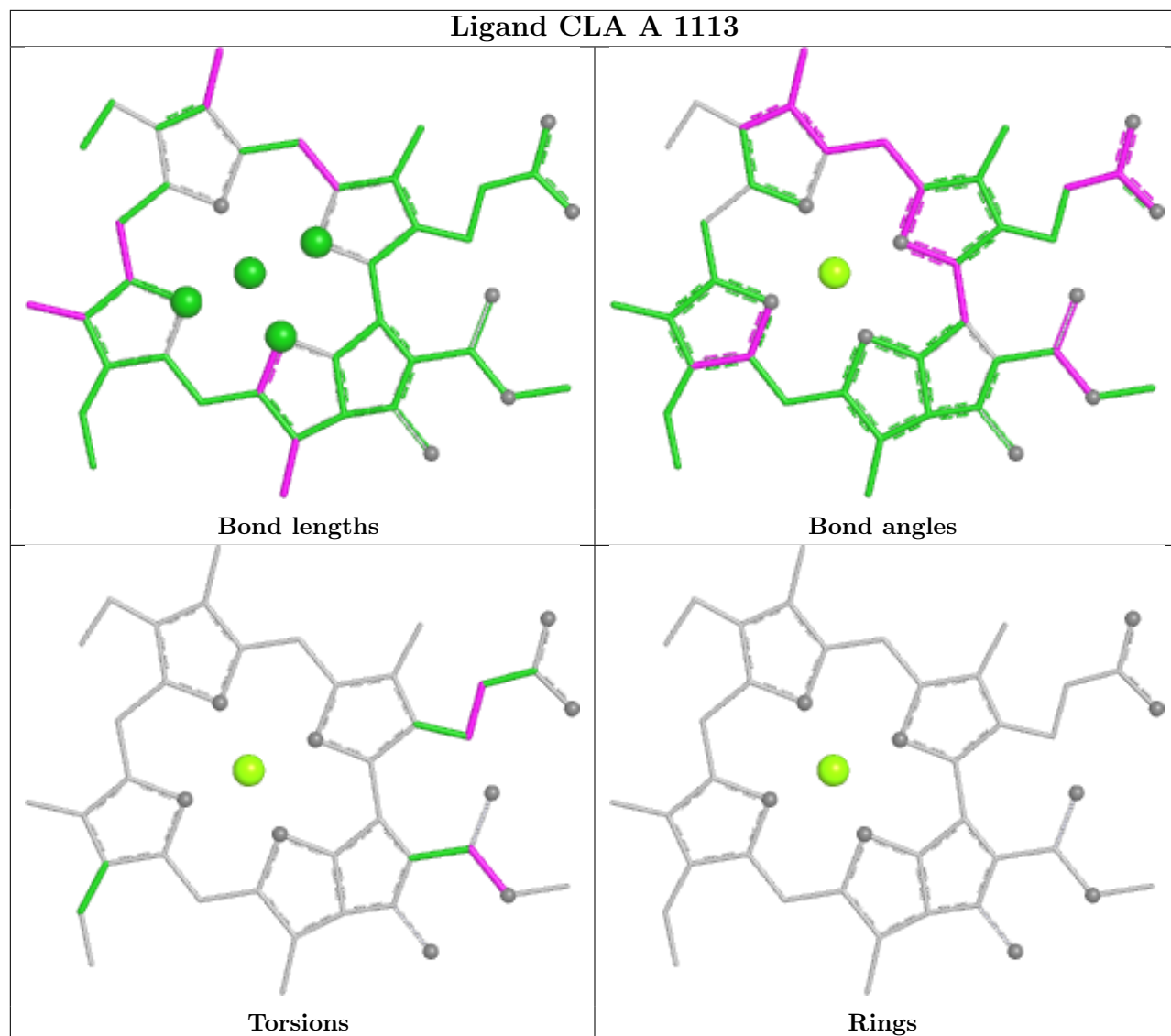
Ligand CLA A 1135



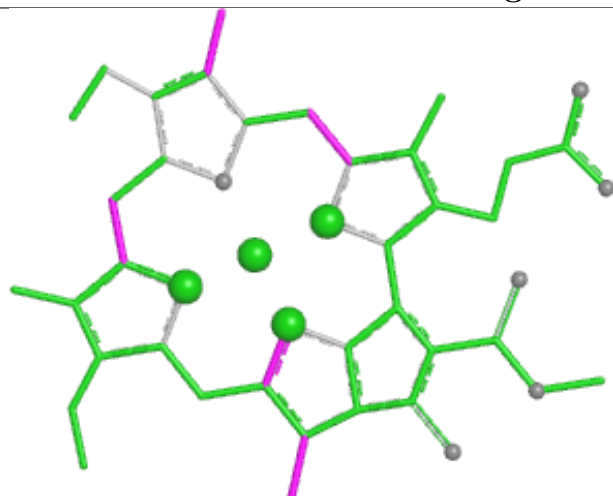
Ligand BCR A 4002



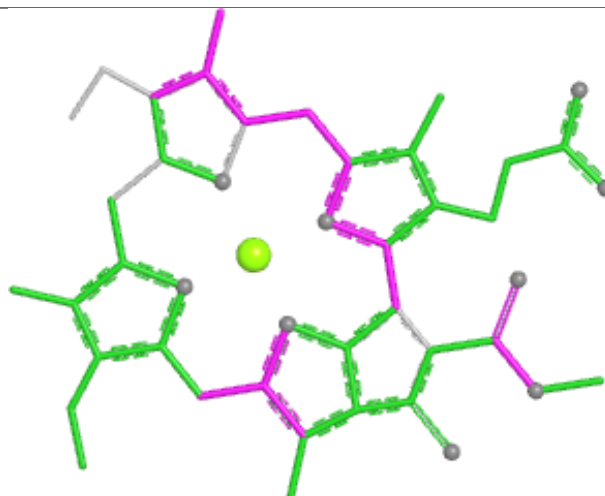
Ligand CLA A 1113



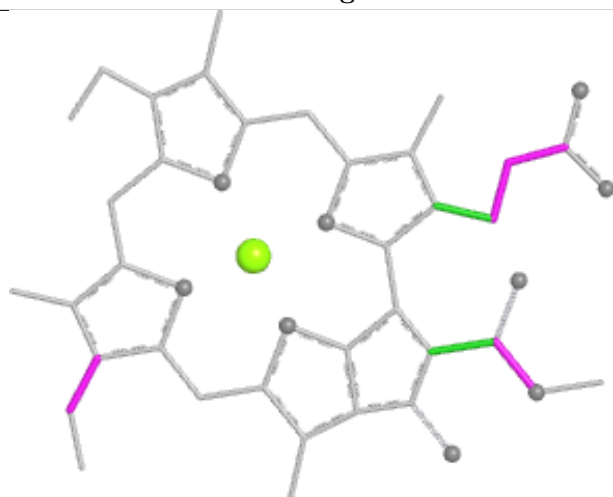
Ligand CLA A 1114



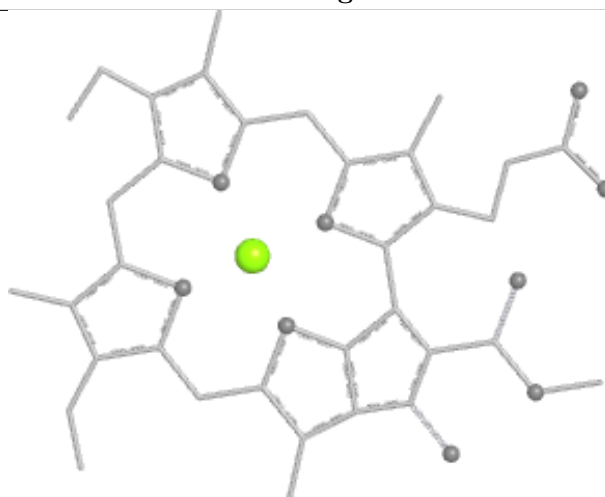
Bond lengths



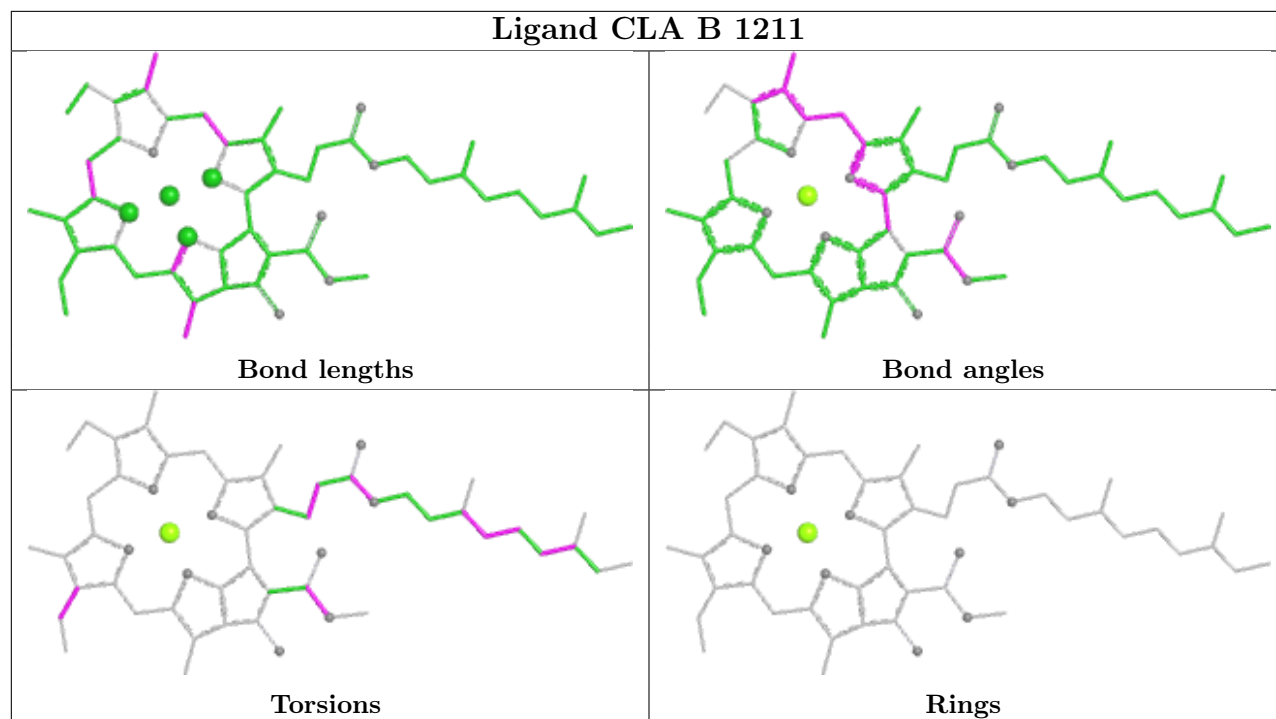
Bond angles



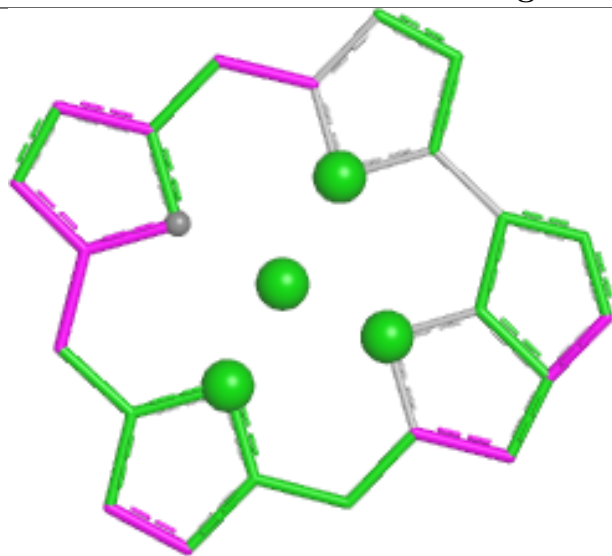
Torsions



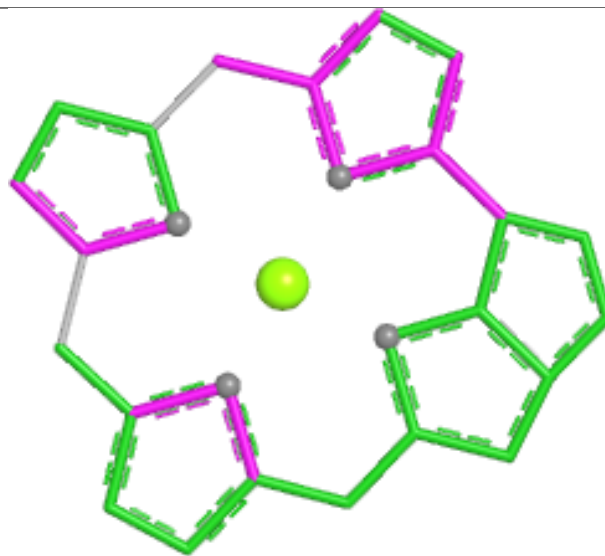
Rings



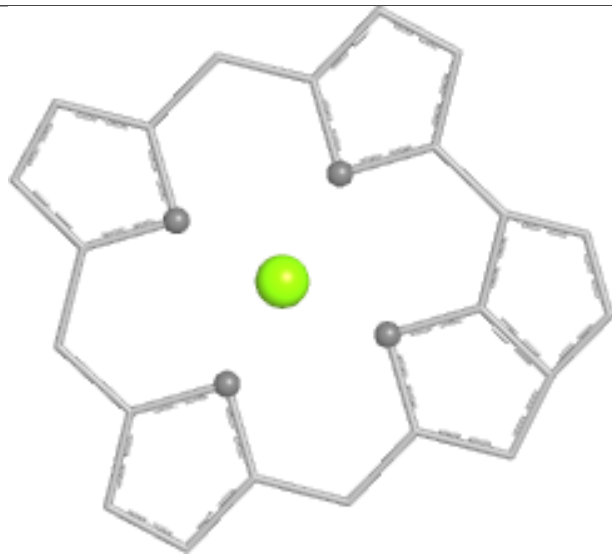
Ligand CLA 3 605



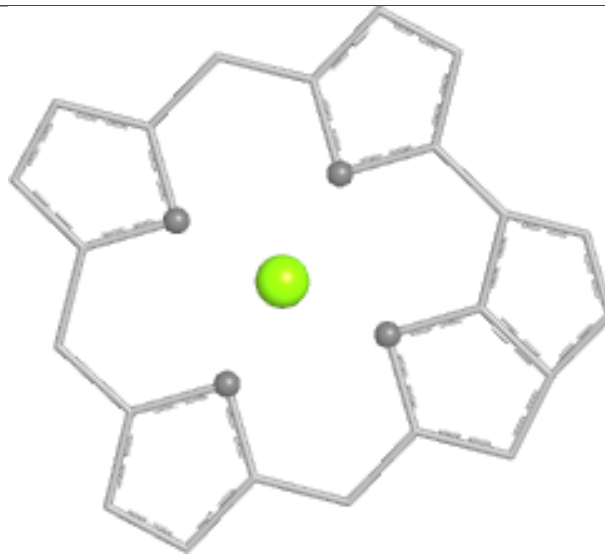
Bond lengths



Bond angles

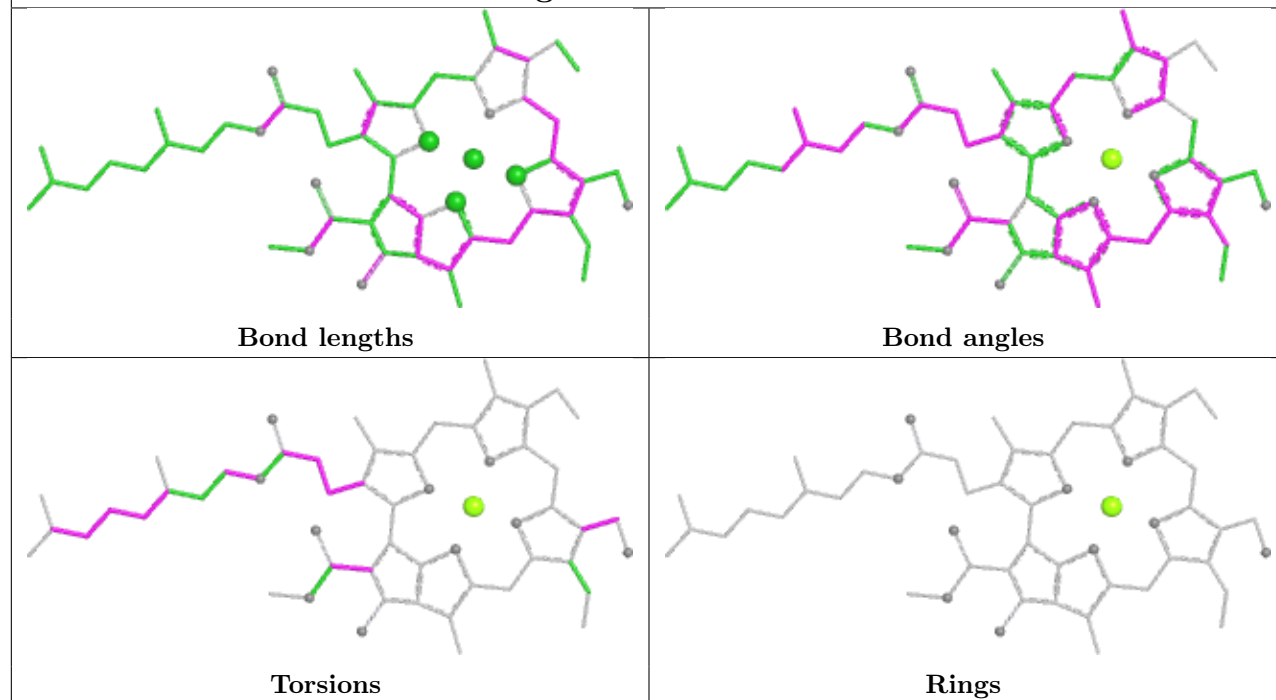


Torsions

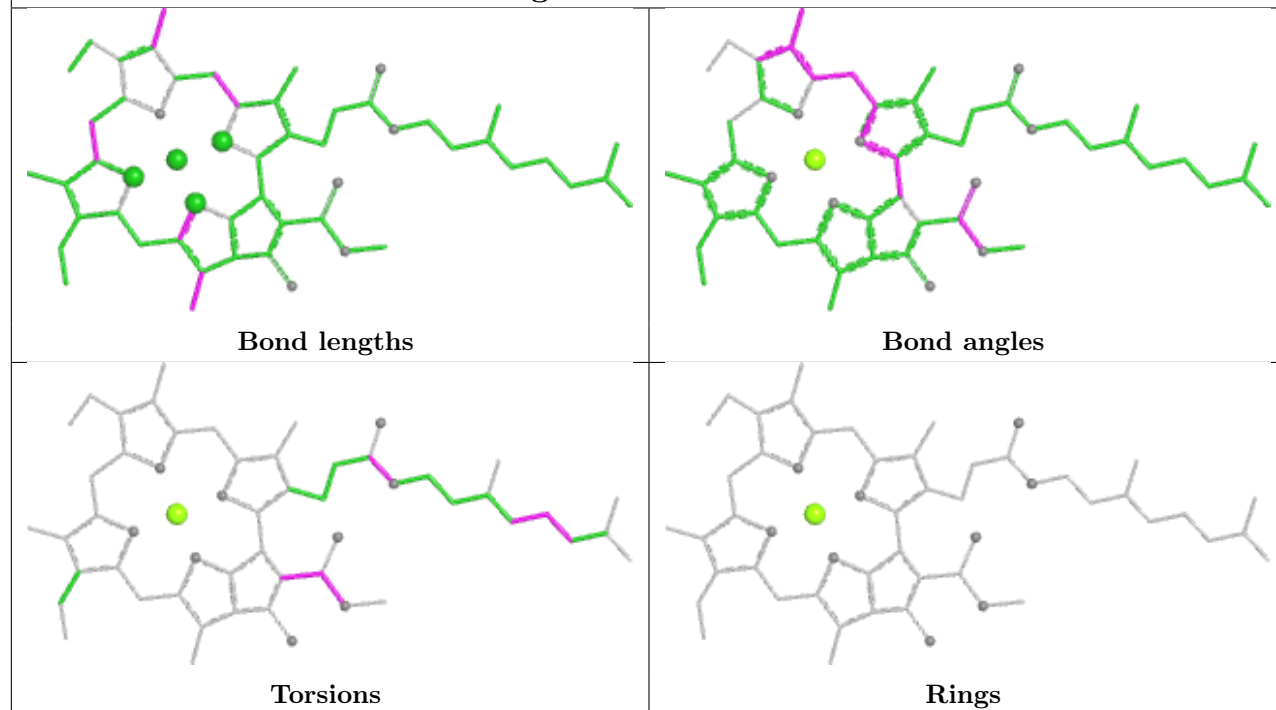


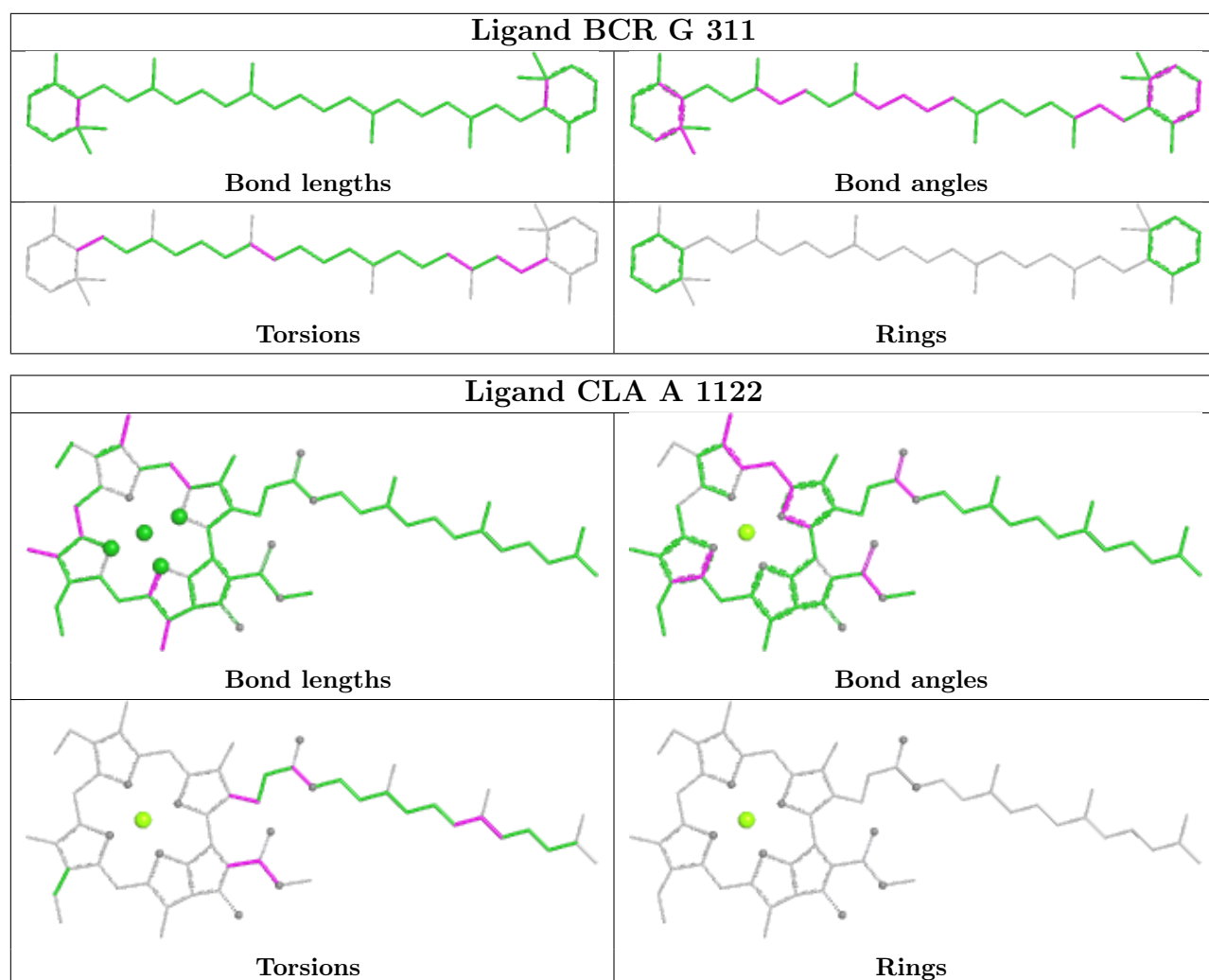
Rings

Ligand CHL 2 602

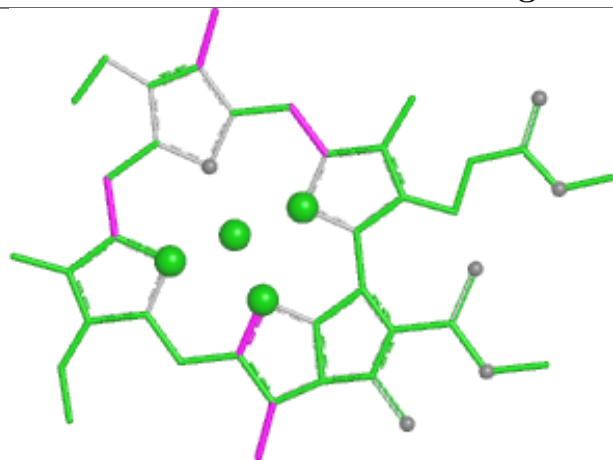


Ligand CLA G 218

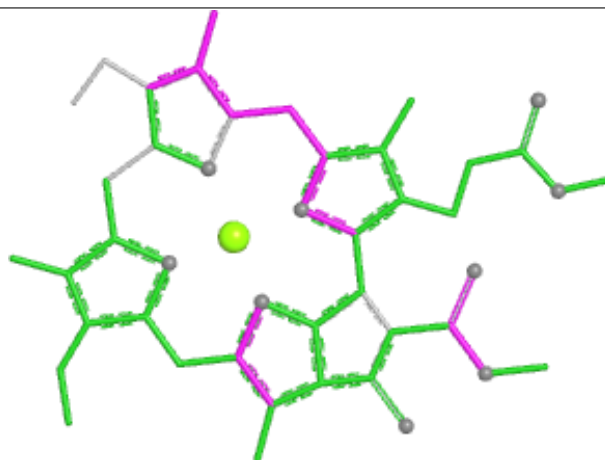




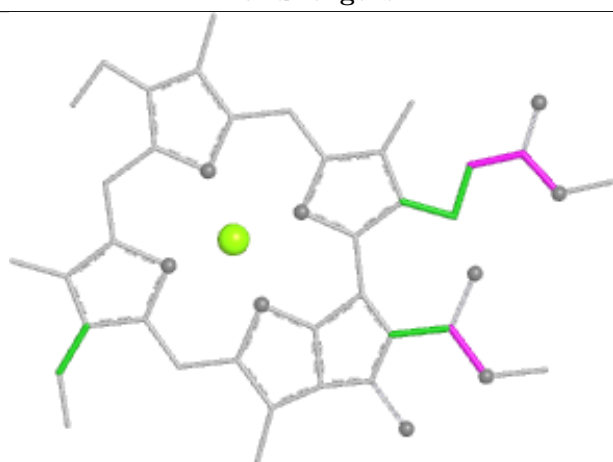
Ligand CLA 2 603



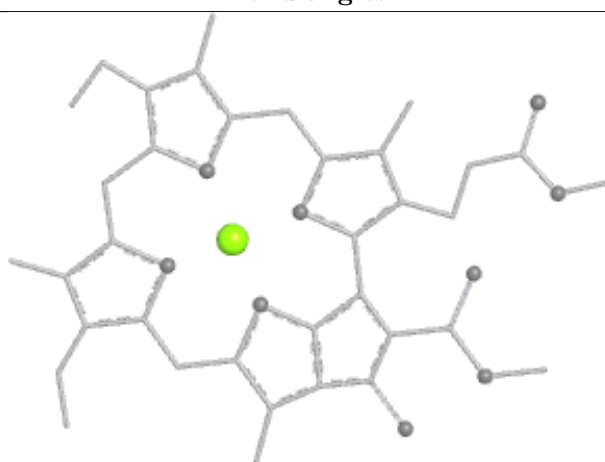
Bond lengths



Bond angles

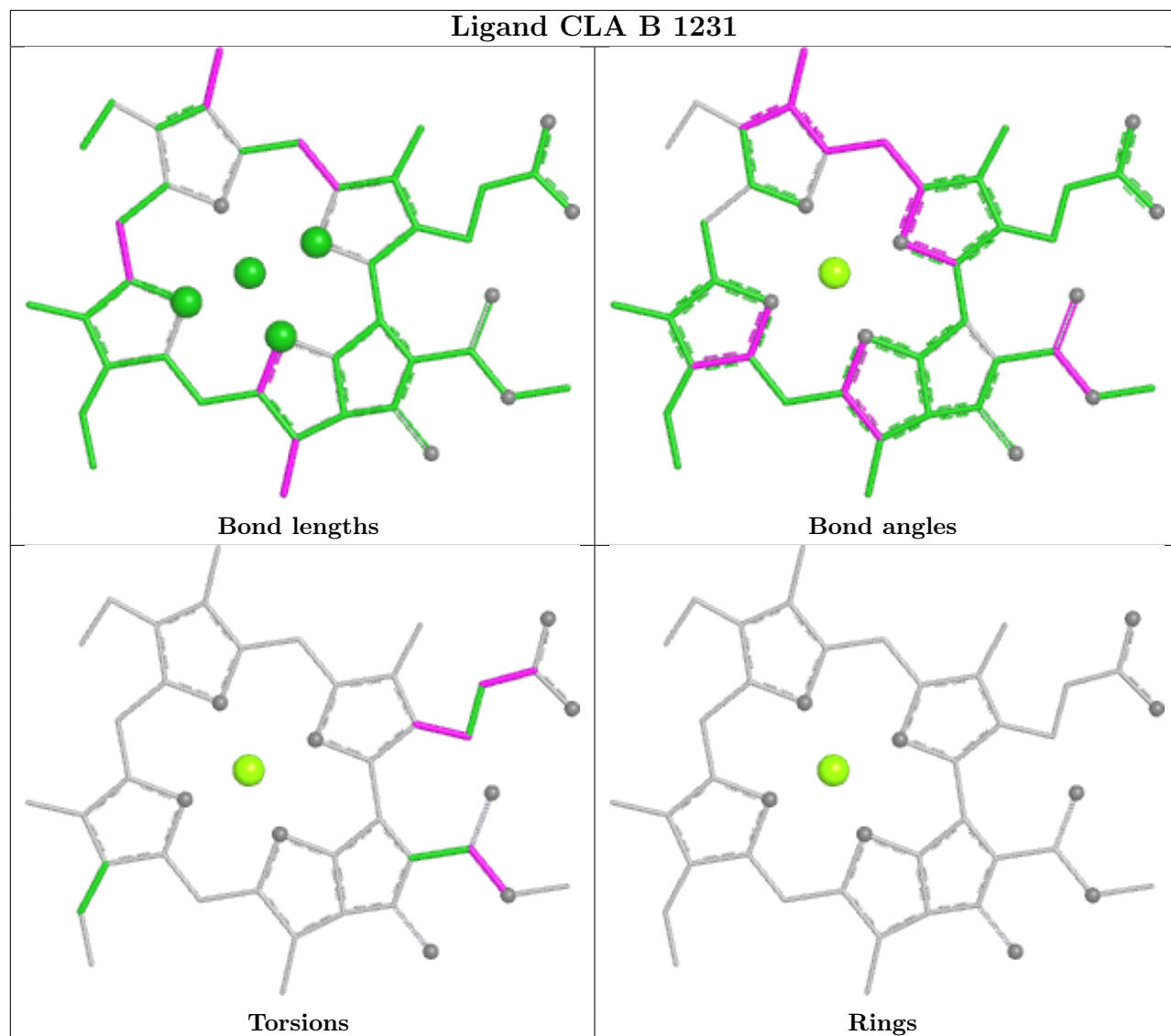


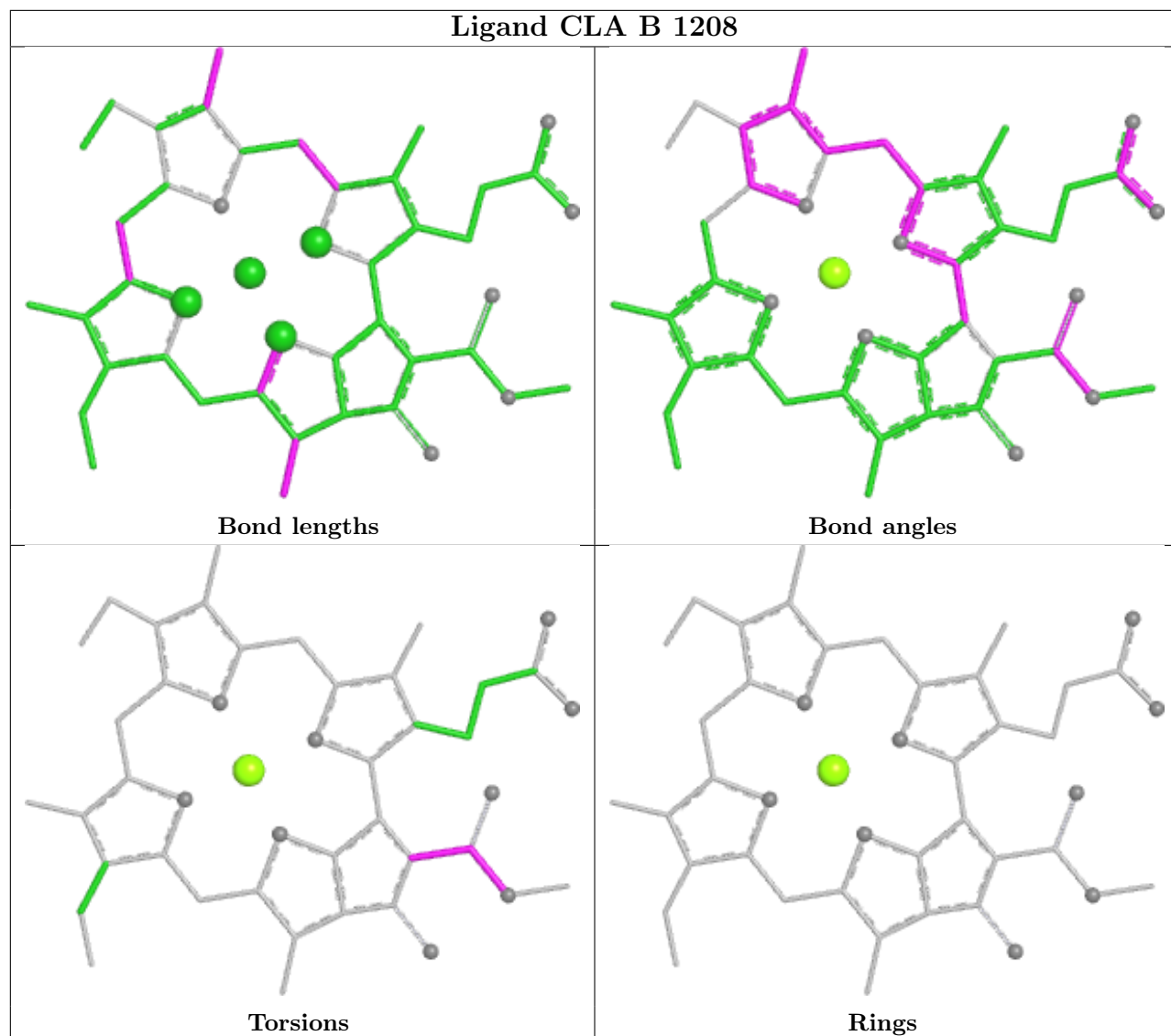
Torsions

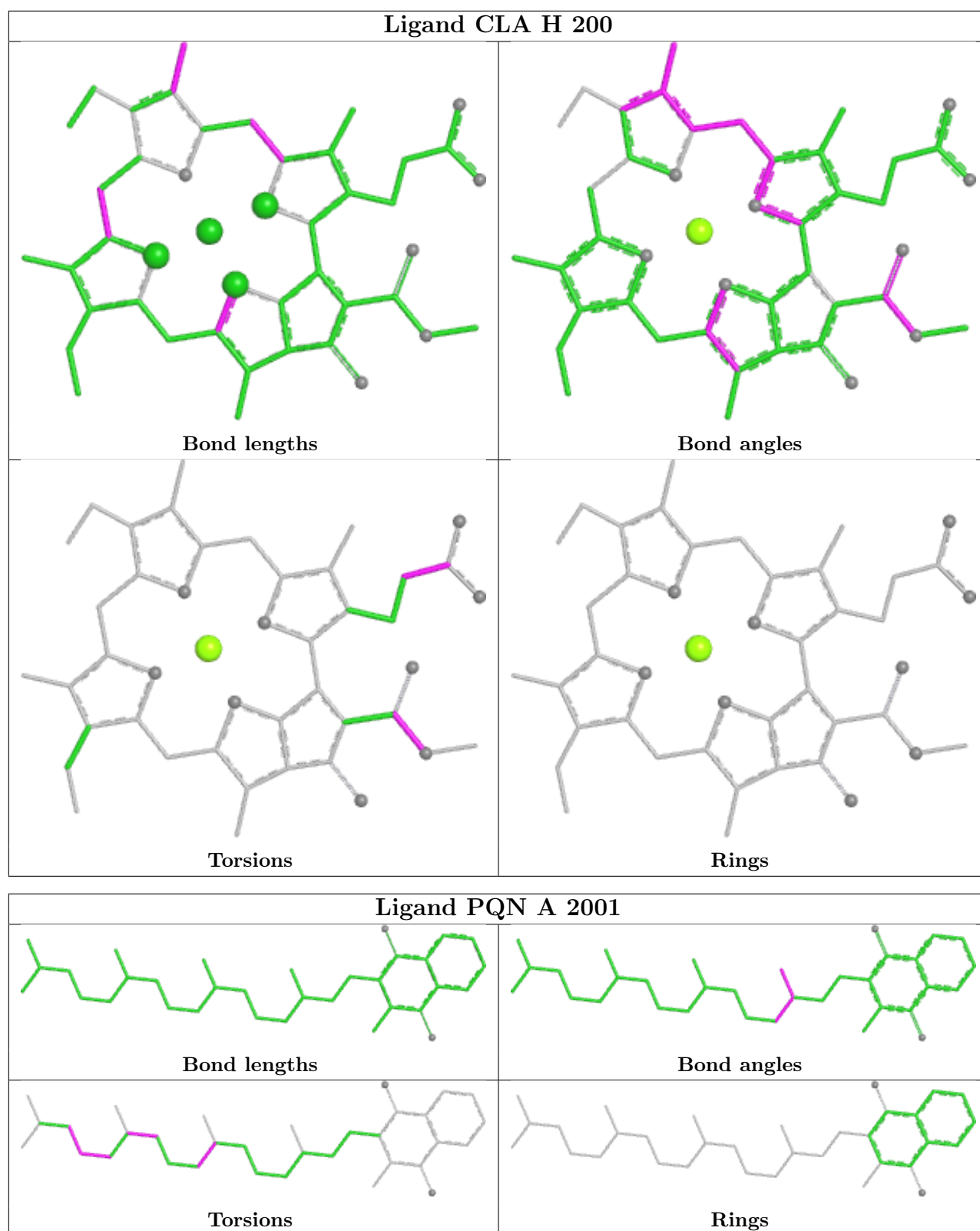


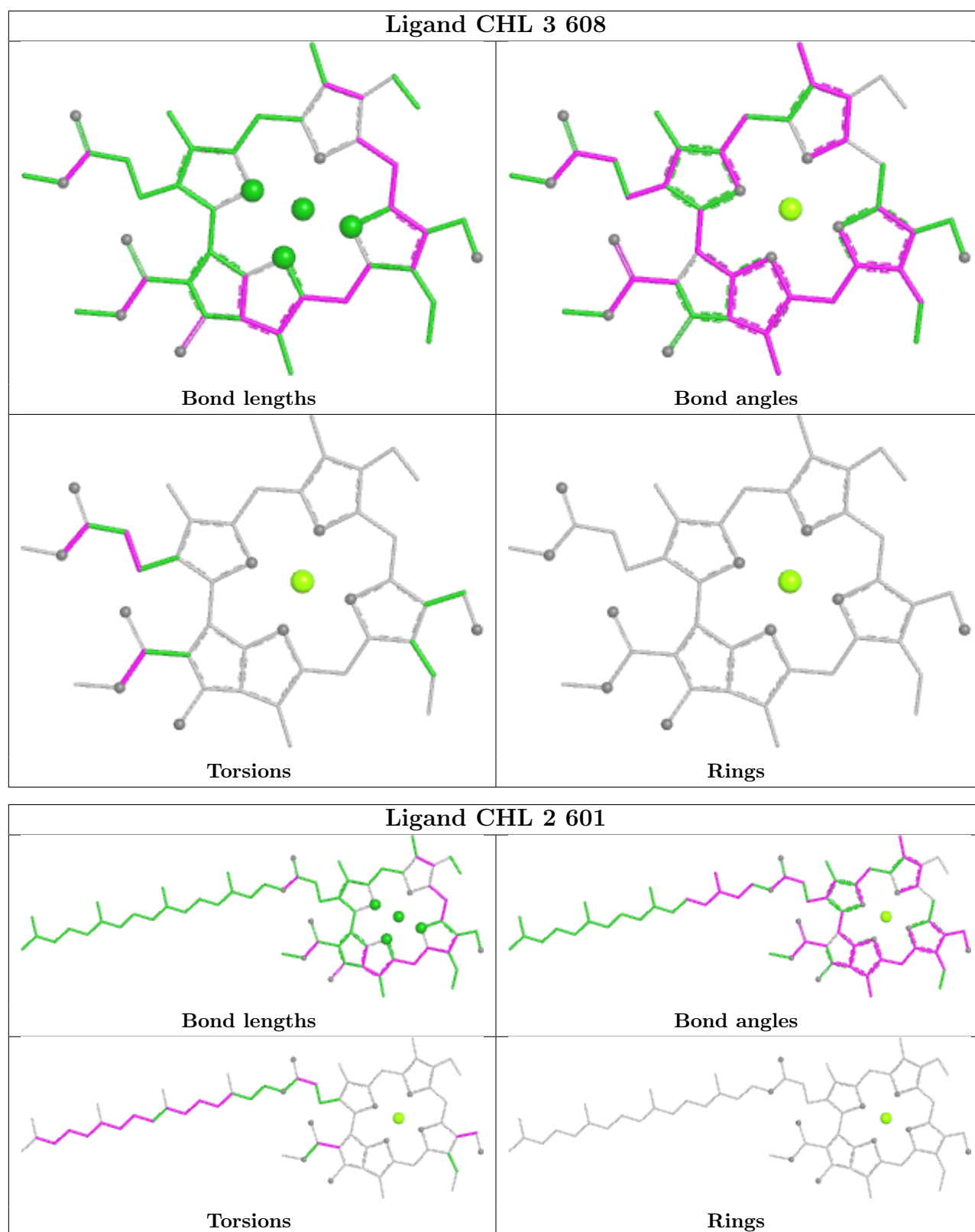
Rings

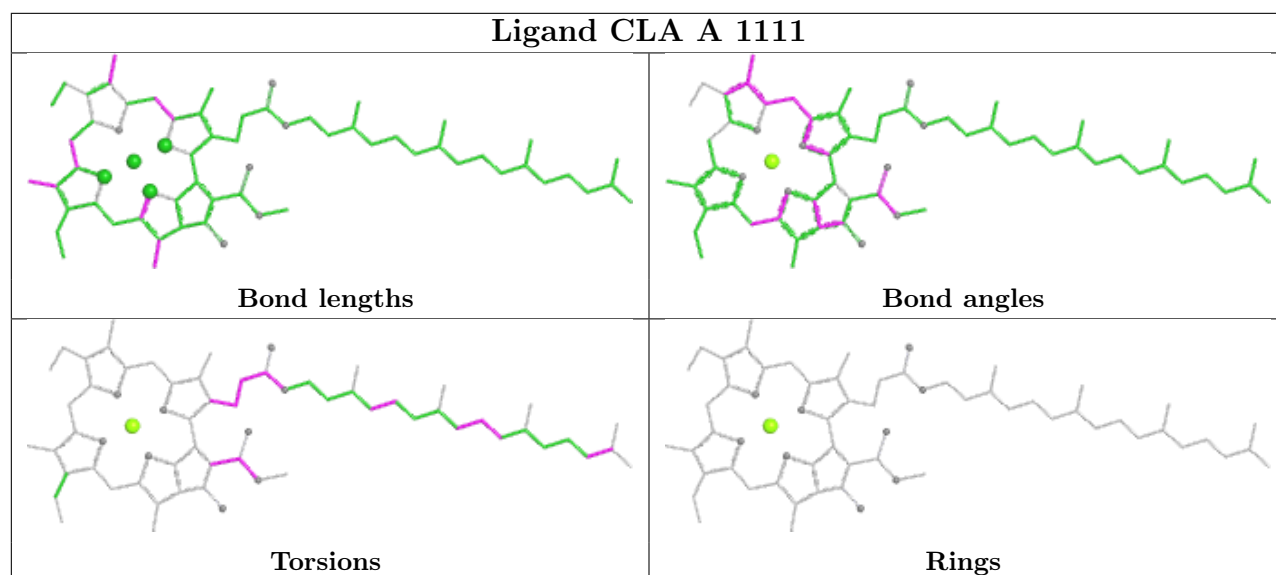
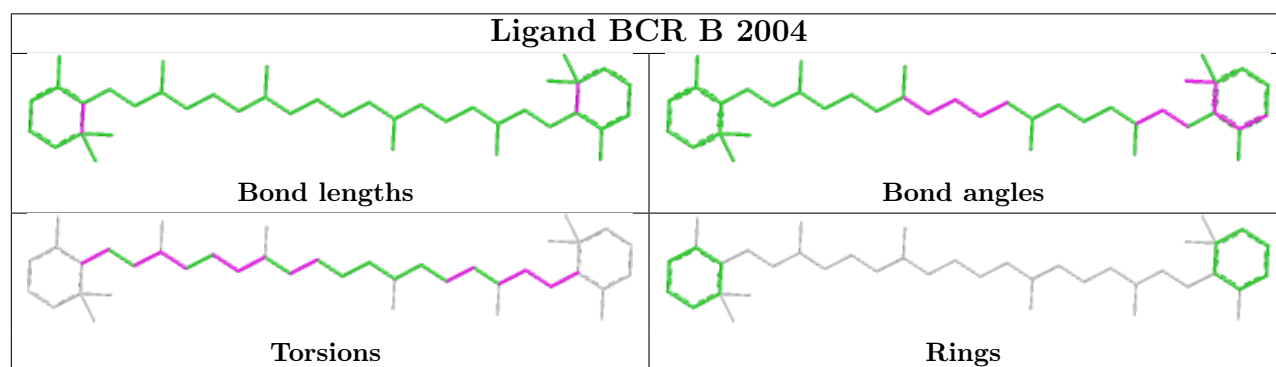
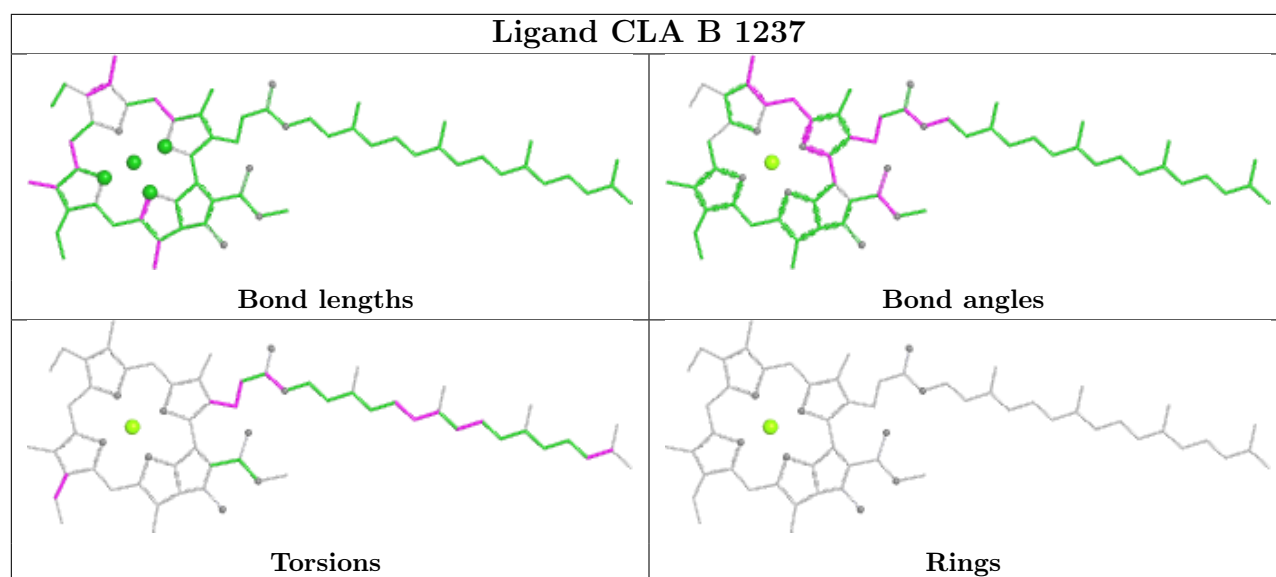
Ligand CLA B 1231

