



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 06:12 AM UTC

PDB ID : 7DKZ / pdb\_00007dkz  
Title : Structure of plant photosystem I-light harvesting complex I supercomplex  
Authors : Wang, J.; Yu, L.J.; Wang, W.  
Deposited on : 2020-11-25  
Resolution : 2.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

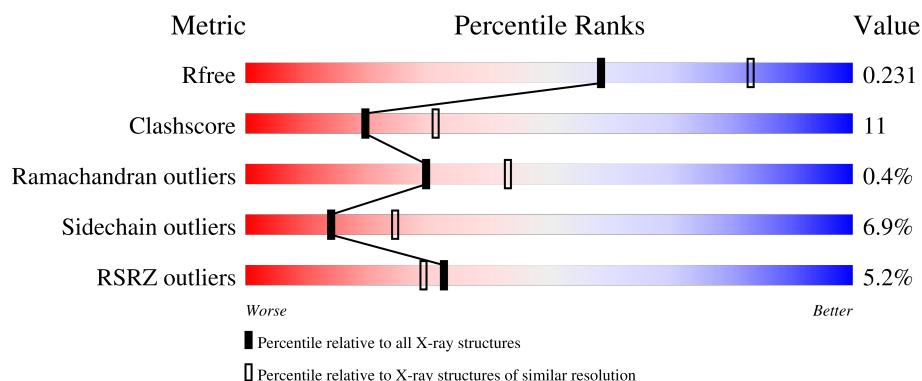
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 4912 (2.40-2.40)                                      |
| Clashscore            | 190562                      | 5391 (2.40-2.40)                                      |
| Ramachandran outliers | 187476                      | 5320 (2.40-2.40)                                      |
| Sidechain outliers    | 187428                      | 5321 (2.40-2.40)                                      |
| RSRZ outliers         | 180081                      | 4916 (2.40-2.40)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                              |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------|
| 1   | 1     | 195    | <div> <div>8%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>.</div> </div> </div>                |
| 2   | 2     | 269    | <div> <div>6%</div> <div> <div></div> <div>54%</div> <div>19%</div> <div>.</div> <div>24%</div> </div> </div> |
| 3   | 3     | 275    | <div> <div>8%</div> <div> <div></div> <div>63%</div> <div>14%</div> <div>.</div> <div>21%</div> </div> </div> |
| 4   | 4     | 198    | <div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>.</div> <div>.</div> </div> </div>   |
| 5   | A     | 758    | <div> <div>3%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>.</div> <div>.</div> </div> </div>   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | B     | 734    |                  |
| 7   | C     | 81     |                  |
| 8   | D     | 143    |                  |
| 9   | E     | 66     |                  |
| 10  | F     | 154    |                  |
| 11  | G     | 97     |                  |
| 12  | H     | 88     |                  |
| 13  | I     | 40     |                  |
| 14  | J     | 42     |                  |
| 15  | L     | 157    |                  |
| 16  | K     | 80     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 17  | CLA  | 1     | 301 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 302 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 303 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 304 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 306 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 307 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 308 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 309 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 310 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 311 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 312 | X         | -        | -       | -                |
| 17  | CLA  | 1     | 313 | X         | -        | -       | -                |
| 17  | CLA  | 2     | 301 | X         | -        | -       | -                |
| 17  | CLA  | 2     | 302 | X         | -        | -       | -                |
| 17  | CLA  | 2     | 303 | X         | -        | -       | -                |
| 17  | CLA  | 2     | 307 | X         | -        | -       | -                |
| 17  | CLA  | 2     | 308 | X         | -        | -       | -                |
| 17  | CLA  | 2     | 309 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 17  | CLA  | 2     | 310 | X         | -        | -       | -                |
| 17  | CLA  | 2     | 311 | X         | -        | -       | -                |
| 17  | CLA  | 2     | 312 | X         | -        | -       | -                |
| 17  | CLA  | 2     | 319 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 602 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 603 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 604 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 605 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 606 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 608 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 609 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 610 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 611 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 612 | X         | -        | -       | -                |
| 17  | CLA  | 3     | 613 | X         | -        | -       | -                |
| 17  | CLA  | 4     | 302 | X         | -        | -       | -                |
| 17  | CLA  | 4     | 304 | X         | -        | -       | -                |
| 17  | CLA  | 4     | 308 | X         | -        | -       | -                |
| 17  | CLA  | 4     | 309 | X         | -        | -       | -                |
| 17  | CLA  | 4     | 310 | X         | -        | -       | -                |
| 17  | CLA  | 4     | 312 | X         | -        | -       | -                |
| 17  | CLA  | 4     | 313 | X         | -        | -       | -                |
| 17  | CLA  | 4     | 314 | X         | -        | -       | -                |
| 17  | CLA  | A     | 801 | X         | -        | -       | -                |
| 17  | CLA  | A     | 802 | X         | -        | -       | -                |
| 17  | CLA  | A     | 803 | X         | -        | -       | -                |
| 17  | CLA  | A     | 804 | X         | -        | -       | -                |
| 17  | CLA  | A     | 805 | X         | -        | -       | -                |
| 17  | CLA  | A     | 806 | X         | -        | -       | -                |
| 17  | CLA  | A     | 807 | X         | -        | -       | -                |
| 17  | CLA  | A     | 808 | X         | -        | -       | -                |
| 17  | CLA  | A     | 809 | X         | -        | -       | -                |
| 17  | CLA  | A     | 810 | X         | -        | -       | -                |
| 17  | CLA  | A     | 811 | X         | -        | -       | -                |
| 17  | CLA  | A     | 812 | X         | -        | -       | -                |
| 17  | CLA  | A     | 813 | X         | -        | -       | -                |
| 17  | CLA  | A     | 814 | X         | -        | -       | -                |
| 17  | CLA  | A     | 815 | X         | -        | -       | -                |
| 17  | CLA  | A     | 816 | X         | -        | -       | -                |
| 17  | CLA  | A     | 817 | X         | -        | -       | -                |
| 17  | CLA  | A     | 818 | X         | -        | -       | -                |
| 17  | CLA  | A     | 819 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 17  | CLA  | A     | 820 | X         | -        | -       | -                |
| 17  | CLA  | A     | 821 | X         | -        | -       | -                |
| 17  | CLA  | A     | 822 | X         | -        | -       | -                |
| 17  | CLA  | A     | 823 | X         | -        | -       | -                |
| 17  | CLA  | A     | 824 | X         | -        | -       | -                |
| 17  | CLA  | A     | 825 | X         | -        | -       | -                |
| 17  | CLA  | A     | 826 | X         | -        | -       | -                |
| 17  | CLA  | A     | 827 | X         | -        | -       | -                |
| 17  | CLA  | A     | 828 | X         | -        | -       | -                |
| 17  | CLA  | A     | 829 | X         | -        | -       | -                |
| 17  | CLA  | A     | 830 | X         | -        | -       | -                |
| 17  | CLA  | A     | 831 | X         | -        | -       | -                |
| 17  | CLA  | A     | 832 | X         | -        | -       | -                |
| 17  | CLA  | A     | 833 | X         | -        | -       | -                |
| 17  | CLA  | A     | 834 | X         | -        | -       | -                |
| 17  | CLA  | A     | 835 | X         | -        | -       | -                |
| 17  | CLA  | A     | 836 | X         | -        | -       | -                |
| 17  | CLA  | A     | 837 | X         | -        | -       | -                |
| 17  | CLA  | A     | 838 | X         | -        | -       | -                |
| 17  | CLA  | A     | 839 | X         | -        | -       | -                |
| 17  | CLA  | A     | 840 | X         | -        | -       | -                |
| 17  | CLA  | A     | 841 | X         | -        | -       | -                |
| 17  | CLA  | A     | 843 | X         | -        | -       | -                |
| 17  | CLA  | A     | 853 | X         | -        | -       | -                |
| 17  | CLA  | B     | 802 | X         | -        | -       | -                |
| 17  | CLA  | B     | 803 | X         | -        | -       | -                |
| 17  | CLA  | B     | 804 | X         | -        | -       | -                |
| 17  | CLA  | B     | 805 | X         | -        | -       | -                |
| 17  | CLA  | B     | 806 | X         | -        | -       | -                |
| 17  | CLA  | B     | 807 | X         | -        | -       | -                |
| 17  | CLA  | B     | 808 | X         | -        | -       | -                |
| 17  | CLA  | B     | 809 | X         | -        | -       | -                |
| 17  | CLA  | B     | 810 | X         | -        | -       | -                |
| 17  | CLA  | B     | 811 | X         | -        | -       | -                |
| 17  | CLA  | B     | 813 | X         | -        | -       | -                |
| 17  | CLA  | B     | 814 | X         | -        | -       | -                |
| 17  | CLA  | B     | 815 | X         | -        | -       | -                |
| 17  | CLA  | B     | 816 | X         | -        | -       | -                |
| 17  | CLA  | B     | 817 | X         | -        | -       | -                |
| 17  | CLA  | B     | 818 | X         | -        | -       | -                |
| 17  | CLA  | B     | 819 | X         | -        | -       | -                |
| 17  | CLA  | B     | 820 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 17  | CLA  | B     | 821 | X         | -        | -       | -                |
| 17  | CLA  | B     | 822 | X         | -        | -       | -                |
| 17  | CLA  | B     | 823 | X         | -        | -       | -                |
| 17  | CLA  | B     | 824 | X         | -        | -       | -                |
| 17  | CLA  | B     | 825 | X         | -        | -       | -                |
| 17  | CLA  | B     | 826 | X         | -        | -       | -                |
| 17  | CLA  | B     | 827 | X         | -        | -       | -                |
| 17  | CLA  | B     | 828 | X         | -        | -       | -                |
| 17  | CLA  | B     | 829 | X         | -        | -       | -                |
| 17  | CLA  | B     | 830 | X         | -        | -       | -                |
| 17  | CLA  | B     | 831 | X         | -        | -       | -                |
| 17  | CLA  | B     | 832 | X         | -        | -       | -                |
| 17  | CLA  | B     | 833 | X         | -        | -       | -                |
| 17  | CLA  | B     | 834 | X         | -        | -       | -                |
| 17  | CLA  | B     | 835 | X         | -        | -       | -                |
| 17  | CLA  | B     | 836 | X         | -        | -       | -                |
| 17  | CLA  | B     | 837 | X         | -        | -       | -                |
| 17  | CLA  | B     | 838 | X         | -        | -       | -                |
| 17  | CLA  | B     | 839 | X         | -        | -       | -                |
| 17  | CLA  | B     | 840 | X         | -        | -       | -                |
| 17  | CLA  | B     | 841 | X         | -        | -       | -                |
| 17  | CLA  | B     | 842 | X         | -        | -       | -                |
| 17  | CLA  | F     | 304 | X         | -        | -       | -                |
| 17  | CLA  | F     | 306 | X         | -        | -       | -                |
| 17  | CLA  | F     | 307 | X         | -        | -       | -                |
| 17  | CLA  | G     | 103 | X         | -        | -       | -                |
| 17  | CLA  | G     | 104 | X         | -        | -       | -                |
| 17  | CLA  | G     | 105 | X         | -        | -       | -                |
| 17  | CLA  | J     | 101 | X         | -        | -       | -                |
| 17  | CLA  | J     | 103 | X         | -        | -       | -                |
| 17  | CLA  | K     | 201 | X         | -        | -       | -                |
| 17  | CLA  | K     | 202 | X         | -        | -       | -                |
| 17  | CLA  | L     | 202 | X         | -        | -       | -                |
| 17  | CLA  | L     | 203 | X         | -        | -       | -                |
| 18  | CHL  | 1     | 305 | X         | -        | -       | -                |
| 18  | CHL  | 2     | 304 | X         | -        | -       | -                |
| 18  | CHL  | 2     | 305 | X         | -        | -       | -                |
| 18  | CHL  | 2     | 306 | X         | -        | -       | -                |
| 18  | CHL  | 2     | 313 | X         | -        | -       | -                |
| 18  | CHL  | 3     | 601 | X         | -        | -       | -                |
| 18  | CHL  | 3     | 607 | X         | -        | -       | -                |
| 18  | CHL  | 4     | 301 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 18  | CHL  | 4     | 305 | X         | -        | -       | -                |
| 18  | CHL  | 4     | 306 | X         | -        | -       | -                |
| 18  | CHL  | 4     | 307 | X         | -        | -       | -                |
| 18  | CHL  | 4     | 315 | X         | -        | -       | -                |
| 19  | LUT  | 4     | 316 | -         | X        | -       | -                |
| 20  | XAT  | 4     | 317 | X         | -        | -       | -                |
| 26  | DGD  | 4     | 323 | -         | -        | X       | -                |

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 36093 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Lhca1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | 1     | 195      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 979 | 252 | 271 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | 2     | 204      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1592  | 1042 | 261 | 285 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | 3     | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1661  | 1088 | 268 | 300 | 5 |         |         |       |

- Molecule 4 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | 4     | 195      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1535  | 1006 | 249 | 277 | 3 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 4     | 89      | LYS      | ARG    | conflict | UNP Q9SQL2 |
| 4     | 128     | ASP      | ALA    | conflict | UNP Q9SQL2 |
| 4     | 149     | PHE      | SER    | conflict | UNP Q9SQL2 |

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 5   | A     | 742      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5852  | 3835 | 997 | 1002 | 18 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| A     | 223     | ILE      | VAL    | conflict | UNP A0A0F6NFW5 |

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 6   | B     | 733      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5856  | 3848 | 998 | 996 | 14 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 611   | 379 | 107 | 114 | 11 |         |         |       |

- Molecule 8 is a protein called PsaD.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | D     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 716 | 191 | 200 | 3 |         |         |       |

- Molecule 9 is a protein called PsaE.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 9   | E     | 63       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 505   | 320 | 89 | 96 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | -1      | PRO      | -      | expression tag | UNP E1C9K6 |
| E     | 0       | PRO      | -      | expression tag | UNP E1C9K6 |
| E     | 14      | GLN      | LYS    | conflict       | UNP E1C9K6 |
| E     | 60      | VAL      | -      | expression tag | UNP E1C9K6 |
| E     | 61      | GLU      | -      | expression tag | UNP E1C9K6 |
| E     | 62      | GLU      | -      | expression tag | UNP E1C9K6 |
| E     | 63      | VAL      | -      | expression tag | UNP E1C9K6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 64      | LYS      | -      | expression tag | UNP E1C9K6 |

- Molecule 10 is a protein called PSI-F.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | F     | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1198  | 777 | 208 | 211 | 2 |         |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| F     | 79      | ALA      | SER    | conflict | UNP A0A0M3KL12 |
| F     | 86      | ASP      | GLU    | conflict | UNP A0A0M3KL12 |
| F     | 107     | LEU      | ILE    | conflict | UNP A0A0M3KL12 |
| F     | 110     | PRO      | ALA    | conflict | UNP A0A0M3KL12 |
| F     | 133     | GLY      | ALA    | conflict | UNP A0A0M3KL12 |
| F     | 187     | ASP      | GLU    | conflict | UNP A0A0M3KL12 |
| F     | 203     | THR      | SER    | conflict | UNP A0A0M3KL12 |

- Molecule 11 is a protein called PsaG.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 11  | G     | 95       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 737   | 477 | 122 | 138 |  |         |         |       |

- Molecule 12 is a protein called PsaH.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 12  | H     | 88       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 673   | 442 | 106 | 125 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 13  | I     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 226   | 156 | 34 | 35 | 1 |         |         |       |

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



| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14  | J     | 39       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 309   | 208 | 48 | 52 | 1 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| J     | 32      | PHE      | LEU    | conflict | UNP D5MAL3 |

- Molecule 15 is a protein called PsaL.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | L     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 737 | 182 | 202 | 1 |         |         |       |

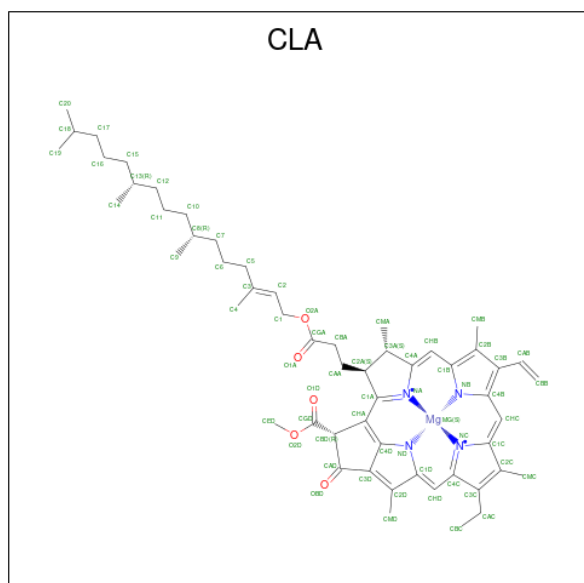
- Molecule 16 is a protein called PSI-K.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 16  | K     | 77       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 515   | 326 | 86 | 100 | 3 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| K     | 85      | ALA      | VAL    | conflict | UNP E1C9L3 |

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 17  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 17  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

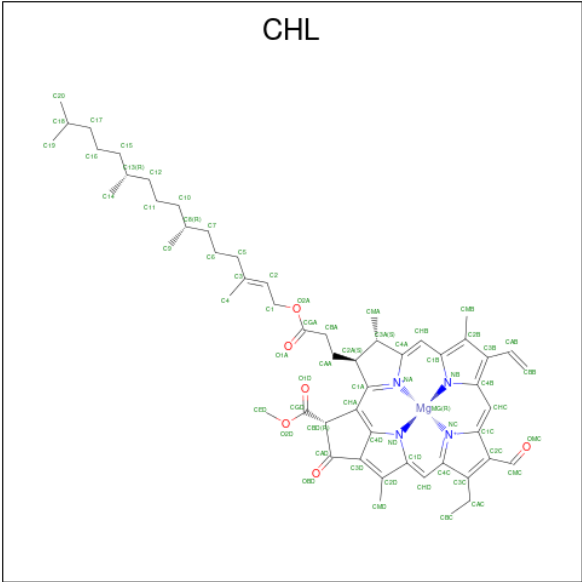
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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17  | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 17  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 17  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 17  | J     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | J     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |         |
| 17  | L     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | L     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 17  | L     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 17  | K     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 17  | K     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |

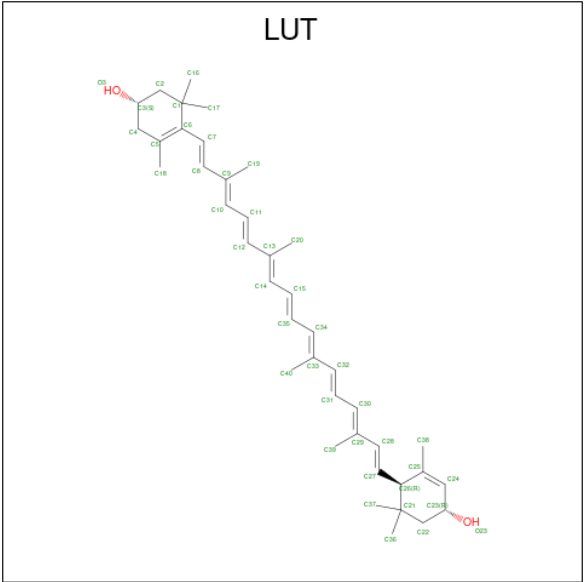
- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).





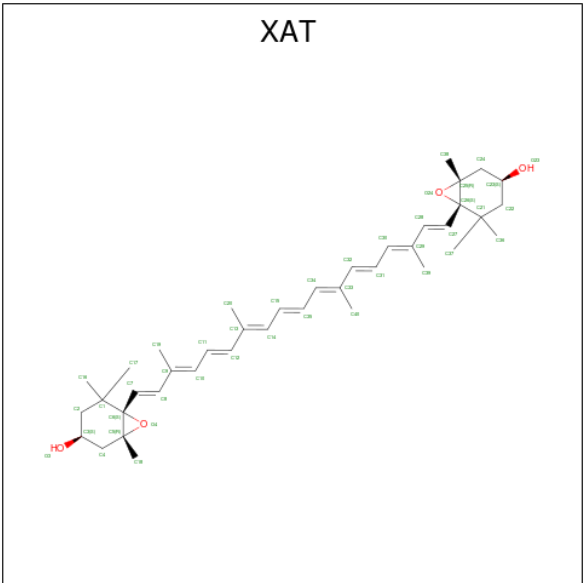
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |         |
| 18  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |         |
| 18  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |         |
| 18  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |         |
| 18  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |         |
| 18  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 19 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



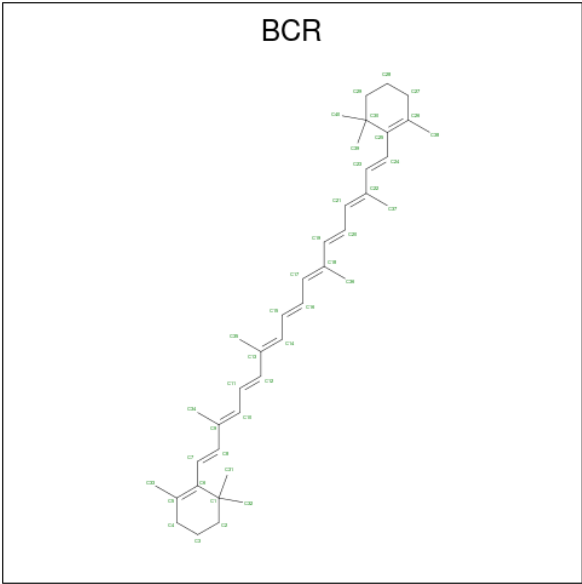
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 19  | 1     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 42    | 40 | 2 |         |         |
| 19  | 2     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 42    | 40 | 2 |         |         |
| 19  | 3     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 42    | 40 | 2 |         |         |
| 19  | 4     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 42    | 40 | 2 |         |         |

- Molecule 20 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 20  | 1     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 20  | 2     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 20  | 3     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 20  | 4     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



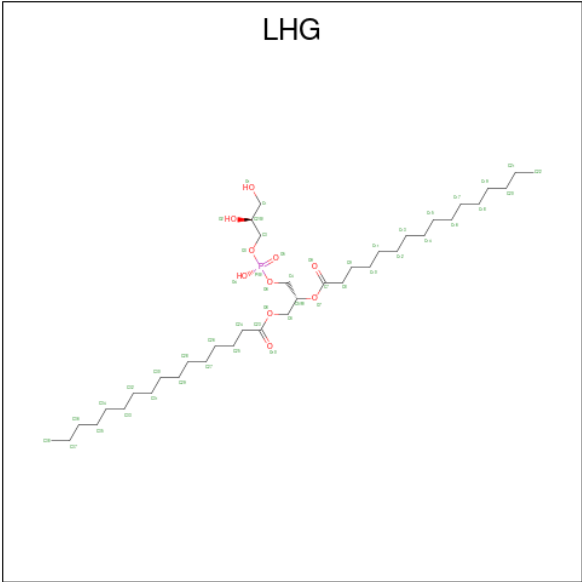
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21  | 1     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 21  | 2     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 21  | 3     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 21  | 4     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 21  | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 21  | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 21  | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 21  | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |

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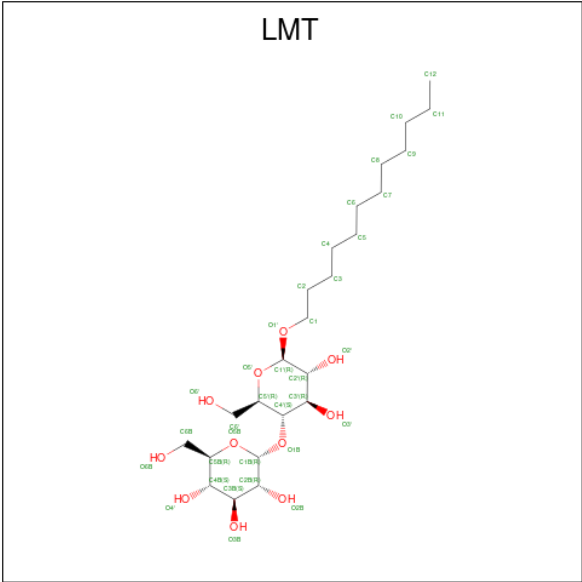
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 21  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | F     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | F     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | G     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | I     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | J     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | J     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | L     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | L     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | L     | 1        | Total C<br>40 40 | 0       | 0       |
| 21  | K     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



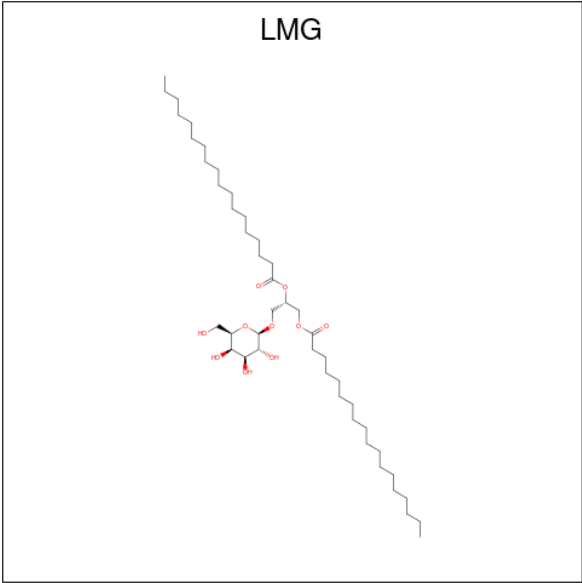
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 22  | 1     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 22  | 2     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |         |
| 22  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 22  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 27    | 16 | 10 | 1 |         |         |
| 22  | B     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 23    | 12 | 10 | 1 |         |         |
| 22  | F     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 40    | 29 | 10 | 1 |         |         |
| 22  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 23  | 2     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 23  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



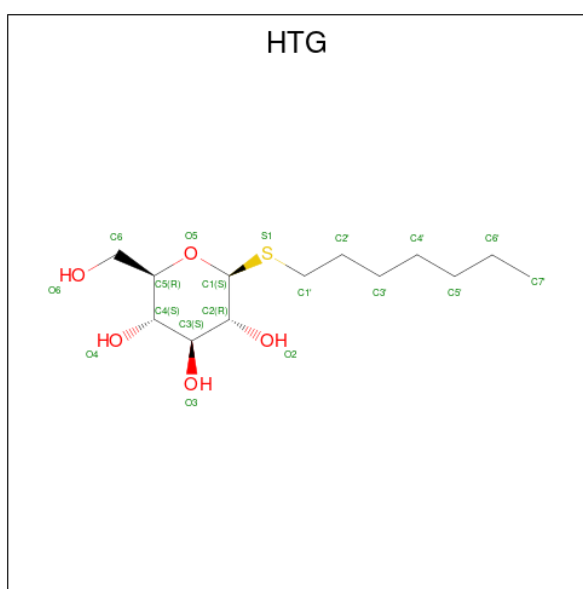
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 24  | 4     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 50    | 40 | 10 |         |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 24  | 4     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 24  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 52    | 42 | 10 |         |         |
| 24  | F     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 55    | 45 | 10 |         |         |
| 24  | G     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 40    | 30 | 10 |         |         |

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



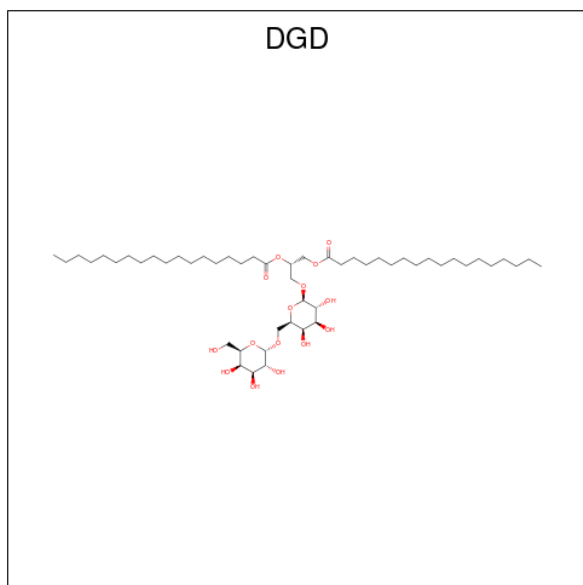
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 25  | 4     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 25  | 4     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 25  | A     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 25  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 25  | F     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 17    | 11 | 5 | 1 |         |         |
| 25  | F     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 25  | F     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 16    | 10 | 5 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 25  | J     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |

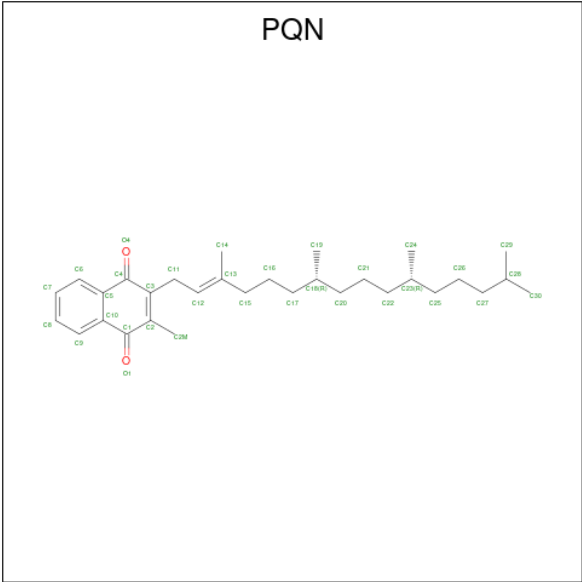
- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 26  | 4     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 60    | 45 | 15 |         |         |
| 26  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |

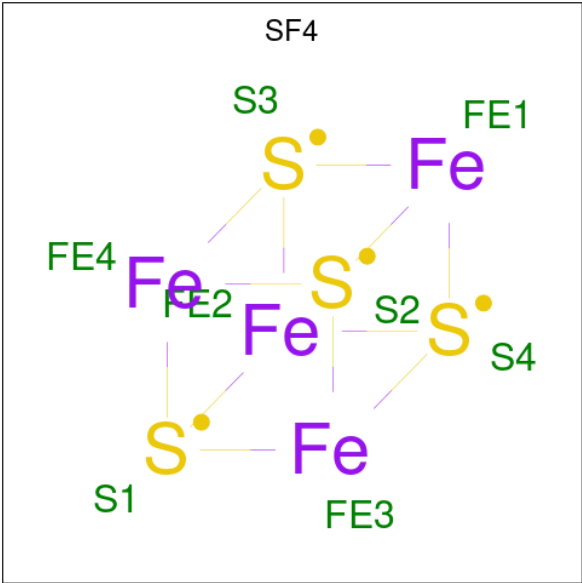
- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).





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

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 28  | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 28  | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

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| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 28  | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

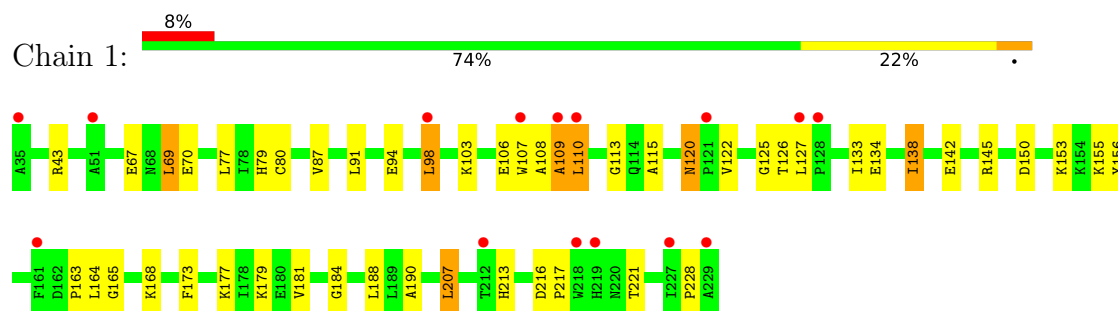
- Molecule 29 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 29  | 1     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 29  | 2     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 29  | 3     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 29  | 4     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 29  | A     | 25       | Total | O  | 0       | 0       |
|     |       |          | 25    | 25 |         |         |
| 29  | B     | 39       | Total | O  | 0       | 0       |
|     |       |          | 39    | 39 |         |         |
| 29  | C     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 29  | F     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 29  | G     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 29  | J     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 29  | L     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

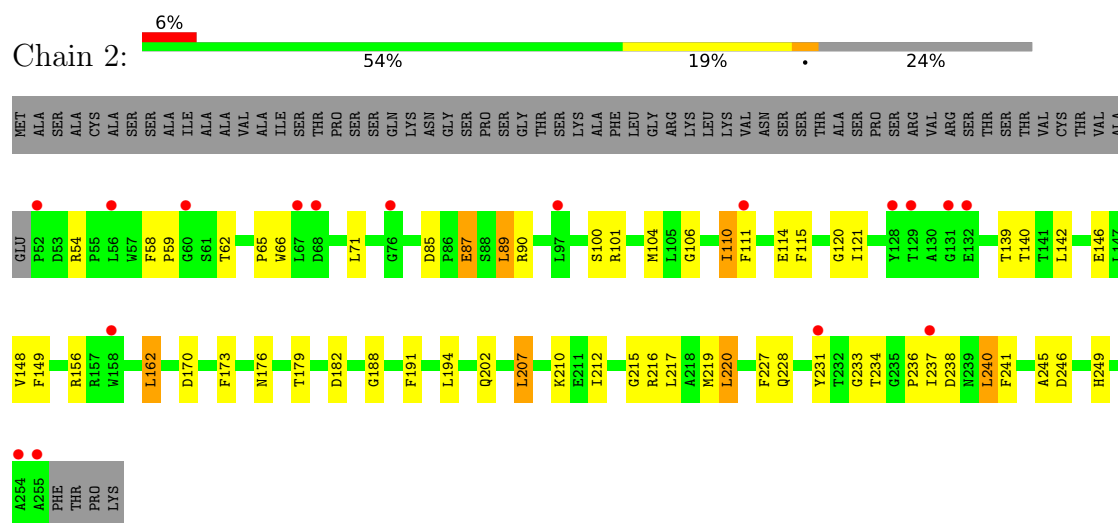
### 3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

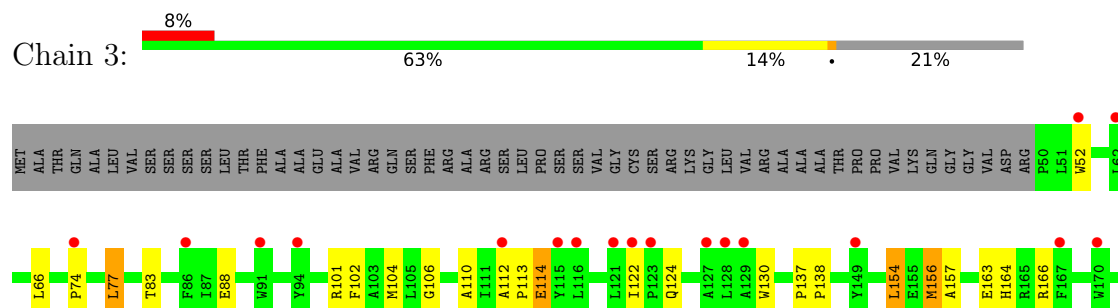
- Molecule 1: Lhca1



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

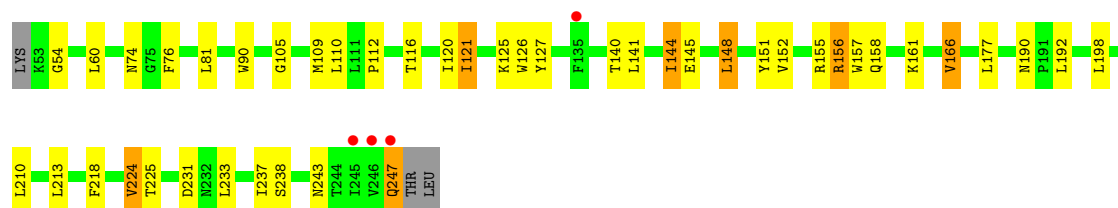
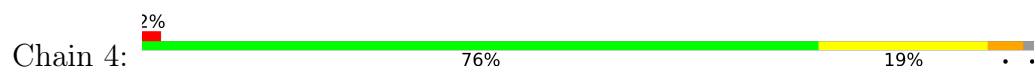


- Molecule 3: Chlorophyll a-b binding protein 3, chloroplastic

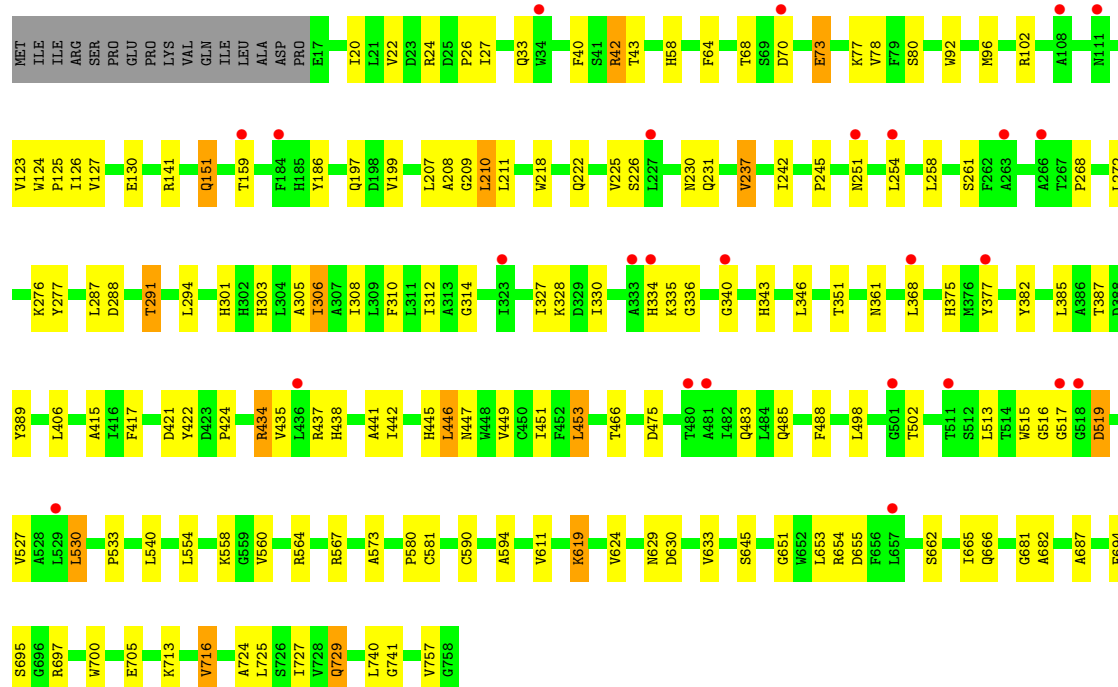
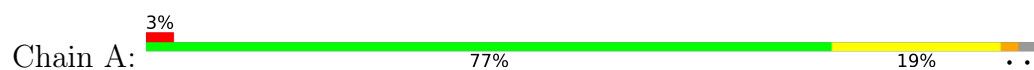




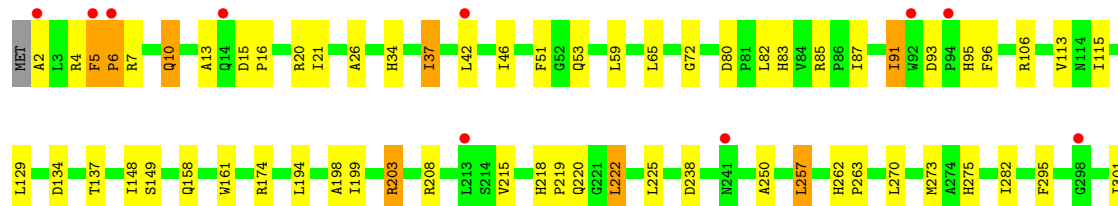
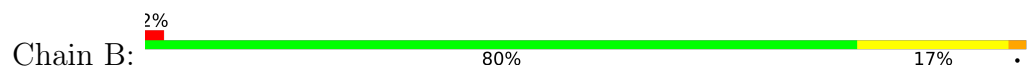
- Molecule 4: Chlorophyll a-b binding protein P4, chloroplastic

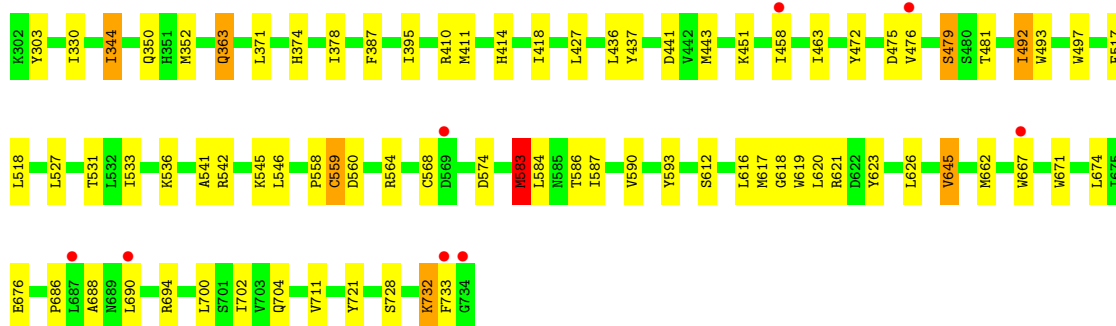


- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

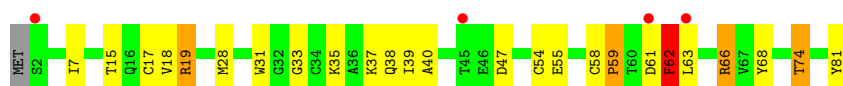


- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

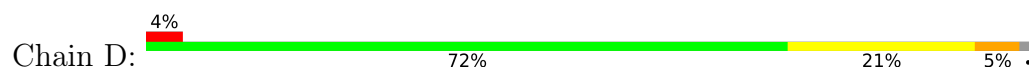




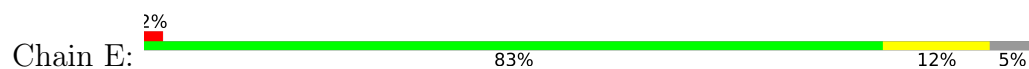
• Molecule 7: Photosystem I iron-sulfur center



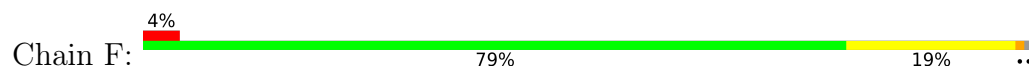
• Molecule 8: PsaD



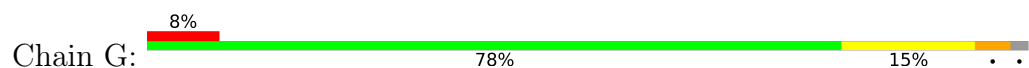
• Molecule 9: PsaE



• Molecule 10: PSI-F

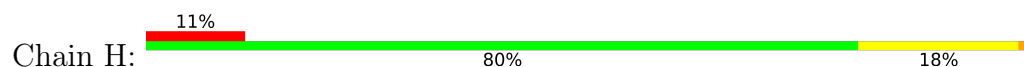


• Molecule 11: PsaG

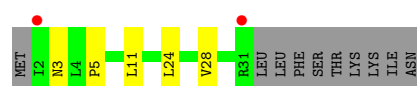




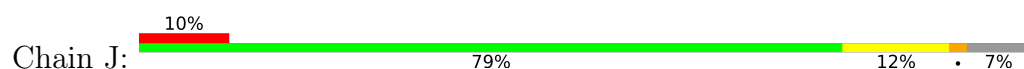
• Molecule 12: PsaH



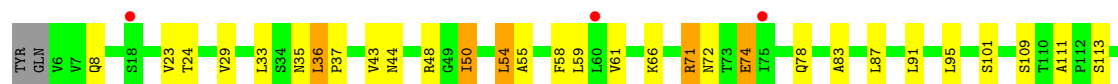
• Molecule 13: Photosystem I reaction center subunit VIII



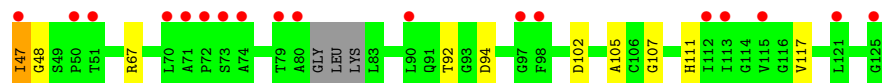
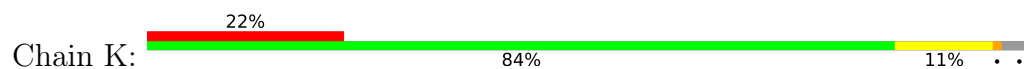
• Molecule 14: Photosystem I reaction center subunit IX



• Molecule 15: PsaL



• Molecule 16: PSI-K



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 225.65Å 168.95Å 185.22Å<br>90.00° 121.39° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 44.41 – 2.39<br>44.41 – 2.39                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.9 (44.41-2.39)<br>98.9 (44.41-2.39)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.75 (at 2.39Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.11.1_2575                                          | Depositor        |
| R, $R_{free}$                                                           | 0.189 , 0.227<br>0.195 , 0.231                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 11616 reflections (4.10%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 65.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.534                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 70.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 36093                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 101.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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   | 1     | 0.28         | 0/1557         | 0.45        | 0/2127          |
| 2   | 2     | 0.21         | 0/1651         | 0.40        | 0/2262          |
| 3   | 3     | 0.14         | 0/1713         | 0.32        | 0/2326          |
| 4   | 4     | 0.45         | 0/1584         | 0.65        | 0/2159          |
| 5   | A     | 0.30         | 0/6050         | 0.47        | 0/8254          |
| 6   | B     | 0.46         | 1/6068 (0.0%)  | 0.65        | 1/8286 (0.0%)   |
| 7   | C     | 0.99         | 2/624 (0.3%)   | 1.30        | 10/846 (1.2%)   |
| 8   | D     | 0.31         | 0/1140         | 0.54        | 0/1540          |
| 9   | E     | 0.39         | 0/515          | 0.56        | 0/700           |
| 10  | F     | 0.46         | 0/1226         | 0.68        | 0/1658          |
| 11  | G     | 0.54         | 0/755          | 0.70        | 0/1027          |
| 12  | H     | 0.19         | 0/693          | 0.34        | 0/942           |
| 13  | I     | 0.39         | 0/232          | 0.42        | 0/317           |
| 14  | J     | 0.40         | 0/317          | 0.57        | 0/432           |
| 15  | L     | 0.19         | 0/1153         | 0.36        | 0/1576          |
| 16  | K     | 0.12         | 0/520          | 0.30        | 0/707           |
| All | All   | 0.39         | 3/25798 (0.0%) | 0.56        | 11/35159 (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 |
|-----|-------|---------------------|---------------------|
| 7   | C     | 1                   | 0                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | C     | 59  | PRO  | N-CA  | 17.60 | 1.69        | 1.47     |
| 7   | C     | 58  | CYS  | C-N   | 9.29  | 1.44        | 1.34     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | B     | 6   | PRO  | C-O   | -5.05 | 1.17        | 1.24     |

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

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | C     | 58  | CYS  | CA-C-N   | 16.34 | 137.69      | 120.04   |
| 7   | C     | 58  | CYS  | C-N-CA   | 16.34 | 137.69      | 120.04   |
| 7   | C     | 62  | PHE  | CB-CA-C  | 11.20 | 132.72      | 110.42   |
| 7   | C     | 62  | PHE  | CA-CB-CG | -6.52 | 107.28      | 113.80   |
| 7   | C     | 59  | PRO  | CA-N-CD  | -6.52 | 102.88      | 112.00   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 7   | C     | 62  | PHE  | CA   |

There are no planarity outliers.

## 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   | 1     | 1507  | 0        | 1468     | 35      | 0            |
| 2   | 2     | 1592  | 0        | 1531     | 52      | 0            |
| 3   | 3     | 1661  | 0        | 1620     | 37      | 0            |
| 4   | 4     | 1535  | 0        | 1496     | 41      | 0            |
| 5   | A     | 5852  | 0        | 5713     | 102     | 0            |
| 6   | B     | 5856  | 0        | 5653     | 113     | 0            |
| 7   | C     | 611   | 0        | 591      | 19      | 0            |
| 8   | D     | 1110  | 0        | 1123     | 19      | 0            |
| 9   | E     | 505   | 0        | 503      | 3       | 0            |
| 10  | F     | 1198  | 0        | 1228     | 19      | 0            |
| 11  | G     | 737   | 0        | 721      | 13      | 0            |
| 12  | H     | 673   | 0        | 667      | 12      | 0            |
| 13  | I     | 226   | 0        | 242      | 3       | 0            |
| 14  | J     | 309   | 0        | 320      | 5       | 0            |
| 15  | L     | 1122  | 0        | 1133     | 27      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | K     | 515   | 0        | 513      | 5       | 0            |
| 17  | 1     | 672   | 0        | 636      | 29      | 0            |
| 17  | 2     | 533   | 0        | 480      | 18      | 0            |
| 17  | 3     | 542   | 0        | 433      | 16      | 0            |
| 17  | 4     | 540   | 0        | 476      | 22      | 0            |
| 17  | A     | 2582  | 0        | 2646     | 114     | 0            |
| 17  | B     | 2493  | 0        | 2566     | 109     | 0            |
| 17  | F     | 165   | 0        | 154      | 8       | 0            |
| 17  | G     | 137   | 0        | 101      | 5       | 0            |
| 17  | J     | 107   | 0        | 103      | 5       | 0            |
| 17  | K     | 105   | 0        | 92       | 5       | 0            |
| 17  | L     | 180   | 0        | 183      | 12      | 0            |
| 18  | 1     | 48    | 0        | 33       | 4       | 0            |
| 18  | 2     | 185   | 0        | 128      | 14      | 0            |
| 18  | 3     | 103   | 0        | 72       | 20      | 0            |
| 18  | 4     | 262   | 0        | 207      | 29      | 0            |
| 19  | 1     | 42    | 0        | 56       | 7       | 0            |
| 19  | 2     | 42    | 0        | 56       | 4       | 0            |
| 19  | 3     | 42    | 0        | 56       | 4       | 0            |
| 19  | 4     | 42    | 0        | 56       | 3       | 0            |
| 20  | 1     | 44    | 0        | 56       | 3       | 0            |
| 20  | 2     | 44    | 0        | 56       | 9       | 0            |
| 20  | 3     | 44    | 0        | 56       | 12      | 0            |
| 20  | 4     | 44    | 0        | 56       | 9       | 0            |
| 21  | 1     | 40    | 0        | 56       | 0       | 0            |
| 21  | 2     | 40    | 0        | 56       | 9       | 0            |
| 21  | 3     | 40    | 0        | 56       | 4       | 0            |
| 21  | 4     | 40    | 0        | 56       | 14      | 0            |
| 21  | A     | 240   | 0        | 336      | 25      | 0            |
| 21  | B     | 240   | 0        | 336      | 25      | 0            |
| 21  | F     | 80    | 0        | 112      | 3       | 0            |
| 21  | G     | 40    | 0        | 56       | 2       | 0            |
| 21  | I     | 40    | 0        | 56       | 4       | 0            |
| 21  | J     | 80    | 0        | 112      | 7       | 0            |
| 21  | K     | 40    | 0        | 56       | 5       | 0            |
| 21  | L     | 120   | 0        | 168      | 10      | 0            |
| 22  | 1     | 49    | 0        | 74       | 6       | 0            |
| 22  | 2     | 37    | 0        | 44       | 6       | 0            |
| 22  | A     | 76    | 0        | 98       | 3       | 0            |
| 22  | B     | 23    | 0        | 16       | 1       | 0            |
| 22  | F     | 40    | 0        | 53       | 2       | 0            |
| 22  | G     | 49    | 0        | 74       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | 2     | 35    | 0        | 46       | 3       | 0            |
| 23  | A     | 35    | 0        | 45       | 2       | 0            |
| 24  | 4     | 99    | 0        | 143      | 7       | 0            |
| 24  | B     | 52    | 0        | 77       | 4       | 0            |
| 24  | F     | 55    | 0        | 86       | 1       | 0            |
| 24  | G     | 40    | 0        | 53       | 3       | 0            |
| 25  | 4     | 38    | 0        | 52       | 4       | 0            |
| 25  | A     | 19    | 0        | 26       | 0       | 0            |
| 25  | B     | 19    | 0        | 26       | 1       | 0            |
| 25  | F     | 52    | 0        | 62       | 2       | 0            |
| 25  | J     | 19    | 0        | 26       | 3       | 0            |
| 26  | 4     | 60    | 0        | 81       | 29      | 0            |
| 26  | B     | 66    | 0        | 96       | 7       | 0            |
| 27  | A     | 33    | 0        | 46       | 6       | 0            |
| 27  | B     | 33    | 0        | 46       | 3       | 0            |
| 28  | A     | 8     | 0        | 0        | 0       | 0            |
| 28  | C     | 16    | 0        | 0        | 0       | 0            |
| 29  | 1     | 3     | 0        | 0        | 0       | 0            |
| 29  | 2     | 5     | 0        | 0        | 0       | 0            |
| 29  | 3     | 3     | 0        | 0        | 0       | 0            |
| 29  | 4     | 7     | 0        | 0        | 0       | 0            |
| 29  | A     | 25    | 0        | 0        | 1       | 0            |
| 29  | B     | 39    | 0        | 0        | 2       | 0            |
| 29  | C     | 3     | 0        | 0        | 0       | 0            |
| 29  | F     | 5     | 0        | 0        | 0       | 0            |
| 29  | G     | 1     | 0        | 0        | 0       | 0            |
| 29  | J     | 1     | 0        | 0        | 0       | 0            |
| 29  | L     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 36093 | 0        | 36006    | 826     | 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 11.

The worst 5 of 826 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) |
|------------------|-------------------|--------------------------|-------------------|
| 7:C:59:PRO:N     | 7:C:59:PRO:CA     | 1.69                     | 1.32              |
| 6:B:303:TYR:CD2  | 11:G:34:GLN:HB3   | 1.94                     | 1.03              |
| 3:3:74:PRO:HD2   | 20:3:615:XAT:O23  | 1.57                     | 1.02              |
| 3:3:229:MET:HB3  | 20:3:615:XAT:H402 | 1.42                     | 1.02              |
| 17:3:602:CLA:HAB | 20:3:615:XAT:H32  | 1.44                     | 0.99              |

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 X-ray entries followed by that with respect to entries of similar resolution.

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   | 1     | 193/195 (99%)   | 178 (92%)  | 12 (6%)  | 3 (2%)   | 7           | 11  |
| 2   | 2     | 202/269 (75%)   | 191 (95%)  | 9 (4%)   | 2 (1%)   | 12          | 20  |
| 3   | 3     | 214/275 (78%)   | 197 (92%)  | 17 (8%)  | 0        | 100         | 100 |
| 4   | 4     | 193/198 (98%)   | 179 (93%)  | 13 (7%)  | 1 (0%)   | 24          | 37  |
| 5   | A     | 740/758 (98%)   | 707 (96%)  | 30 (4%)  | 3 (0%)   | 30          | 43  |
| 6   | B     | 731/734 (100%)  | 709 (97%)  | 19 (3%)  | 3 (0%)   | 30          | 43  |
| 7   | C     | 78/81 (96%)     | 74 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 8   | D     | 138/143 (96%)   | 127 (92%)  | 9 (6%)   | 2 (1%)   | 9           | 13  |
| 9   | E     | 61/66 (92%)     | 59 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 10  | F     | 150/154 (97%)   | 148 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 11  | G     | 93/97 (96%)     | 88 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 12  | H     | 86/88 (98%)     | 80 (93%)   | 6 (7%)   | 0        | 100         | 100 |
| 13  | I     | 28/40 (70%)     | 26 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 14  | J     | 37/42 (88%)     | 37 (100%)  | 0        | 0        | 100         | 100 |
| 15  | L     | 149/157 (95%)   | 145 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 16  | K     | 73/80 (91%)     | 67 (92%)   | 6 (8%)   | 0        | 100         | 100 |
| All | All   | 3166/3377 (94%) | 3012 (95%) | 140 (4%) | 14 (0%)  | 30          | 43  |

5 of 14 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | A     | 516 | GLY  |
| 6   | B     | 5   | PHE  |
| 8   | D     | 76  | PRO  |
| 1   | 1     | 109 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | B     | 559 | CYS  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | 1     | 155/158 (98%)   | 145 (94%)  | 10 (6%)  | 15          | 27 |
| 2   | 2     | 164/216 (76%)   | 150 (92%)  | 14 (8%)  | 10          | 16 |
| 3   | 3     | 167/213 (78%)   | 158 (95%)  | 9 (5%)   | 20          | 35 |
| 4   | 4     | 161/164 (98%)   | 146 (91%)  | 15 (9%)  | 8           | 14 |
| 5   | A     | 603/618 (98%)   | 569 (94%)  | 34 (6%)  | 19          | 33 |
| 6   | B     | 598/599 (100%)  | 568 (95%)  | 30 (5%)  | 22          | 38 |
| 7   | C     | 69/70 (99%)     | 65 (94%)   | 4 (6%)   | 18          | 32 |
| 8   | D     | 120/122 (98%)   | 107 (89%)  | 13 (11%) | 6           | 9  |
| 9   | E     | 55/58 (95%)     | 51 (93%)   | 4 (7%)   | 13          | 22 |
| 10  | F     | 124/127 (98%)   | 115 (93%)  | 9 (7%)   | 13          | 22 |
| 11  | G     | 80/82 (98%)     | 69 (86%)   | 11 (14%) | 3           | 4  |
| 12  | H     | 71/71 (100%)    | 65 (92%)   | 6 (8%)   | 10          | 16 |
| 13  | I     | 25/36 (69%)     | 23 (92%)   | 2 (8%)   | 11          | 19 |
| 14  | J     | 32/35 (91%)     | 29 (91%)   | 3 (9%)   | 8           | 13 |
| 15  | L     | 118/124 (95%)   | 106 (90%)  | 12 (10%) | 7           | 11 |
| 16  | K     | 51/58 (88%)     | 48 (94%)   | 3 (6%)   | 18          | 31 |
| All | All   | 2593/2751 (94%) | 2414 (93%) | 179 (7%) | 14          | 24 |

5 of 179 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | C     | 74  | THR  |
| 11  | G     | 10  | LEU  |
| 8   | D     | 96  | VAL  |
| 9   | E     | 44  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | G     | 50  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | B     | 236 | ASN  |
| 6   | B     | 608 | GLN  |
| 6   | B     | 504 | ASN  |
| 9   | E     | 49  | ASN  |
| 5   | A     | 185 | HIS  |