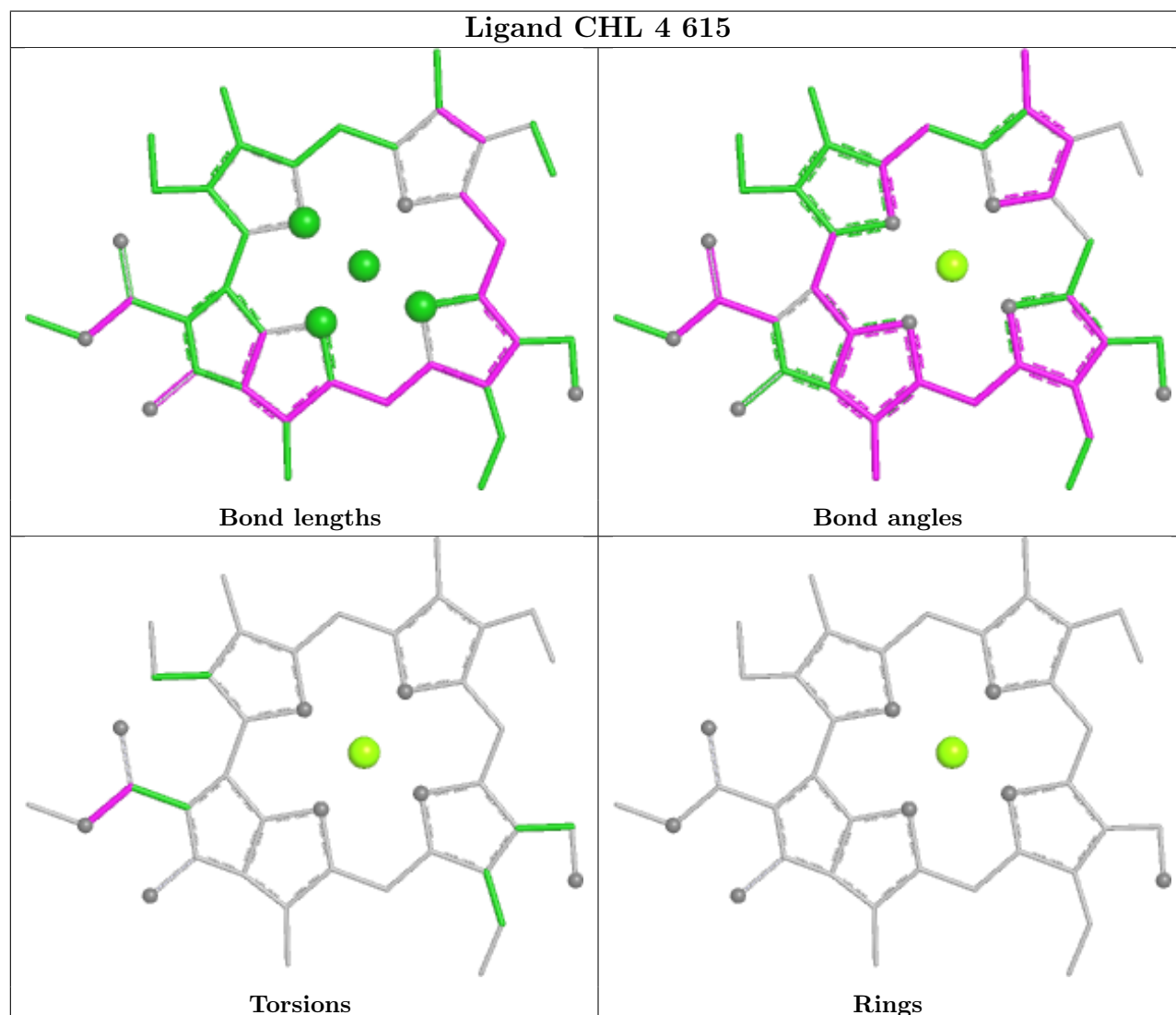
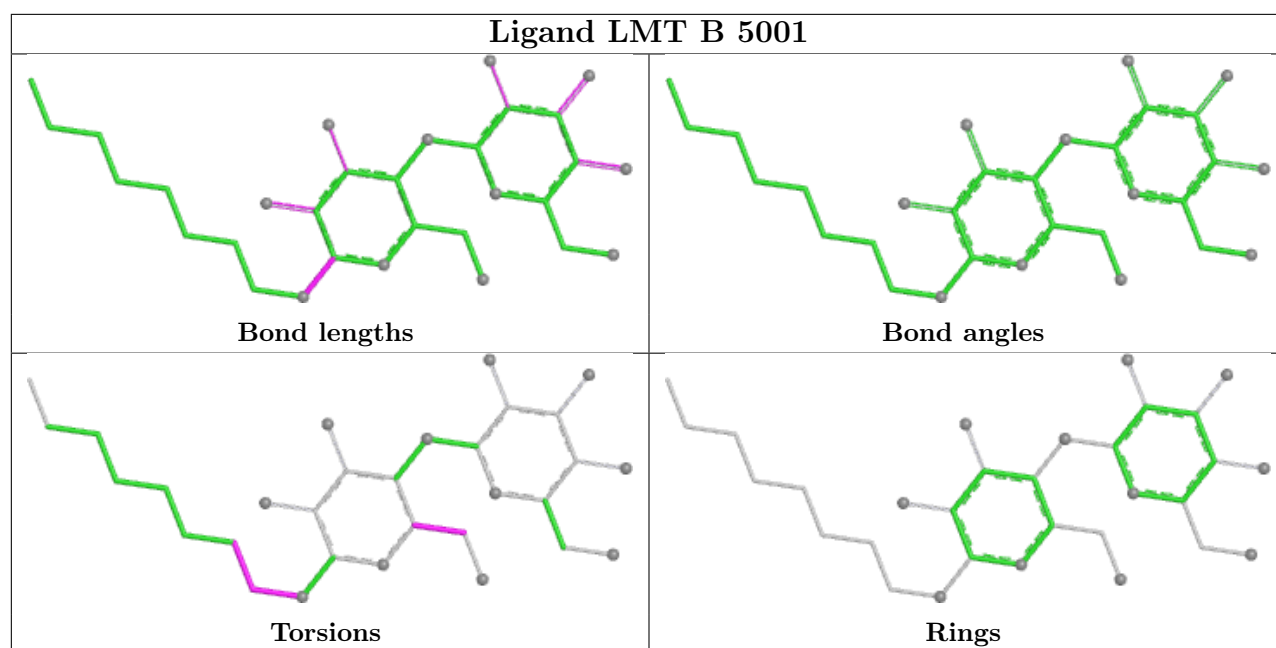




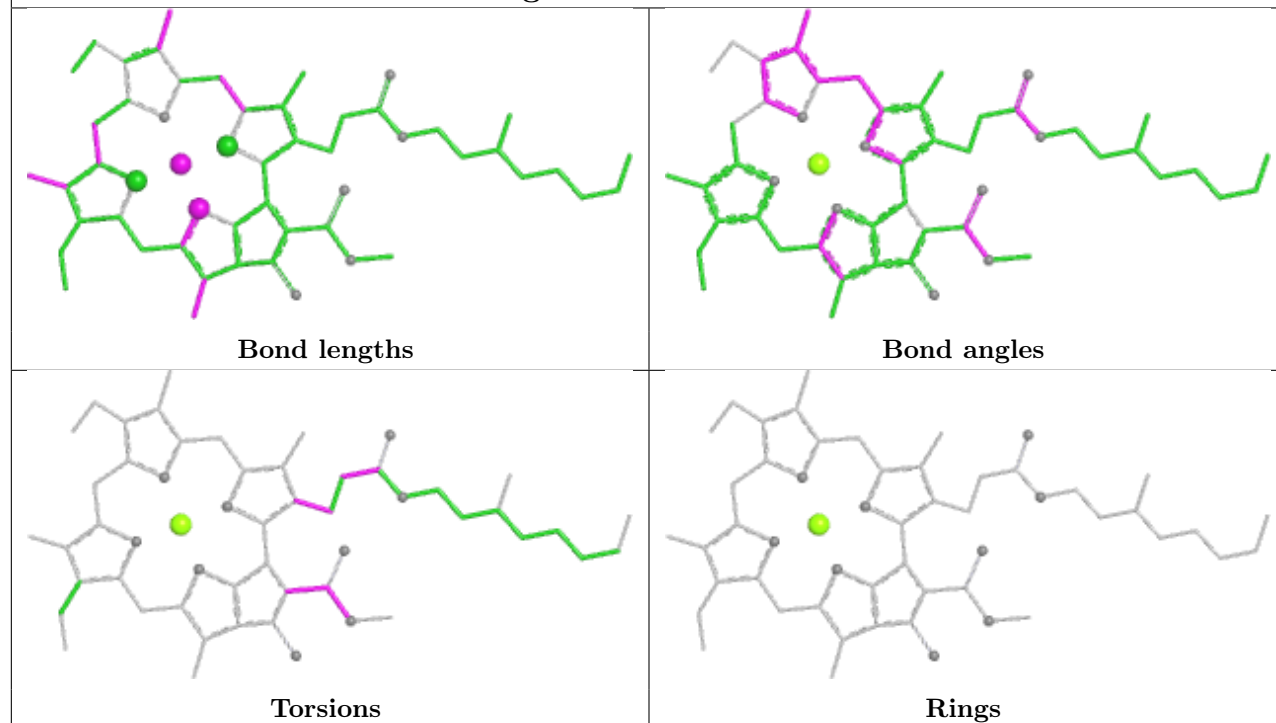




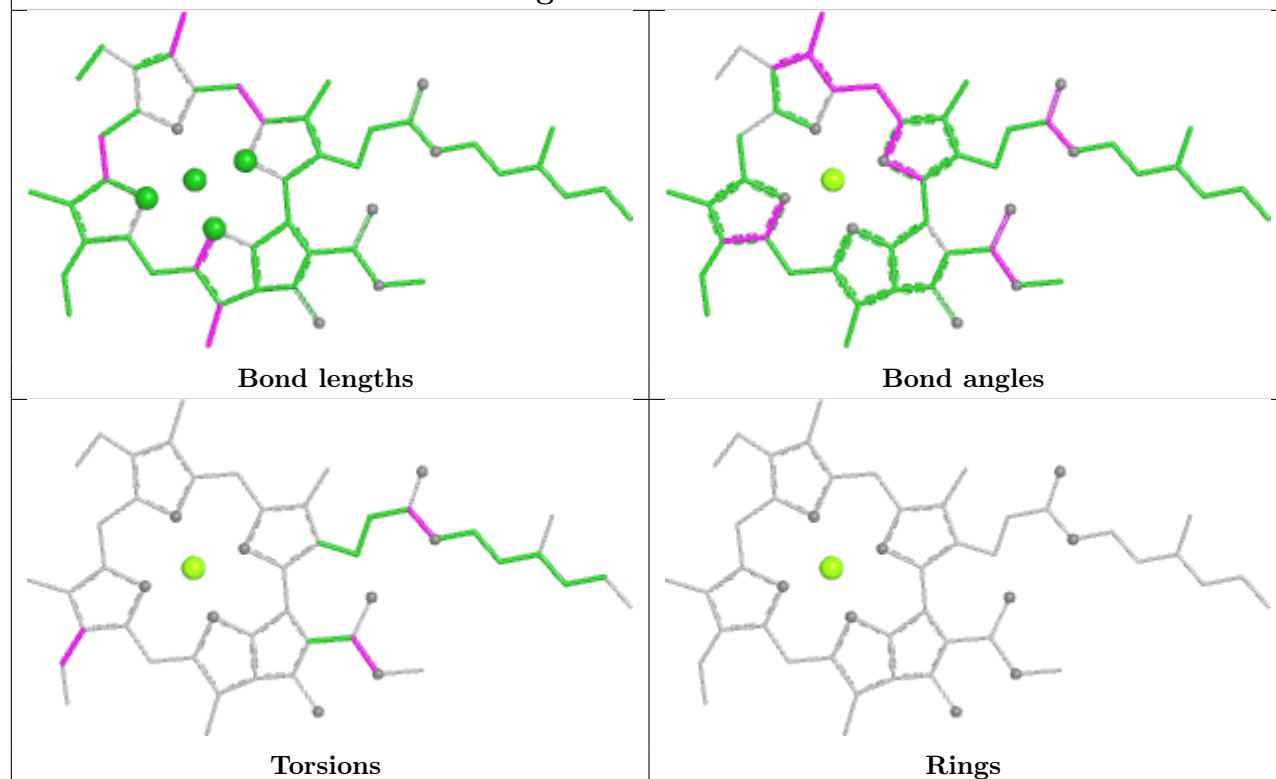


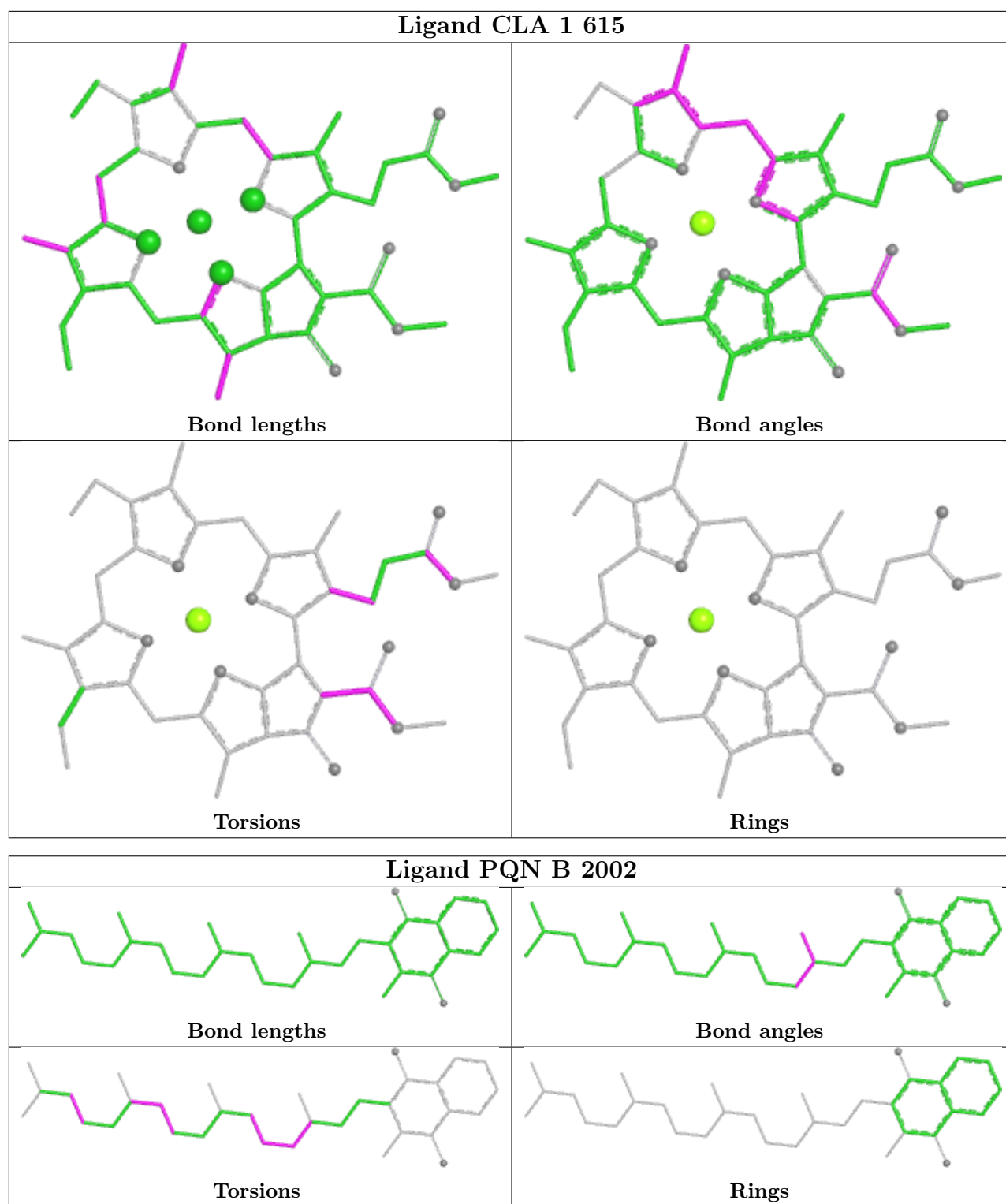


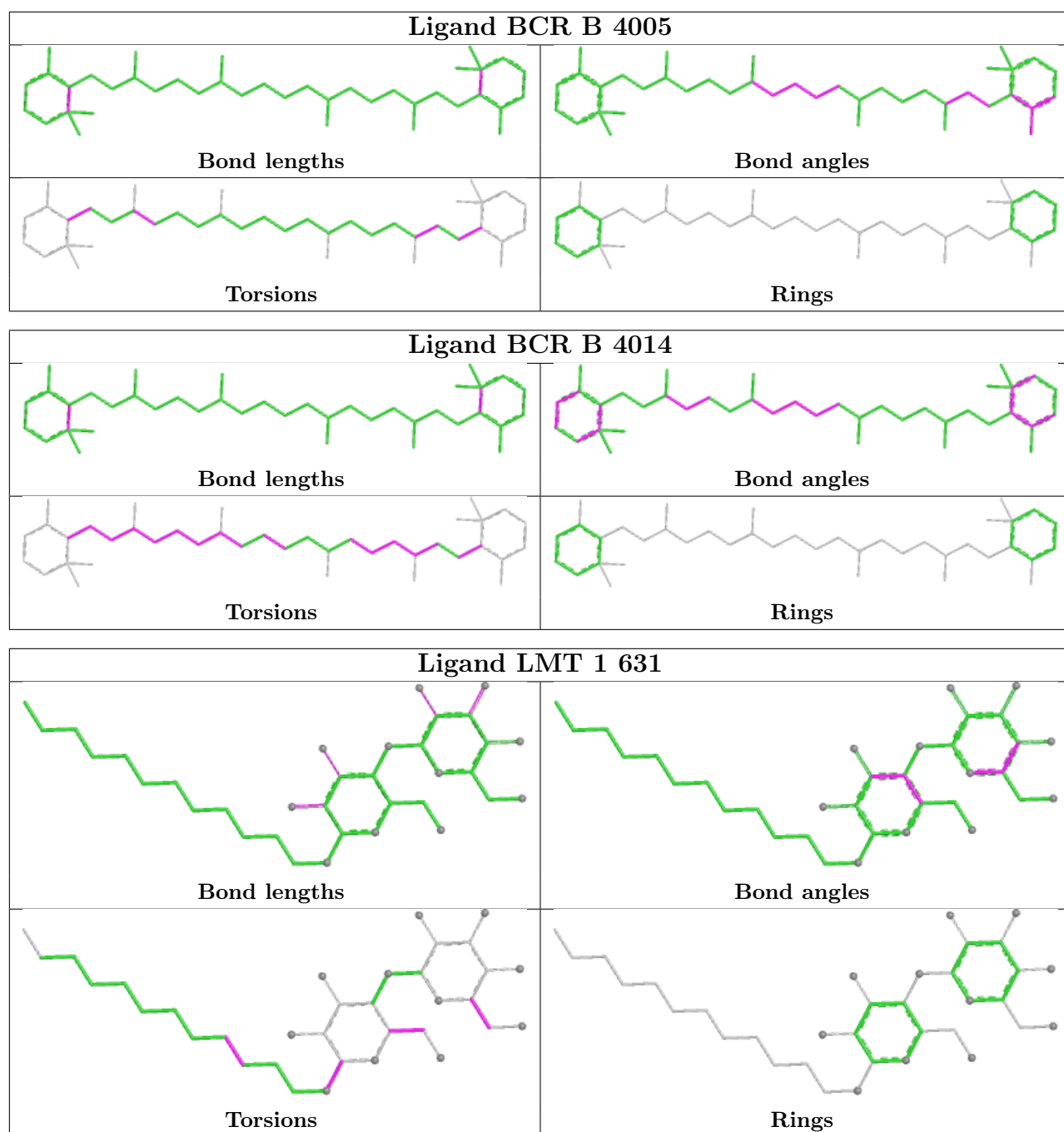
Ligand CLA A 1116

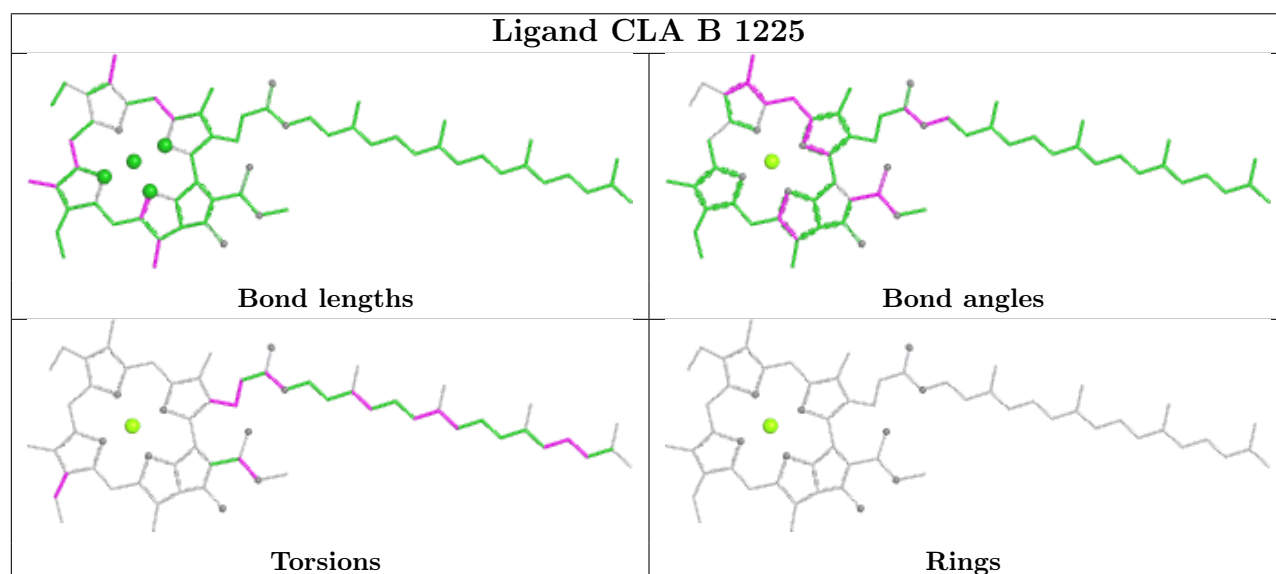
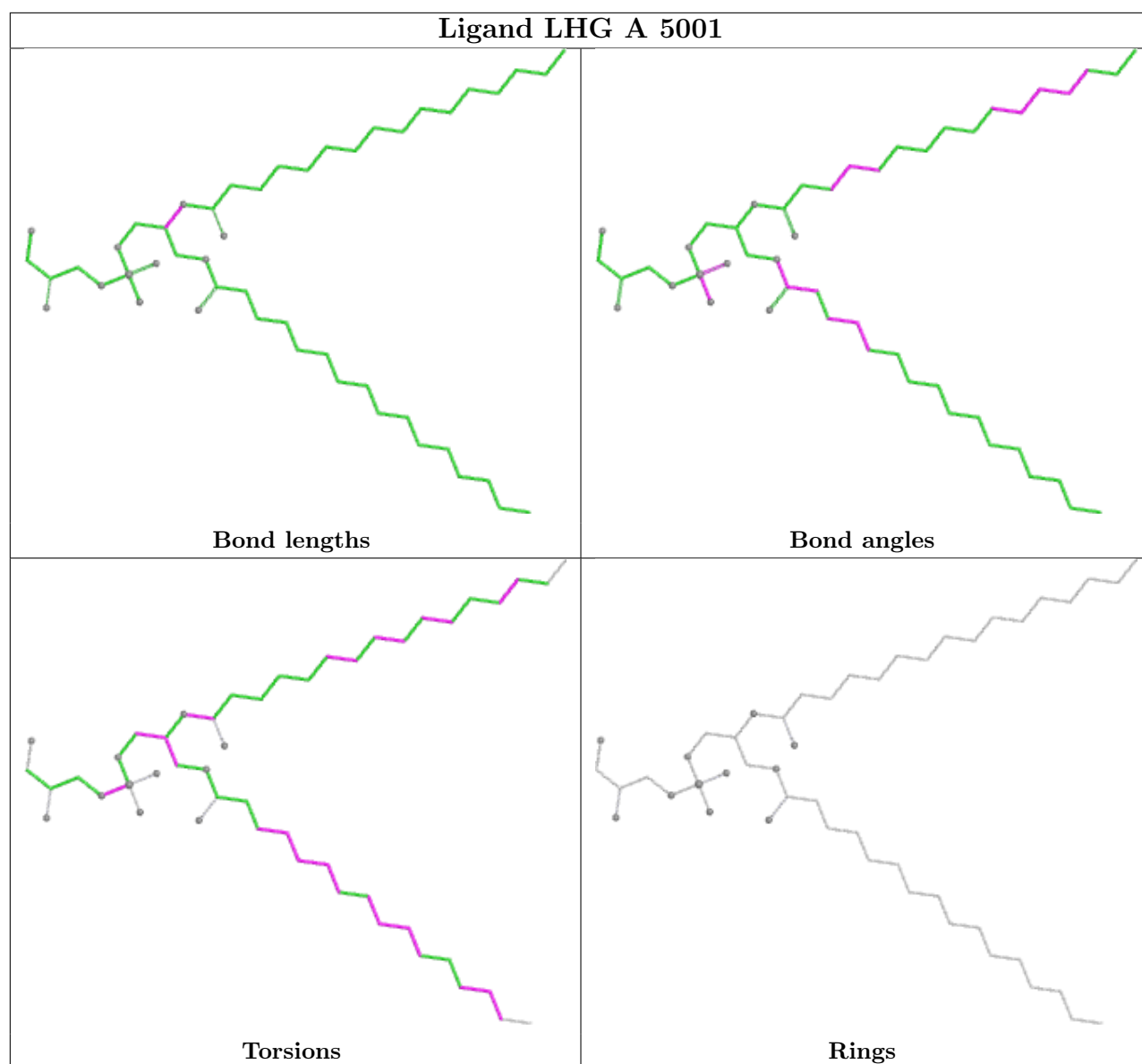


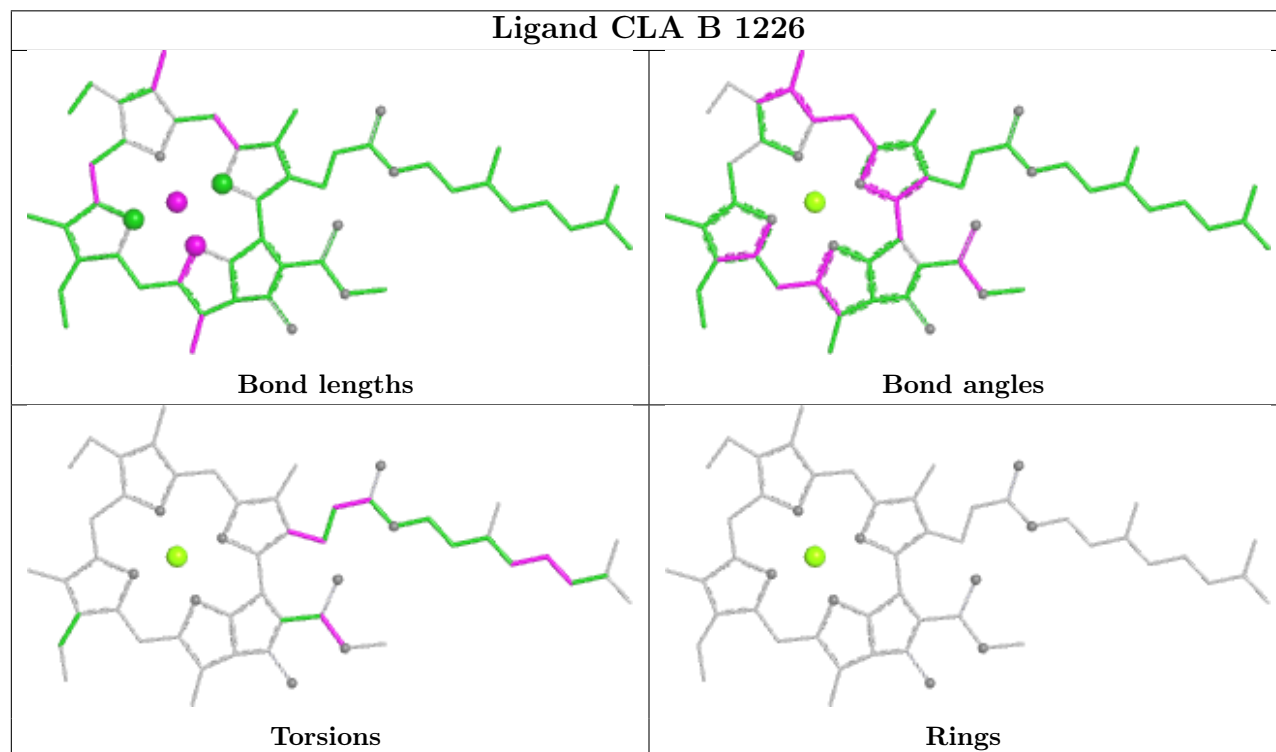
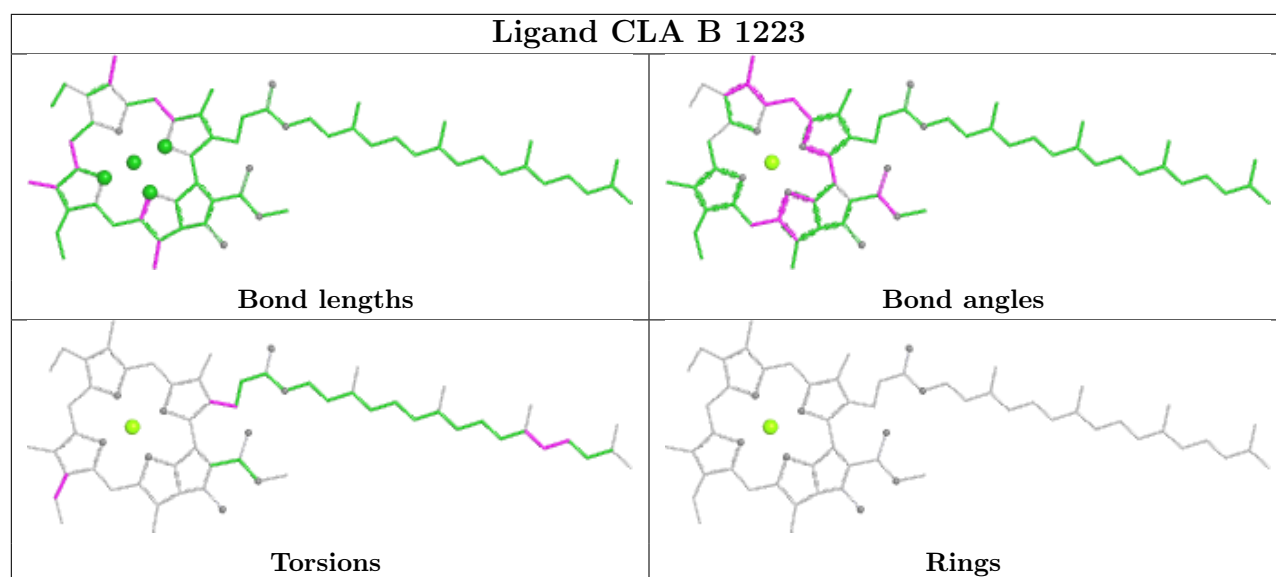
Ligand CLA 2 612

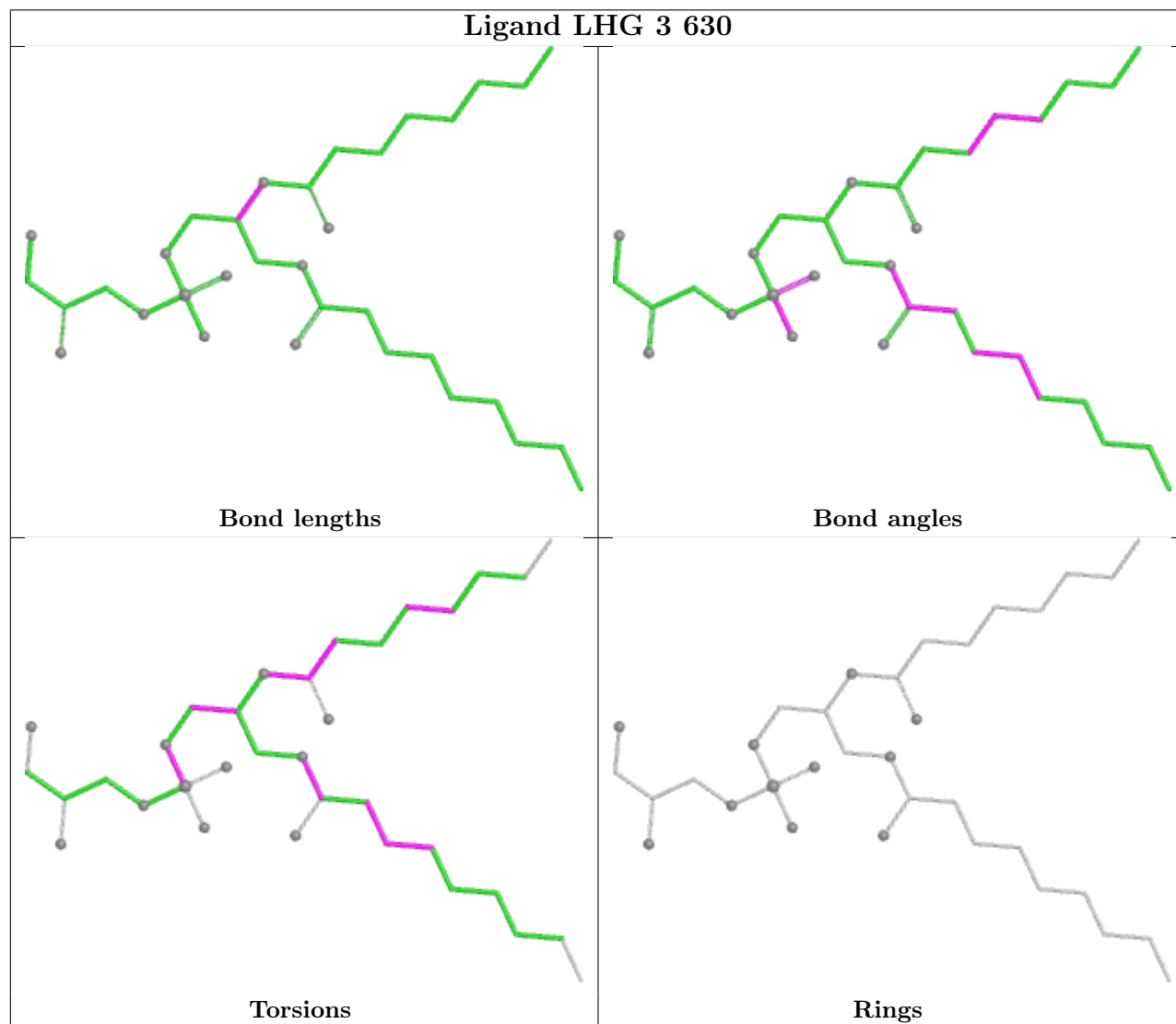
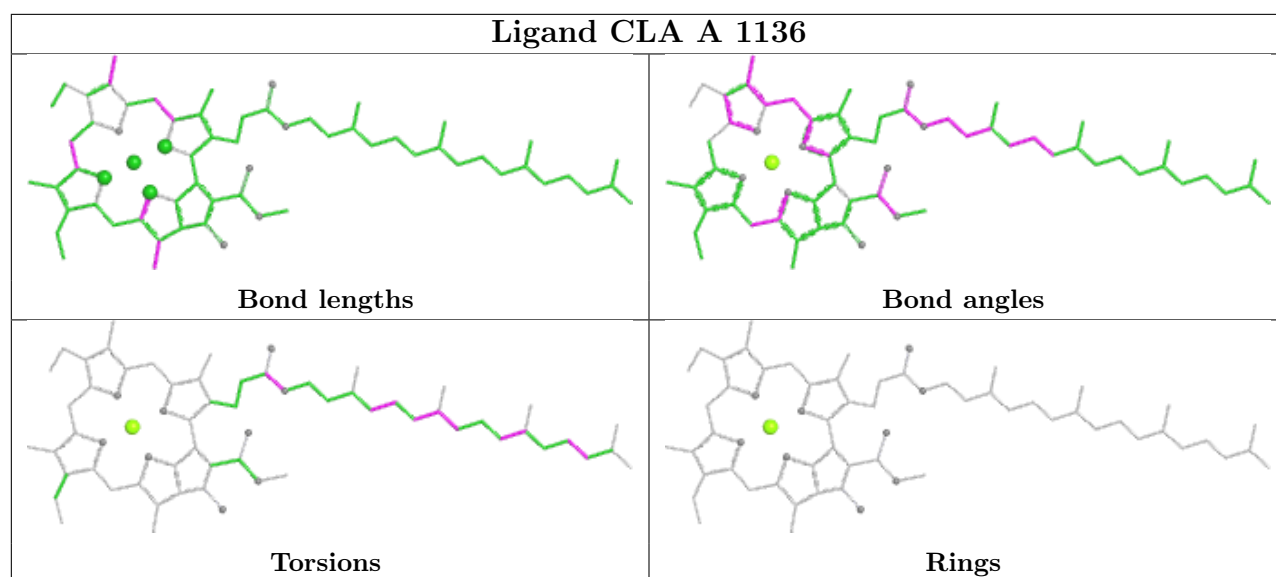


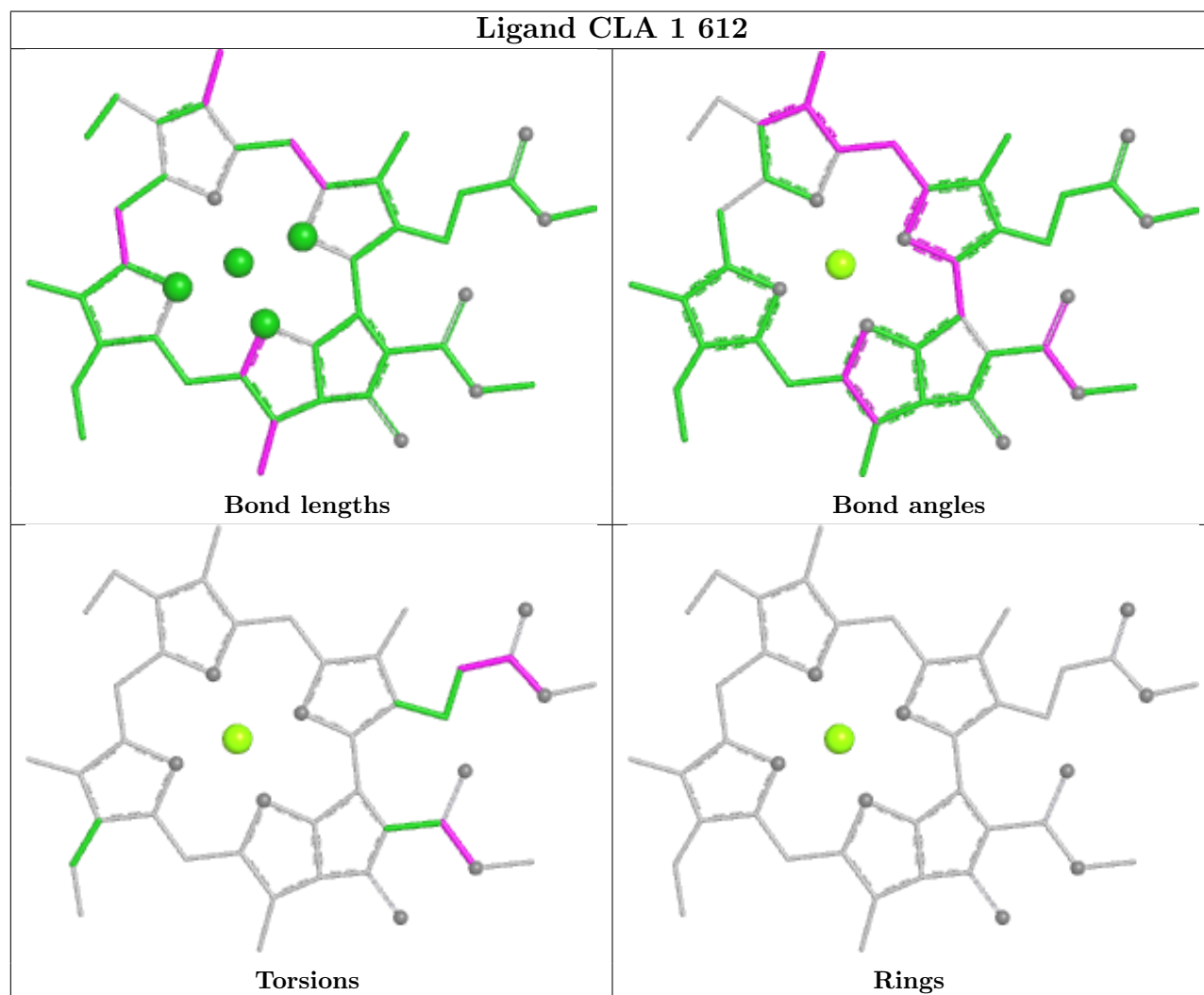
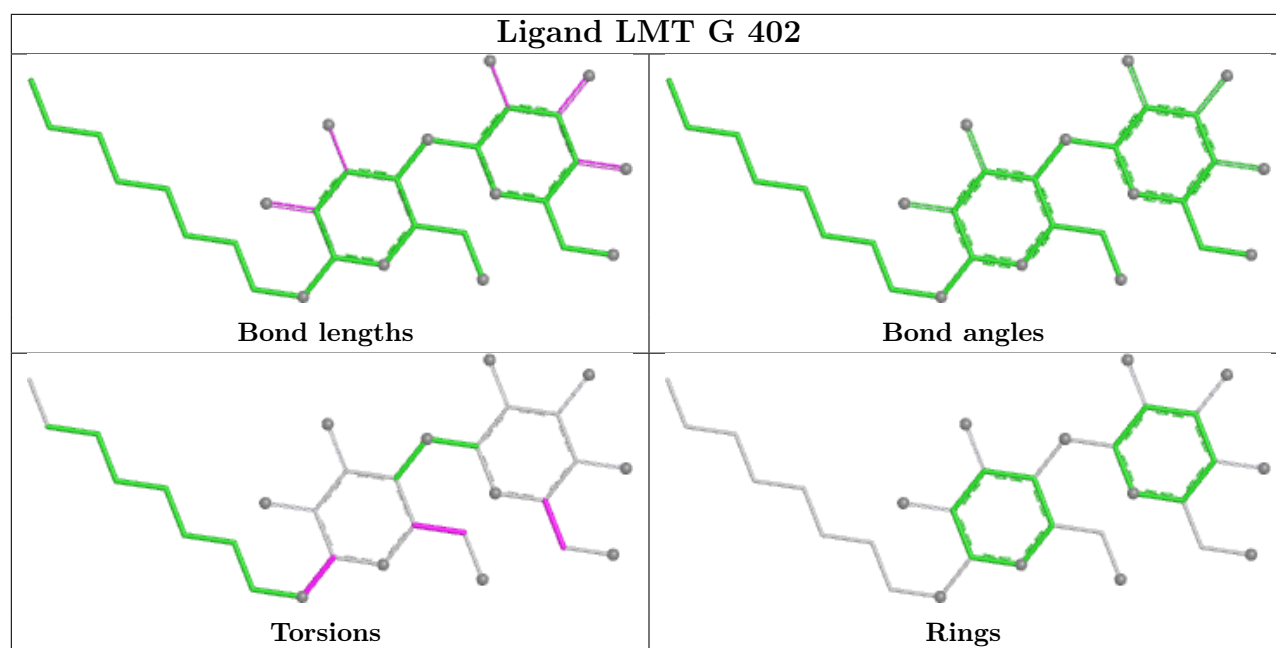


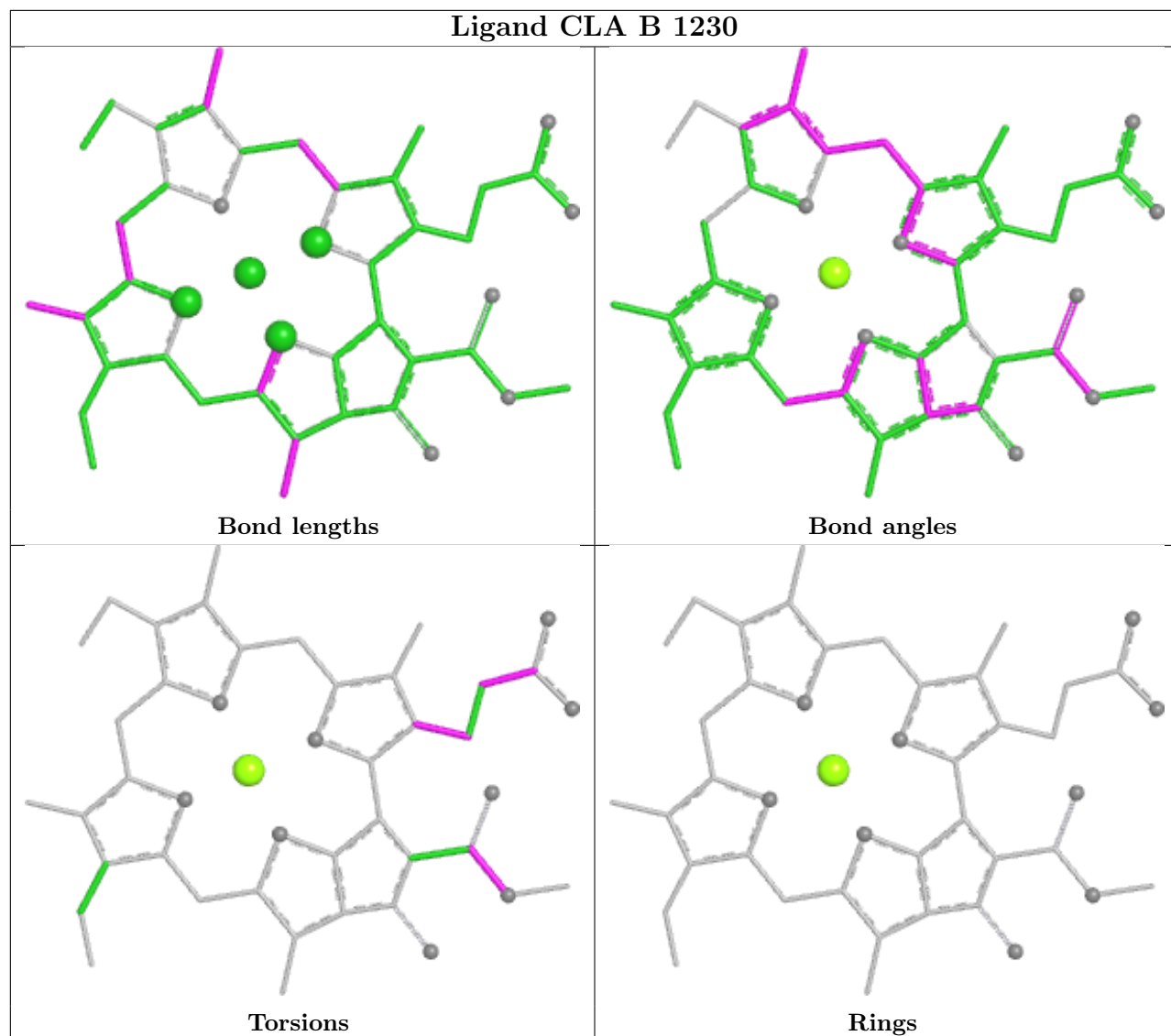


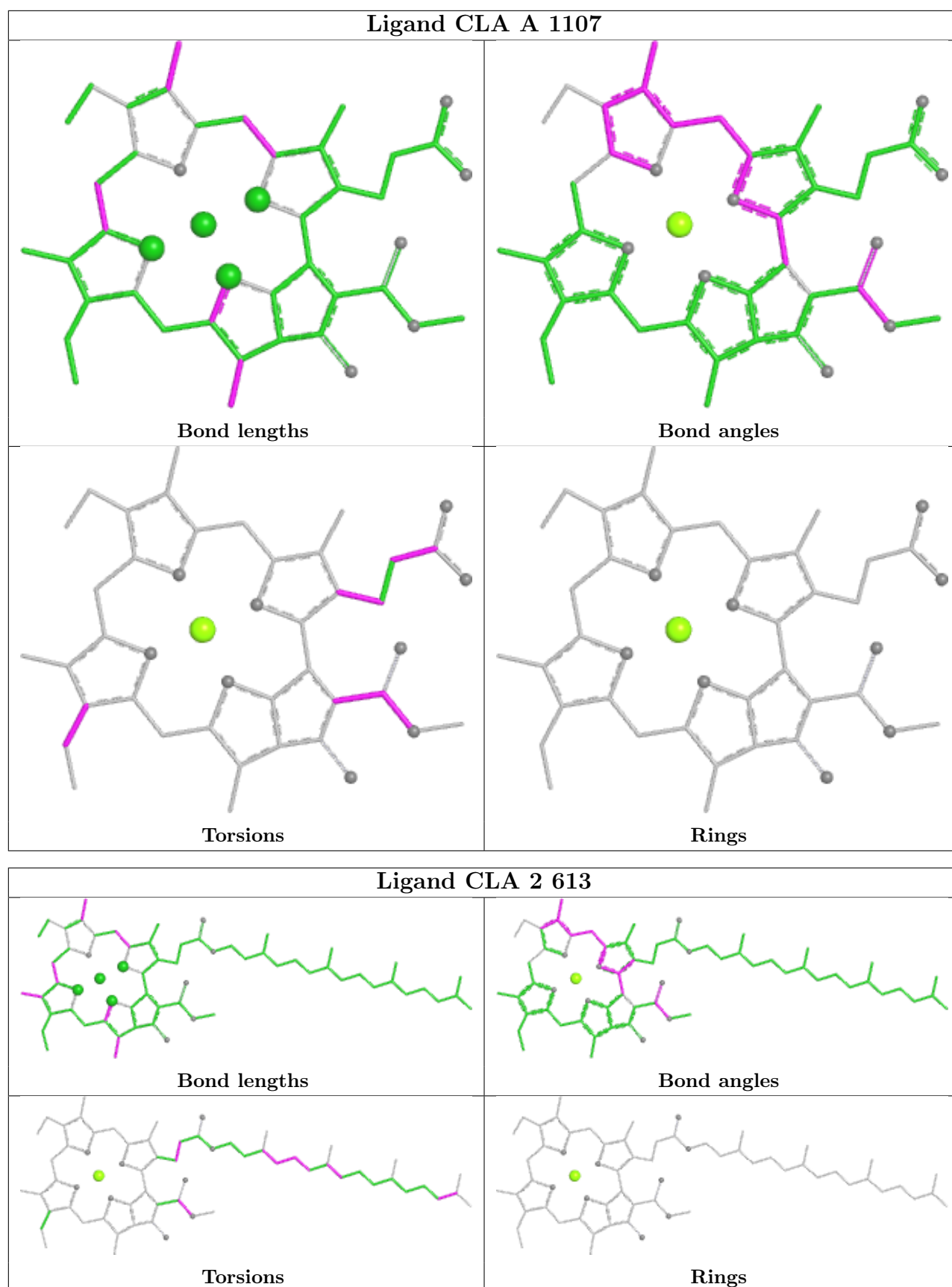


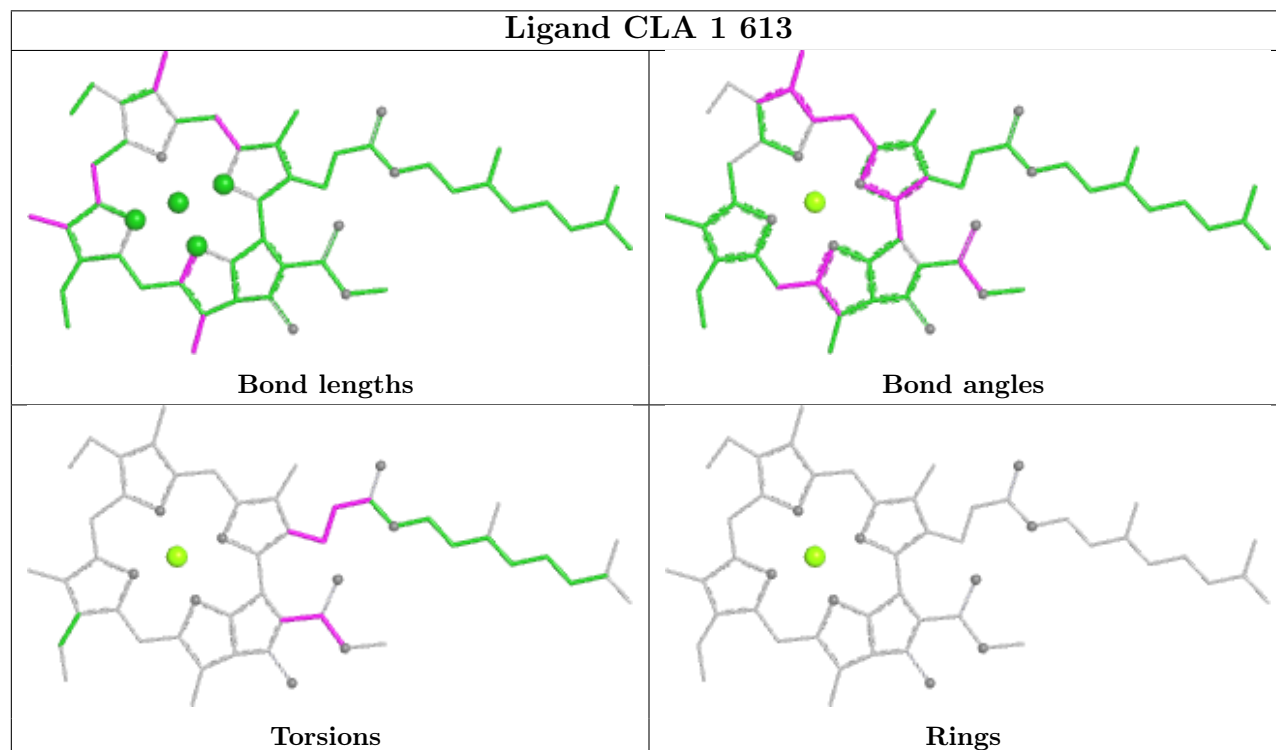
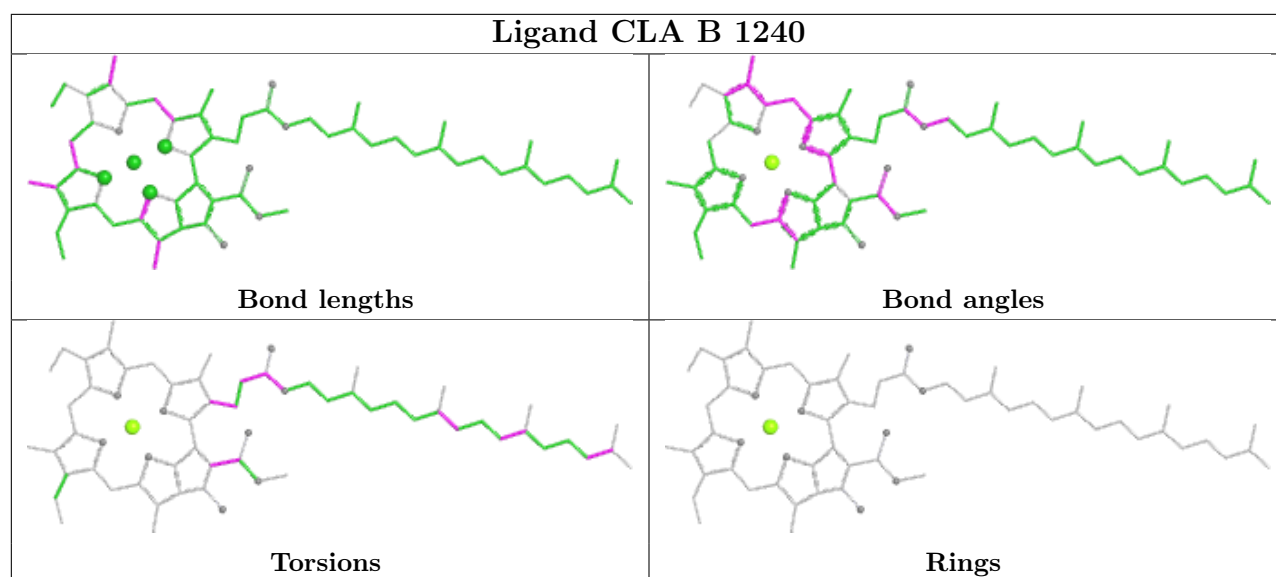




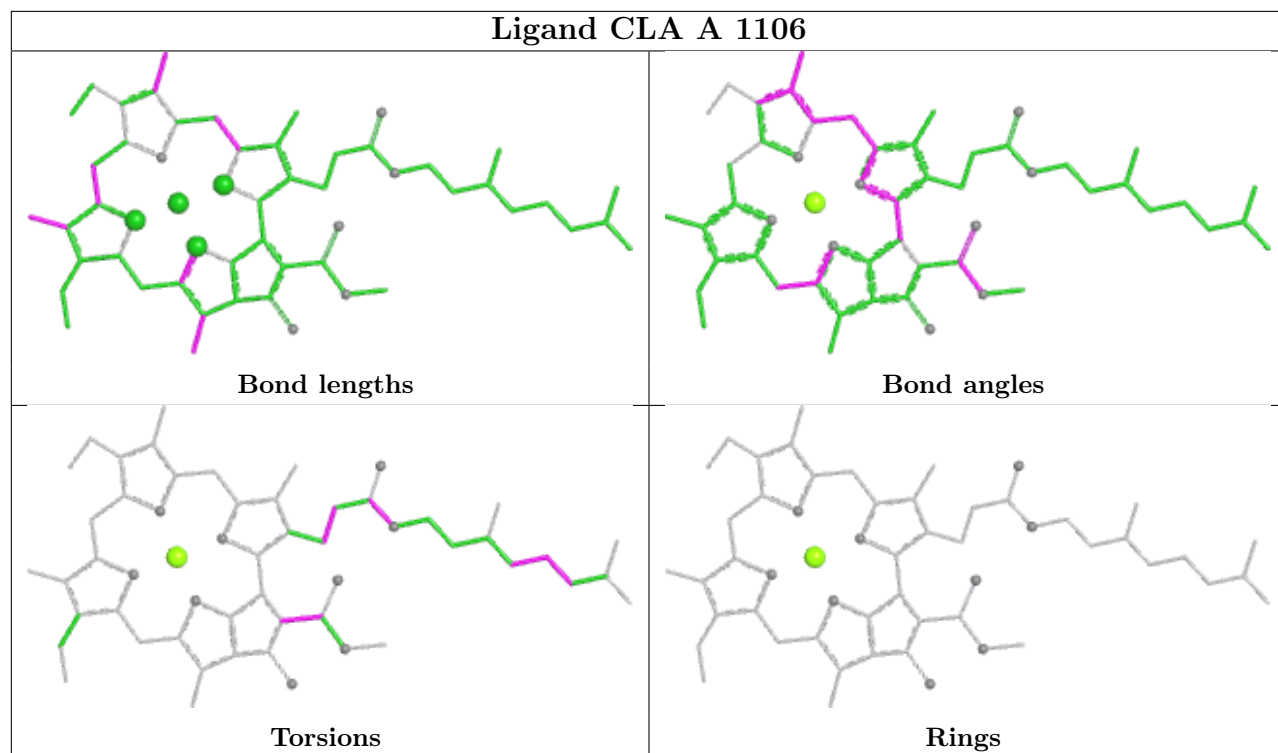




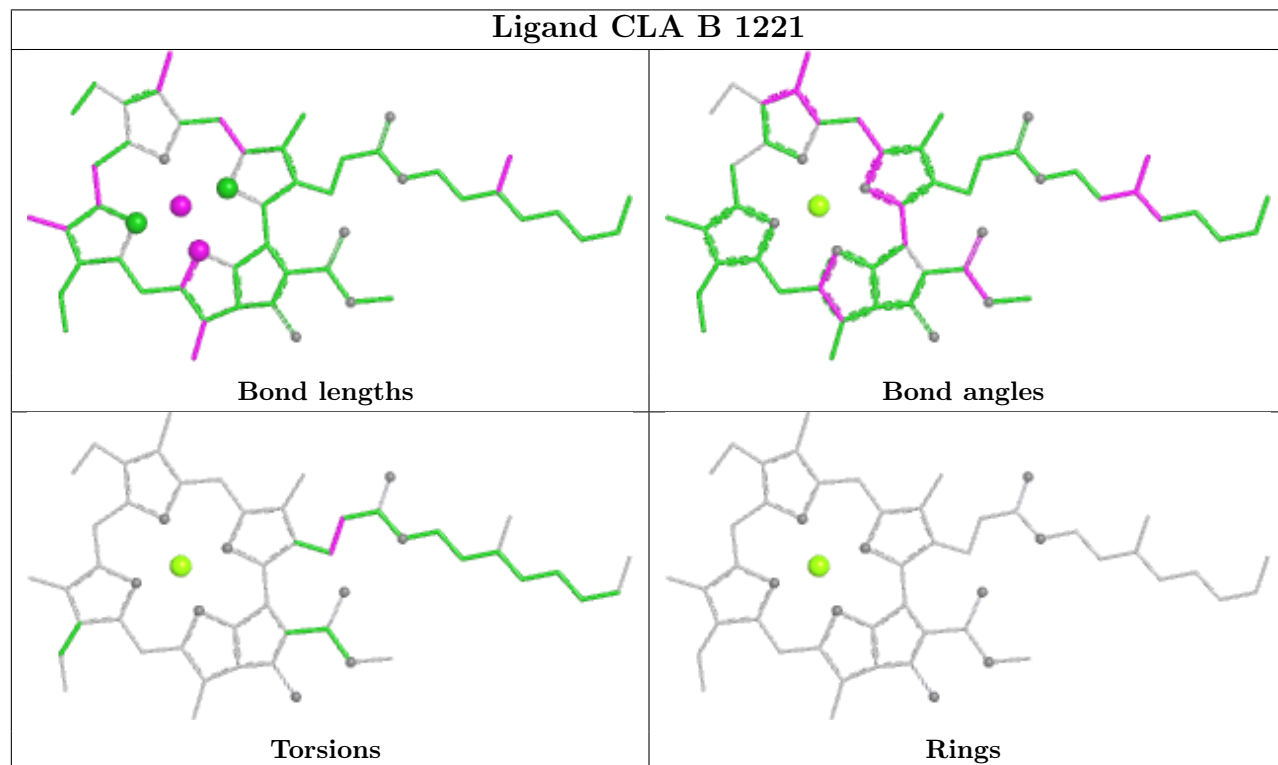


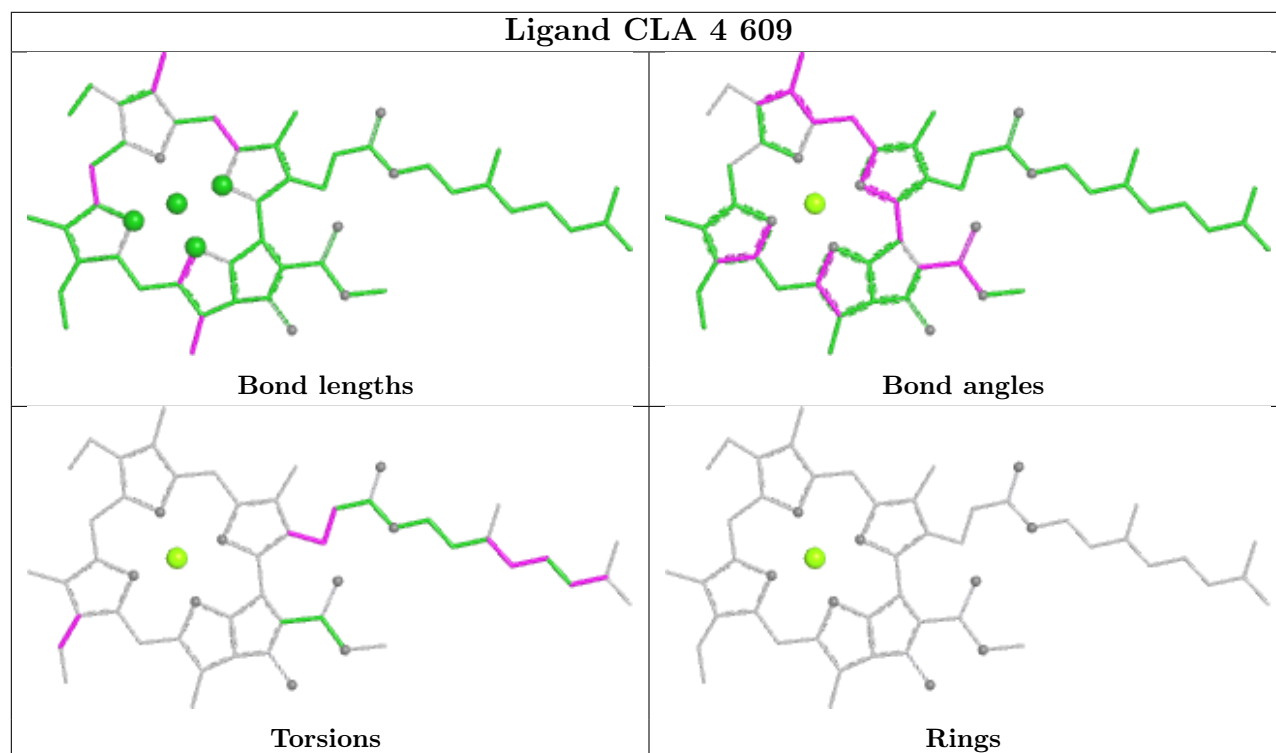
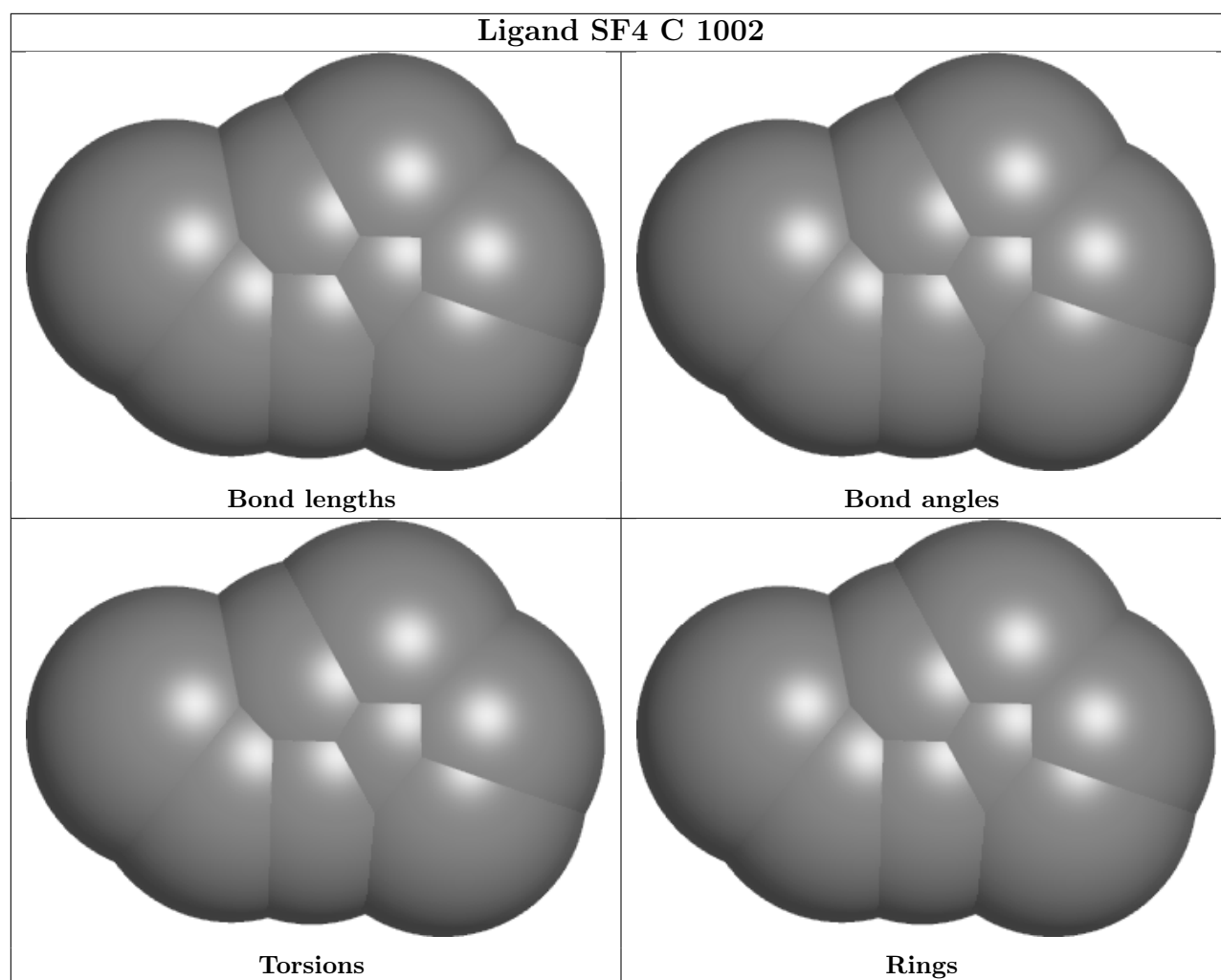


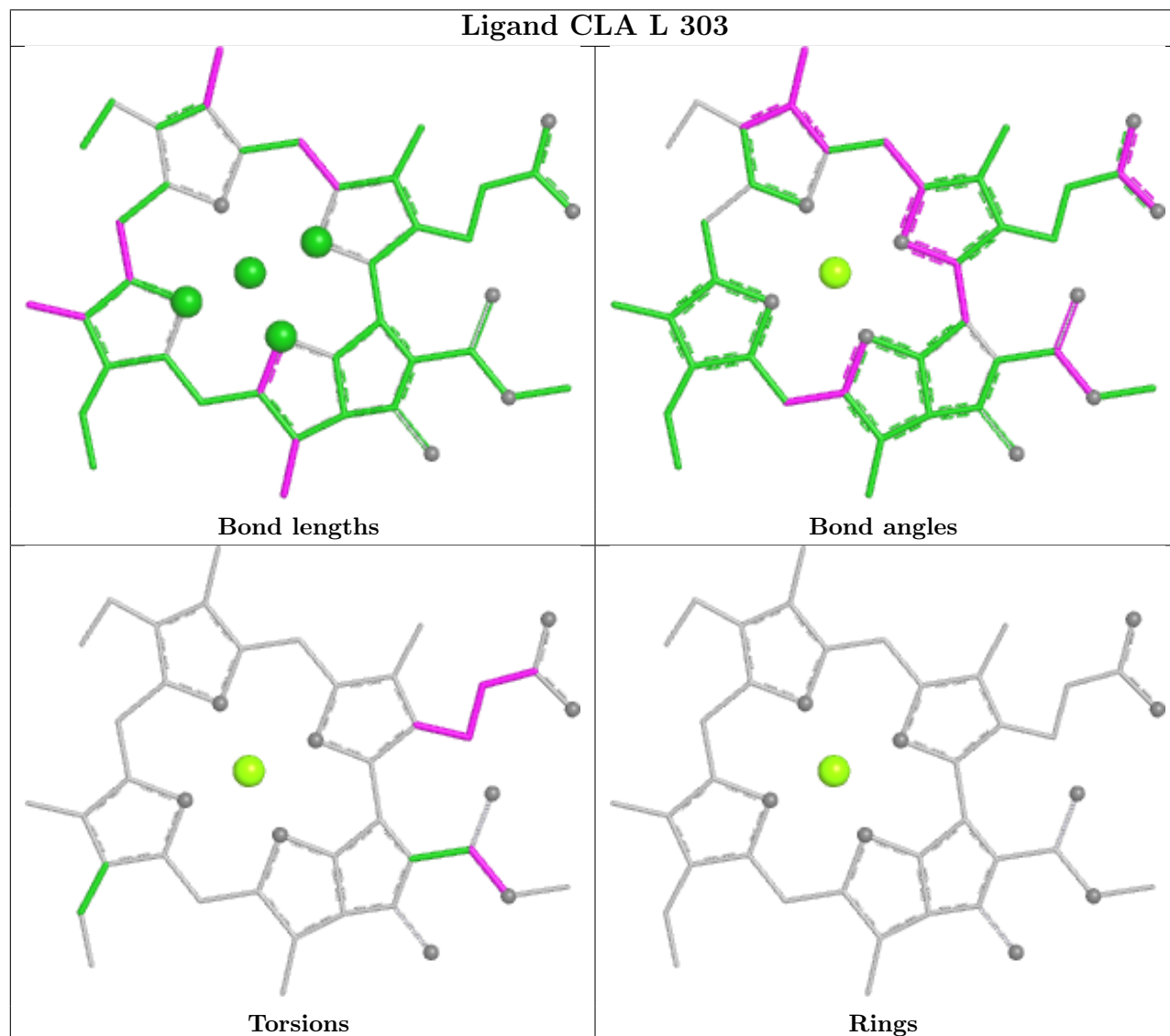
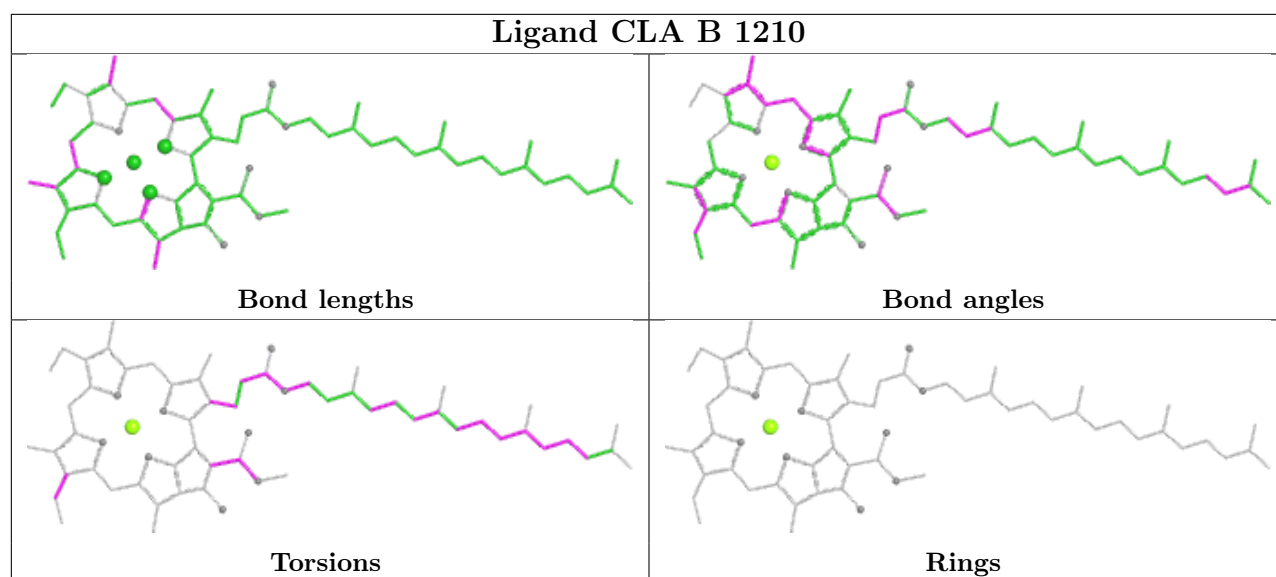
Ligand CLA A 1106

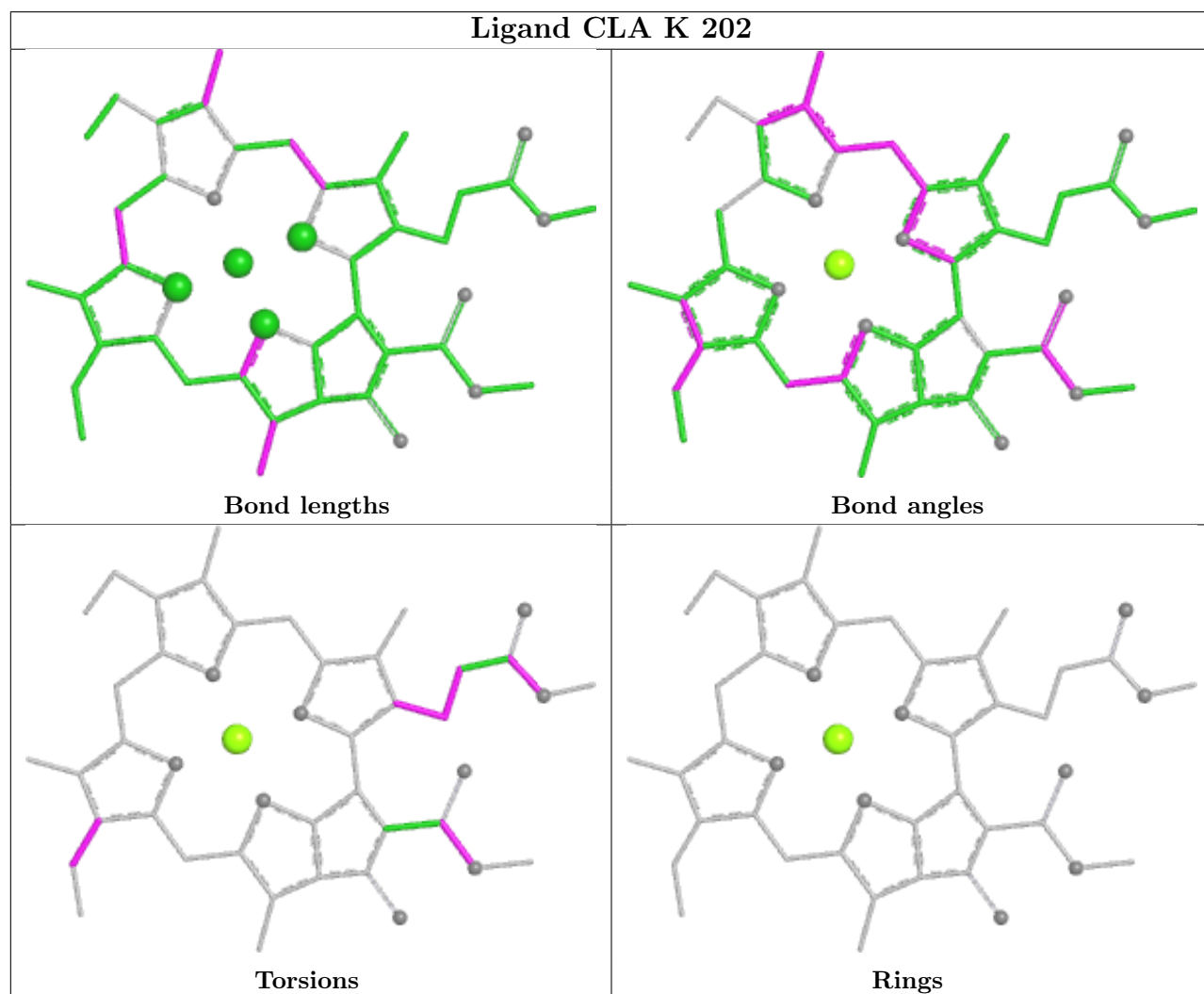
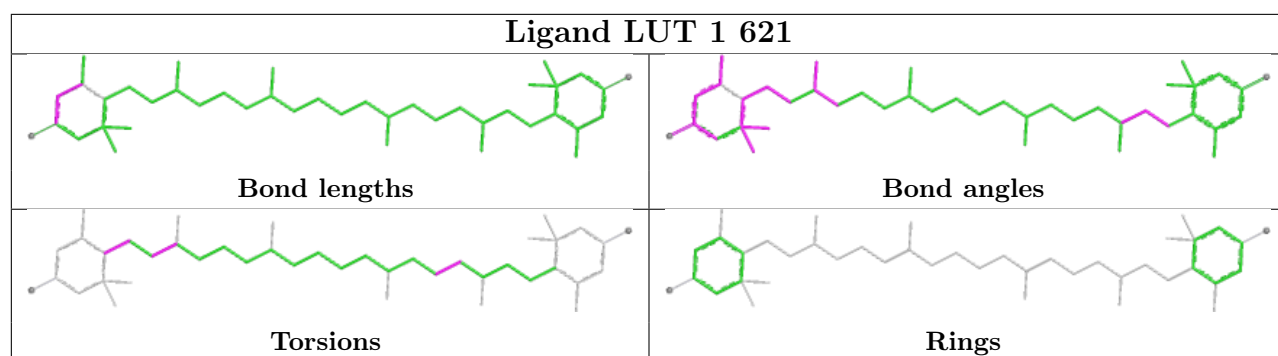