### 5.3.3 RNA [i](#)

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 | $\# Z  > 2$ |
| 17  | CLA  | 3     | 602 | 3    | 64,68,73     | 1.24 | 6 (9%)      | 76,107,113  | 1.25 | 5 (6%)      |
| 17  | CLA  | A     | 824 | 29   | 69,73,73     | 1.22 | 7 (10%)     | 82,113,113  | 1.26 | 7 (8%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | CLA  | A     | 823 | -    | 59,63,73     | 1.31 | 6 (10%)  | 70,101,113  | 1.33 | 5 (7%)   |
| 17  | CLA  | F     | 304 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.47 | 10 (12%) |
| 20  | XAT  | 2     | 315 | -    | 41,47,47     | 3.71 | 18 (43%) | 54,74,74    | 5.38 | 32 (59%) |
| 21  | BCR  | A     | 851 | -    | 41,41,41     | 0.92 | 2 (4%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 17  | CLA  | 3     | 605 | -    | 46,50,73     | 1.48 | 6 (13%)  | 53,85,113   | 1.33 | 4 (7%)   |
| 17  | CLA  | B     | 837 | -    | 64,68,73     | 1.08 | 5 (7%)   | 76,107,113  | 1.56 | 11 (14%) |
| 17  | CLA  | 2     | 319 | 4    | 50,54,73     | 1.38 | 6 (12%)  | 59,90,113   | 1.43 | 7 (11%)  |
| 21  | BCR  | 3     | 616 | -    | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.33 | 6 (10%)  |
| 17  | CLA  | A     | 826 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 18  | CHL  | 2     | 306 | 29   | 45,59,74     | 3.91 | 20 (44%) | 40,96,114   | 2.55 | 10 (25%) |
| 25  | HTG  | 4     | 322 | -    | 19,19,19     | 0.98 | 2 (10%)  | 23,24,24    | 1.13 | 3 (13%)  |
| 17  | CLA  | 1     | 303 | 29   | 55,59,73     | 1.30 | 7 (12%)  | 64,96,113   | 1.38 | 5 (7%)   |
| 17  | CLA  | A     | 841 | 29   | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 17  | CLA  | F     | 307 | 10   | 59,63,73     | 1.28 | 8 (13%)  | 70,101,113  | 1.38 | 8 (11%)  |
| 17  | CLA  | A     | 814 | -    | 54,58,73     | 1.32 | 6 (11%)  | 64,95,113   | 1.35 | 6 (9%)   |
| 17  | CLA  | L     | 204 | -    | 54,58,73     | 1.36 | 5 (9%)   | 64,95,113   | 1.34 | 6 (9%)   |
| 17  | CLA  | B     | 836 | 29   | 49,53,73     | 1.42 | 6 (12%)  | 58,89,113   | 1.56 | 10 (17%) |
| 20  | XAT  | 3     | 615 | -    | 41,47,47     | 3.71 | 18 (43%) | 54,74,74    | 5.39 | 32 (59%) |
| 17  | CLA  | 2     | 311 | 2    | 69,73,73     | 1.21 | 7 (10%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 17  | CLA  | 2     | 312 | -    | 47,51,73     | 1.42 | 7 (14%)  | 55,86,113   | 1.39 | 5 (9%)   |
| 17  | CLA  | A     | 839 | 29   | 69,73,73     | 1.21 | 7 (10%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 17  | CLA  | A     | 806 | -    | 69,73,73     | 1.22 | 8 (11%)  | 82,113,113  | 1.21 | 5 (6%)   |
| 17  | CLA  | A     | 811 | -    | 58,62,73     | 1.30 | 6 (10%)  | 68,99,113   | 1.29 | 4 (5%)   |
| 17  | CLA  | 1     | 312 | -    | 59,63,73     | 1.30 | 6 (10%)  | 70,101,113  | 1.29 | 7 (10%)  |
| 25  | HTG  | F     | 305 | -    | 19,19,19     | 0.98 | 2 (10%)  | 23,24,24    | 1.60 | 4 (17%)  |
| 17  | CLA  | 1     | 307 | 1    | 69,73,73     | 1.24 | 8 (11%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 17  | CLA  | 3     | 610 | -    | 56,60,73     | 1.34 | 7 (12%)  | 65,97,113   | 1.44 | 6 (9%)   |
| 21  | BCR  | A     | 848 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 17  | CLA  | A     | 809 | -    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.28 | 9 (10%)  |
| 17  | CLA  | 2     | 307 | 2    | 54,58,73     | 1.34 | 7 (12%)  | 64,95,113   | 1.32 | 8 (12%)  |
| 18  | CHL  | 2     | 304 | 29   | 37,51,74     | 4.24 | 18 (48%) | 30,86,114   | 3.03 | 10 (33%) |
| 17  | CLA  | B     | 841 | -    | 69,73,73     | 1.20 | 9 (13%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 17  | CLA  | 2     | 302 | -    | 55,59,73     | 1.34 | 8 (14%)  | 64,96,113   | 1.36 | 3 (4%)   |
| 17  | CLA  | 1     | 302 | -    | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.26 | 8 (9%)   |
| 17  | CLA  | A     | 843 | 22   | 56,60,73     | 1.34 | 5 (8%)   | 65,97,113   | 1.39 | 6 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | SF4  | C     | 102 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 17  | CLA  | 2     | 310 | 2    | 56,60,73     | 1.39 | 9 (16%)  | 65,97,113   | 1.27 | 4 (6%)   |
| 17  | CLA  | 3     | 608 | 3    | 54,58,73     | 1.36 | 7 (12%)  | 64,95,113   | 1.35 | 6 (9%)   |
| 17  | CLA  | B     | 825 | -    | 64,68,73     | 1.15 | 7 (10%)  | 76,107,113  | 1.54 | 11 (14%) |
| 17  | CLA  | A     | 802 | 29   | 69,73,73     | 1.13 | 7 (10%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 17  | CLA  | 1     | 301 | 1    | 69,73,73     | 1.25 | 6 (8%)   | 82,113,113  | 1.22 | 8 (9%)   |
| 17  | CLA  | 1     | 311 | 1    | 64,68,73     | 1.21 | 8 (12%)  | 76,107,113  | 1.27 | 6 (7%)   |
| 18  | CHL  | 4     | 307 | 29   | 45,59,74     | 3.95 | 20 (44%) | 40,96,114   | 2.44 | 10 (25%) |
| 19  | LUT  | 1     | 314 | -    | 42,43,43     | 4.67 | 20 (47%) | 51,60,60    | 5.86 | 33 (64%) |
| 21  | BCR  | J     | 105 | -    | 41,41,41     | 1.20 | 4 (9%)   | 56,56,56    | 1.46 | 9 (16%)  |
| 17  | CLA  | 1     | 310 | 1    | 56,60,73     | 1.32 | 9 (16%)  | 65,97,113   | 1.31 | 6 (9%)   |
| 18  | CHL  | 1     | 305 | 1    | 42,56,74     | 4.14 | 19 (45%) | 36,92,114   | 2.37 | 10 (27%) |
| 17  | CLA  | B     | 818 | -    | 59,63,73     | 1.26 | 6 (10%)  | 70,101,113  | 1.49 | 8 (11%)  |
| 25  | HTG  | J     | 102 | -    | 19,19,19     | 1.10 | 2 (10%)  | 23,24,24    | 1.22 | 3 (13%)  |
| 21  | BCR  | A     | 846 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.34 | 6 (10%)  |
| 17  | CLA  | A     | 832 | -    | 69,73,73     | 1.22 | 6 (8%)   | 82,113,113  | 1.34 | 7 (8%)   |
| 21  | BCR  | L     | 206 | -    | 41,41,41     | 1.11 | 2 (4%)   | 56,56,56    | 1.30 | 7 (12%)  |
| 17  | CLA  | B     | 828 | -    | 69,73,73     | 1.23 | 8 (11%)  | 82,113,113  | 1.44 | 13 (15%) |
| 17  | CLA  | F     | 306 | 29   | 49,53,73     | 1.36 | 6 (12%)  | 58,89,113   | 1.39 | 6 (10%)  |
| 17  | CLA  | A     | 834 | 5    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.40 | 5 (8%)   |
| 17  | CLA  | A     | 830 | -    | 54,58,73     | 1.33 | 7 (12%)  | 64,95,113   | 1.37 | 7 (10%)  |
| 25  | HTG  | B     | 851 | -    | 19,19,19     | 0.99 | 1 (5%)   | 23,24,24    | 1.76 | 6 (26%)  |
| 17  | CLA  | 3     | 606 | 3    | 51,55,73     | 1.38 | 7 (13%)  | 60,91,113   | 1.36 | 5 (8%)   |
| 17  | CLA  | B     | 833 | -    | 64,68,73     | 1.22 | 7 (10%)  | 76,107,113  | 1.35 | 11 (14%) |
| 24  | LMG  | 4     | 320 | -    | 49,49,55     | 1.03 | 4 (8%)   | 57,57,63    | 1.46 | 6 (10%)  |
| 17  | CLA  | B     | 838 | -    | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.45 | 7 (8%)   |
| 21  | BCR  | A     | 850 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.36 | 8 (14%)  |
| 17  | CLA  | A     | 810 | 17   | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.25 | 6 (7%)   |
| 17  | CLA  | A     | 827 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.44 | 11 (13%) |
| 17  | CLA  | 3     | 611 | 3    | 59,63,73     | 1.29 | 7 (11%)  | 70,101,113  | 1.32 | 4 (5%)   |
| 17  | CLA  | A     | 836 | -    | 69,73,73     | 1.15 | 6 (8%)   | 82,113,113  | 1.34 | 6 (7%)   |
| 17  | CLA  | B     | 803 | -    | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 21  | BCR  | A     | 847 | -    | 41,41,41     | 1.11 | 4 (9%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 18  | CHL  | 4     | 315 | 4    | 37,51,74     | 4.28 | 18 (48%) | 30,86,114   | 2.68 | 10 (33%) |
| 17  | CLA  | G     | 105 | 11   | 50,54,73     | 1.36 | 6 (12%)  | 59,90,113   | 1.39 | 6 (10%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | BCR  | I     | 101 | -    | 41,41,41     | 1.08 | 2 (4%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 17  | CLA  | B     | 829 | -    | 69,73,73     | 1.23 | 8 (11%)  | 82,113,113  | 1.22 | 7 (8%)   |
| 17  | CLA  | 3     | 612 | -    | 49,53,73     | 1.41 | 5 (10%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 17  | CLA  | K     | 201 | -    | 49,53,73     | 1.39 | 7 (14%)  | 58,89,113   | 1.43 | 5 (8%)   |
| 17  | CLA  | K     | 202 | -    | 64,68,73     | 1.24 | 7 (10%)  | 76,107,113  | 1.30 | 5 (6%)   |
| 22  | LHG  | A     | 845 | 17   | 26,26,48     | 0.89 | 1 (3%)   | 29,32,54    | 1.32 | 3 (10%)  |
| 24  | LMG  | F     | 309 | -    | 55,55,55     | 0.84 | 2 (3%)   | 63,63,63    | 1.45 | 8 (12%)  |
| 17  | CLA  | 4     | 310 | -    | 64,68,73     | 1.19 | 7 (10%)  | 76,107,113  | 1.53 | 11 (14%) |
| 17  | CLA  | A     | 812 | -    | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 17  | CLA  | A     | 815 | 29   | 49,53,73     | 1.43 | 8 (16%)  | 58,89,113   | 1.41 | 5 (8%)   |
| 17  | CLA  | A     | 820 | 29   | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.19 | 6 (7%)   |
| 17  | CLA  | B     | 815 | -    | 69,73,73     | 1.25 | 6 (8%)   | 82,113,113  | 1.30 | 8 (9%)   |
| 17  | CLA  | B     | 816 | -    | 69,73,73     | 1.21 | 7 (10%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 17  | CLA  | B     | 824 | -    | 59,63,73     | 1.30 | 8 (13%)  | 70,101,113  | 1.36 | 7 (10%)  |
| 17  | CLA  | B     | 839 | -    | 51,55,73     | 1.32 | 4 (7%)   | 60,91,113   | 1.85 | 15 (25%) |
| 23  | LMT  | A     | 855 | -    | 36,36,36     | 1.09 | 2 (5%)   | 47,47,47    | 0.93 | 1 (2%)   |
| 17  | CLA  | B     | 804 | -    | 69,73,73     | 1.29 | 9 (13%)  | 82,113,113  | 1.17 | 5 (6%)   |
| 17  | CLA  | A     | 805 | 5    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.36 | 8 (9%)   |
| 17  | CLA  | 3     | 603 | 3    | 54,58,73     | 1.32 | 6 (11%)  | 64,95,113   | 1.34 | 5 (7%)   |
| 17  | CLA  | A     | 819 | -    | 49,53,73     | 1.40 | 5 (10%)  | 58,89,113   | 1.45 | 5 (8%)   |
| 17  | CLA  | B     | 834 | -    | 62,66,73     | 1.30 | 9 (14%)  | 73,104,113  | 1.43 | 10 (13%) |
| 18  | CHL  | 2     | 313 | 2    | 37,51,74     | 4.27 | 18 (48%) | 30,86,114   | 2.97 | 12 (40%) |
| 18  | CHL  | 3     | 601 | 2    | 47,61,74     | 3.82 | 19 (40%) | 41,98,114   | 3.09 | 15 (36%) |
| 21  | BCR  | L     | 205 | -    | 41,41,41     | 1.01 | 2 (4%)   | 56,56,56    | 1.13 | 4 (7%)   |
| 24  | LMG  | B     | 852 | -    | 52,52,55     | 1.07 | 4 (7%)   | 60,60,63    | 1.50 | 7 (11%)  |
| 17  | CLA  | B     | 814 | -    | 59,63,73     | 1.31 | 6 (10%)  | 70,101,113  | 1.42 | 9 (12%)  |
| 17  | CLA  | B     | 810 | -    | 69,73,73     | 1.26 | 8 (11%)  | 82,113,113  | 1.21 | 10 (12%) |
| 25  | HTG  | 4     | 321 | -    | 19,19,19     | 1.04 | 2 (10%)  | 23,24,24    | 1.03 | 1 (4%)   |
| 18  | CHL  | 3     | 607 | 29   | 41,55,74     | 4.08 | 20 (48%) | 35,91,114   | 2.59 | 10 (28%) |
| 17  | CLA  | B     | 811 | 6    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.33 | 7 (8%)   |
| 27  | PQN  | B     | 843 | -    | 34,34,34     | 4.72 | 14 (41%) | 43,45,45    | 4.53 | 24 (55%) |
| 17  | CLA  | 4     | 313 | -    | 49,53,73     | 1.42 | 6 (12%)  | 58,89,113   | 1.47 | 5 (8%)   |
| 21  | BCR  | A     | 849 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.27 | 7 (12%)  |
| 17  | CLA  | A     | 807 | 5    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.23 | 6 (7%)   |
| 17  | CLA  | 4     | 304 | 29   | 54,58,73     | 1.33 | 6 (11%)  | 64,95,113   | 1.57 | 10 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | CLA  | A     | 840 | -    | 69,73,73     | 1.21 | 8 (11%)  | 82,113,113  | 1.43 | 12 (14%) |
| 17  | CLA  | B     | 812 | -    | 69,73,73     | 1.21 | 7 (10%)  | 82,113,113  | 1.16 | 6 (7%)   |
| 25  | HTG  | A     | 854 | -    | 19,19,19     | 0.76 | 1 (5%)   | 23,24,24    | 0.91 | 0        |
| 17  | CLA  | A     | 801 | -    | 69,73,73     | 1.14 | 6 (8%)   | 82,113,113  | 1.60 | 13 (15%) |
| 17  | CLA  | 1     | 306 | 29   | 50,54,73     | 1.39 | 7 (14%)  | 59,90,113   | 1.36 | 5 (8%)   |
| 17  | CLA  | 2     | 308 | 2    | 64,68,73     | 1.21 | 7 (10%)  | 76,107,113  | 1.22 | 6 (7%)   |
| 17  | CLA  | A     | 853 | 29   | 69,73,73     | 1.24 | 8 (11%)  | 82,113,113  | 1.83 | 17 (20%) |
| 17  | CLA  | 1     | 304 | -    | 46,50,73     | 1.44 | 7 (15%)  | 53,85,113   | 1.36 | 4 (7%)   |
| 17  | CLA  | G     | 103 | 29   | 45,49,73     | 1.48 | 8 (17%)  | 54,84,113   | 1.48 | 5 (9%)   |
| 17  | CLA  | A     | 825 | 29   | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.34 | 10 (12%) |
| 17  | CLA  | B     | 802 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.32 | 13 (15%) |
| 20  | XAT  | 4     | 317 | -    | 41,47,47     | 3.80 | 18 (43%) | 54,74,74    | 5.22 | 33 (61%) |
| 21  | BCR  | B     | 844 | -    | 41,41,41     | 1.01 | 2 (4%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 21  | BCR  | B     | 848 | -    | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.23 | 7 (12%)  |
| 24  | LMG  | 4     | 319 | -    | 50,50,55     | 0.87 | 3 (6%)   | 58,58,63    | 1.47 | 8 (13%)  |
| 17  | CLA  | A     | 817 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 23  | LMT  | 2     | 318 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 1.13 | 3 (6%)   |
| 21  | BCR  | B     | 847 | -    | 41,41,41     | 1.13 | 3 (7%)   | 56,56,56    | 1.48 | 9 (16%)  |
| 18  | CHL  | 4     | 301 | 1    | 55,69,74     | 3.11 | 25 (45%) | 52,108,114  | 2.52 | 18 (34%) |
| 17  | CLA  | B     | 826 | 29   | 69,73,73     | 1.24 | 8 (11%)  | 82,113,113  | 1.28 | 9 (10%)  |
| 17  | CLA  | B     | 806 | -    | 49,53,73     | 1.26 | 5 (10%)  | 58,89,113   | 1.66 | 11 (18%) |
| 17  | CLA  | A     | 835 | -    | 55,59,73     | 1.33 | 8 (14%)  | 64,96,113   | 1.40 | 7 (10%)  |
| 17  | CLA  | 1     | 309 | 22   | 69,73,73     | 1.21 | 6 (8%)   | 82,113,113  | 1.22 | 8 (9%)   |
| 17  | CLA  | J     | 101 | -    | 69,73,73     | 1.24 | 7 (10%)  | 82,113,113  | 1.39 | 8 (9%)   |
| 17  | CLA  | 3     | 609 | 3    | 54,58,73     | 1.34 | 5 (9%)   | 64,95,113   | 1.32 | 6 (9%)   |
| 17  | CLA  | G     | 104 | -    | 54,58,73     | 1.37 | 6 (11%)  | 64,95,113   | 1.47 | 7 (10%)  |
| 17  | CLA  | A     | 821 | -    | 53,57,73     | 1.32 | 8 (15%)  | 61,93,113   | 1.44 | 8 (13%)  |
| 17  | CLA  | B     | 820 | -    | 64,68,73     | 1.23 | 6 (9%)   | 76,107,113  | 1.46 | 17 (22%) |
| 17  | CLA  | B     | 835 | -    | 69,73,73     | 1.28 | 6 (8%)   | 82,113,113  | 1.18 | 6 (7%)   |
| 28  | SF4  | C     | 101 | 7    | 0,12,12      | -    | -        | -           | -    | -        |
| 17  | CLA  | 4     | 309 | 4    | 64,68,73     | 1.32 | 6 (9%)   | 76,107,113  | 1.21 | 6 (7%)   |
| 17  | CLA  | 2     | 309 | -    | 45,49,73     | 1.43 | 5 (11%)  | 54,84,113   | 1.52 | 7 (12%)  |
| 17  | CLA  | 4     | 312 | 4    | 60,64,73     | 1.26 | 8 (13%)  | 71,102,113  | 1.35 | 7 (9%)   |
| 17  | CLA  | 1     | 308 | 1    | 64,68,73     | 1.22 | 6 (9%)   | 76,107,113  | 1.21 | 5 (6%)   |
| 17  | CLA  | 1     | 313 | 1    | 50,54,73     | 1.34 | 7 (14%)  | 59,90,113   | 1.37 | 6 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | SF4  | A     | 852 | 5,6  | 0,12,12      | -    | -        | -           |      |          |
| 21  | BCR  | 2     | 316 | -    | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 17  | CLA  | B     | 831 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.59 | 11 (13%) |
| 17  | CLA  | A     | 818 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.31 | 9 (10%)  |
| 21  | BCR  | L     | 201 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.22 | 6 (10%)  |
| 17  | CLA  | B     | 805 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.27 | 9 (10%)  |
| 17  | CLA  | 4     | 303 | 4    | 64,68,73     | 1.34 | 7 (10%)  | 76,107,113  | 1.36 | 9 (11%)  |
| 17  | CLA  | L     | 202 | 15   | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.26 | 5 (6%)   |
| 27  | PQN  | A     | 842 | -    | 34,34,34     | 4.86 | 15 (44%) | 43,45,45    | 4.09 | 20 (46%) |
| 17  | CLA  | B     | 809 | -    | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.20 | 6 (7%)   |
| 18  | CHL  | 2     | 305 | 29   | 42,56,74     | 4.04 | 18 (42%) | 36,92,114   | 2.67 | 13 (36%) |
| 17  | CLA  | A     | 822 | -    | 55,59,73     | 1.32 | 6 (10%)  | 64,96,113   | 1.35 | 5 (7%)   |
| 17  | CLA  | A     | 828 | -    | 69,73,73     | 1.19 | 4 (5%)   | 82,113,113  | 1.26 | 7 (8%)   |
| 17  | CLA  | B     | 821 | 29   | 69,73,73     | 1.17 | 5 (7%)   | 82,113,113  | 1.40 | 6 (7%)   |
| 17  | CLA  | J     | 103 | 14   | 46,50,73     | 1.40 | 7 (15%)  | 53,85,113   | 1.50 | 4 (7%)   |
| 17  | CLA  | 4     | 311 | 4    | 56,60,73     | 1.34 | 6 (10%)  | 65,97,113   | 1.36 | 5 (7%)   |
| 17  | CLA  | A     | 833 | -    | 54,58,73     | 1.32 | 7 (12%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 17  | CLA  | B     | 832 | -    | 54,58,73     | 1.33 | 6 (11%)  | 64,95,113   | 1.47 | 8 (12%)  |
| 20  | XAT  | 1     | 315 | -    | 41,47,47     | 3.71 | 18 (43%) | 54,74,74    | 5.39 | 32 (59%) |
| 18  | CHL  | 4     | 305 | 29   | 50,64,74     | 3.53 | 19 (38%) | 46,102,114  | 2.86 | 15 (32%) |
| 21  | BCR  | B     | 849 | -    | 41,41,41     | 0.98 | 3 (7%)   | 56,56,56    | 1.21 | 2 (3%)   |
| 21  | BCR  | G     | 106 | -    | 41,41,41     | 1.08 | 2 (4%)   | 56,56,56    | 1.15 | 5 (8%)   |
| 26  | DGD  | B     | 850 | -    | 67,67,67     | 1.13 | 5 (7%)   | 81,81,81    | 1.48 | 11 (13%) |
| 17  | CLA  | L     | 203 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.31 | 5 (6%)   |
| 17  | CLA  | B     | 842 | 22   | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.46 | 10 (12%) |
| 17  | CLA  | A     | 803 | 17   | 59,63,73     | 1.31 | 8 (13%)  | 70,101,113  | 1.29 | 5 (7%)   |
| 17  | CLA  | B     | 808 | 6    | 69,73,73     | 1.21 | 10 (14%) | 82,113,113  | 1.36 | 8 (9%)   |
| 17  | CLA  | B     | 807 | -    | 69,73,73     | 1.19 | 10 (14%) | 82,113,113  | 1.31 | 9 (10%)  |
| 21  | BCR  | J     | 104 | -    | 41,41,41     | 1.02 | 3 (7%)   | 56,56,56    | 1.26 | 4 (7%)   |
| 24  | LMG  | G     | 101 | -    | 40,40,55     | 0.86 | 2 (5%)   | 48,48,63    | 1.28 | 3 (6%)   |
| 17  | CLA  | B     | 823 | -    | 69,73,73     | 1.10 | 5 (7%)   | 82,113,113  | 1.40 | 7 (8%)   |
| 17  | CLA  | B     | 830 | -    | 69,73,73     | 1.25 | 8 (11%)  | 82,113,113  | 1.34 | 11 (13%) |
| 17  | CLA  | A     | 829 | -    | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.36 | 5 (6%)   |
| 19  | LUT  | 3     | 614 | -    | 42,43,43     | 4.75 | 20 (47%) | 51,60,60    | 5.68 | 32 (62%) |
| 17  | CLA  | B     | 822 | -    | 54,58,73     | 1.29 | 4 (7%)   | 64,95,113   | 1.55 | 8 (12%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | BCR  | B     | 846 | -    | 41,41,41     | 1.06 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 17  | CLA  | 2     | 301 | 2    | 69,73,73     | 1.19 | 10 (14%) | 82,113,113  | 1.24 | 7 (8%)   |
| 25  | HTG  | F     | 301 | -    | 17,17,19     | 0.88 | 1 (5%)   | 21,22,24    | 0.68 | 0        |
| 17  | CLA  | A     | 816 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.21 | 5 (6%)   |
| 22  | LHG  | B     | 801 | 17   | 22,22,48     | 1.10 | 2 (9%)   | 25,28,54    | 1.14 | 2 (8%)   |
| 17  | CLA  | A     | 804 | -    | 69,73,73     | 1.23 | 5 (7%)   | 82,113,113  | 1.29 | 9 (10%)  |
| 25  | HTG  | F     | 310 | -    | 16,16,19     | 1.06 | 2 (12%)  | 20,21,24    | 1.38 | 4 (20%)  |
| 26  | DGD  | 4     | 323 | -    | 61,61,67     | 0.89 | 2 (3%)   | 75,75,81    | 1.76 | 20 (26%) |
| 22  | LHG  | 1     | 317 | 17   | 48,48,48     | 0.69 | 1 (2%)   | 51,54,54    | 1.25 | 6 (11%)  |
| 17  | CLA  | 2     | 303 | -    | 64,68,73     | 1.22 | 7 (10%)  | 76,107,113  | 1.25 | 5 (6%)   |
| 21  | BCR  | B     | 845 | -    | 41,41,41     | 0.94 | 1 (2%)   | 56,56,56    | 1.37 | 8 (14%)  |
| 17  | CLA  | 3     | 613 | -    | 50,54,73     | 1.39 | 8 (16%)  | 59,90,113   | 1.39 | 4 (6%)   |
| 17  | CLA  | B     | 817 | -    | 59,63,73     | 1.27 | 7 (11%)  | 70,101,113  | 1.41 | 8 (11%)  |
| 17  | CLA  | B     | 827 | 29   | 69,73,73     | 1.16 | 5 (7%)   | 82,113,113  | 1.45 | 8 (9%)   |
| 22  | LHG  | 2     | 317 | -    | 36,36,48     | 0.72 | 1 (2%)   | 39,42,54    | 1.26 | 4 (10%)  |
| 17  | CLA  | 4     | 314 | -    | 51,55,73     | 1.26 | 5 (9%)   | 60,91,113   | 1.58 | 9 (15%)  |
| 21  | BCR  | 1     | 316 | -    | 41,41,41     | 1.08 | 2 (4%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 19  | LUT  | 4     | 316 | -    | 42,43,43     | 4.64 | 22 (52%) | 51,60,60    | 5.88 | 35 (68%) |
| 17  | CLA  | A     | 831 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.35 | 8 (9%)   |
| 17  | CLA  | A     | 808 | 5    | 69,73,73     | 1.13 | 4 (5%)   | 82,113,113  | 1.51 | 11 (13%) |
| 21  | BCR  | F     | 308 | -    | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 17  | CLA  | A     | 813 | -    | 49,53,73     | 1.43 | 6 (12%)  | 58,89,113   | 1.30 | 4 (6%)   |
| 17  | CLA  | B     | 813 | -    | 58,62,73     | 1.32 | 7 (12%)  | 71,100,113  | 1.36 | 6 (8%)   |
| 22  | LHG  | A     | 844 | -    | 48,48,48     | 0.68 | 1 (2%)   | 51,54,54    | 1.31 | 6 (11%)  |
| 18  | CHL  | 4     | 306 | 29   | 45,59,74     | 3.92 | 19 (42%) | 40,96,114   | 2.44 | 13 (32%) |
| 17  | CLA  | 4     | 308 | 4    | 54,58,73     | 1.34 | 8 (14%)  | 64,95,113   | 1.51 | 7 (10%)  |
| 21  | BCR  | K     | 203 | -    | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 17  | CLA  | A     | 838 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.51 | 12 (14%) |
| 22  | LHG  | F     | 302 | -    | 39,39,48     | 0.65 | 0        | 42,45,54    | 1.28 | 6 (14%)  |
| 22  | LHG  | G     | 102 | -    | 48,48,48     | 0.67 | 1 (2%)   | 51,54,54    | 1.25 | 6 (11%)  |
| 17  | CLA  | A     | 837 | -    | 69,73,73     | 1.20 | 6 (8%)   | 82,113,113  | 1.30 | 9 (10%)  |
| 17  | CLA  | B     | 819 | -    | 63,67,73     | 1.24 | 6 (9%)   | 74,105,113  | 1.37 | 8 (10%)  |
| 21  | BCR  | 4     | 318 | -    | 41,41,41     | 0.99 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 21  | BCR  | F     | 303 | -    | 41,41,41     | 0.95 | 2 (4%)   | 56,56,56    | 1.41 | 12 (21%) |
| 19  | LUT  | 2     | 314 | -    | 42,43,43     | 4.72 | 20 (47%) | 51,60,60    | 5.81 | 33 (64%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | CLA  | B     | 840 | 29   | 69,73,73     | 1.14 | 6 (8%)   | 82,113,113  | 1.28 | 6 (7%)   |
| 17  | CLA  | 3     | 604 | -    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.38 | 6 (10%)  |
| 17  | CLA  | 4     | 302 | 4    | 64,68,73     | 1.30 | 8 (12%)  | 76,107,113  | 1.37 | 8 (10%)  |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 17  | CLA  | 3     | 602 | 3    | 1/1/14/20 | 5/33/109/115  | -       |
| 17  | CLA  | A     | 824 | 29   | 1/1/15/20 | 10/39/115/115 | -       |
| 17  | CLA  | A     | 823 | -    | 1/1/13/20 | 7/27/103/115  | -       |
| 17  | CLA  | F     | 304 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 20  | XAT  | 2     | 315 | -    | -         | 13/31/93/93   | 0/4/4/4 |
| 21  | BCR  | A     | 851 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 17  | CLA  | 3     | 605 | -    | 1/1/10/20 | 2/12/88/115   | -       |
| 17  | CLA  | B     | 837 | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 17  | CLA  | 2     | 319 | 4    | 1/1/11/20 | 2/17/93/115   | -       |
| 21  | BCR  | 3     | 616 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 17  | CLA  | A     | 826 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 18  | CHL  | 2     | 306 | 29   | 3/3/17/26 | 5/21/119/137  | -       |
| 25  | HTG  | 4     | 322 | -    | -         | 1/10/30/30    | 0/1/1/1 |
| 17  | CLA  | 1     | 303 | 29   | 1/1/12/20 | 8/23/99/115   | -       |
| 17  | CLA  | A     | 841 | 29   | 1/1/15/20 | 12/39/115/115 | -       |
| 17  | CLA  | F     | 307 | 10   | 1/1/13/20 | 8/27/103/115  | -       |
| 17  | CLA  | A     | 814 | -    | 1/1/12/20 | 9/21/97/115   | -       |
| 17  | CLA  | L     | 204 | -    | -         | 7/21/97/115   | -       |
| 17  | CLA  | B     | 836 | 29   | 1/1/11/20 | 4/15/91/115   | -       |
| 20  | XAT  | 3     | 615 | -    | -         | 13/31/93/93   | 0/4/4/4 |
| 17  | CLA  | 2     | 311 | 2    | 1/1/15/20 | 14/39/115/115 | -       |
| 17  | CLA  | 2     | 312 | -    | 1/1/10/20 | 0/13/89/115   | -       |
| 17  | CLA  | A     | 839 | 29   | 1/1/15/20 | 16/39/115/115 | -       |
| 17  | CLA  | A     | 806 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | CLA  | A     | 811 | -    | 1/1/12/20 | 5/26/102/115  | -       |
| 17  | CLA  | 1     | 312 | -    | 1/1/13/20 | 9/27/103/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | HTG  | F     | 305 | -    | -         | 3/10/30/30    | 0/1/1/1 |
| 17  | CLA  | 1     | 307 | 1    | 1/1/15/20 | 13/39/115/115 | -       |
| 17  | CLA  | 3     | 610 | -    | 1/1/12/20 | 10/24/100/115 | -       |
| 21  | BCR  | A     | 848 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 17  | CLA  | A     | 809 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 17  | CLA  | 2     | 307 | 2    | 1/1/12/20 | 1/21/97/115   | -       |
| 18  | CHL  | 2     | 304 | 29   | 3/3/15/26 | 5/12/110/137  | -       |
| 17  | CLA  | B     | 841 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 17  | CLA  | 2     | 302 | -    | 1/1/12/20 | 2/23/99/115   | -       |
| 17  | CLA  | 1     | 302 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 17  | CLA  | A     | 843 | 22   | 1/1/12/20 | 11/24/100/115 | -       |
| 28  | SF4  | C     | 102 | 7    | -         | -             | 0/6/5/5 |
| 17  | CLA  | 2     | 310 | 2    | 1/1/12/20 | 6/24/100/115  | -       |
| 17  | CLA  | 3     | 608 | 3    | 1/1/12/20 | 4/21/97/115   | -       |
| 17  | CLA  | B     | 825 | -    | 1/1/14/20 | 8/33/109/115  | -       |
| 17  | CLA  | A     | 802 | 29   | 1/1/15/20 | 6/39/115/115  | -       |
| 17  | CLA  | 1     | 301 | 1    | 1/1/15/20 | 9/39/115/115  | -       |
| 17  | CLA  | 1     | 311 | 1    | 1/1/14/20 | 8/33/109/115  | -       |
| 18  | CHL  | 4     | 307 | 29   | 3/3/17/26 | 2/21/119/137  | -       |
| 19  | LUT  | 1     | 314 | -    | -         | 12/29/67/67   | 0/2/2/2 |
| 21  | BCR  | J     | 105 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 17  | CLA  | 1     | 310 | 1    | 1/1/12/20 | 9/24/100/115  | -       |
| 18  | CHL  | 1     | 305 | 1    | 3/3/16/26 | 5/18/116/137  | -       |
| 17  | CLA  | B     | 818 | -    | 1/1/13/20 | 5/27/103/115  | -       |
| 25  | HTG  | J     | 102 | -    | -         | 6/10/30/30    | 0/1/1/1 |
| 21  | BCR  | A     | 846 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 17  | CLA  | A     | 832 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 21  | BCR  | L     | 206 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 17  | CLA  | B     | 828 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 17  | CLA  | F     | 306 | 29   | 1/1/11/20 | 0/15/91/115   | -       |
| 17  | CLA  | A     | 834 | 5    | 1/1/11/20 | 6/15/91/115   | -       |
| 17  | CLA  | A     | 830 | -    | 1/1/12/20 | 5/21/97/115   | -       |
| 25  | HTG  | B     | 851 | -    | -         | 7/10/30/30    | 0/1/1/1 |
| 17  | CLA  | 3     | 606 | 3    | 1/1/11/20 | 8/18/94/115   | -       |
| 17  | CLA  | B     | 833 | -    | 1/1/14/20 | 5/33/109/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24  | LMG  | 4     | 320 | -    | -         | 21/44/64/70   | 0/1/1/1 |
| 17  | CLA  | B     | 838 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 21  | BCR  | A     | 850 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 17  | CLA  | A     | 810 | 17   | 1/1/15/20 | 13/39/115/115 | -       |
| 17  | CLA  | A     | 827 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 17  | CLA  | 3     | 611 | 3    | 1/1/13/20 | 10/27/103/115 | -       |
| 17  | CLA  | A     | 836 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 17  | CLA  | B     | 803 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 21  | BCR  | A     | 847 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 18  | CHL  | 4     | 315 | 4    | 3/3/15/26 | 4/12/110/137  | -       |
| 17  | CLA  | G     | 105 | 11   | 1/1/11/20 | 6/17/93/115   | -       |
| 21  | BCR  | I     | 101 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 17  | CLA  | B     | 829 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 17  | CLA  | 3     | 612 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 17  | CLA  | K     | 201 | -    | 1/1/11/20 | 3/15/91/115   | -       |
| 17  | CLA  | K     | 202 | -    | 1/1/14/20 | 14/33/109/115 | -       |
| 22  | LHG  | A     | 845 | 17   | -         | 14/31/31/53   | -       |
| 24  | LMG  | F     | 309 | -    | -         | 20/50/70/70   | 0/1/1/1 |
| 17  | CLA  | 4     | 310 | -    | 1/1/14/20 | 15/33/109/115 | -       |
| 17  | CLA  | A     | 812 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 17  | CLA  | A     | 815 | 29   | 1/1/11/20 | 4/15/91/115   | -       |
| 17  | CLA  | A     | 820 | 29   | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | CLA  | B     | 815 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 17  | CLA  | B     | 816 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | CLA  | B     | 824 | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 17  | CLA  | B     | 839 | -    | 1/1/11/20 | 2/18/94/115   | -       |
| 23  | LMT  | A     | 855 | -    | -         | 14/21/61/61   | 0/2/2/2 |
| 17  | CLA  | B     | 804 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 17  | CLA  | A     | 805 | 5    | 1/1/15/20 | 21/39/115/115 | -       |
| 17  | CLA  | 3     | 603 | 3    | 1/1/12/20 | 2/21/97/115   | -       |
| 17  | CLA  | A     | 819 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 17  | CLA  | B     | 834 | -    | 1/1/13/20 | 13/31/107/115 | -       |
| 18  | CHL  | 2     | 313 | 2    | 3/3/15/26 | 2/12/110/137  | -       |
| 18  | CHL  | 3     | 601 | 2    | 3/3/17/26 | 5/24/122/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 21  | BCR  | L     | 205 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 24  | LMG  | B     | 852 | -    | -         | 21/47/67/70   | 0/1/1/1 |
| 17  | CLA  | B     | 814 | -    | 1/1/13/20 | 6/27/103/115  | -       |
| 17  | CLA  | B     | 810 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | HTG  | 4     | 321 | -    | -         | 3/10/30/30    | 0/1/1/1 |
| 18  | CHL  | 3     | 607 | 29   | 3/3/16/26 | 4/17/115/137  | -       |
| 17  | CLA  | B     | 811 | 6    | 1/1/15/20 | 9/39/115/115  | -       |
| 27  | PQN  | B     | 843 | -    | -         | 3/23/43/43    | 0/2/2/2 |
| 17  | CLA  | 4     | 313 | -    | 1/1/11/20 | 8/15/91/115   | -       |
| 21  | BCR  | A     | 849 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 17  | CLA  | A     | 807 | 5    | 1/1/15/20 | 18/39/115/115 | -       |
| 17  | CLA  | 4     | 304 | 29   | 1/1/12/20 | 6/21/97/115   | -       |
| 17  | CLA  | A     | 840 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 17  | CLA  | B     | 812 | -    | -         | 17/39/115/115 | -       |
| 25  | HTG  | A     | 854 | -    | -         | 2/10/30/30    | 0/1/1/1 |
| 17  | CLA  | A     | 801 | -    | 2/2/15/20 | 8/39/115/115  | -       |
| 17  | CLA  | 1     | 306 | 29   | 1/1/11/20 | 1/17/93/115   | -       |
| 17  | CLA  | 2     | 308 | 2    | 1/1/14/20 | 10/33/109/115 | -       |
| 17  | CLA  | A     | 853 | 29   | 1/1/15/20 | 13/39/115/115 | -       |
| 17  | CLA  | 1     | 304 | -    | 1/1/10/20 | 4/12/88/115   | -       |
| 17  | CLA  | G     | 103 | 29   | 1/1/10/20 | 4/10/86/115   | -       |
| 17  | CLA  | A     | 825 | 29   | 1/1/15/20 | 5/39/115/115  | -       |
| 17  | CLA  | B     | 802 | -    | 1/1/15/20 | 2/39/115/115  | -       |
| 20  | XAT  | 4     | 317 | -    | 3/3/12/26 | 11/31/93/93   | 0/4/4/4 |
| 21  | BCR  | B     | 844 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 21  | BCR  | B     | 848 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 24  | LMG  | 4     | 319 | -    | -         | 15/45/65/70   | 0/1/1/1 |
| 17  | CLA  | A     | 817 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 23  | LMT  | 2     | 318 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 21  | BCR  | B     | 847 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 18  | CHL  | 4     | 301 | 1    | 4/4/19/26 | 16/33/131/137 | -       |
| 17  | CLA  | B     | 826 | 29   | 1/1/15/20 | 16/39/115/115 | -       |
| 17  | CLA  | B     | 806 | -    | 1/1/11/20 | 1/15/91/115   | -       |
| 17  | CLA  | A     | 835 | -    | 1/1/12/20 | 9/23/99/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 17  | CLA  | 1     | 309 | 22   | 1/1/15/20 | 16/39/115/115 | -       |
| 17  | CLA  | J     | 101 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | CLA  | 3     | 609 | 3    | 1/1/12/20 | 3/21/97/115   | -       |
| 17  | CLA  | G     | 104 | -    | 1/1/12/20 | 4/21/97/115   | -       |
| 17  | CLA  | A     | 821 | -    | 1/1/11/20 | 8/20/96/115   | -       |
| 17  | CLA  | B     | 820 | -    | 1/1/14/20 | 14/33/109/115 | -       |
| 17  | CLA  | B     | 835 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 28  | SF4  | C     | 101 | 7    | -         | -             | 0/6/5/5 |
| 17  | CLA  | 4     | 309 | 4    | 1/1/14/20 | 8/33/109/115  | -       |
| 17  | CLA  | 2     | 309 | -    | 1/1/10/20 | 2/10/86/115   | -       |
| 17  | CLA  | 4     | 312 | 4    | 1/1/13/20 | 7/29/105/115  | -       |
| 17  | CLA  | 1     | 308 | 1    | 1/1/14/20 | 9/33/109/115  | -       |
| 17  | CLA  | 1     | 313 | 1    | 1/1/11/20 | 4/17/93/115   | -       |
| 28  | SF4  | A     | 852 | 5,6  | -         | -             | 0/6/5/5 |
| 21  | BCR  | 2     | 316 | -    | -         | 17/29/63/63   | 0/2/2/2 |
| 17  | CLA  | B     | 831 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 17  | CLA  | A     | 818 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 21  | BCR  | L     | 201 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 17  | CLA  | B     | 805 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 17  | CLA  | 4     | 303 | 4    | -         | 15/33/109/115 | -       |
| 17  | CLA  | L     | 202 | 15   | 1/1/15/20 | 14/39/115/115 | -       |
| 27  | PQN  | A     | 842 | -    | -         | 6/23/43/43    | 0/2/2/2 |
| 17  | CLA  | B     | 809 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 18  | CHL  | 2     | 305 | 29   | 3/3/16/26 | 3/18/116/137  | -       |
| 17  | CLA  | A     | 822 | -    | 1/1/12/20 | 11/23/99/115  | -       |
| 17  | CLA  | A     | 828 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | CLA  | B     | 821 | 29   | 1/1/15/20 | 5/39/115/115  | -       |
| 17  | CLA  | J     | 103 | 14   | 1/1/10/20 | 6/12/88/115   | -       |
| 17  | CLA  | 4     | 311 | 4    | -         | 4/24/100/115  | -       |
| 17  | CLA  | A     | 833 | -    | 1/1/12/20 | 4/21/97/115   | -       |
| 17  | CLA  | B     | 832 | -    | 1/1/12/20 | 2/21/97/115   | -       |
| 20  | XAT  | 1     | 315 | -    | -         | 13/31/93/93   | 0/4/4/4 |
| 18  | CHL  | 4     | 305 | 29   | 4/4/18/26 | 9/27/125/137  | -       |
| 21  | BCR  | B     | 849 | -    | -         | 8/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 21  | BCR  | G     | 106 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 26  | DGD  | B     | 850 | -    | -         | 24/55/95/95   | 0/2/2/2 |
| 17  | CLA  | L     | 203 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 17  | CLA  | B     | 842 | 22   | 1/1/15/20 | 5/39/115/115  | -       |
| 17  | CLA  | A     | 803 | 17   | 1/1/13/20 | 9/27/103/115  | -       |
| 17  | CLA  | B     | 808 | 6    | 1/1/15/20 | 12/39/115/115 | -       |
| 17  | CLA  | B     | 807 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 21  | BCR  | J     | 104 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 24  | LMG  | G     | 101 | -    | -         | 16/35/55/70   | 0/1/1/1 |
| 17  | CLA  | B     | 823 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 17  | CLA  | B     | 830 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 17  | CLA  | A     | 829 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | LUT  | 3     | 614 | -    | -         | 12/29/67/67   | 0/2/2/2 |
| 17  | CLA  | B     | 822 | -    | 1/1/12/20 | 4/21/97/115   | -       |
| 21  | BCR  | B     | 846 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 17  | CLA  | 2     | 301 | 2    | 1/1/15/20 | 5/39/115/115  | -       |
| 25  | HTG  | F     | 301 | -    | -         | 4/8/28/30     | 0/1/1/1 |
| 17  | CLA  | A     | 816 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | LHG  | B     | 801 | 17   | -         | 10/26/26/53   | -       |
| 17  | CLA  | A     | 804 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 25  | HTG  | F     | 310 | -    | -         | 3/7/27/30     | 0/1/1/1 |
| 26  | DGD  | 4     | 323 | -    | -         | 27/49/89/95   | 0/2/2/2 |
| 22  | LHG  | 1     | 317 | 17   | -         | 20/53/53/53   | -       |
| 17  | CLA  | 2     | 303 | -    | 1/1/14/20 | 15/33/109/115 | -       |
| 21  | BCR  | B     | 845 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 17  | CLA  | 3     | 613 | -    | 1/1/11/20 | 2/17/93/115   | -       |
| 17  | CLA  | B     | 817 | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 17  | CLA  | B     | 827 | 29   | 1/1/15/20 | 8/39/115/115  | -       |
| 22  | LHG  | 2     | 317 | -    | -         | 19/41/41/53   | -       |
| 17  | CLA  | 4     | 314 | -    | 1/1/11/20 | 4/18/94/115   | -       |
| 21  | BCR  | 1     | 316 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 19  | LUT  | 4     | 316 | -    | -         | 13/29/67/67   | 0/2/2/2 |
| 17  | CLA  | A     | 831 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 17  | CLA  | A     | 808 | 5    | 1/1/15/20 | 8/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 21  | BCR  | F     | 308 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 17  | CLA  | A     | 813 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 17  | CLA  | B     | 813 | -    | 1/1/13/20 | 9/25/101/115  | -       |
| 22  | LHG  | A     | 844 | -    | -         | 27/53/53/53   | -       |
| 18  | CHL  | 4     | 306 | 29   | 3/3/17/26 | 9/21/119/137  | -       |
| 17  | CLA  | 4     | 308 | 4    | 1/1/12/20 | 3/21/97/115   | -       |
| 21  | BCR  | K     | 203 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 17  | CLA  | A     | 838 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | LHG  | F     | 302 | -    | -         | 30/44/44/53   | -       |
| 22  | LHG  | G     | 102 | -    | -         | 26/53/53/53   | -       |
| 17  | CLA  | A     | 837 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 17  | CLA  | B     | 819 | -    | 1/1/13/20 | 6/32/108/115  | -       |
| 21  | BCR  | 4     | 318 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 21  | BCR  | F     | 303 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 19  | LUT  | 2     | 314 | -    | -         | 13/29/67/67   | 0/2/2/2 |
| 17  | CLA  | B     | 840 | 29   | 1/1/15/20 | 14/39/115/115 | -       |
| 17  | CLA  | 3     | 604 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 17  | CLA  | 4     | 302 | 4    | 1/1/14/20 | 6/33/109/115  | -       |

The worst 5 of 1473 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | 1     | 314 | LUT  | C24-C25 | 16.50 | 1.52        | 1.33     |
| 19  | 2     | 314 | LUT  | C24-C25 | 16.25 | 1.52        | 1.33     |
| 19  | 3     | 614 | LUT  | C24-C25 | 16.14 | 1.52        | 1.33     |
| 19  | 4     | 316 | LUT  | C24-C25 | 15.71 | 1.51        | 1.33     |
| 19  | 3     | 614 | LUT  | C5-C6   | 11.31 | 1.53        | 1.34     |

The worst 5 of 1764 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 27  | A     | 842 | PQN  | C6-C5-C10   | -13.48 | 104.14      | 119.26   |
| 18  | 3     | 601 | CHL  | O2D-CGD-CBD | 12.29  | 124.45      | 110.95   |
| 27  | A     | 842 | PQN  | C9-C10-C5   | -12.25 | 105.51      | 119.26   |
| 19  | 4     | 316 | LUT  | C31-C30-C29 | -12.02 | 110.43      | 127.28   |
| 19  | 4     | 316 | LUT  | C11-C10-C9  | -11.98 | 110.48      | 127.28   |

5 of 178 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 17  | 1     | 301 | CLA  | ND   |
| 17  | 1     | 302 | CLA  | ND   |
| 17  | 1     | 303 | CLA  | ND   |
| 17  | 1     | 304 | CLA  | ND   |
| 17  | 1     | 306 | CLA  | ND   |

5 of 1883 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | 1     | 301 | CLA  | CHA-CBD-CGD-O1D |
| 17  | 1     | 301 | CLA  | CHA-CBD-CGD-O2D |
| 17  | 1     | 307 | CLA  | CBA-CGA-O2A-C1  |
| 17  | 1     | 307 | CLA  | O1A-CGA-O2A-C1  |
| 17  | 1     | 309 | CLA  | C1A-C2A-CAA-CBA |

There are no ring outliers.

190 monomers are involved in 543 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | 3     | 602 | CLA  | 6       | 0            |
| 17  | A     | 824 | CLA  | 1       | 0            |
| 17  | A     | 823 | CLA  | 4       | 0            |
| 17  | F     | 304 | CLA  | 2       | 0            |
| 20  | 2     | 315 | XAT  | 9       | 0            |
| 21  | A     | 851 | BCR  | 5       | 0            |
| 17  | 3     | 605 | CLA  | 1       | 0            |
| 17  | B     | 837 | CLA  | 7       | 0            |
| 21  | 3     | 616 | BCR  | 4       | 0            |
| 17  | A     | 826 | CLA  | 1       | 0            |
| 18  | 2     | 306 | CHL  | 6       | 0            |
| 25  | 4     | 322 | HTG  | 2       | 0            |
| 17  | 1     | 303 | CLA  | 2       | 0            |
| 17  | A     | 841 | CLA  | 4       | 0            |
| 17  | F     | 307 | CLA  | 2       | 0            |
| 17  | A     | 814 | CLA  | 4       | 0            |
| 17  | L     | 204 | CLA  | 2       | 0            |
| 17  | B     | 836 | CLA  | 2       | 0            |
| 20  | 3     | 615 | XAT  | 12      | 0            |
| 17  | 2     | 311 | CLA  | 4       | 0            |
| 17  | 2     | 312 | CLA  | 1       | 0            |
| 17  | A     | 839 | CLA  | 3       | 0            |
| 17  | A     | 806 | CLA  | 1       | 0            |
| 17  | A     | 811 | CLA  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | 1     | 312 | CLA  | 2       | 0            |
| 25  | F     | 305 | HTG  | 1       | 0            |
| 17  | 1     | 307 | CLA  | 3       | 0            |
| 17  | 3     | 610 | CLA  | 1       | 0            |
| 21  | A     | 848 | BCR  | 3       | 0            |
| 17  | A     | 809 | CLA  | 3       | 0            |
| 17  | 2     | 307 | CLA  | 1       | 0            |
| 18  | 2     | 304 | CHL  | 2       | 0            |
| 17  | B     | 841 | CLA  | 1       | 0            |
| 17  | 1     | 302 | CLA  | 2       | 0            |
| 17  | A     | 843 | CLA  | 6       | 0            |
| 17  | 2     | 310 | CLA  | 1       | 0            |
| 17  | 3     | 608 | CLA  | 3       | 0            |
| 17  | B     | 825 | CLA  | 3       | 0            |
| 17  | 1     | 301 | CLA  | 1       | 0            |
| 17  | 1     | 311 | CLA  | 6       | 0            |
| 18  | 4     | 307 | CHL  | 4       | 0            |
| 19  | 1     | 314 | LUT  | 7       | 0            |
| 21  | J     | 105 | BCR  | 5       | 0            |
| 17  | 1     | 310 | CLA  | 3       | 0            |
| 18  | 1     | 305 | CHL  | 4       | 0            |
| 17  | B     | 818 | CLA  | 2       | 0            |
| 25  | J     | 102 | HTG  | 3       | 0            |
| 21  | A     | 846 | BCR  | 10      | 0            |
| 17  | A     | 832 | CLA  | 2       | 0            |
| 21  | L     | 206 | BCR  | 4       | 0            |
| 17  | B     | 828 | CLA  | 2       | 0            |
| 17  | F     | 306 | CLA  | 4       | 0            |
| 17  | A     | 834 | CLA  | 2       | 0            |
| 25  | B     | 851 | HTG  | 1       | 0            |
| 17  | B     | 833 | CLA  | 1       | 0            |
| 24  | 4     | 320 | LMG  | 7       | 0            |
| 17  | B     | 838 | CLA  | 4       | 0            |
| 21  | A     | 850 | BCR  | 3       | 0            |
| 17  | A     | 810 | CLA  | 7       | 0            |
| 17  | A     | 827 | CLA  | 1       | 0            |
| 17  | A     | 836 | CLA  | 3       | 0            |
| 17  | B     | 803 | CLA  | 6       | 0            |
| 21  | A     | 847 | BCR  | 1       | 0            |
| 18  | 4     | 315 | CHL  | 4       | 0            |
| 17  | G     | 105 | CLA  | 1       | 0            |
| 21  | I     | 101 | BCR  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | B     | 829 | CLA  | 6       | 0            |
| 17  | K     | 201 | CLA  | 3       | 0            |
| 17  | K     | 202 | CLA  | 2       | 0            |
| 22  | A     | 845 | LHG  | 1       | 0            |
| 24  | F     | 309 | LMG  | 1       | 0            |
| 17  | 4     | 310 | CLA  | 1       | 0            |
| 17  | A     | 812 | CLA  | 2       | 0            |
| 17  | A     | 815 | CLA  | 1       | 0            |
| 17  | A     | 820 | CLA  | 6       | 0            |
| 17  | B     | 815 | CLA  | 2       | 0            |
| 17  | B     | 816 | CLA  | 3       | 0            |
| 17  | B     | 824 | CLA  | 2       | 0            |
| 17  | B     | 839 | CLA  | 2       | 0            |
| 23  | A     | 855 | LMT  | 2       | 0            |
| 17  | B     | 804 | CLA  | 2       | 0            |
| 17  | A     | 805 | CLA  | 3       | 0            |
| 17  | 3     | 603 | CLA  | 2       | 0            |
| 17  | A     | 819 | CLA  | 4       | 0            |
| 17  | B     | 834 | CLA  | 2       | 0            |
| 18  | 2     | 313 | CHL  | 5       | 0            |
| 18  | 3     | 601 | CHL  | 18      | 0            |
| 21  | L     | 205 | BCR  | 4       | 0            |
| 24  | B     | 852 | LMG  | 4       | 0            |
| 17  | B     | 810 | CLA  | 6       | 0            |
| 25  | 4     | 321 | HTG  | 2       | 0            |
| 18  | 3     | 607 | CHL  | 2       | 0            |
| 17  | B     | 811 | CLA  | 5       | 0            |
| 27  | B     | 843 | PQN  | 3       | 0            |
| 21  | A     | 849 | BCR  | 3       | 0            |
| 17  | A     | 807 | CLA  | 2       | 0            |
| 17  | 4     | 304 | CLA  | 5       | 0            |
| 17  | A     | 840 | CLA  | 4       | 0            |
| 17  | B     | 812 | CLA  | 3       | 0            |
| 17  | A     | 801 | CLA  | 1       | 0            |
| 17  | 2     | 308 | CLA  | 5       | 0            |
| 17  | A     | 853 | CLA  | 7       | 0            |
| 17  | 1     | 304 | CLA  | 4       | 0            |
| 17  | G     | 103 | CLA  | 1       | 0            |
| 17  | A     | 825 | CLA  | 4       | 0            |
| 17  | B     | 802 | CLA  | 3       | 0            |
| 20  | 4     | 317 | XAT  | 9       | 0            |
| 21  | B     | 844 | BCR  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | B     | 848 | BCR  | 4       | 0            |
| 17  | A     | 817 | CLA  | 5       | 0            |
| 23  | 2     | 318 | LMT  | 3       | 0            |
| 21  | B     | 847 | BCR  | 8       | 0            |
| 18  | 4     | 301 | CHL  | 11      | 0            |
| 17  | B     | 826 | CLA  | 7       | 0            |
| 17  | B     | 806 | CLA  | 2       | 0            |
| 17  | A     | 835 | CLA  | 3       | 0            |
| 17  | 1     | 309 | CLA  | 5       | 0            |
| 17  | J     | 101 | CLA  | 5       | 0            |
| 17  | 3     | 609 | CLA  | 2       | 0            |
| 17  | G     | 104 | CLA  | 3       | 0            |
| 17  | A     | 821 | CLA  | 1       | 0            |
| 17  | B     | 820 | CLA  | 2       | 0            |
| 17  | B     | 835 | CLA  | 3       | 0            |
| 17  | 4     | 309 | CLA  | 1       | 0            |
| 17  | 2     | 309 | CLA  | 1       | 0            |
| 17  | 1     | 308 | CLA  | 6       | 0            |
| 21  | 2     | 316 | BCR  | 9       | 0            |
| 17  | B     | 831 | CLA  | 2       | 0            |
| 17  | A     | 818 | CLA  | 3       | 0            |
| 21  | L     | 201 | BCR  | 2       | 0            |
| 17  | B     | 805 | CLA  | 3       | 0            |
| 17  | 4     | 303 | CLA  | 4       | 0            |
| 17  | L     | 202 | CLA  | 5       | 0            |
| 27  | A     | 842 | PQN  | 6       | 0            |
| 17  | B     | 809 | CLA  | 6       | 0            |
| 18  | 2     | 305 | CHL  | 2       | 0            |
| 17  | A     | 822 | CLA  | 1       | 0            |
| 17  | A     | 828 | CLA  | 3       | 0            |
| 17  | B     | 821 | CLA  | 2       | 0            |
| 17  | 4     | 311 | CLA  | 2       | 0            |
| 17  | B     | 832 | CLA  | 3       | 0            |
| 20  | 1     | 315 | XAT  | 3       | 0            |
| 18  | 4     | 305 | CHL  | 5       | 0            |
| 21  | B     | 849 | BCR  | 3       | 0            |
| 21  | G     | 106 | BCR  | 2       | 0            |
| 26  | B     | 850 | DGD  | 7       | 0            |
| 17  | L     | 203 | CLA  | 5       | 0            |
| 17  | B     | 842 | CLA  | 3       | 0            |
| 17  | A     | 803 | CLA  | 7       | 0            |
| 17  | B     | 808 | CLA  | 1       | 0            |

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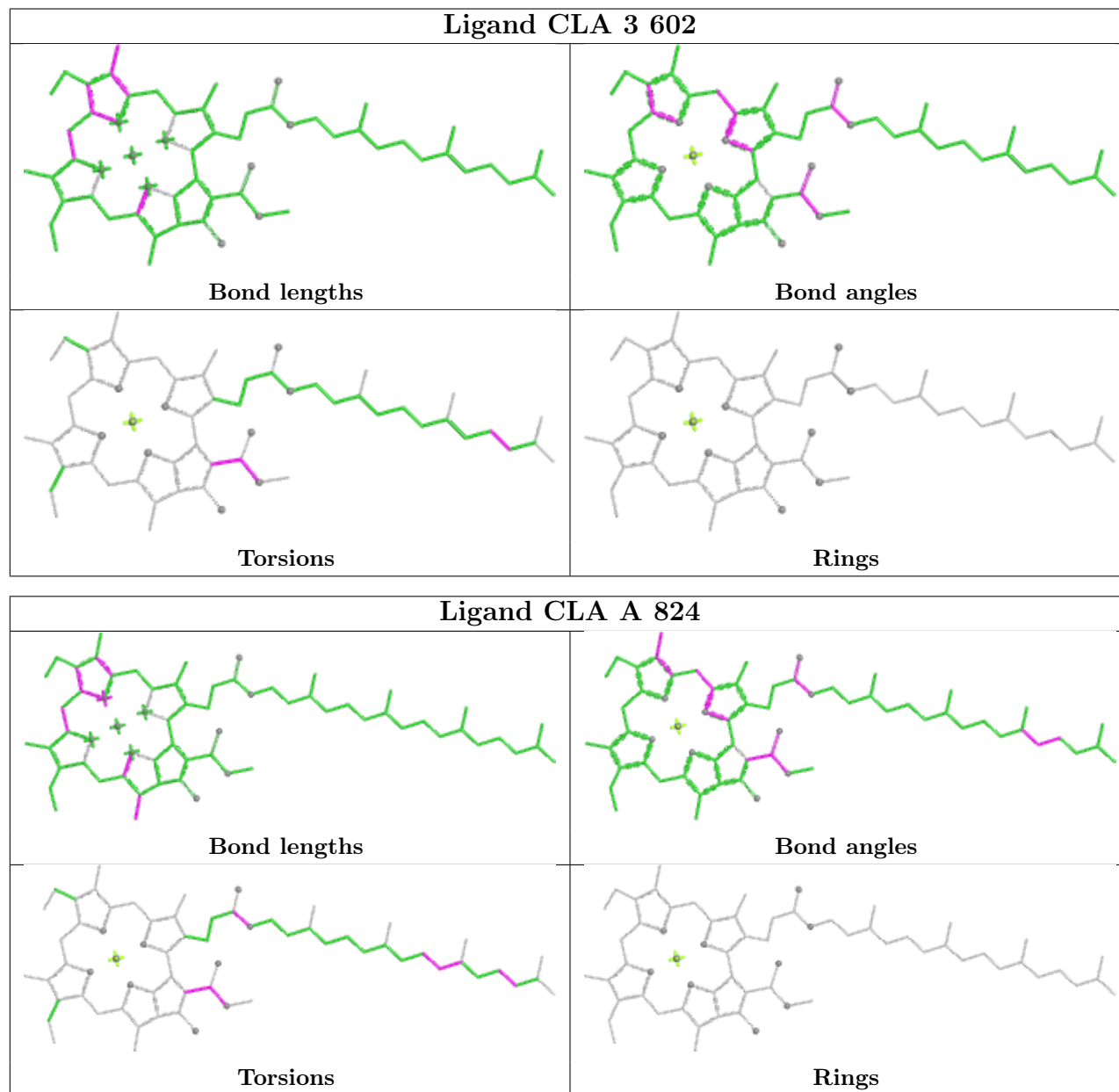
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | B     | 807 | CLA  | 3       | 0            |
| 21  | J     | 104 | BCR  | 2       | 0            |
| 24  | G     | 101 | LMG  | 3       | 0            |
| 17  | B     | 823 | CLA  | 4       | 0            |
| 17  | B     | 830 | CLA  | 2       | 0            |
| 17  | A     | 829 | CLA  | 2       | 0            |
| 19  | 3     | 614 | LUT  | 4       | 0            |
| 17  | B     | 822 | CLA  | 2       | 0            |
| 21  | B     | 846 | BCR  | 3       | 0            |
| 17  | 2     | 301 | CLA  | 4       | 0            |
| 17  | A     | 816 | CLA  | 4       | 0            |
| 22  | B     | 801 | LHG  | 1       | 0            |
| 17  | A     | 804 | CLA  | 6       | 0            |
| 25  | F     | 310 | HTG  | 1       | 0            |
| 26  | 4     | 323 | DGD  | 29      | 0            |
| 22  | 1     | 317 | LHG  | 6       | 0            |
| 17  | 2     | 303 | CLA  | 1       | 0            |
| 21  | B     | 845 | BCR  | 4       | 0            |
| 17  | 3     | 613 | CLA  | 2       | 0            |
| 17  | B     | 817 | CLA  | 1       | 0            |
| 17  | B     | 827 | CLA  | 9       | 0            |
| 22  | 2     | 317 | LHG  | 6       | 0            |
| 17  | 4     | 314 | CLA  | 2       | 0            |
| 19  | 4     | 316 | LUT  | 3       | 0            |
| 17  | A     | 831 | CLA  | 2       | 0            |
| 17  | A     | 808 | CLA  | 5       | 0            |
| 21  | F     | 308 | BCR  | 3       | 0            |
| 17  | A     | 813 | CLA  | 1       | 0            |
| 22  | A     | 844 | LHG  | 2       | 0            |
| 18  | 4     | 306 | CHL  | 7       | 0            |
| 17  | 4     | 308 | CLA  | 1       | 0            |
| 21  | K     | 203 | BCR  | 5       | 0            |
| 17  | A     | 838 | CLA  | 4       | 0            |
| 22  | F     | 302 | LHG  | 2       | 0            |
| 22  | G     | 102 | LHG  | 2       | 0            |
| 17  | A     | 837 | CLA  | 6       | 0            |
| 17  | B     | 819 | CLA  | 6       | 0            |
| 21  | 4     | 318 | BCR  | 14      | 0            |
| 19  | 2     | 314 | LUT  | 4       | 0            |
| 17  | 4     | 302 | CLA  | 6       | 0            |

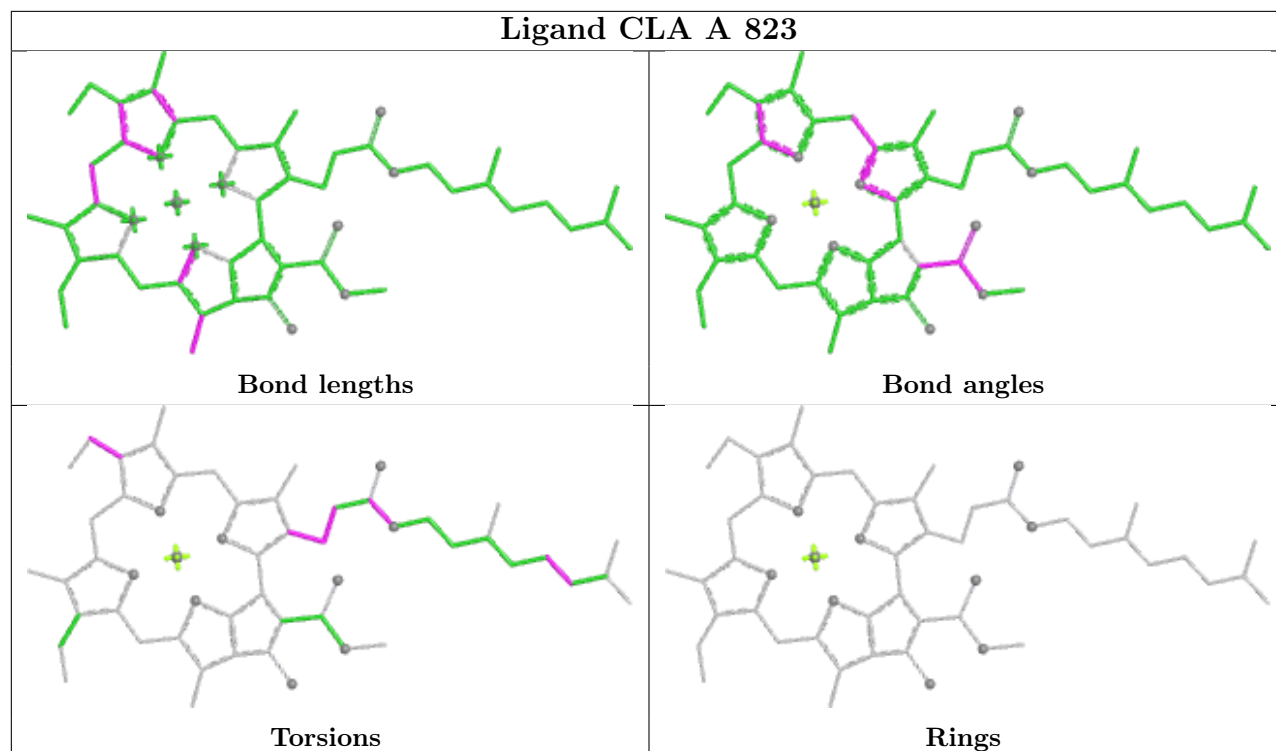
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In



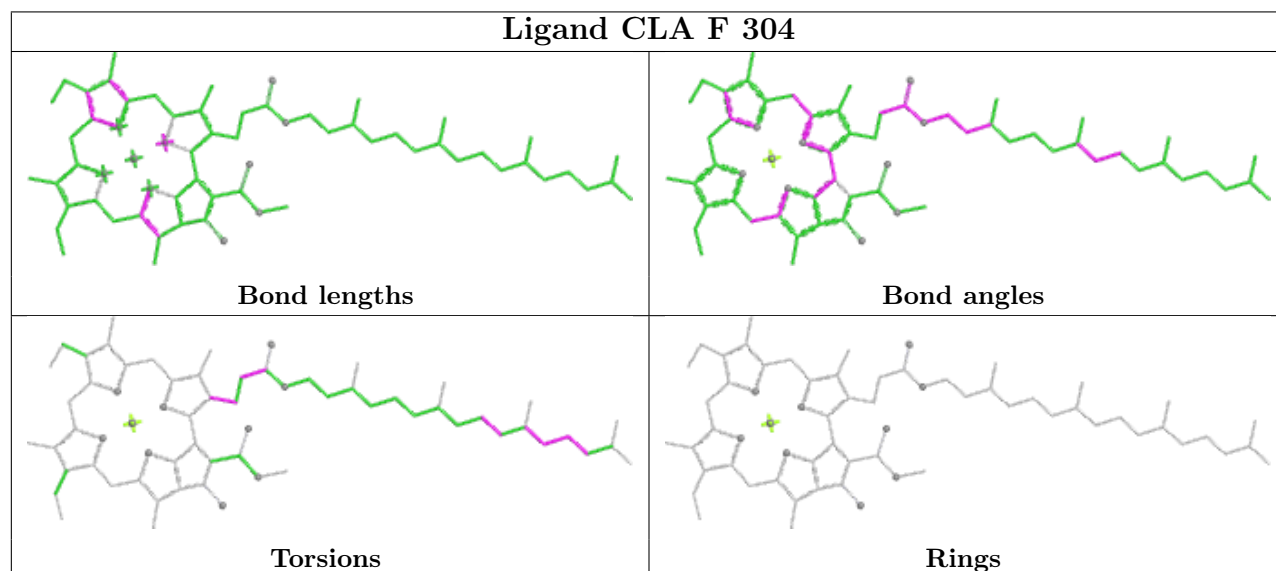
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



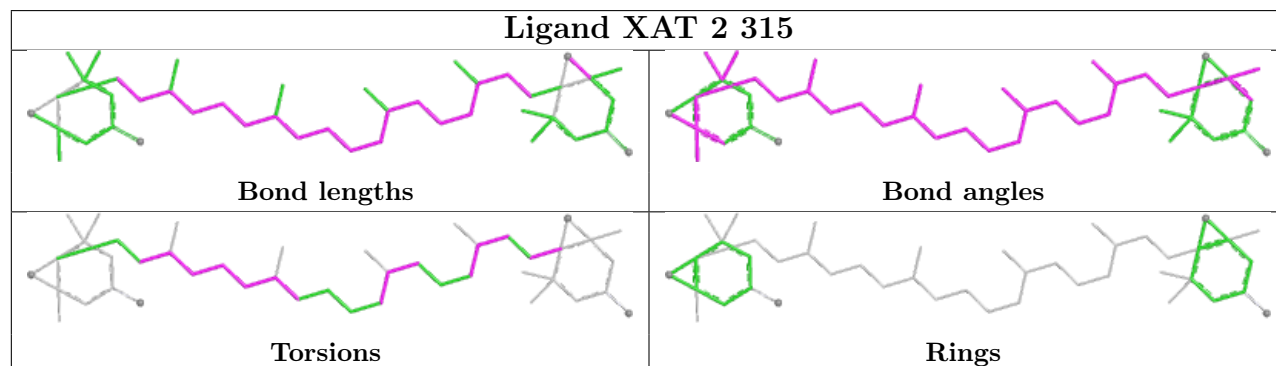
## Ligand CLA A 823

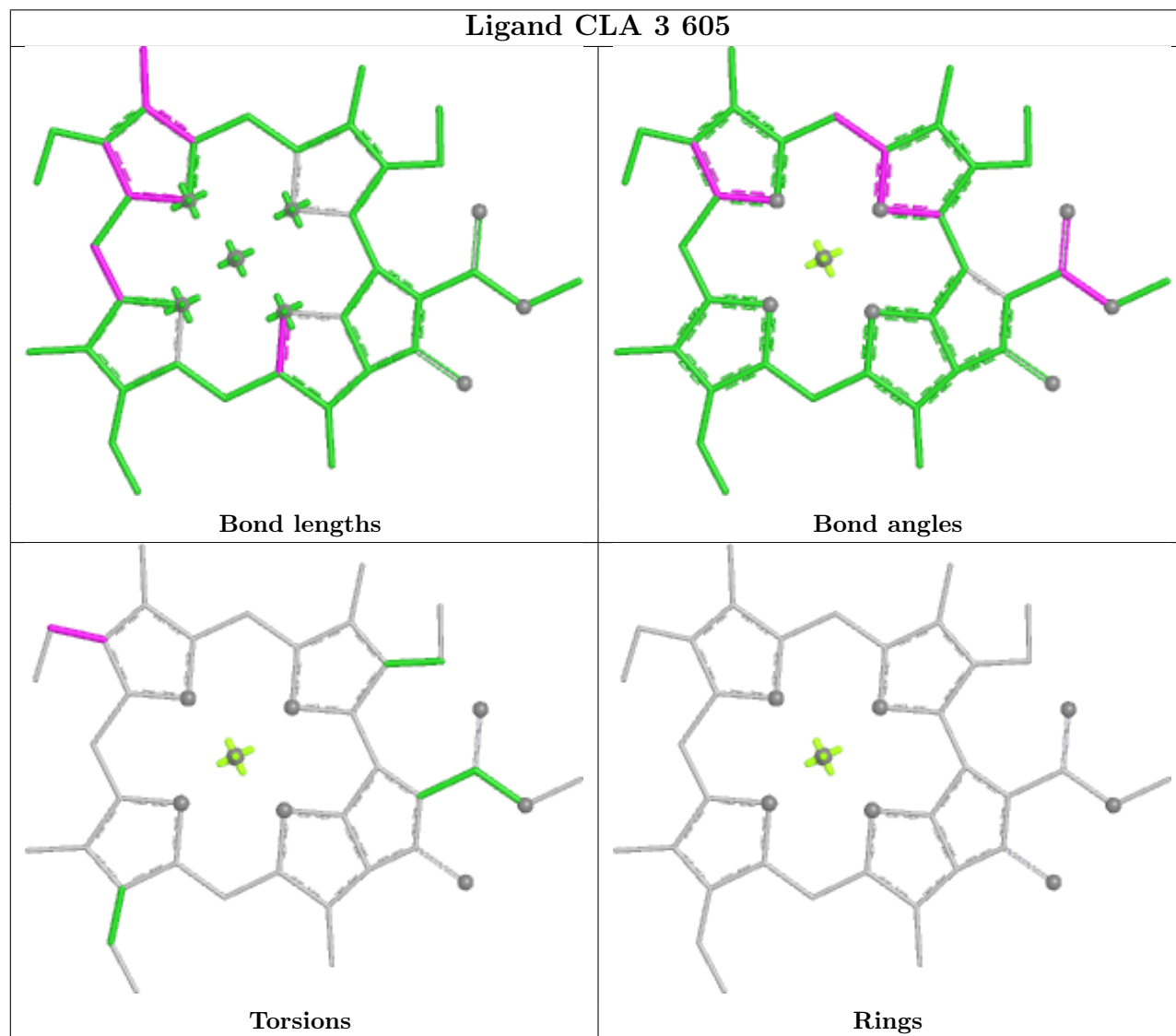
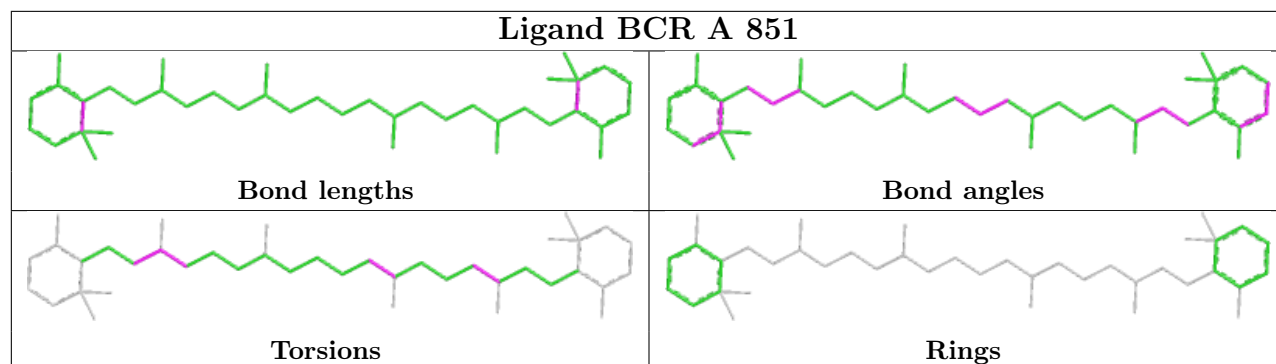