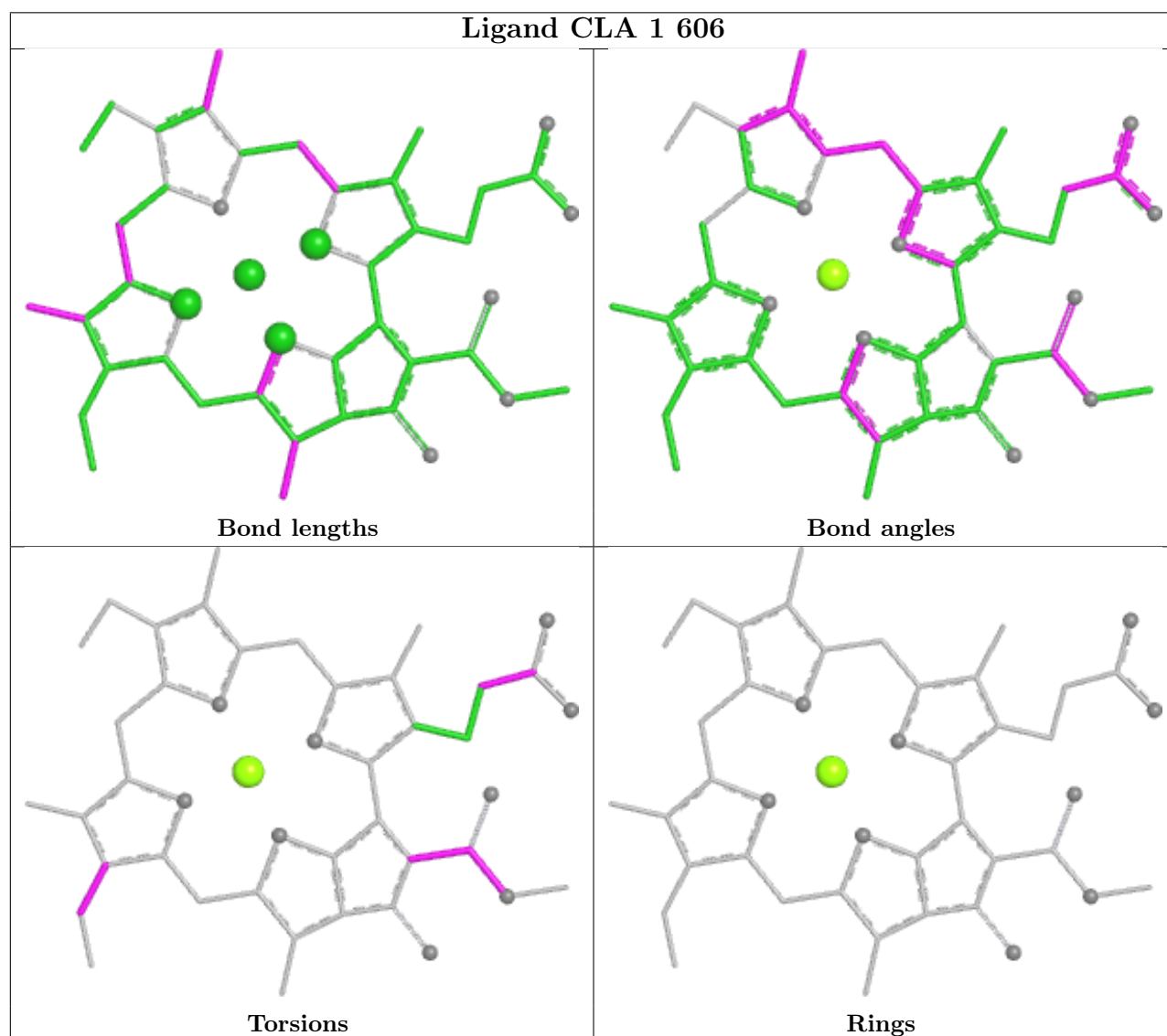
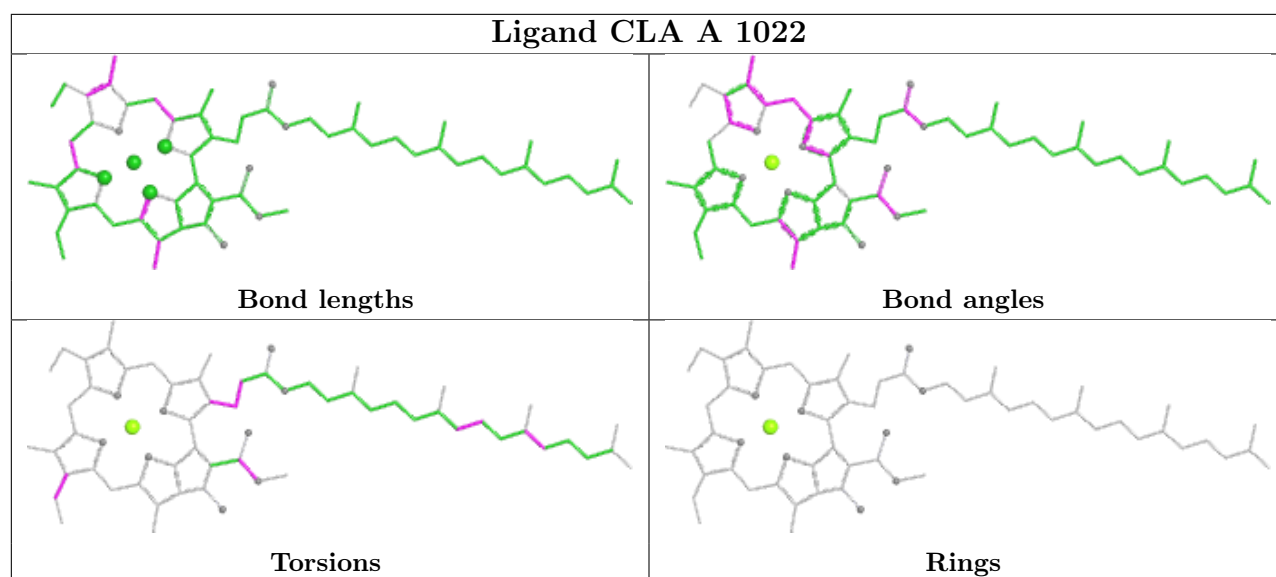
Ligand CLA B 1221

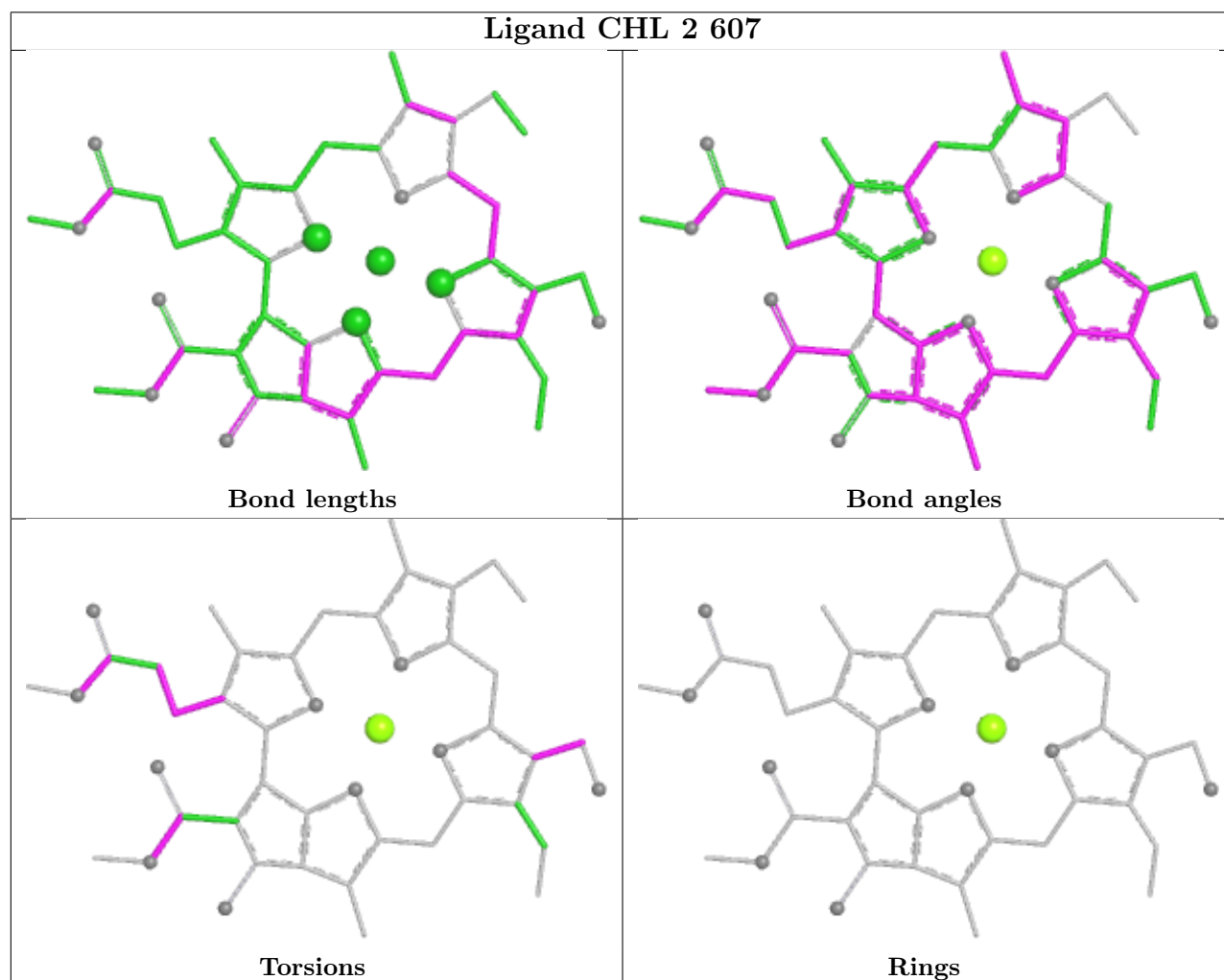
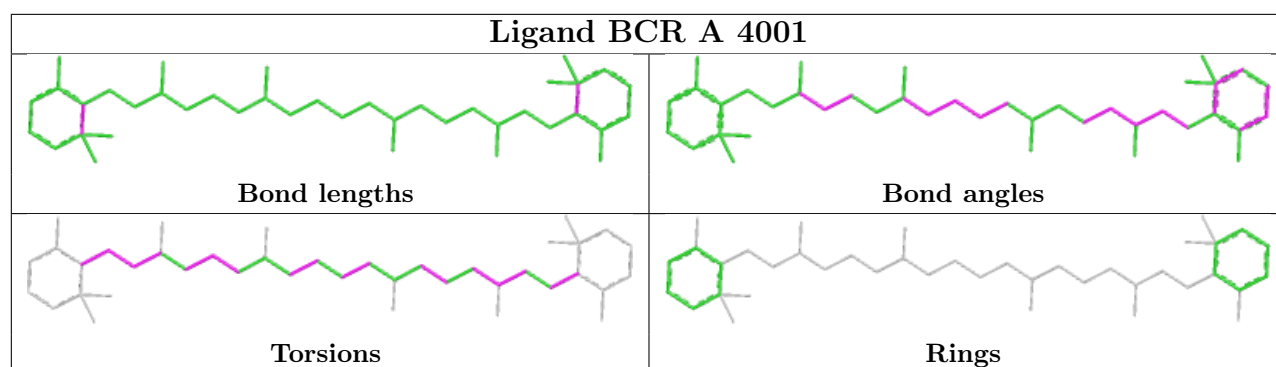




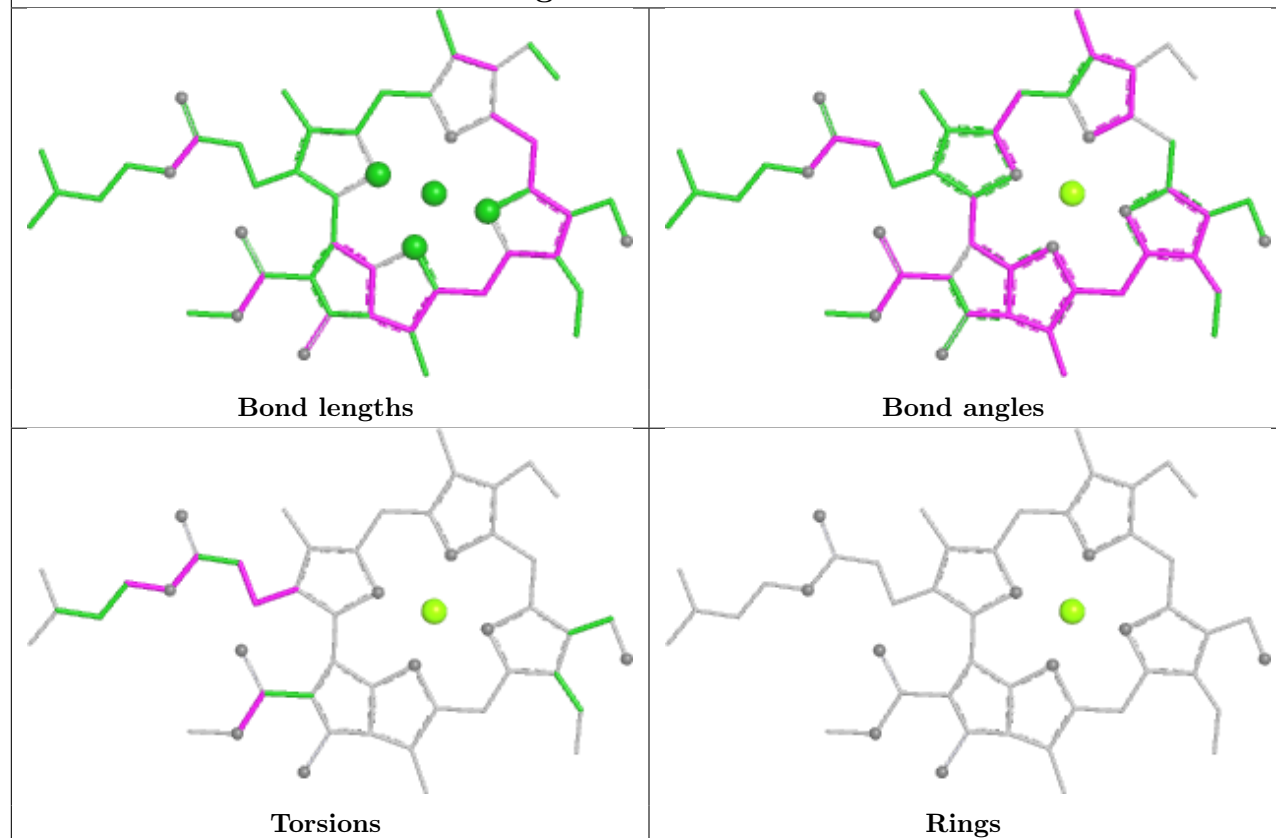




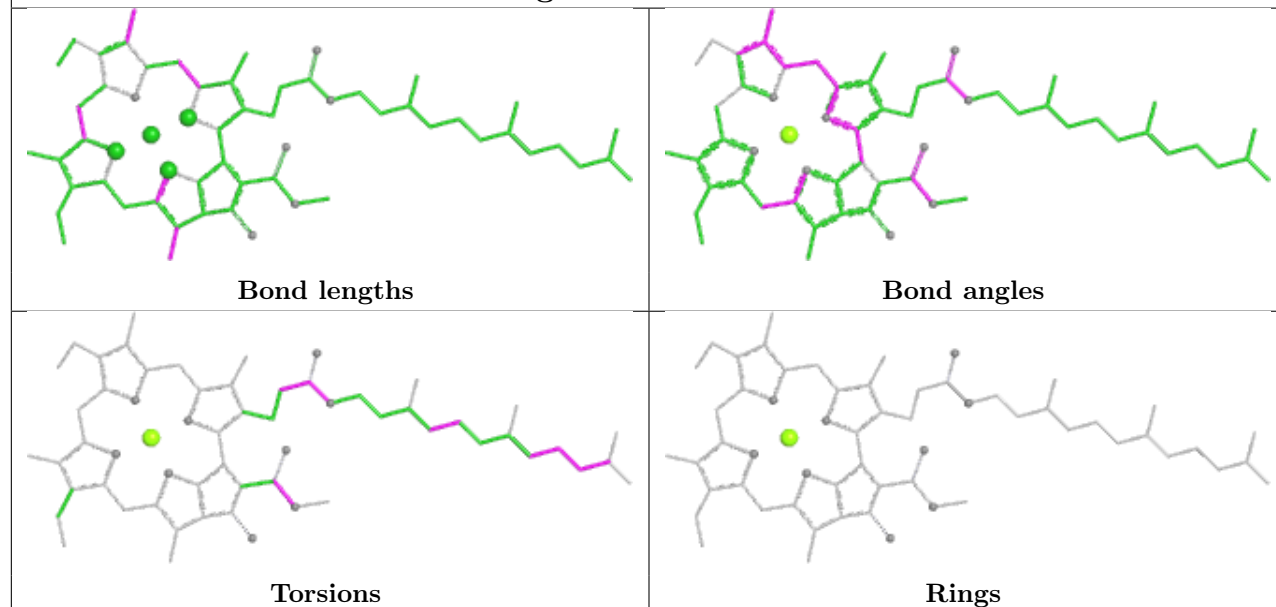


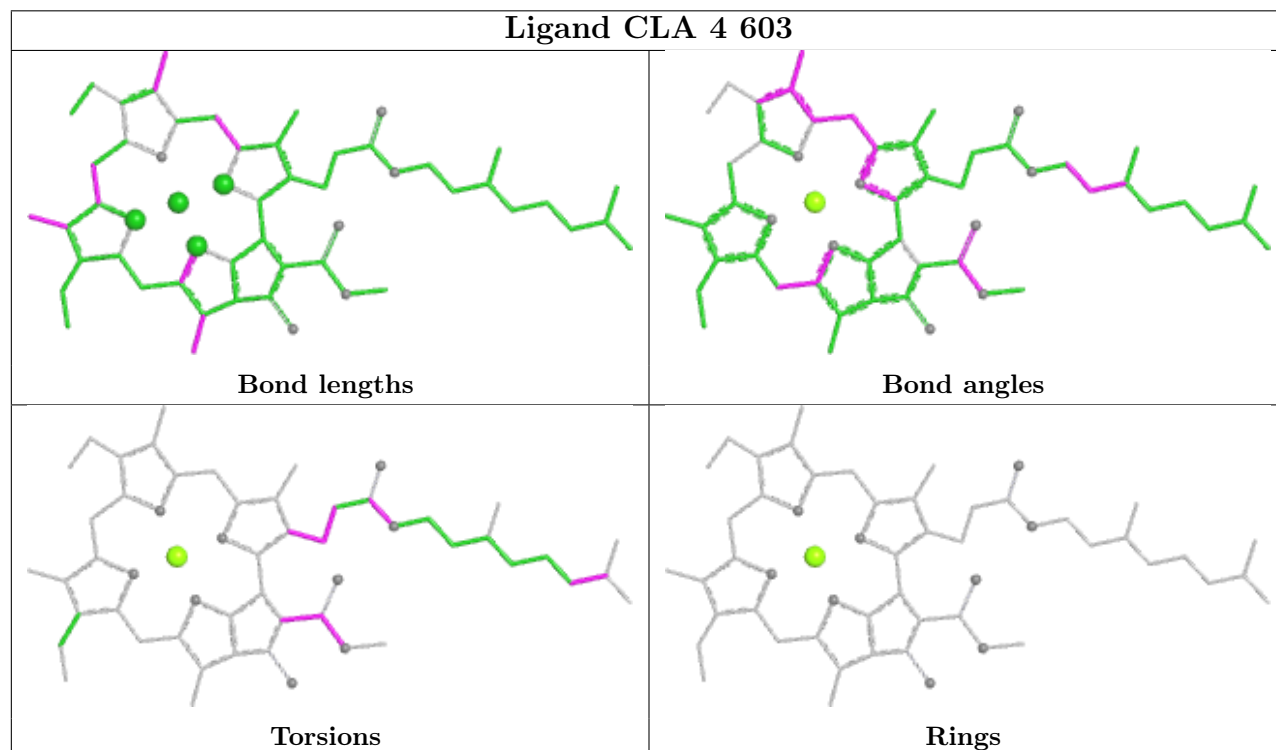
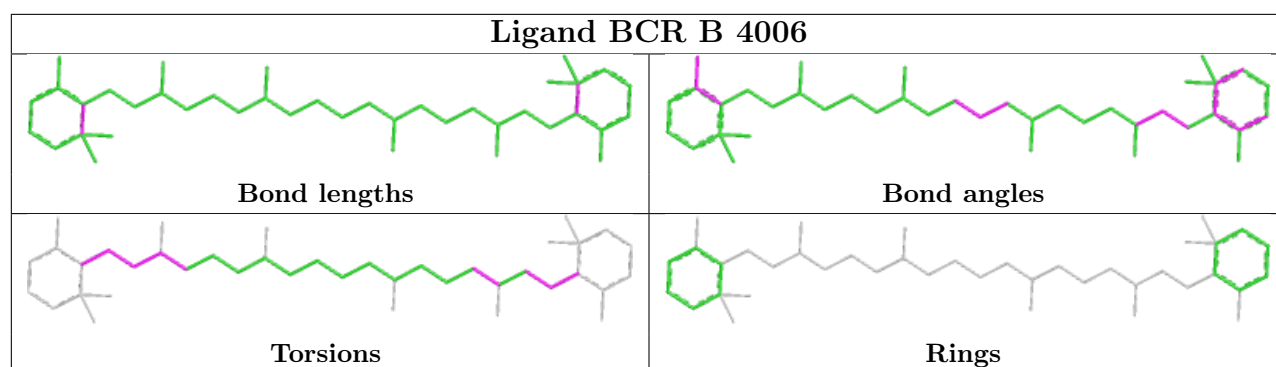


Ligand CHL 4 608

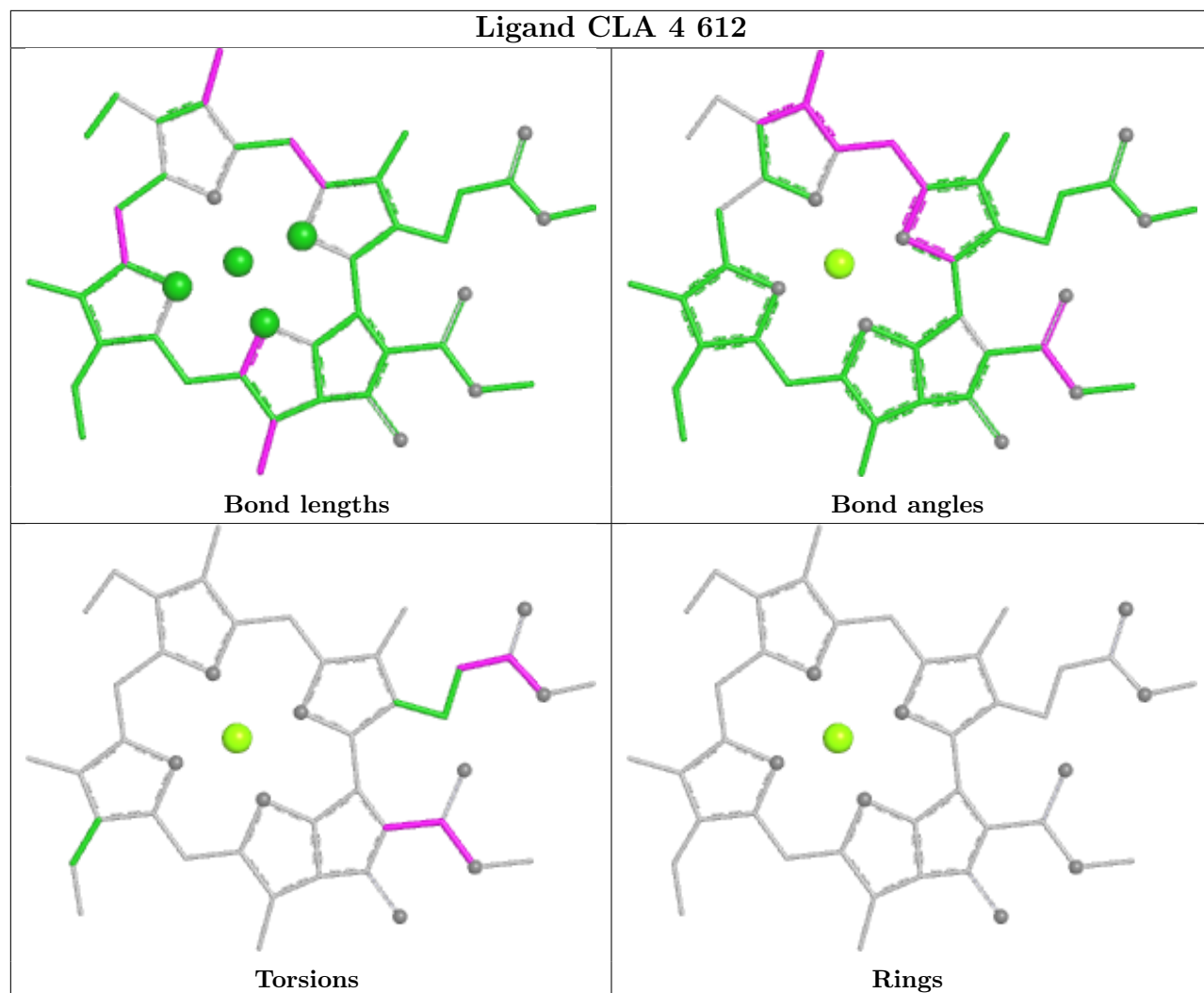


Ligand CLA 3 609

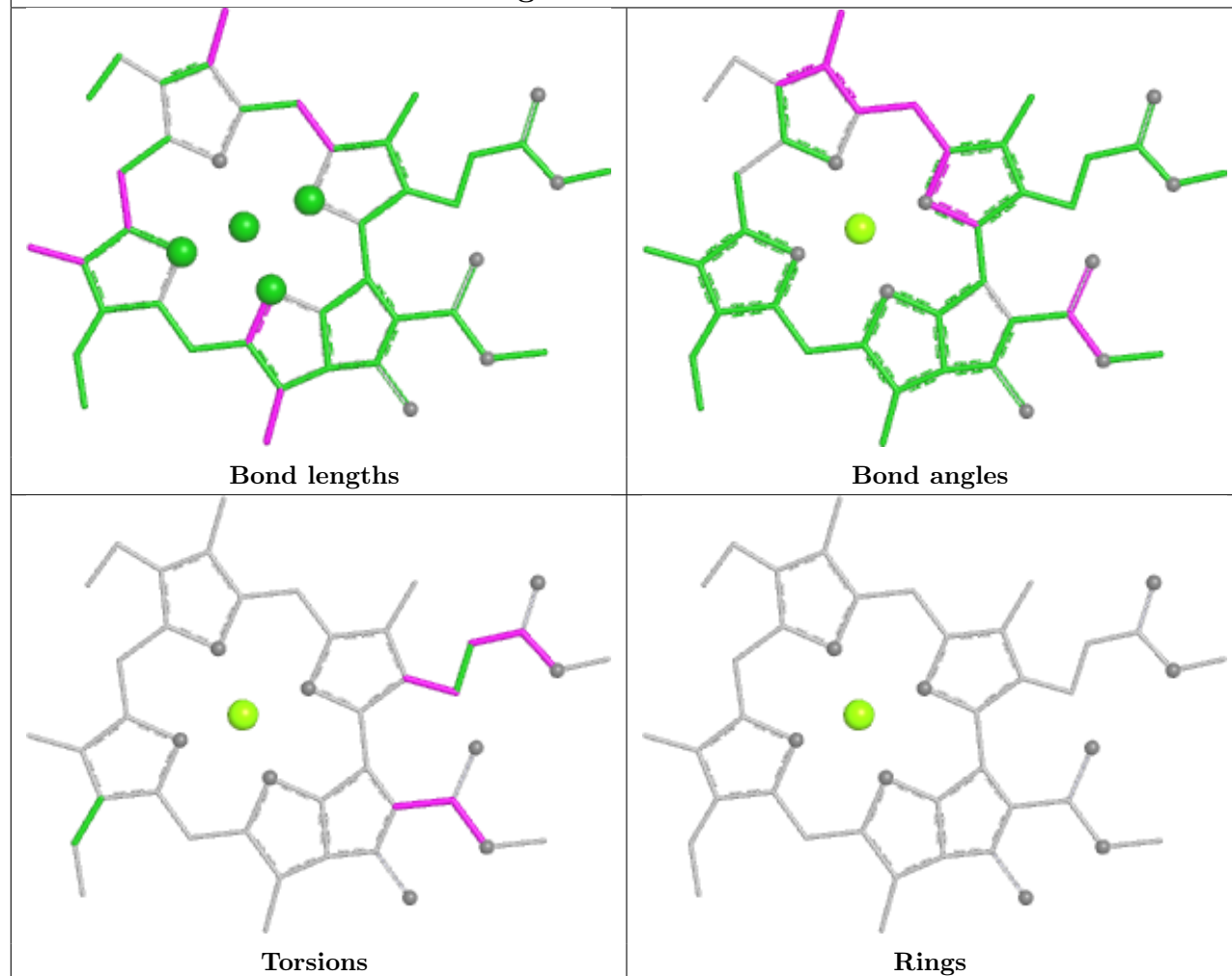




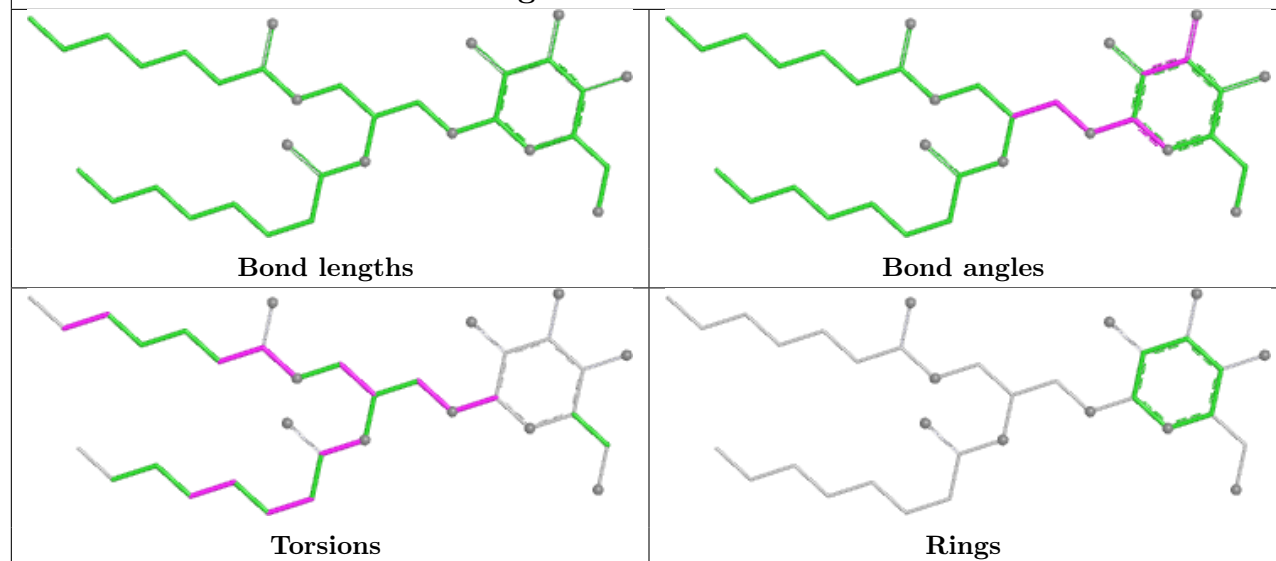
Ligand CLA 4 612

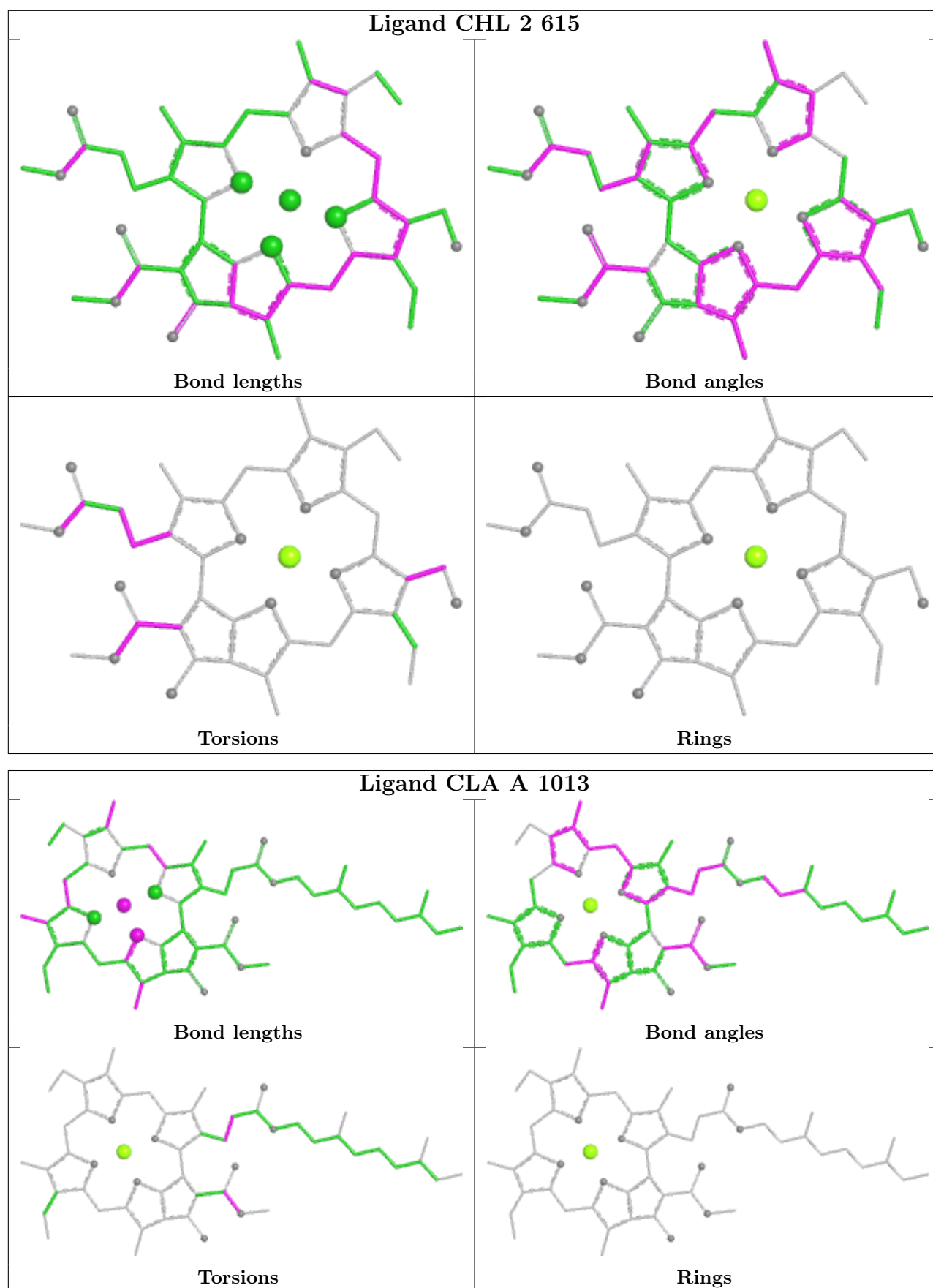


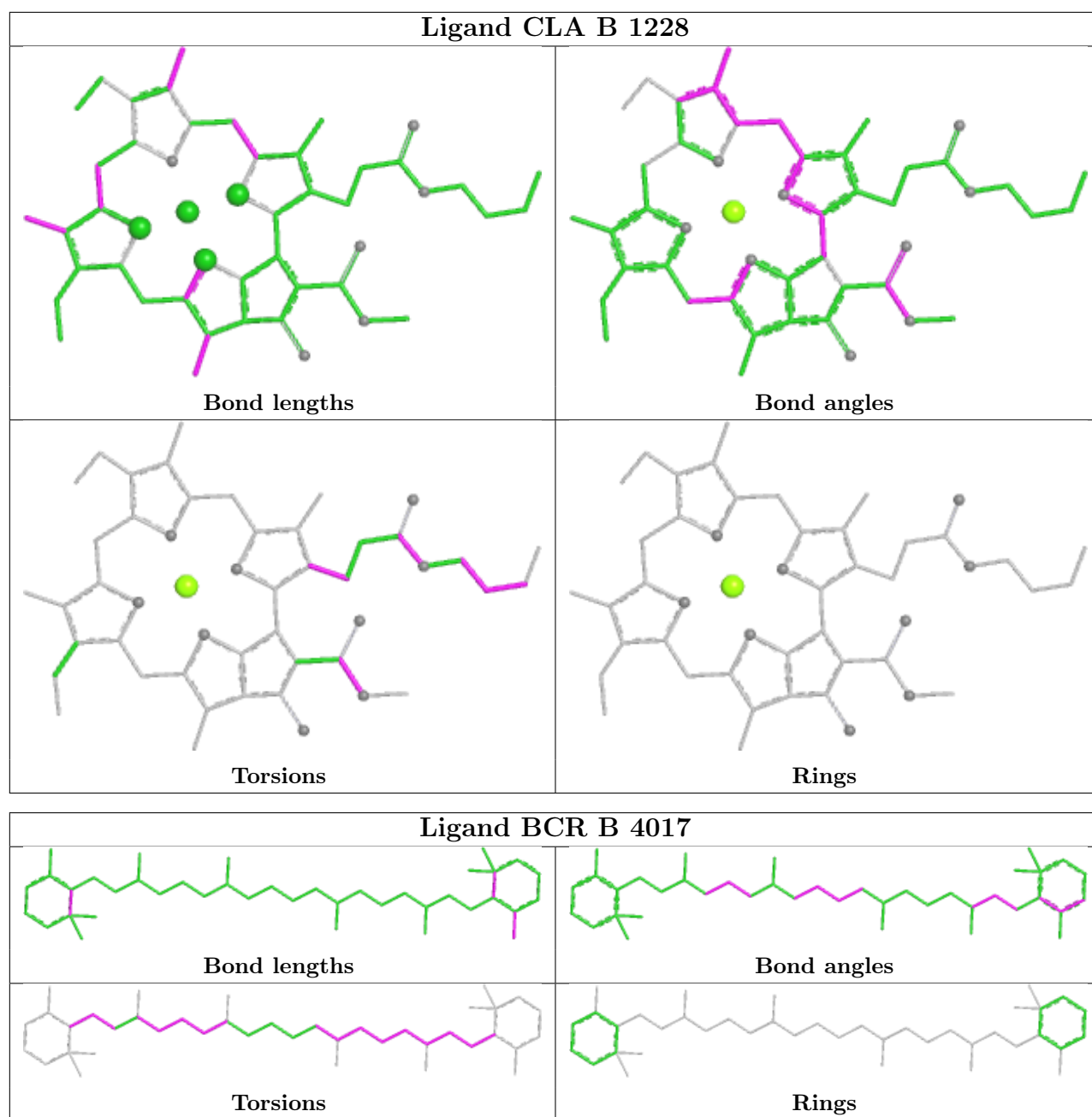
Ligand CLA 3 606

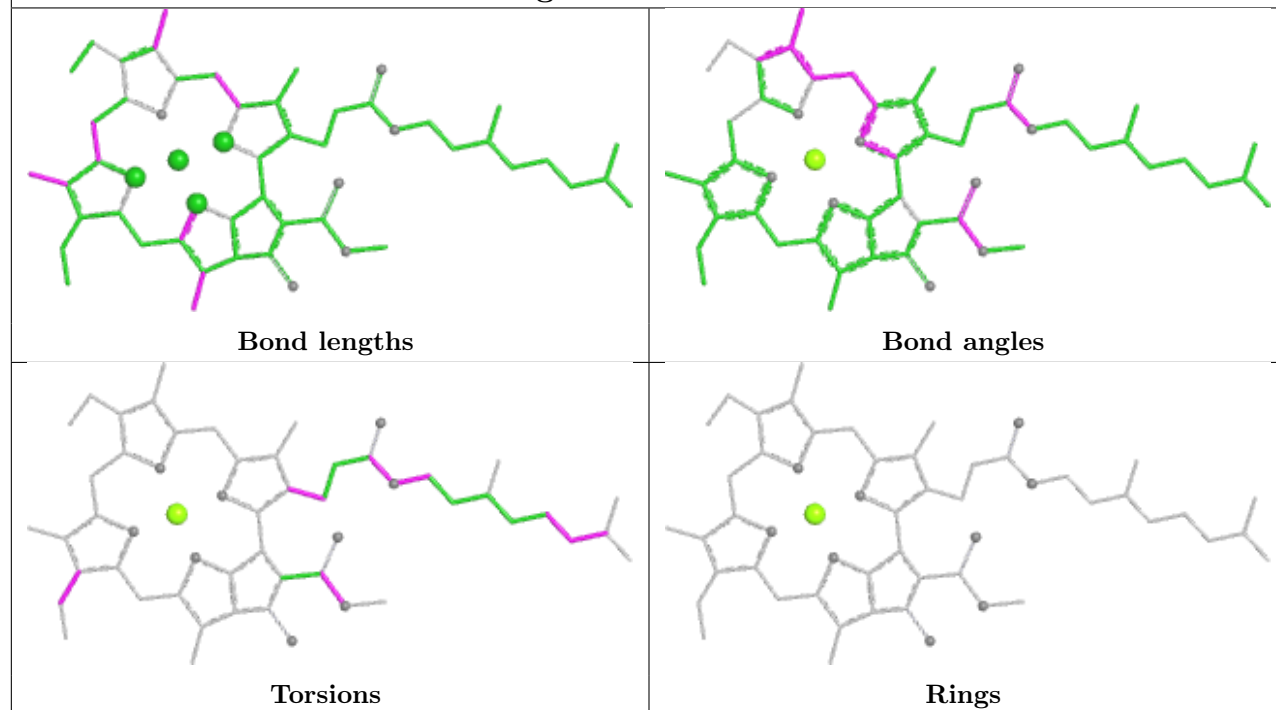
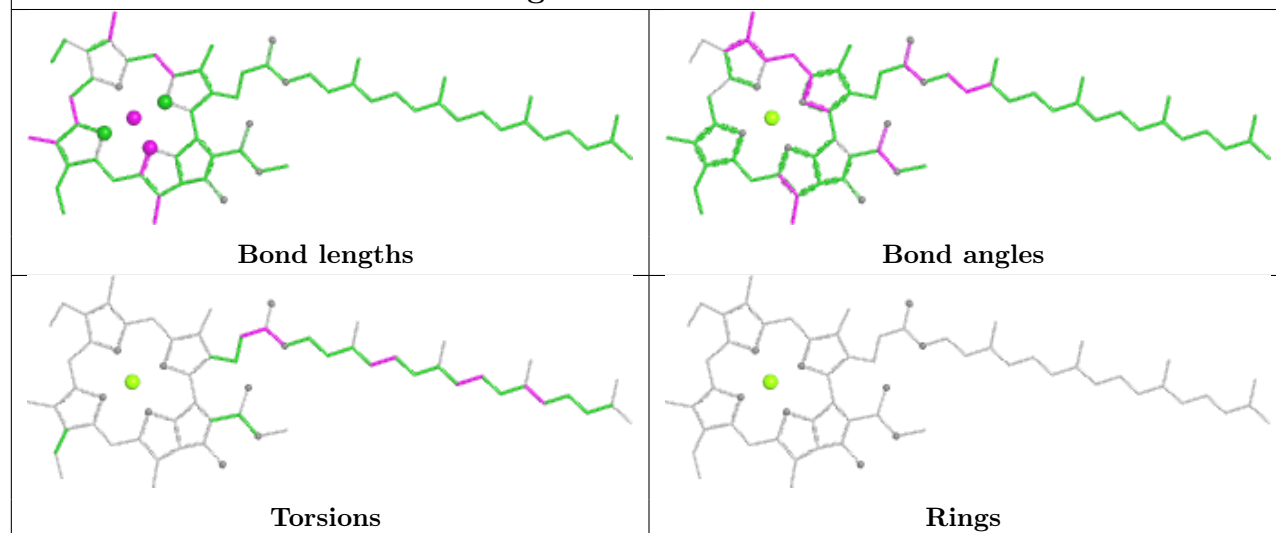