## Ligand CLA F 304

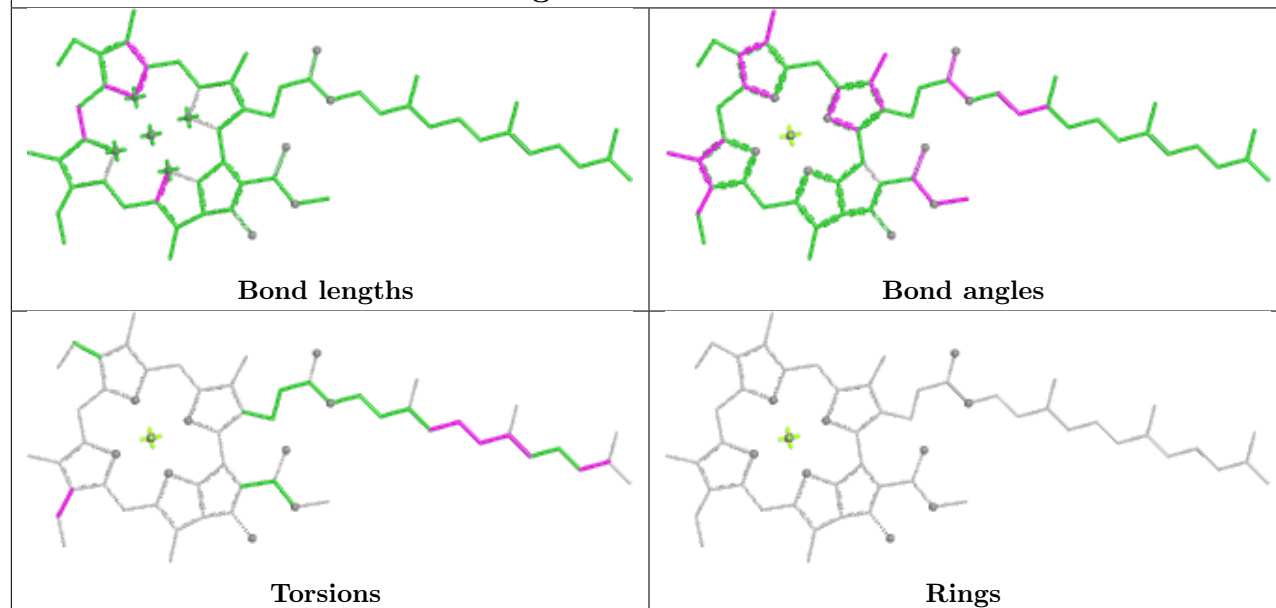


## Ligand XAT 2 315

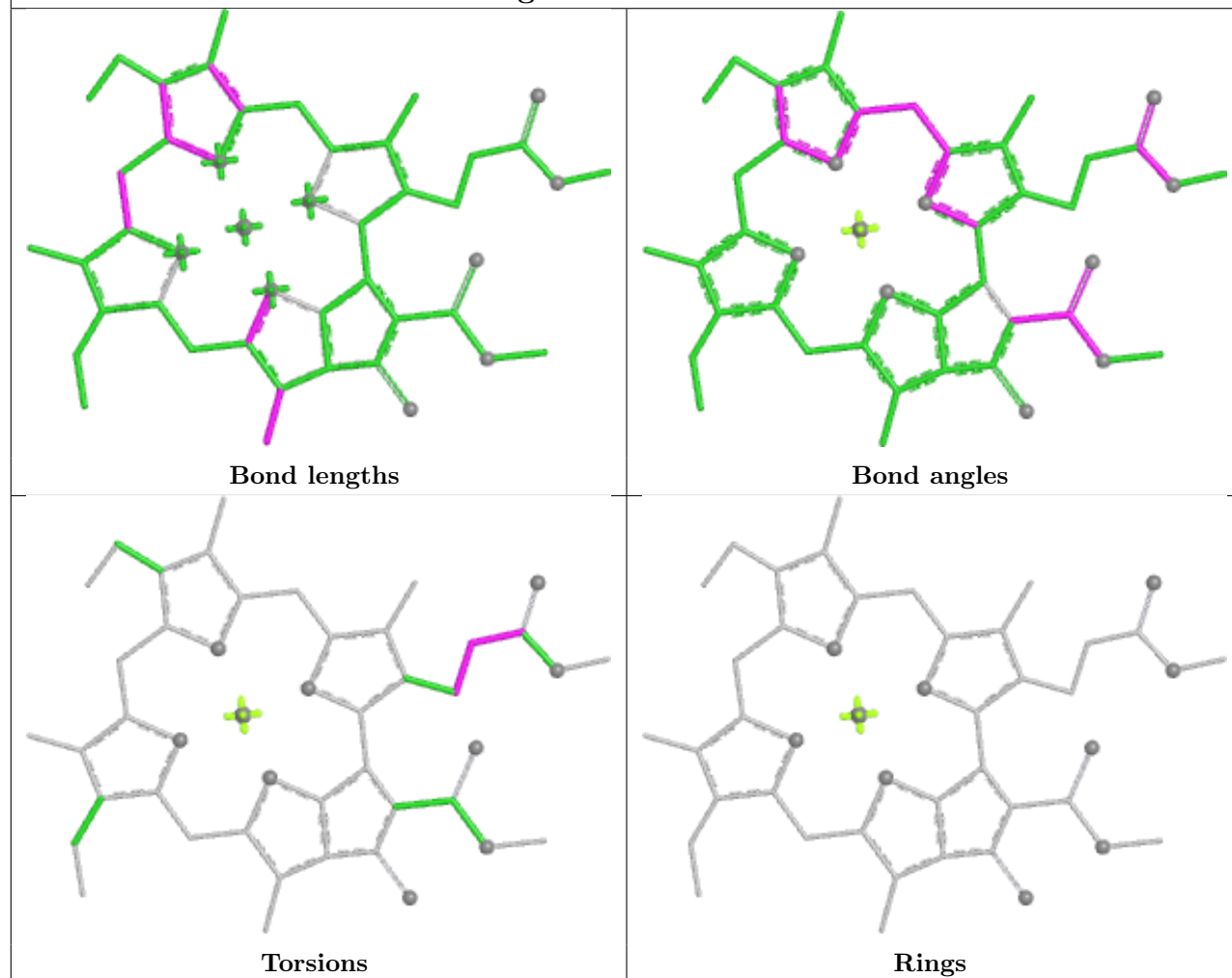


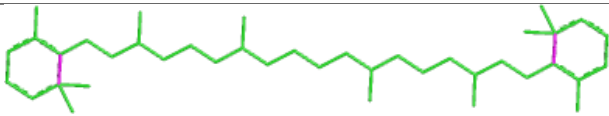
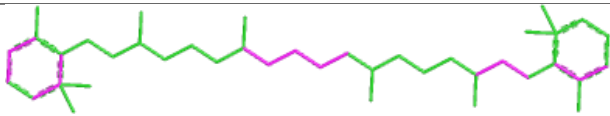
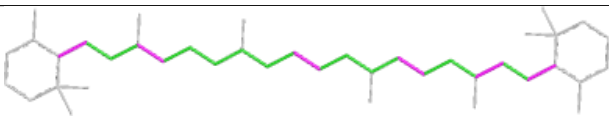
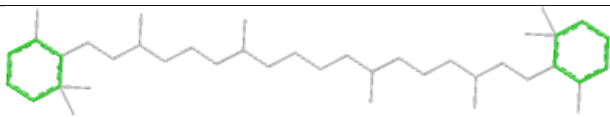


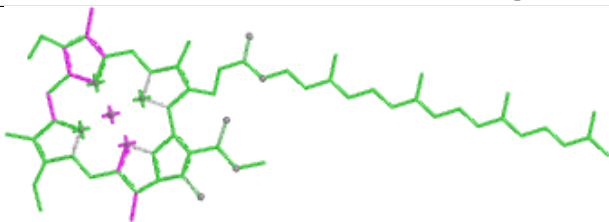
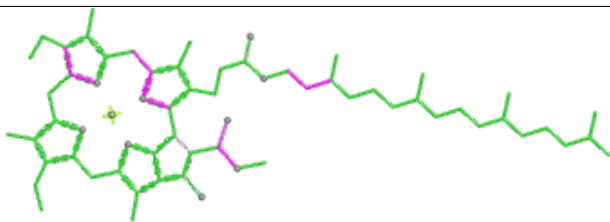
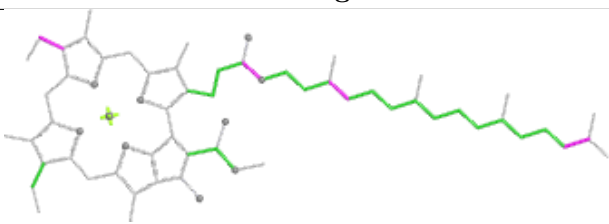
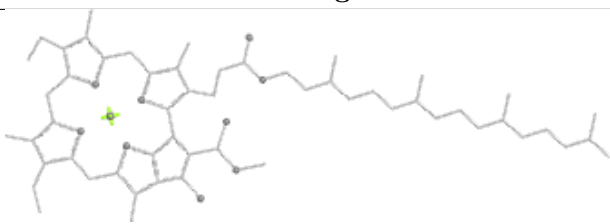
## Ligand CLA B 837



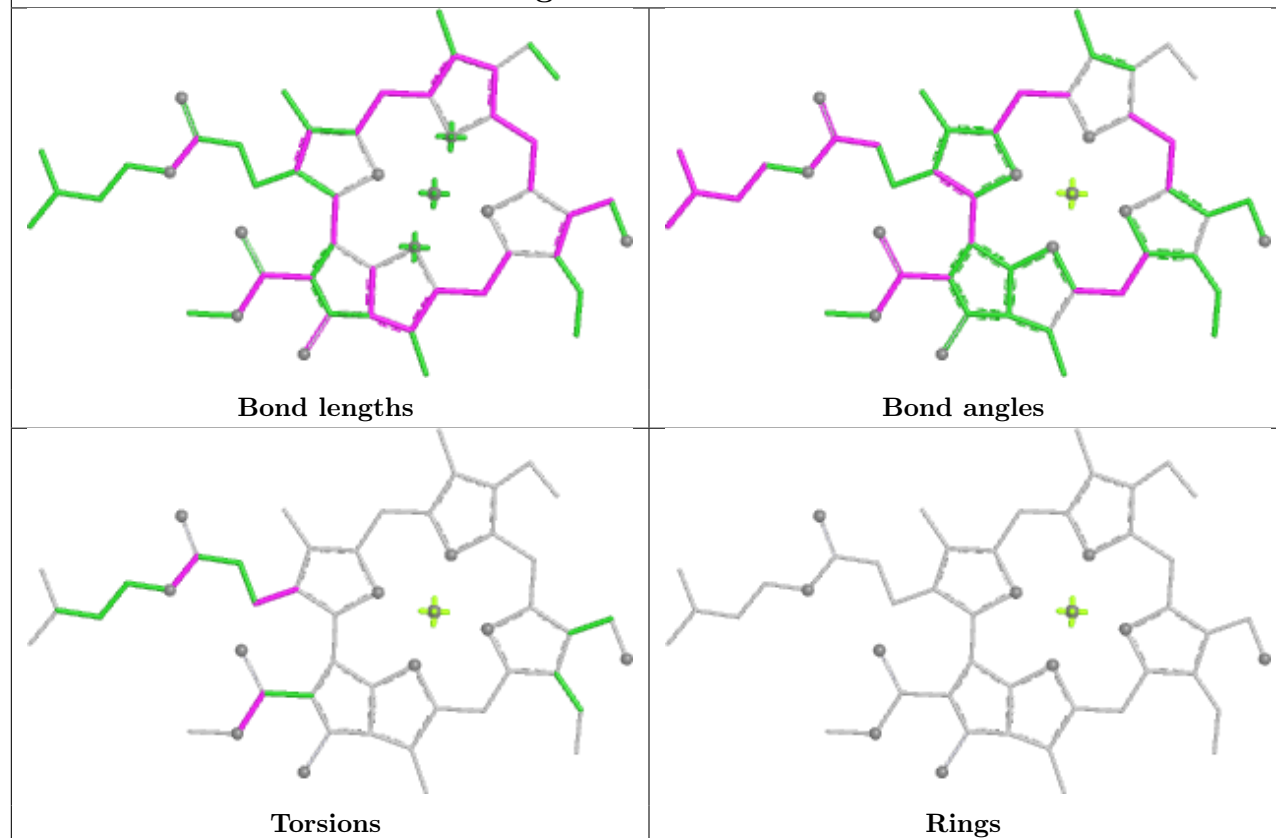
## Ligand CLA 2 319



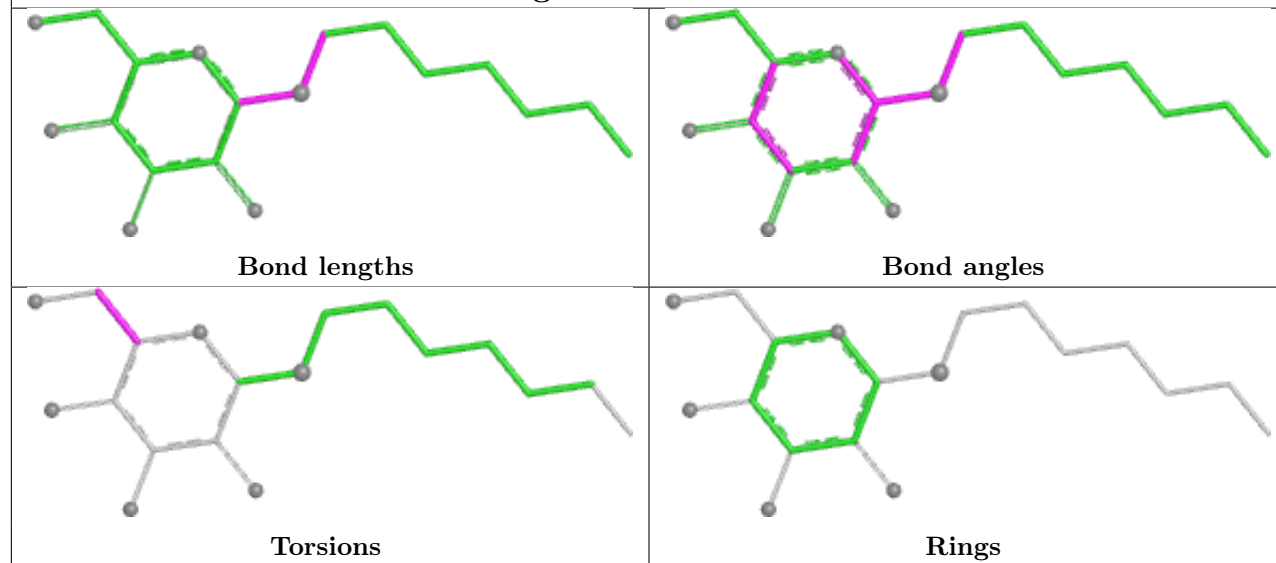
| Ligand BCR 3 616                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA A 826                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

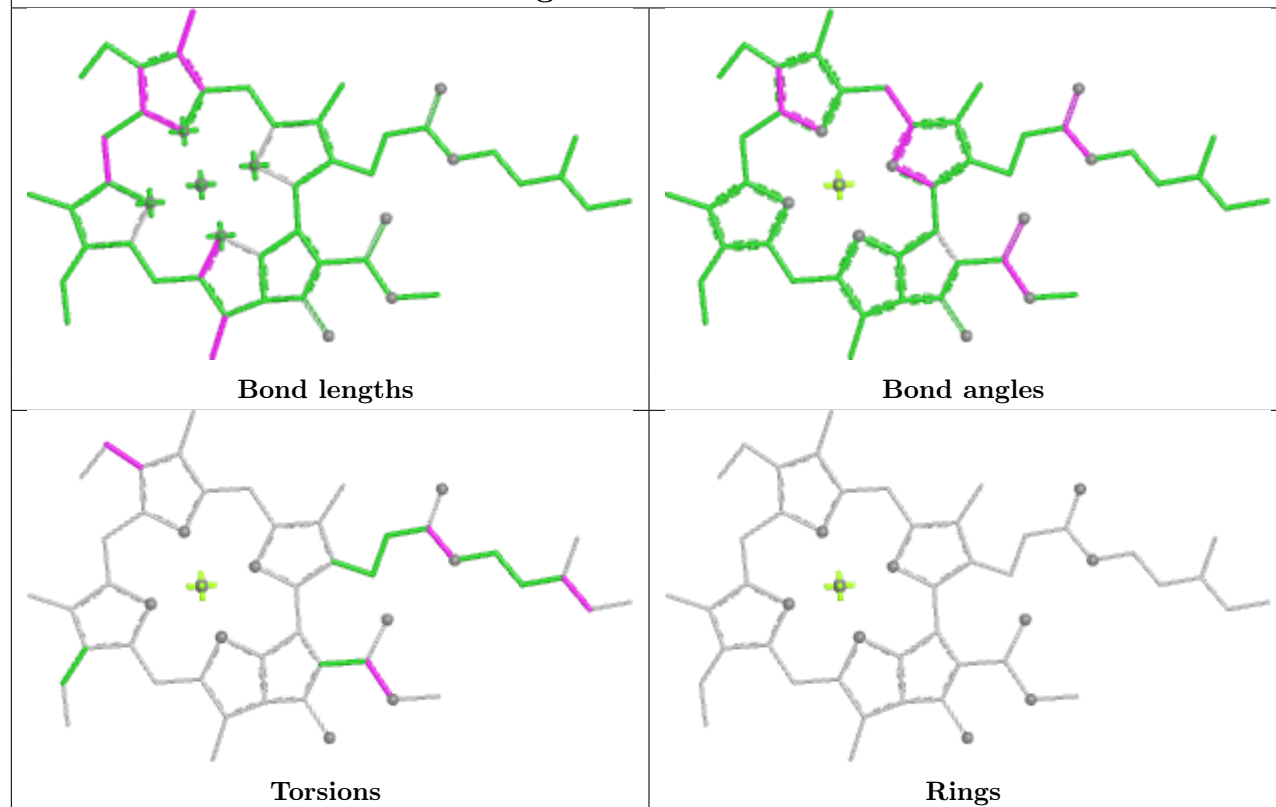
## Ligand CHL 2 306



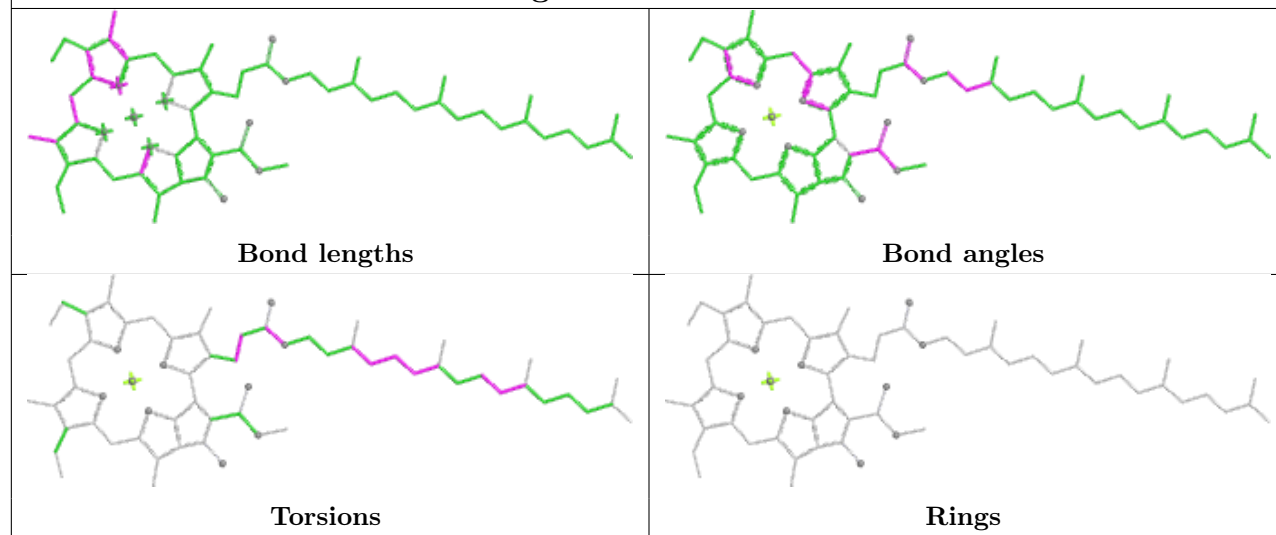
## Ligand HTG 4 322



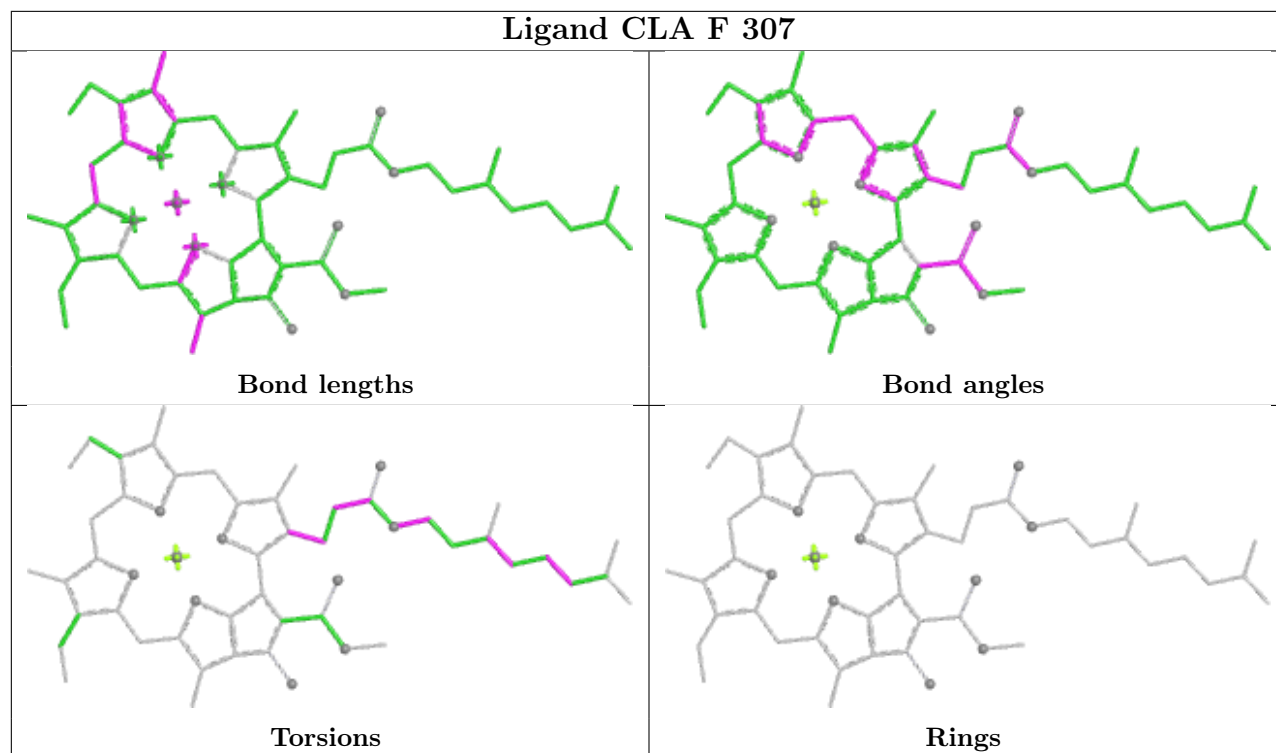
## Ligand CLA 1 303



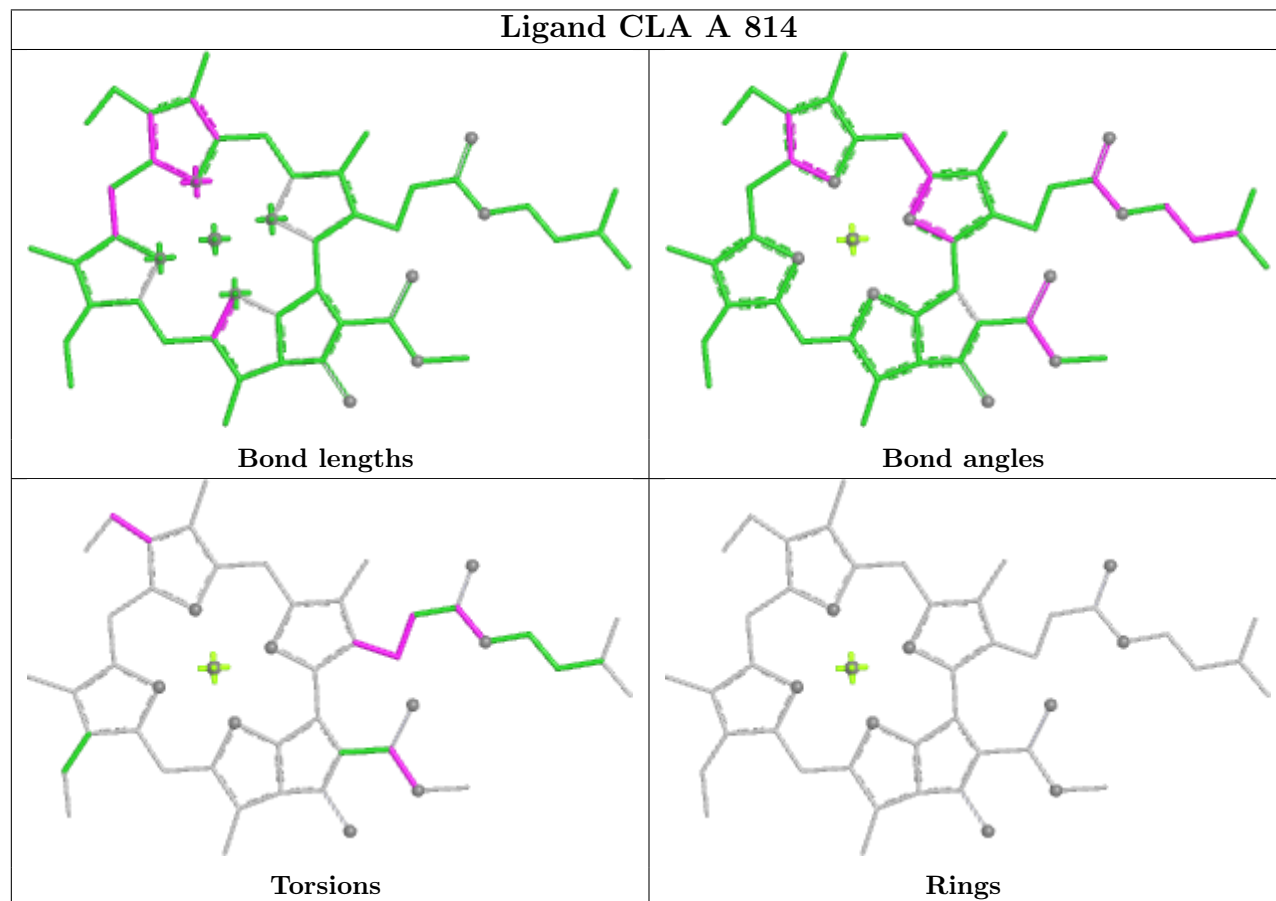
## Ligand CLA A 841



## Ligand CLA F 307

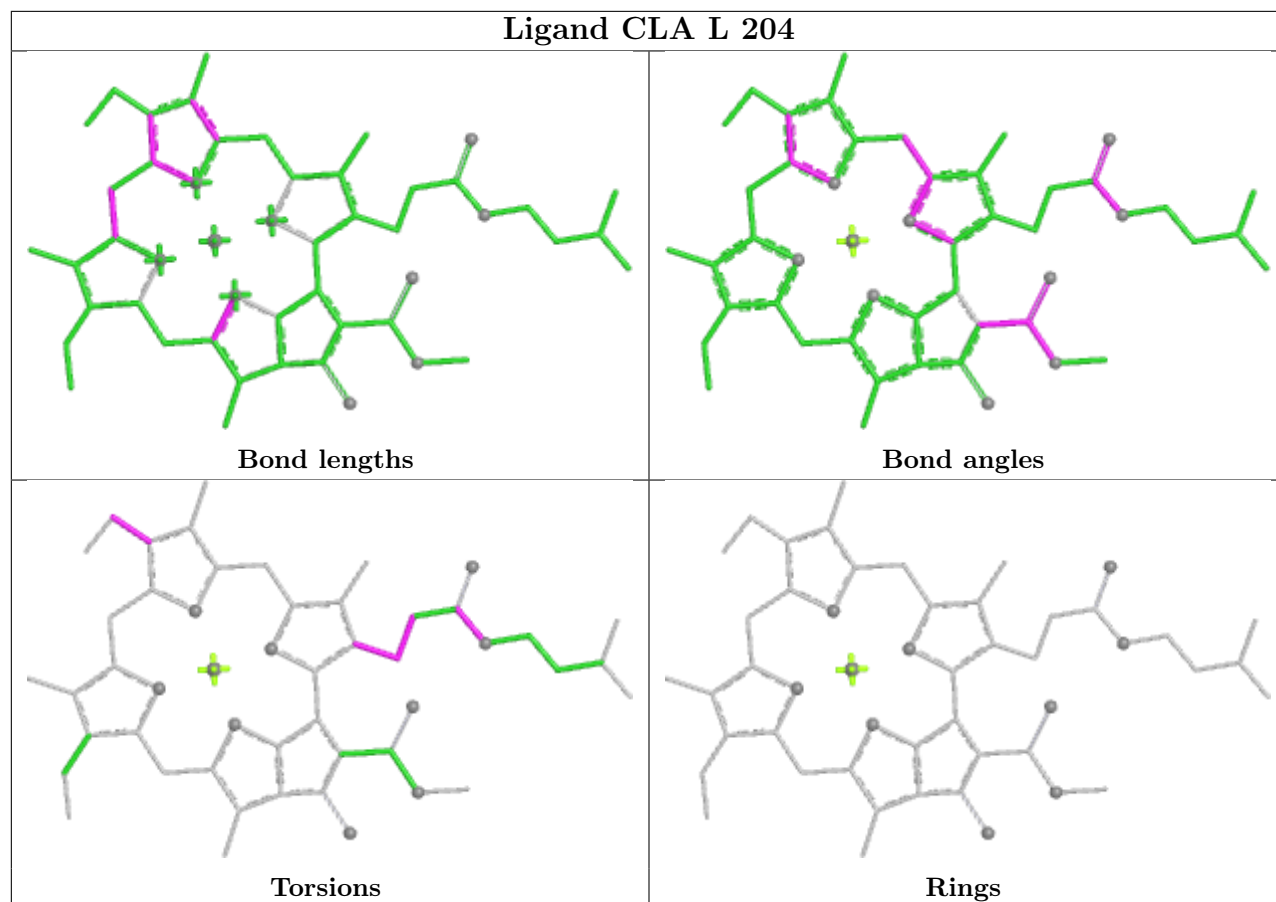


## Ligand CLA A 814

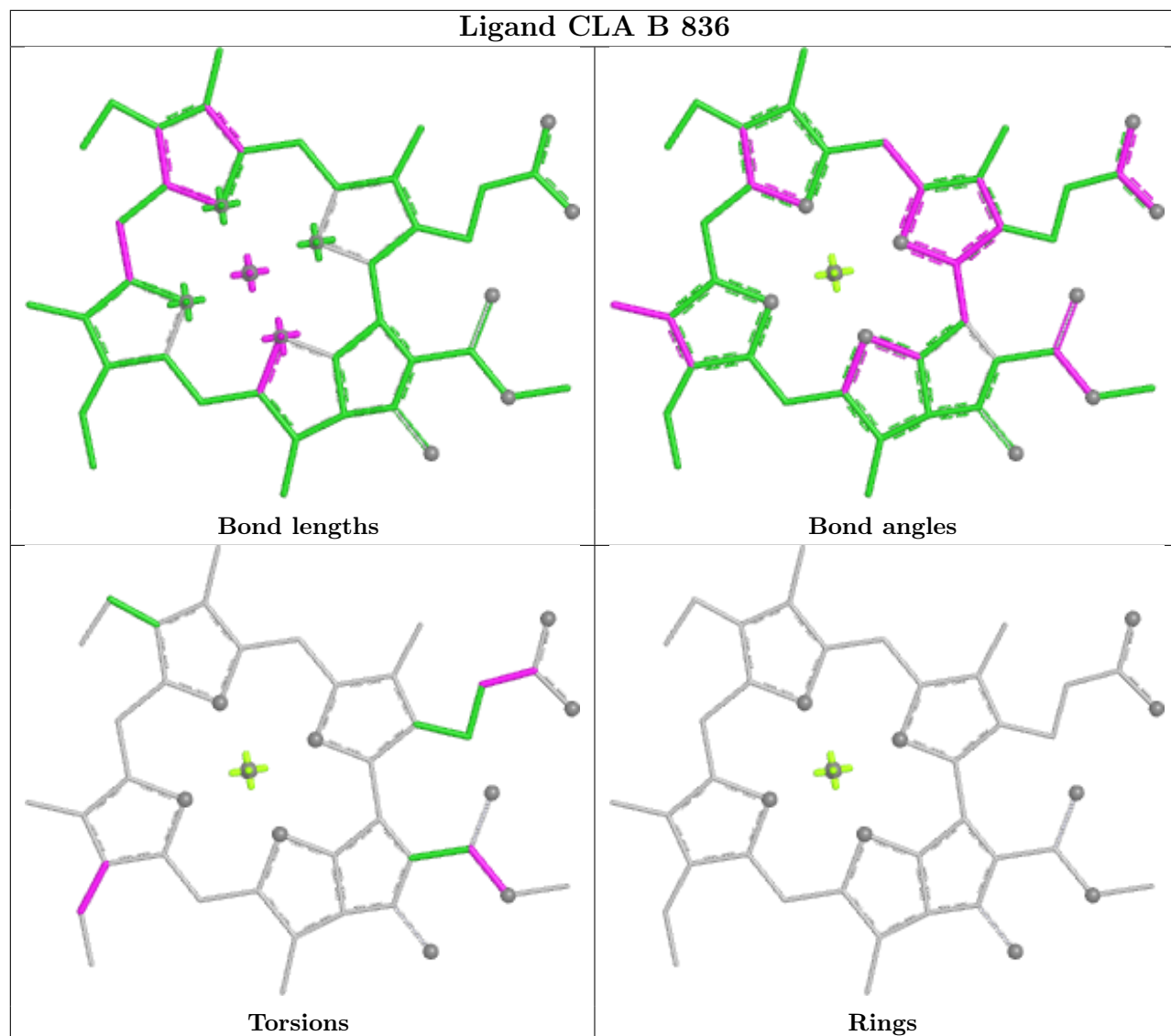




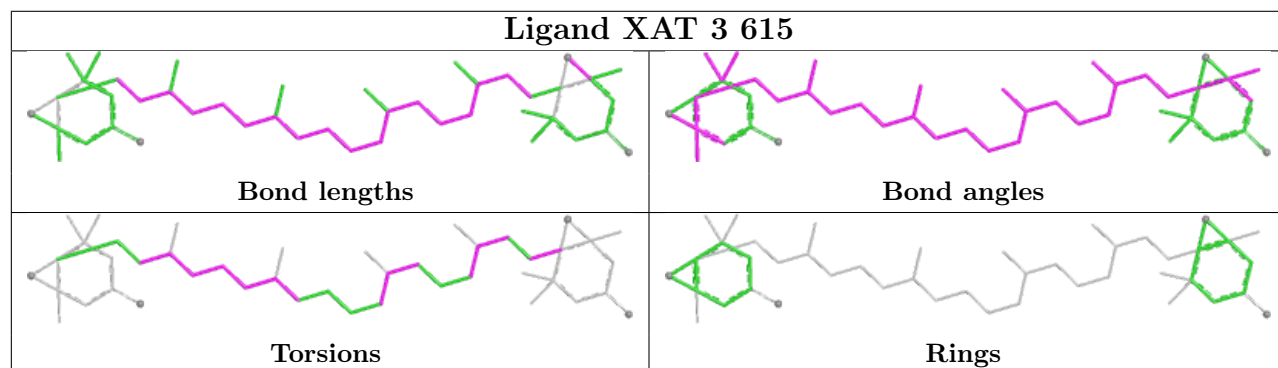
## Ligand CLA L 204



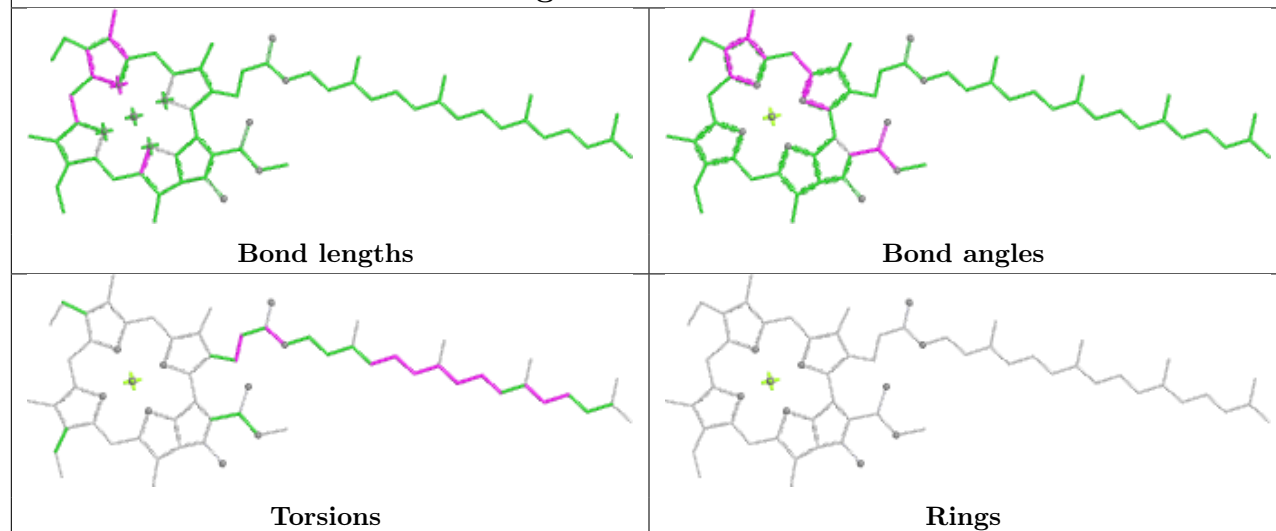
## Ligand CLA B 836



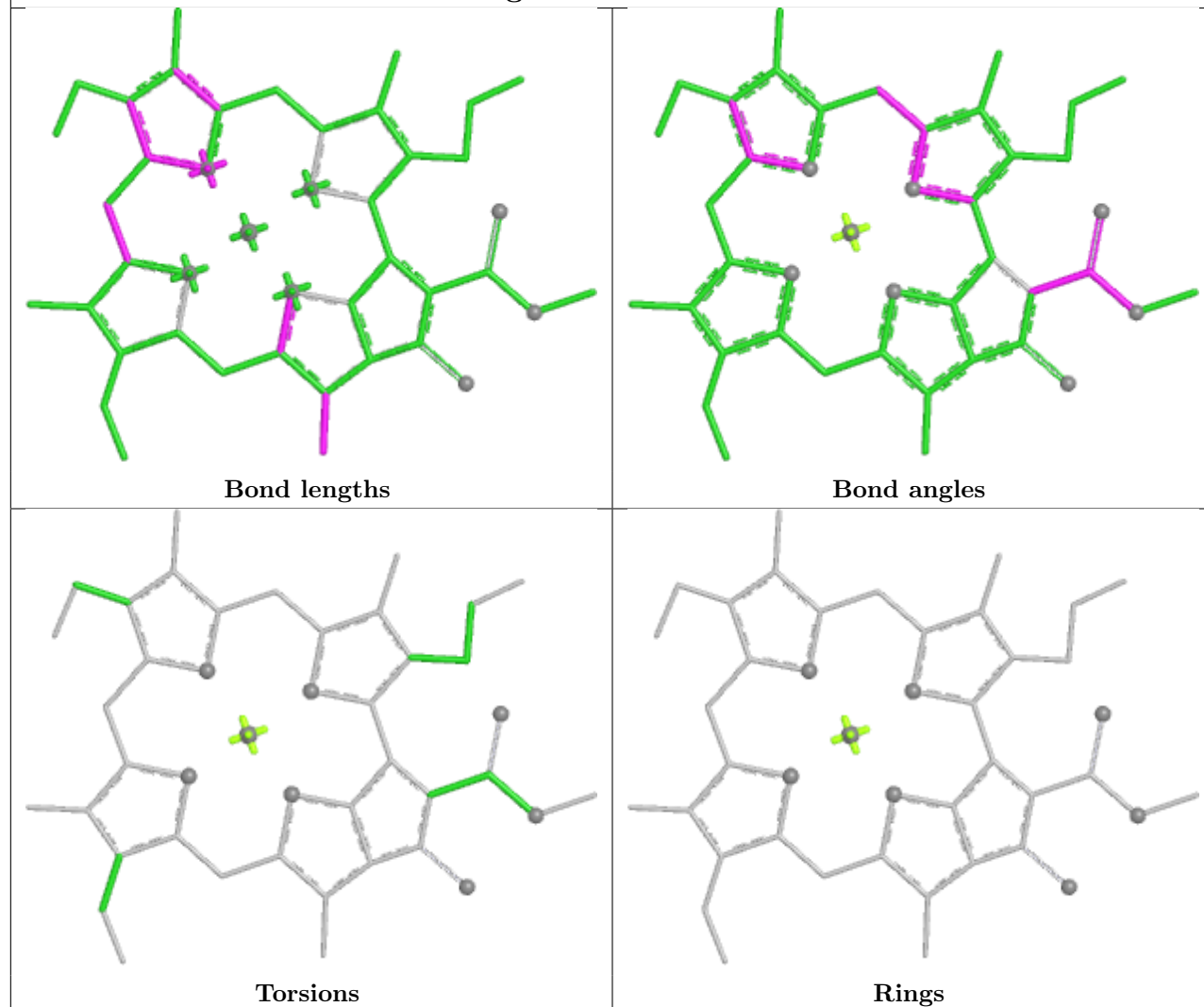
## Ligand XAT 3 615

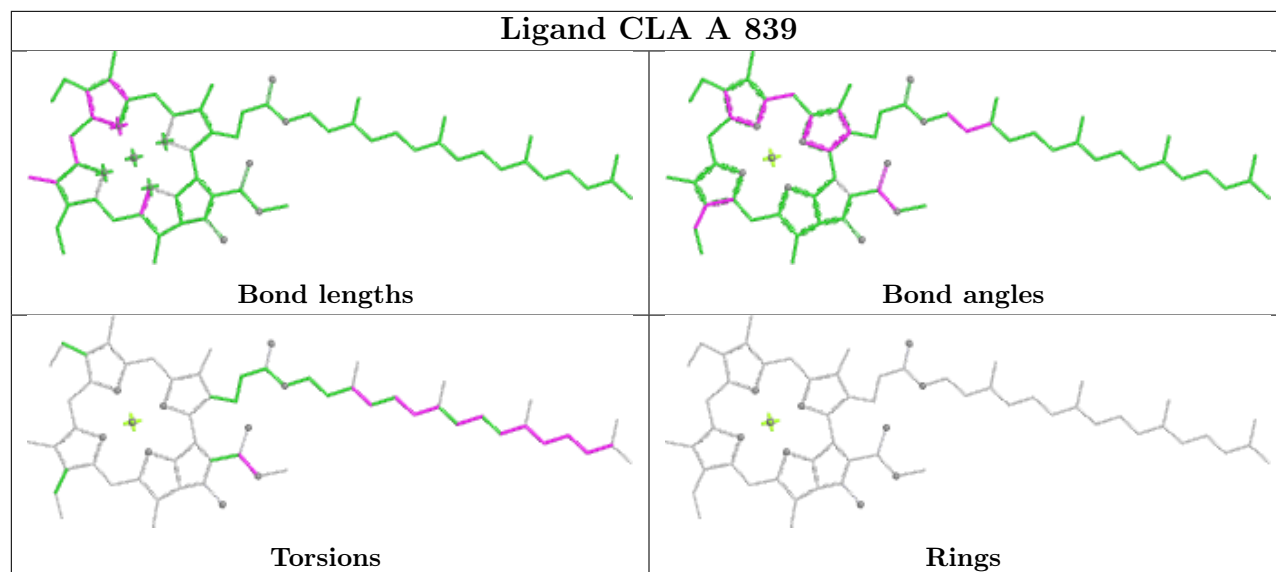
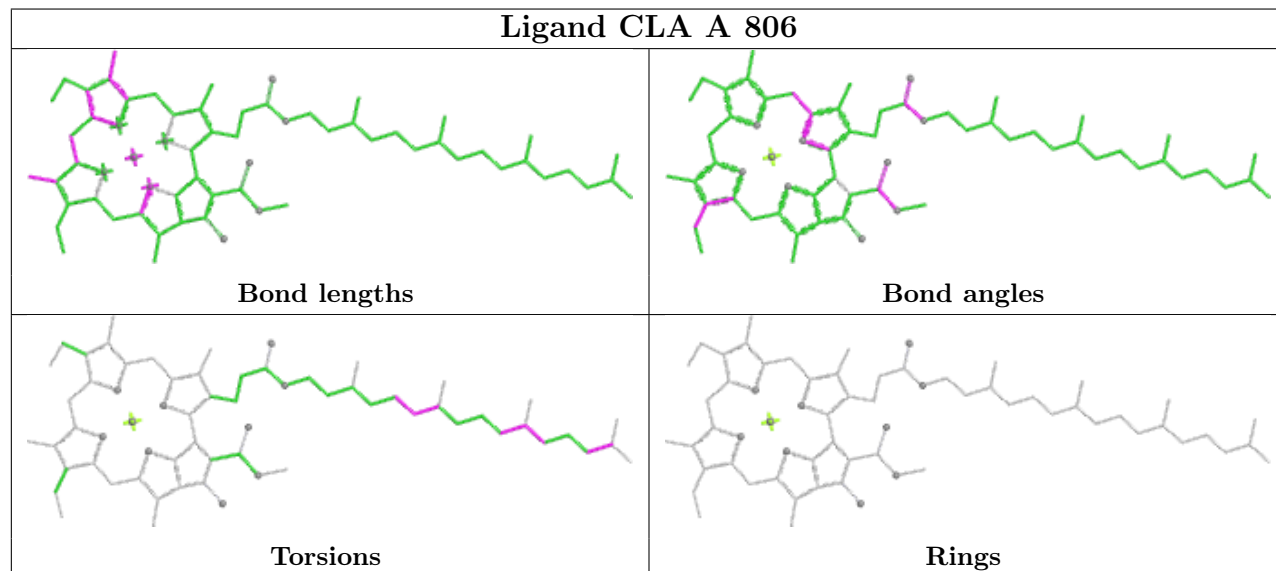


## Ligand CLA 2 311

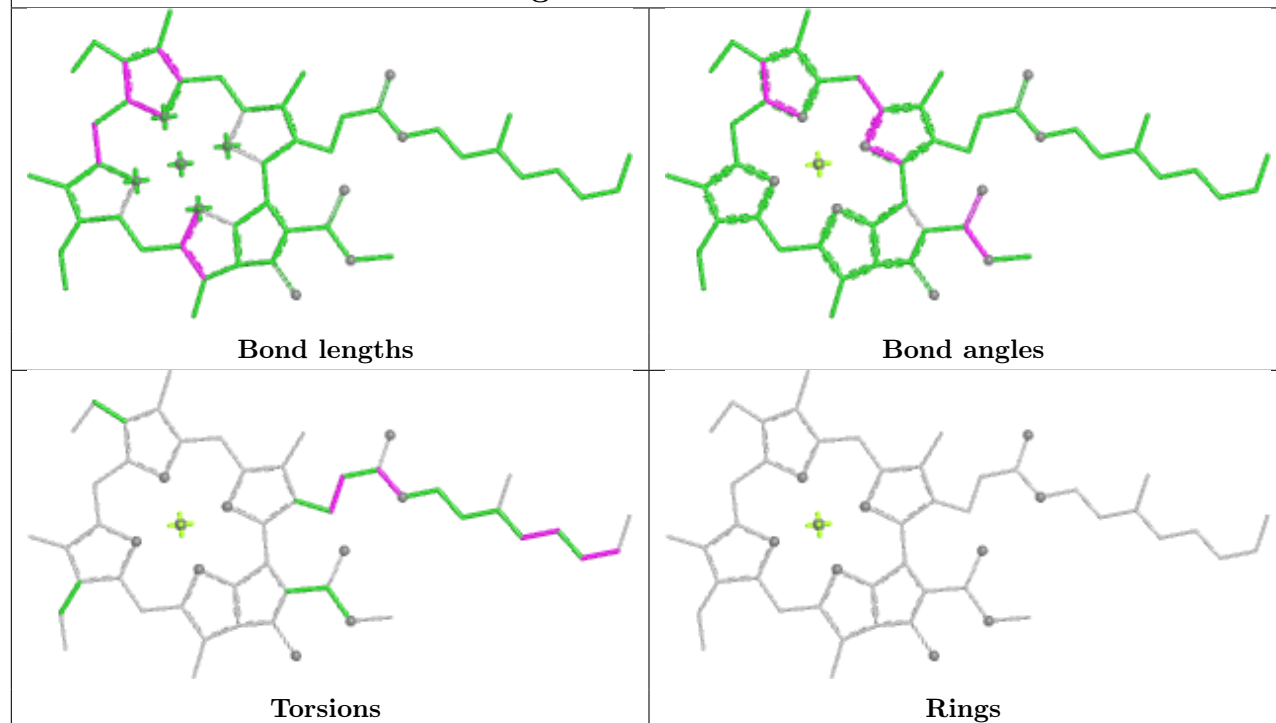


## Ligand CLA 2 312

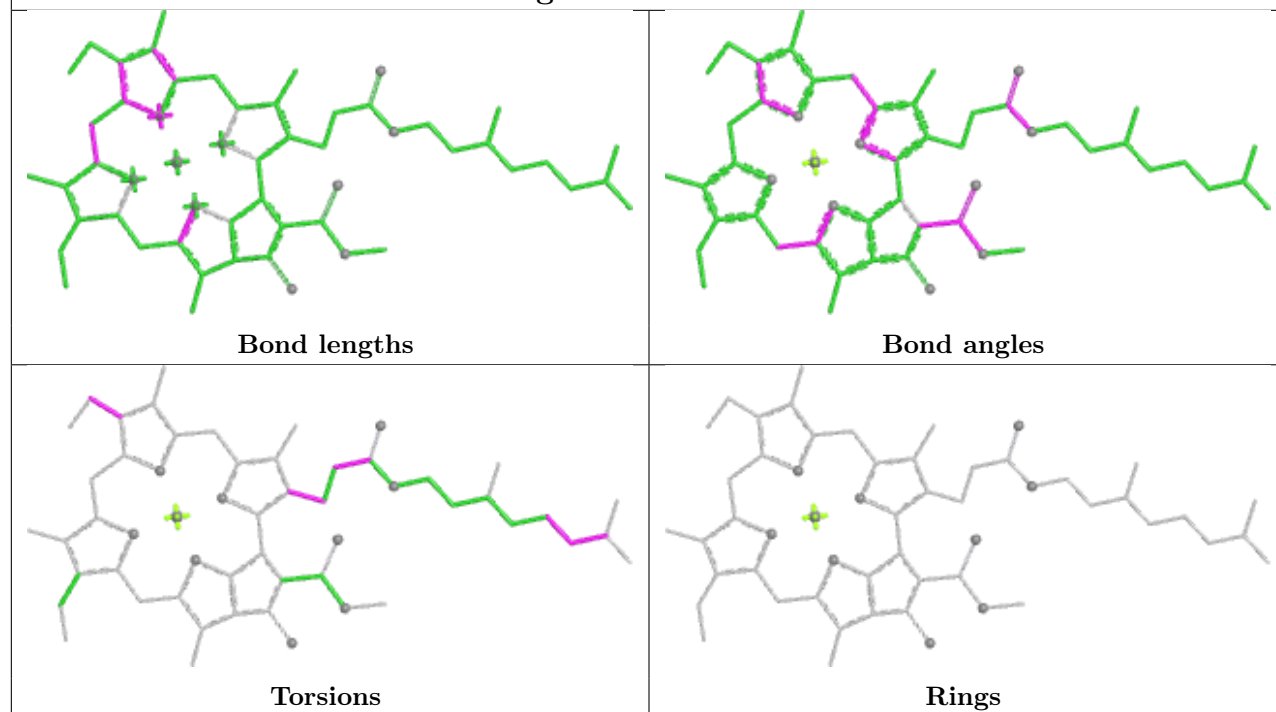


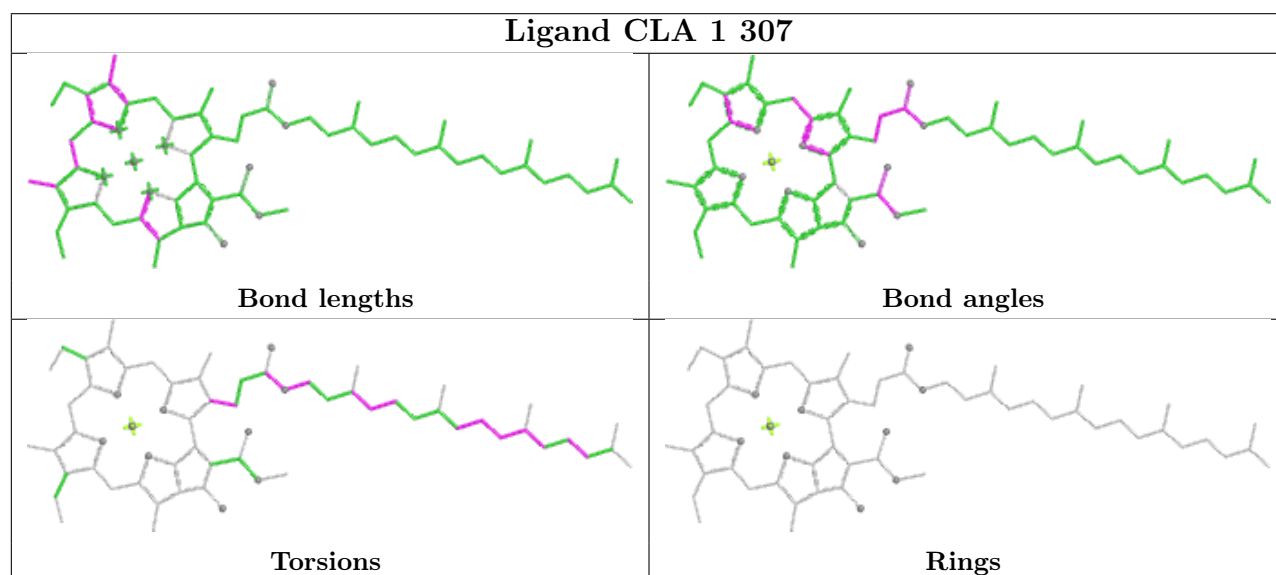
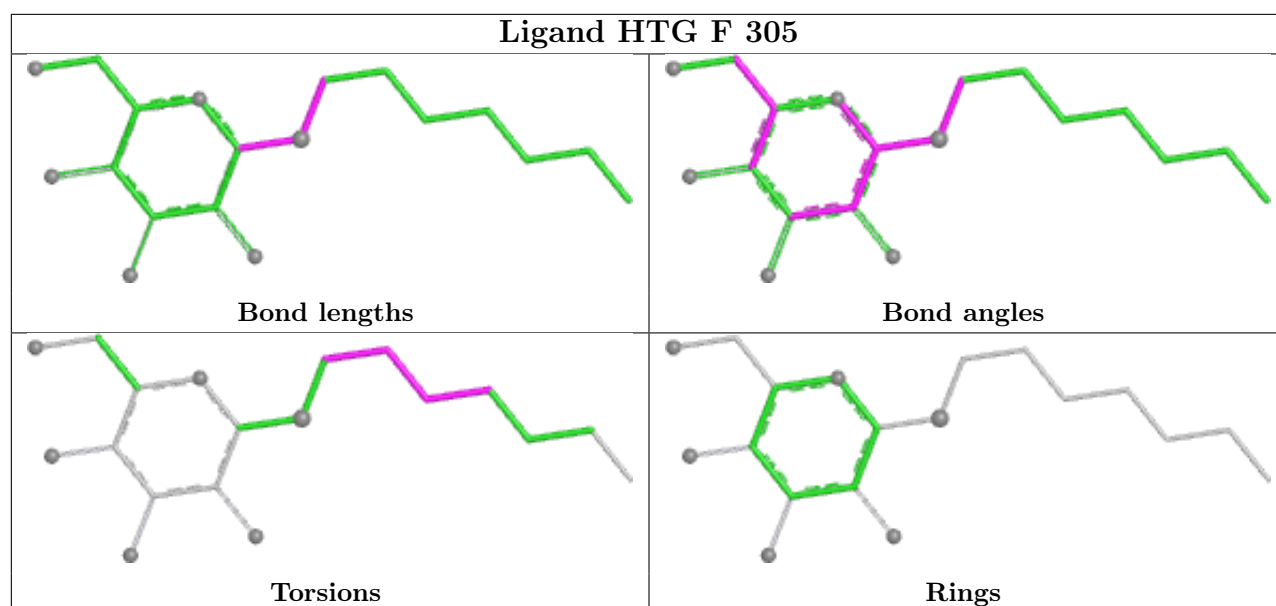
**Ligand CLA A 839****Ligand CLA A 806**