Ligand LMG A 5002

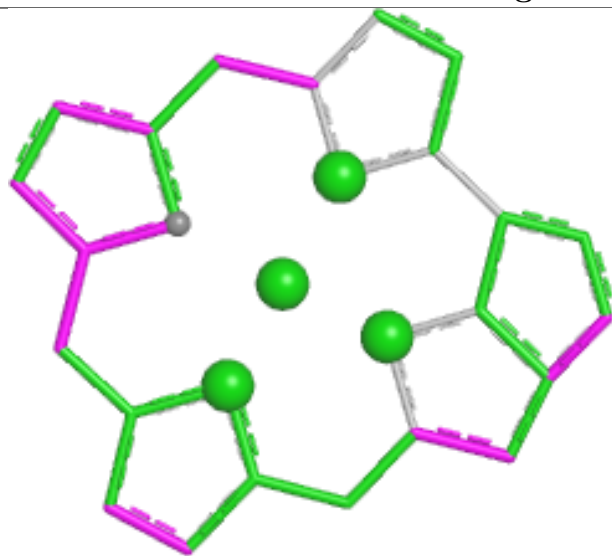




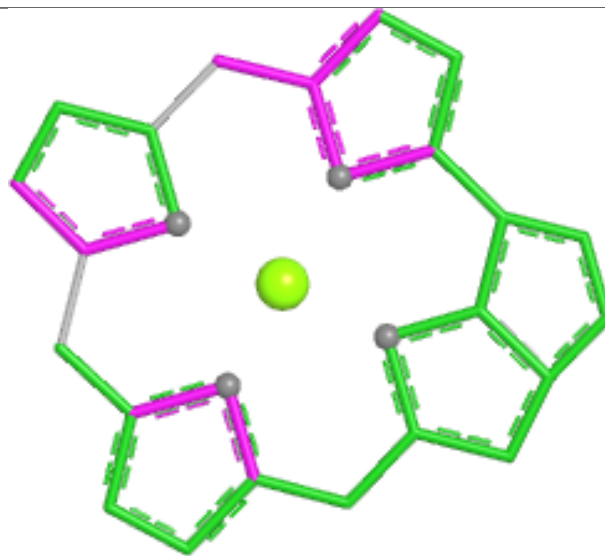


Ligand CLA 3 603**Ligand CL0 A 1011**

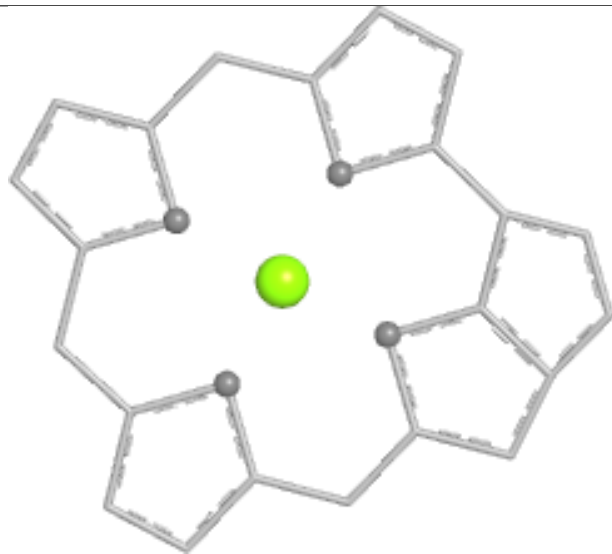
Ligand CLA F 303



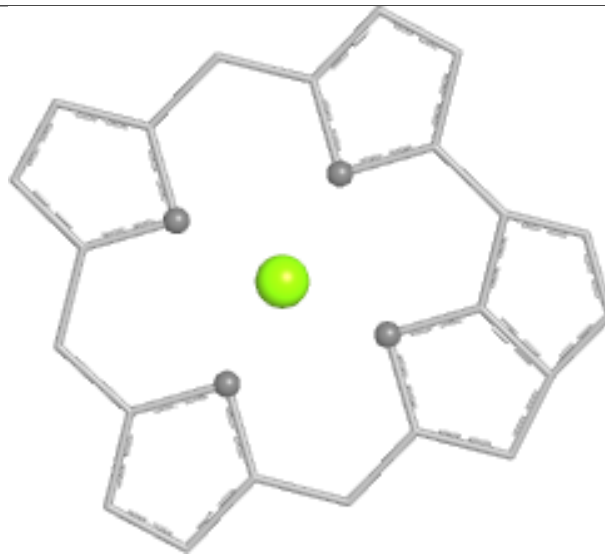
Bond lengths



Bond angles

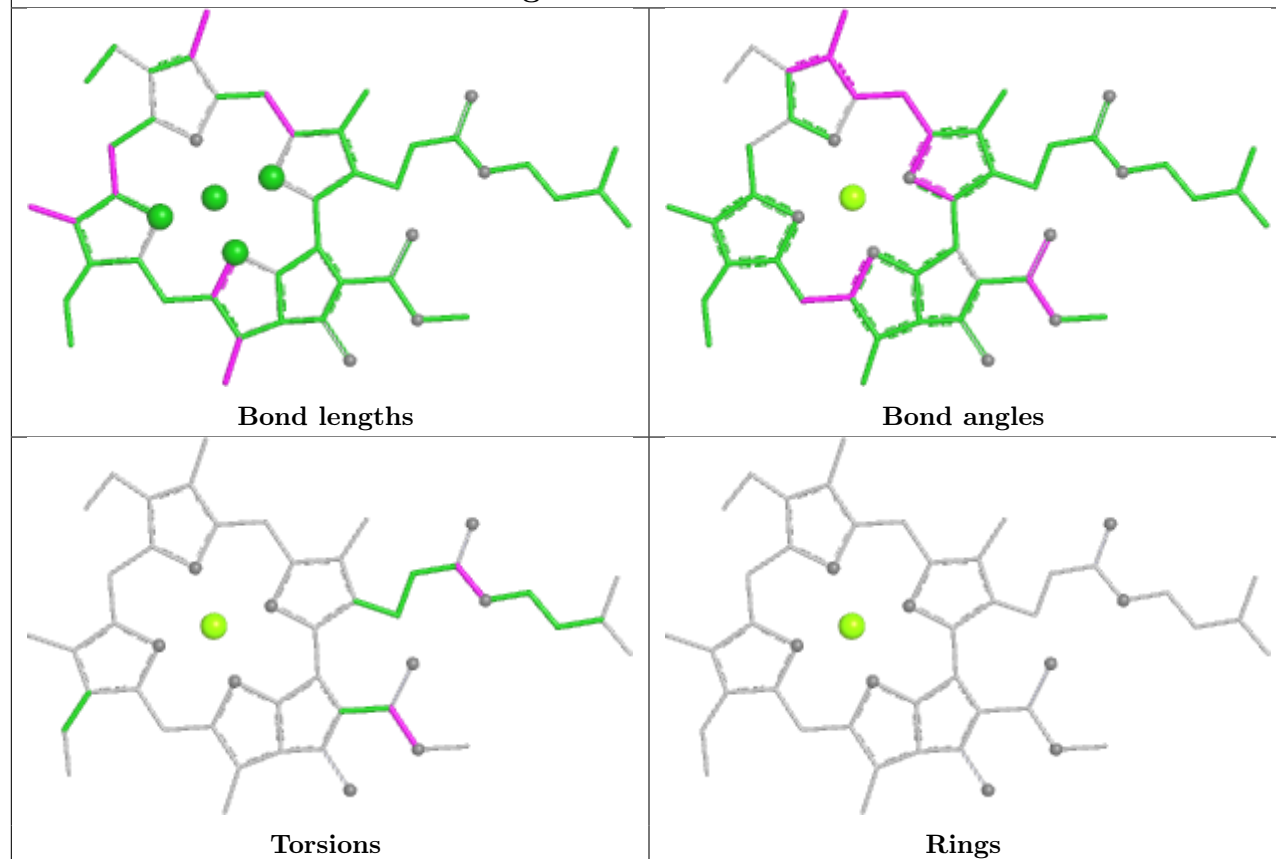


Torsions

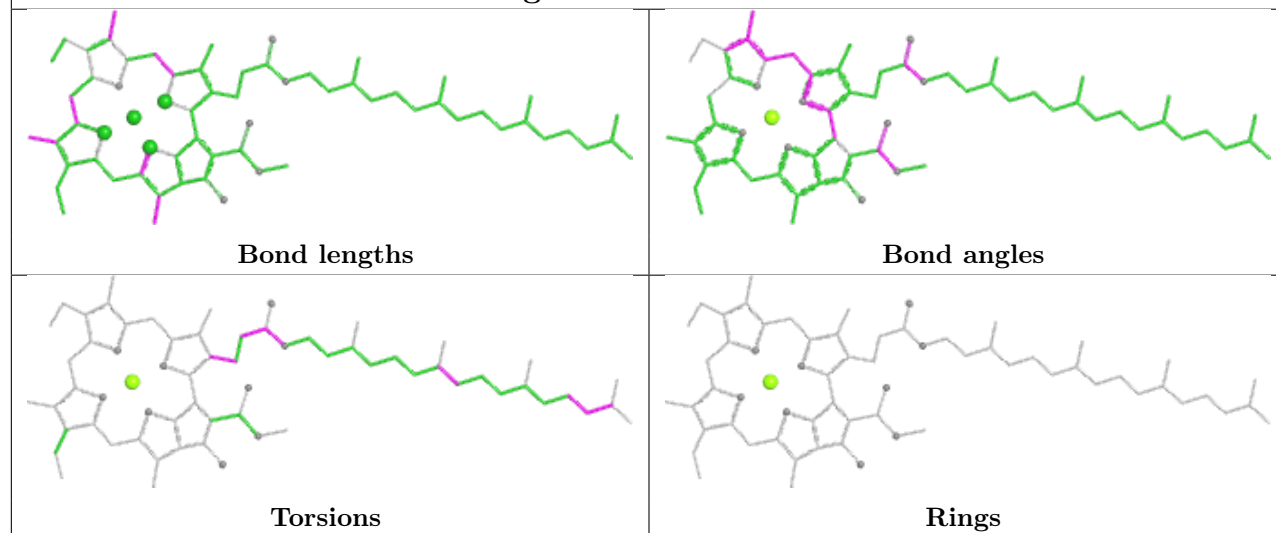


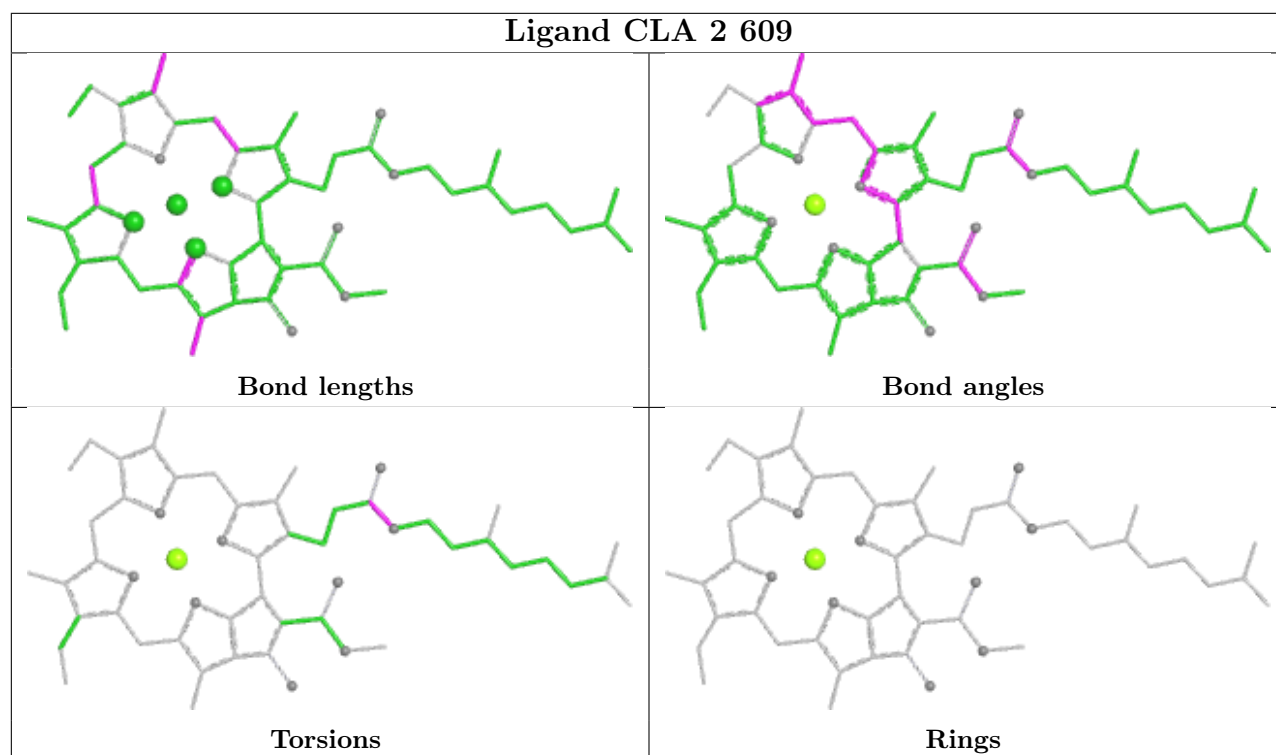
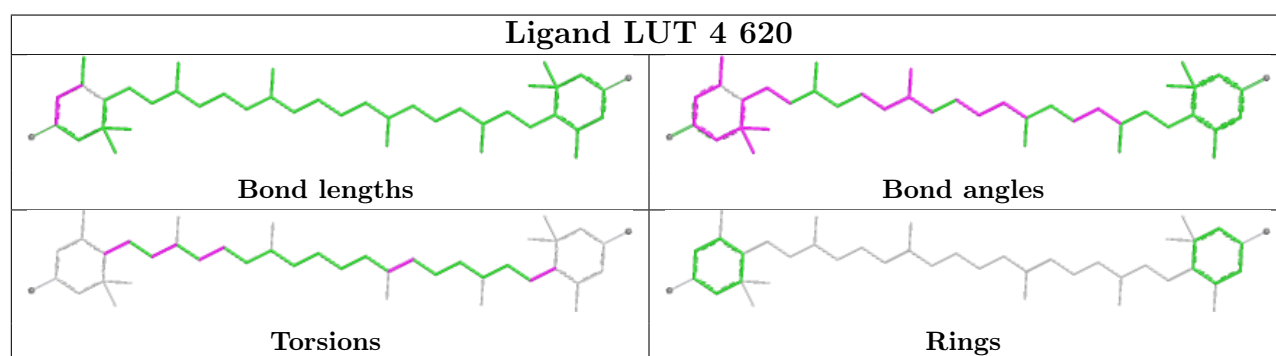
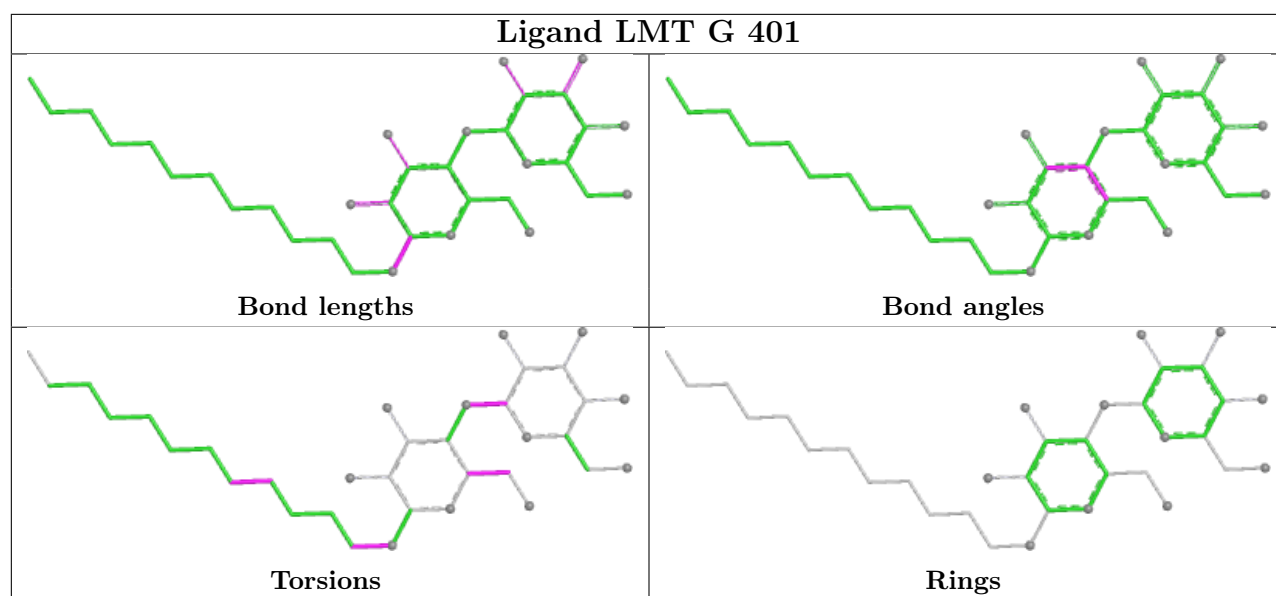
Rings

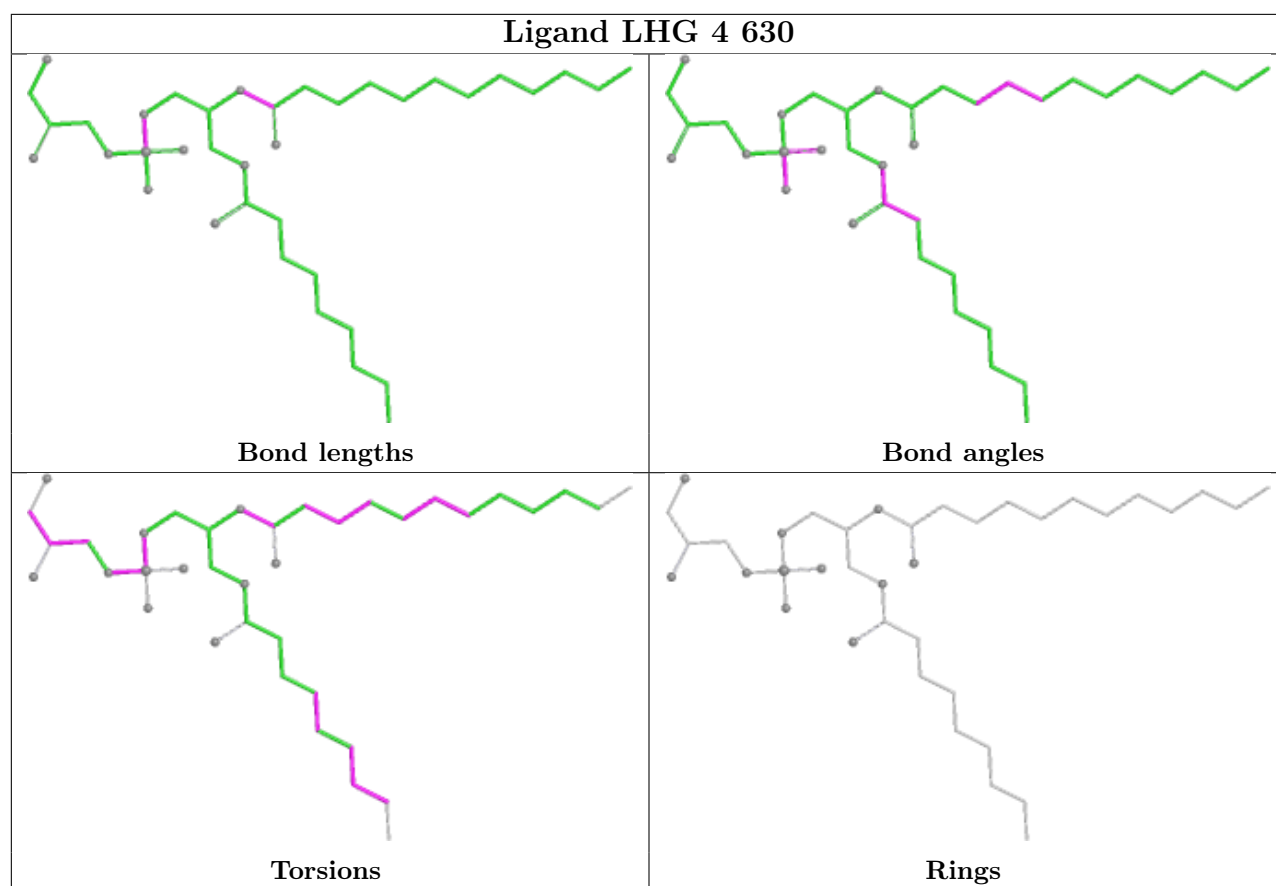
Ligand CLA A 1139



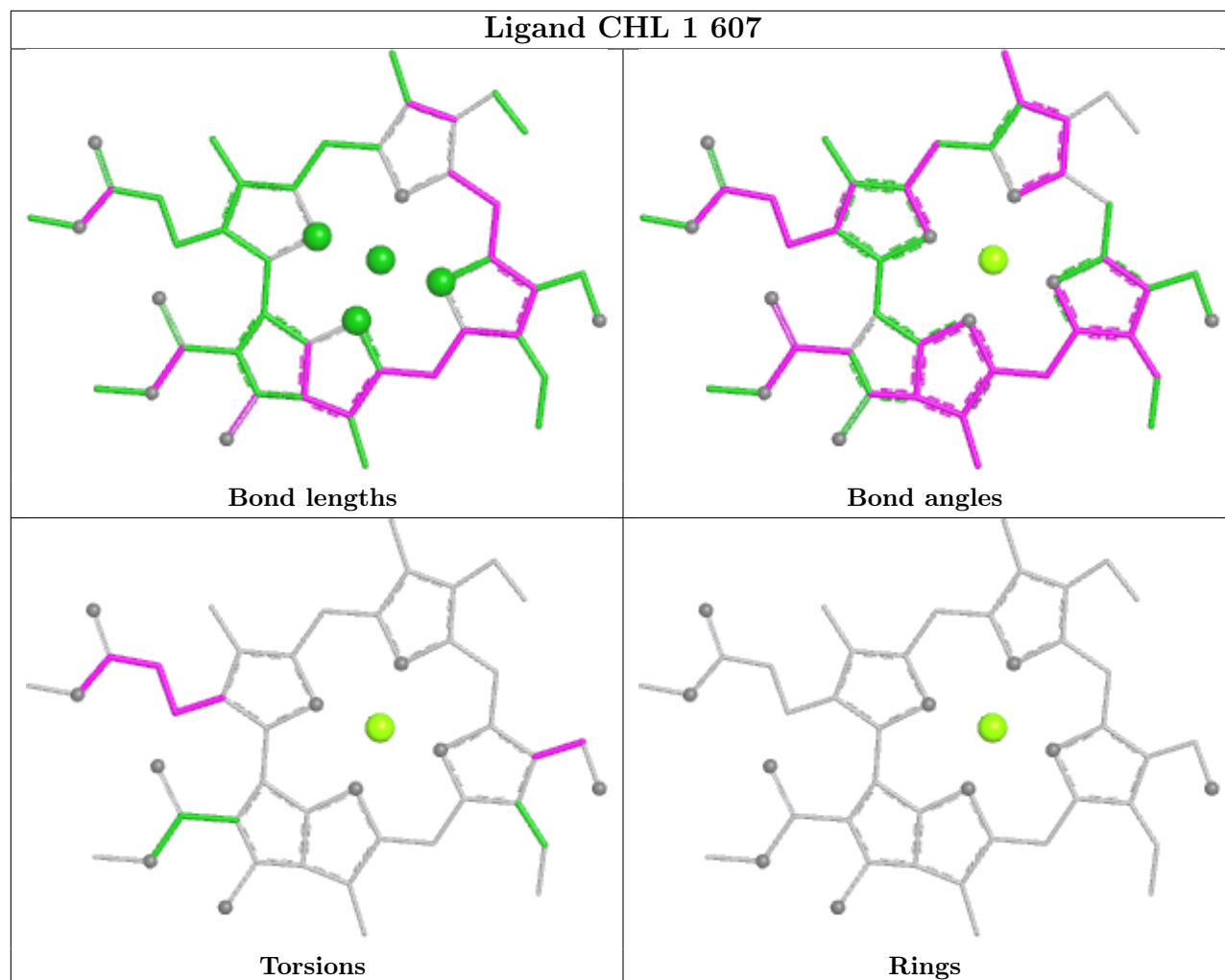
Ligand CLA B 1202



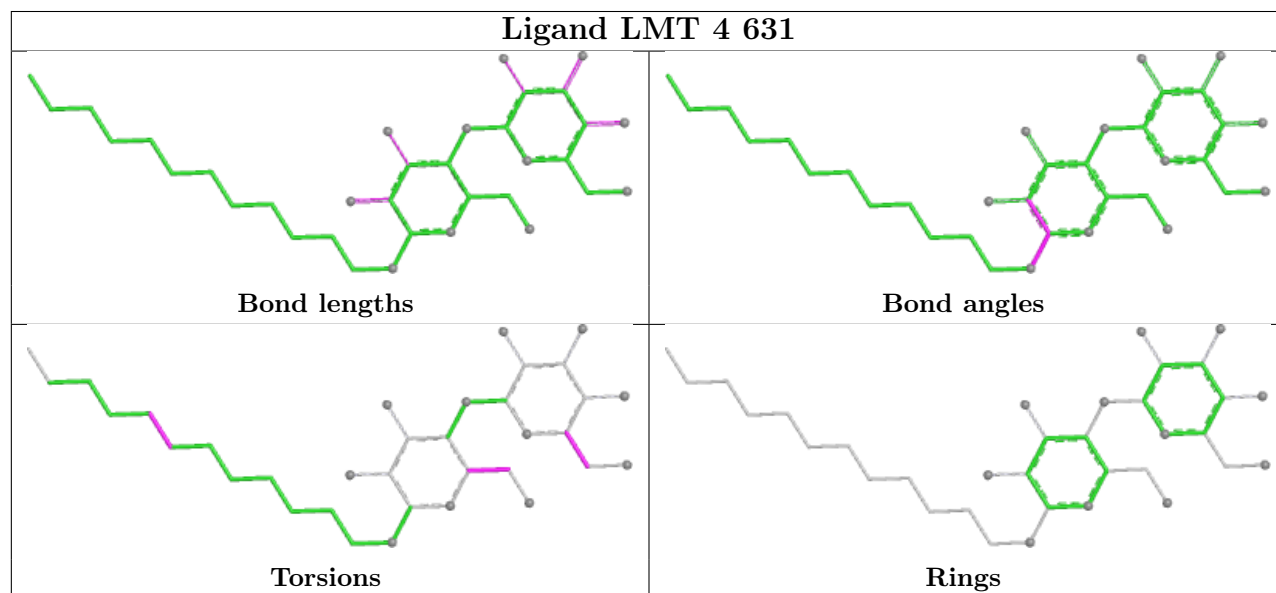


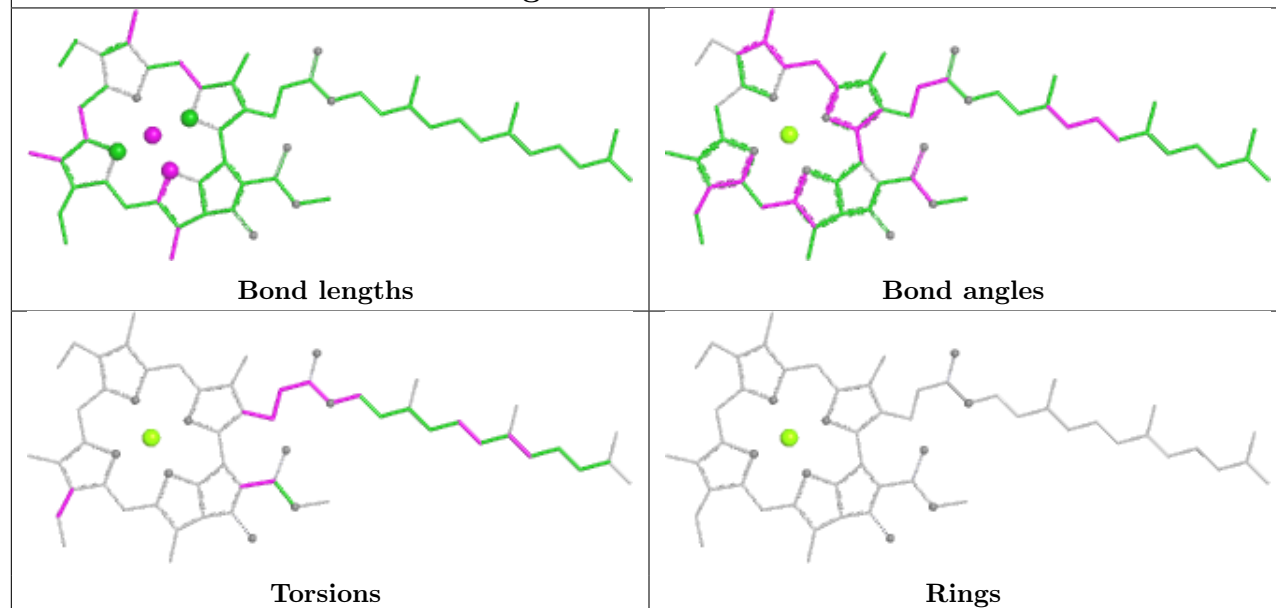
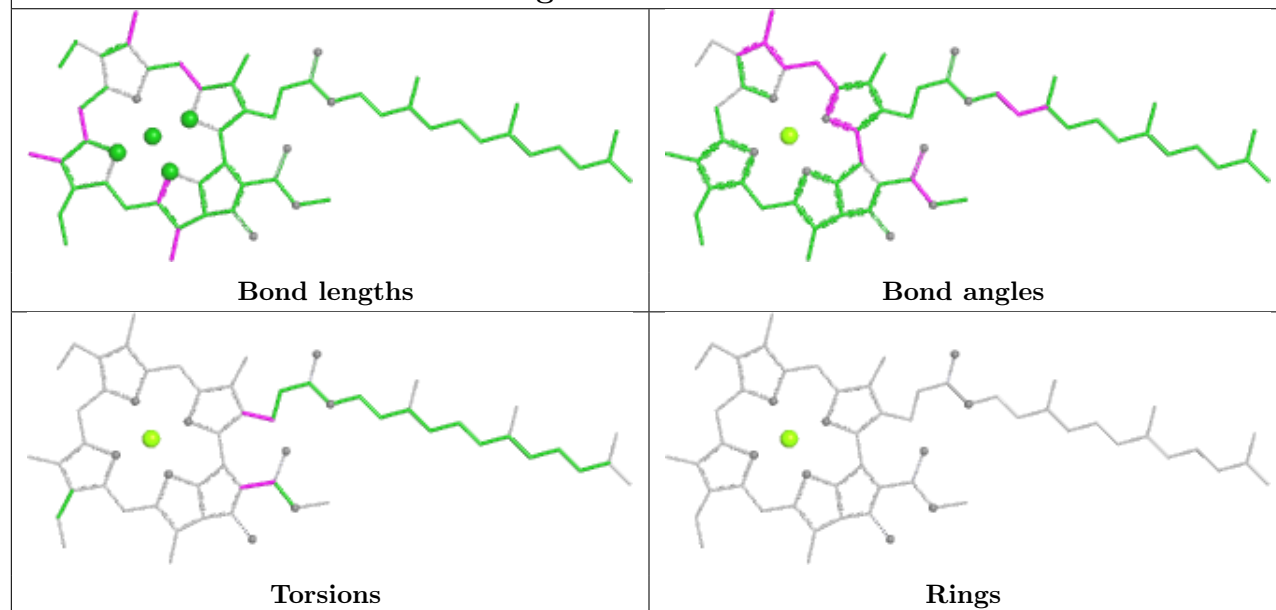


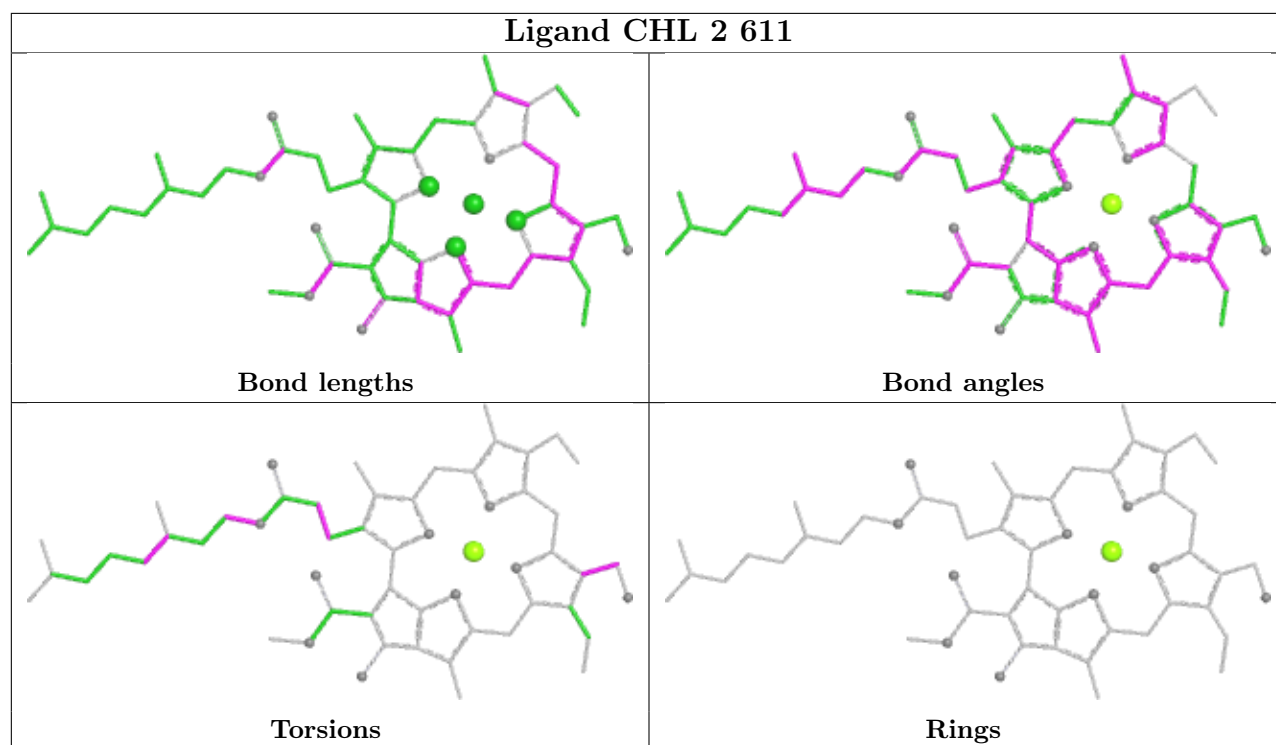
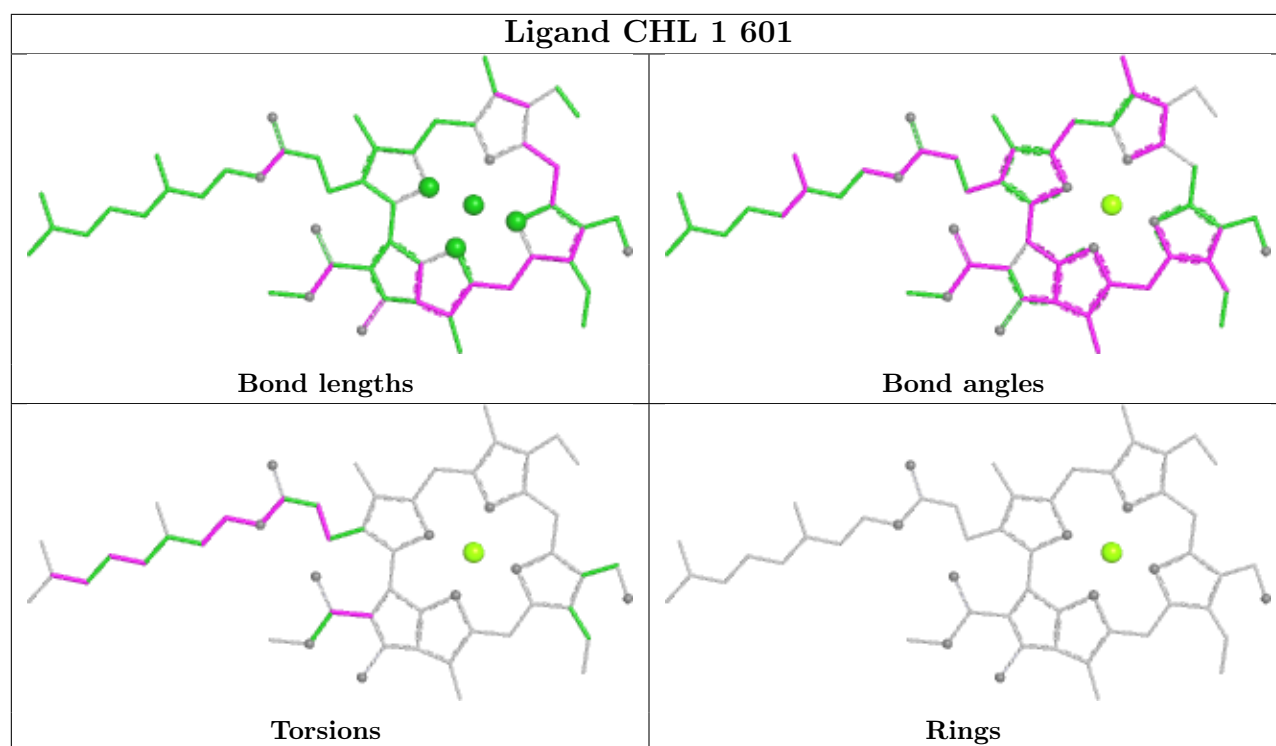
Ligand CHL 1 607