## Ligand CLA A 811

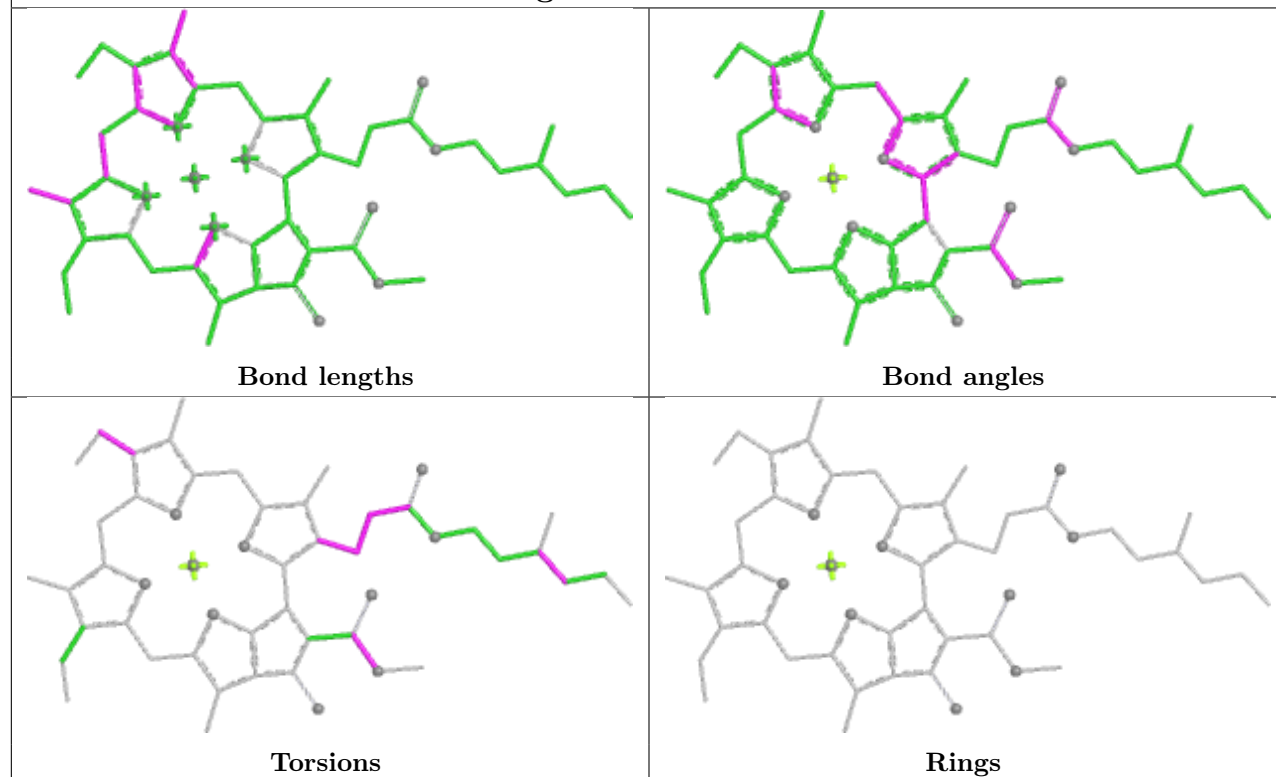


## Ligand CLA 1 312

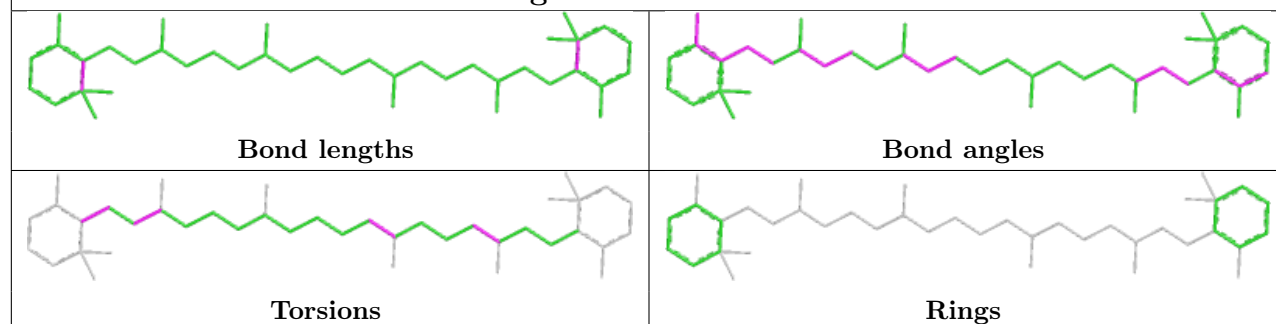




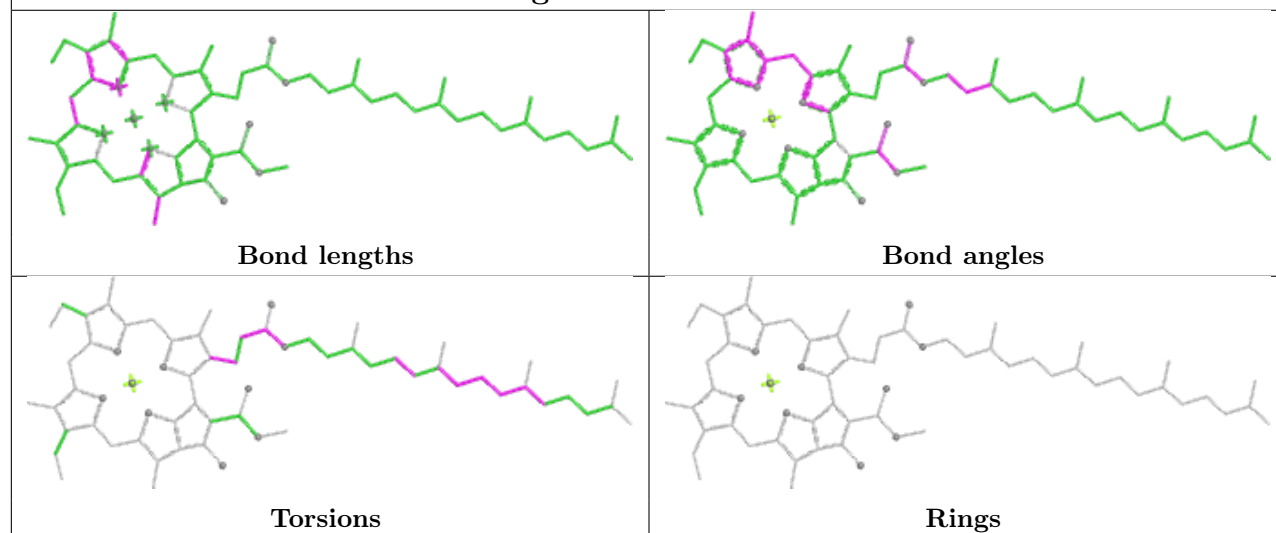
## Ligand CLA 3 610



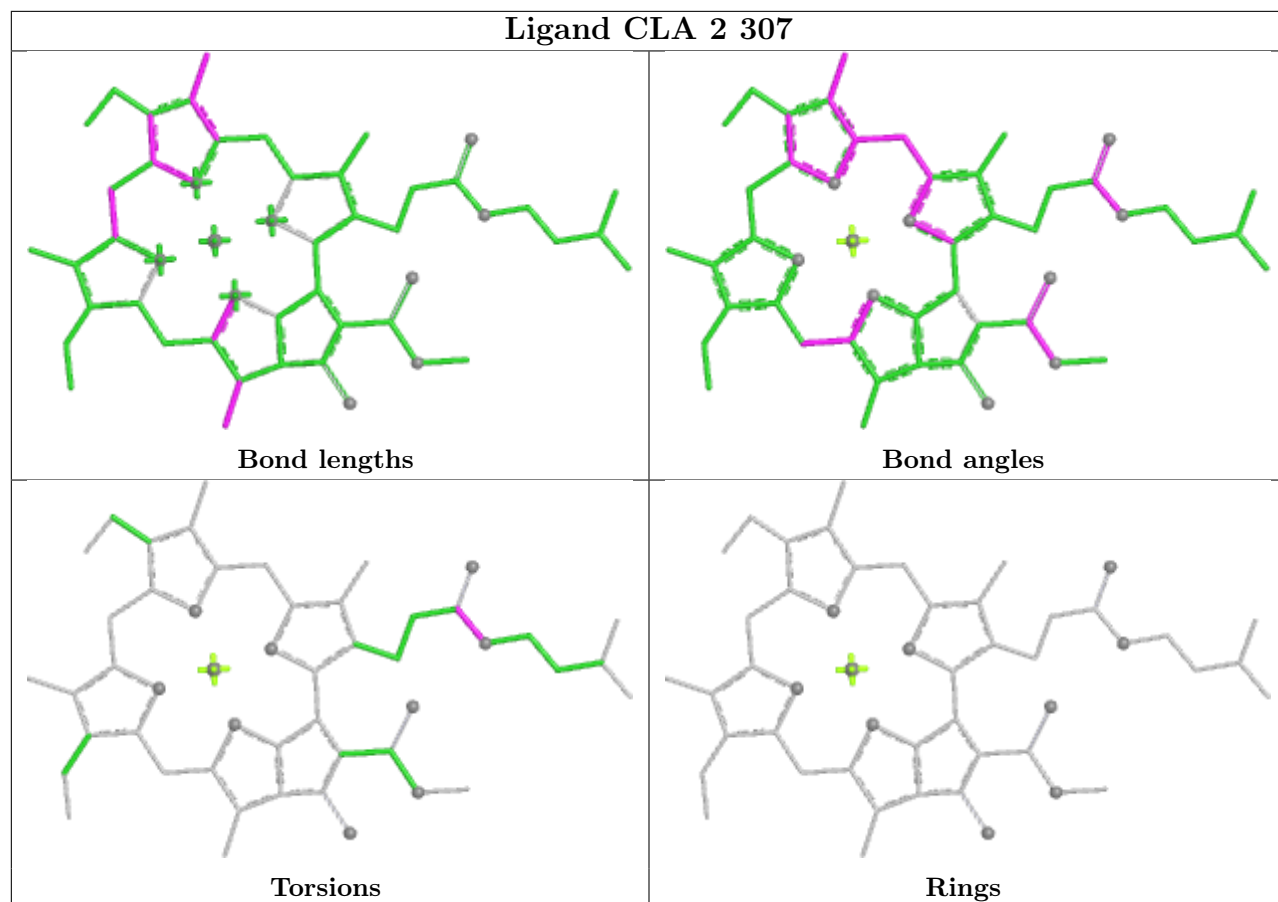
## Ligand BCR A 848



## Ligand CLA A 809

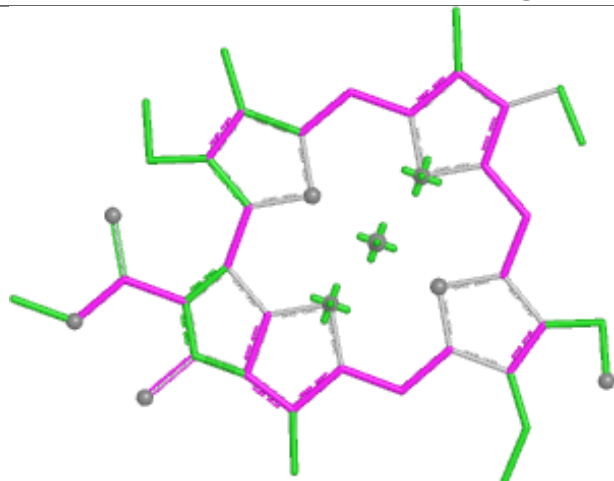


## Ligand CLA 2 307

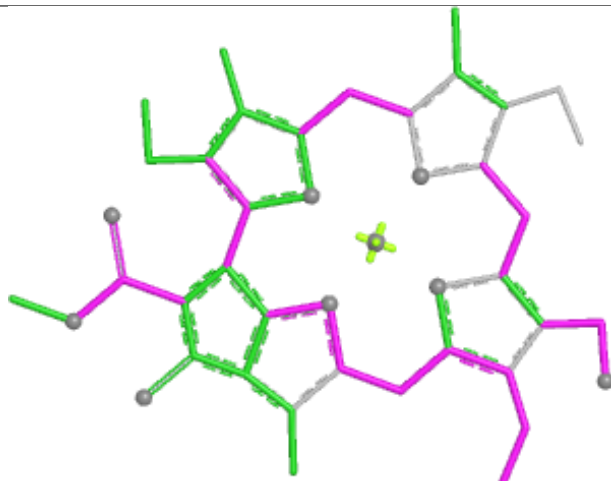




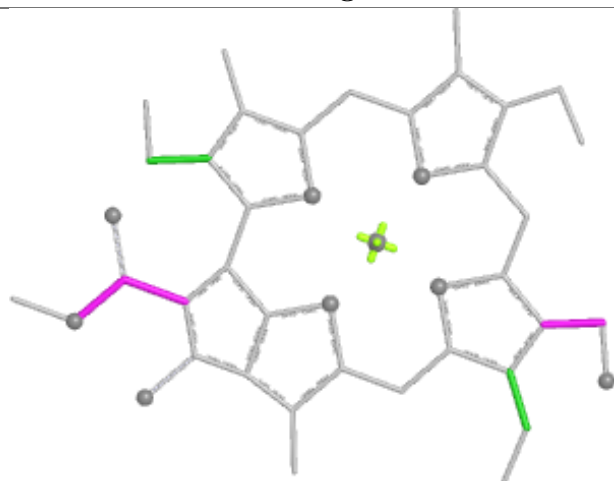
## Ligand CHL 2 304



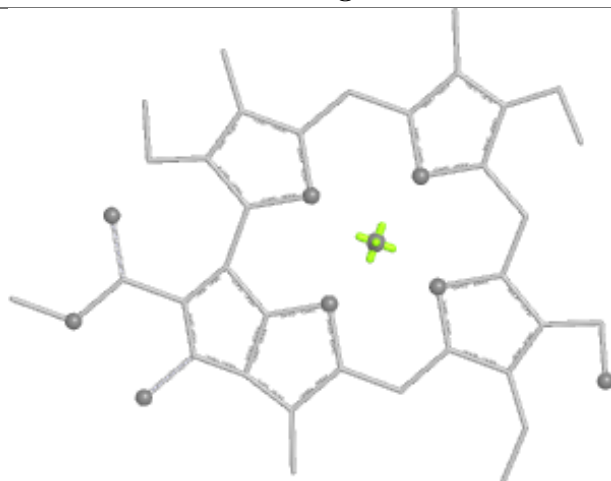
Bond lengths



Bond angles

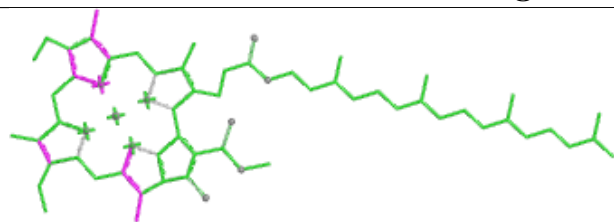


Torsions

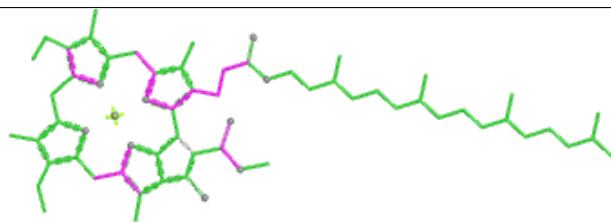


Rings

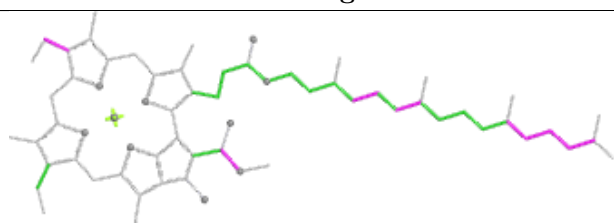
## Ligand CLA B 841



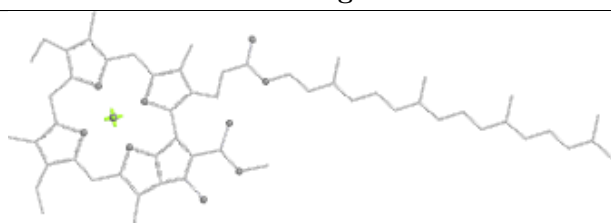
Bond lengths



Bond angles

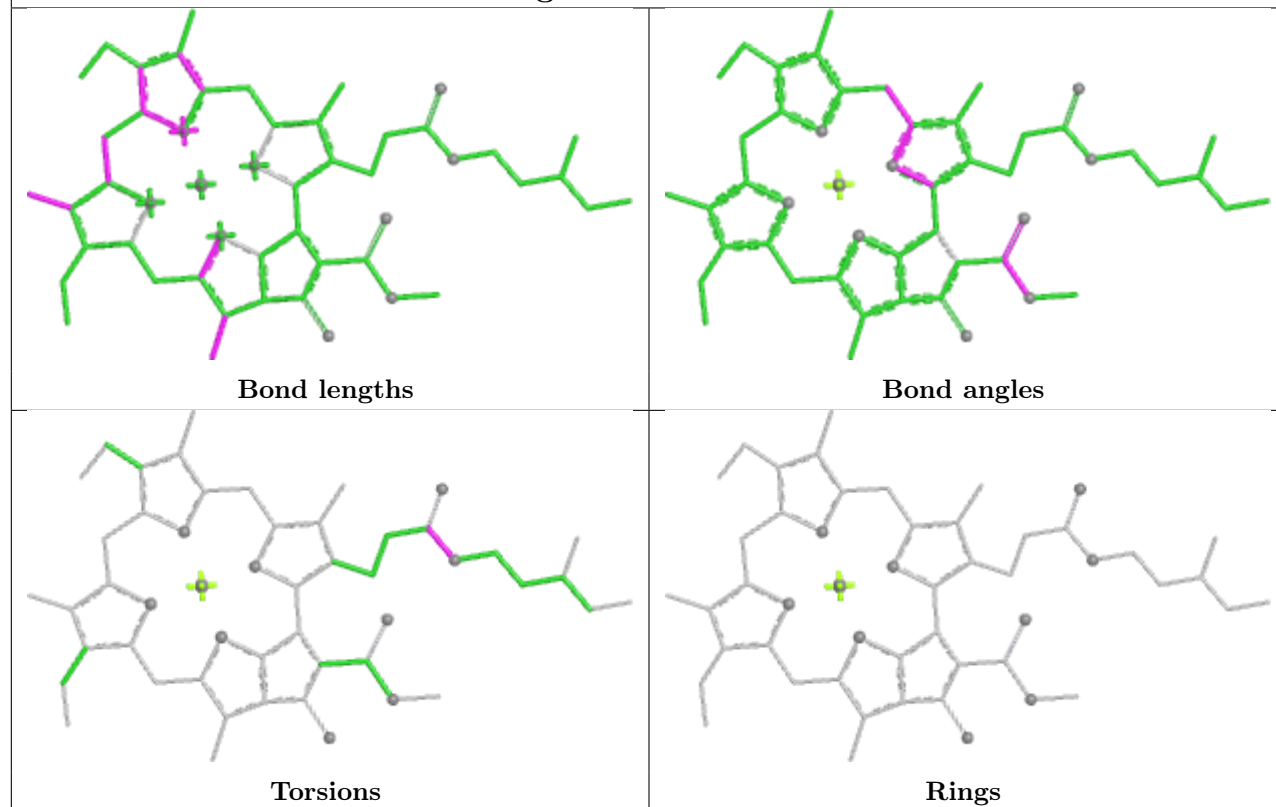


Torsions

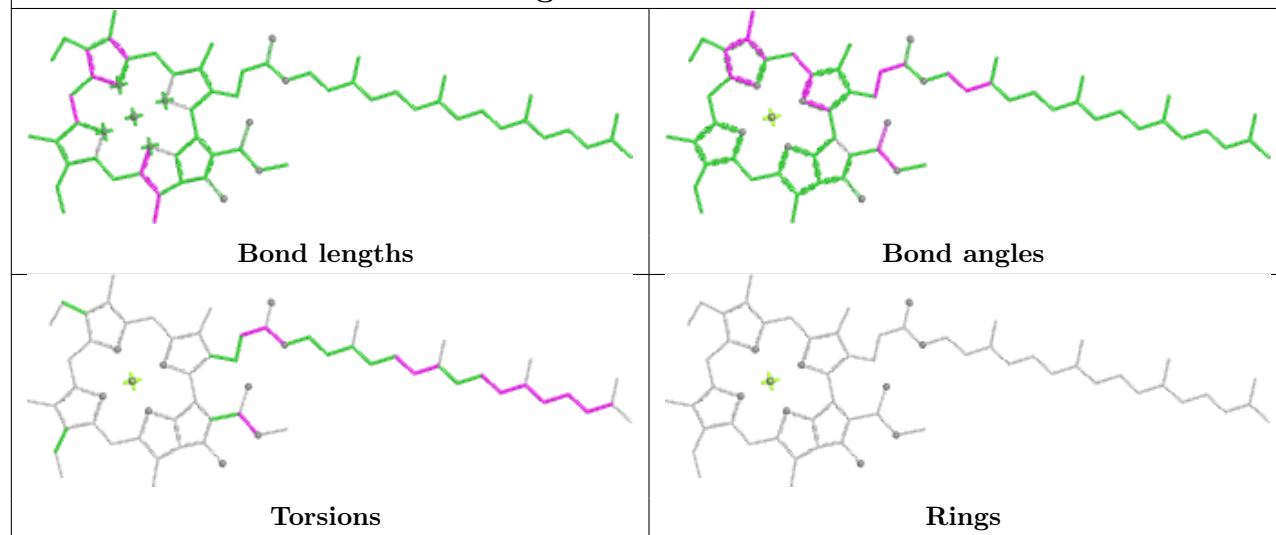


Rings

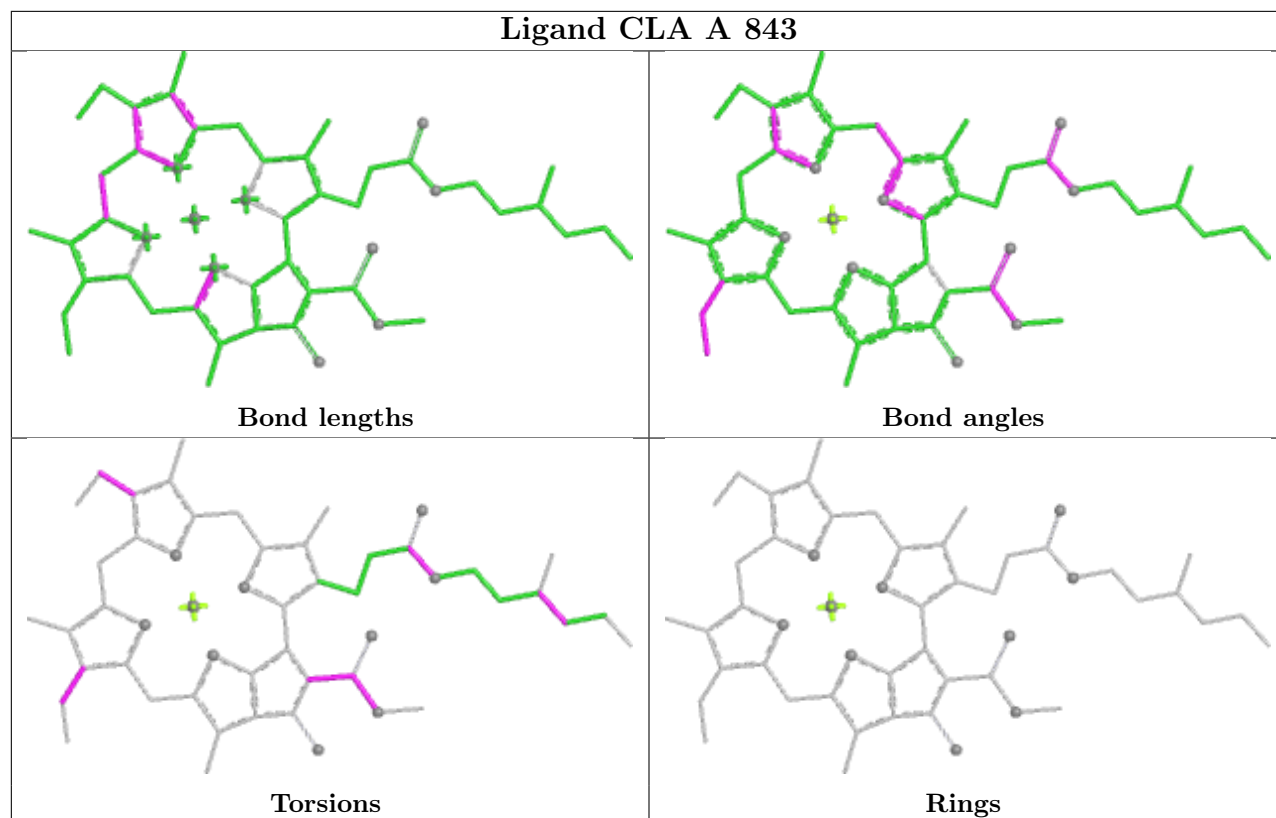
## Ligand CLA 2 302



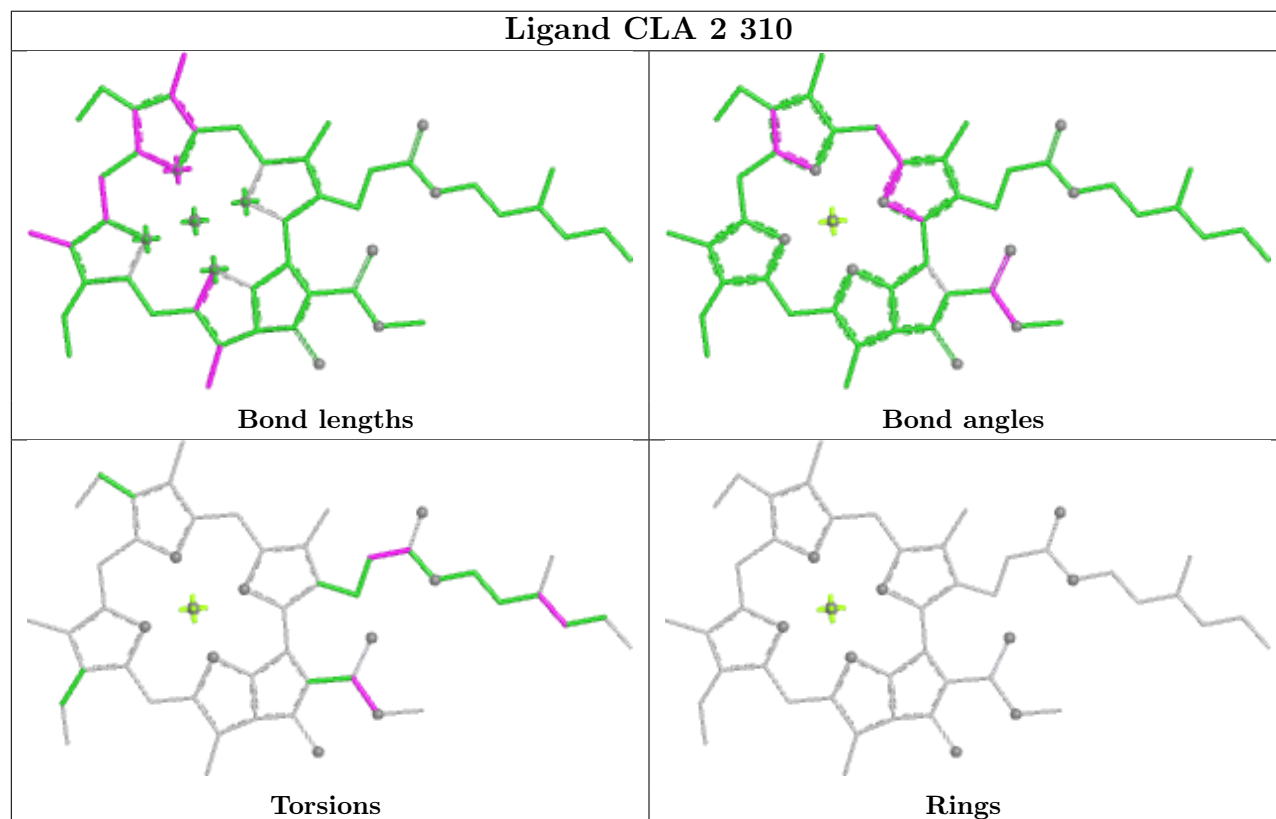
## Ligand CLA 1 302



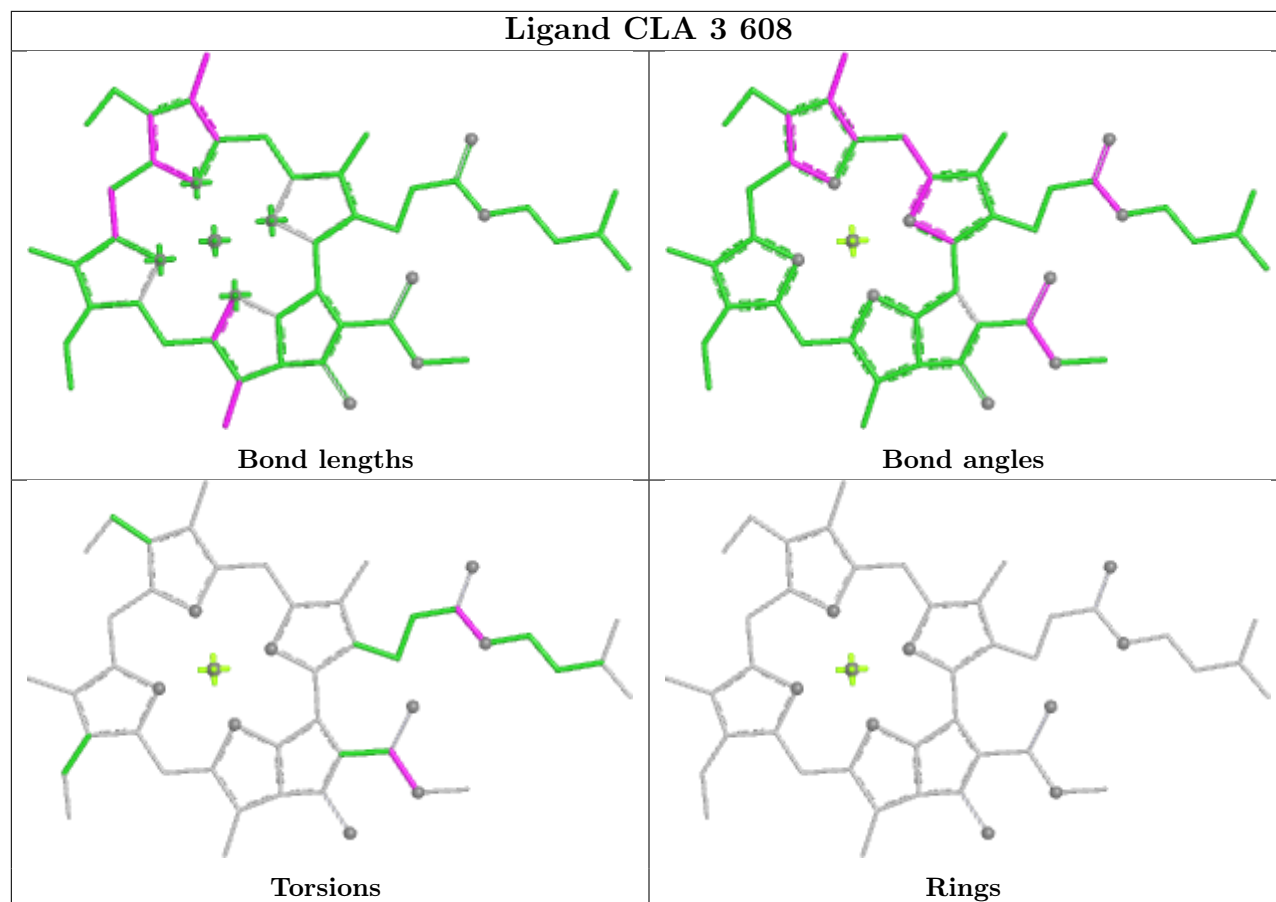
## Ligand CLA A 843



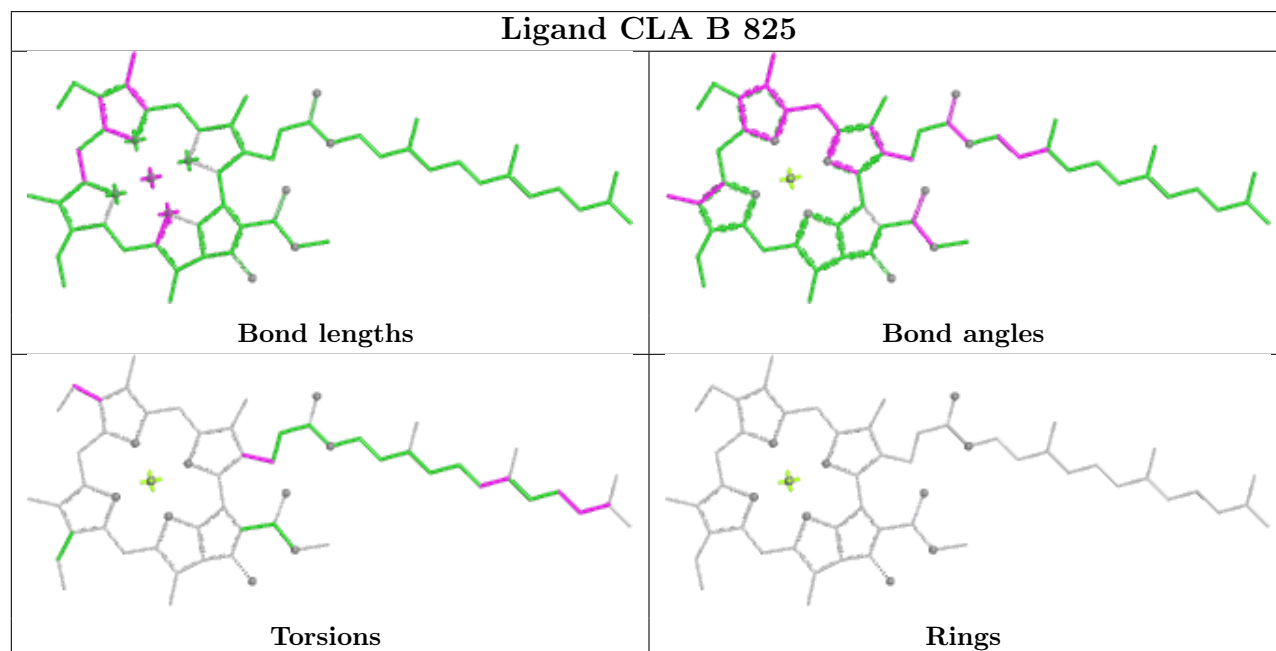
## Ligand CLA 2 310

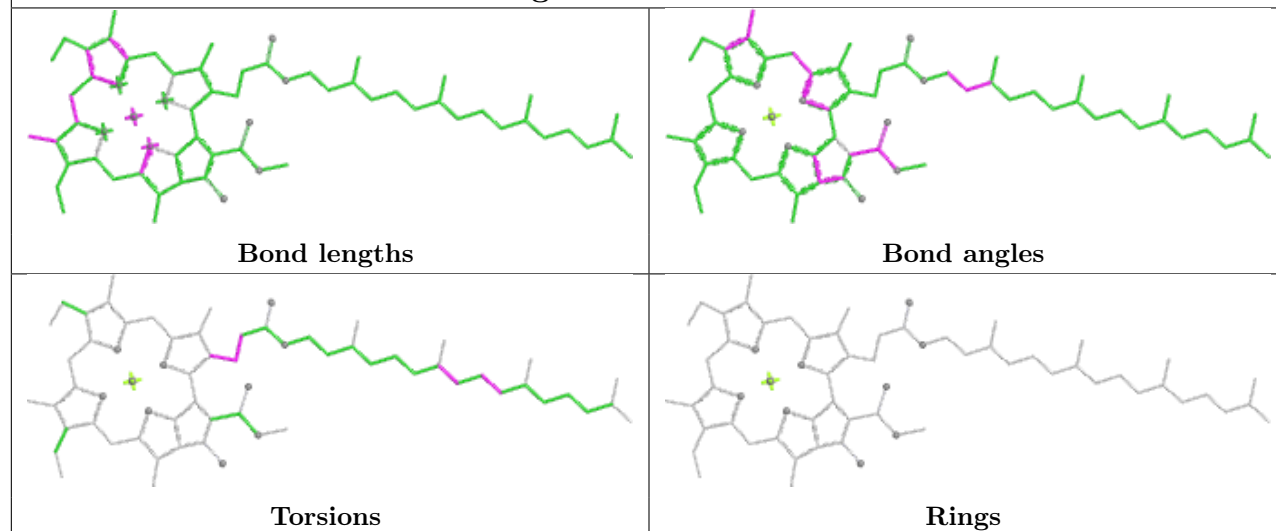
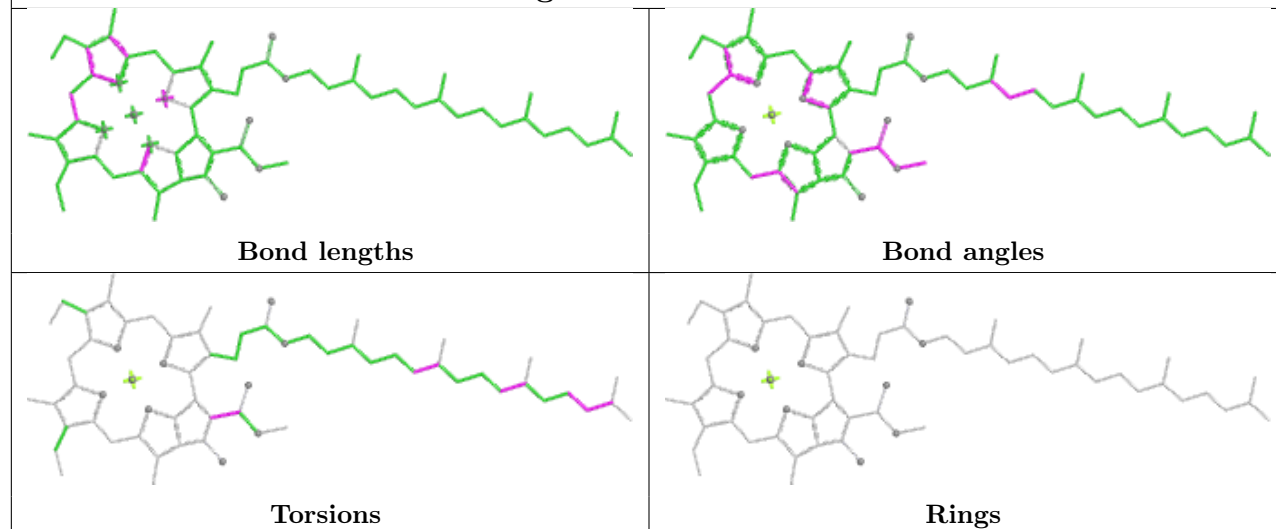


## Ligand CLA 3 608

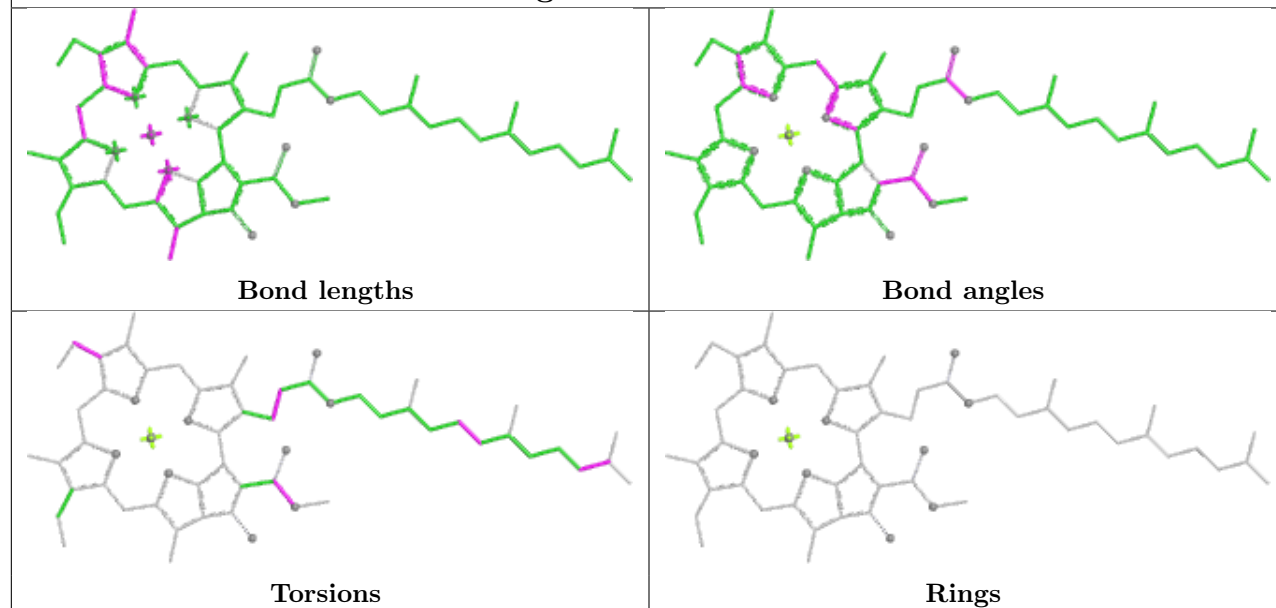


## Ligand CLA B 825

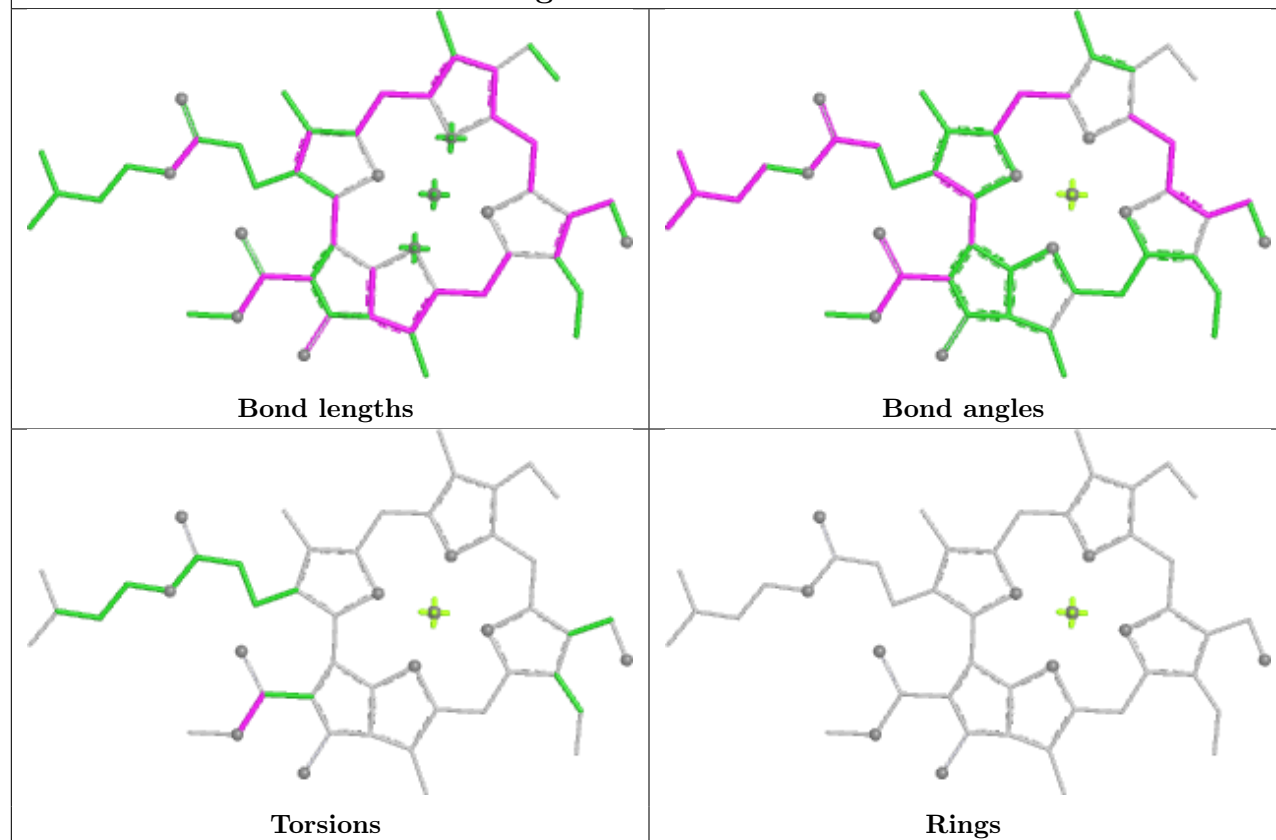


**Ligand CLA A 802****Ligand CLA 1 301**

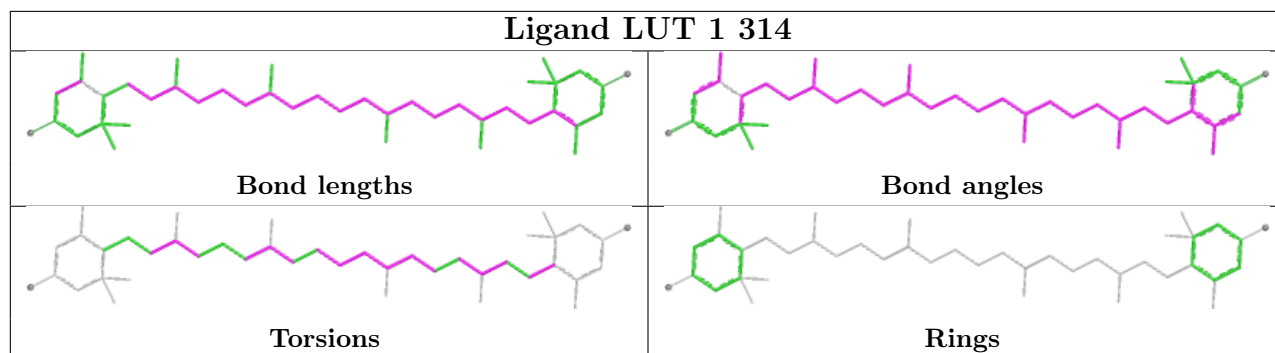
## Ligand CLA 1 311



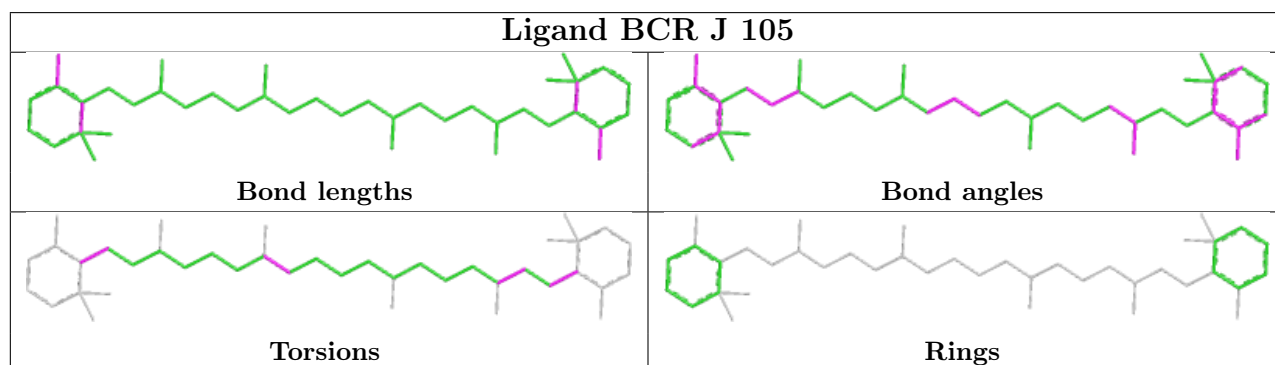
## Ligand CHL 4 307



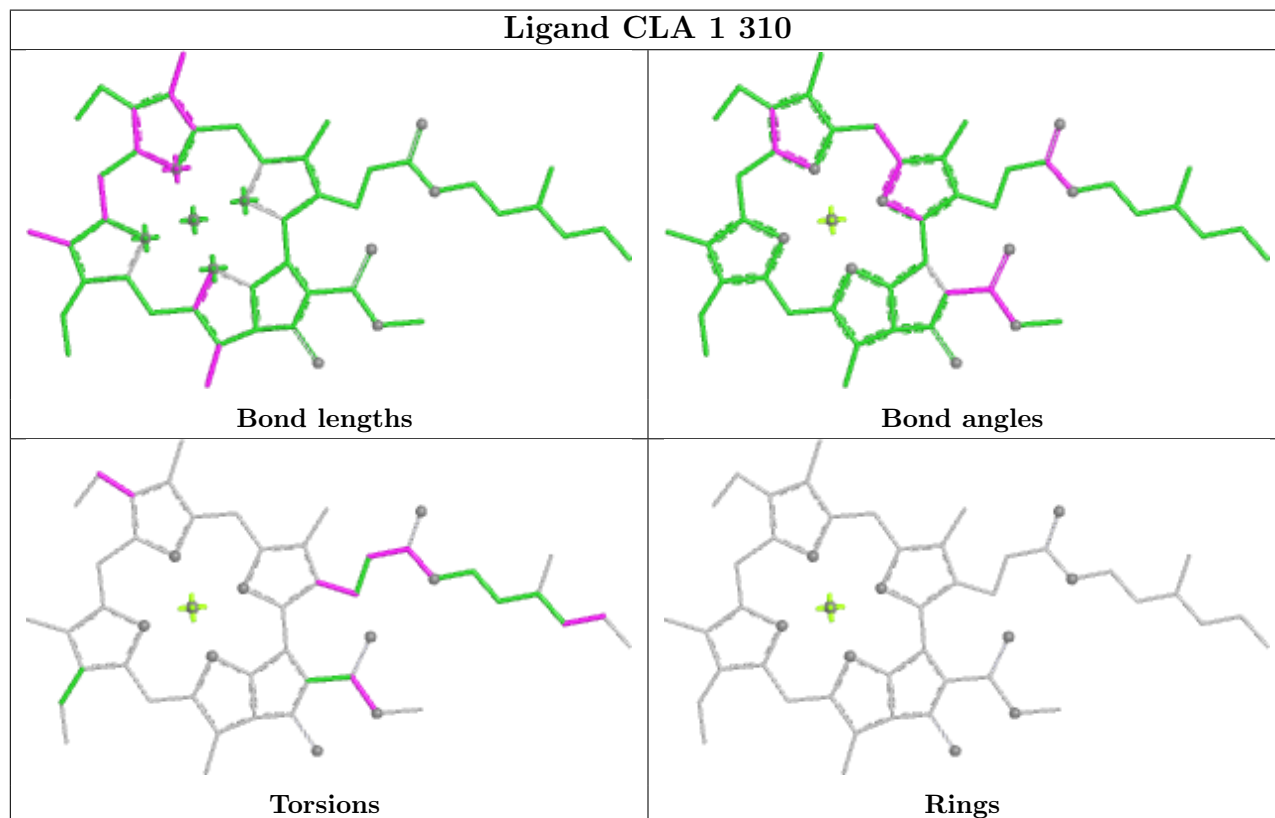
## Ligand LUT 1 314



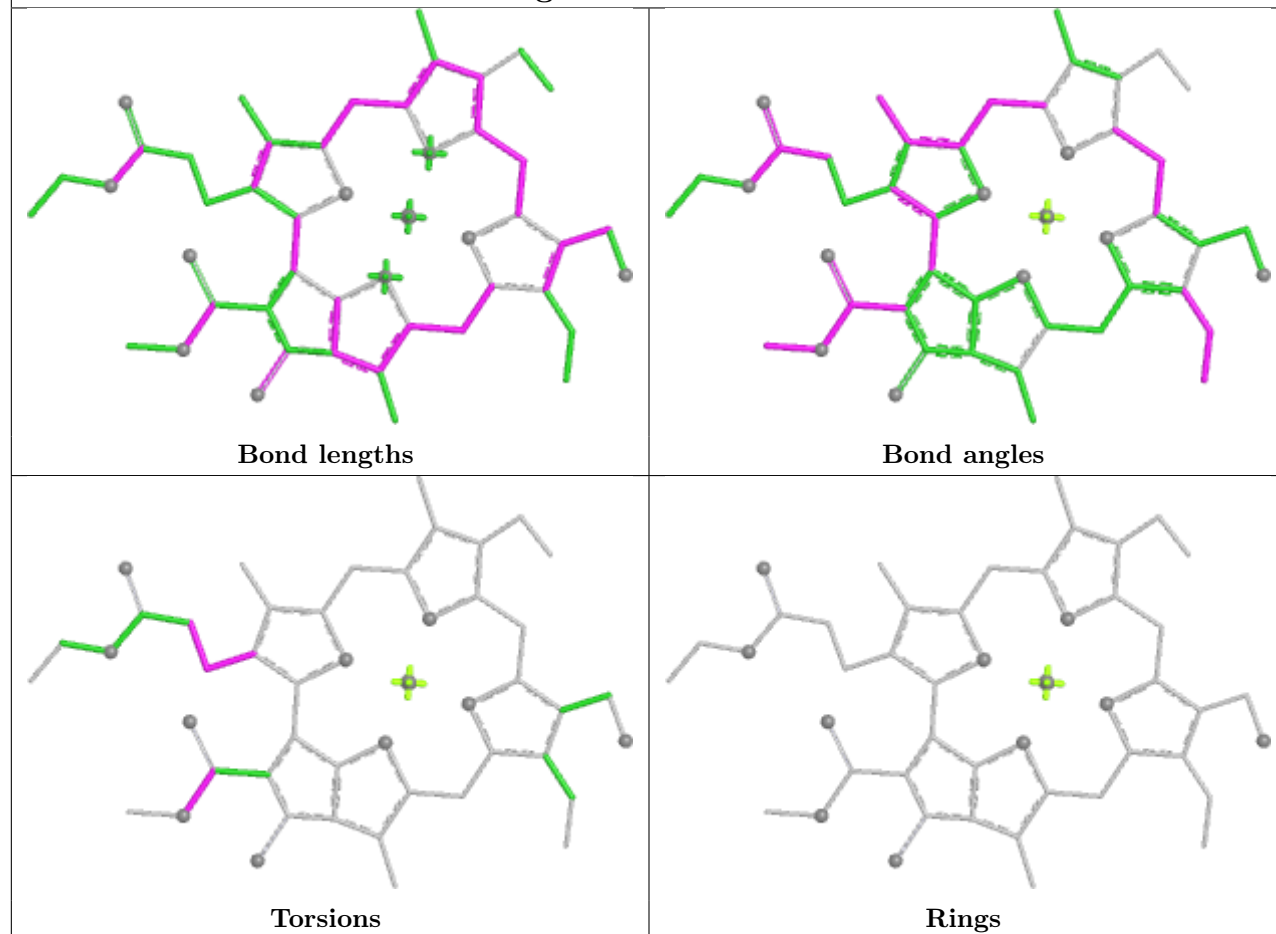
## Ligand BCR J 105



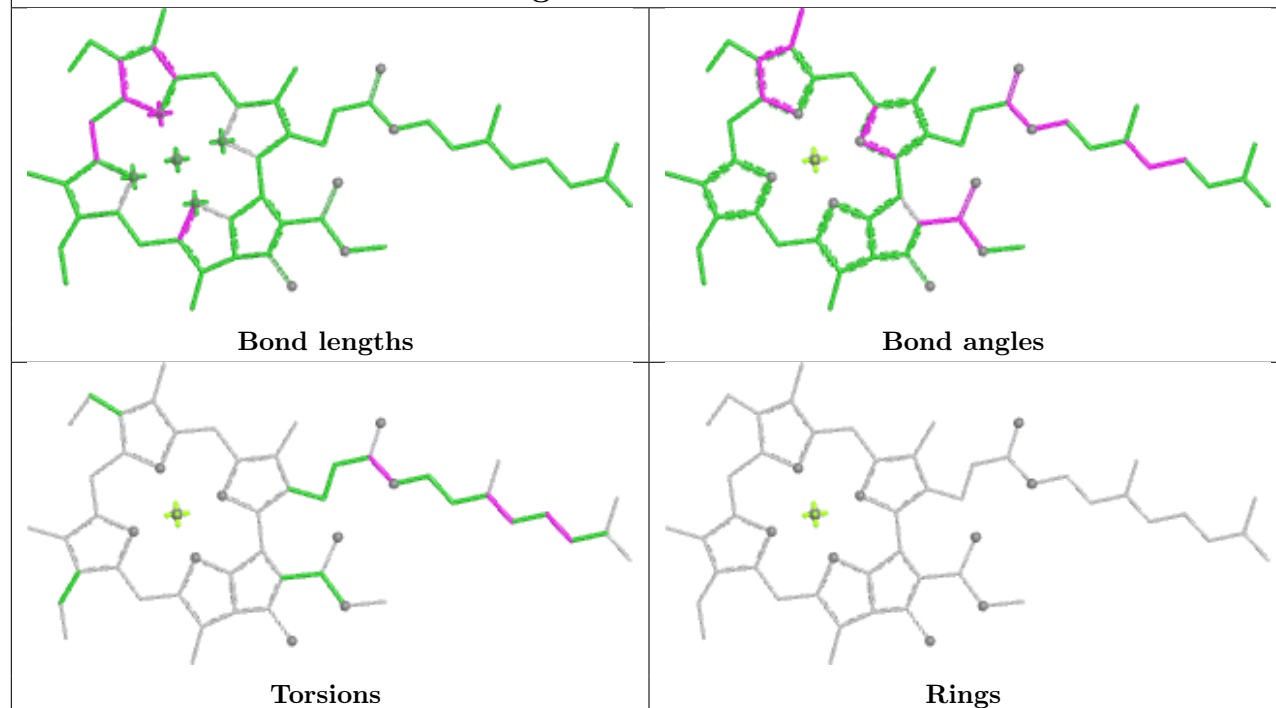
## Ligand CLA 1 310



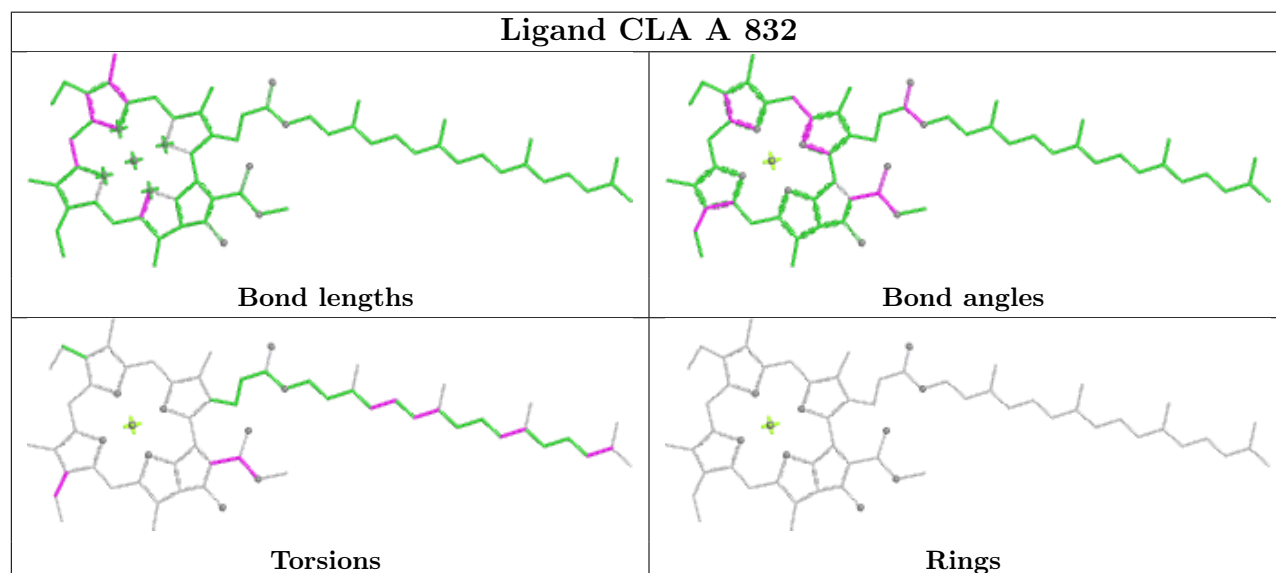
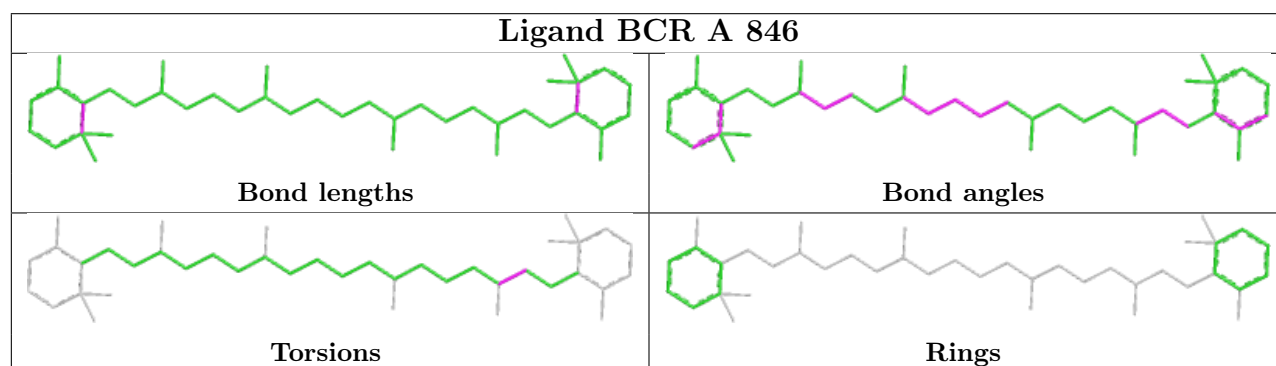
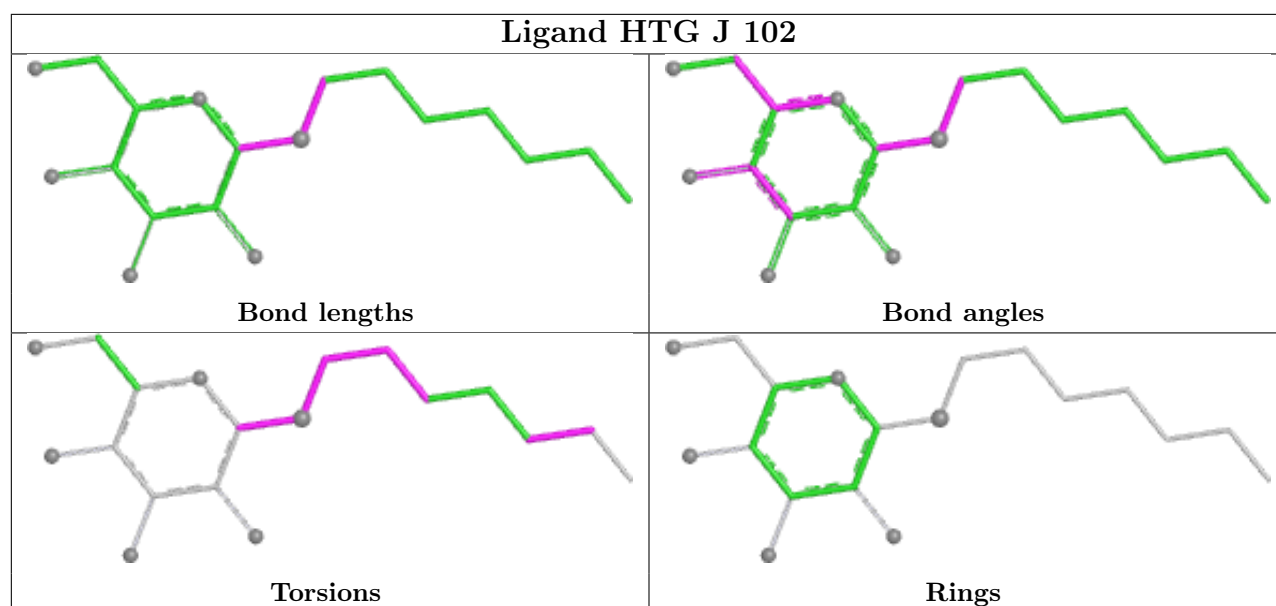
## Ligand CHL 1 305