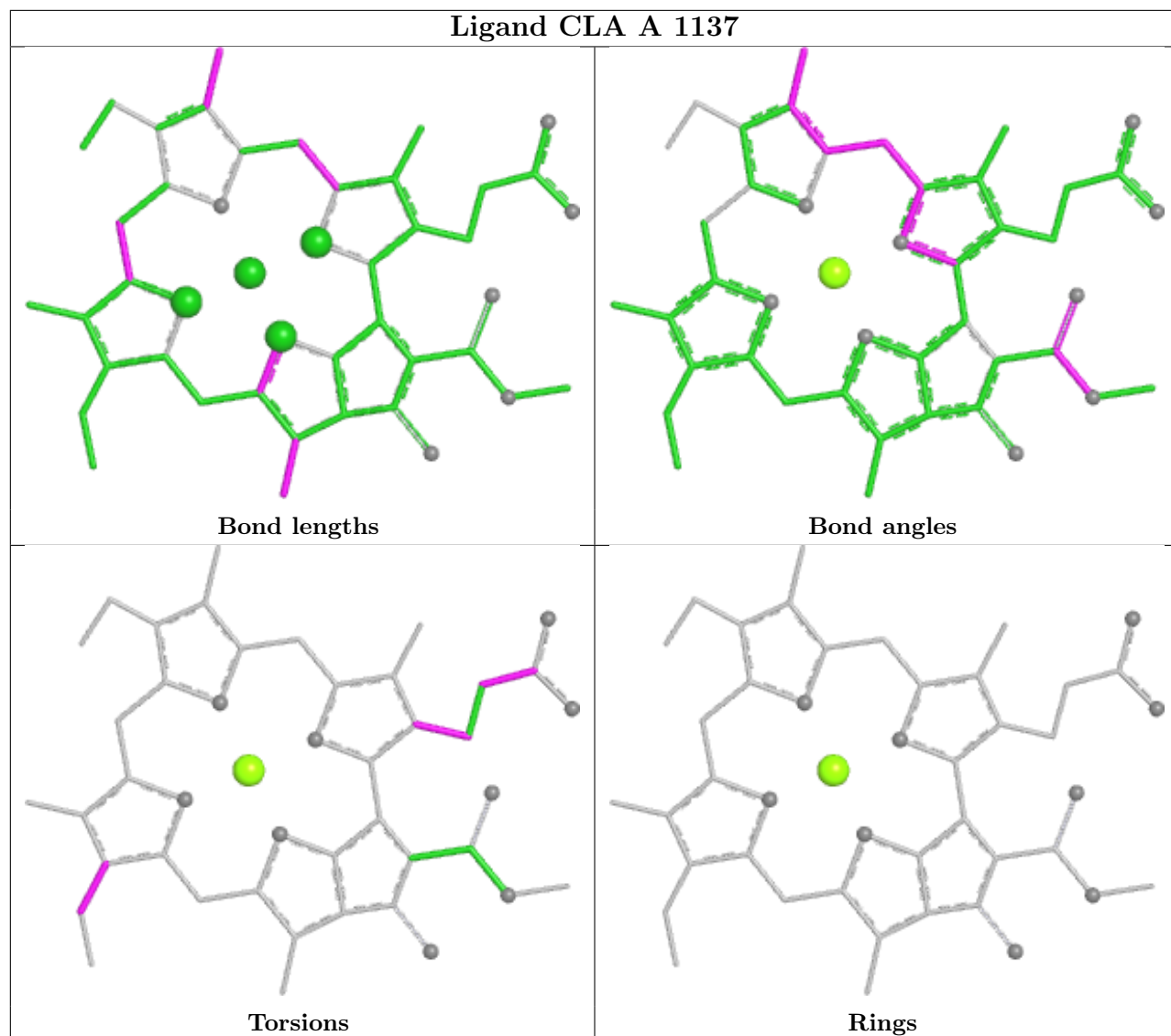
Ligand LMT 4 631



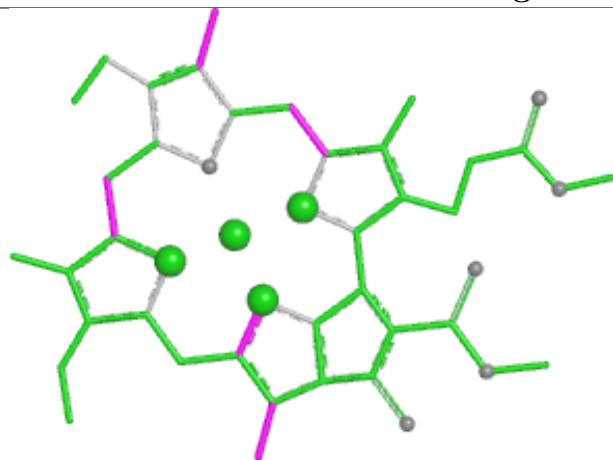
Ligand CLA A 1125**Ligand CLA 1 602**



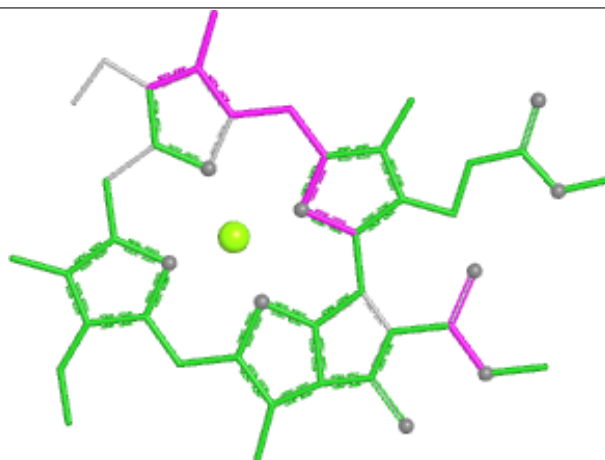
Ligand CLA A 1137



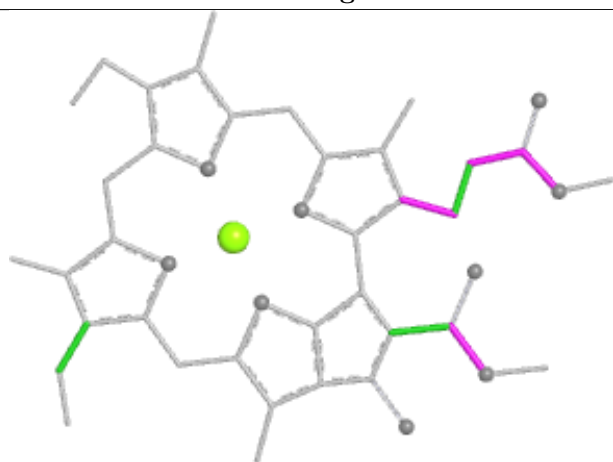
Ligand CLA G 202



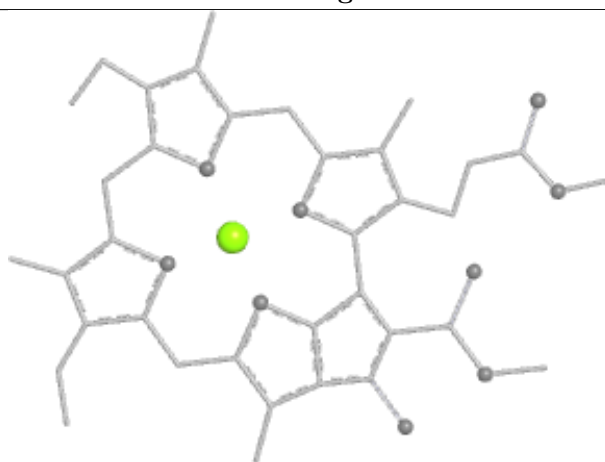
Bond lengths



Bond angles

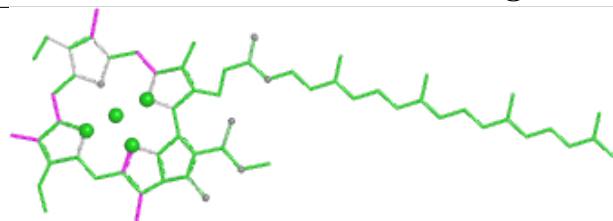


Torsions

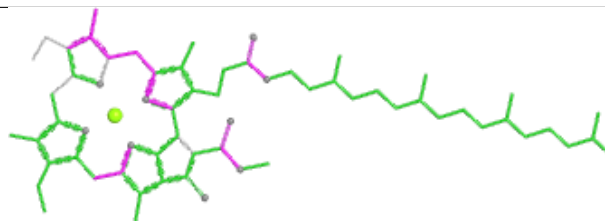


Rings

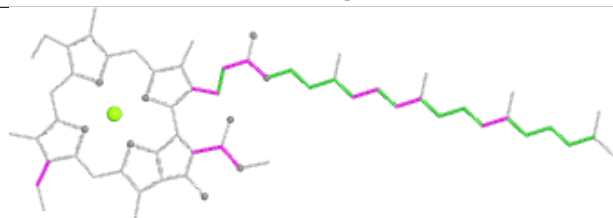
Ligand CLA A 1103



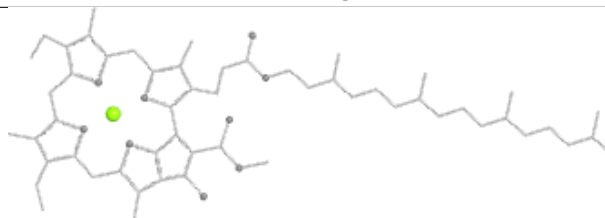
Bond lengths



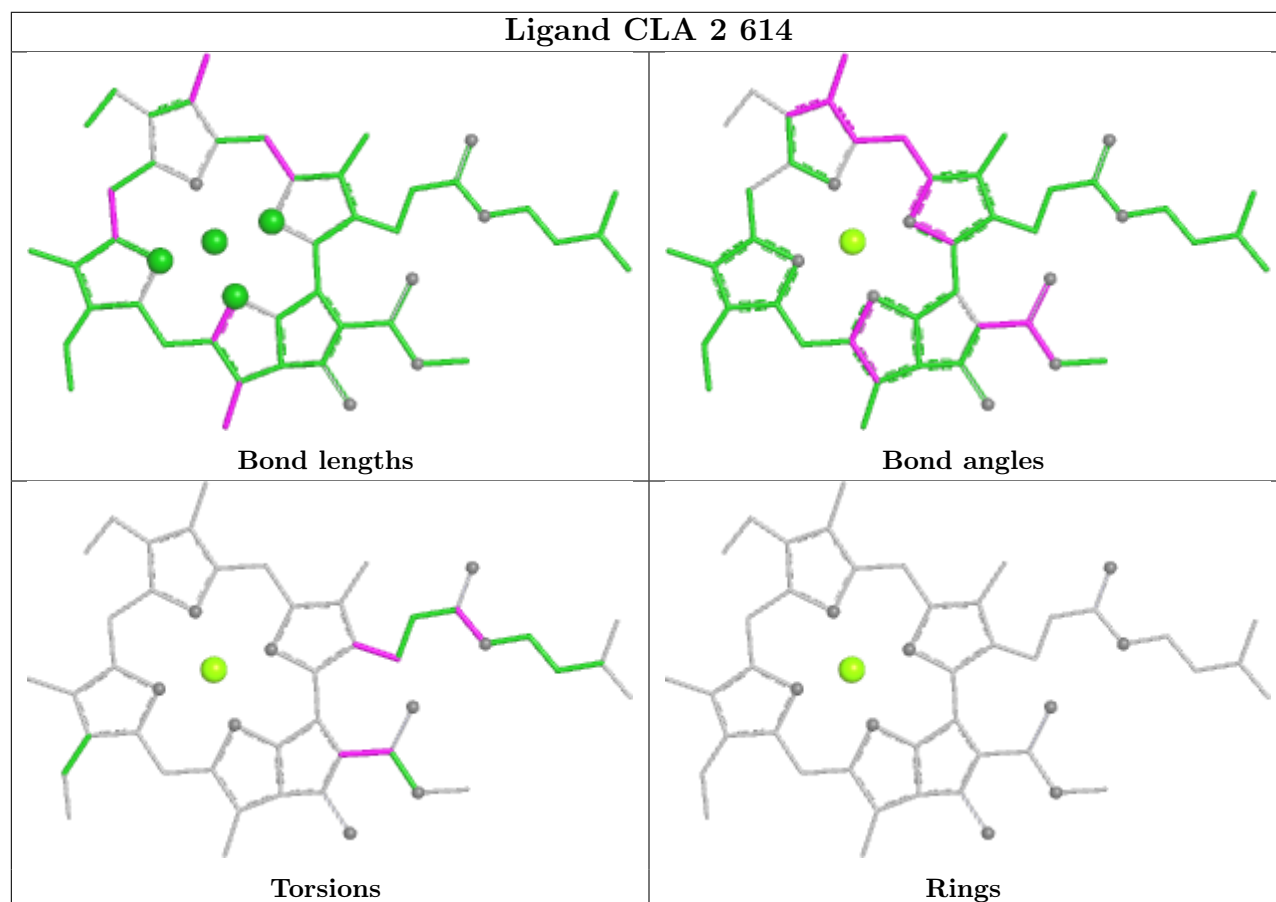
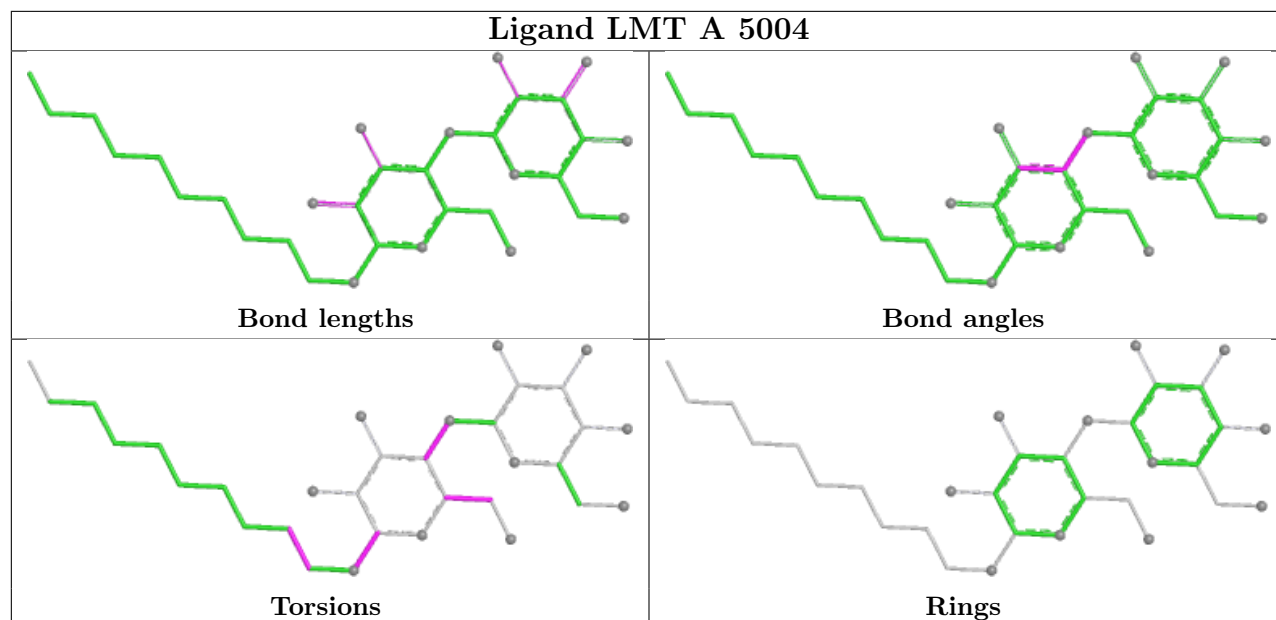
Bond angles

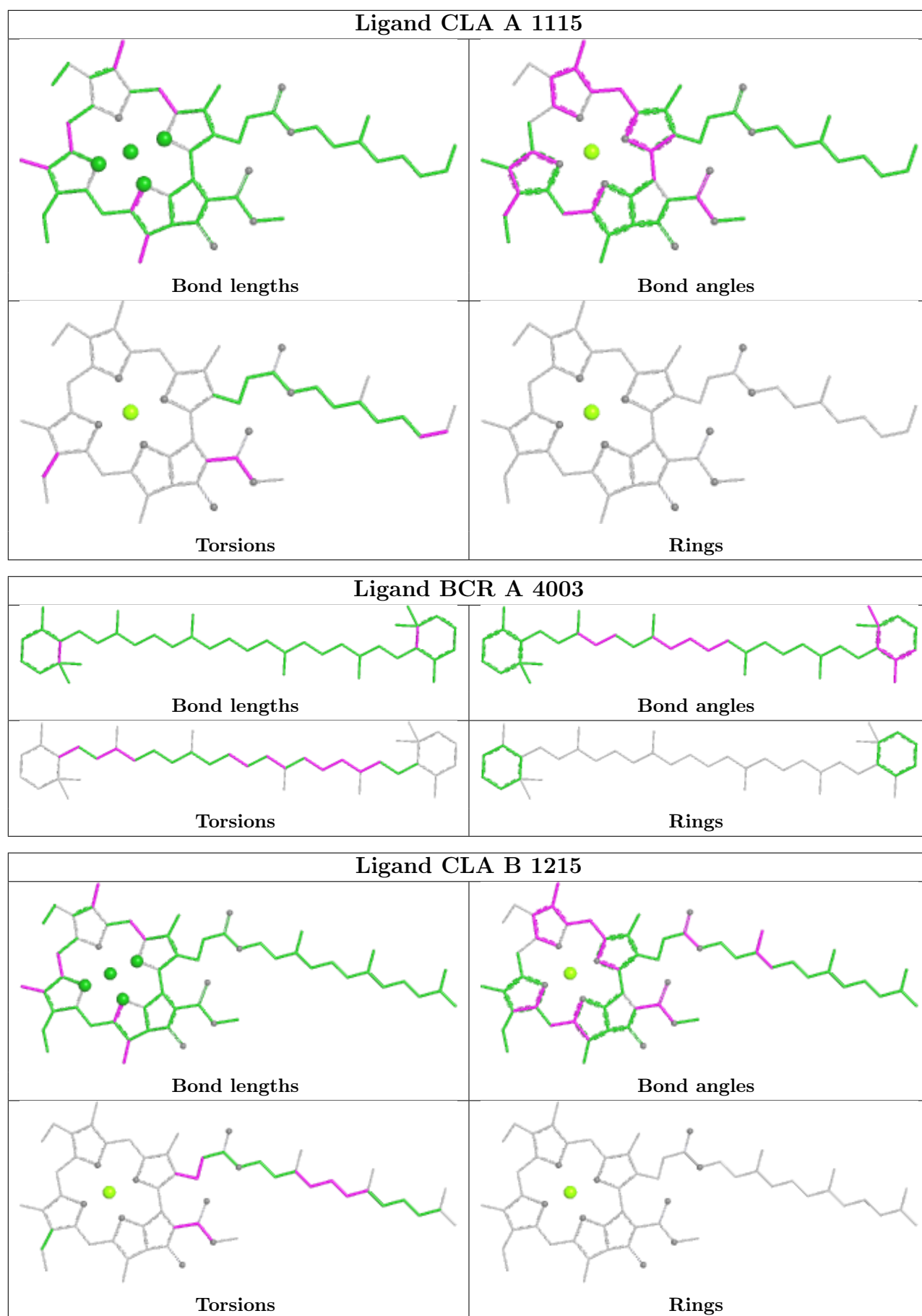


Torsions

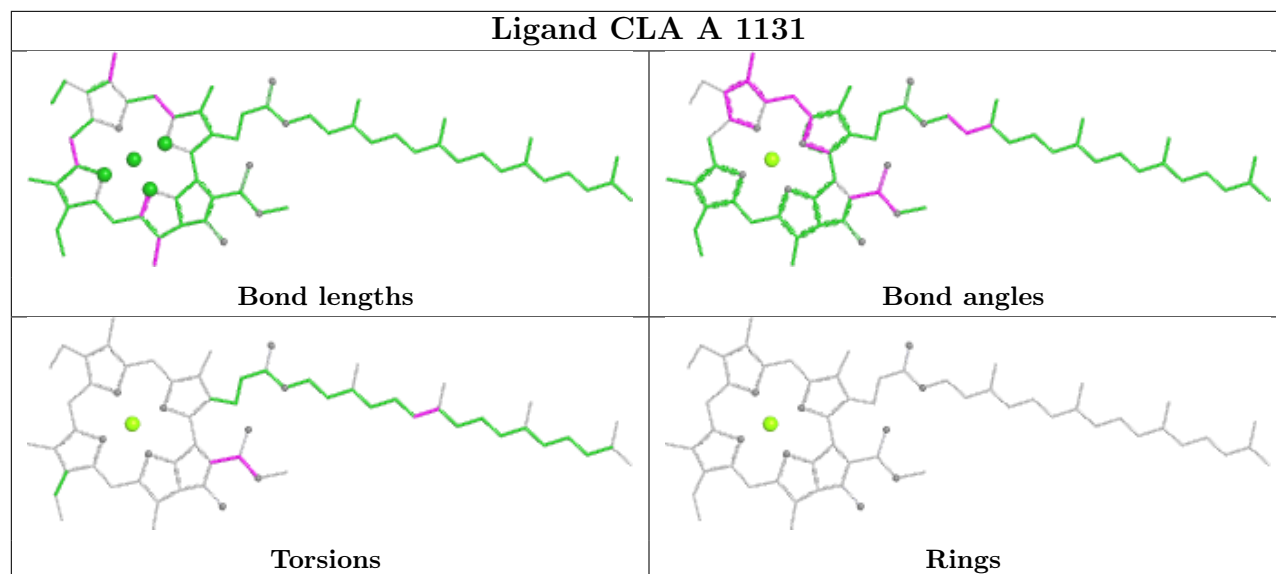


Rings

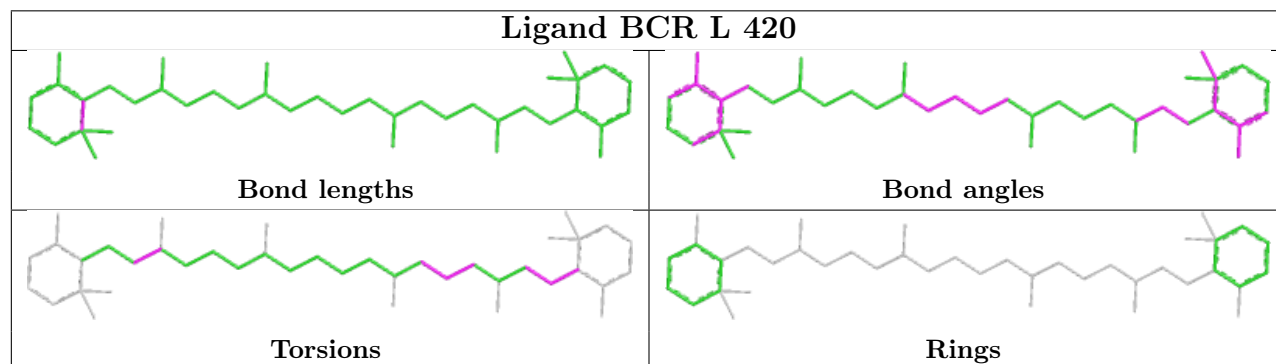




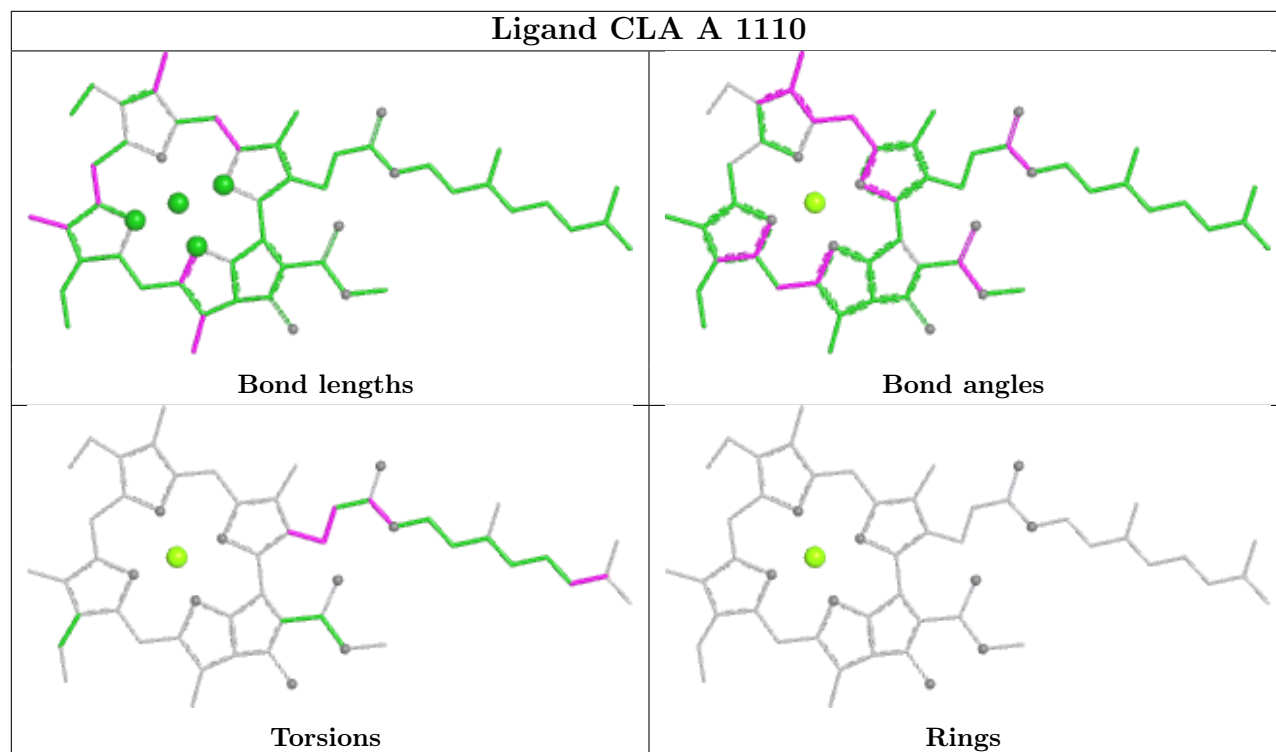
Ligand CLA A 1131

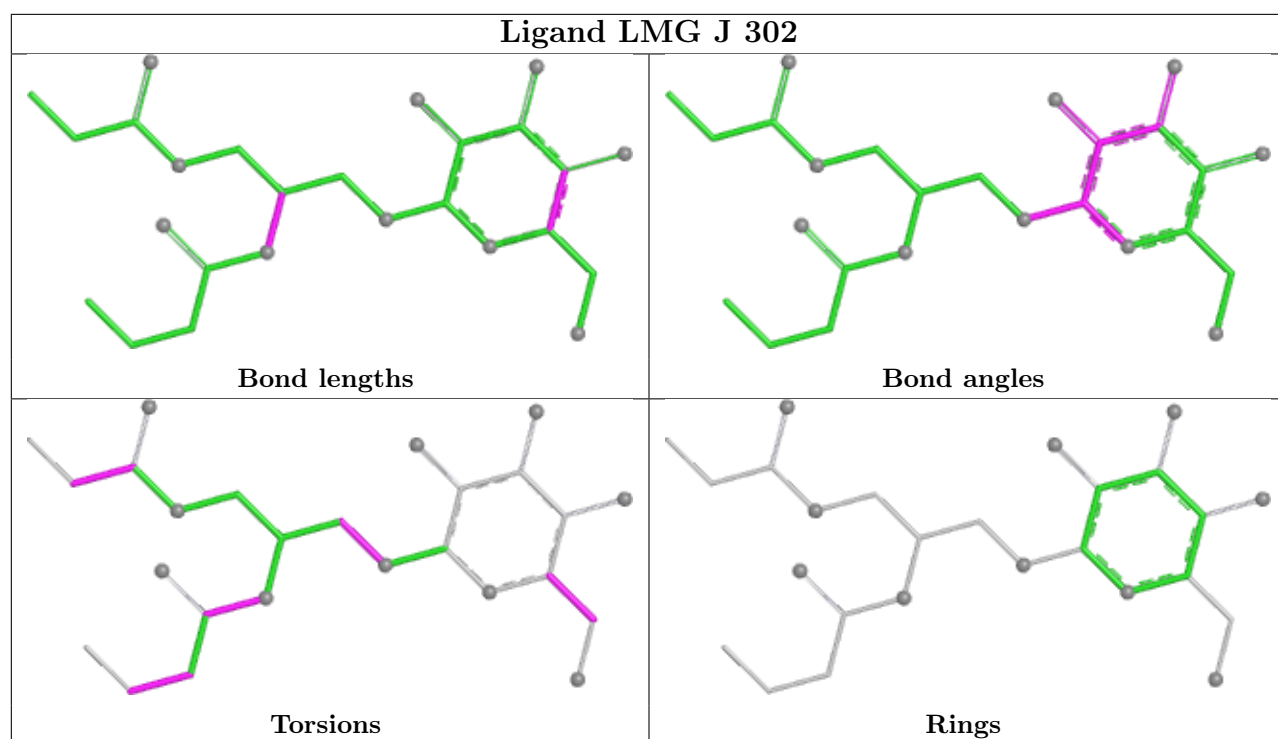


Ligand BCR L 420

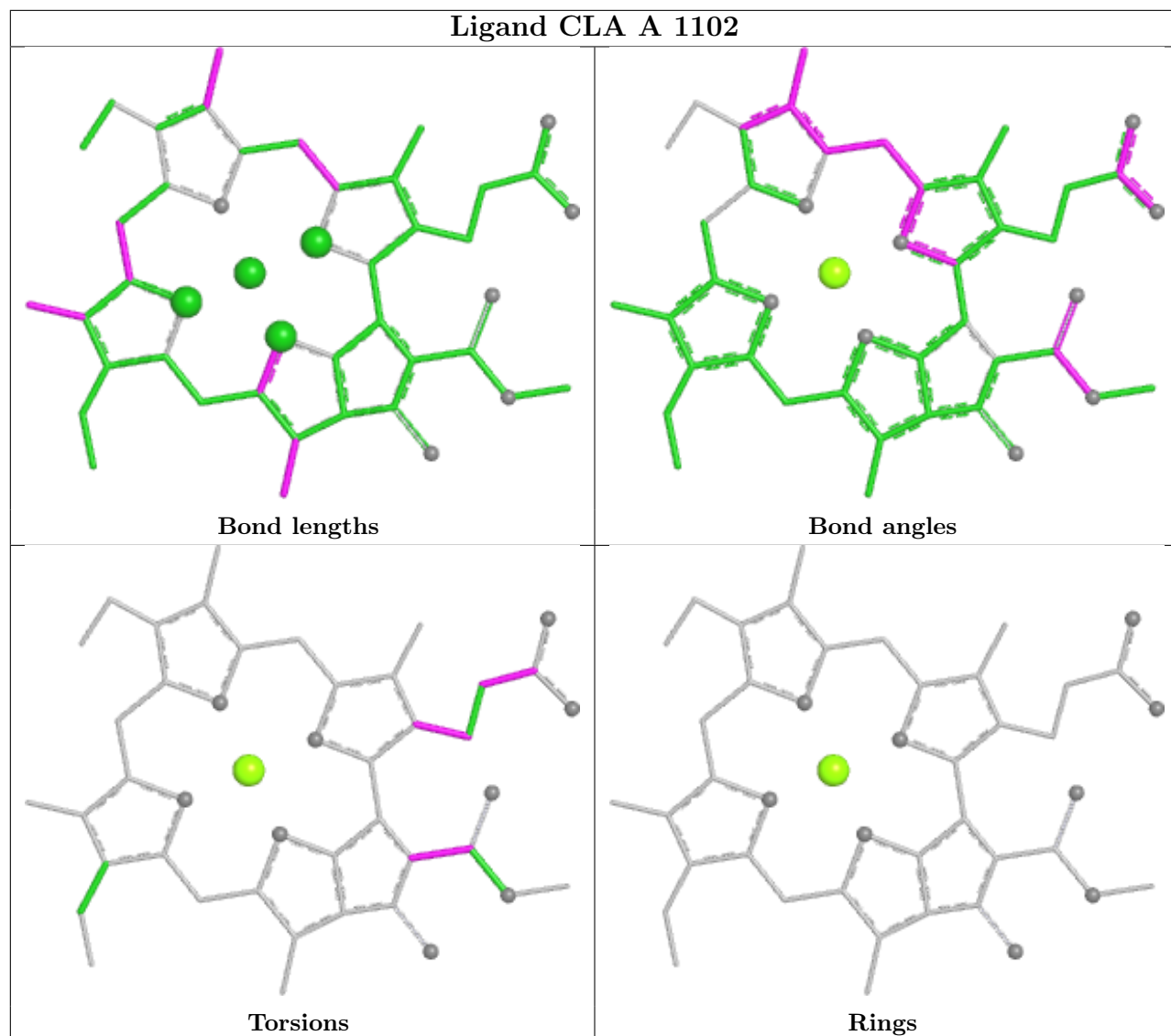


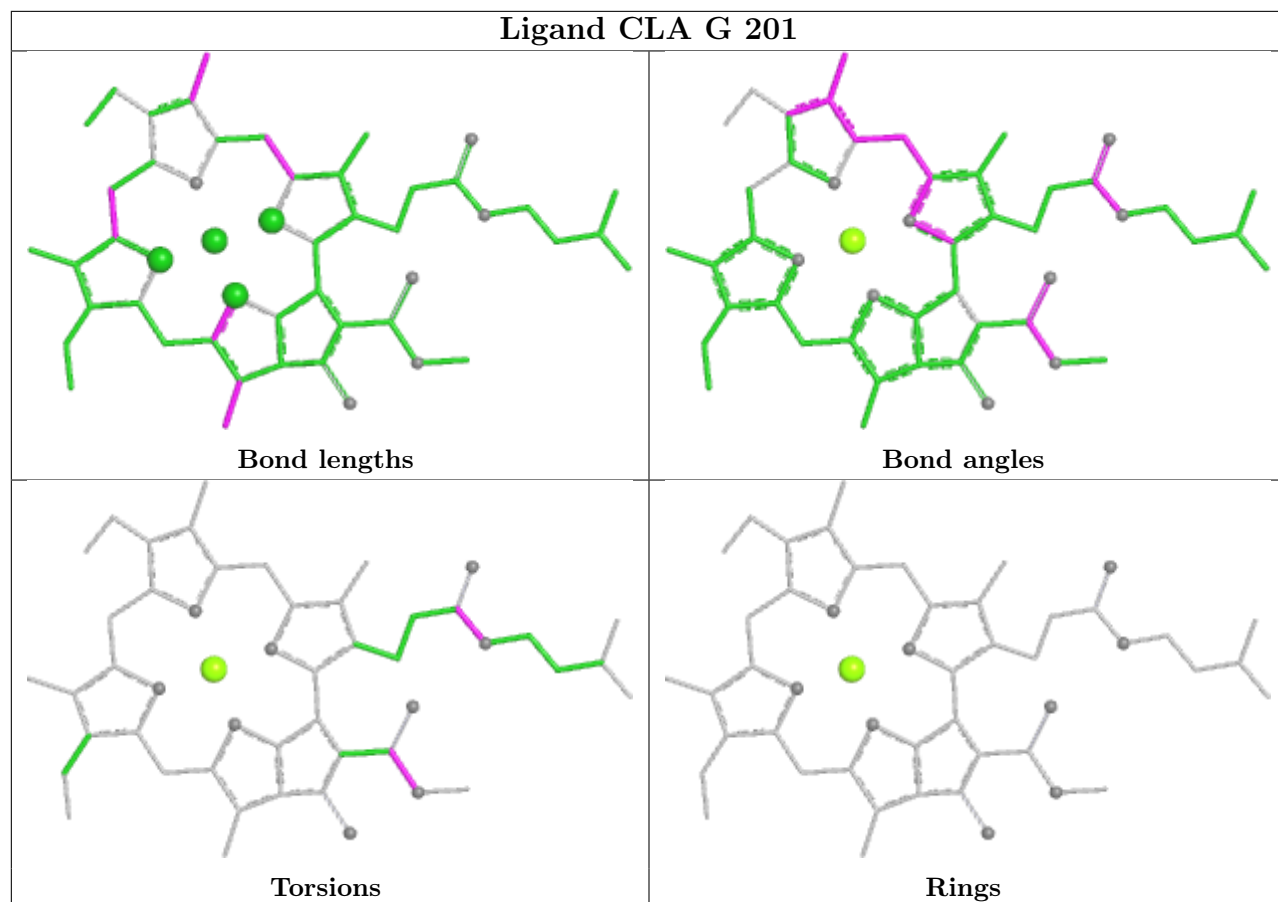
Ligand CLA A 1110

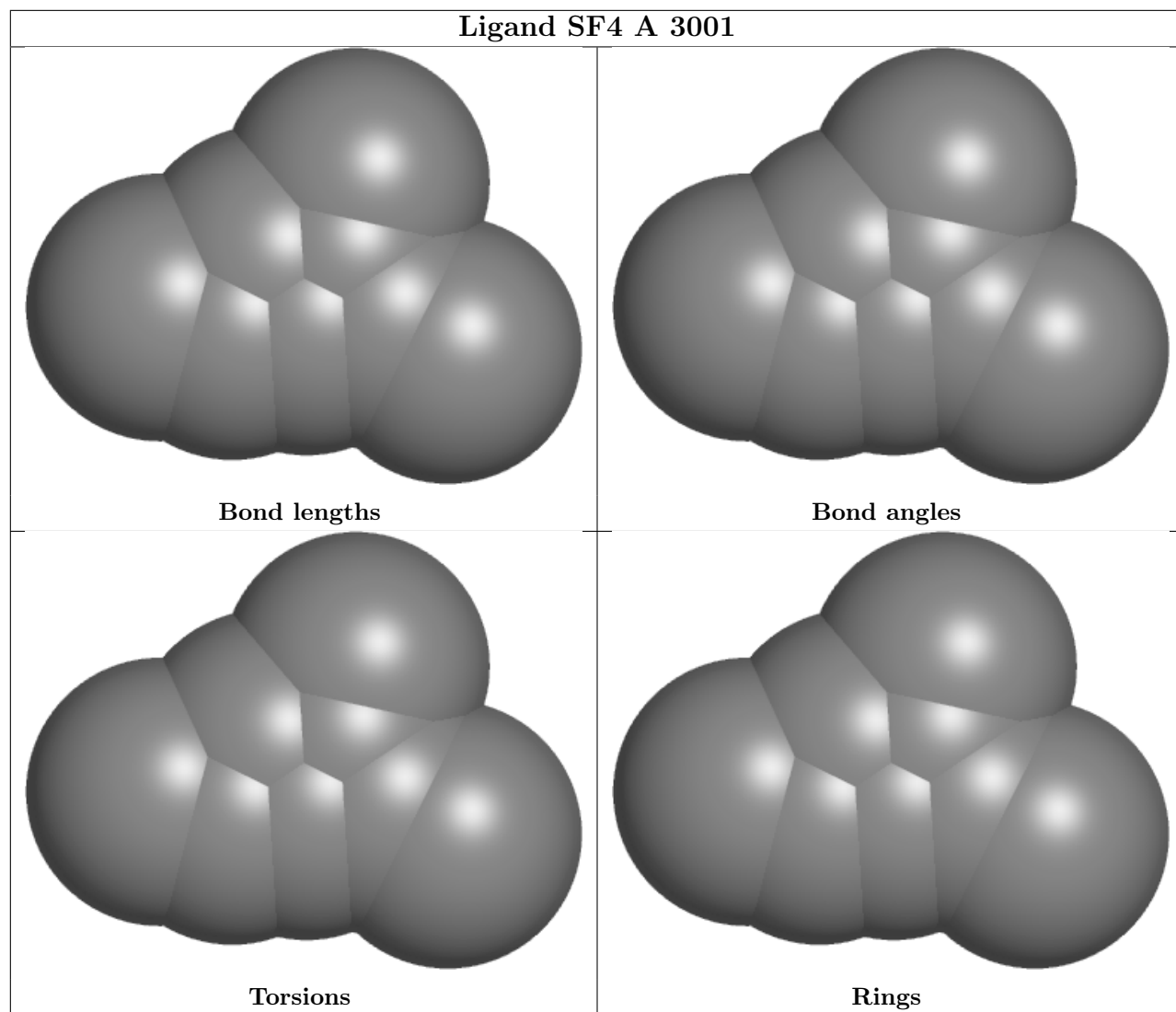




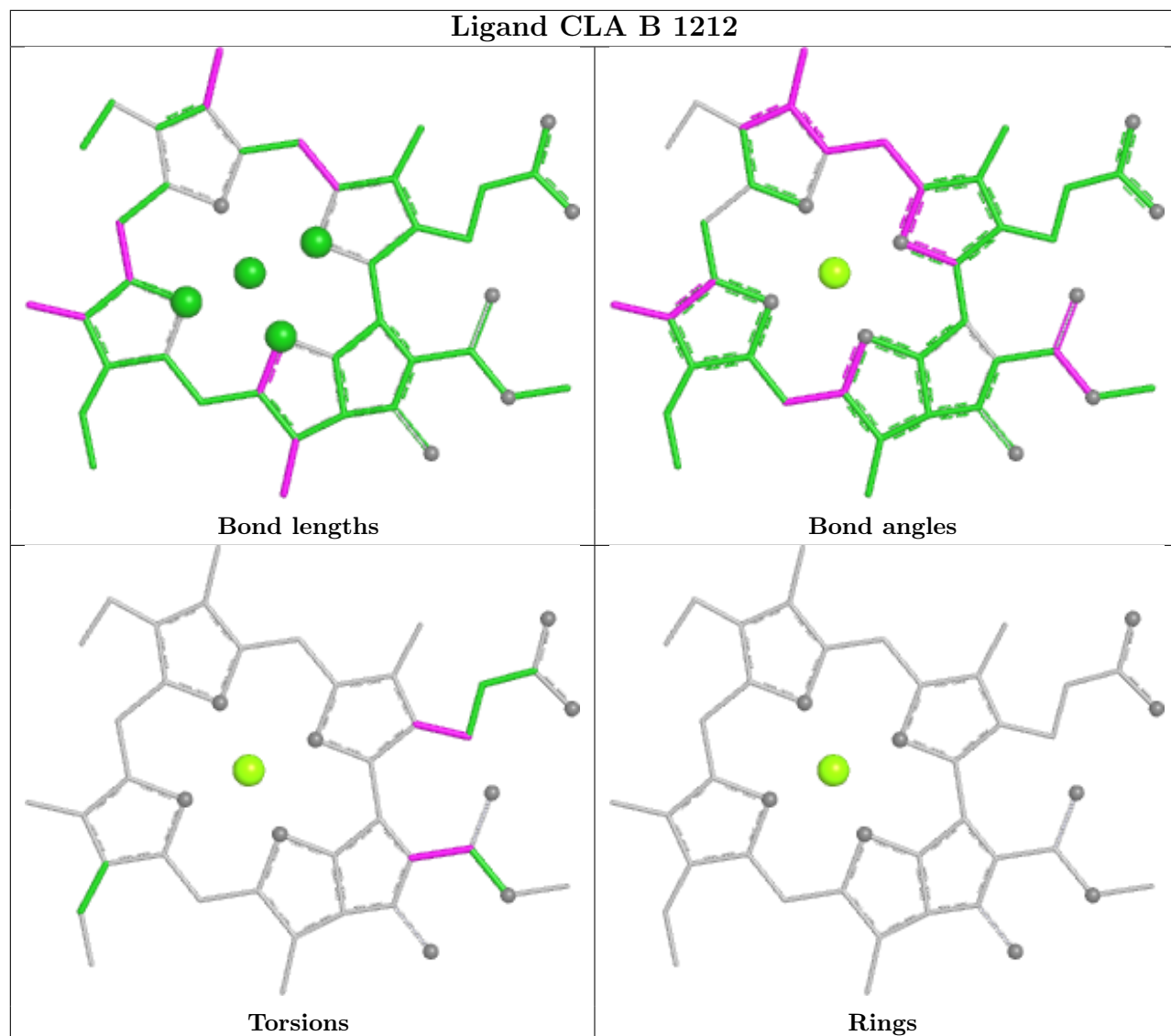
Ligand CLA A 1102



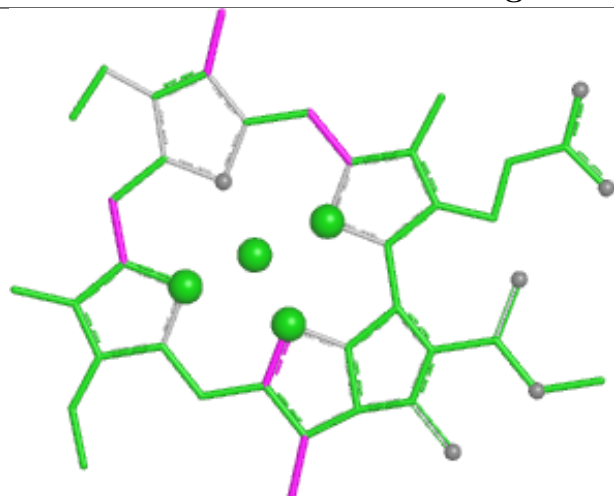




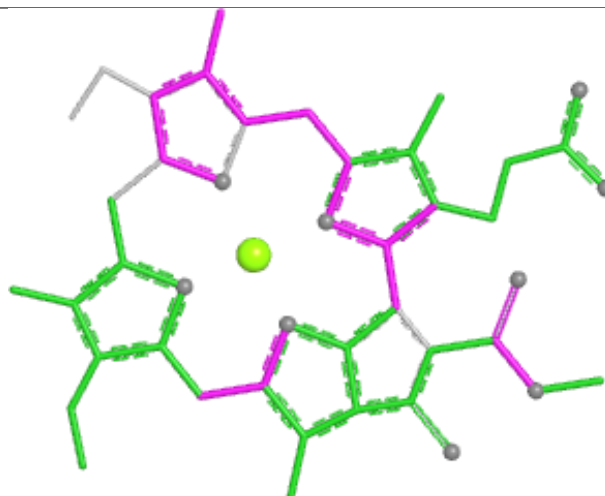
Ligand CLA B 1212



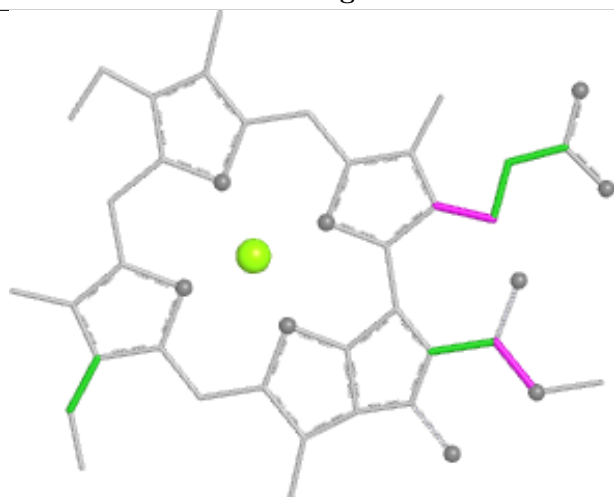
Ligand CLA B 1232



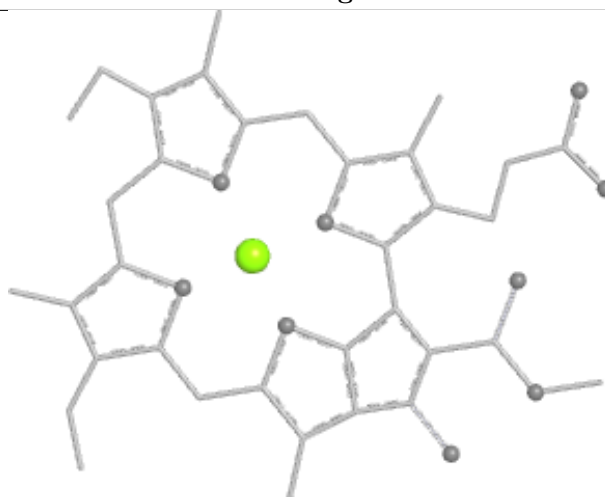
Bond lengths



Bond angles

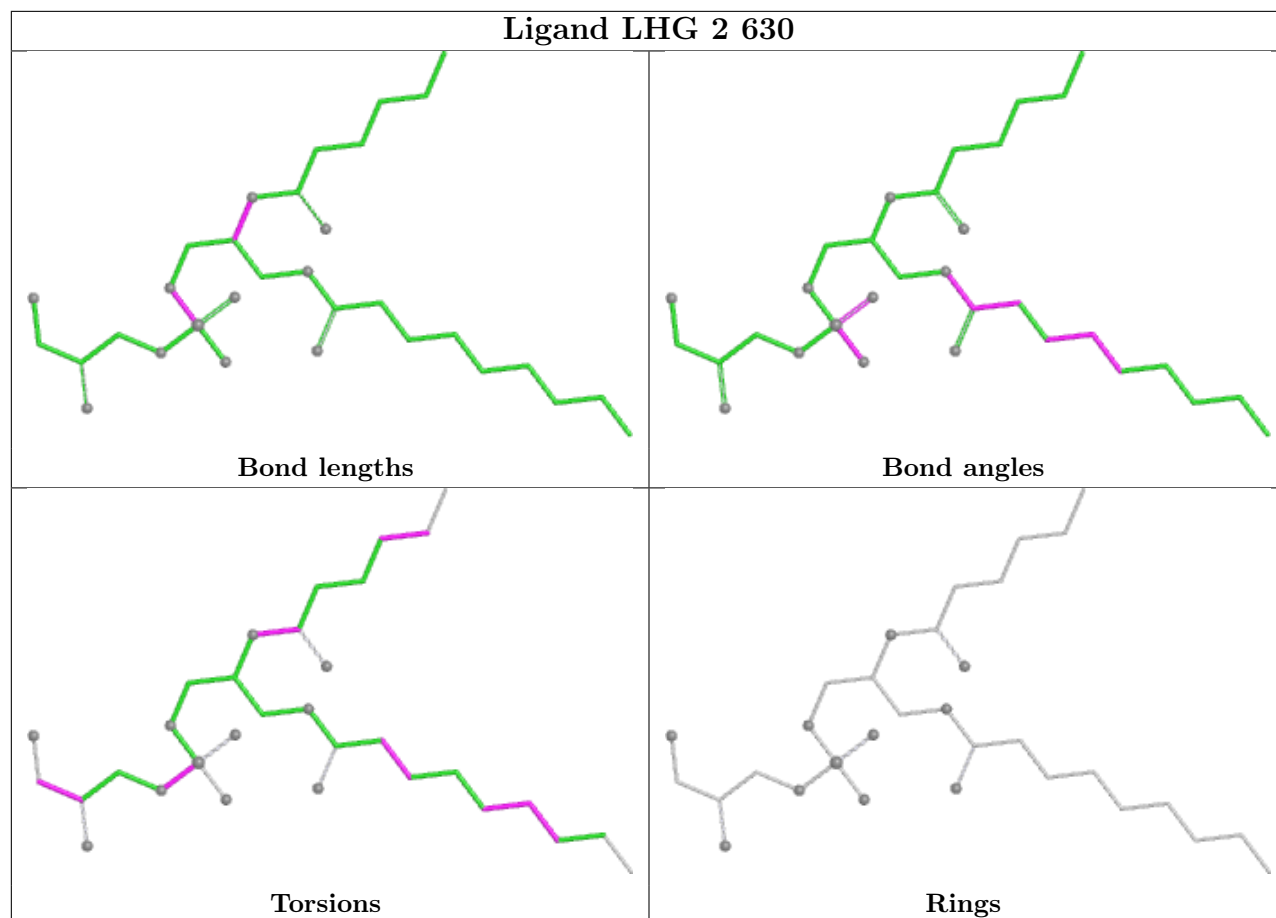


Torsions

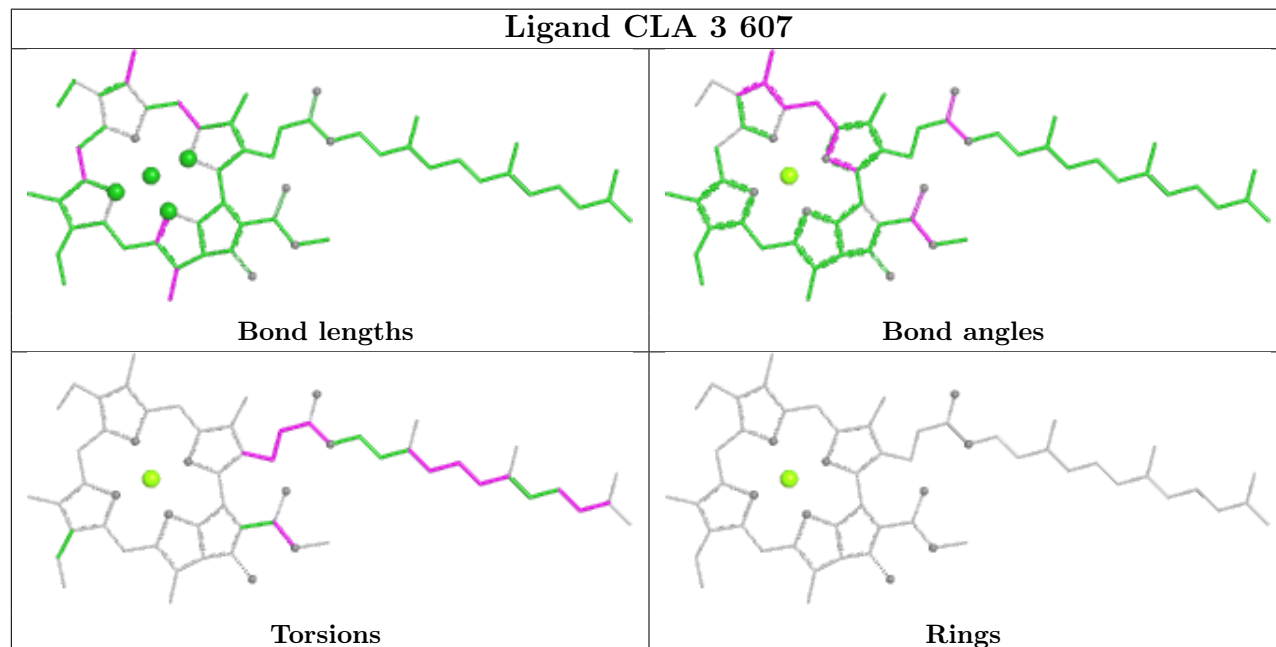


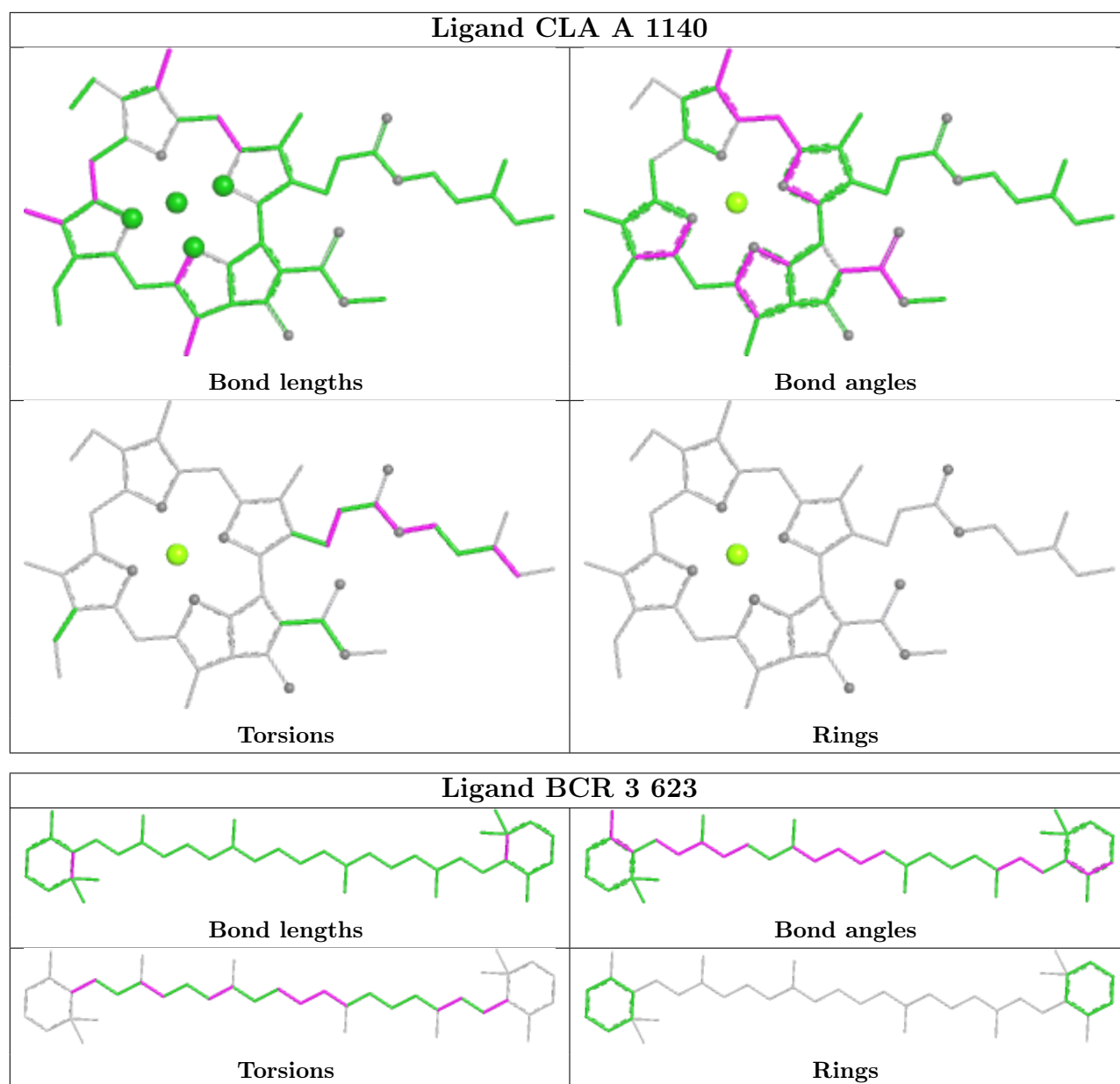
Rings

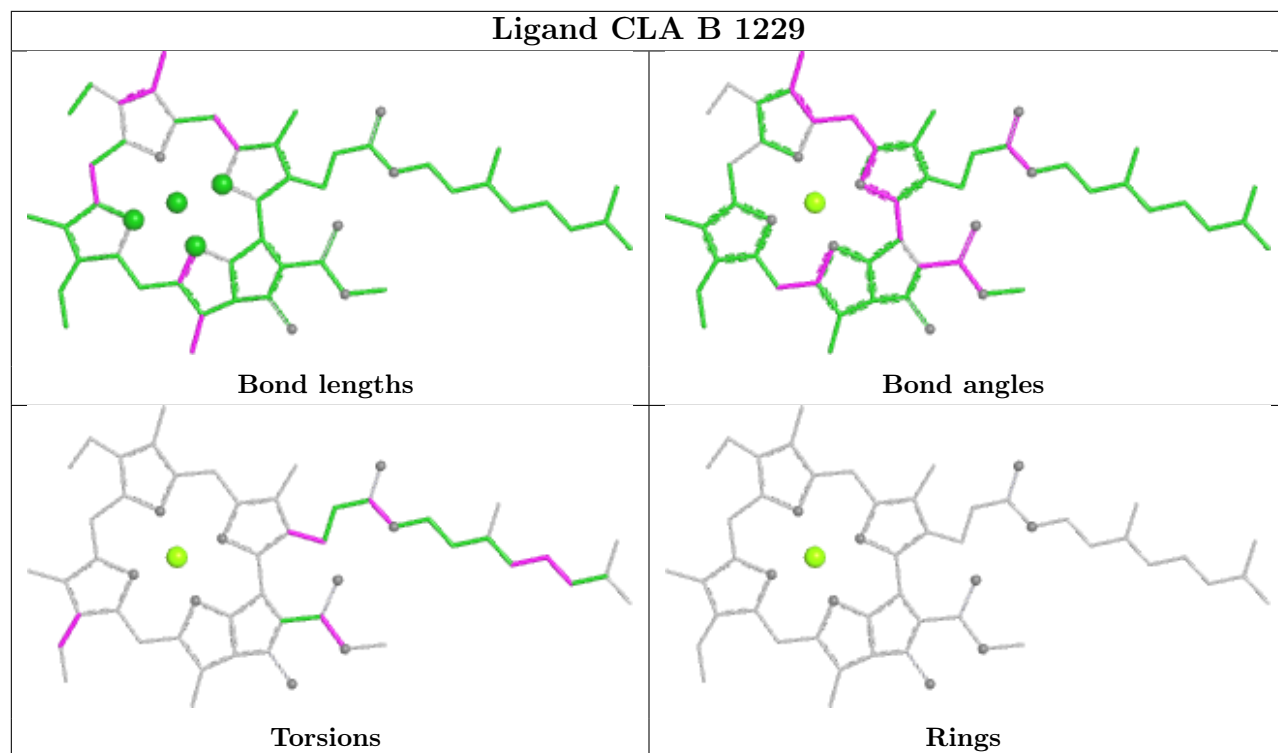
Ligand LHG 2 630



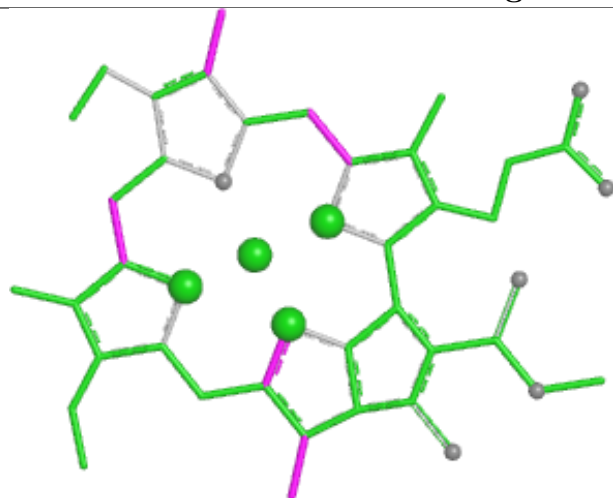
Ligand CLA 3 607



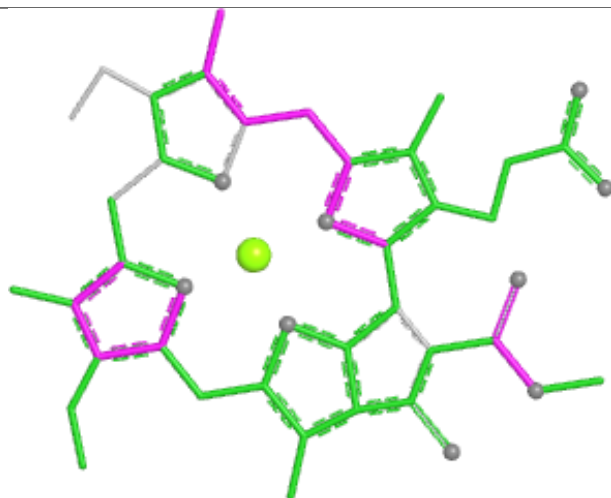




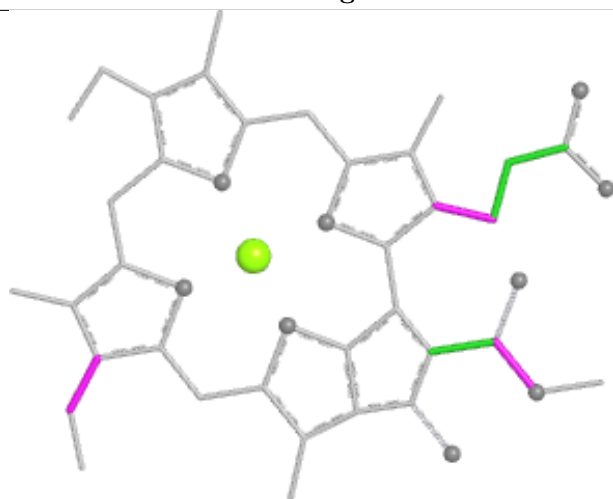
Ligand CLA B 1239



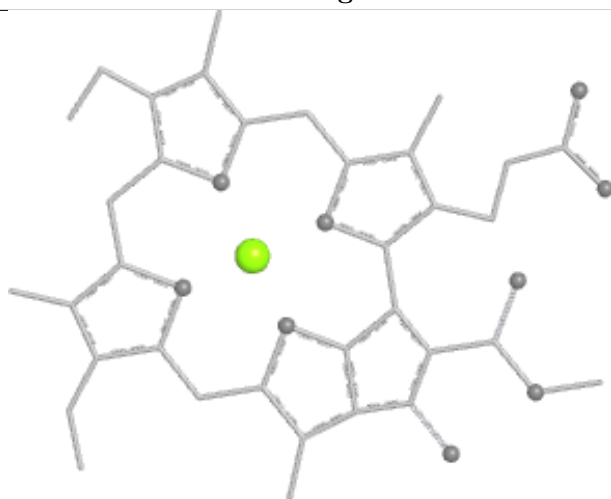
Bond lengths



Bond angles

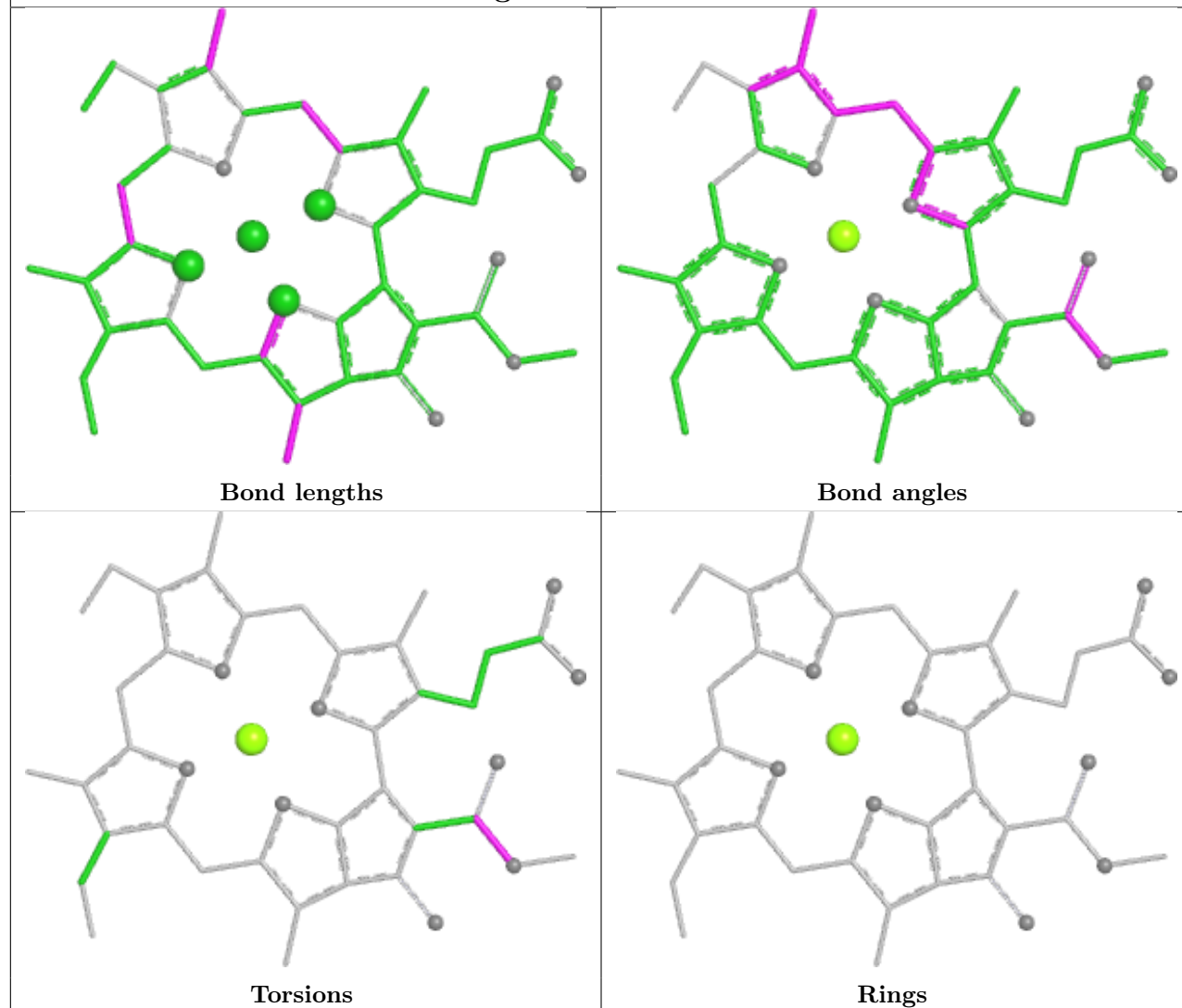


Torsions

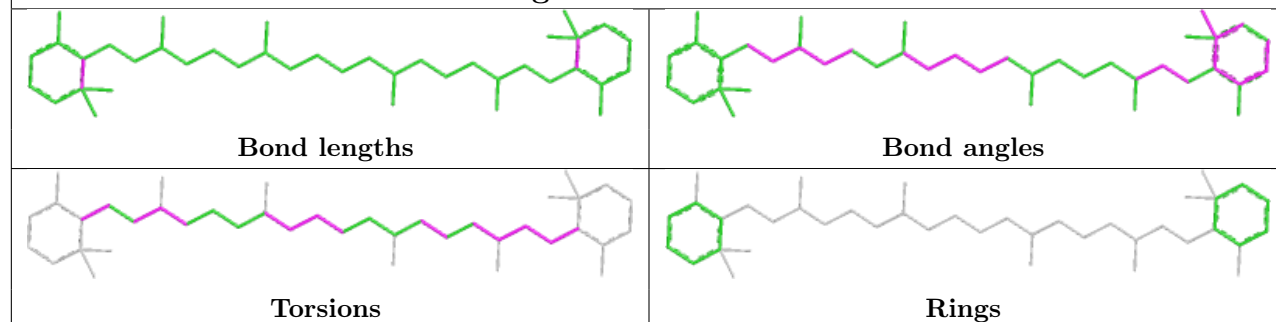


Rings

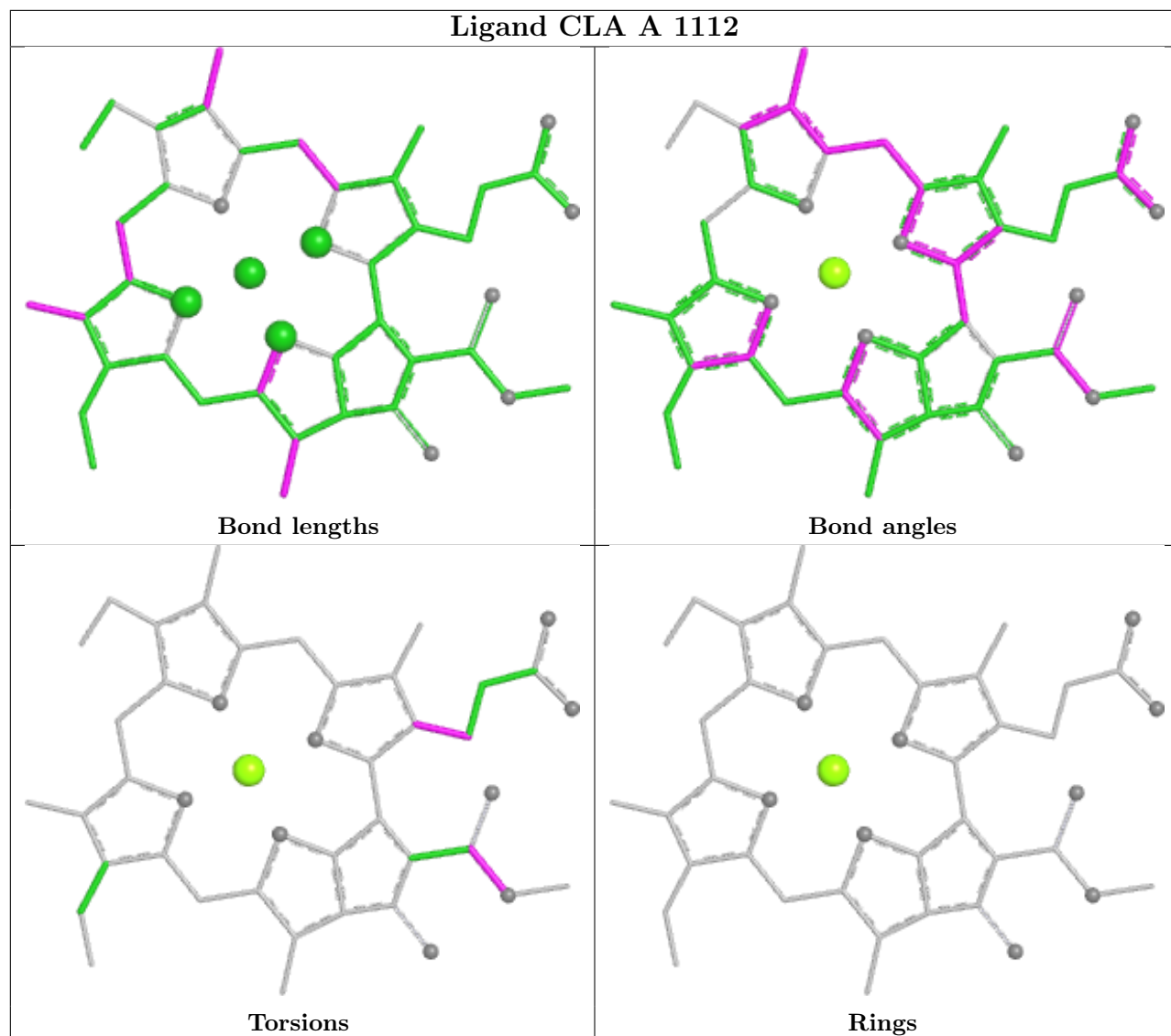
Ligand CLA F 301



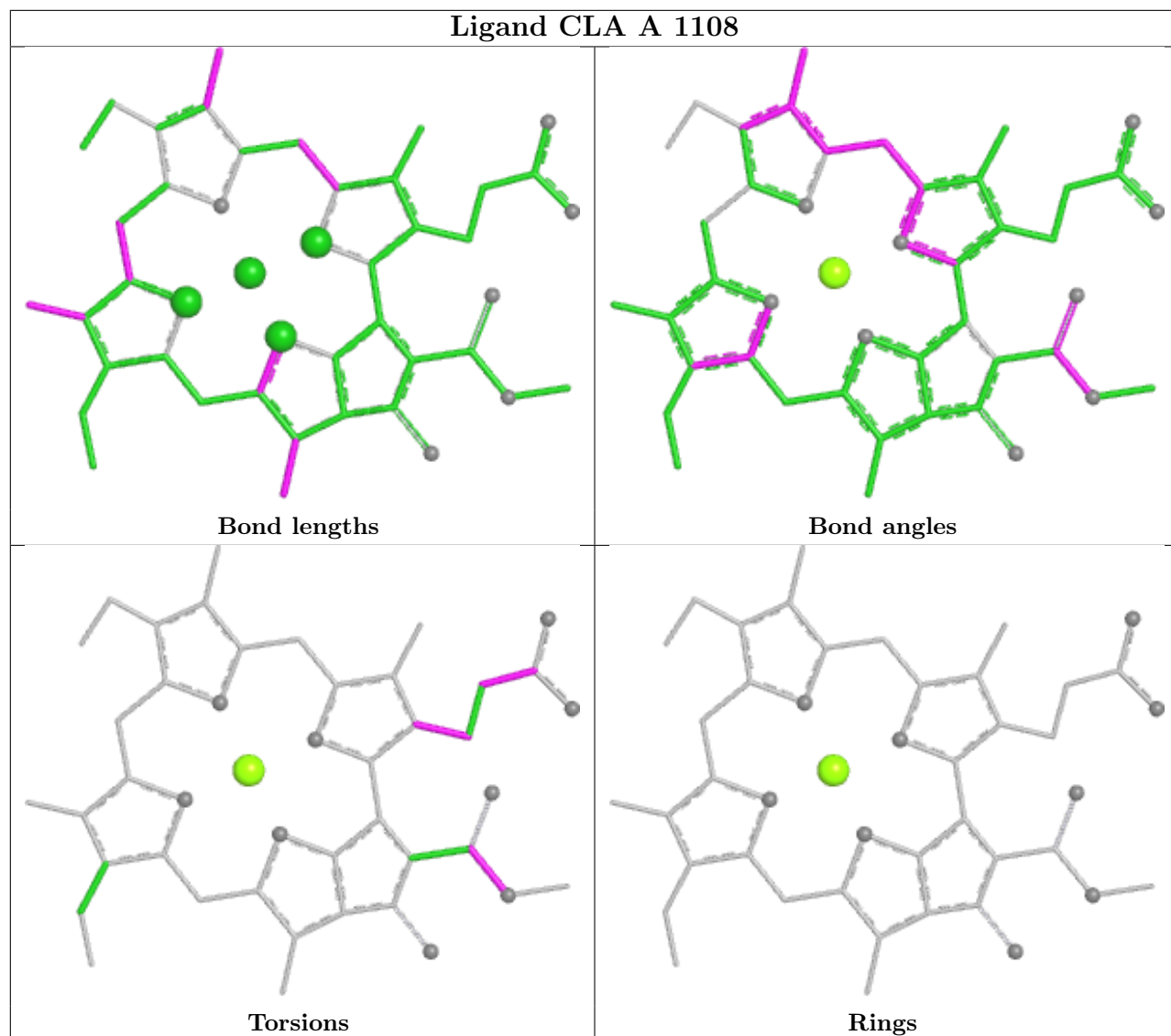
Ligand BCR F 416

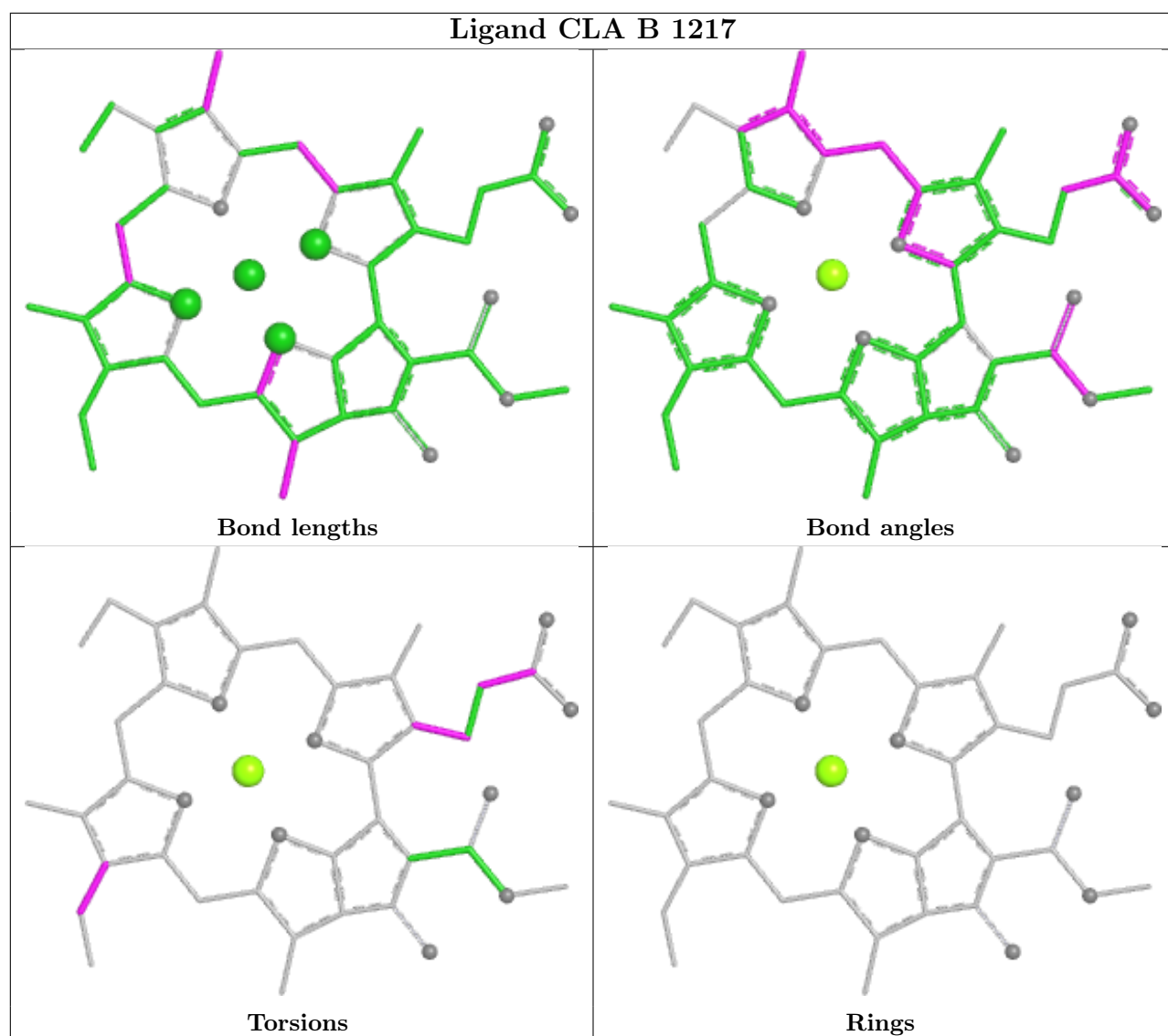


Ligand CLA A 1112

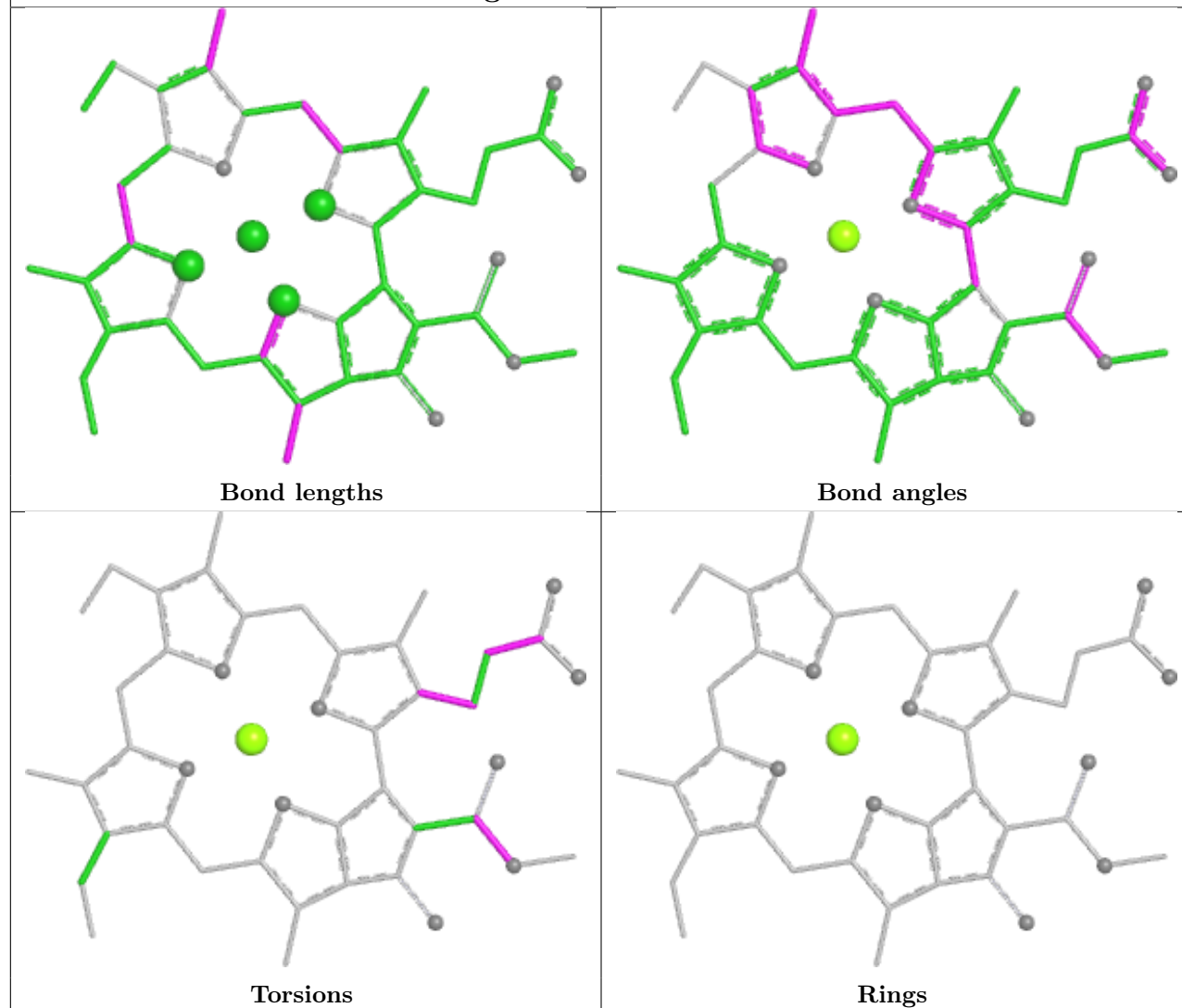


Ligand CLA A 1108

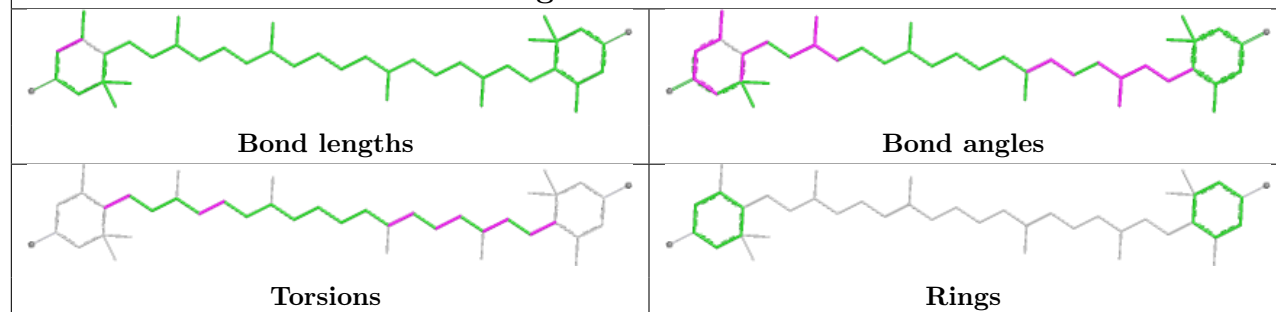




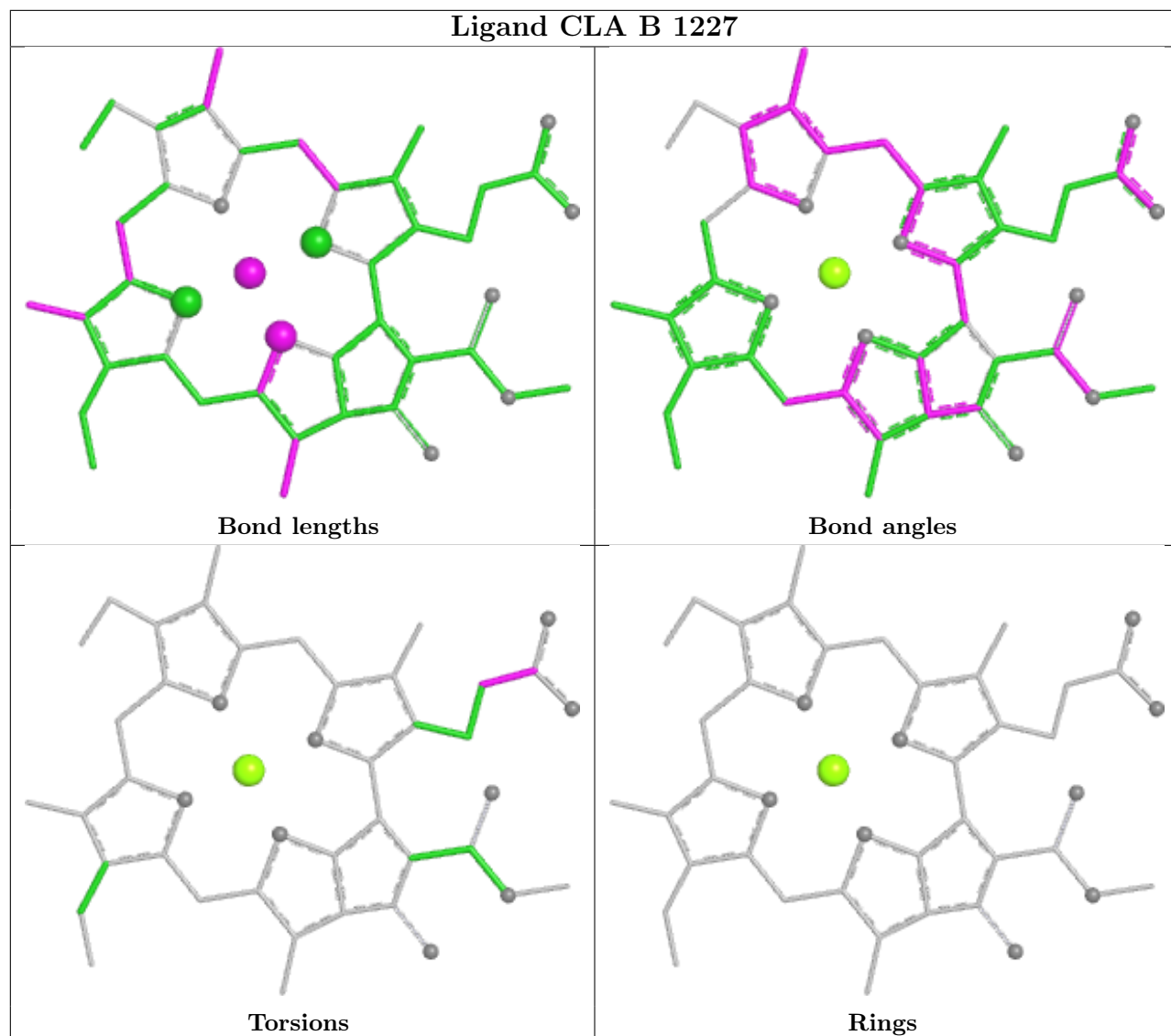
Ligand CLA A 1134

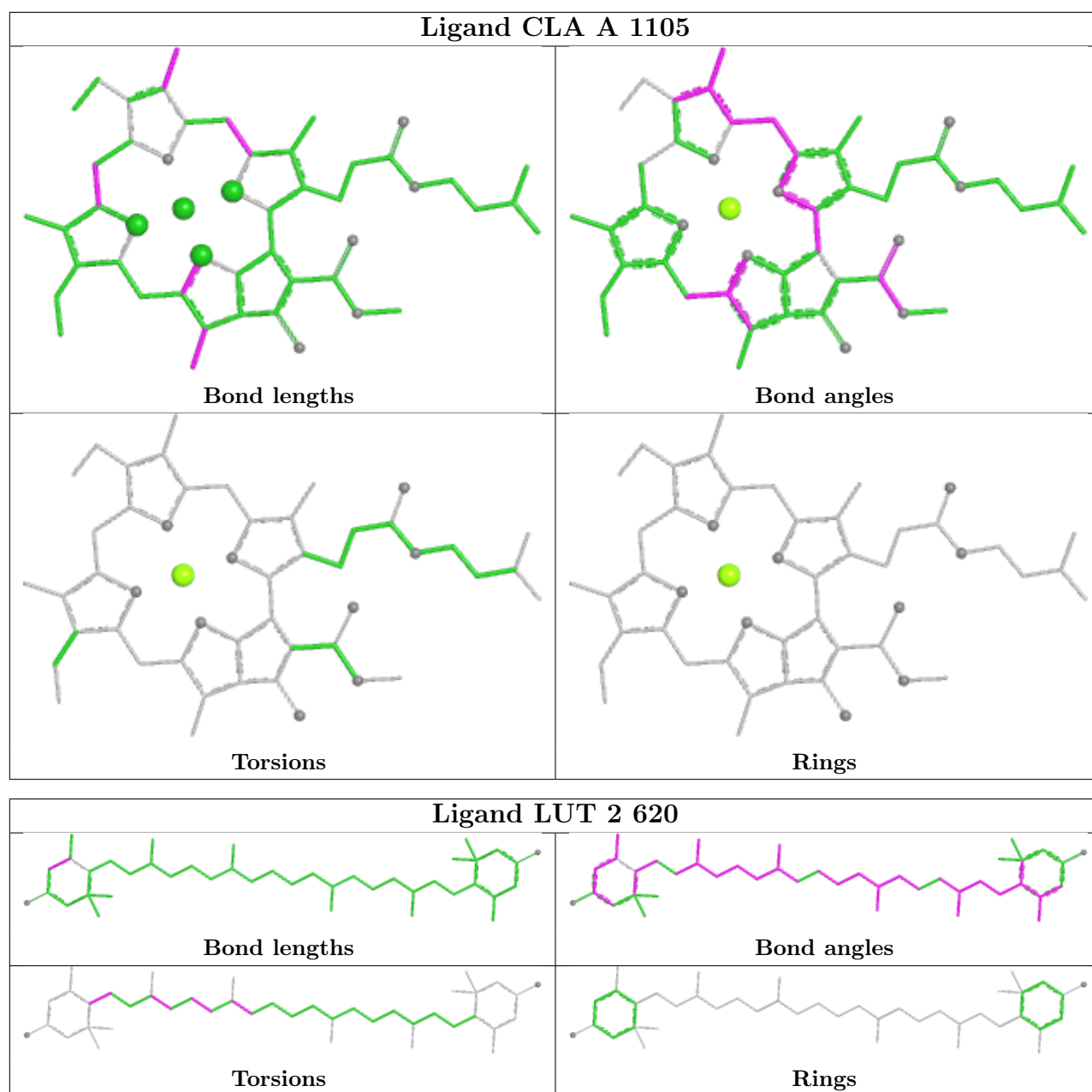


Ligand LUT 2 623

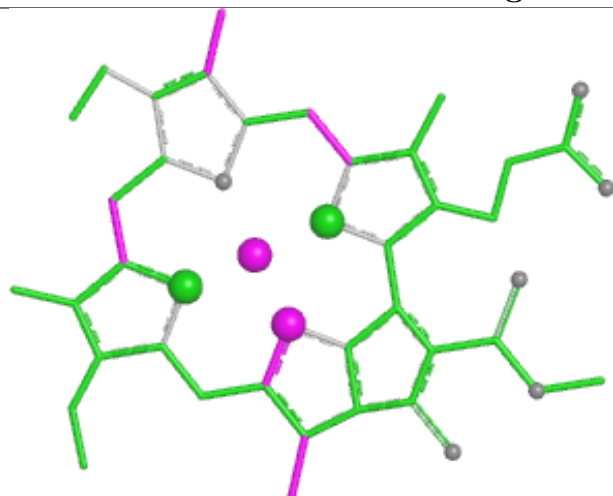


Ligand CLA B 1227

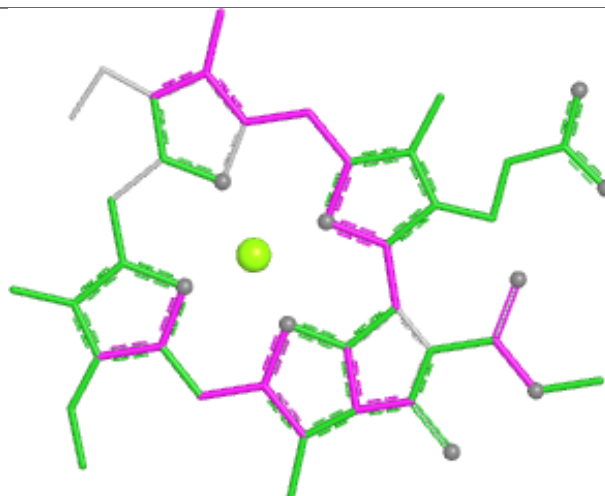




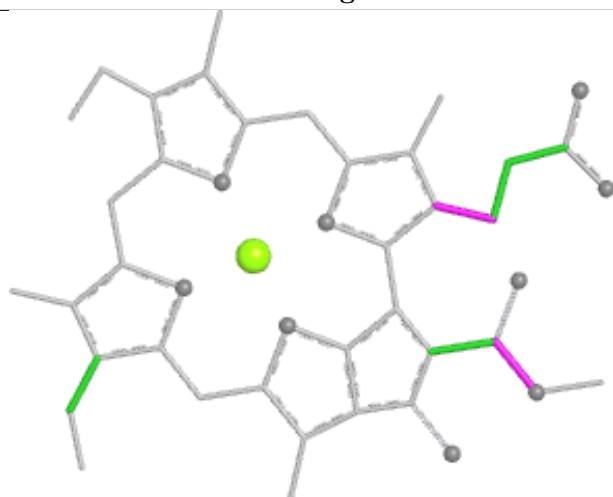
Ligand CLA B 1219



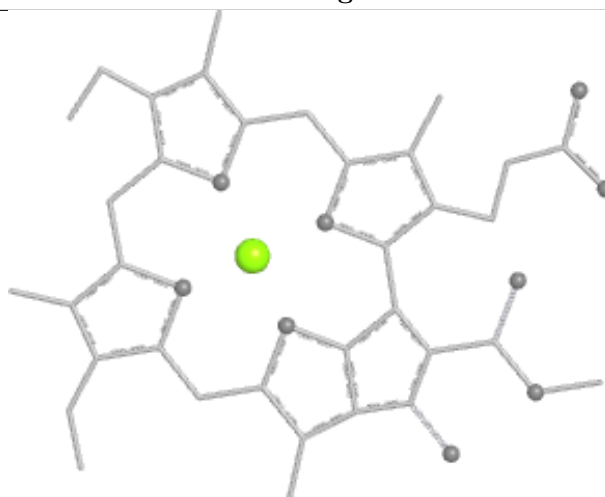
Bond lengths



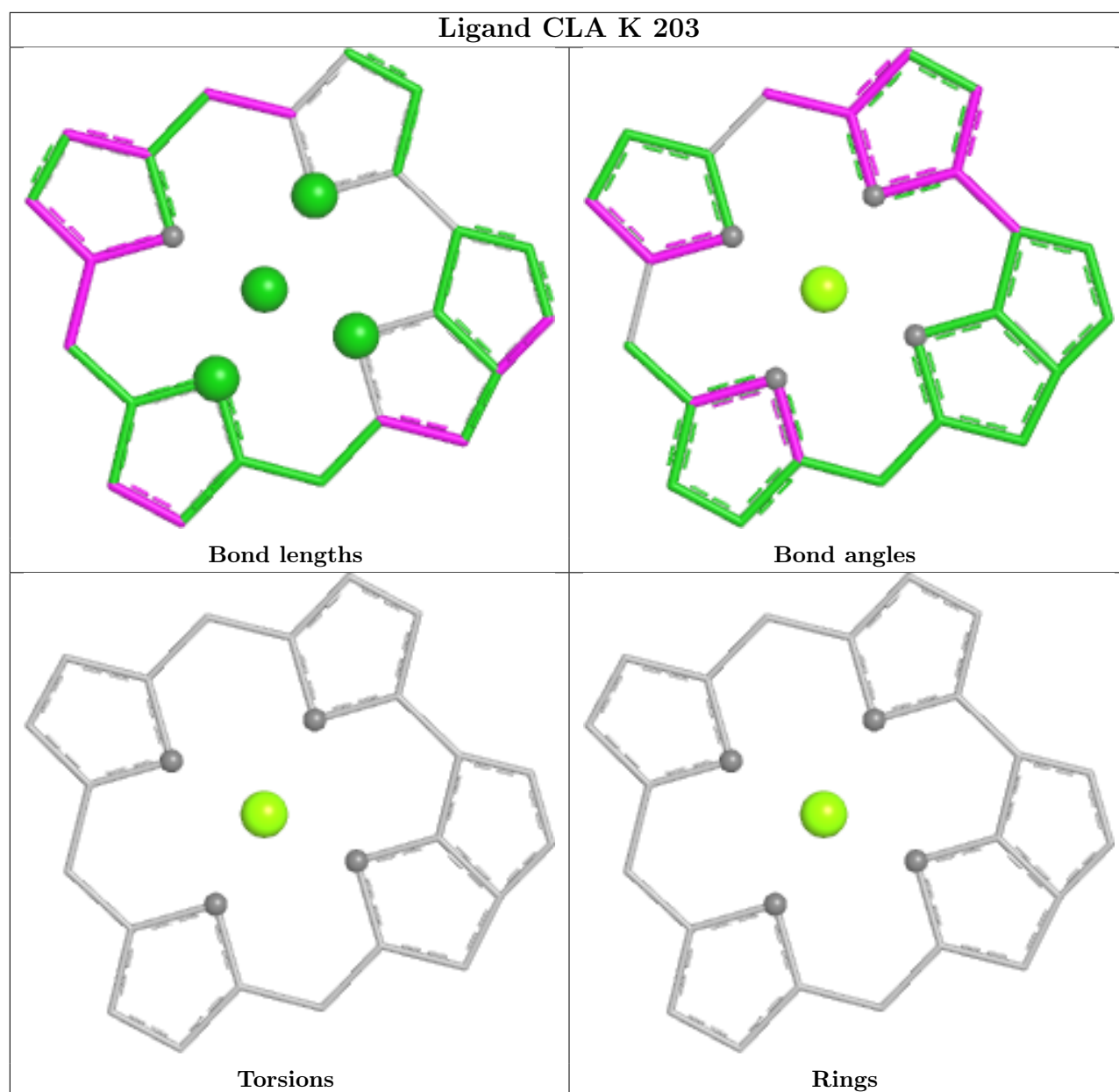
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

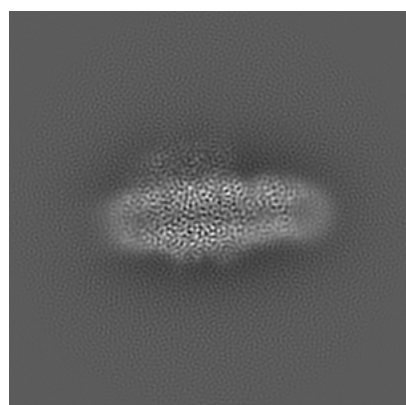
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23040. These allow visual inspection of the internal detail of the map and identification of artifacts.

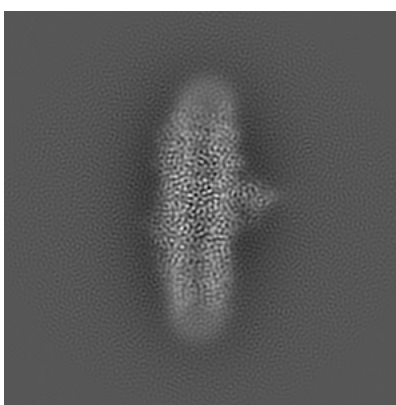
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

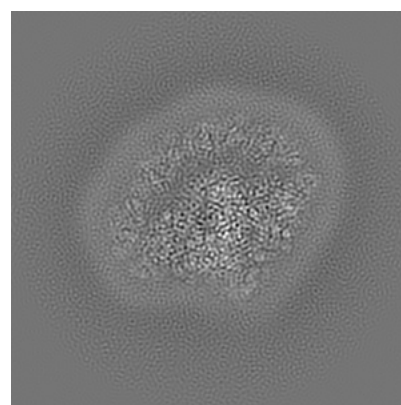
6.1.1 Primary map



X



Y

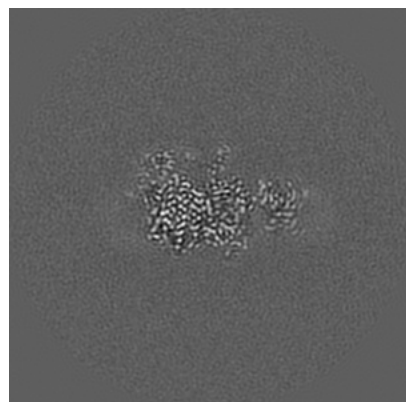


Z

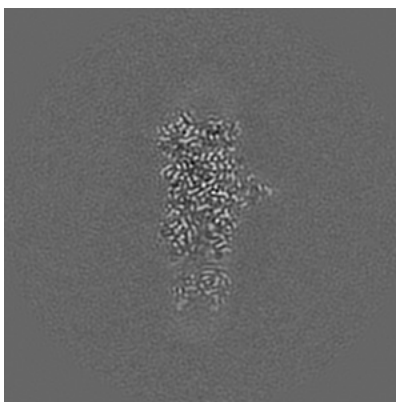
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

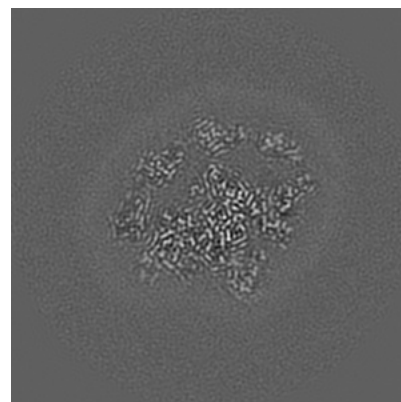
6.2.1 Primary map