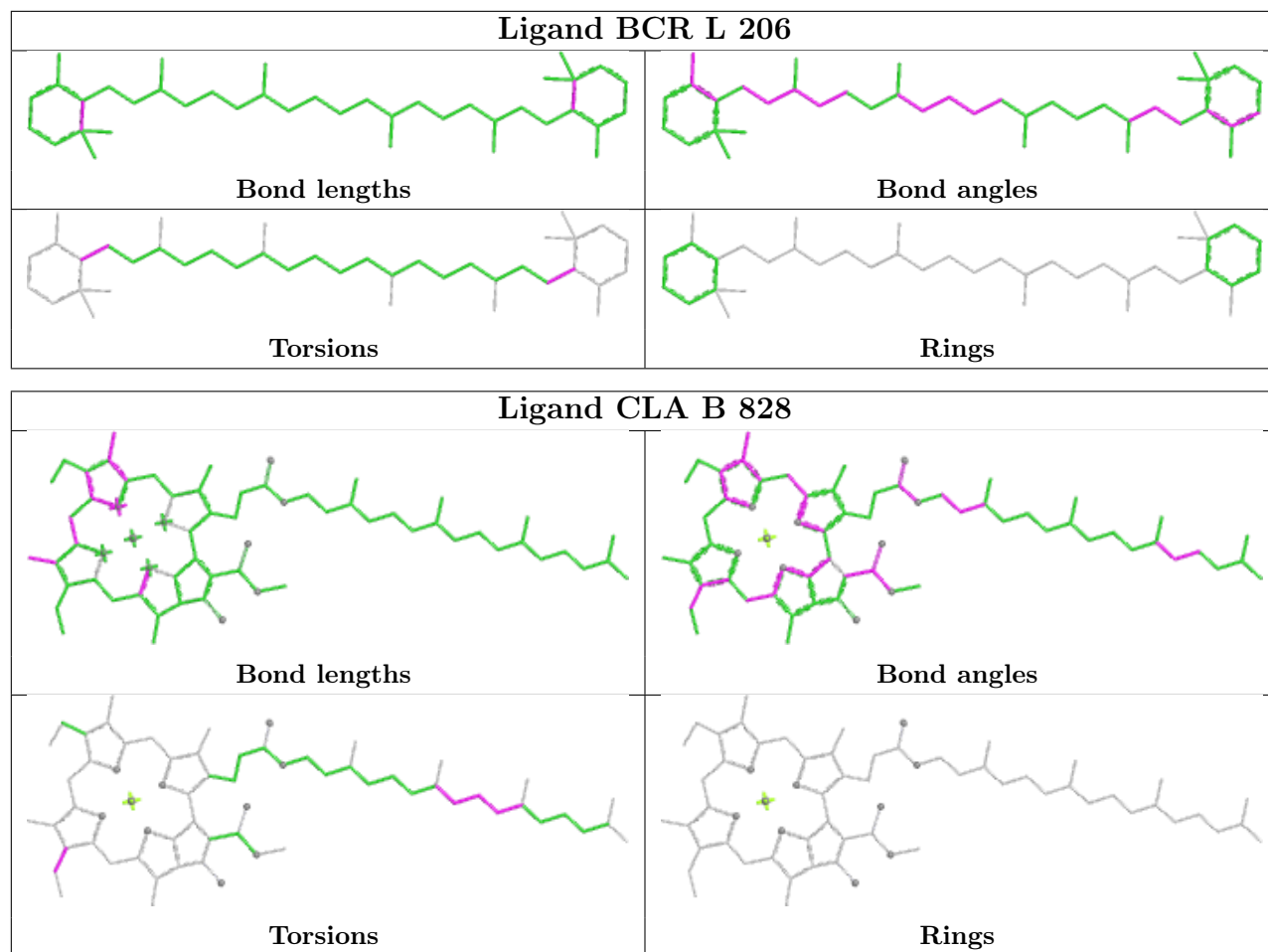


## Ligand CLA B 818

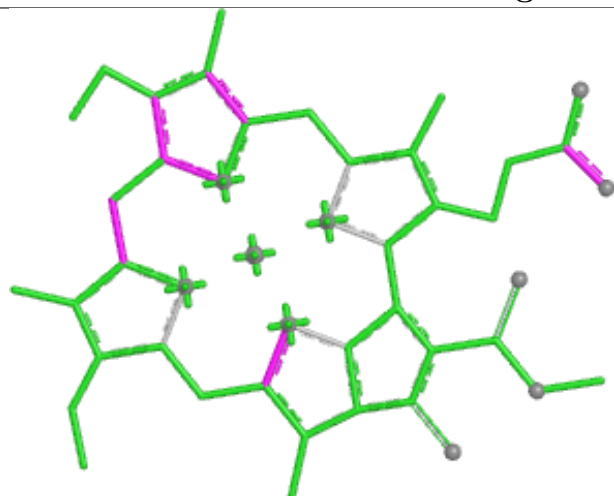




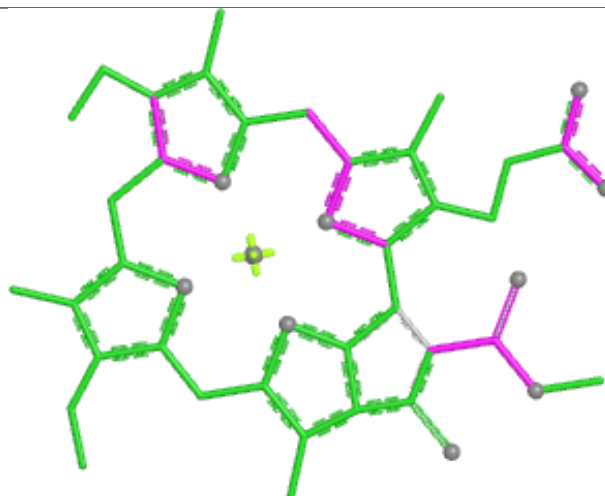




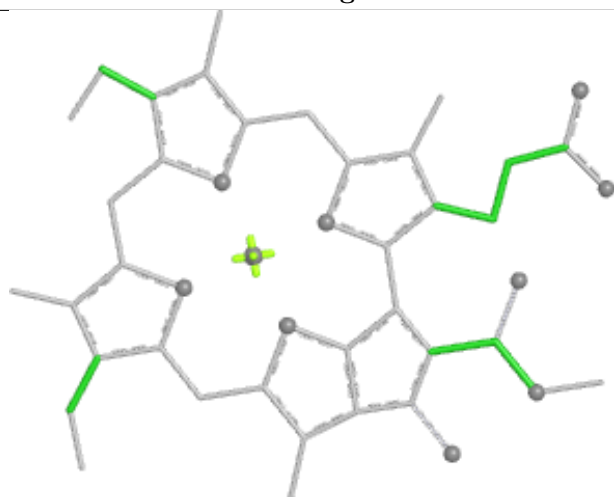
## Ligand CLA F 306



Bond lengths



Bond angles

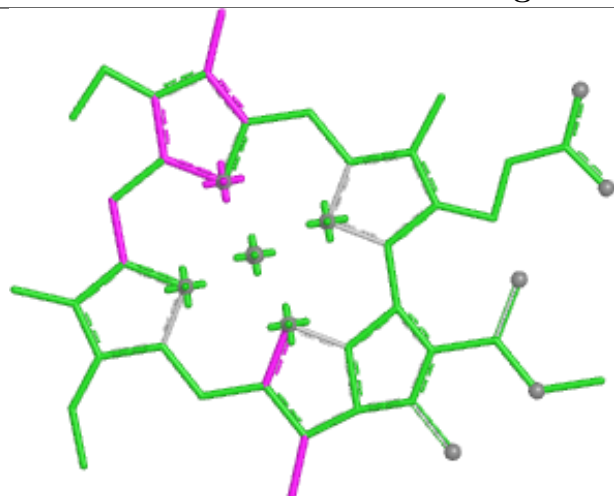


Torsions

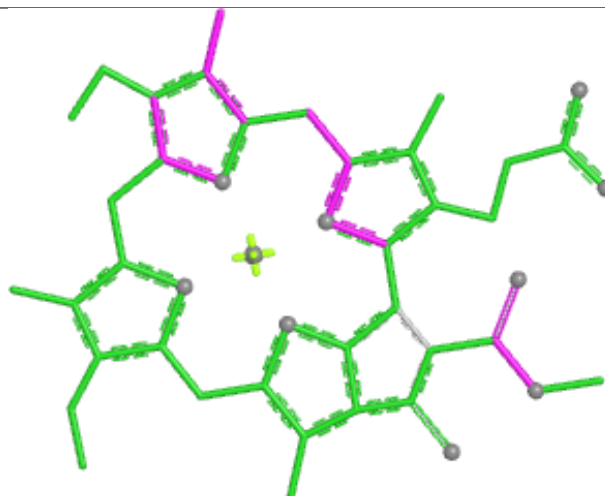


Rings

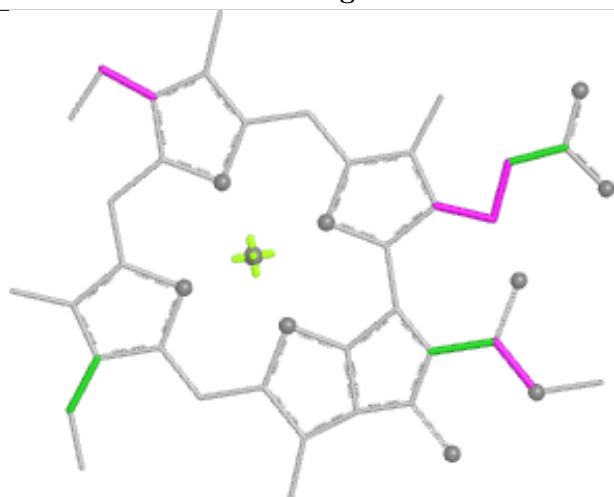
## Ligand CLA A 834



Bond lengths



Bond angles

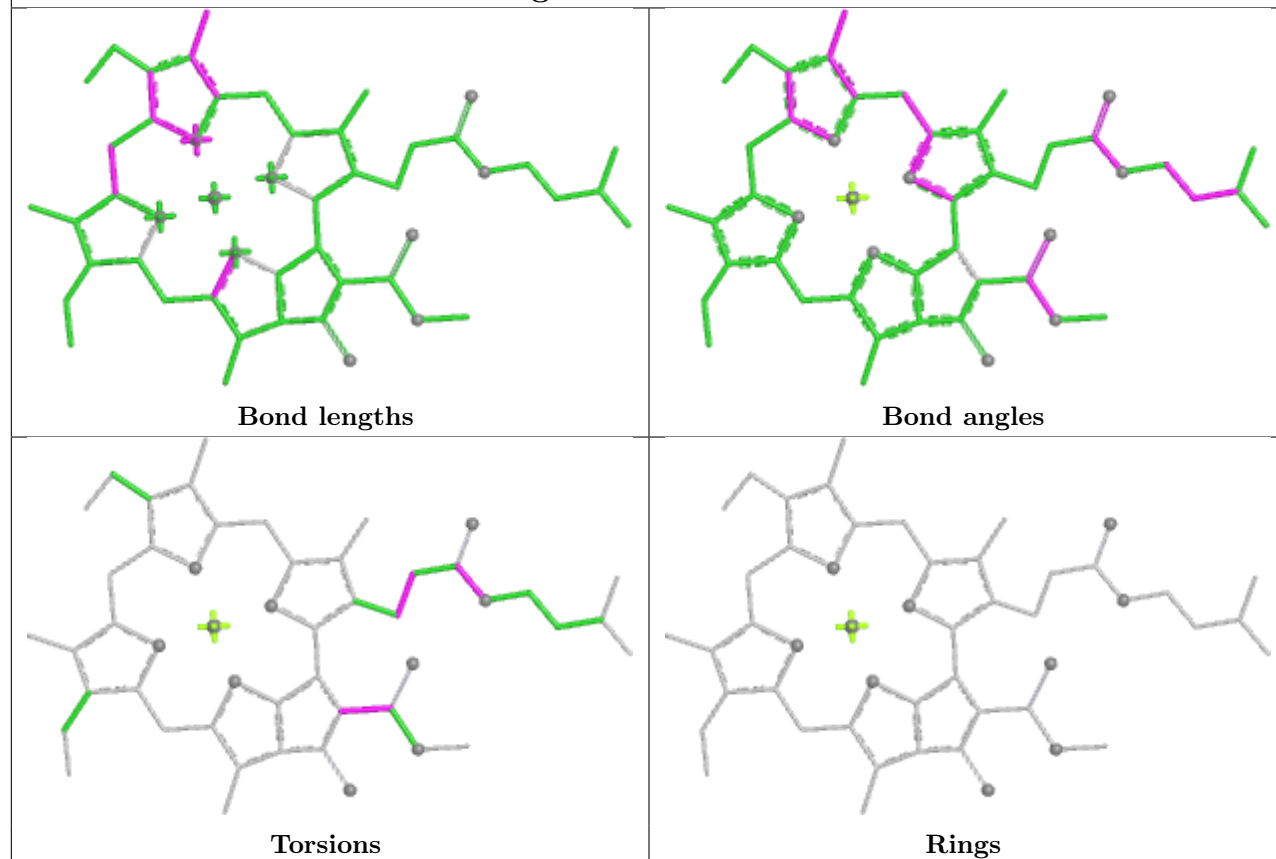


Torsions

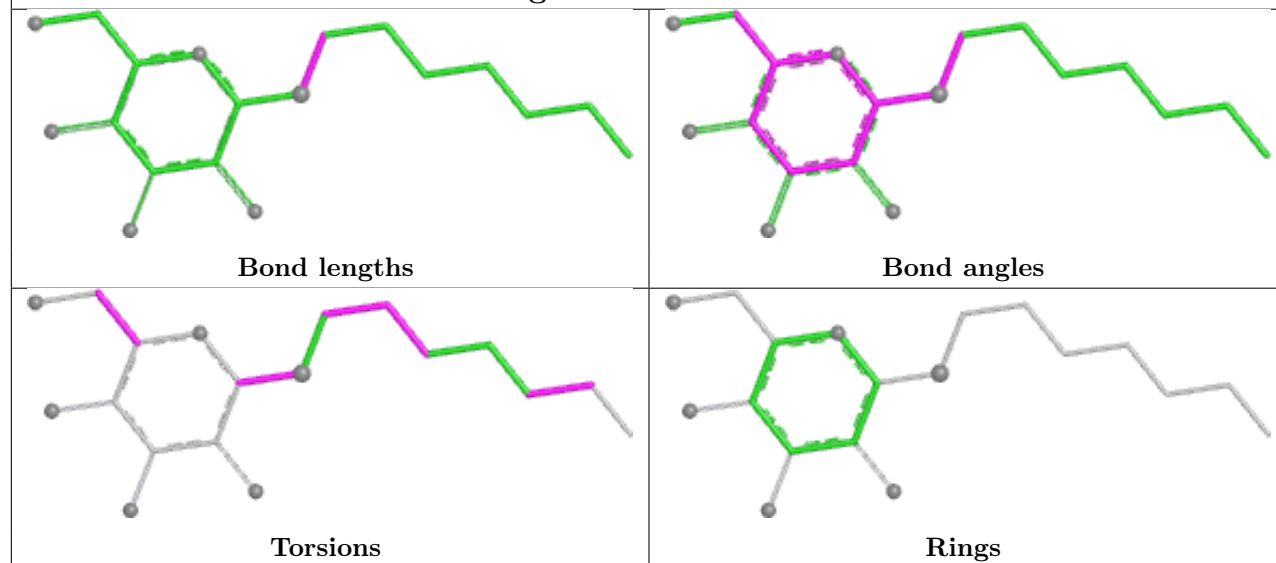


Rings

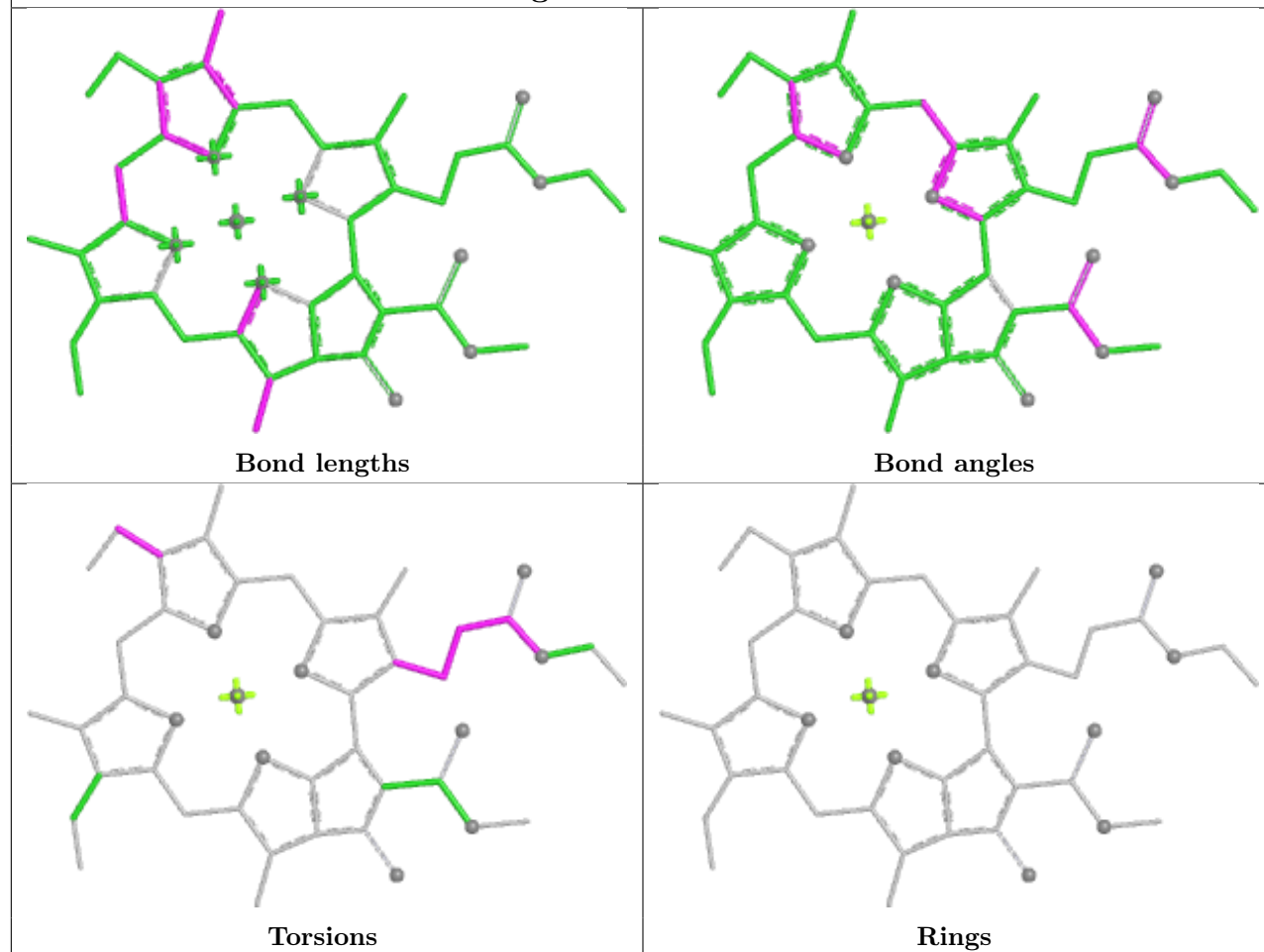
## Ligand CLA A 830



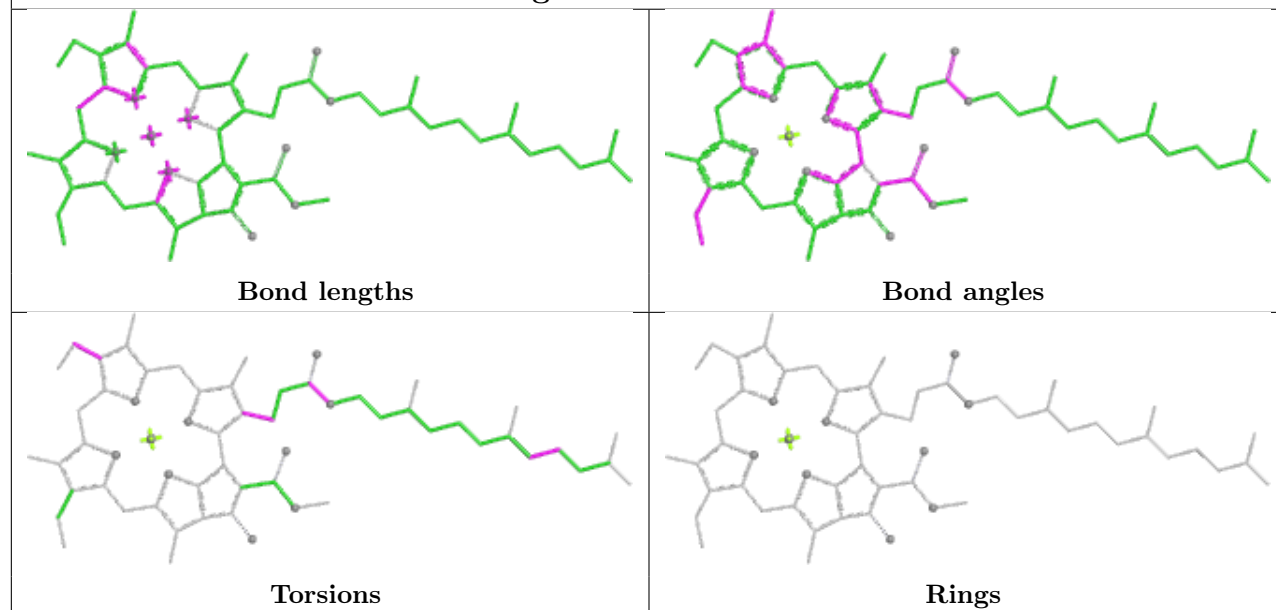
## Ligand HTG B 851

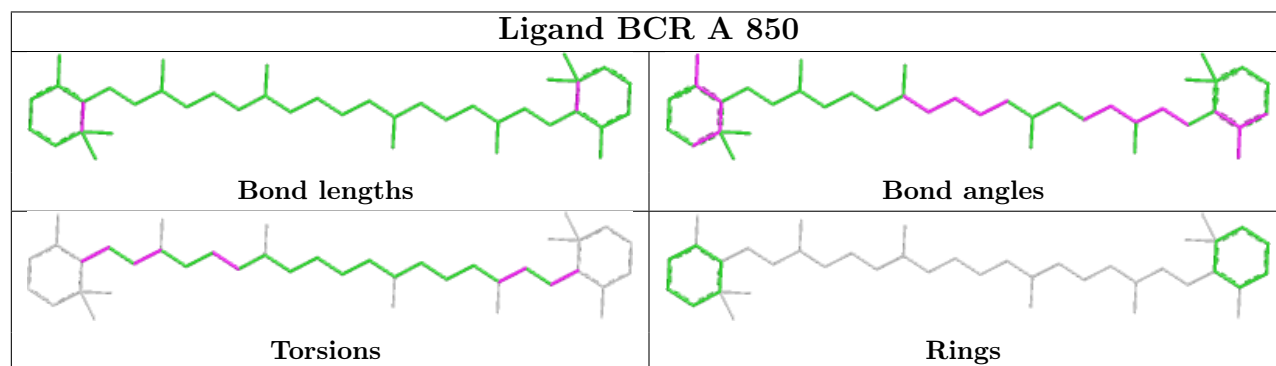
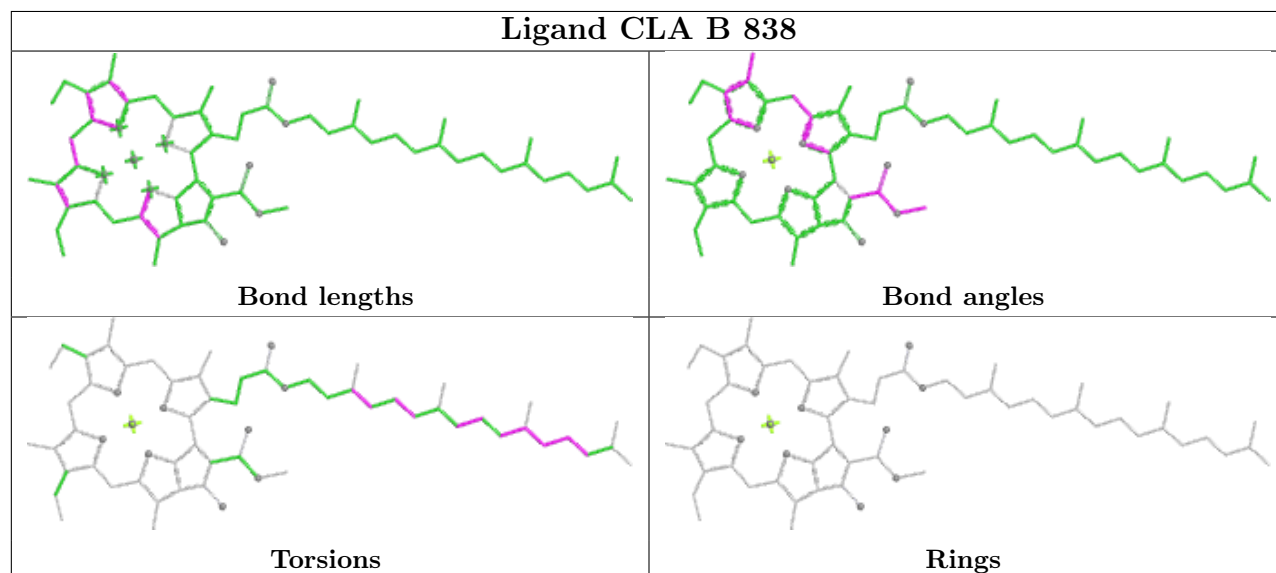
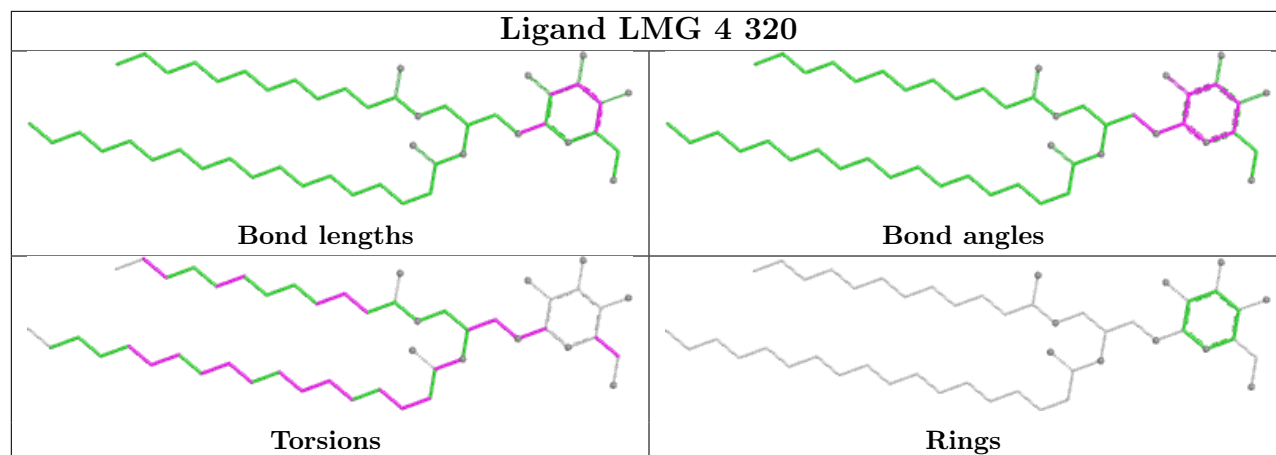


## Ligand CLA 3 606

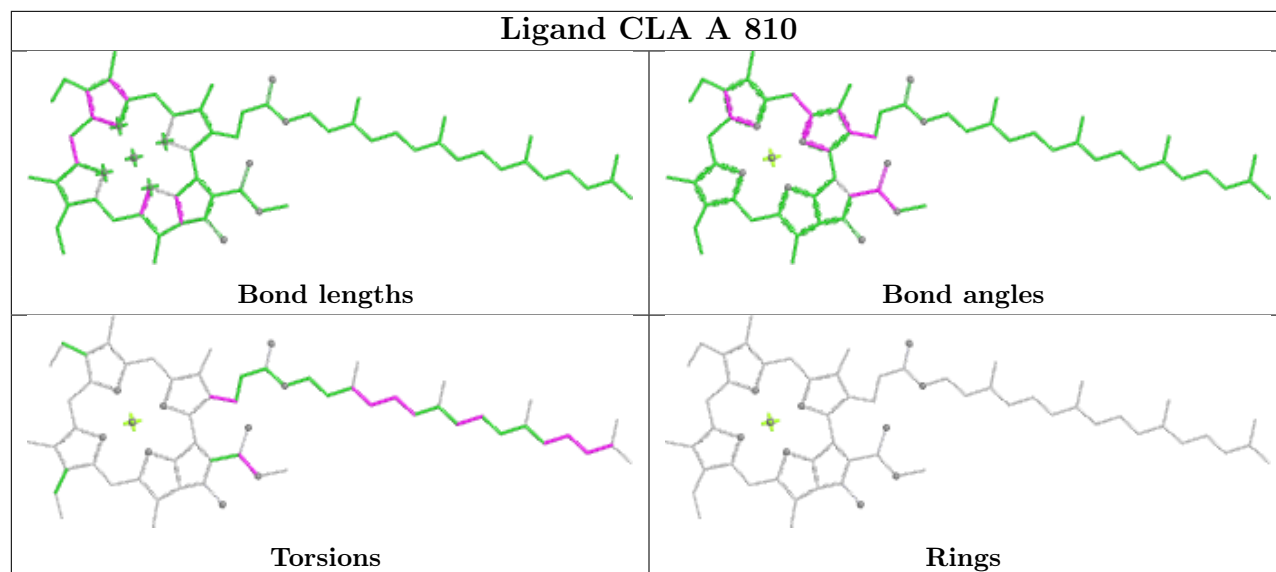


## Ligand CLA B 833

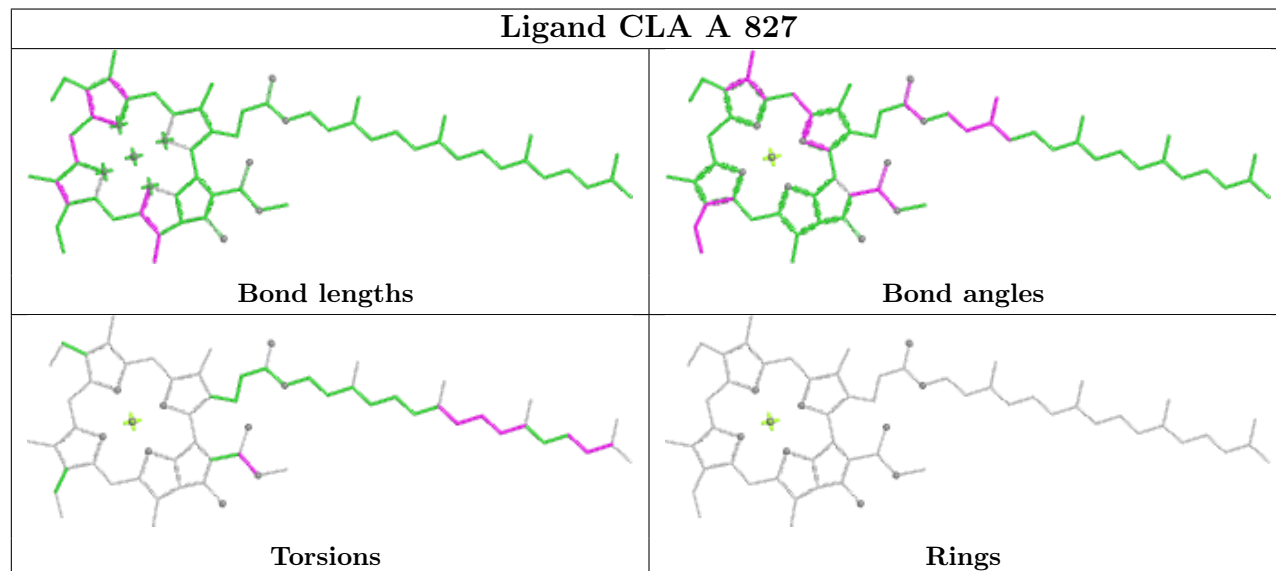




## Ligand CLA A 810

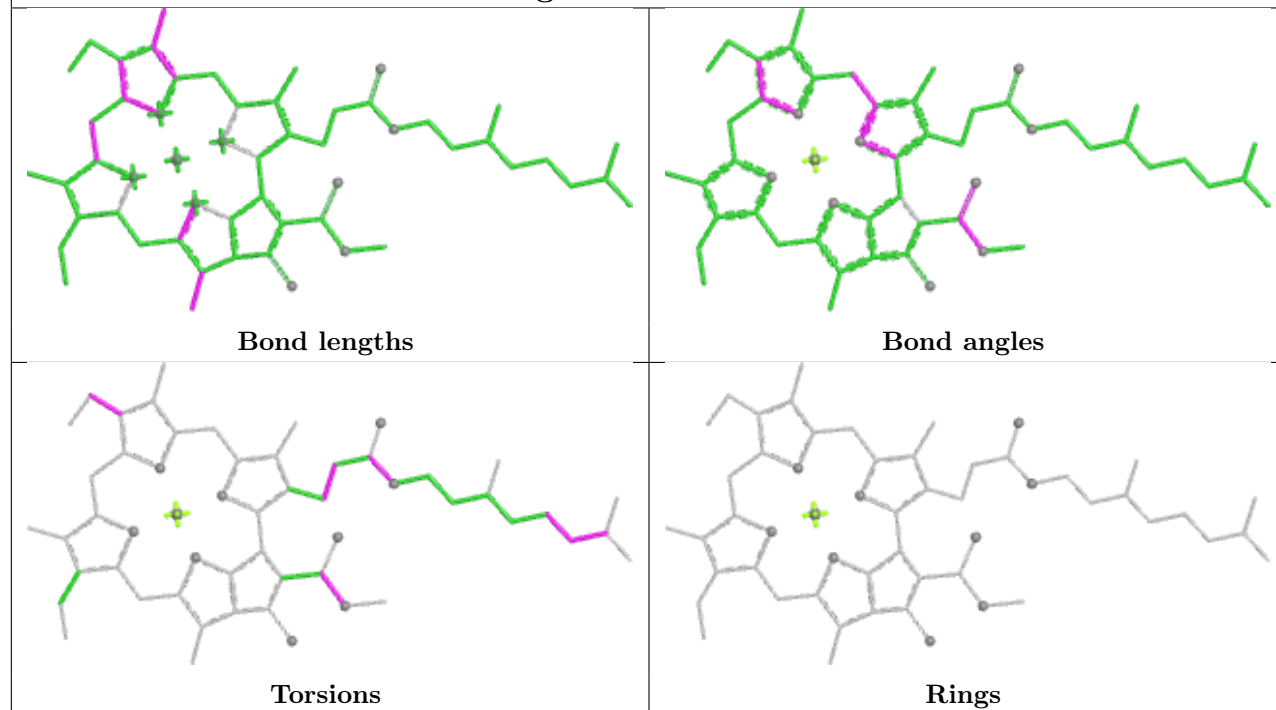


## Ligand CLA A 827

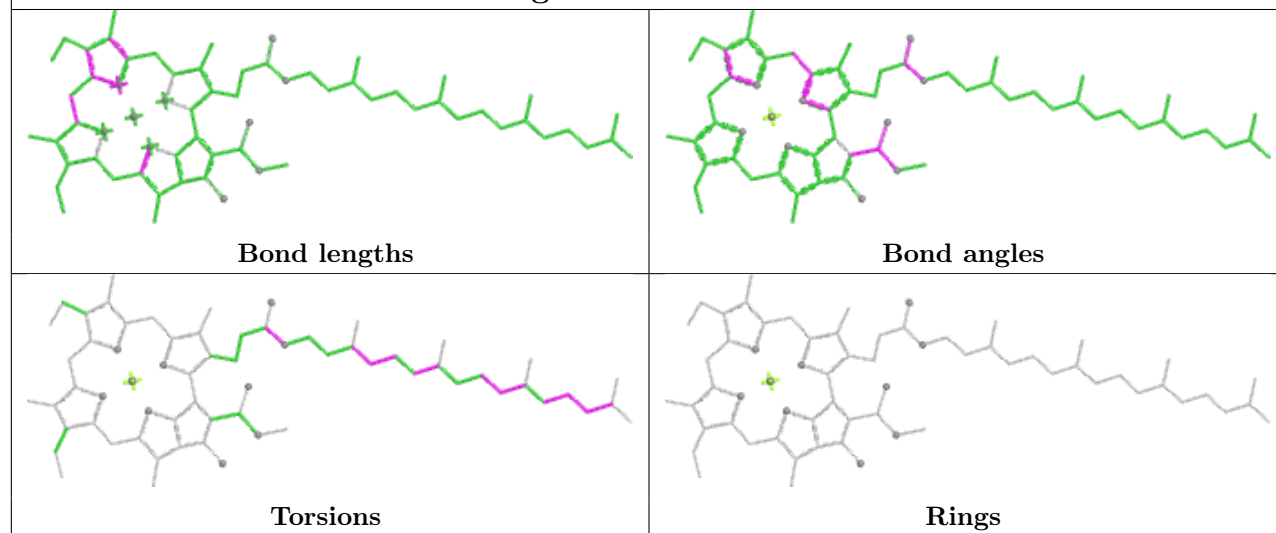


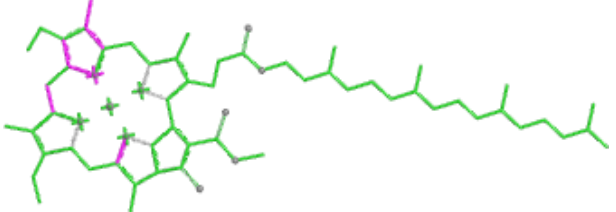
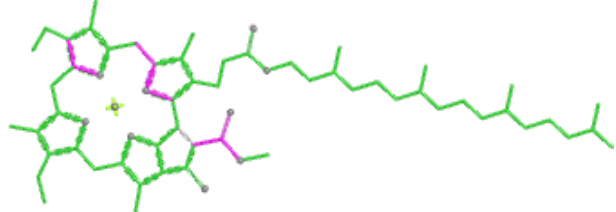
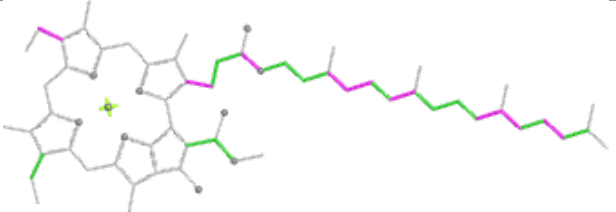
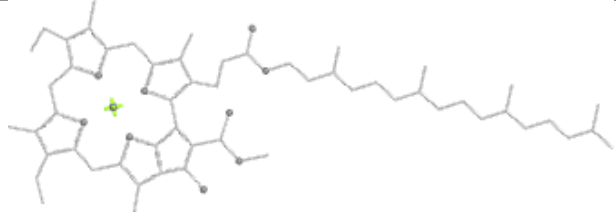


## Ligand CLA 3 611

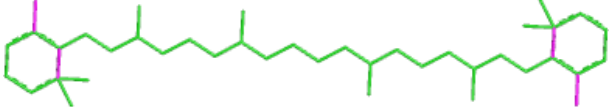
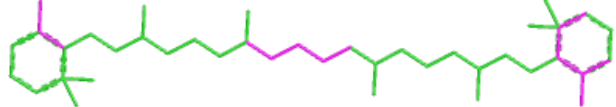
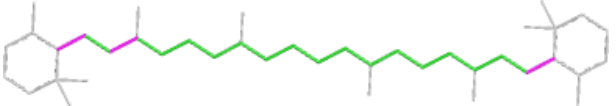
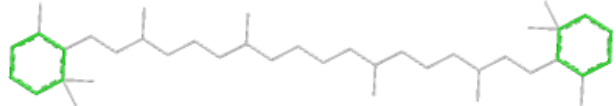


## Ligand CLA A 836

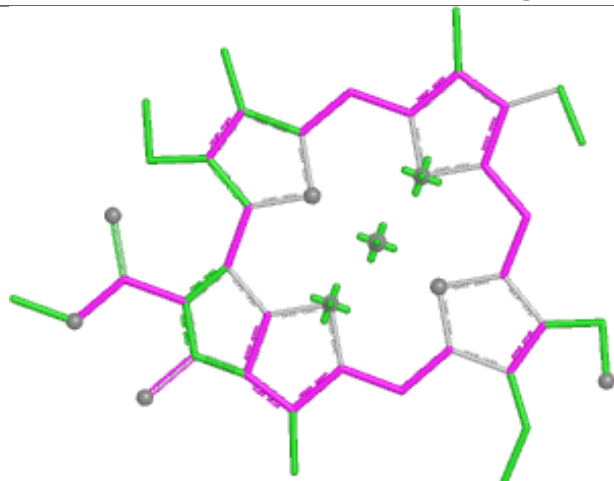


| Ligand CLA B 803                                                                  |                                                                                    |  |  |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|--|--|
|  |  |  |  |
| Bond lengths                                                                      | Bond angles                                                                        |  |  |
|  |  |  |  |
| Torsions                                                                          | Rings                                                                              |  |  |

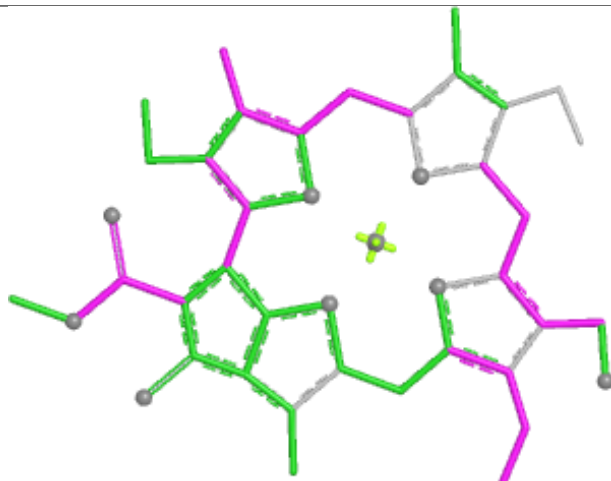
  

| Ligand BCR A 847                                                                   |                                                                                     |  |  |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|--|--|
|   |   |  |  |
| Bond lengths                                                                       | Bond angles                                                                         |  |  |
|  |  |  |  |
| Torsions                                                                           | Rings                                                                               |  |  |

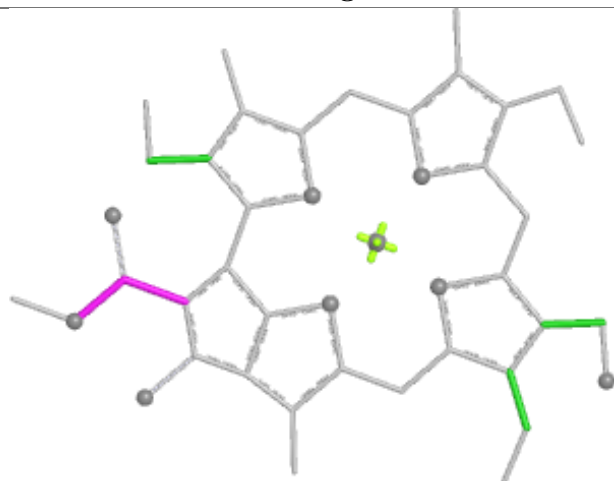
## Ligand CHL 4 315



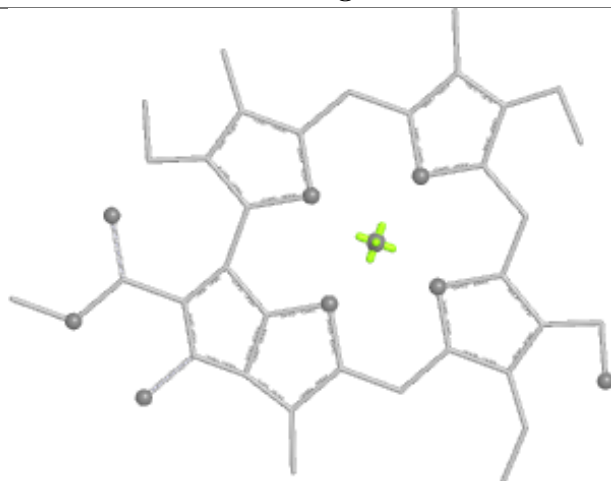
Bond lengths



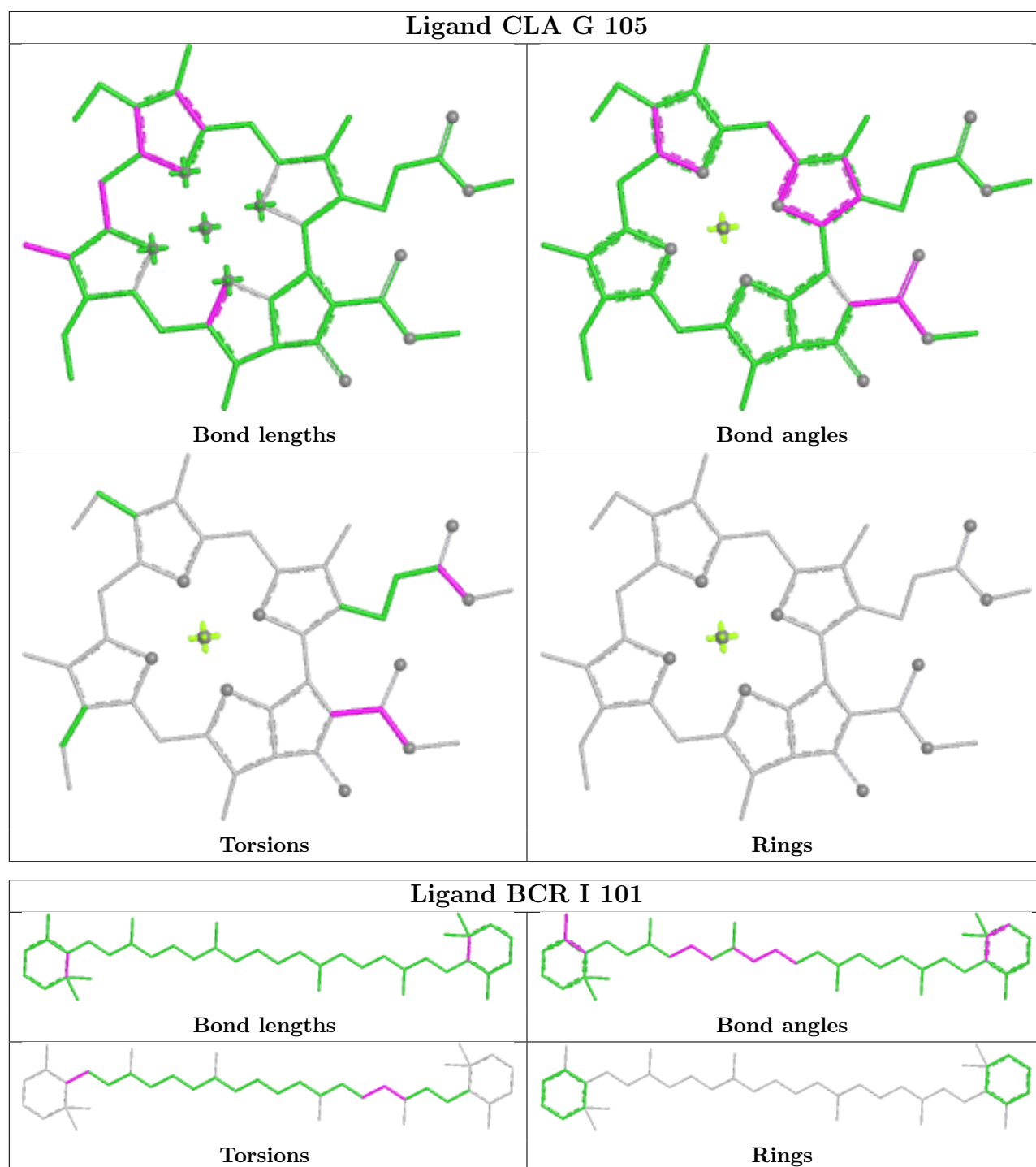
Bond angles



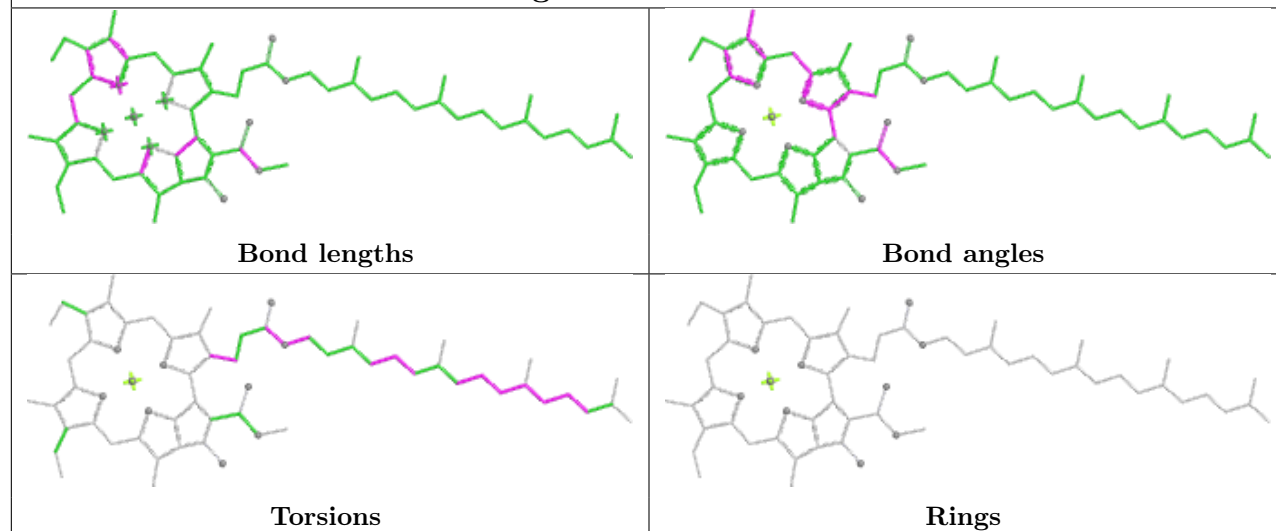
Torsions



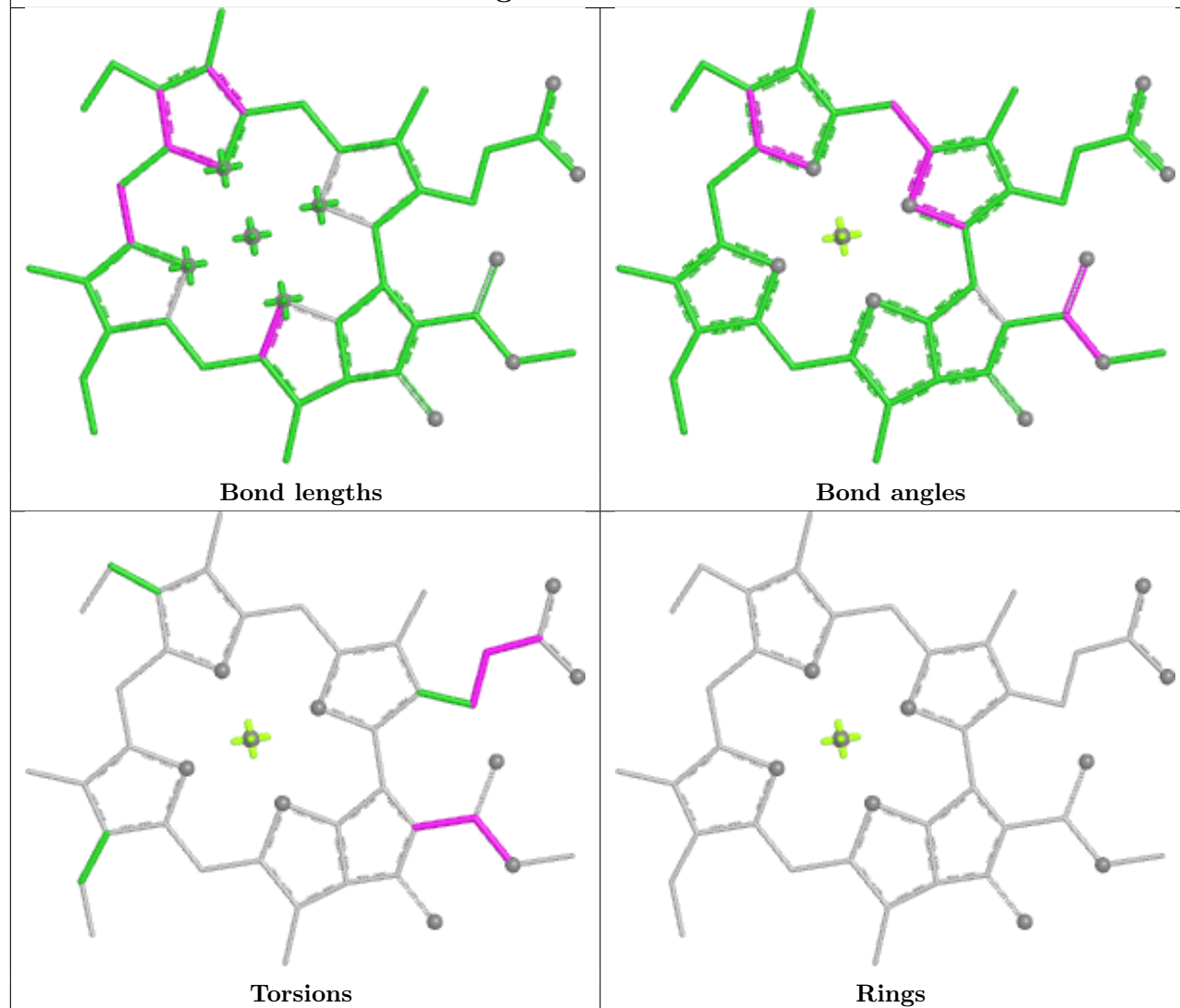
Rings



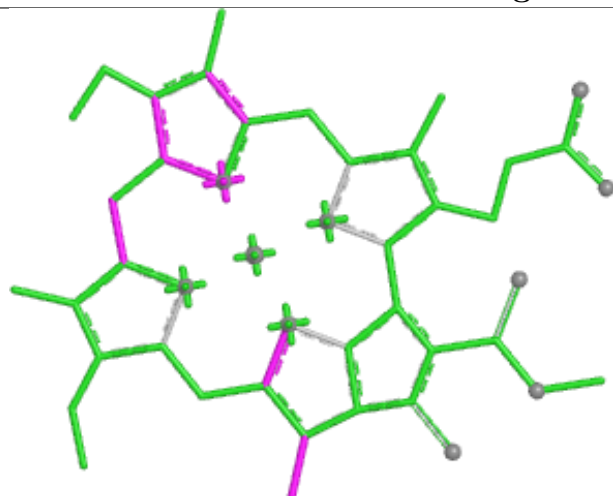
## Ligand CLA B 829



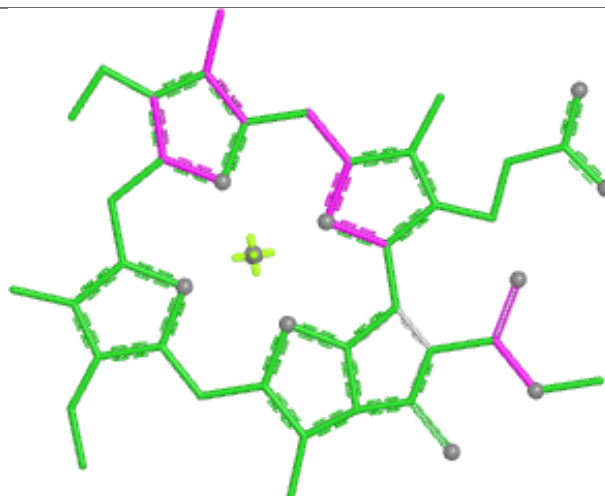
## Ligand CLA 3 612



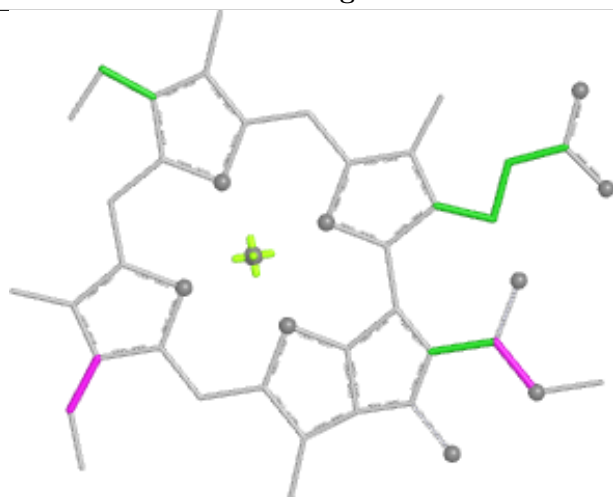
## Ligand CLA K 201



Bond lengths



Bond angles

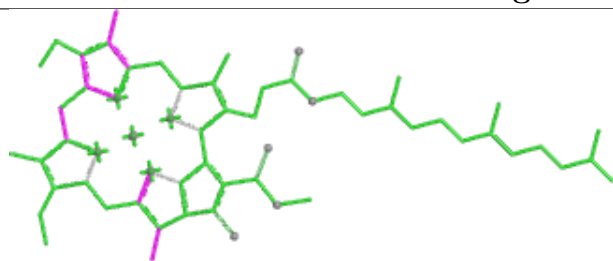


Torsions

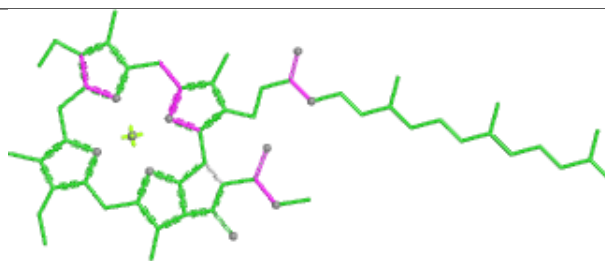


Rings

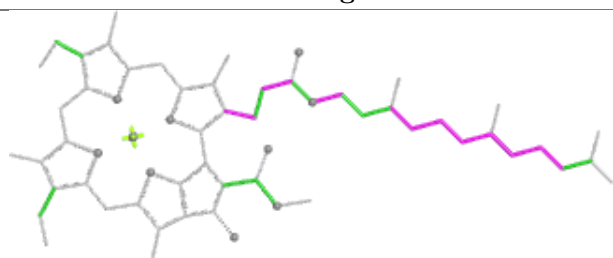
## Ligand CLA K 202



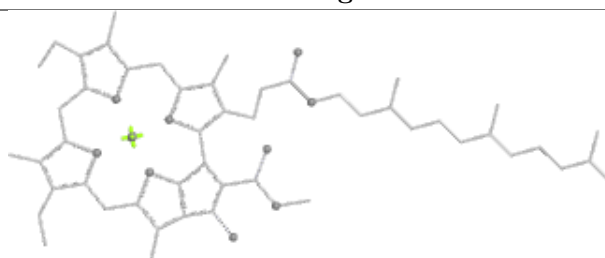
Bond lengths



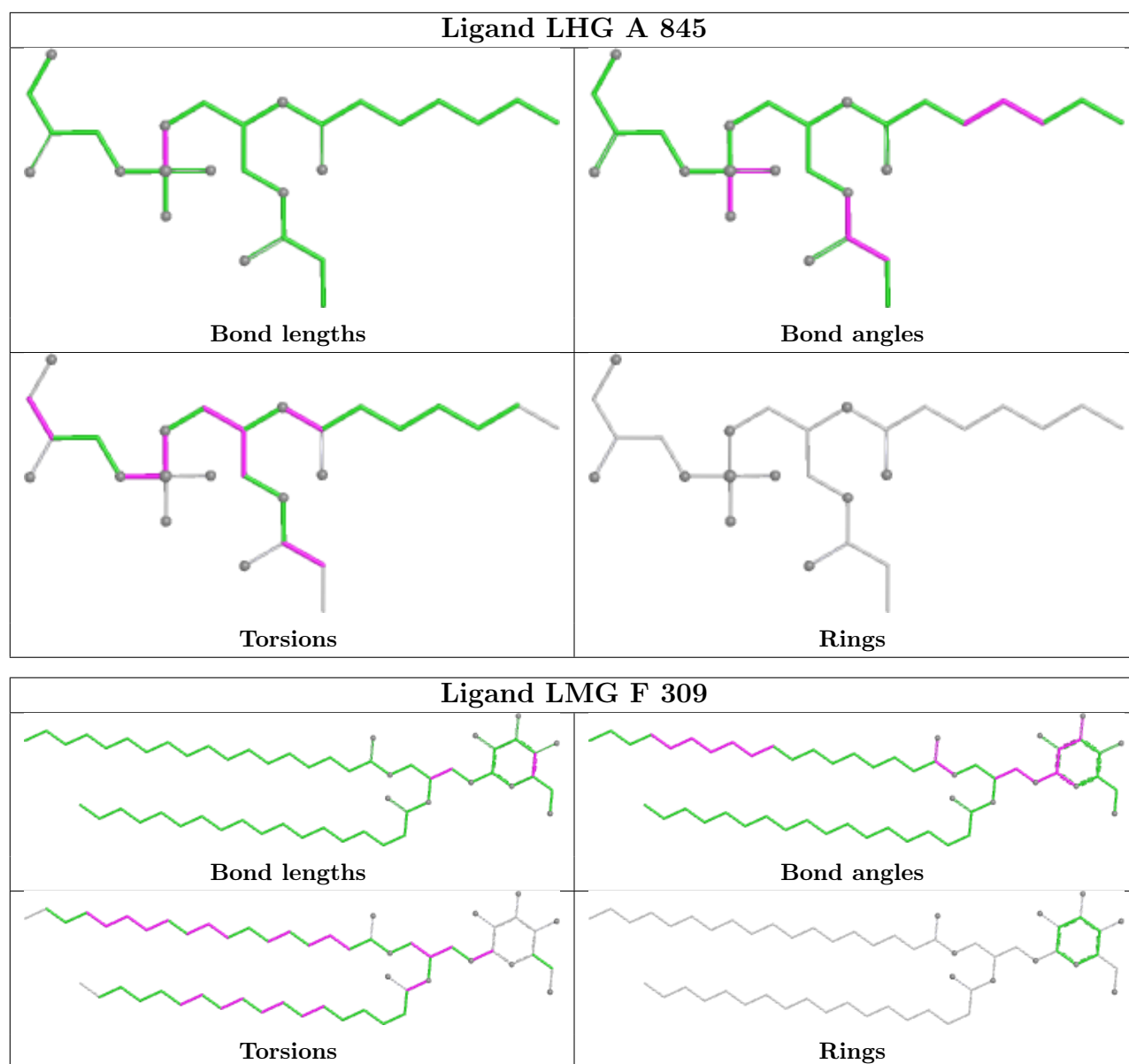
Bond angles

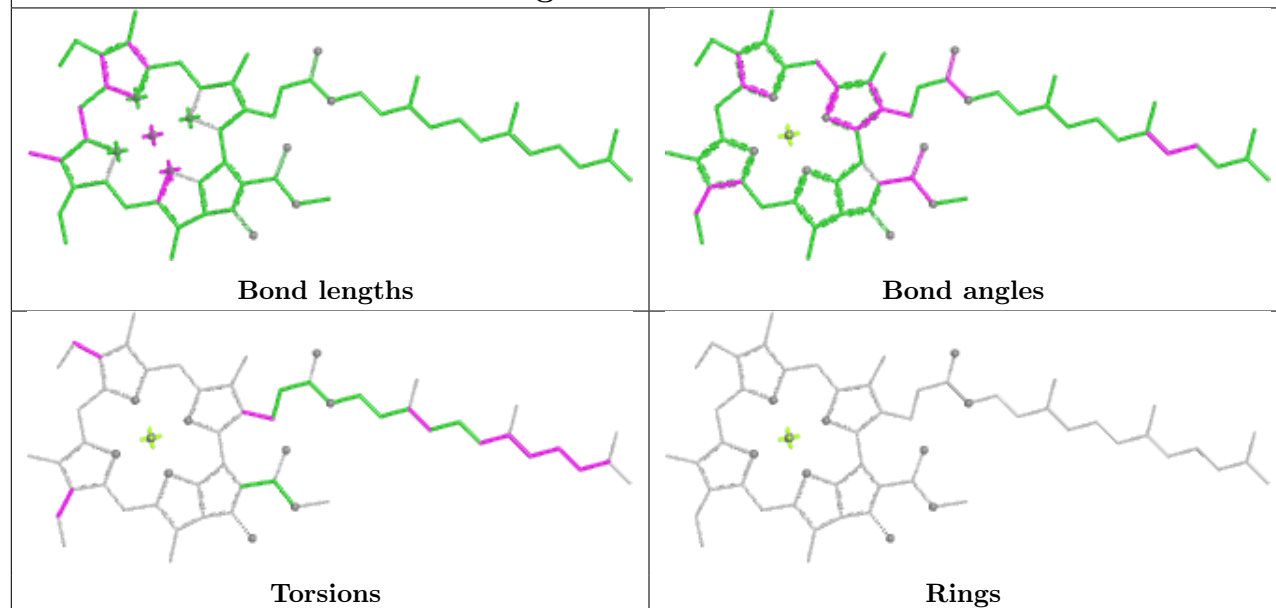
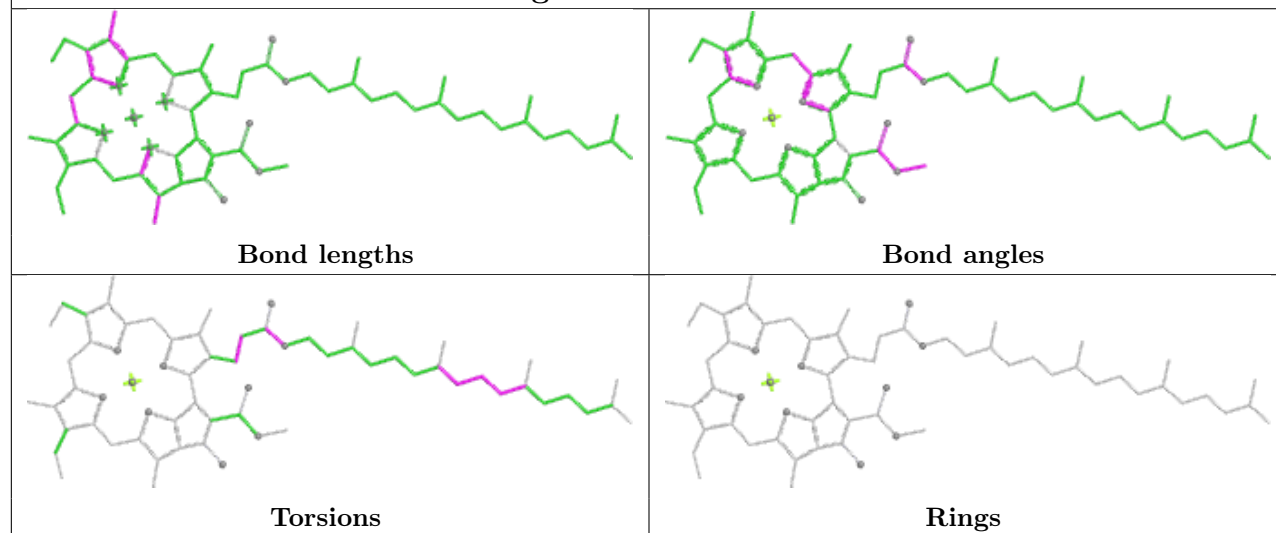


Torsions



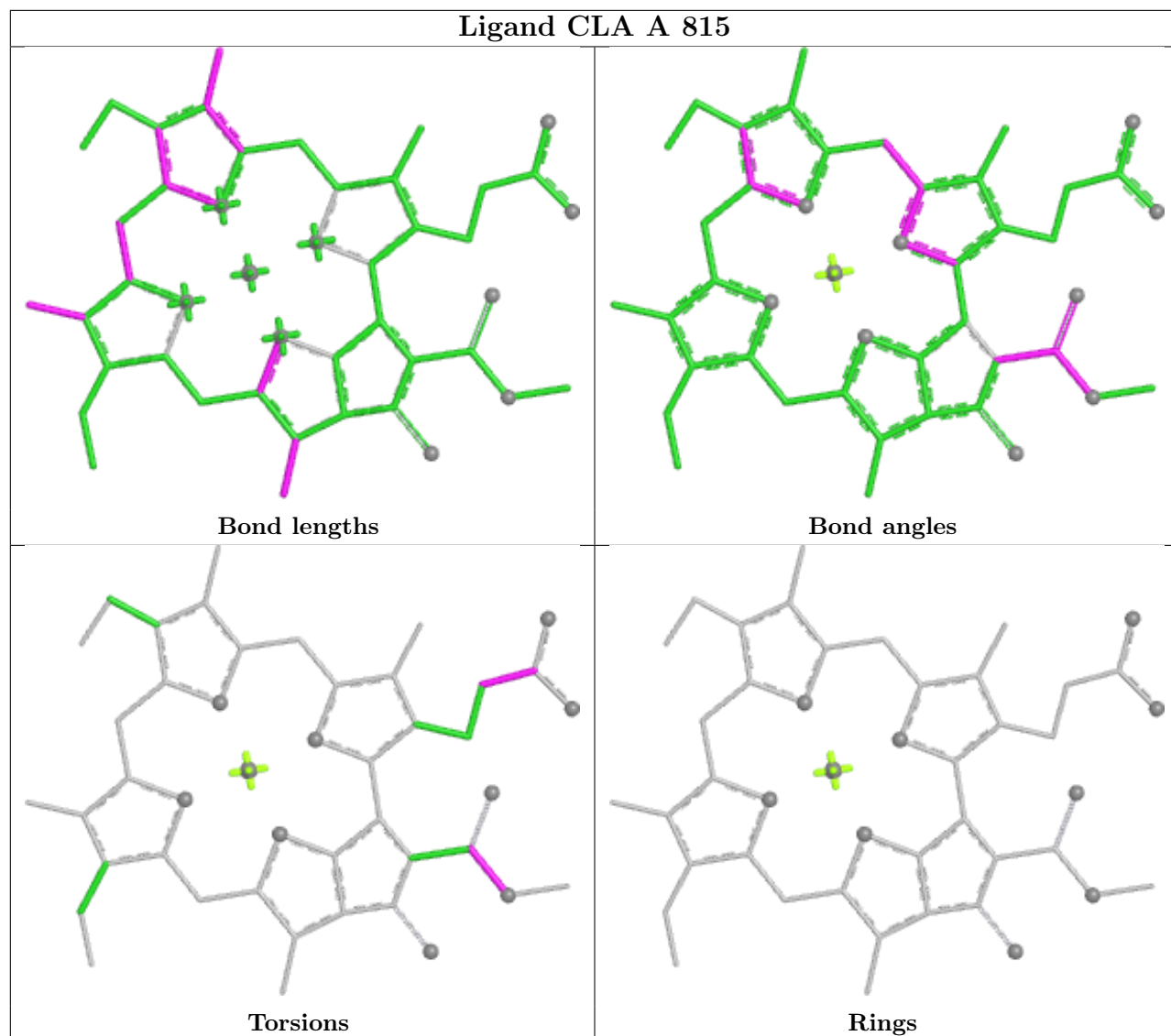
Rings



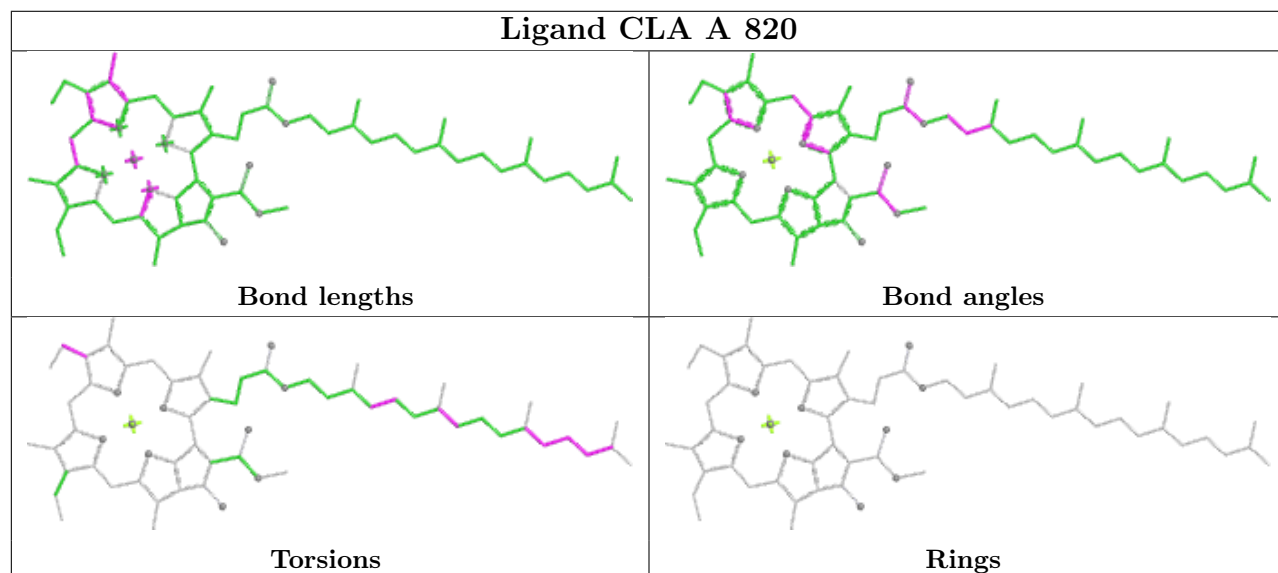
**Ligand CLA 4 310****Ligand CLA A 812**

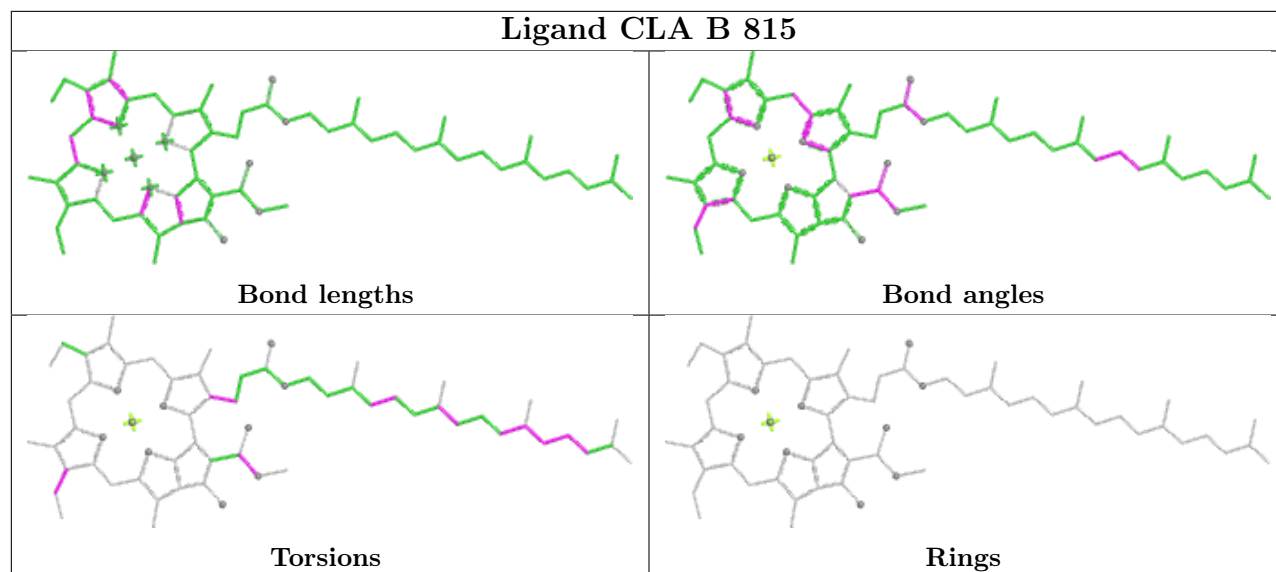
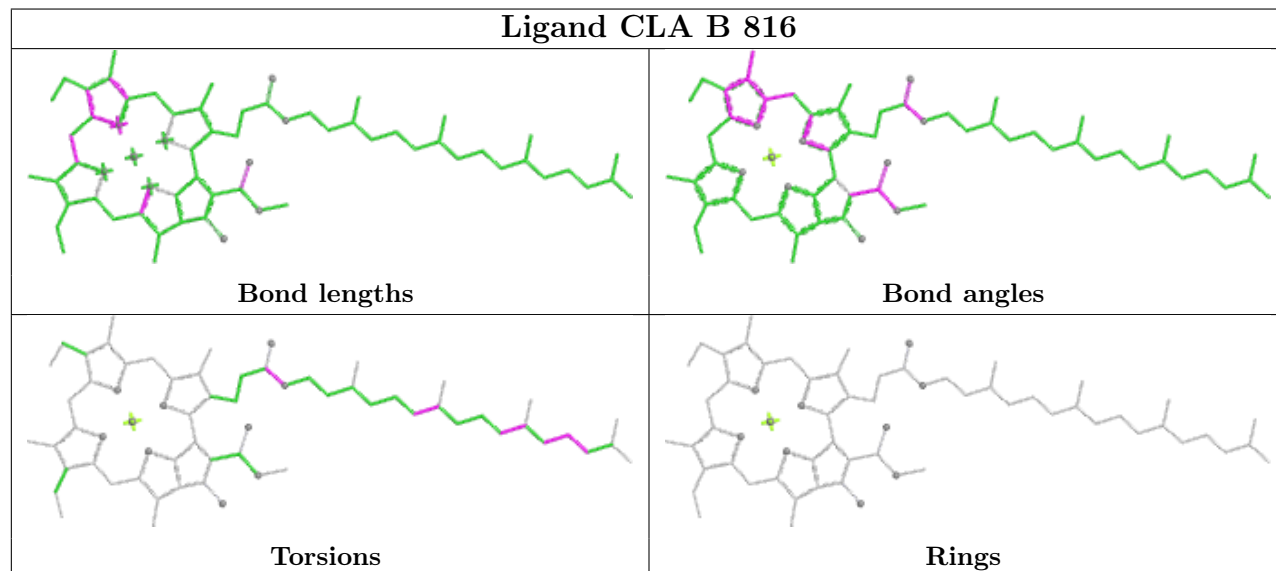


## Ligand CLA A 815

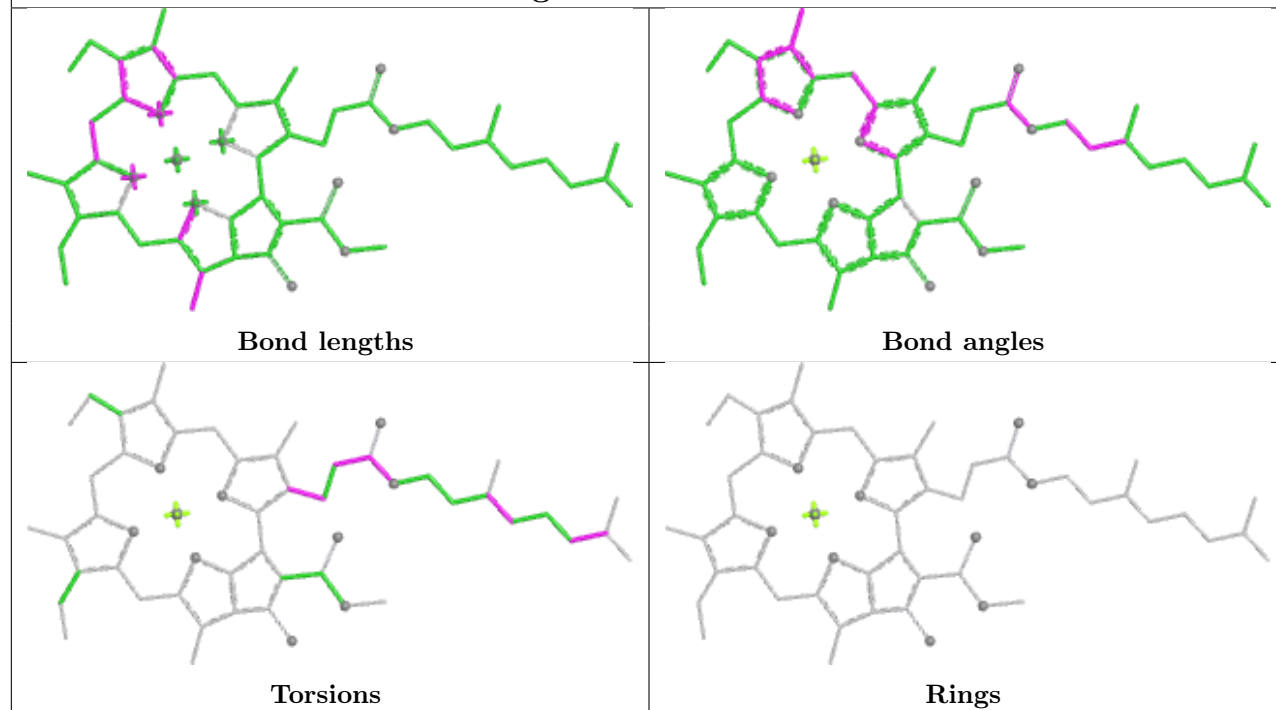


## Ligand CLA A 820

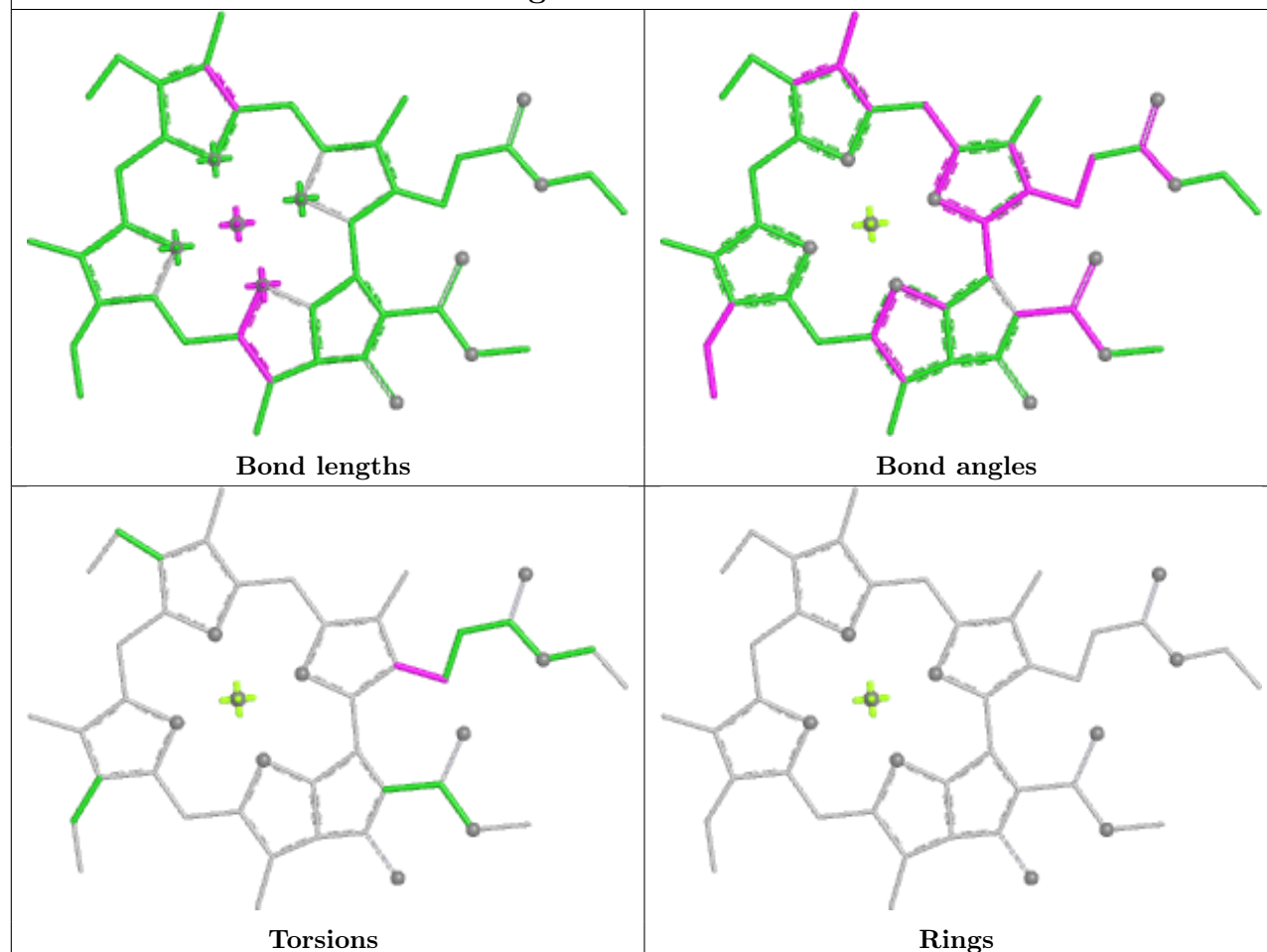


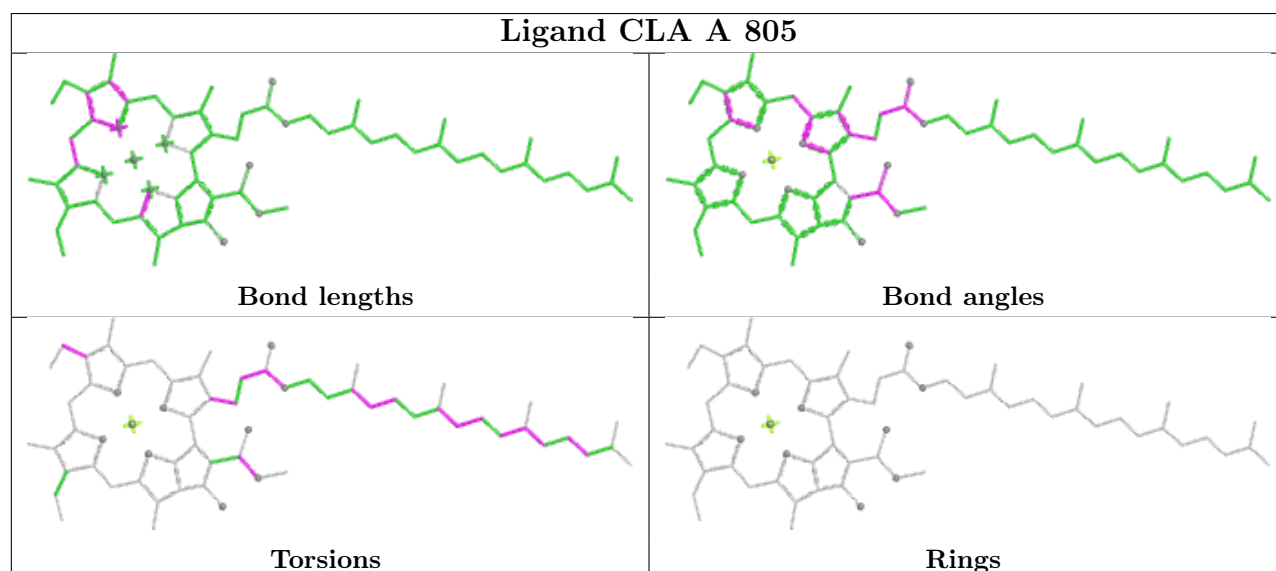
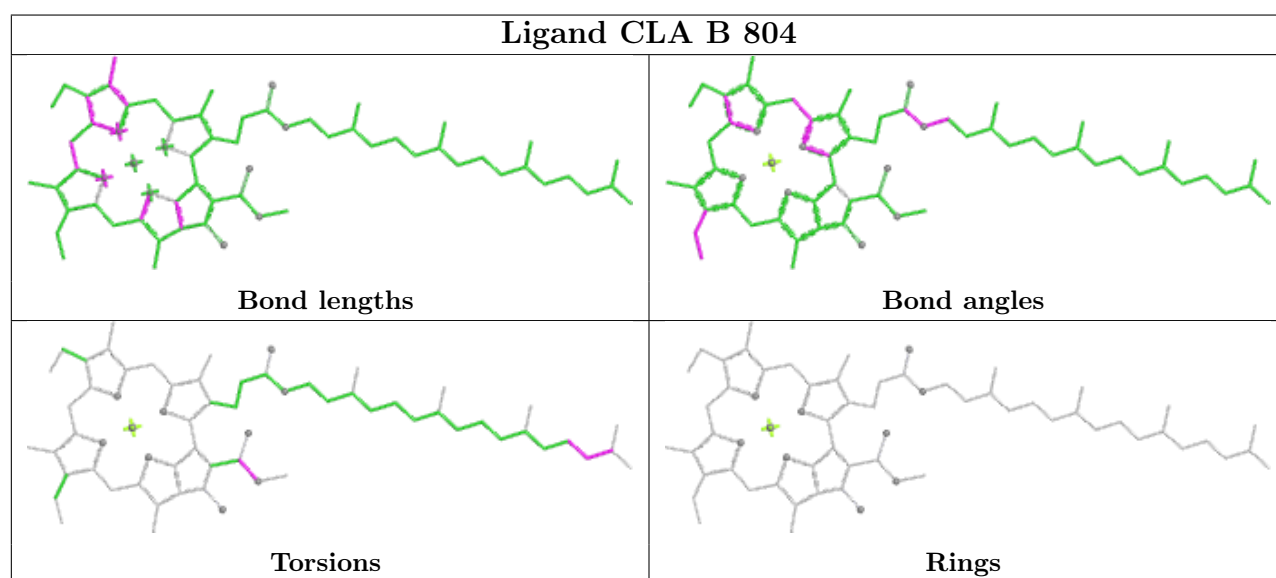
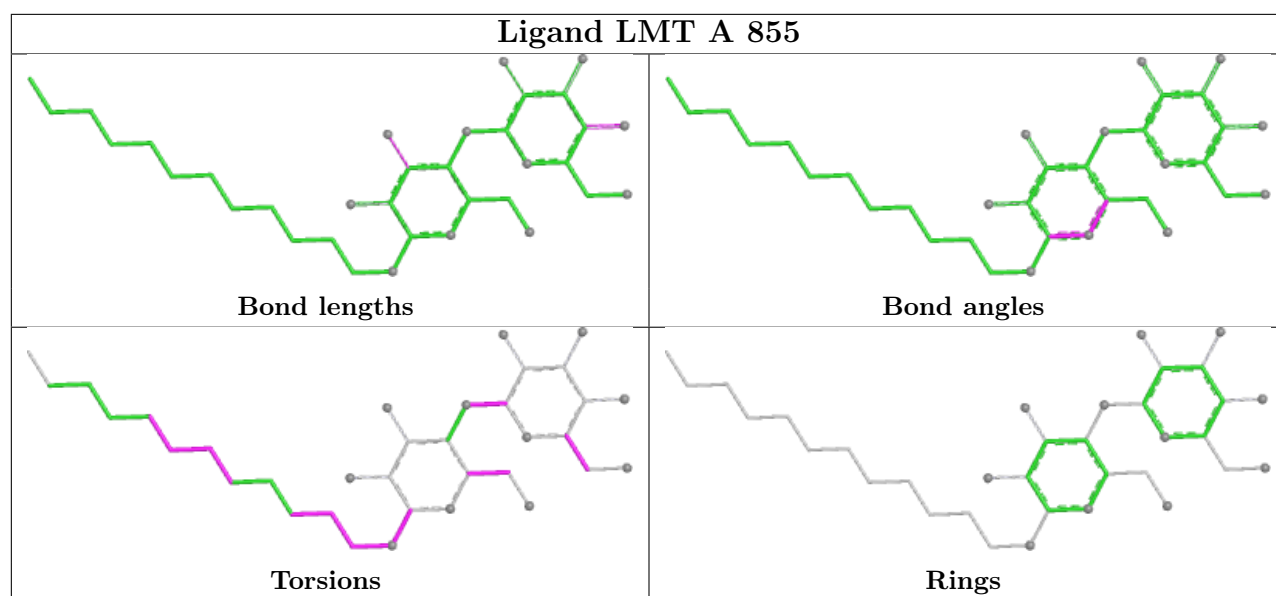
**Ligand CLA B 815****Ligand CLA B 816**

## Ligand CLA B 824

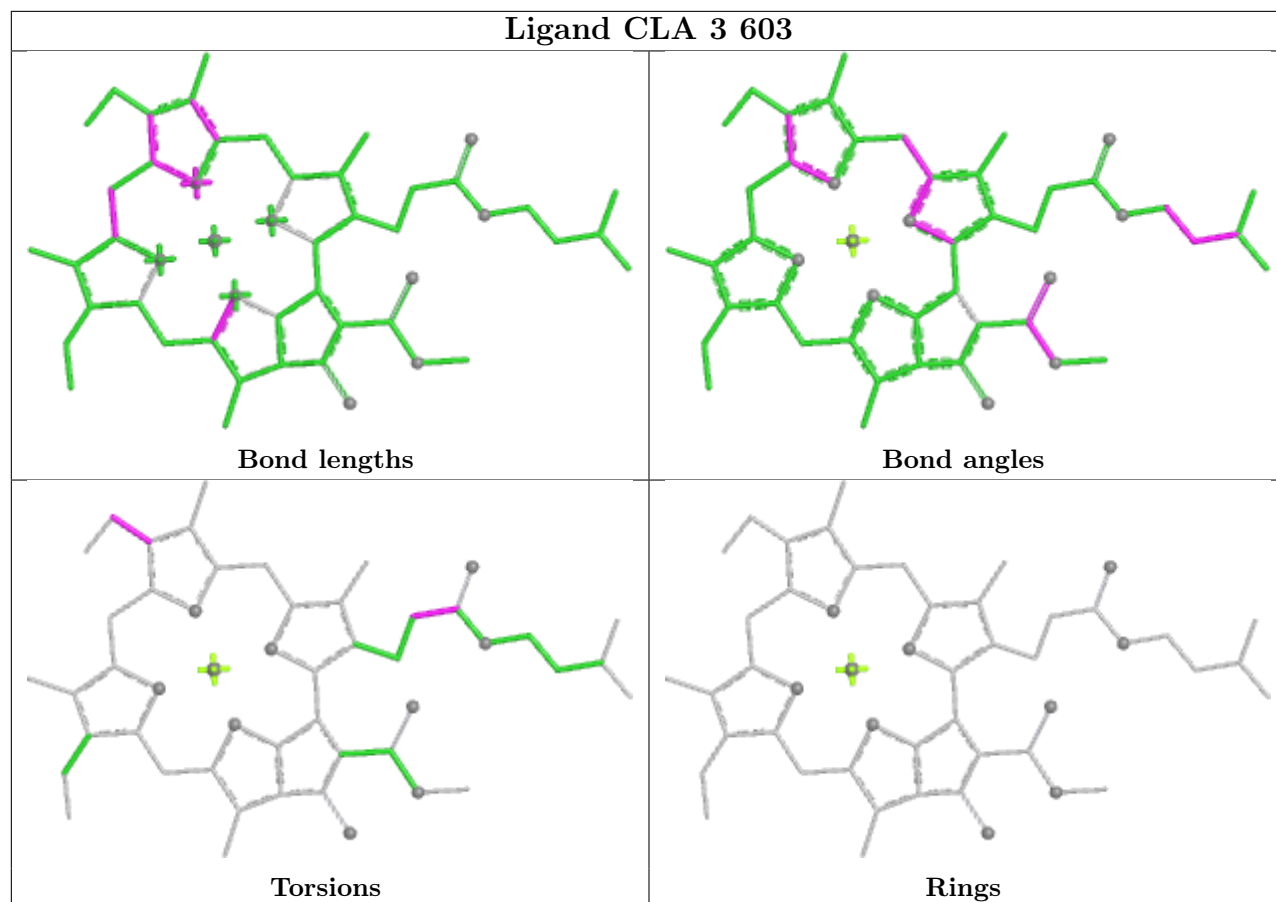


## Ligand CLA B 839

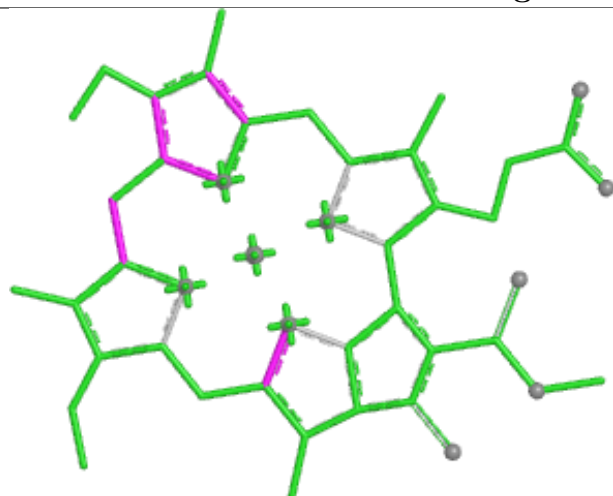




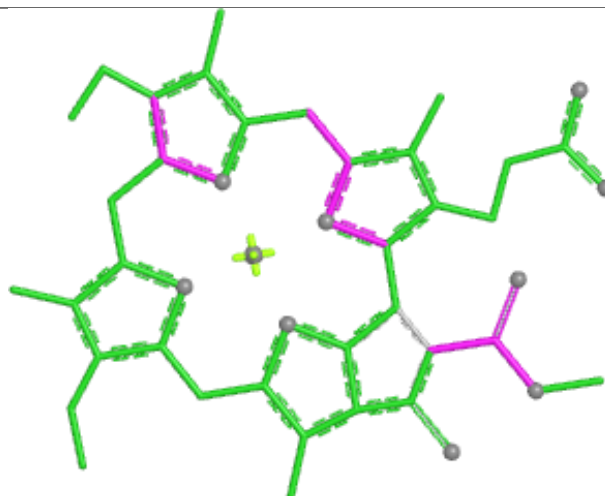
## Ligand CLA 3 603



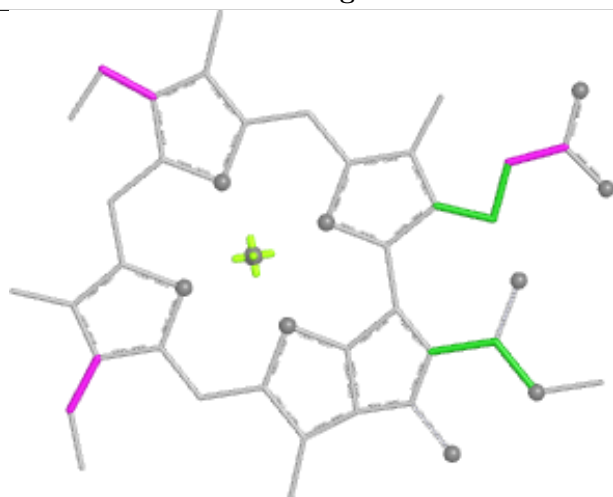
## Ligand CLA A 819



Bond lengths



Bond angles

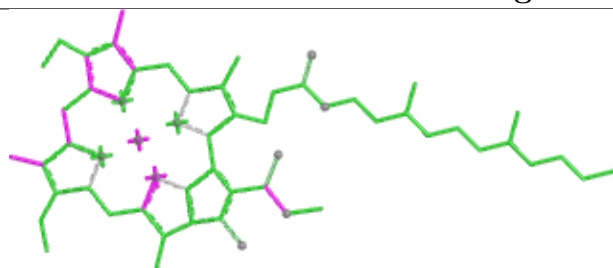


Torsions

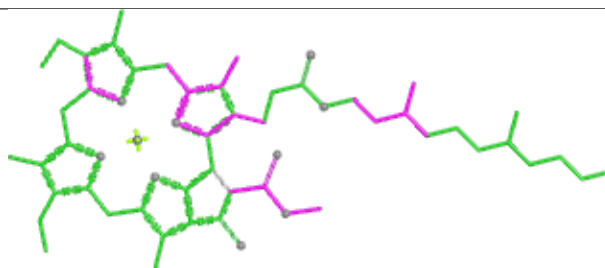


Rings

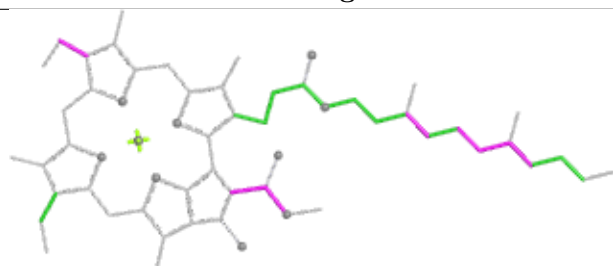
## Ligand CLA B 834



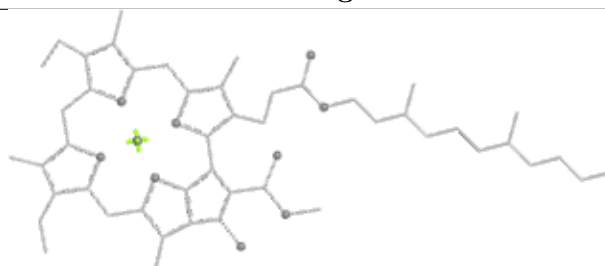
Bond lengths



Bond angles

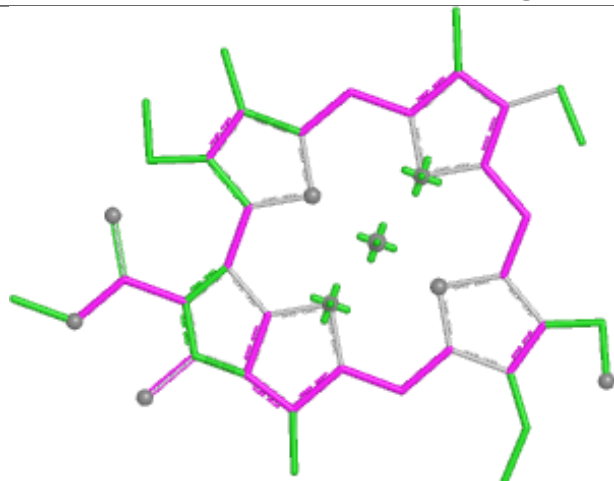


Torsions

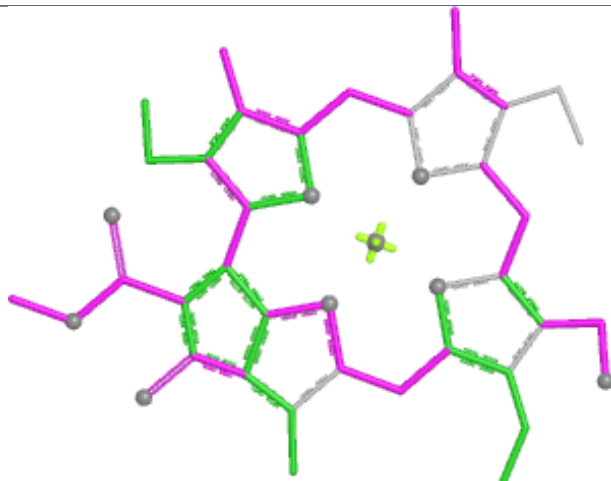


Rings

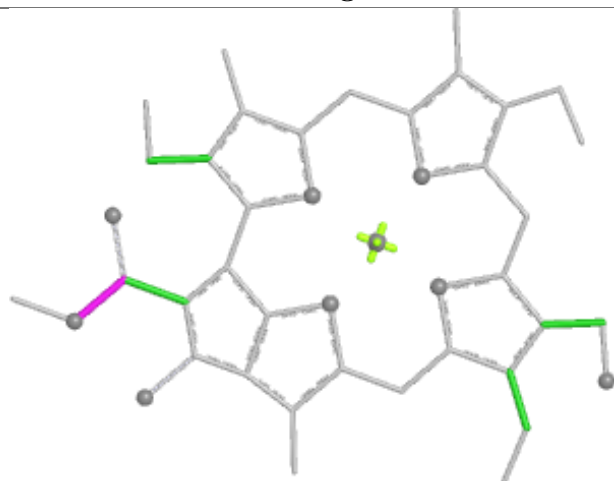
## Ligand CHL 2 313



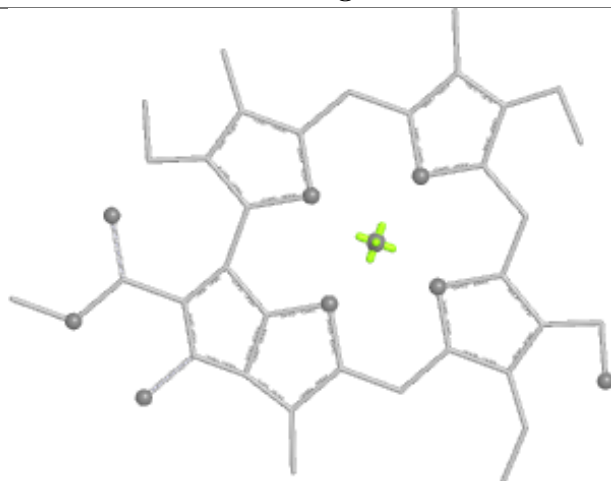
Bond lengths



Bond angles

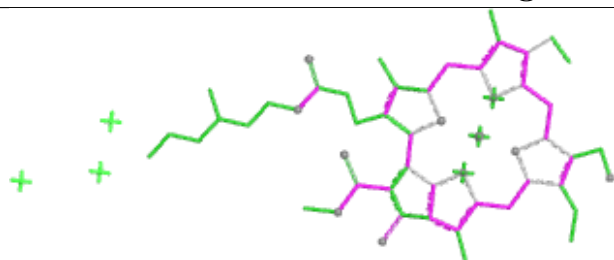


Torsions

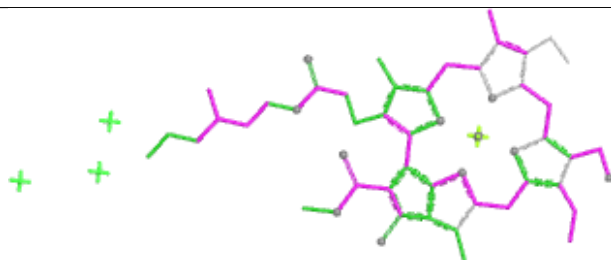


Rings

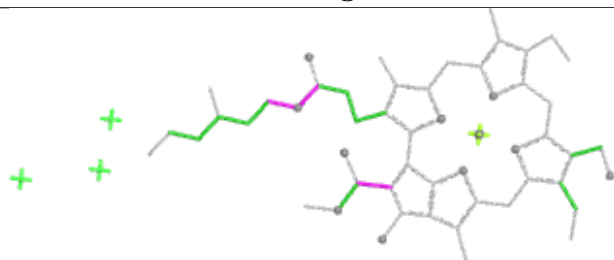
## Ligand CHL 3 601



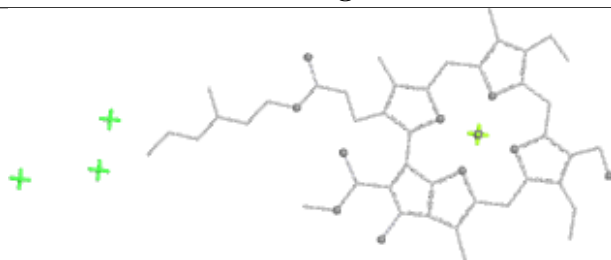
Bond lengths



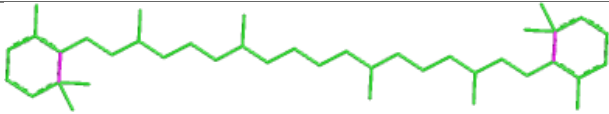
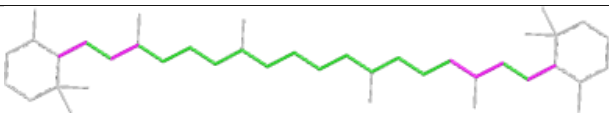
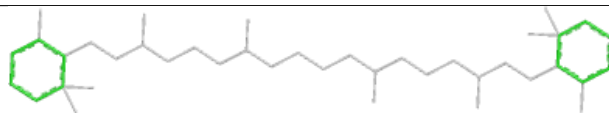
Bond angles

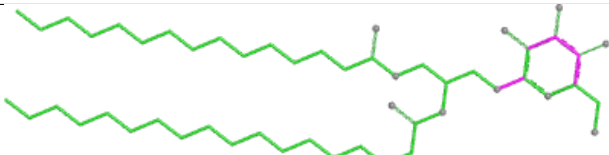
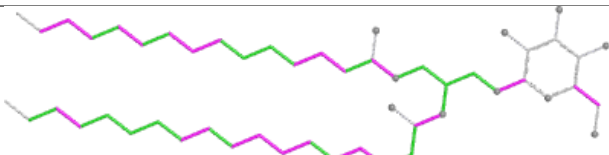
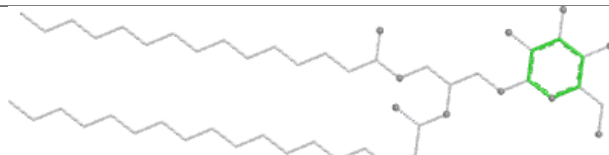


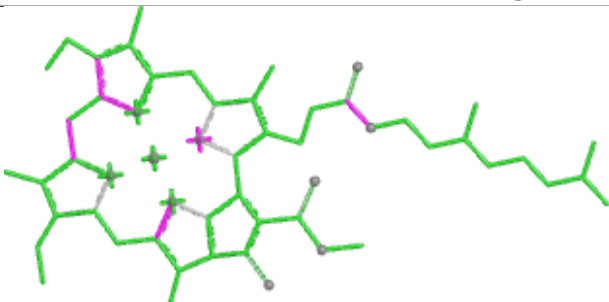
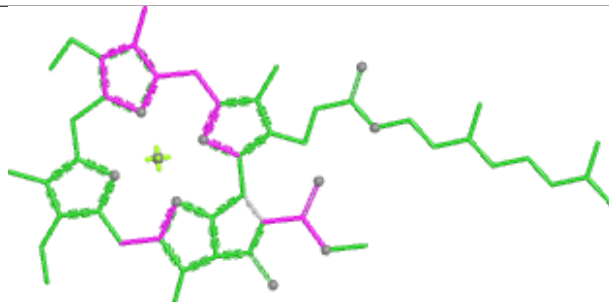
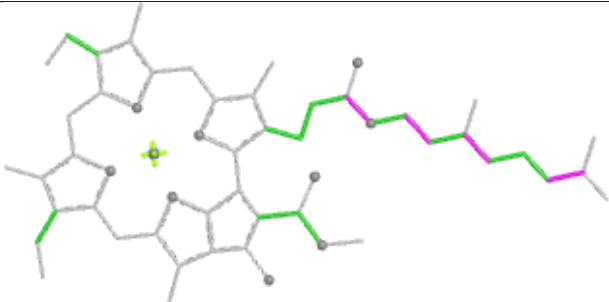
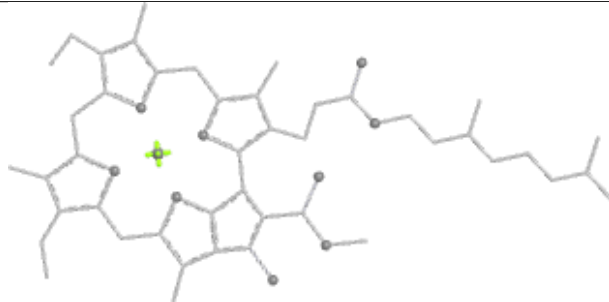
Torsions



Rings

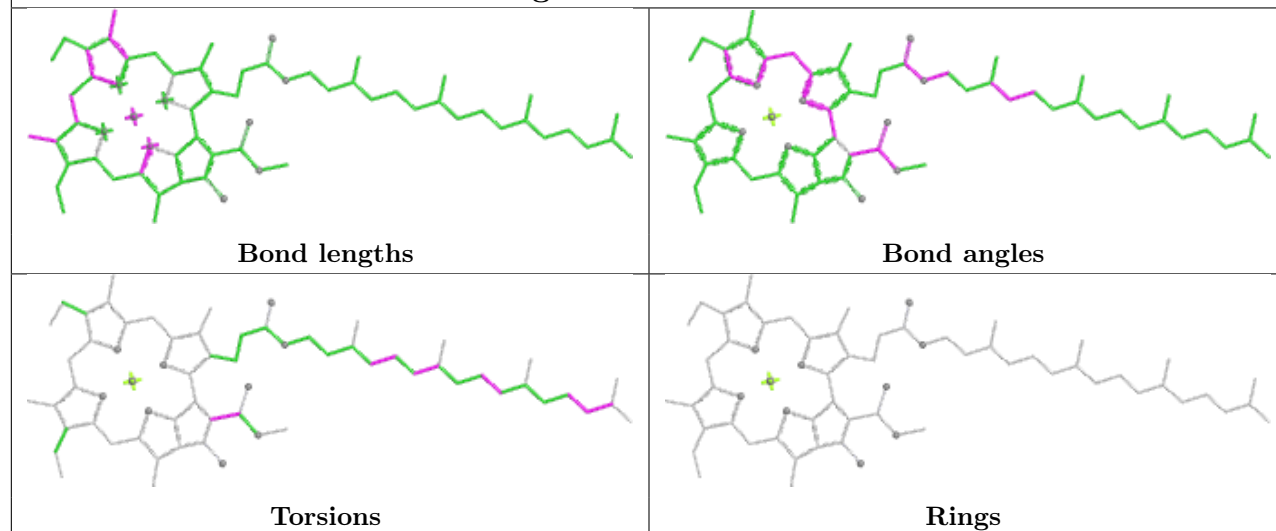
| Ligand BCR L 205                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand LMG B 852                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

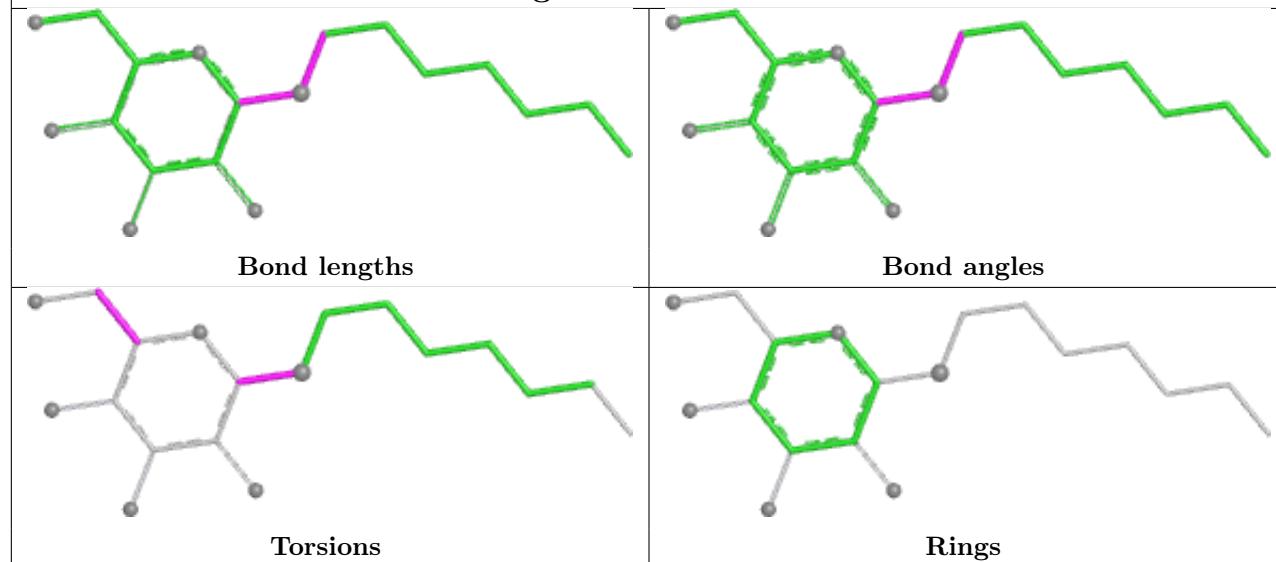
| Ligand CLA B 814                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



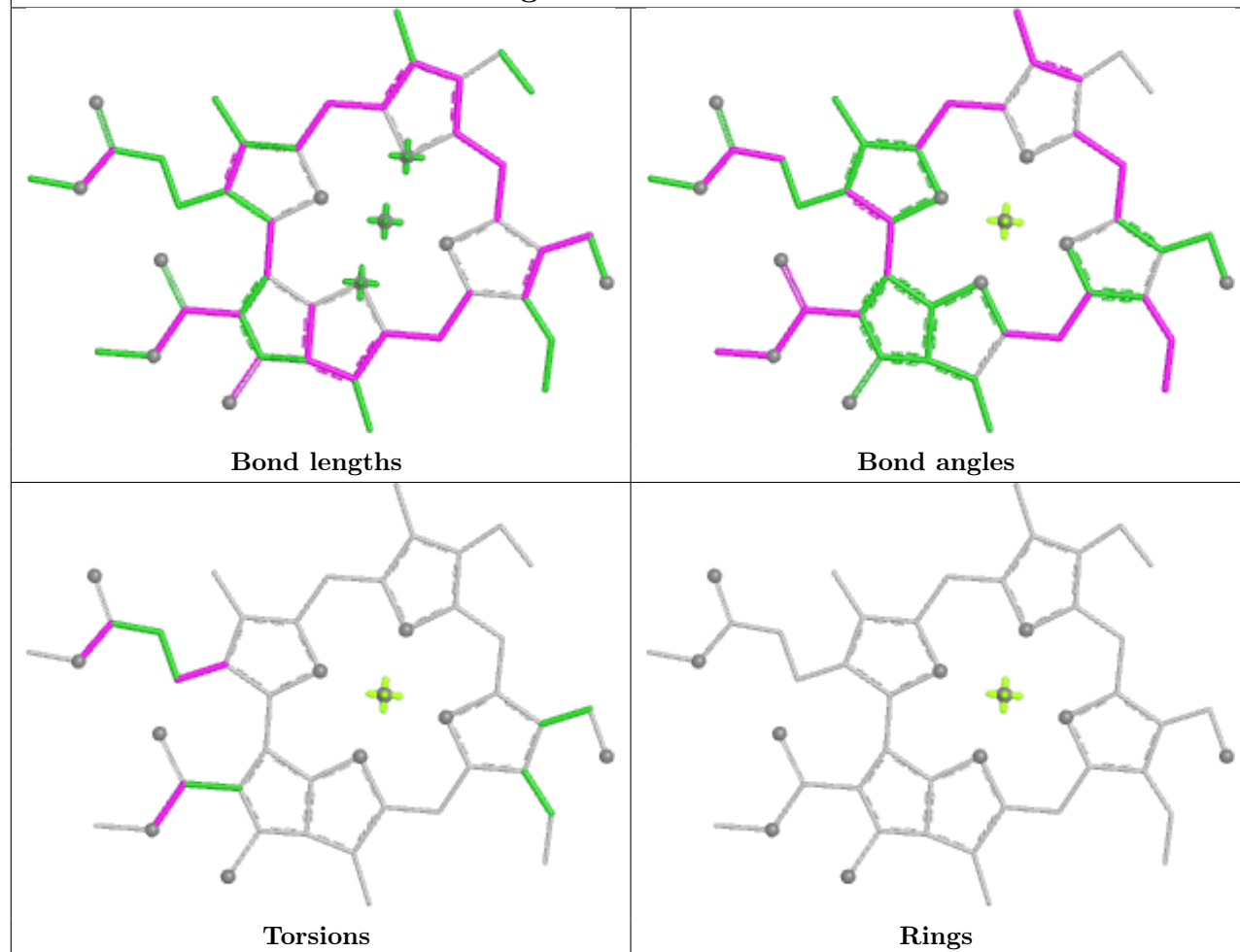
## Ligand CLA B 810



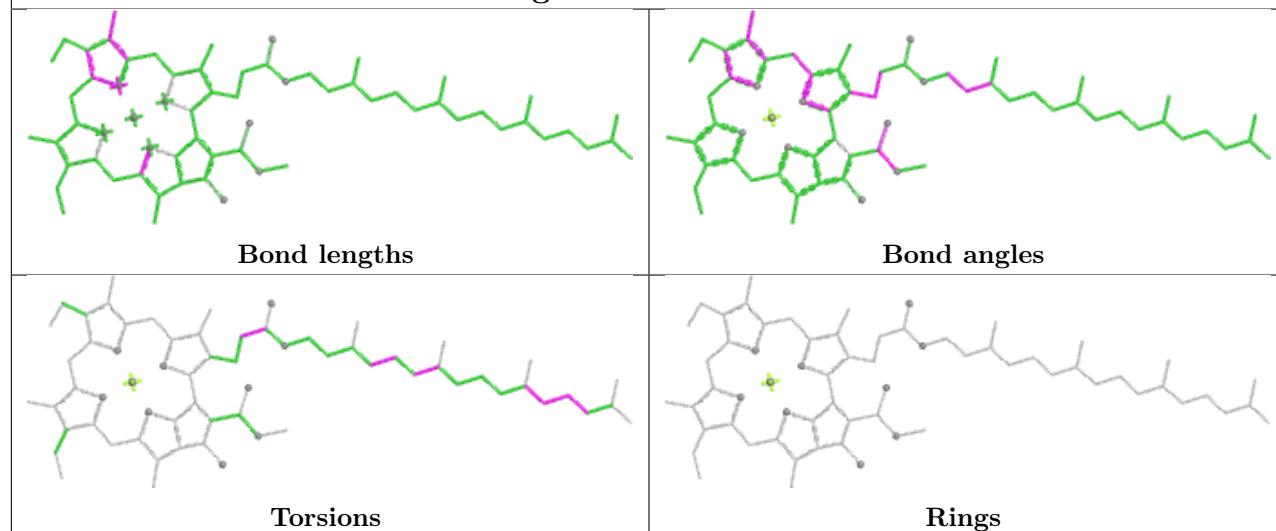
## Ligand HTG 4 321

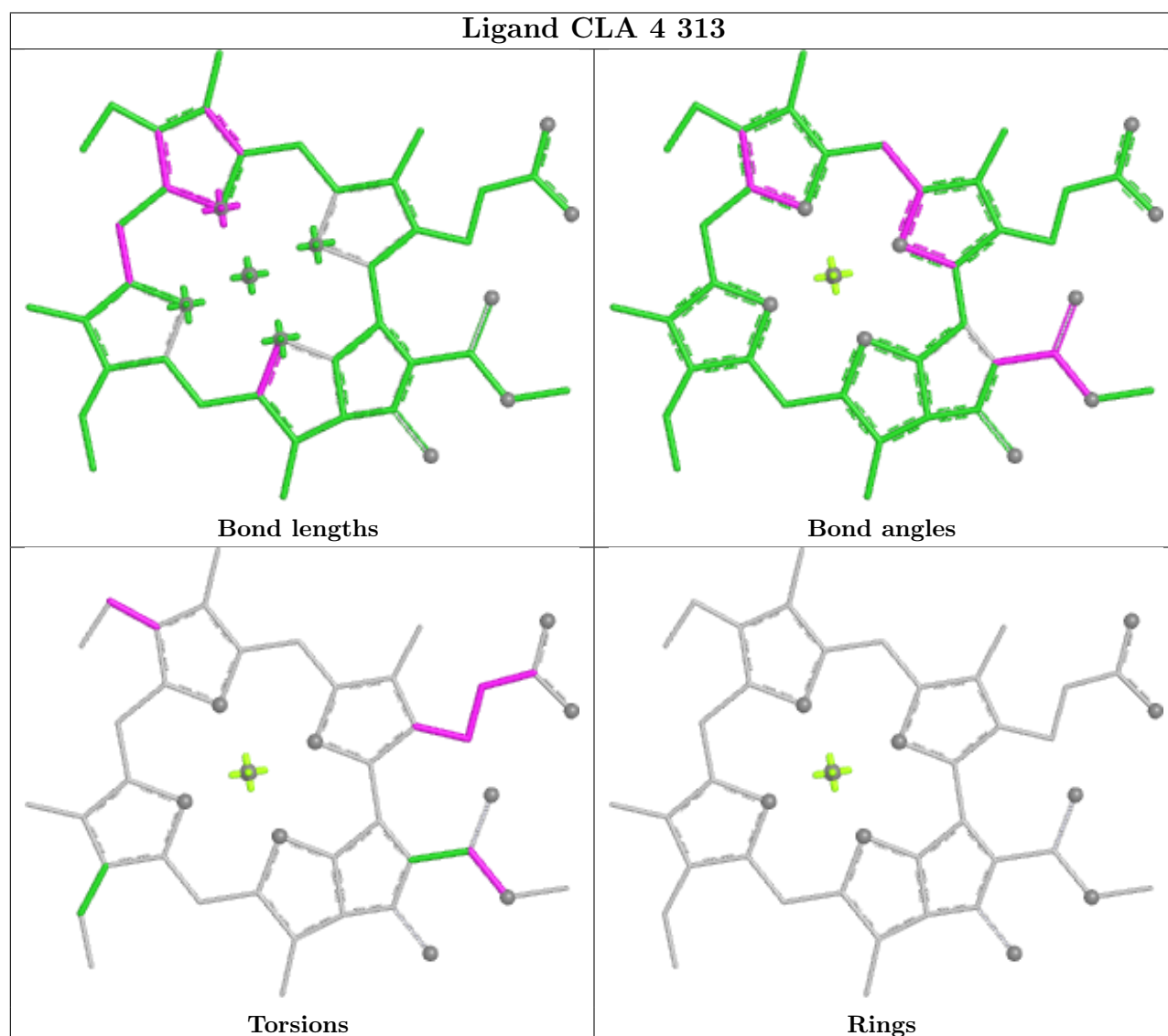
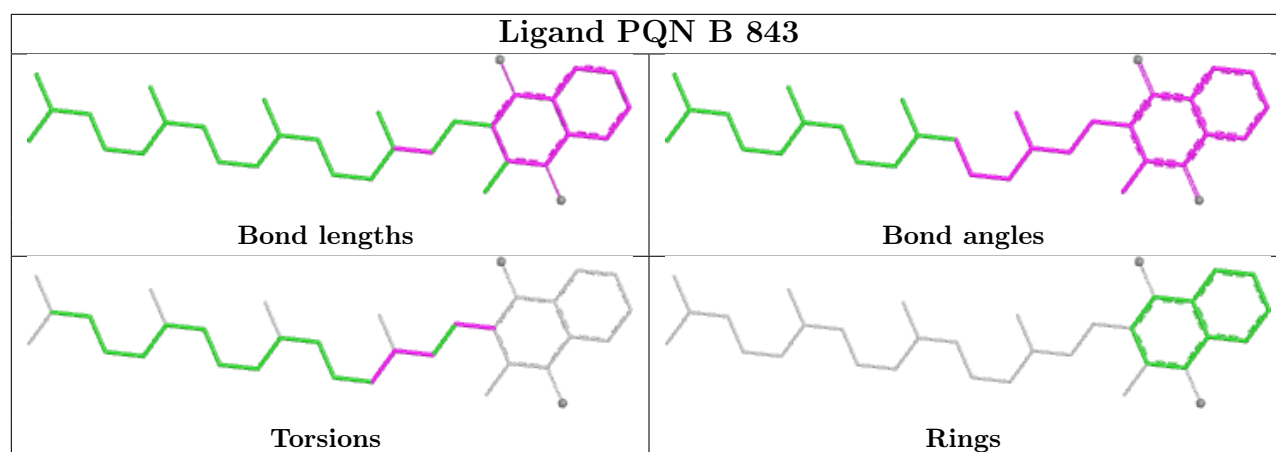


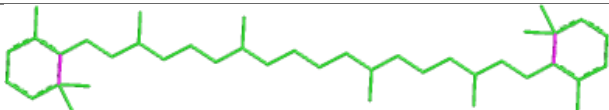
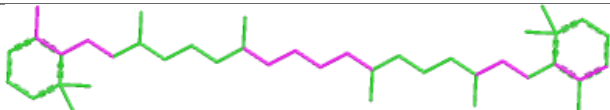
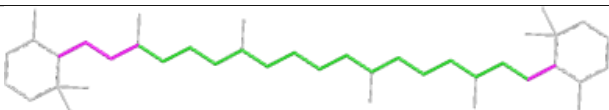
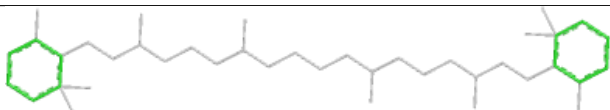
## Ligand CHL 3 607

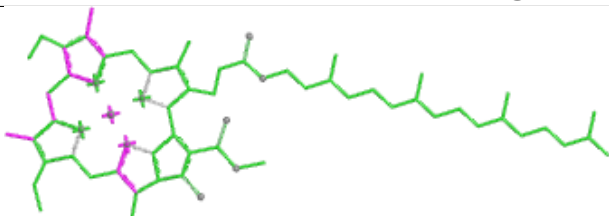
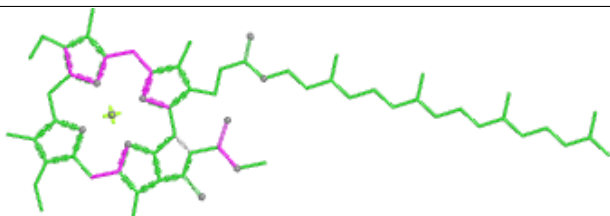
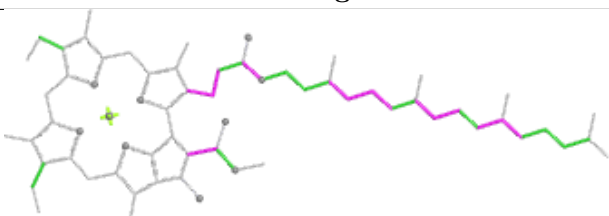
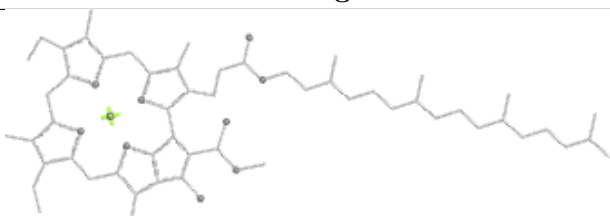


## Ligand CLA B 811

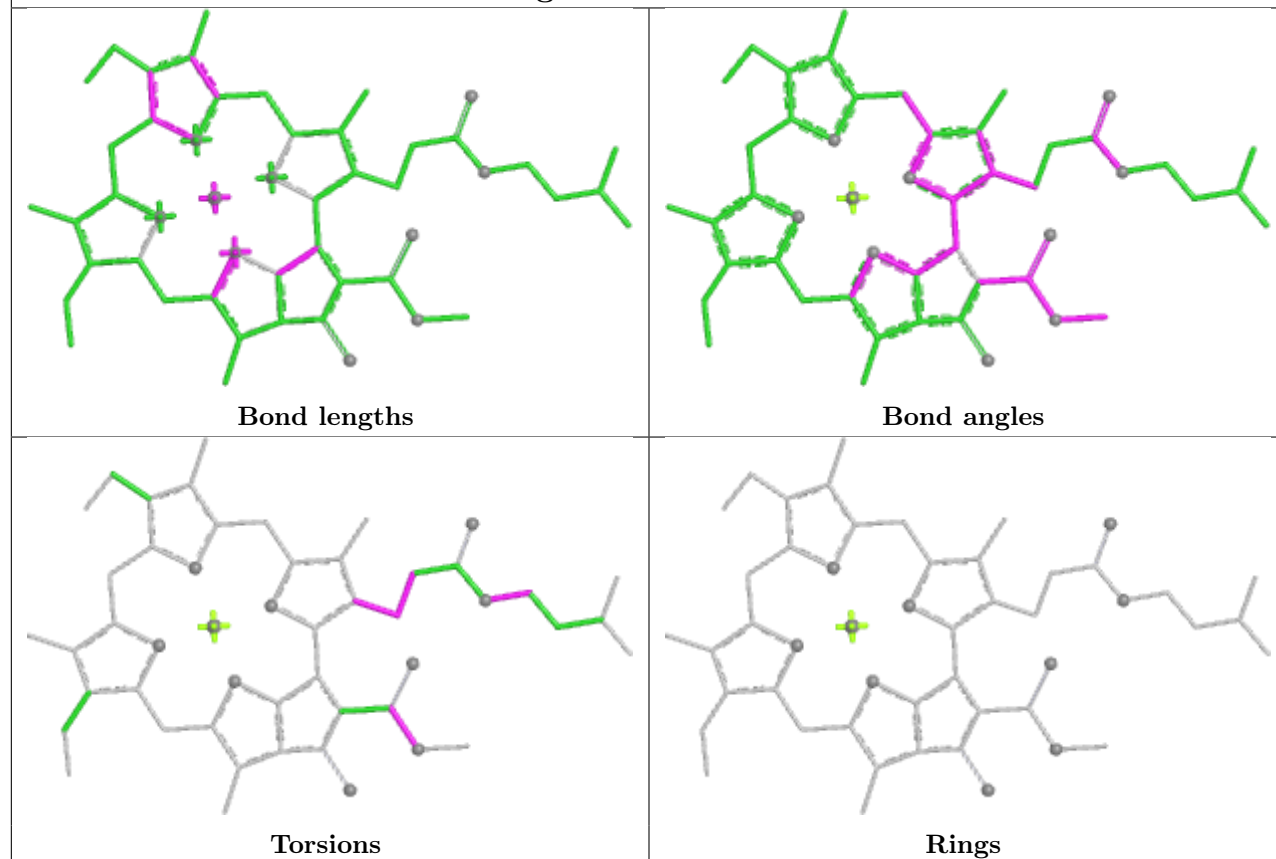




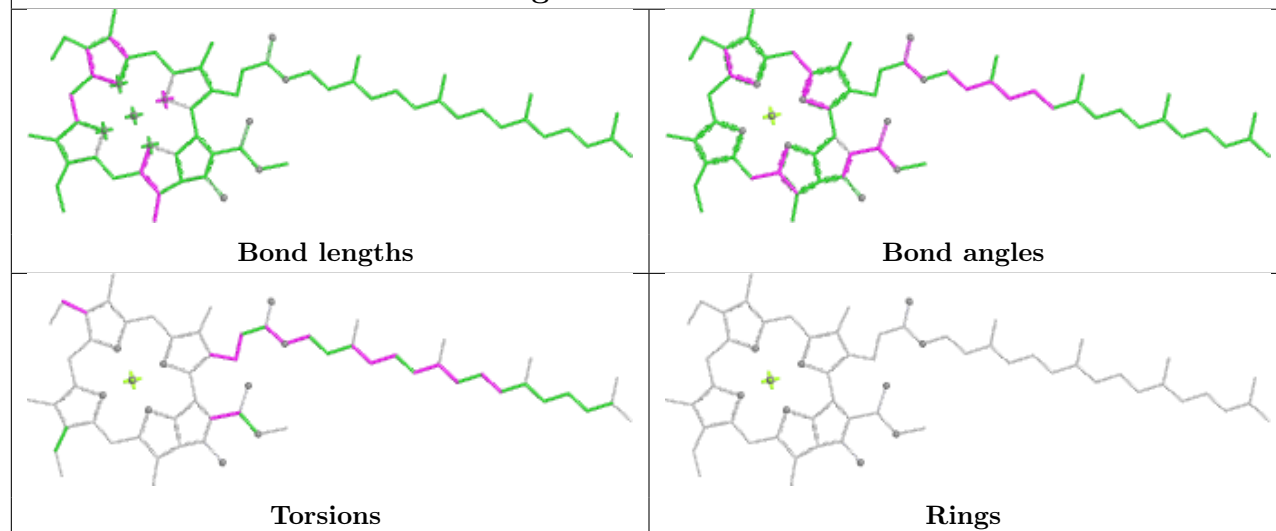
| Ligand BCR A 849                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA A 807                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