X Index: 140



Y Index: 140

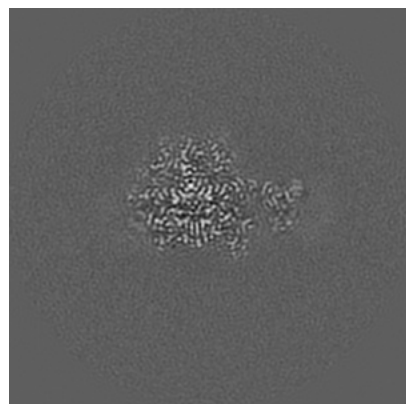


Z Index: 140

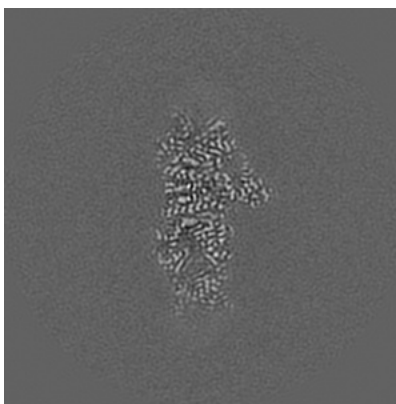
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

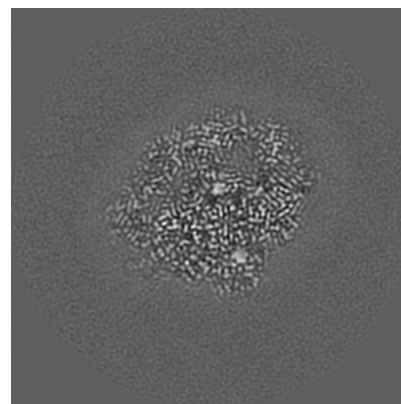
6.3.1 Primary map



X Index: 150



Y Index: 129

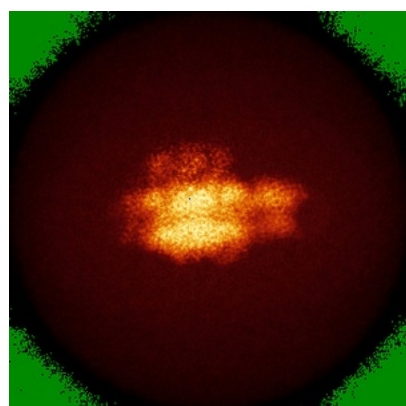


Z Index: 148

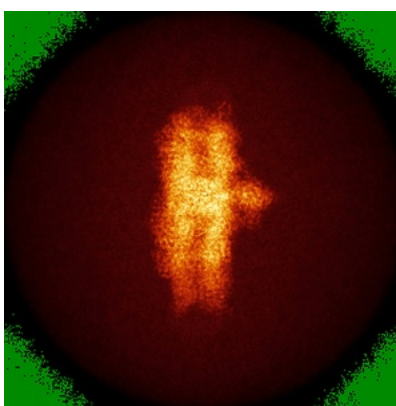
The images above show the largest variance slices of the map in three orthogonal directions.

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

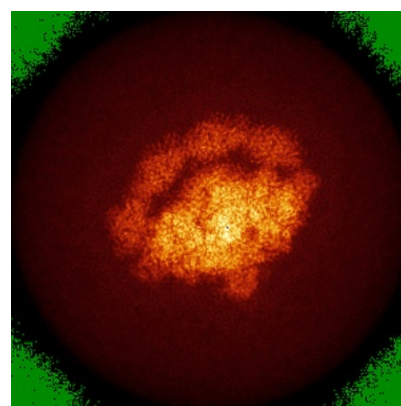
6.4.1 Primary map



X



Y

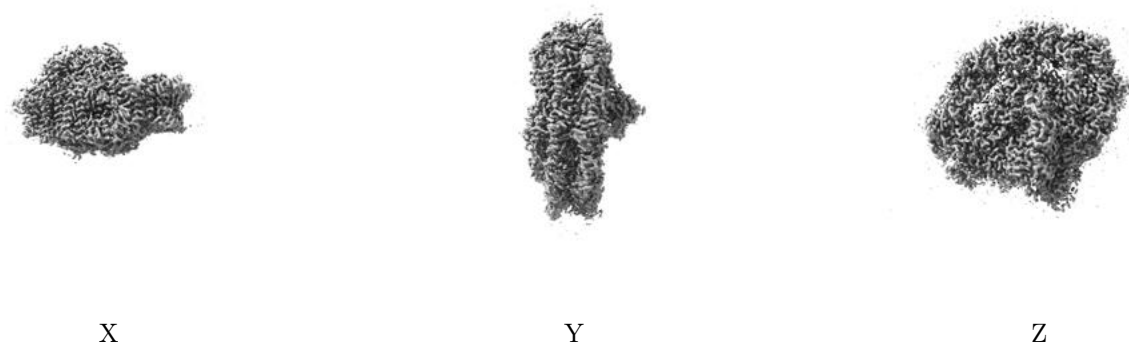


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

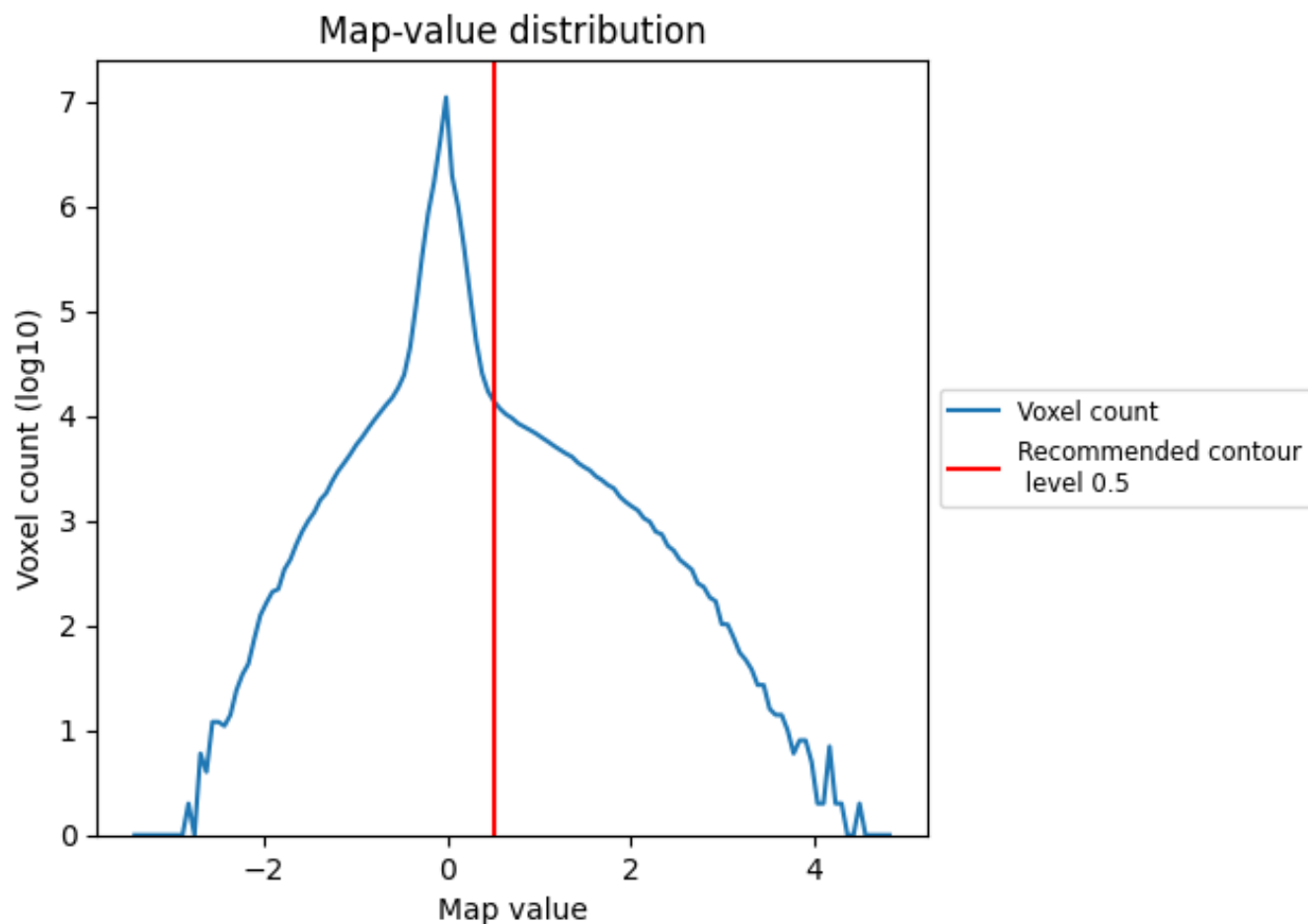
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

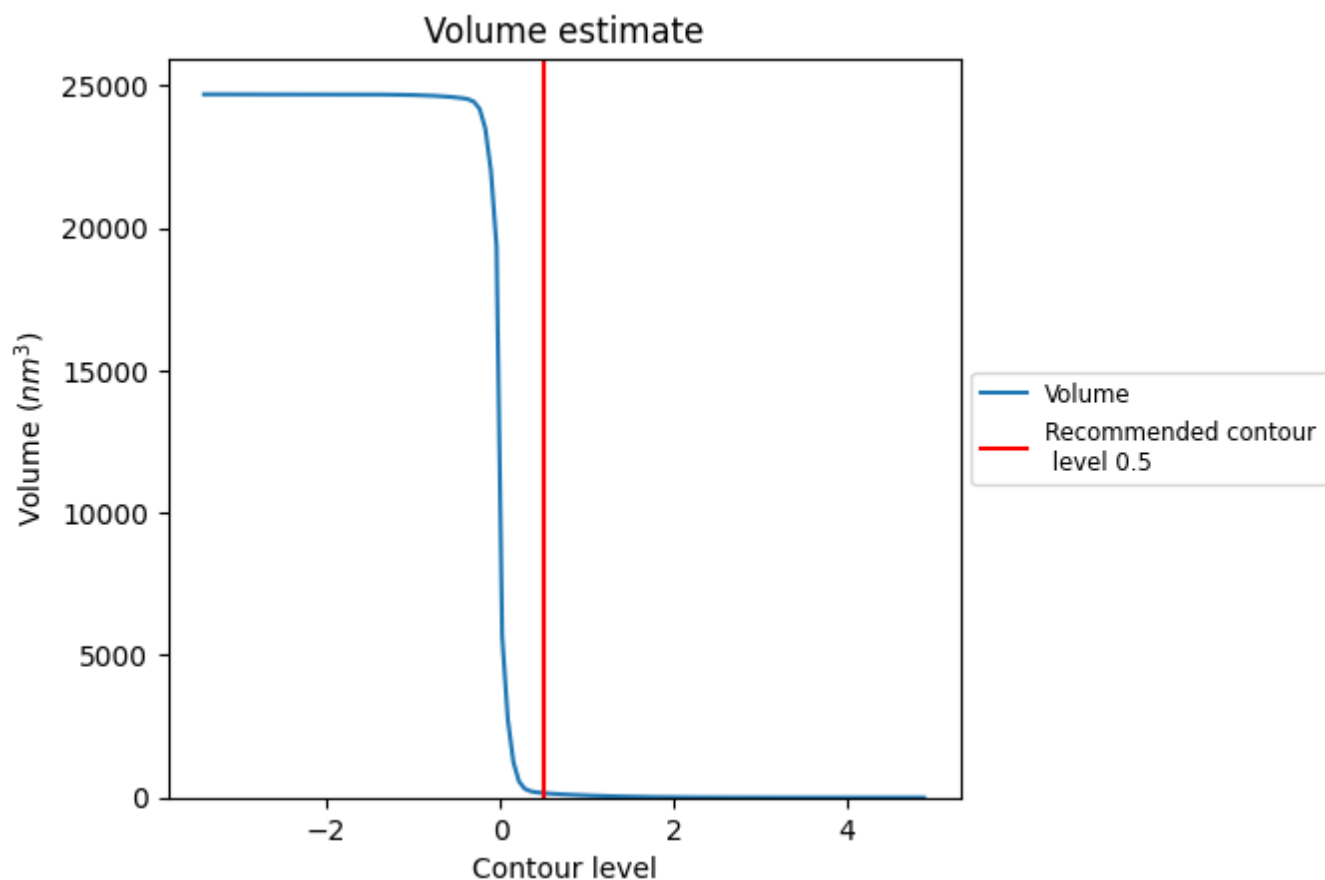
This section contains the results of statistical analysis of the map.

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.

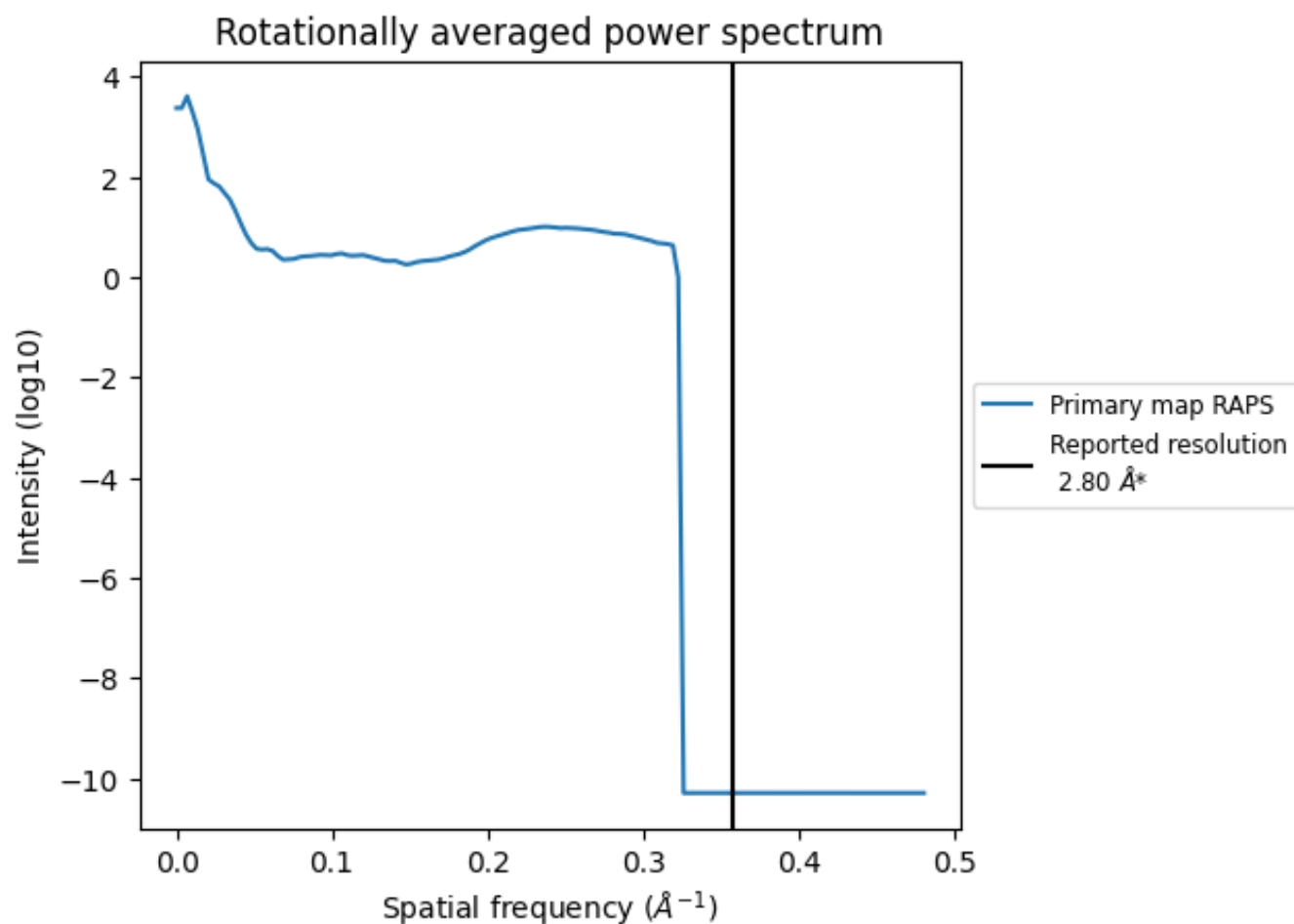
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm^3 ; this corresponds to an approximate mass of 143 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 0.357 Å⁻¹

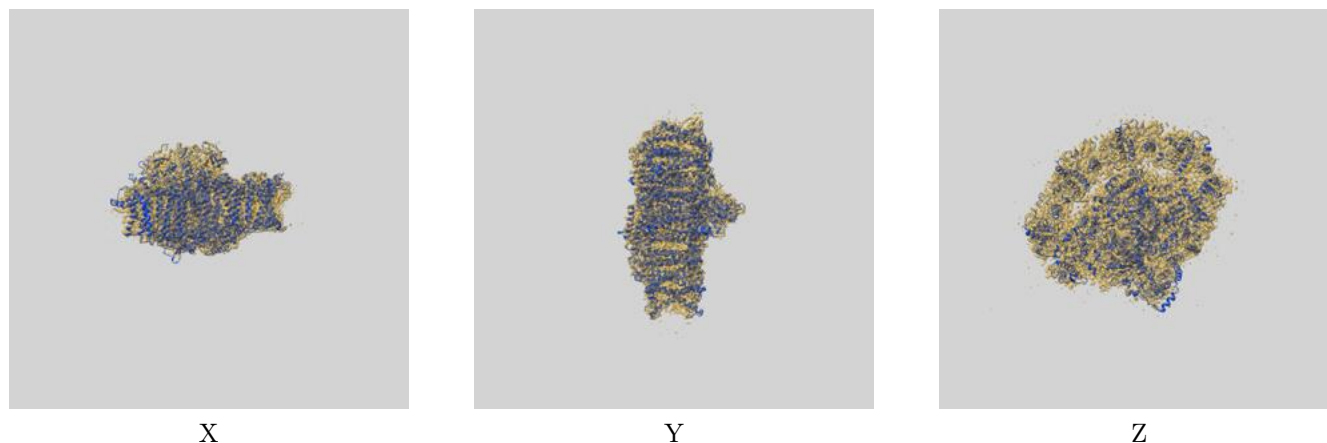
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

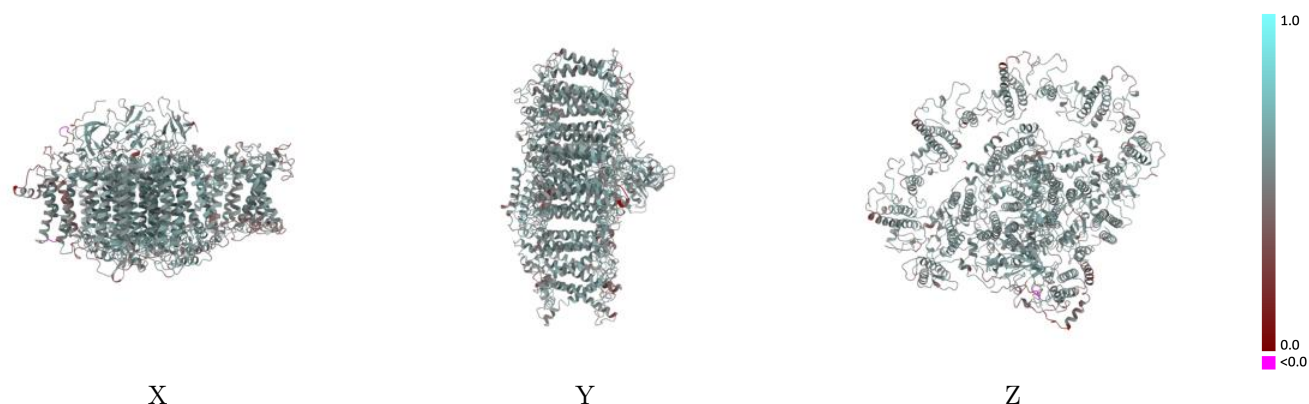
This section contains information regarding the fit between EMDB map EMD-23040 and PDB model 7KUX. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



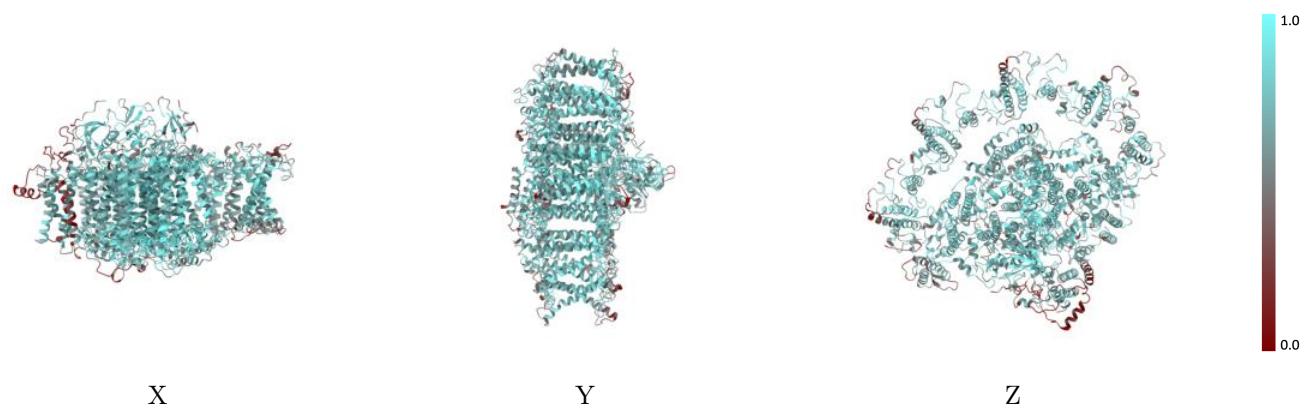
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



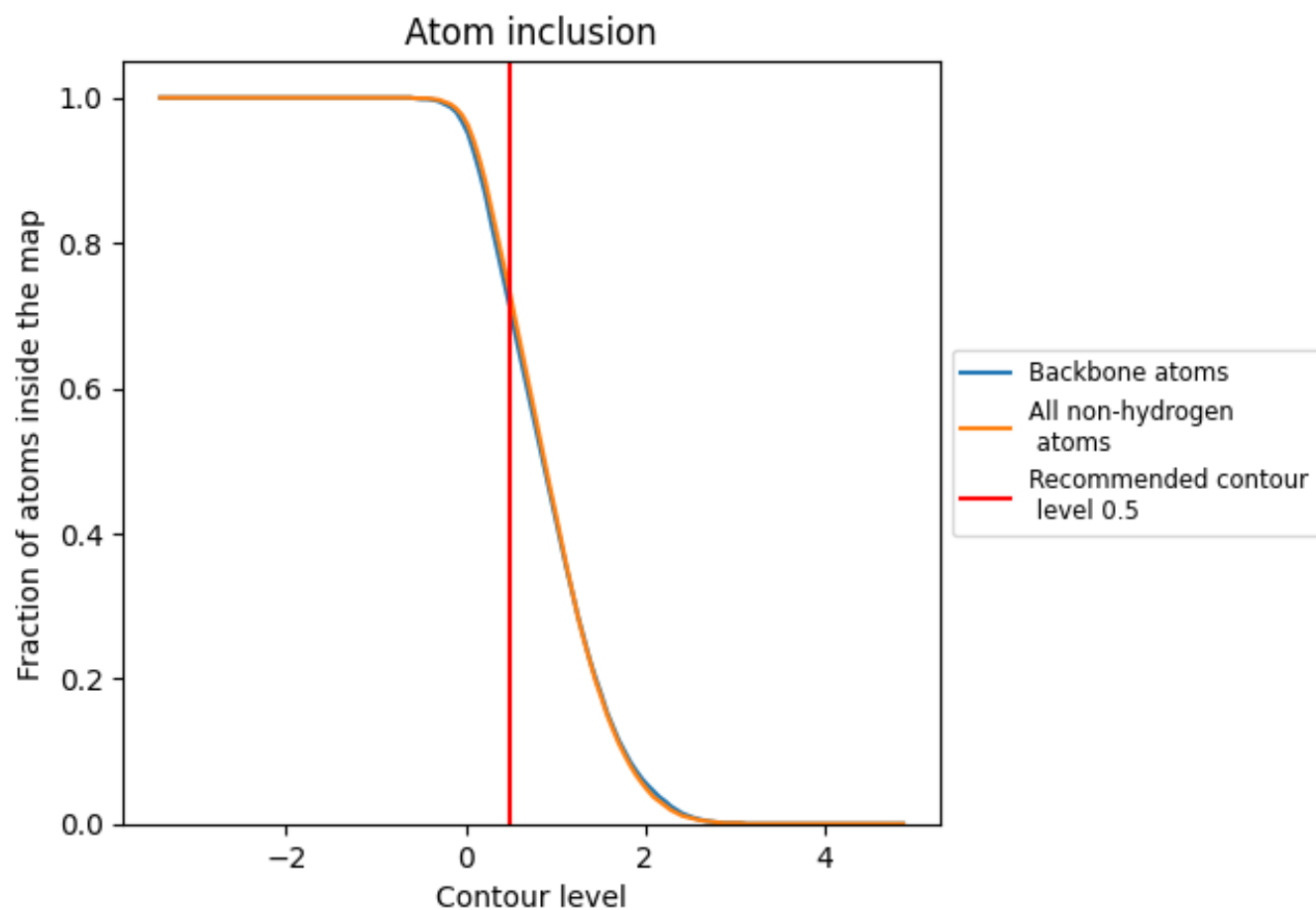
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------|--------------------|
| All | <div></div> 0.7280 | <div></div> 0.5460 |
| 1 | <div></div> 0.6710 | <div></div> 0.5260 |
| 2 | <div></div> 0.6570 | <div></div> 0.5240 |
| 3 | <div></div> 0.6500 | <div></div> 0.5290 |
| 4 | <div></div> 0.6710 | <div></div> 0.5180 |
| A | <div></div> 0.8050 | <div></div> 0.5680 |
| B | <div></div> 0.8170 | <div></div> 0.5730 |
| C | <div></div> 0.8060 | <div></div> 0.5680 |
| D | <div></div> 0.6760 | <div></div> 0.5320 |
| E | <div></div> 0.6970 | <div></div> 0.5370 |
| F | <div></div> 0.7070 | <div></div> 0.5490 |
| G | <div></div> 0.6660 | <div></div> 0.5370 |
| H | <div></div> 0.2460 | <div></div> 0.3980 |
| I | <div></div> 0.7040 | <div></div> 0.5450 |
| J | <div></div> 0.7580 | <div></div> 0.5580 |
| K | <div></div> 0.5540 | <div></div> 0.5000 |
| L | <div></div> 0.5940 | <div></div> 0.5040 |
| M | <div></div> 0.6310 | <div></div> 0.5120 |