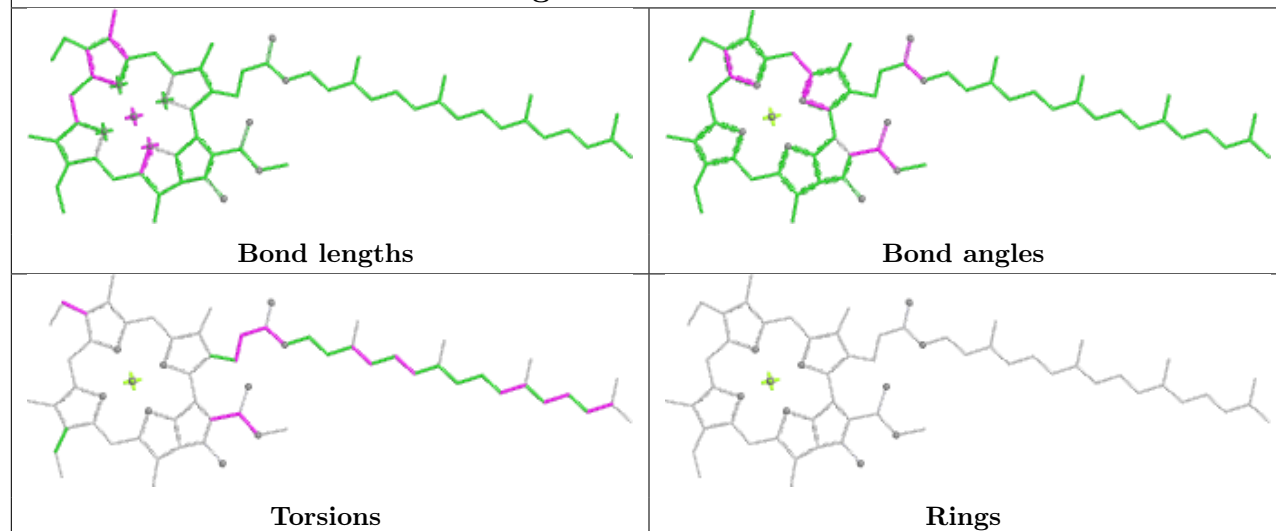
## Ligand CLA 4 304



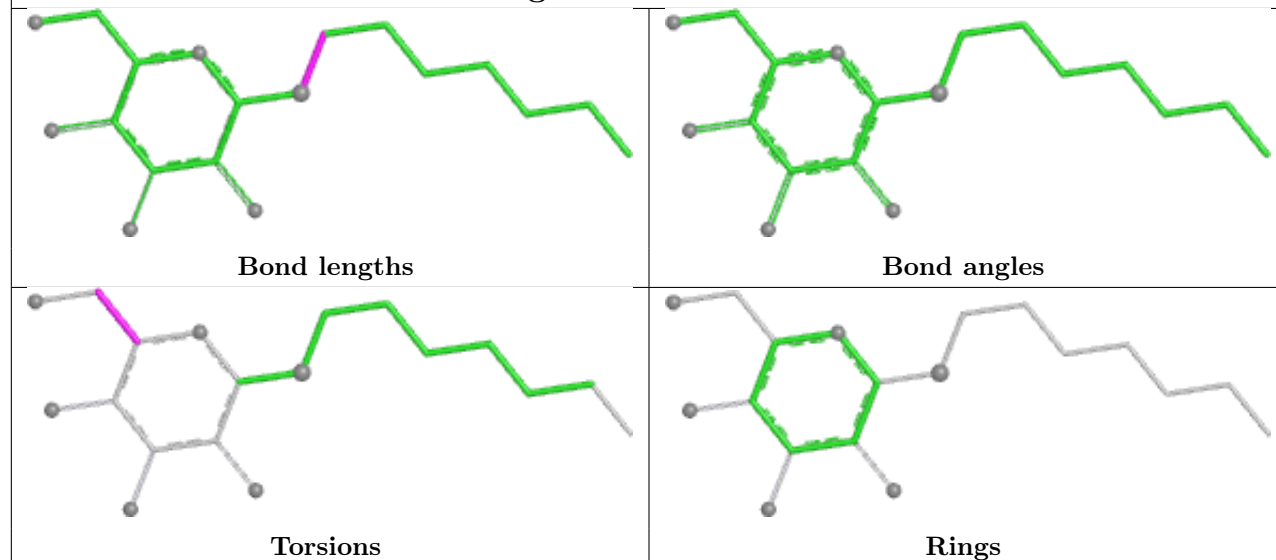
## Ligand CLA A 840



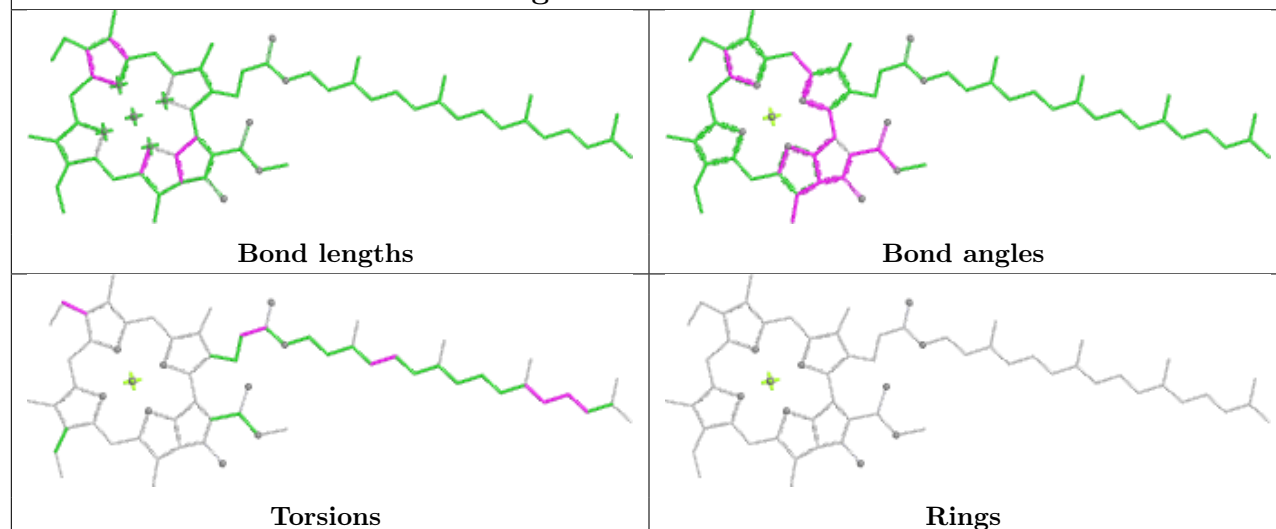
## Ligand CLA B 812



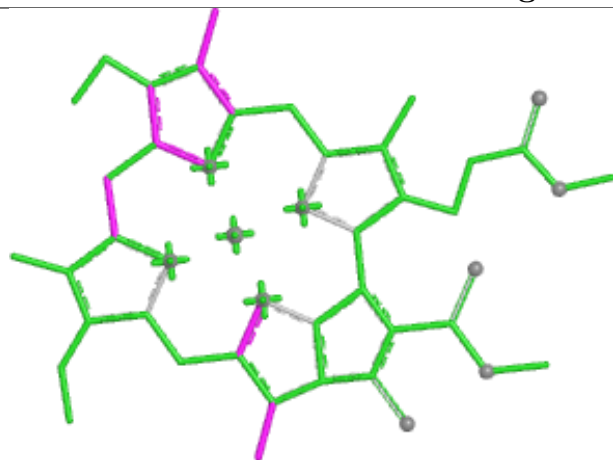
## Ligand HTG A 854



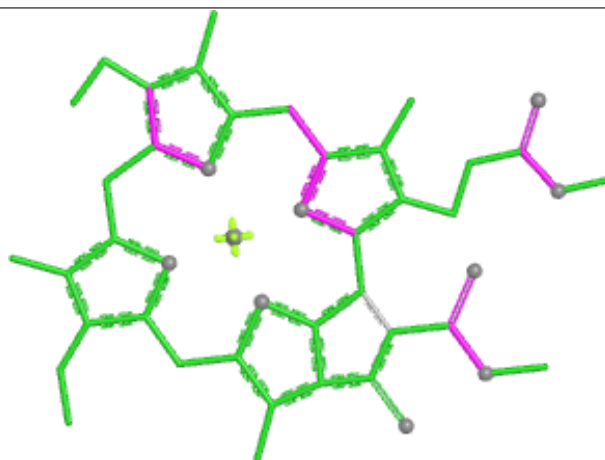
## Ligand CLA A 801



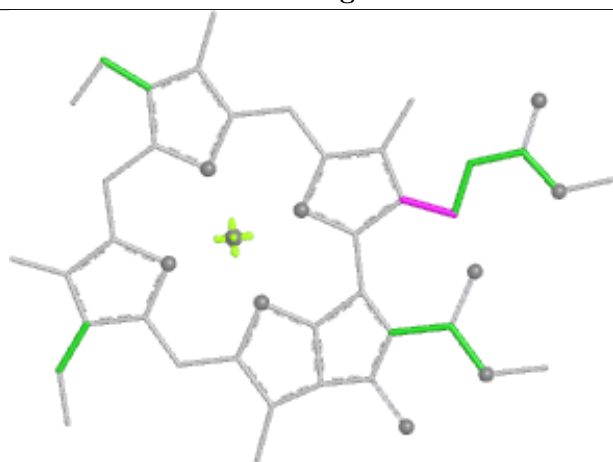
## Ligand CLA 1 306



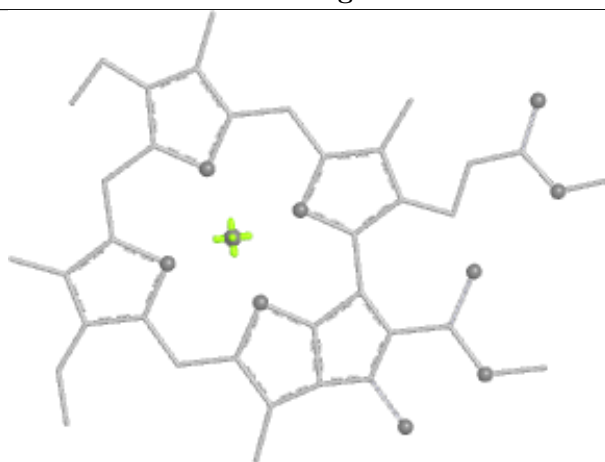
Bond lengths



Bond angles

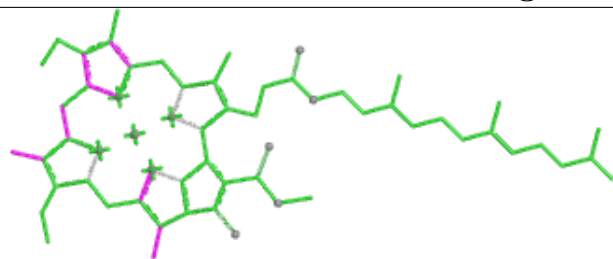


Torsions

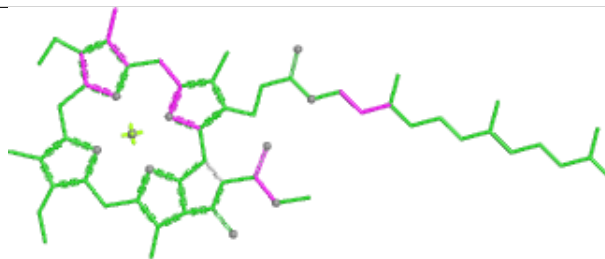


Rings

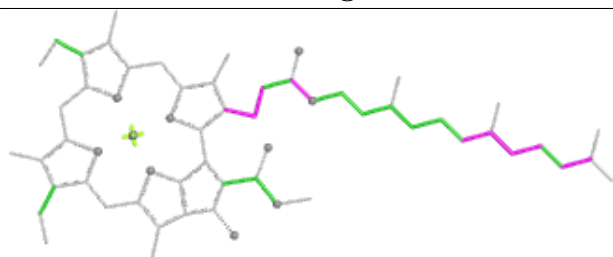
## Ligand CLA 2 308



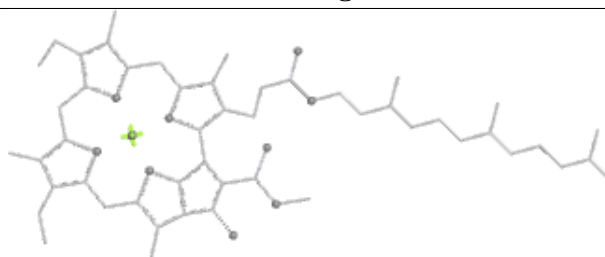
Bond lengths



Bond angles

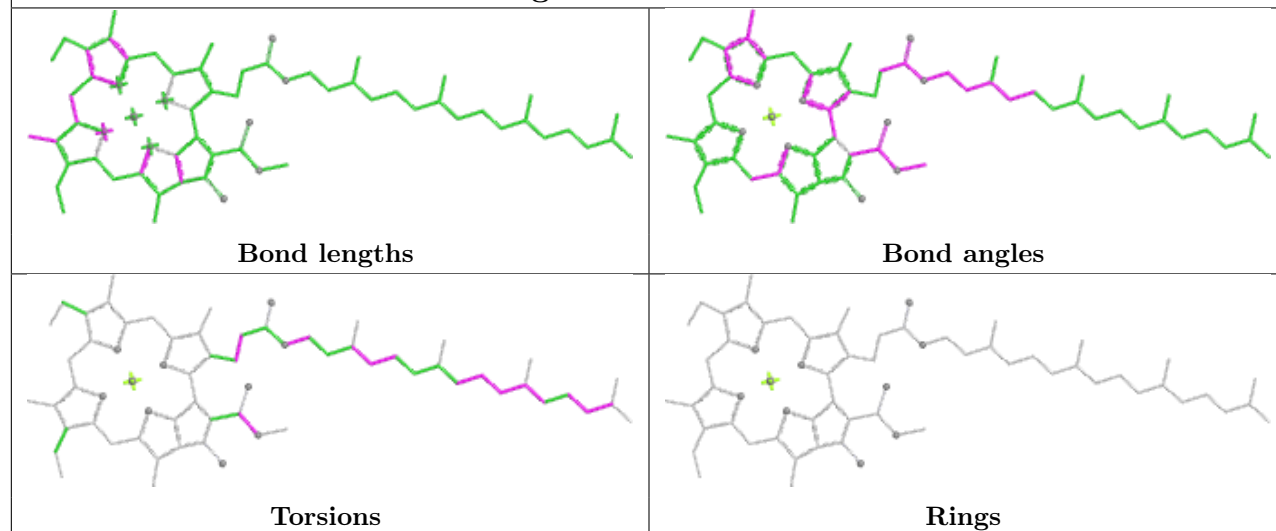


Torsions

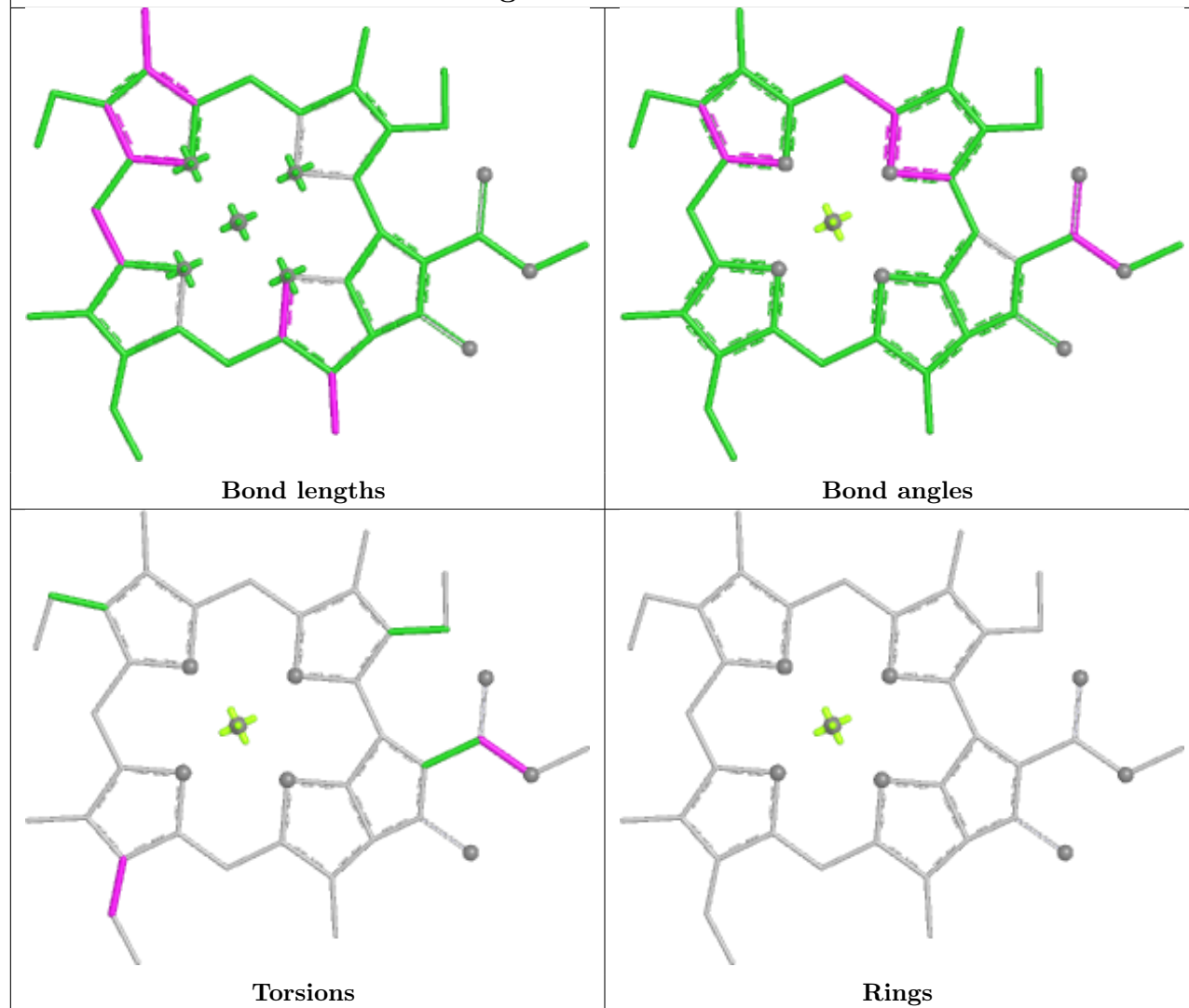


Rings

## Ligand CLA A 853

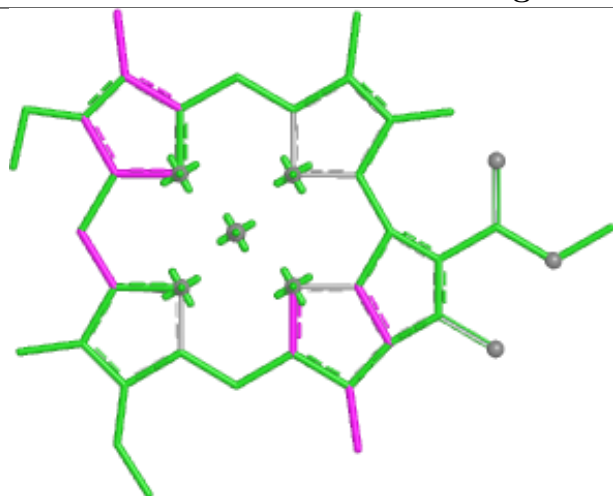


## Ligand CLA 1 304

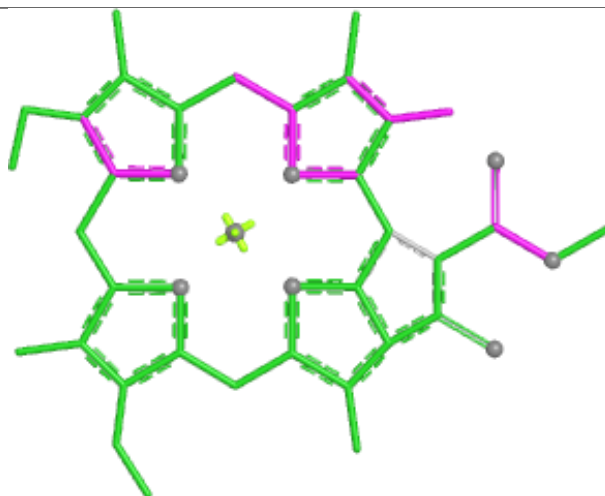




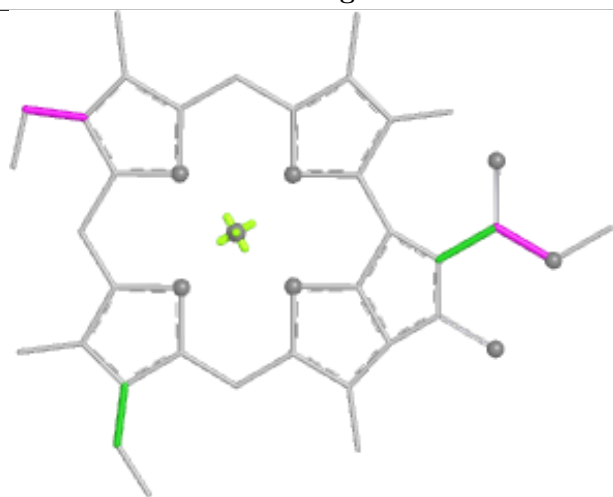
## Ligand CLA G 103



Bond lengths



Bond angles

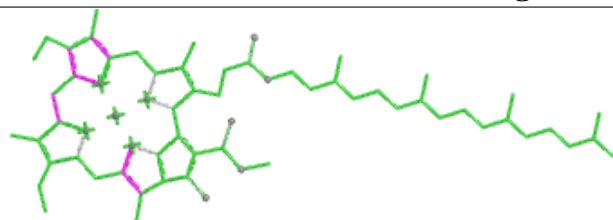


Torsions

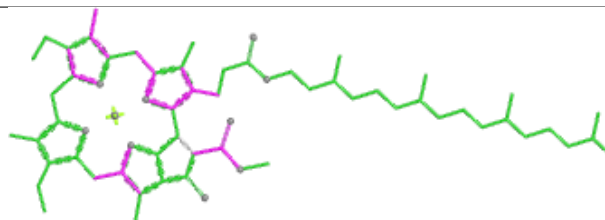


Rings

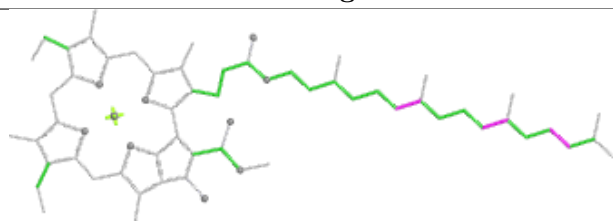
## Ligand CLA A 825



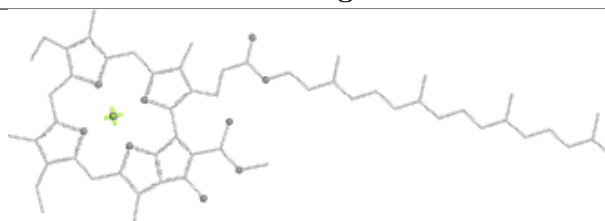
Bond lengths



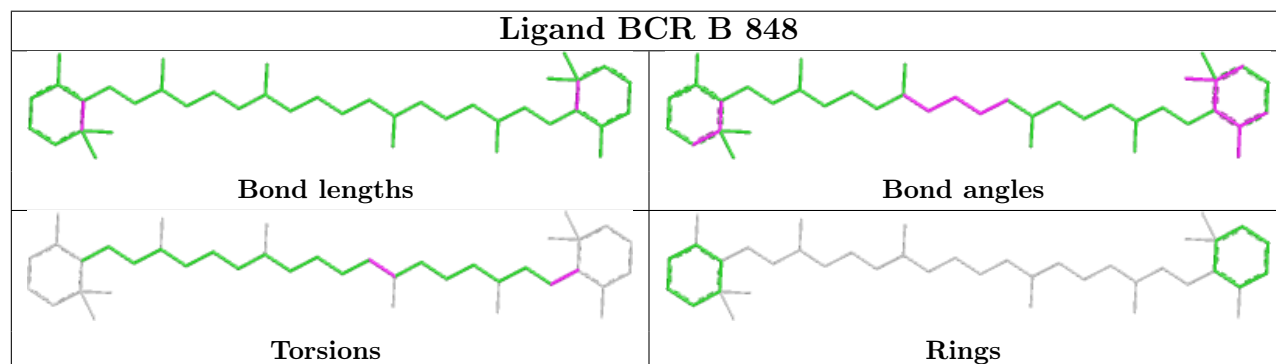
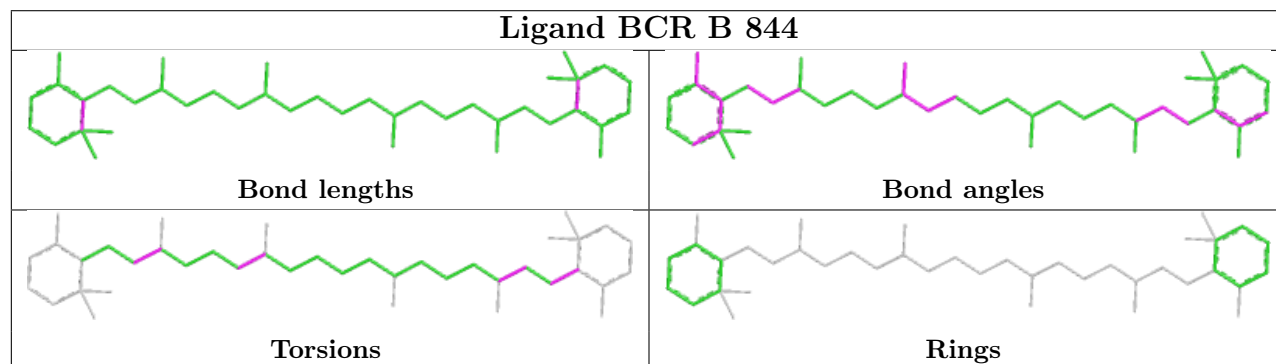
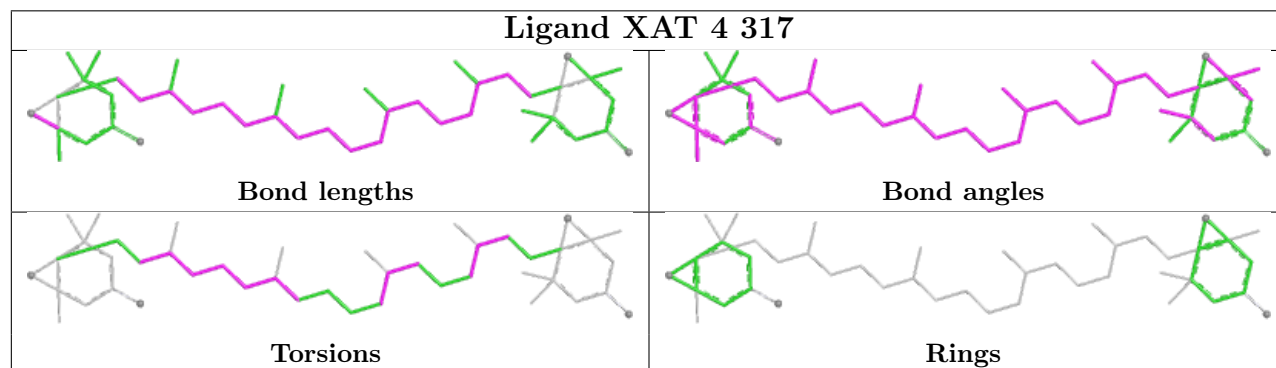
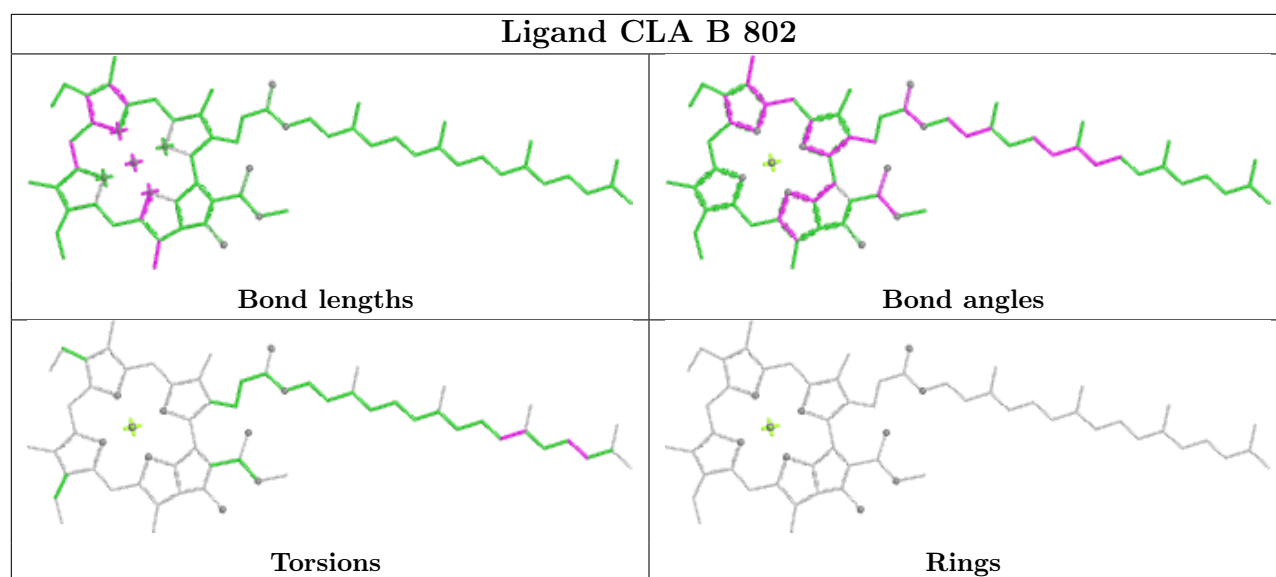
Bond angles

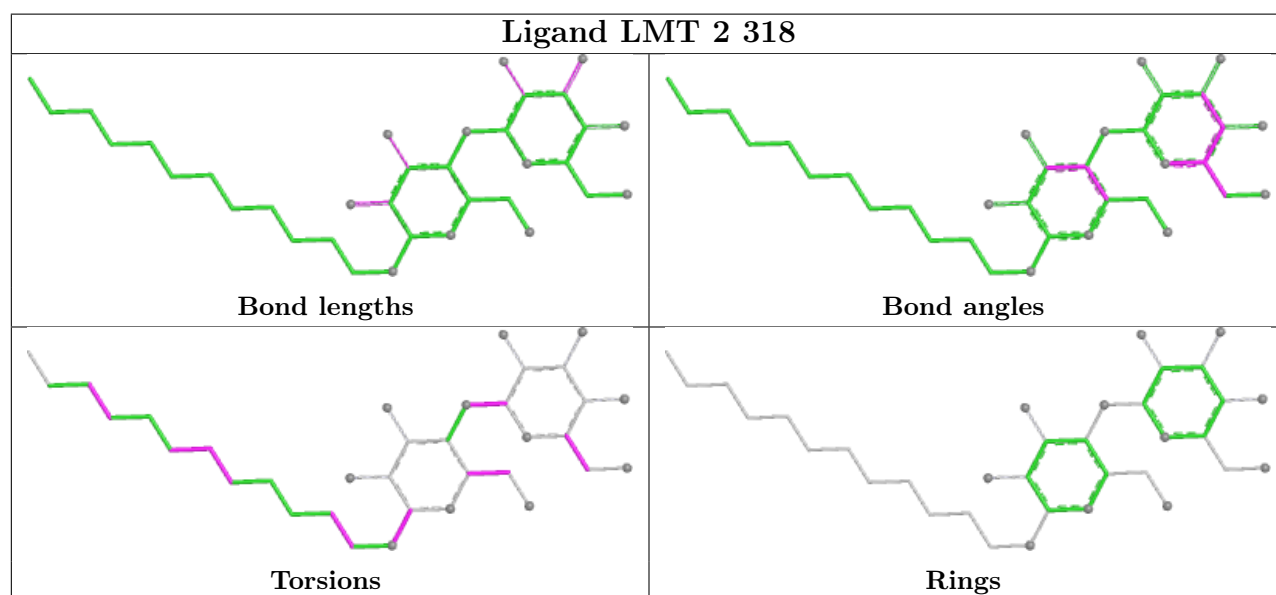
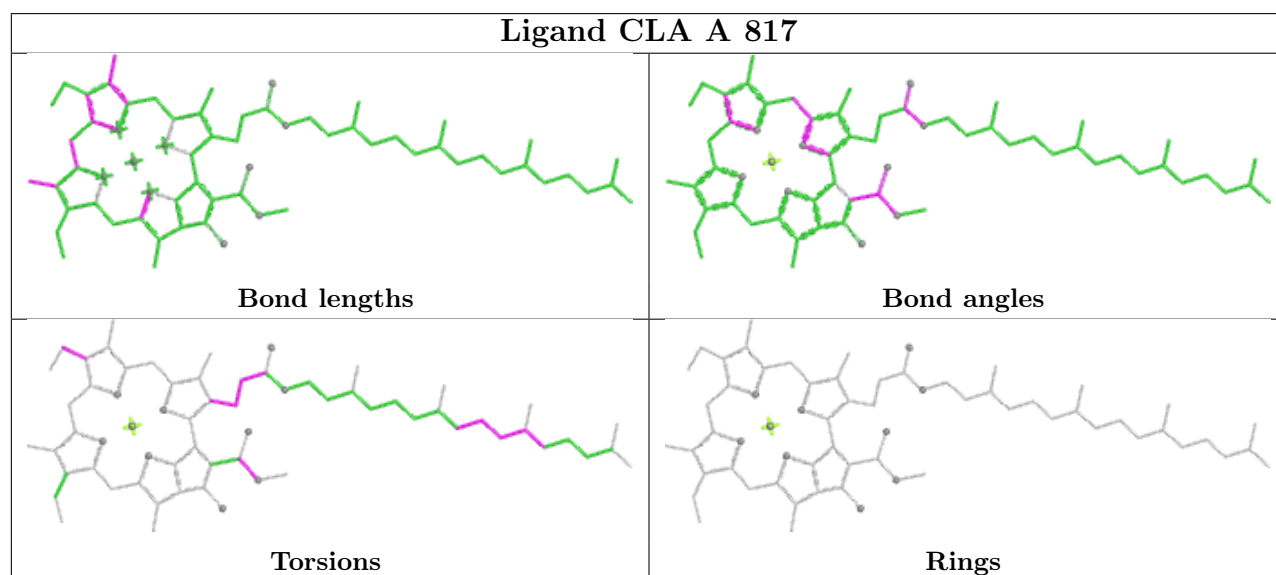
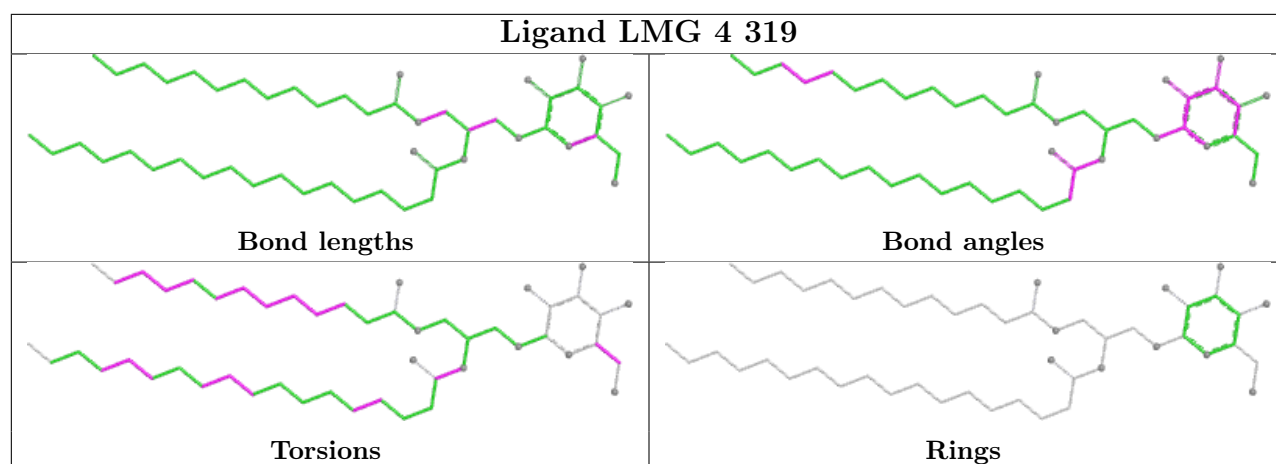


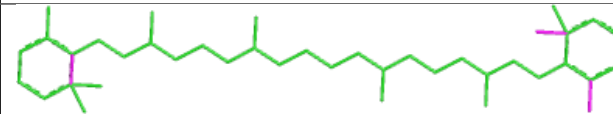
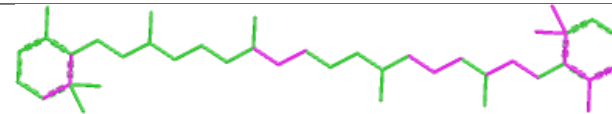
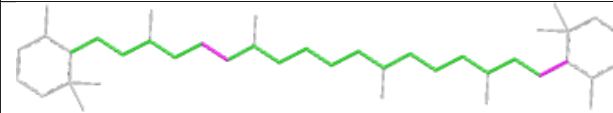
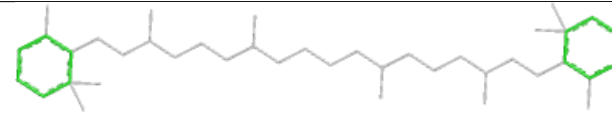
Torsions

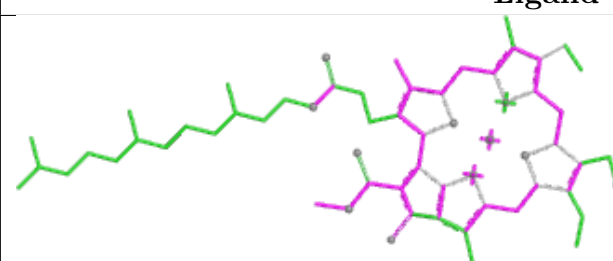
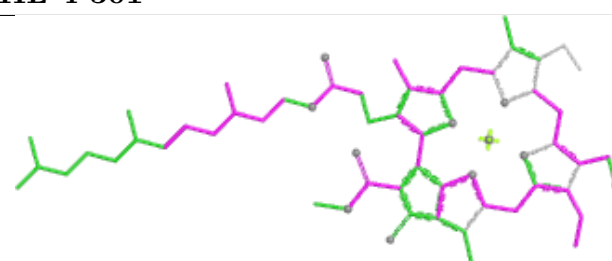
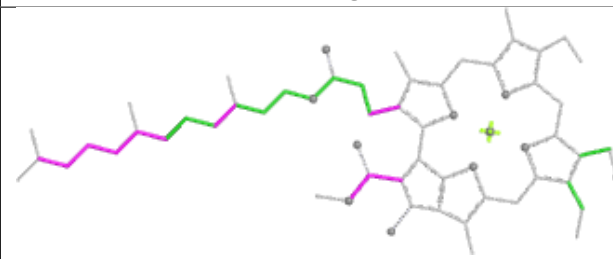
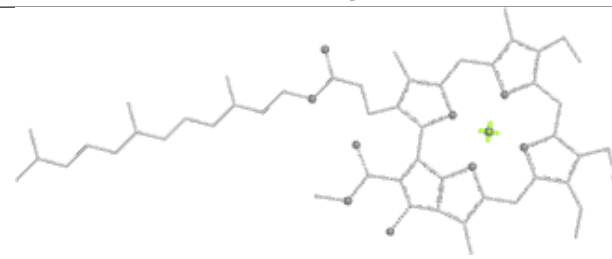


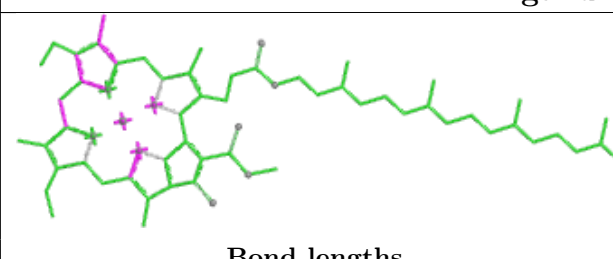
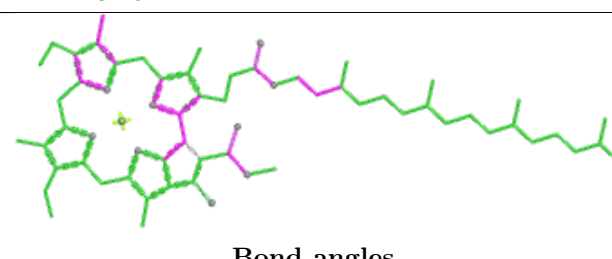
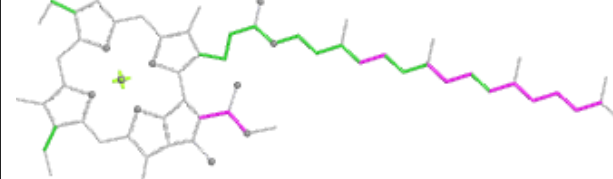
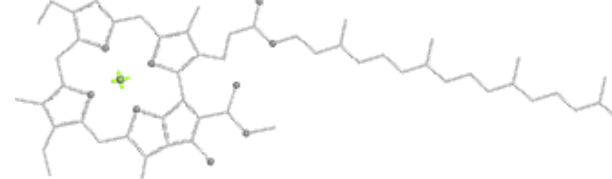
Rings



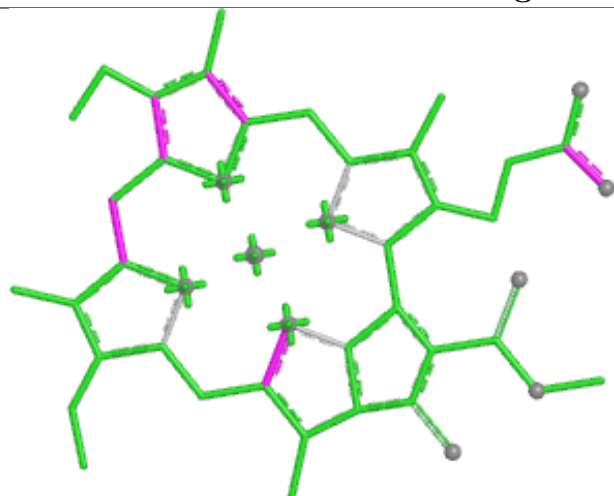


| Ligand BCR B 847                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

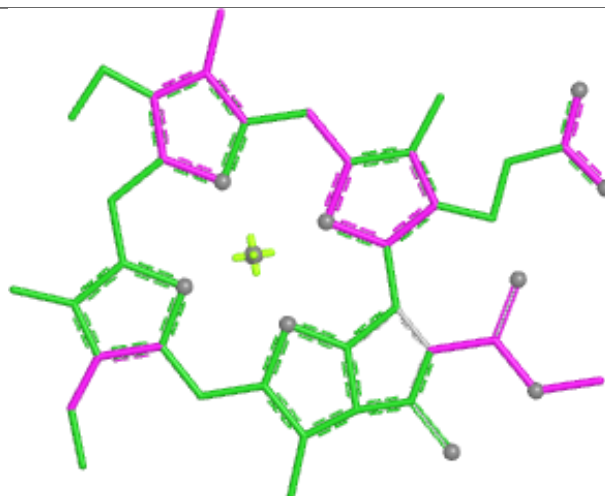
| Ligand CHL 4 301                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

| Ligand CLA B 826                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

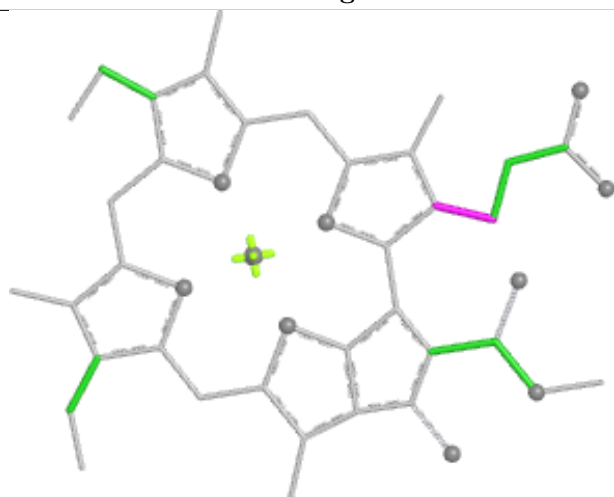
## Ligand CLA B 806



Bond lengths



Bond angles

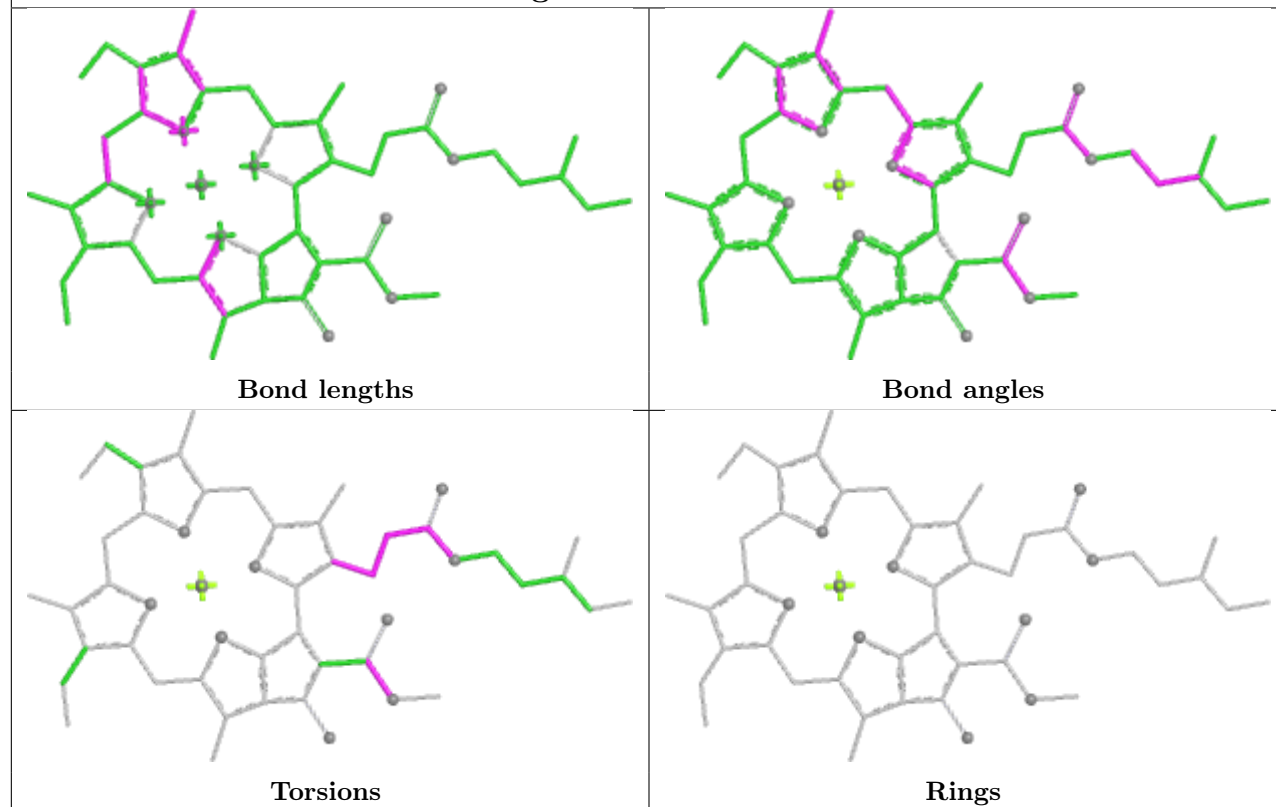


Torsions

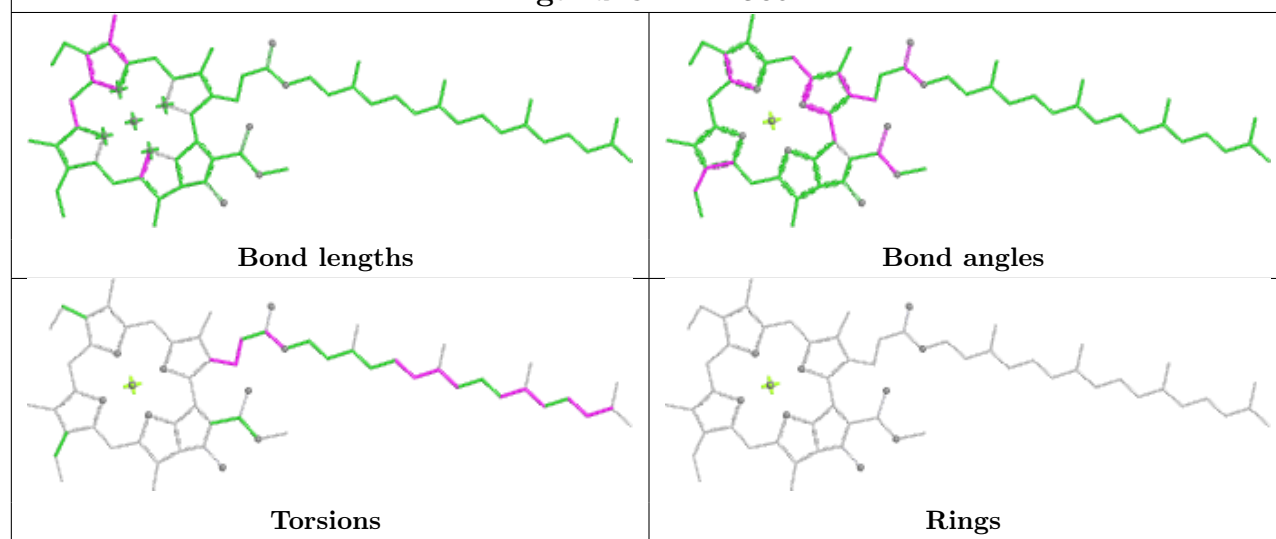


Rings

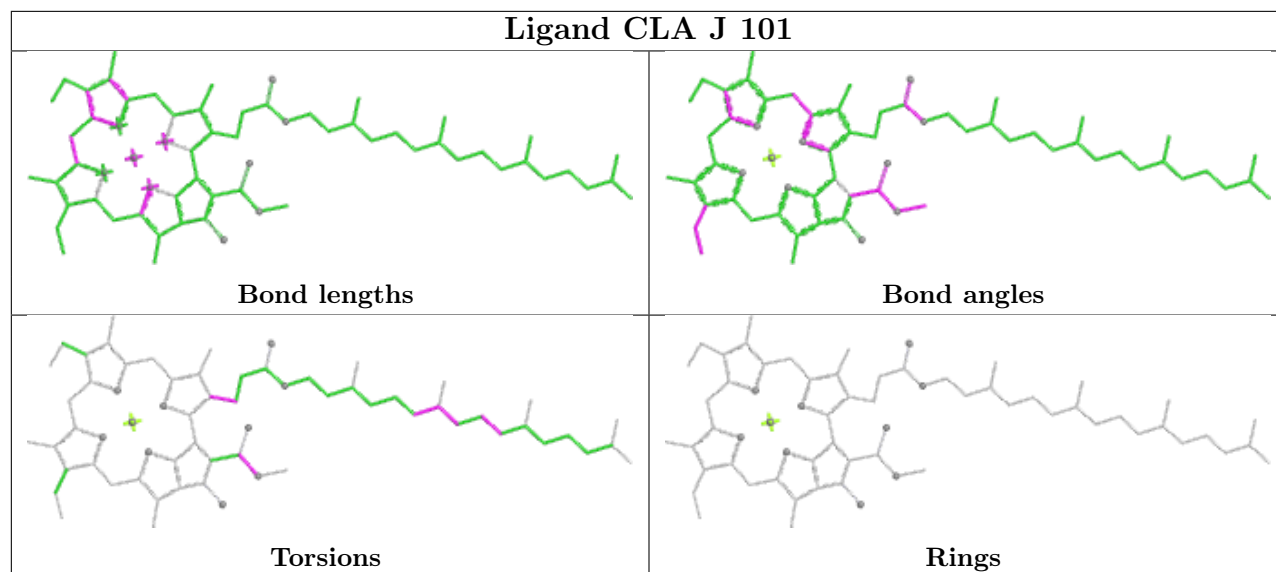
## Ligand CLA A 835



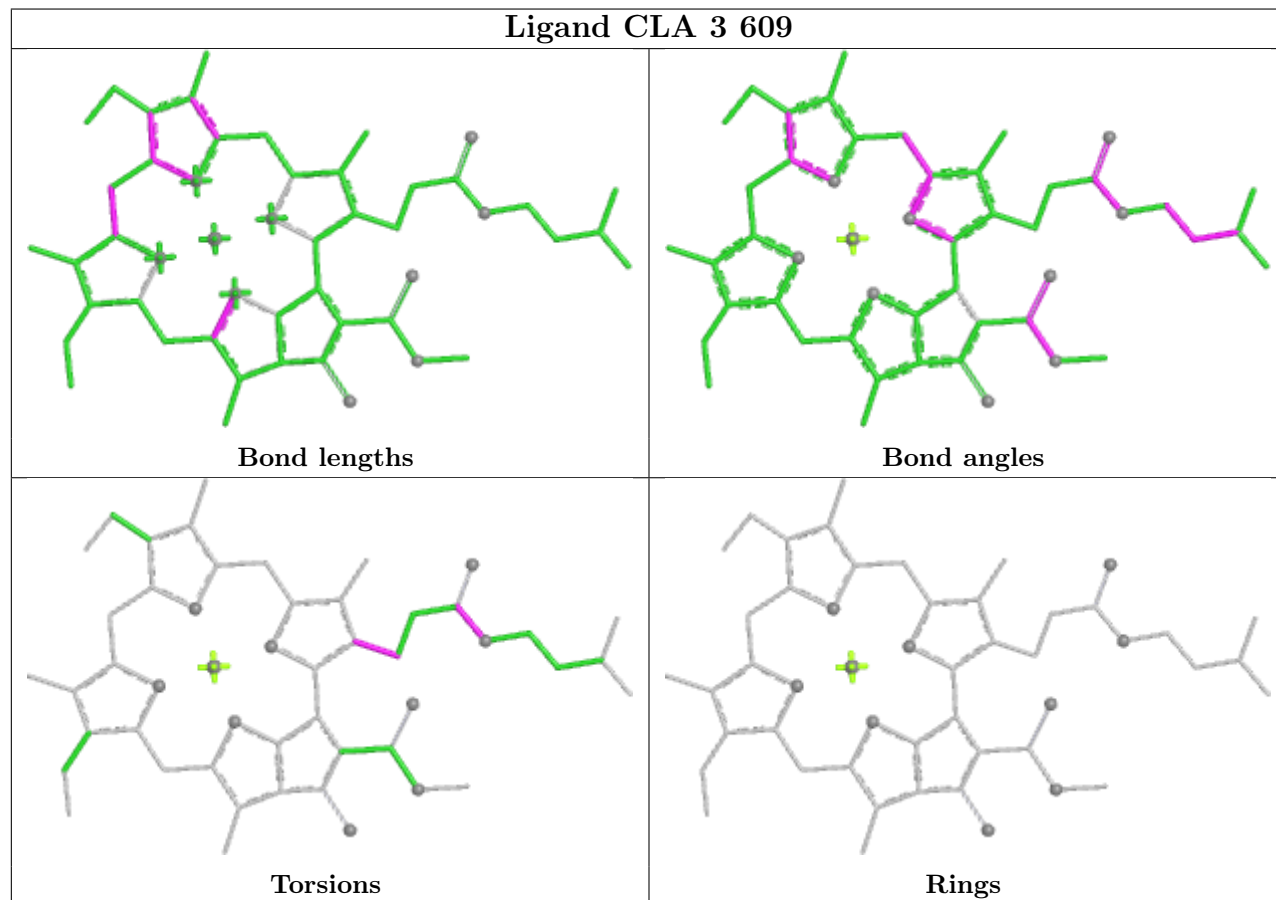
## Ligand CLA 1 309



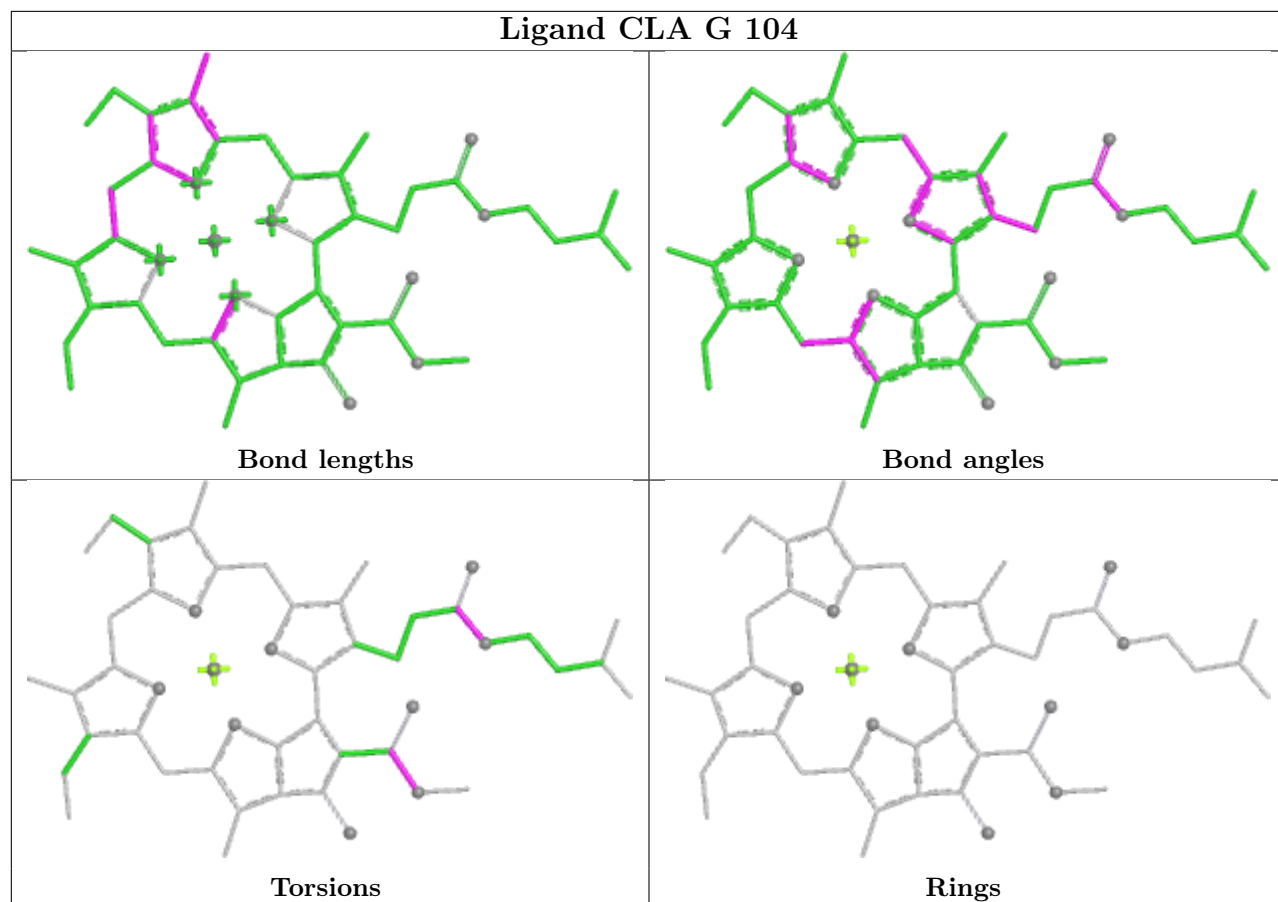
## Ligand CLA J 101



## Ligand CLA 3 609

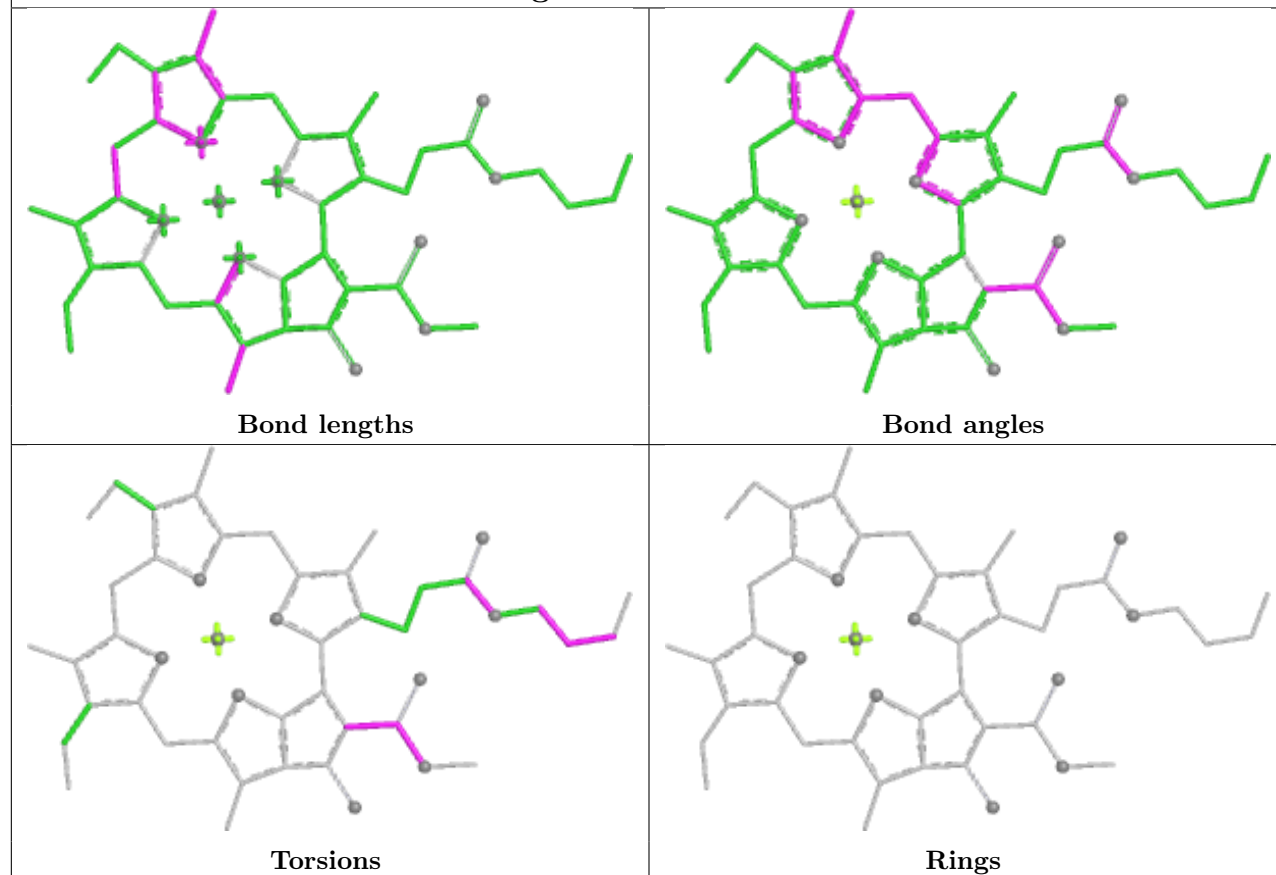


## Ligand CLA G 104

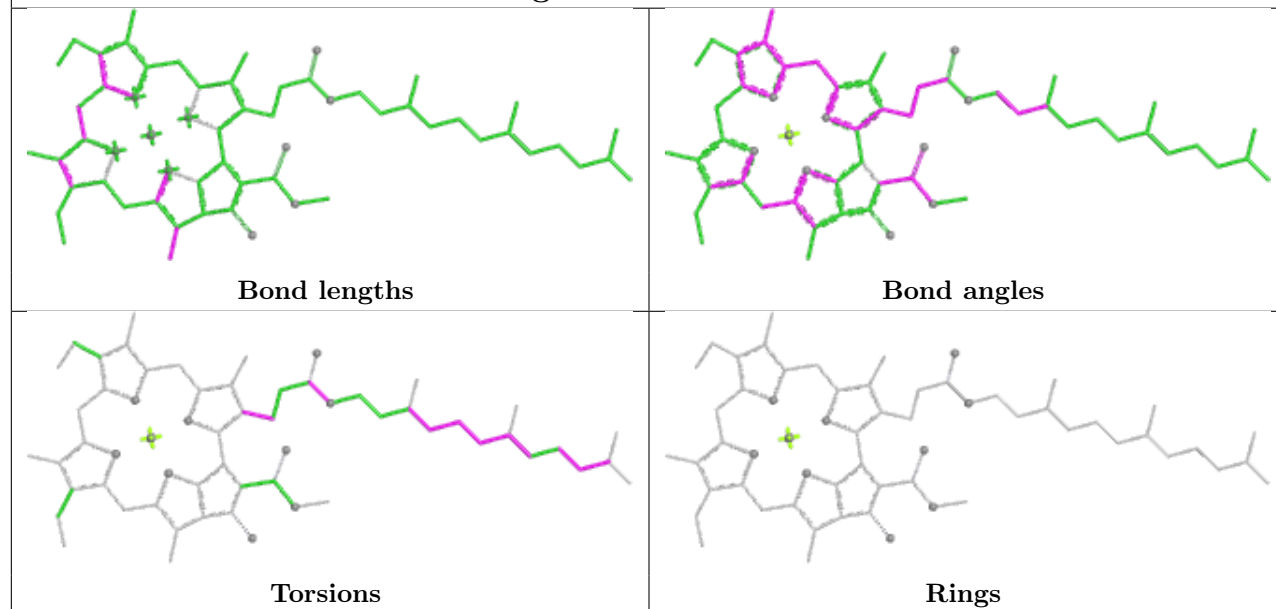


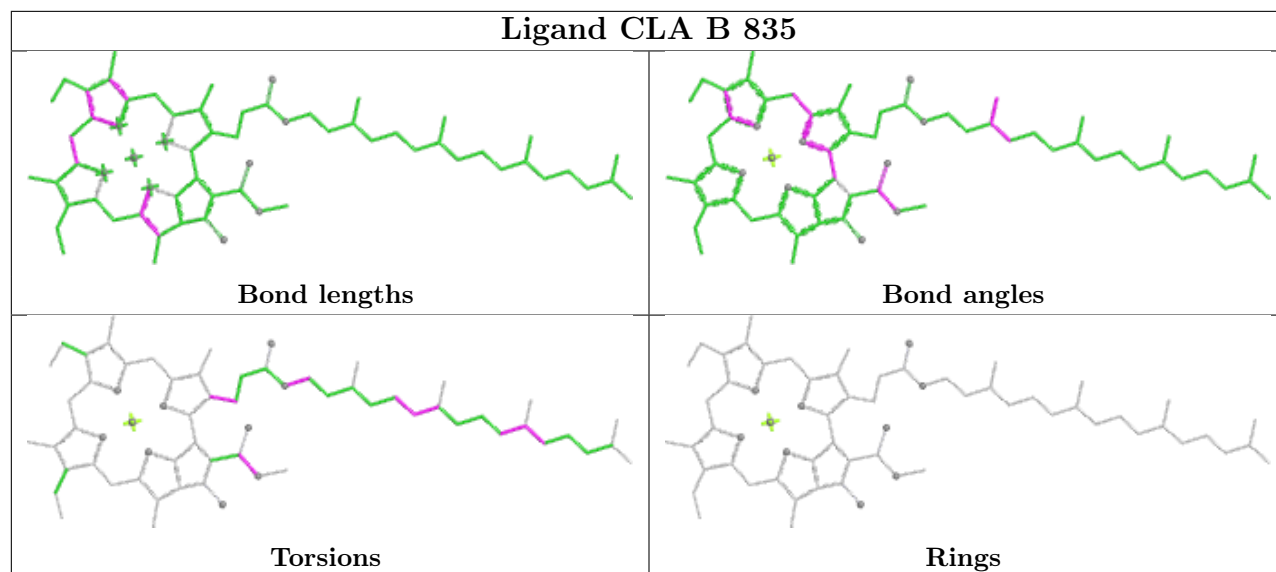
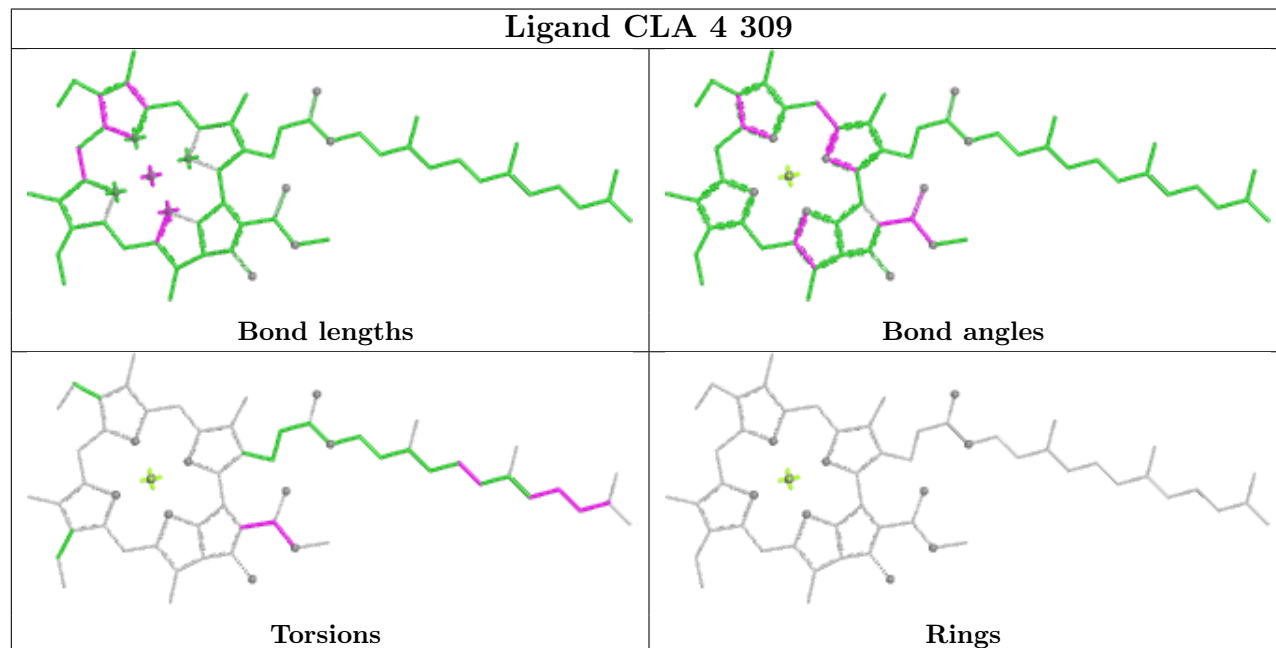


## Ligand CLA A 821

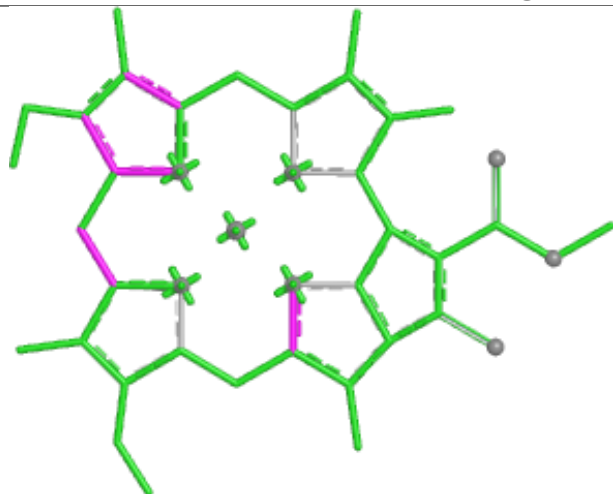


## Ligand CLA B 820

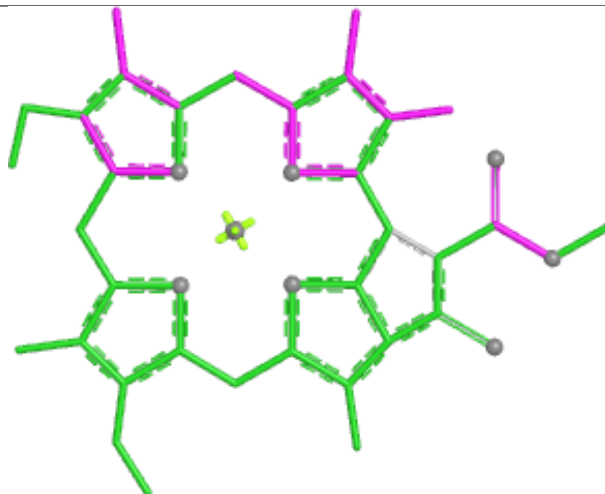


**Ligand CLA B 835****Ligand CLA 4 309**

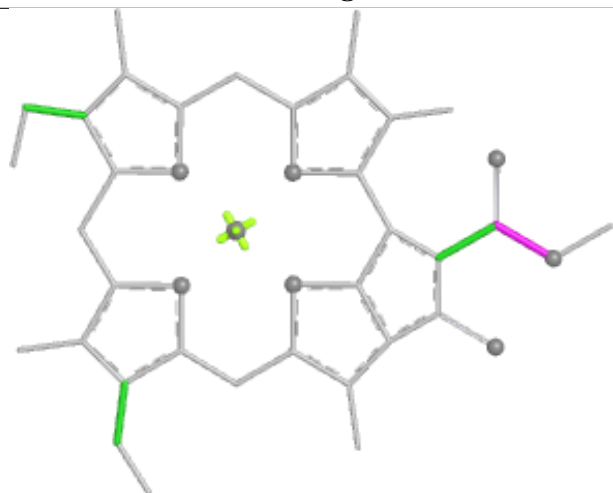
## Ligand CLA 2 309



Bond lengths



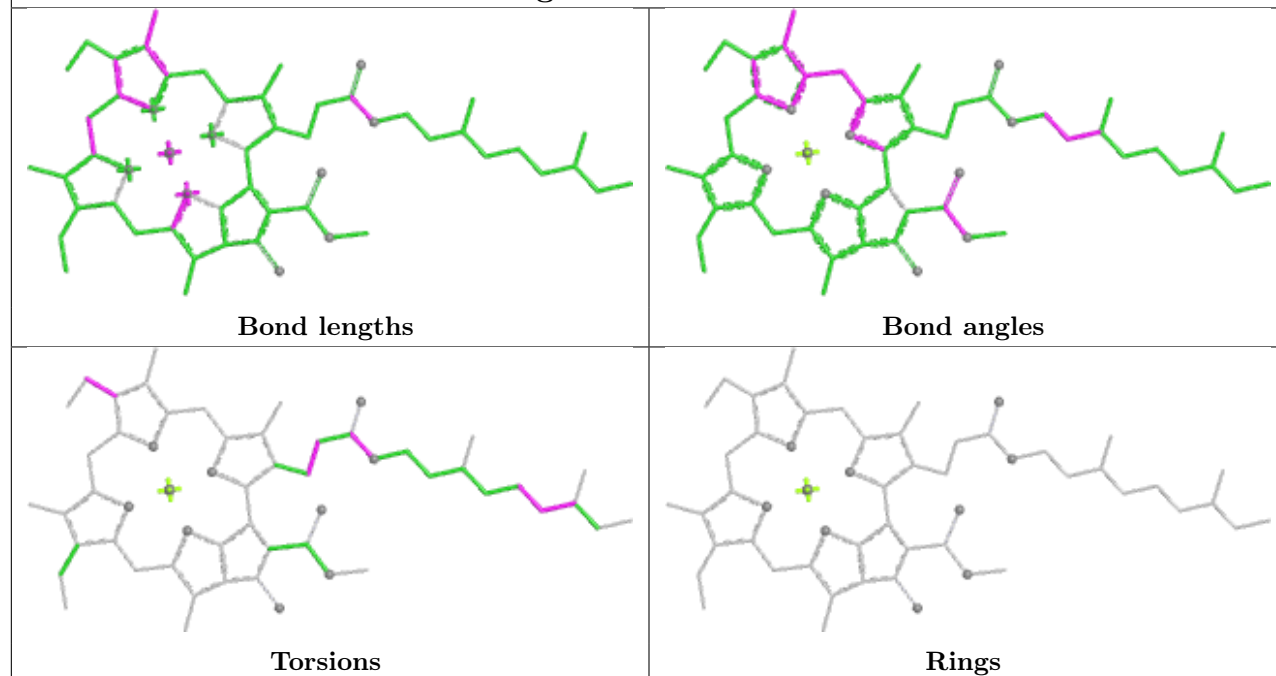
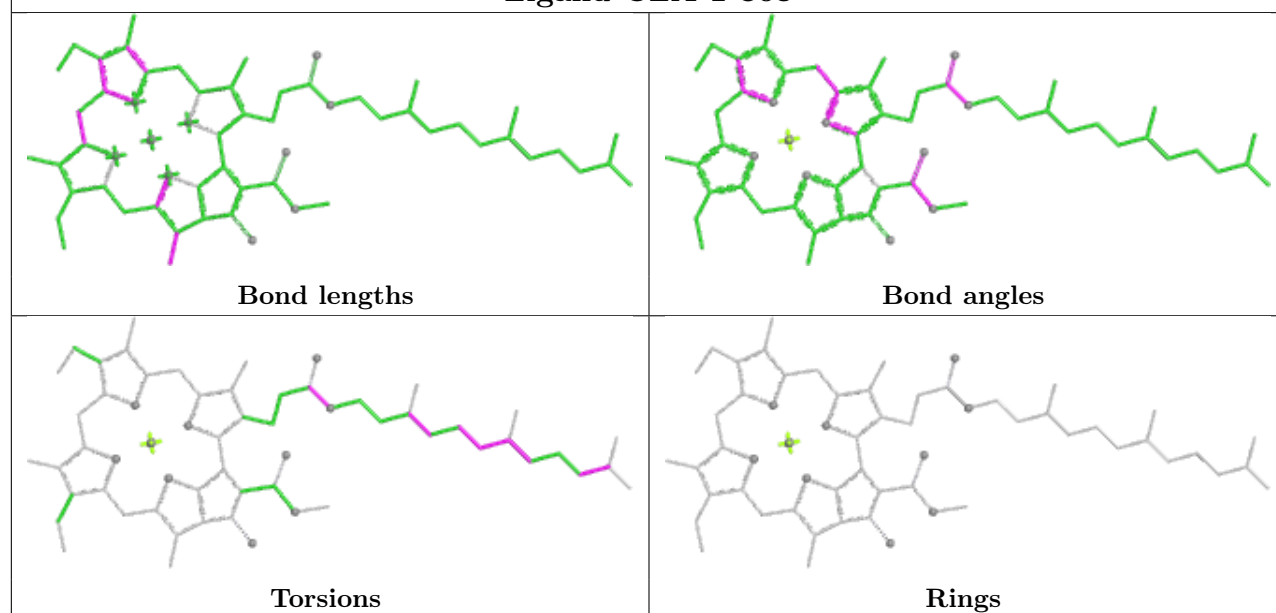
Bond angles



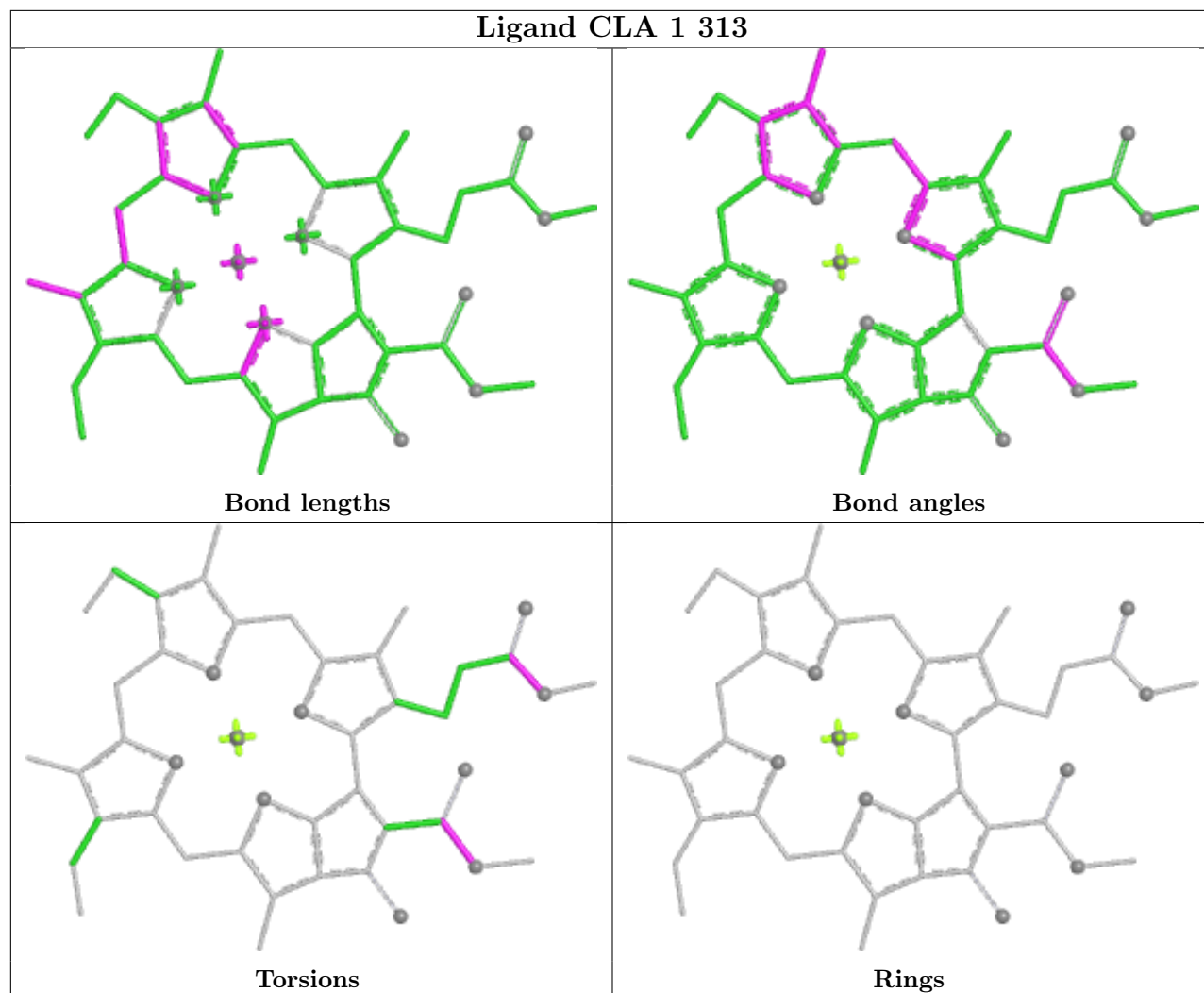
Torsions



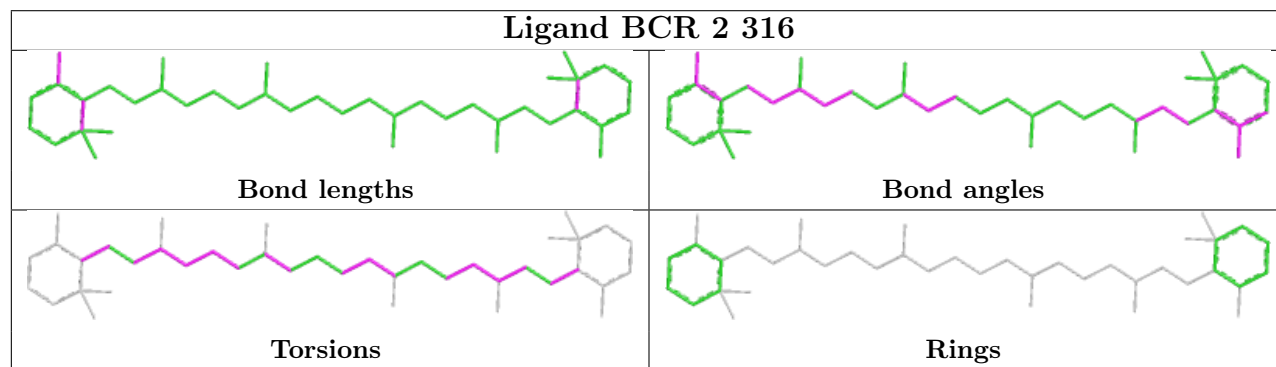
Rings

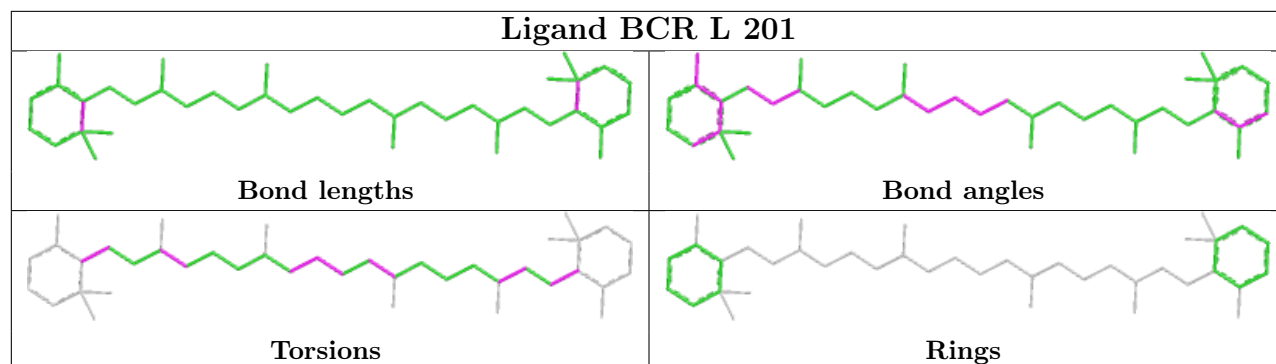
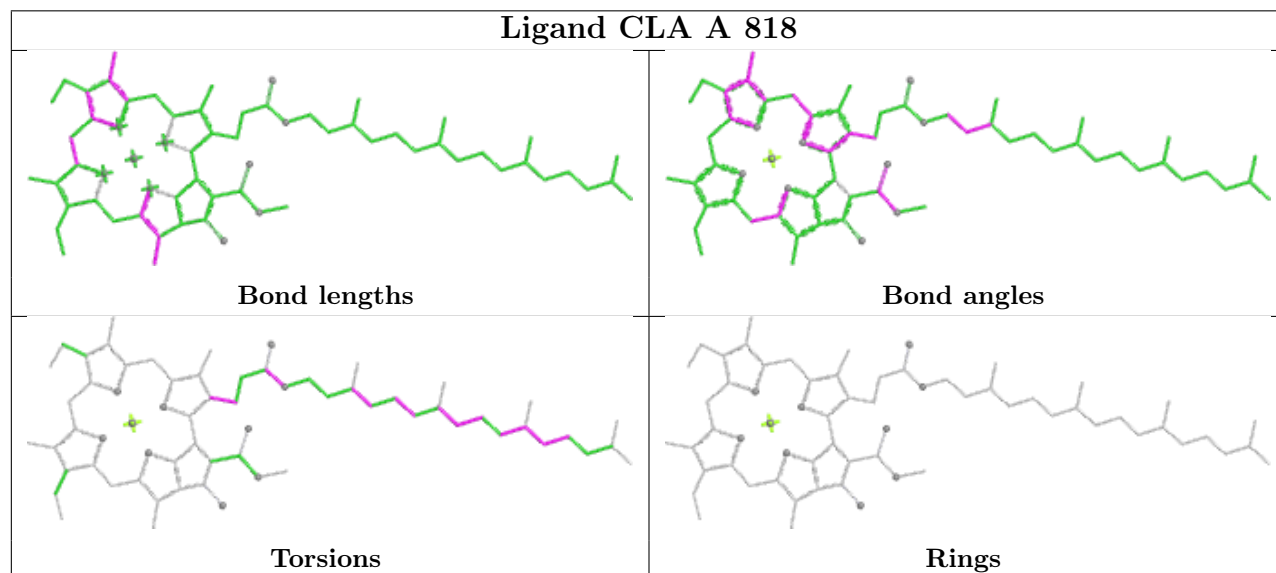
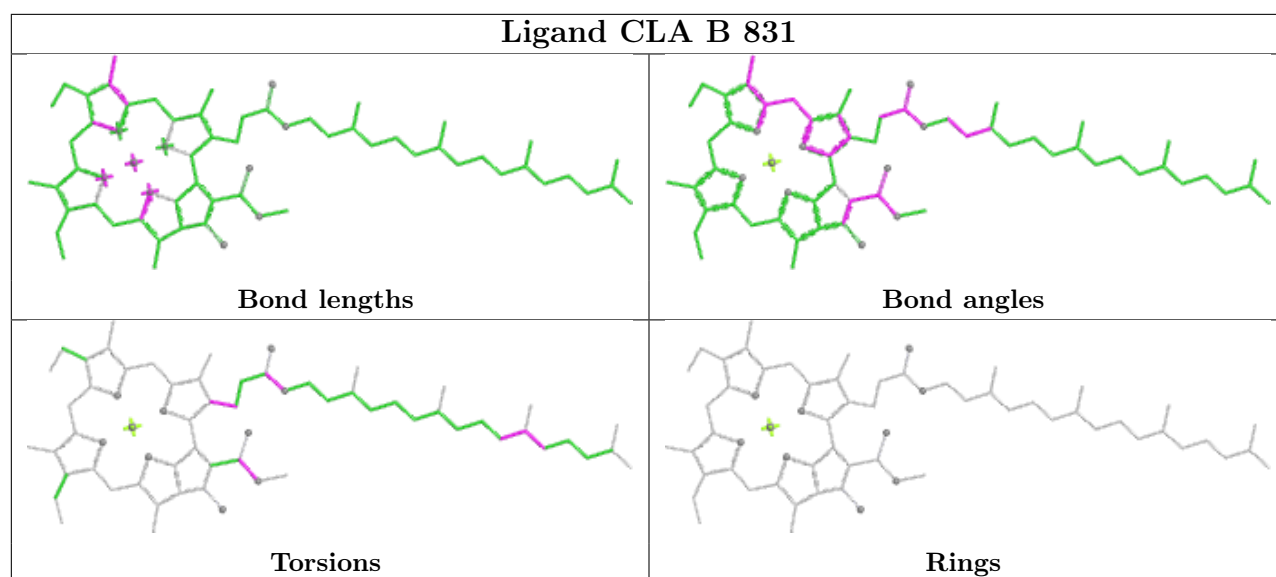
**Ligand CLA 4 312****Ligand CLA 1 308**

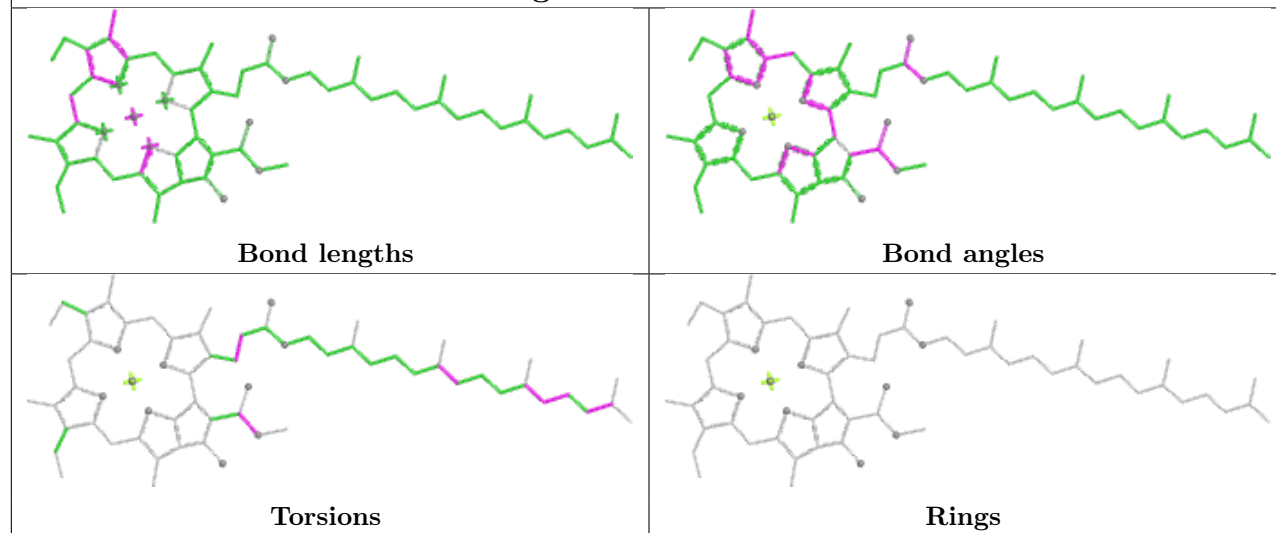
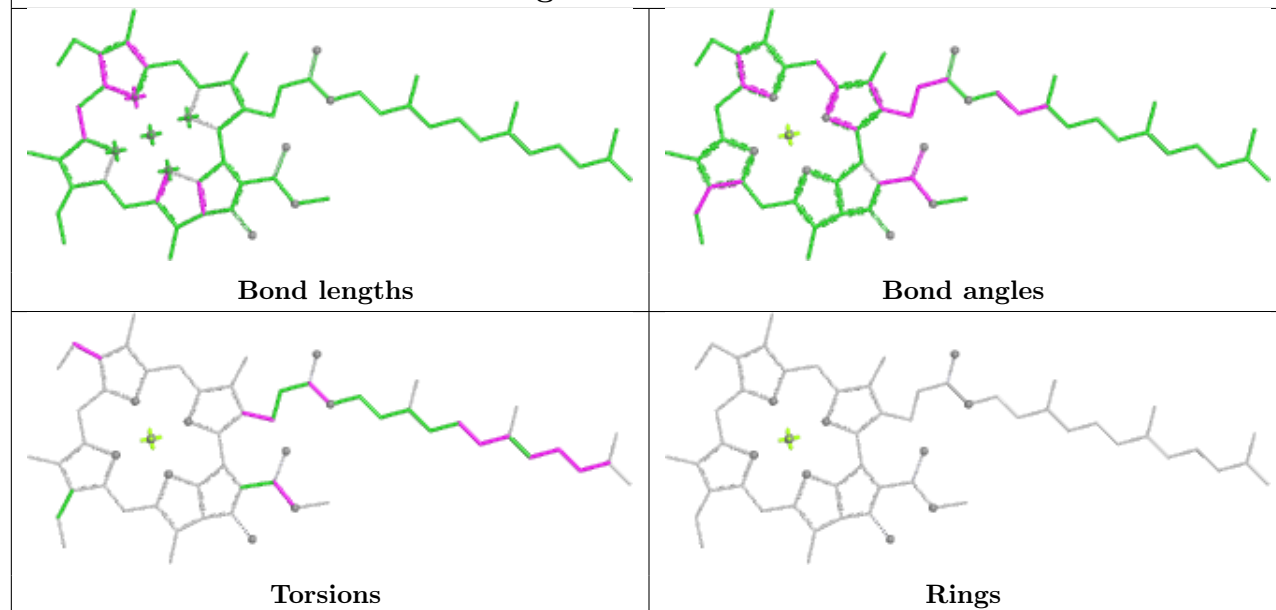
## Ligand CLA 1 313



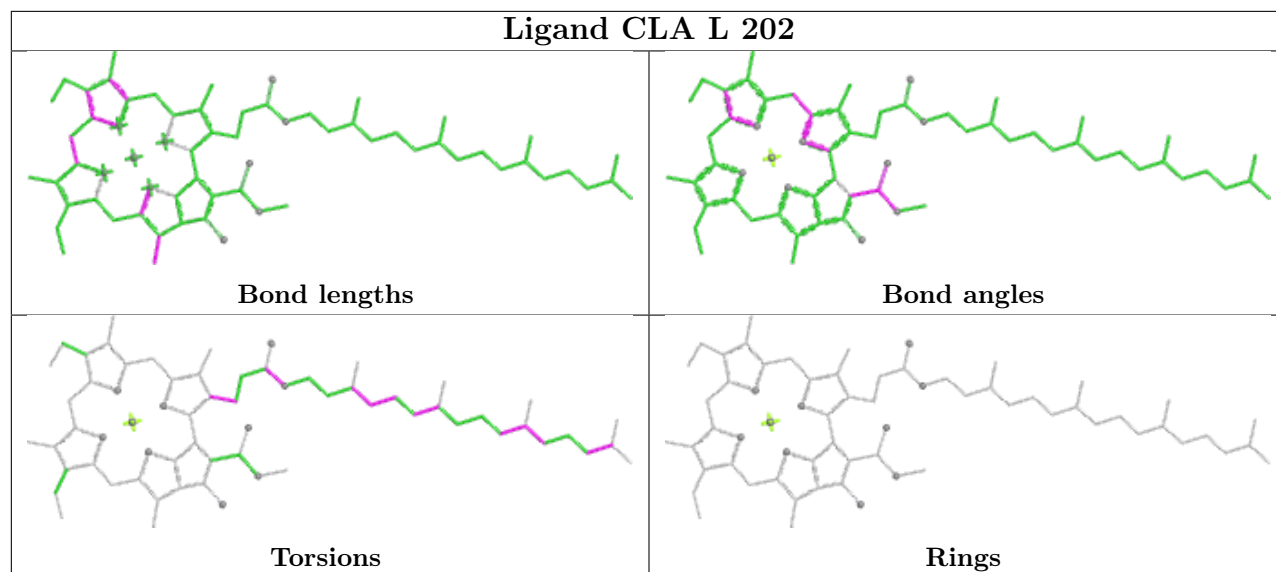
## Ligand BCR 2 316



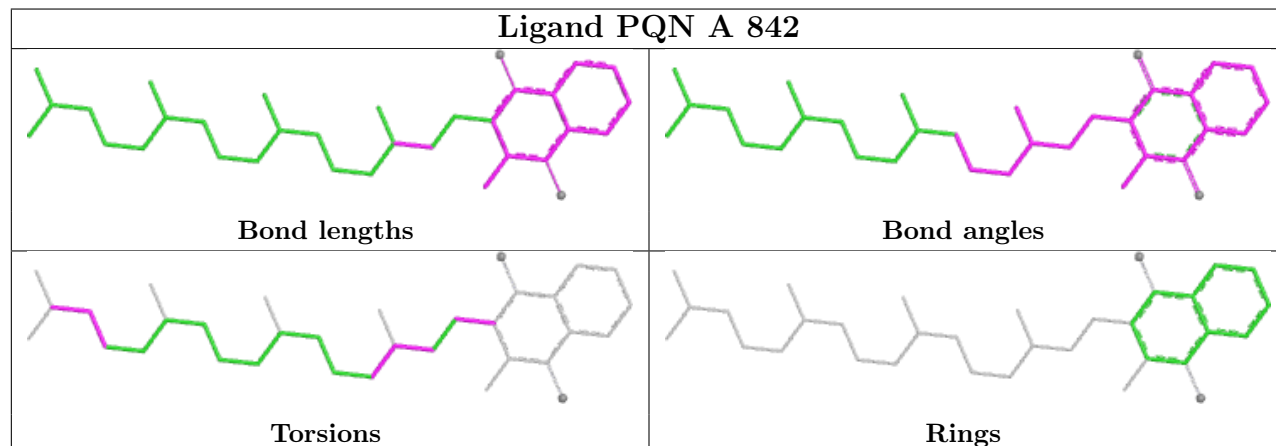


**Ligand CLA B 805****Ligand CLA 4 303**

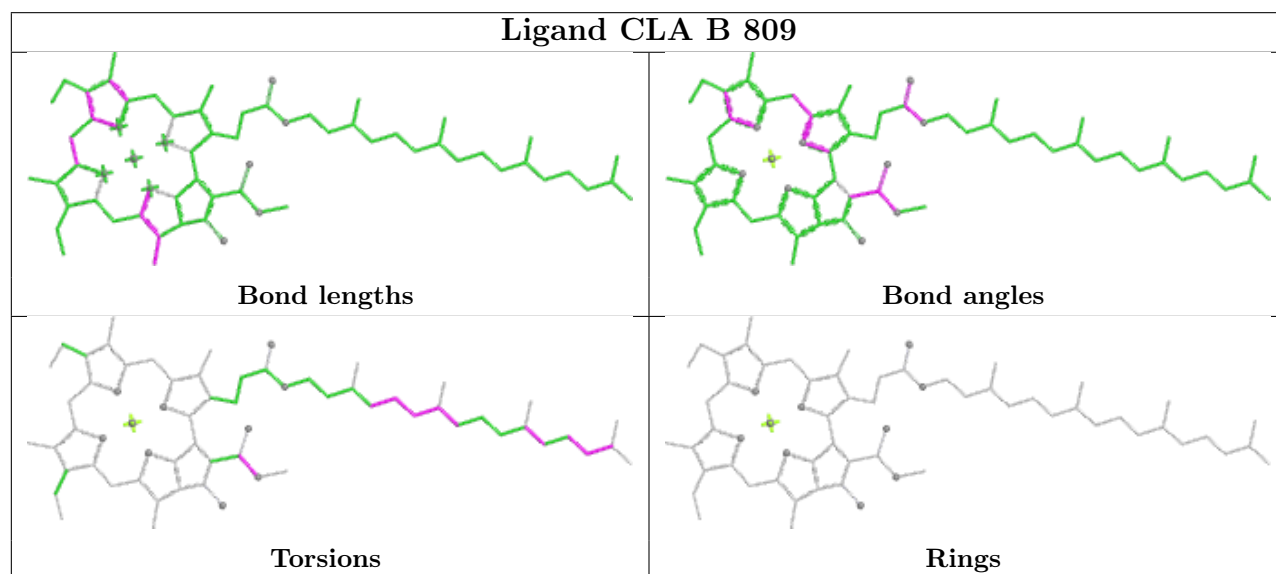
## Ligand CLA L 202



## Ligand PQN A 842

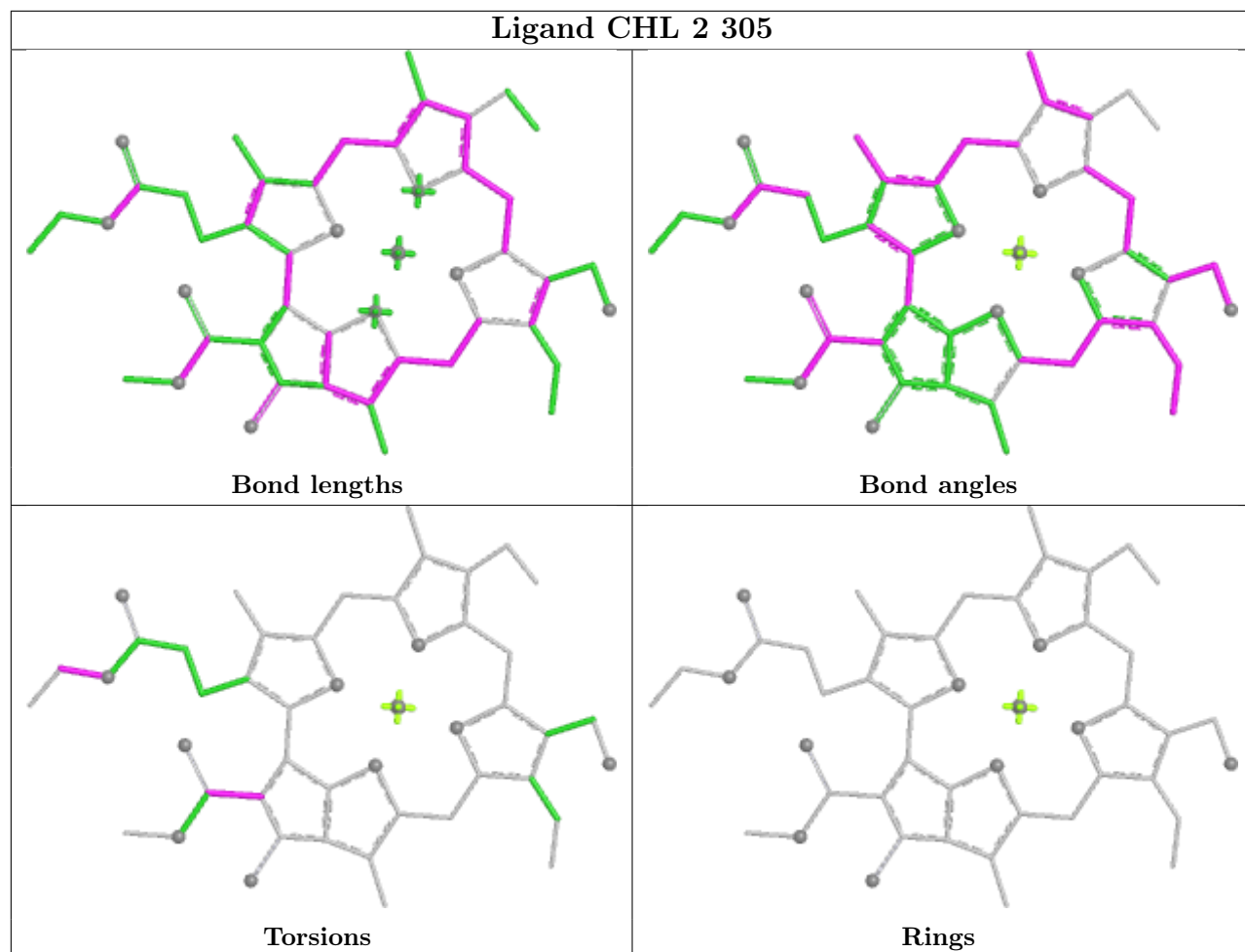


## Ligand CLA B 809

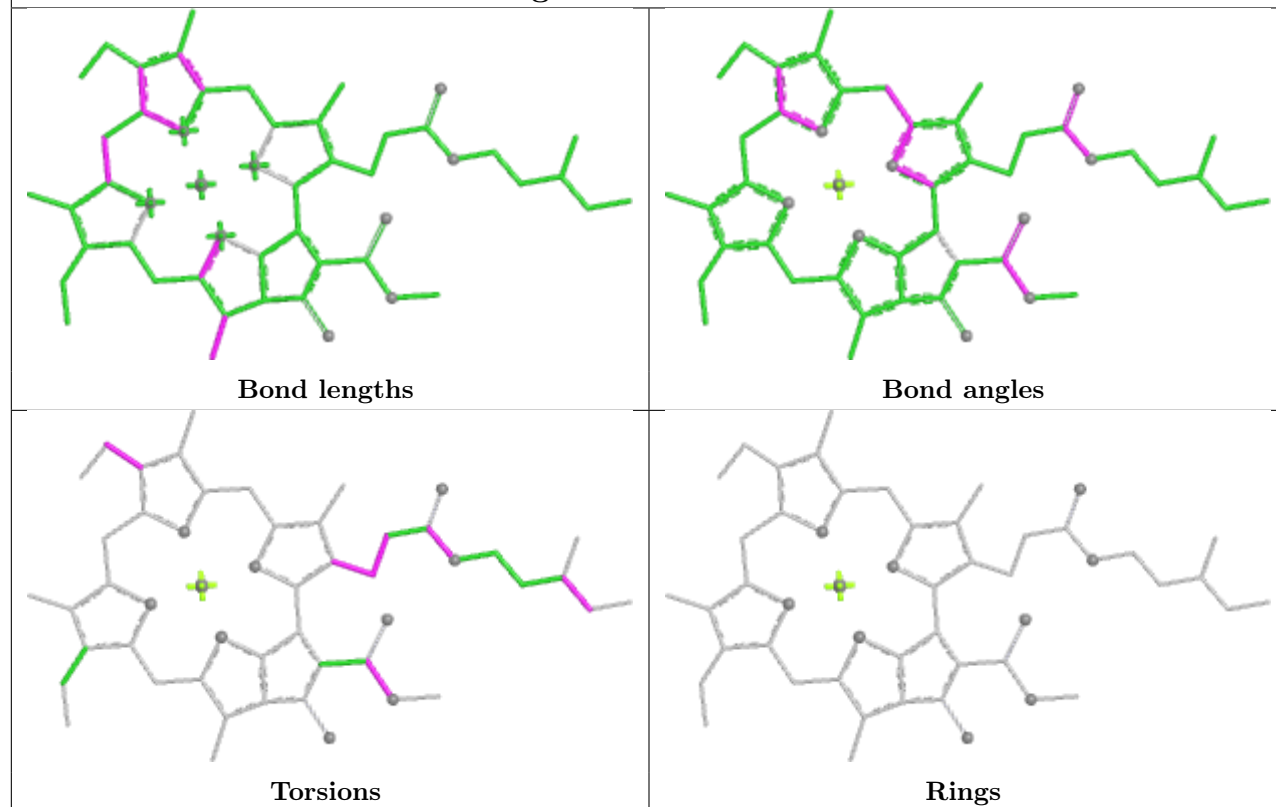




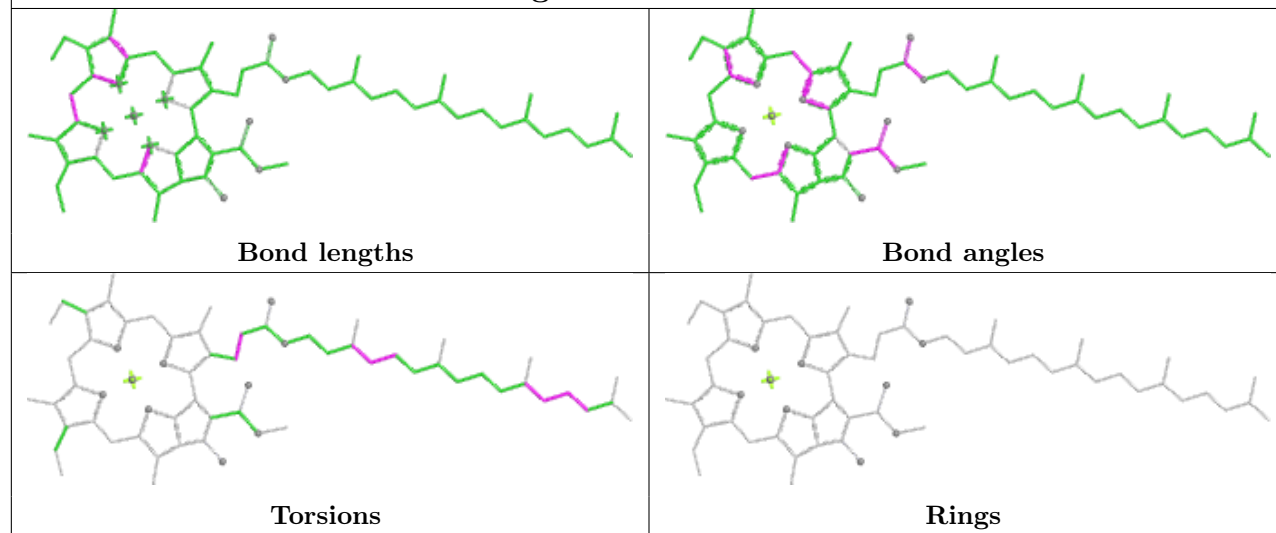
## Ligand CHL 2 305



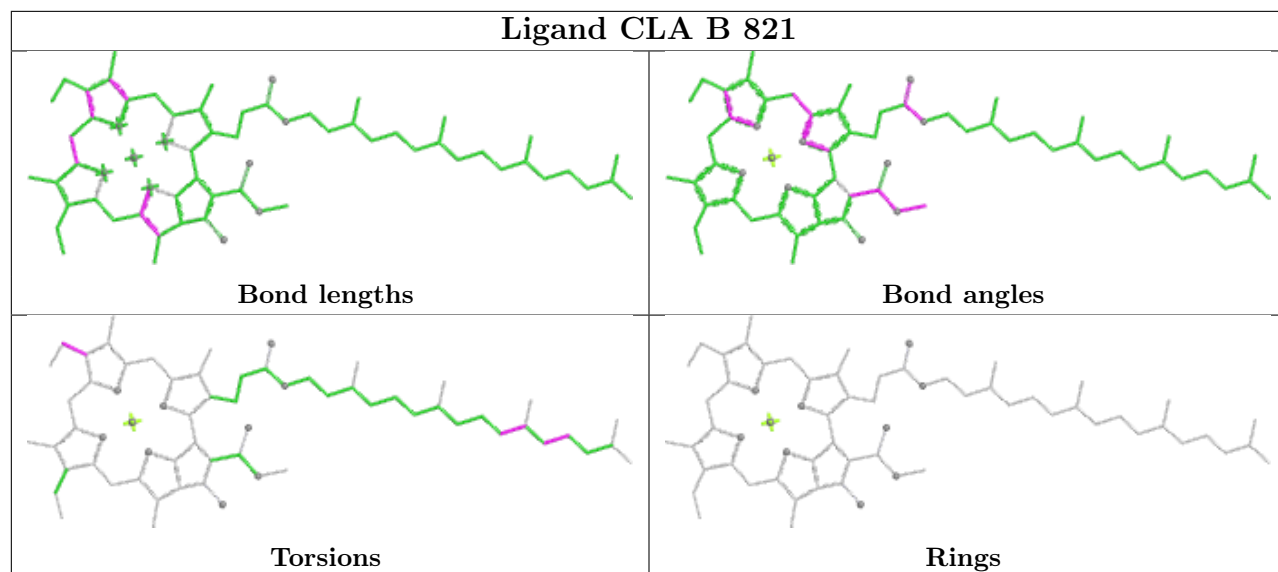
## Ligand CLA A 822



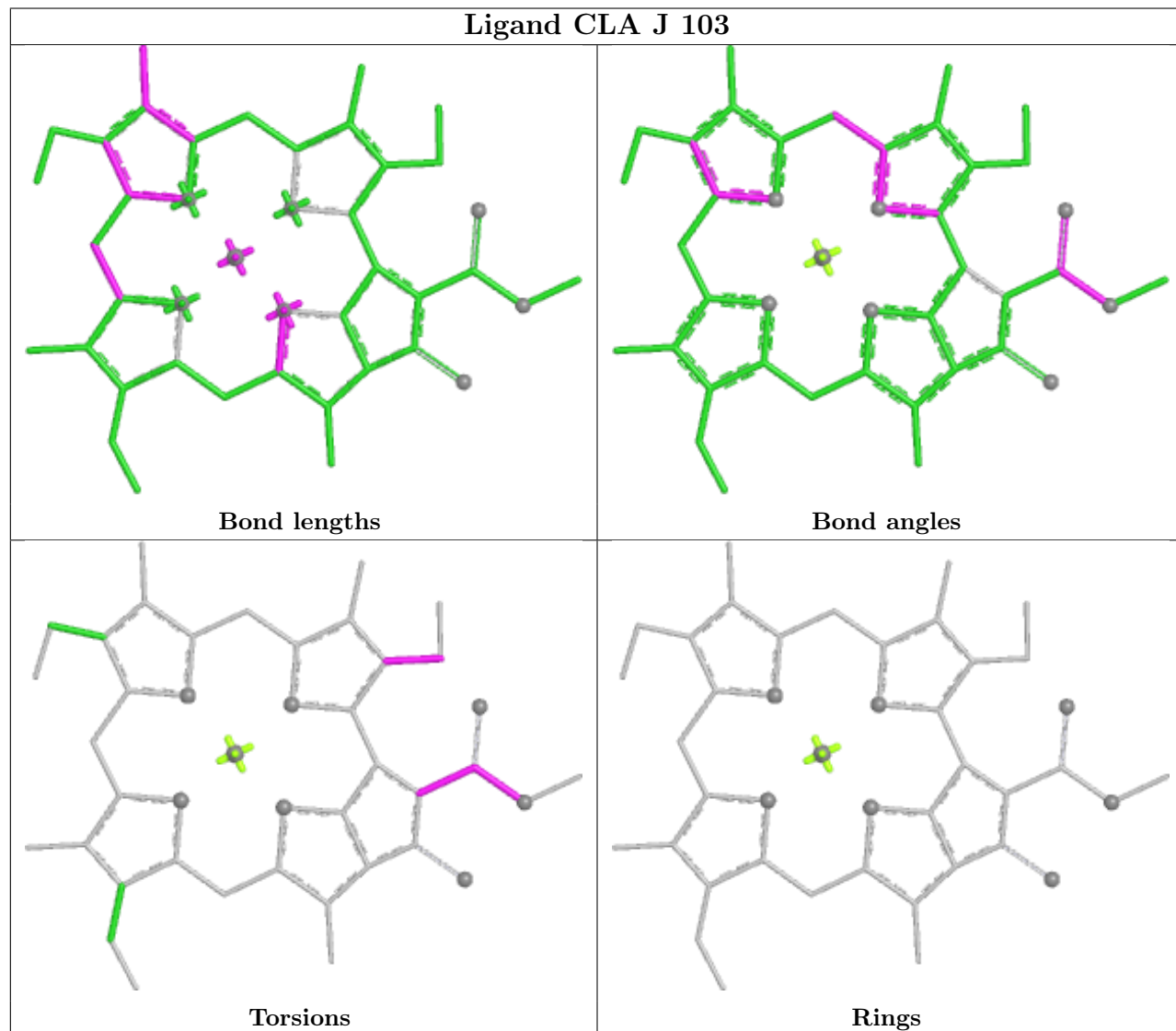
## Ligand CLA A 828



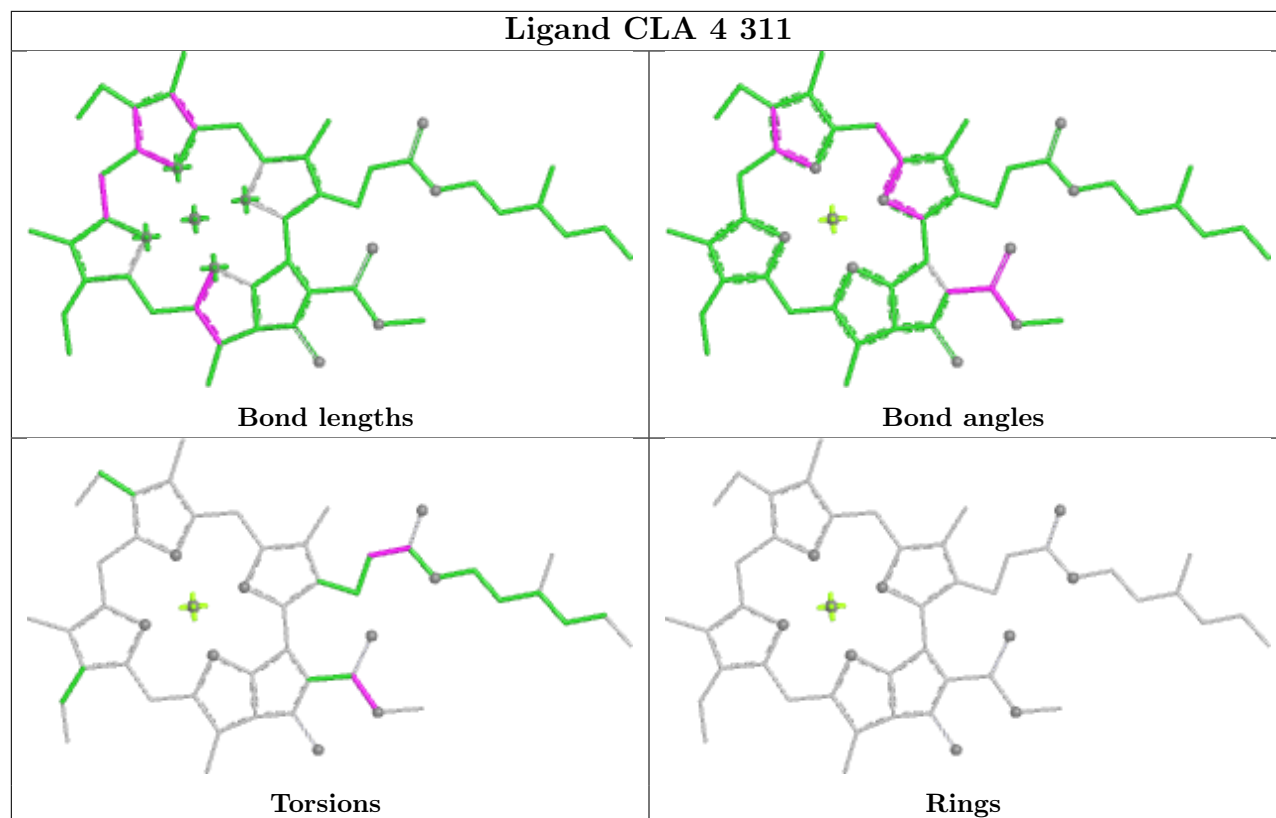
## Ligand CLA B 821



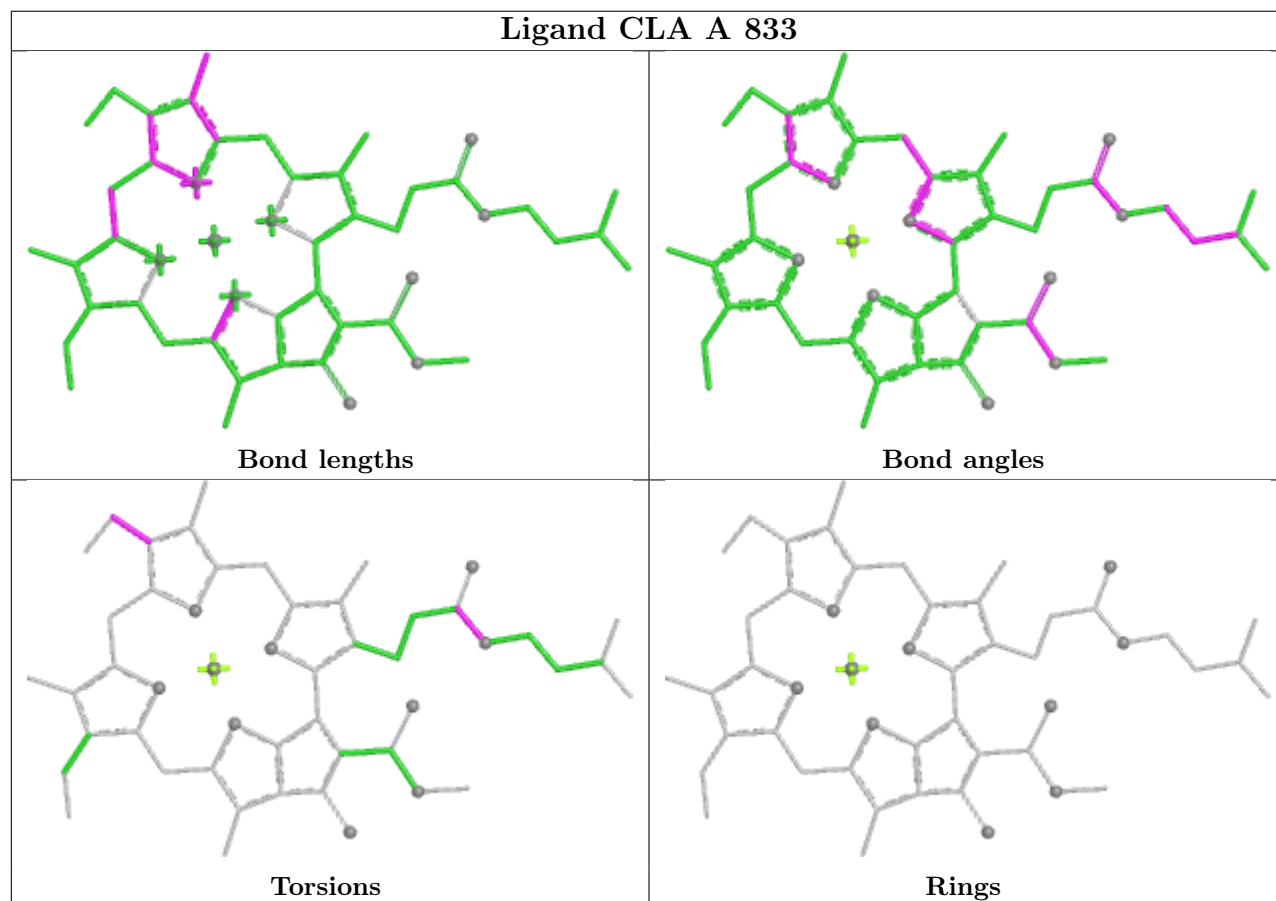
## Ligand CLA J 103



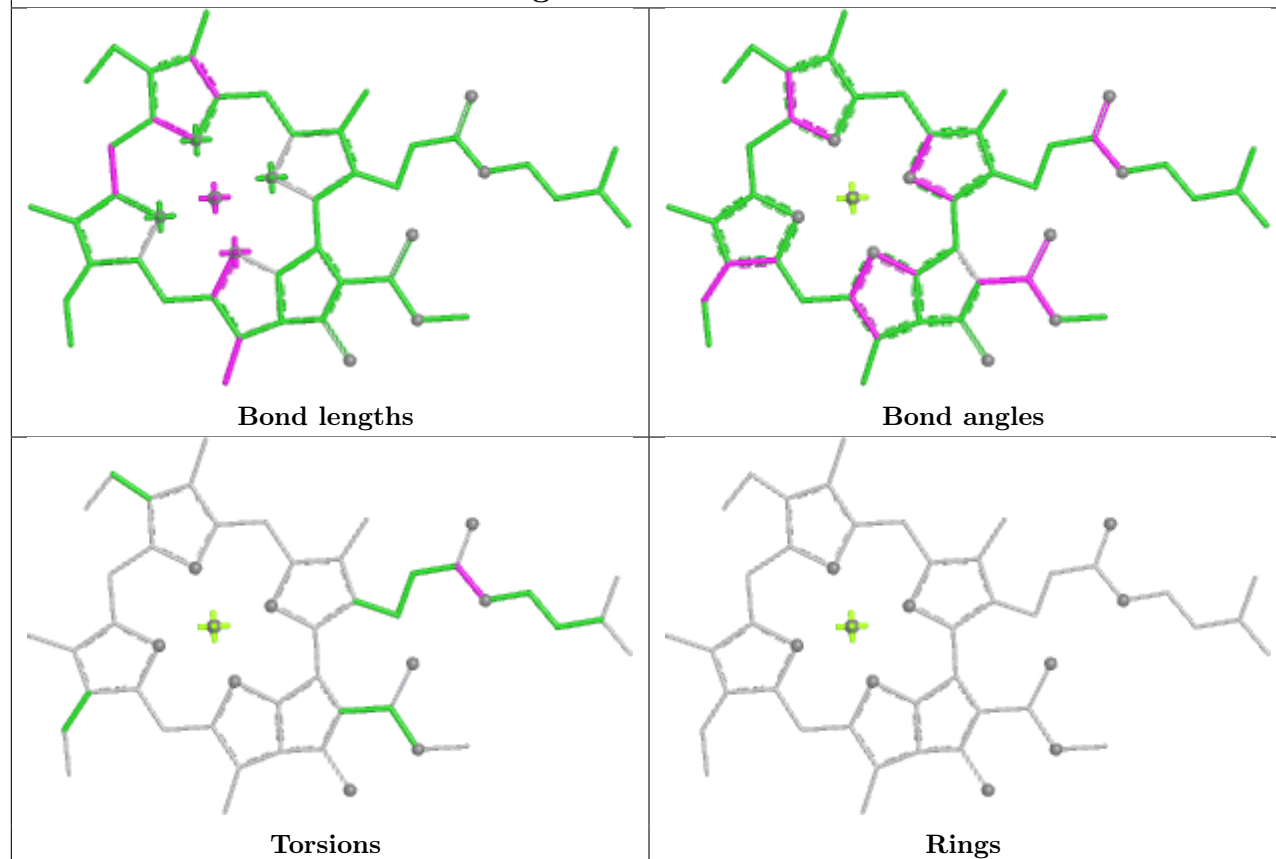
## Ligand CLA 4 311



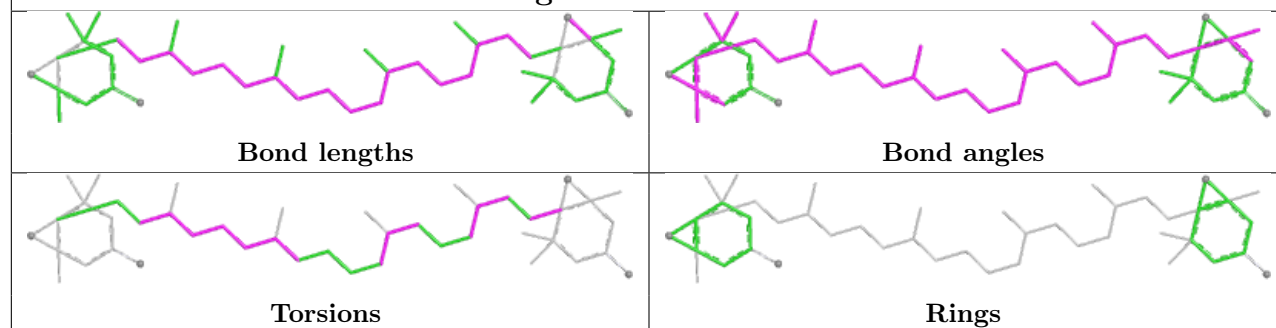
## Ligand CLA A 833

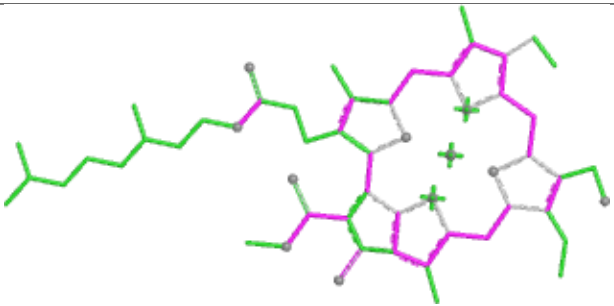
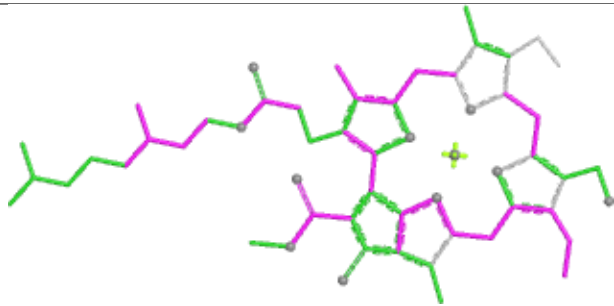
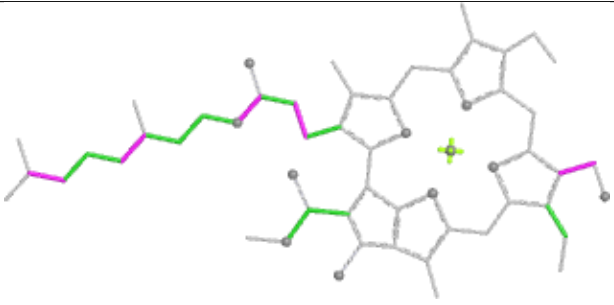
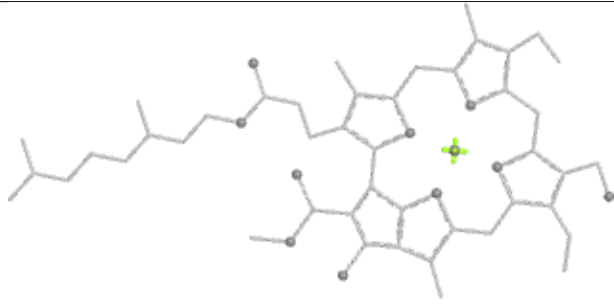


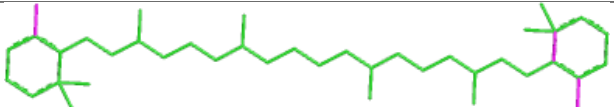
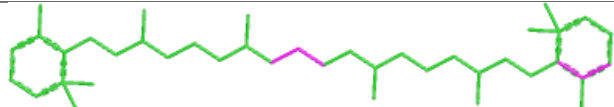
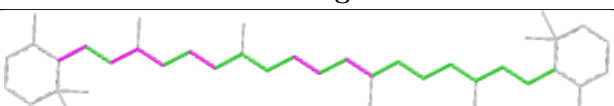
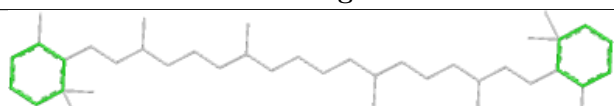
## Ligand CLA B 832

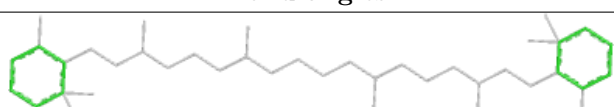


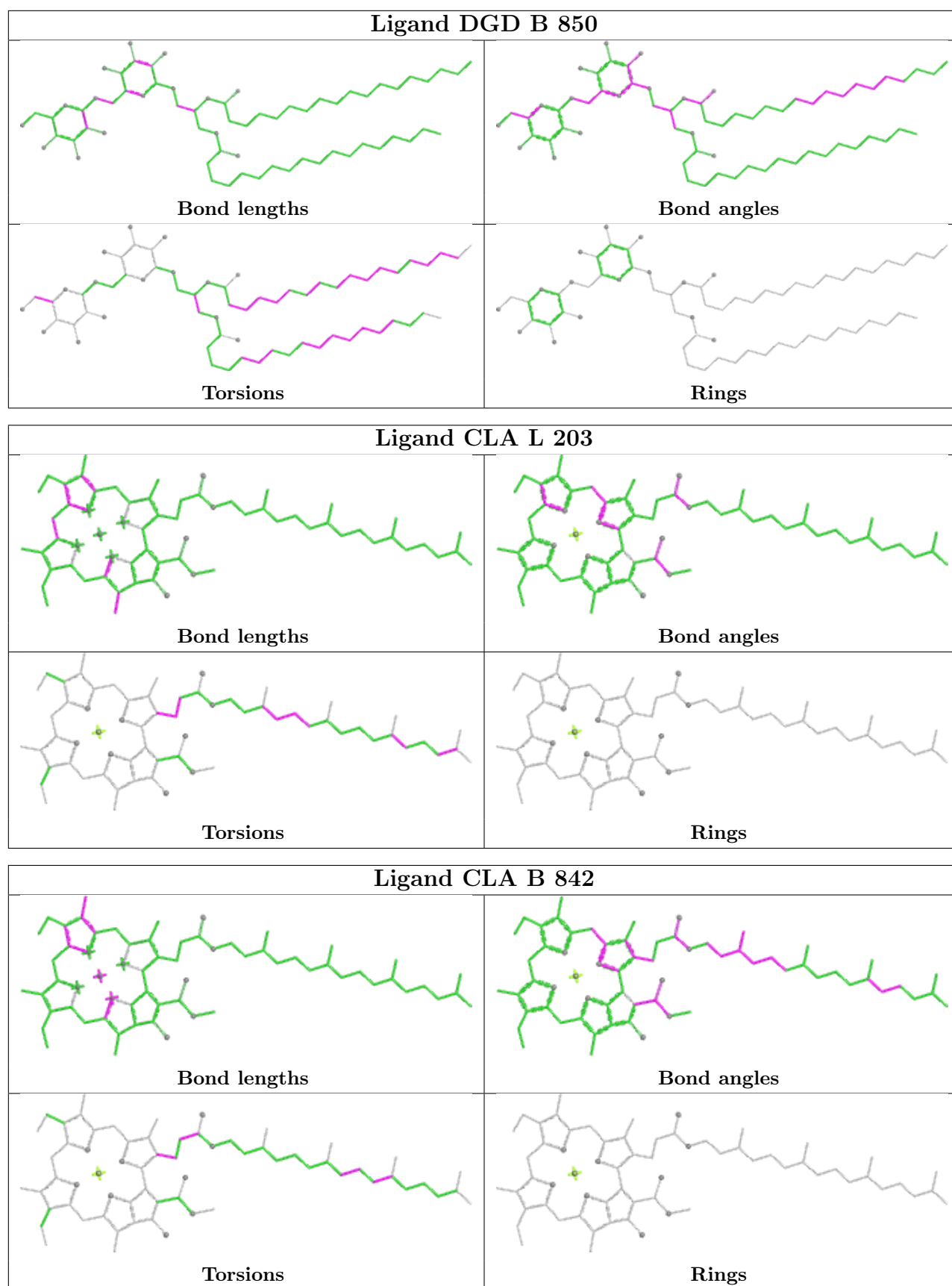
## Ligand XAT 1 315

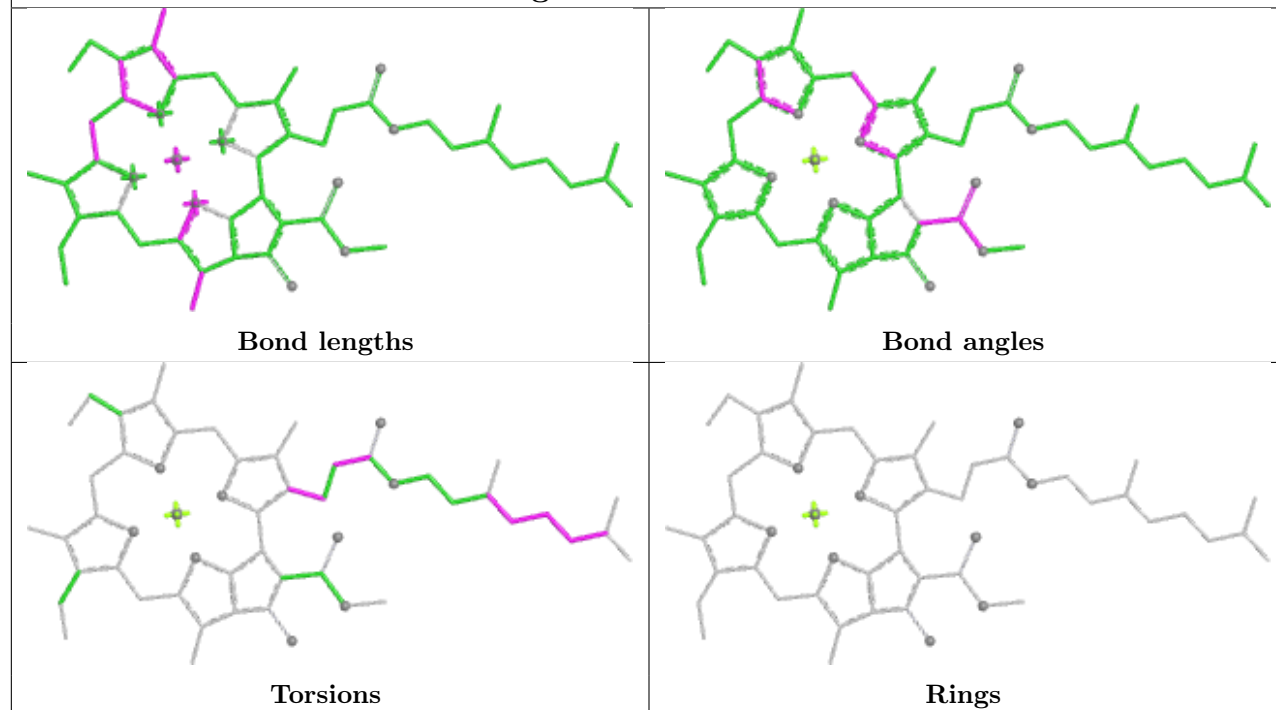
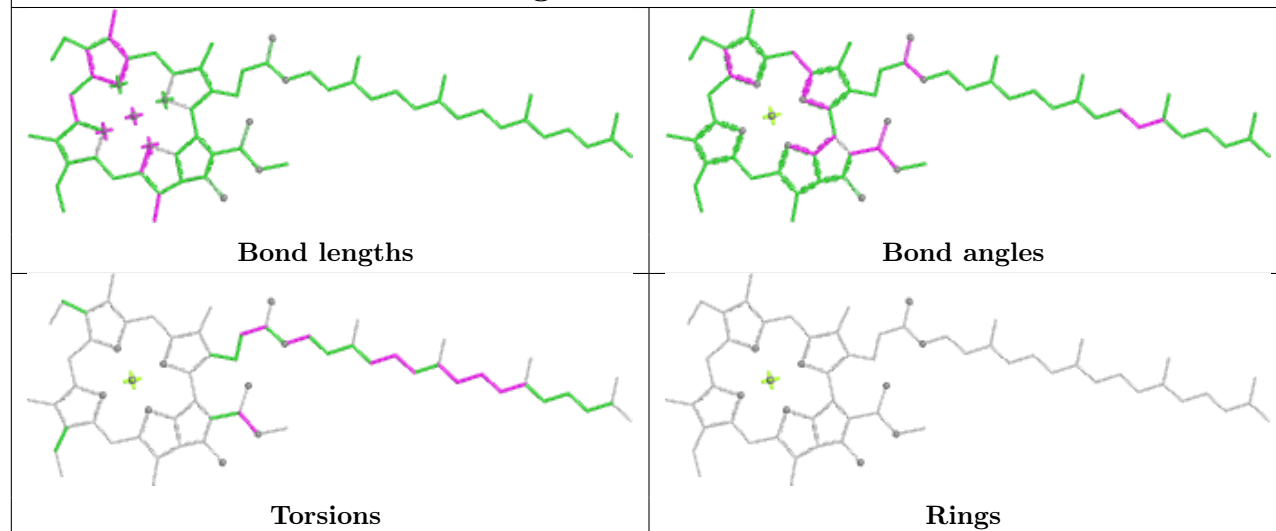


| Ligand CHL 4 305                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

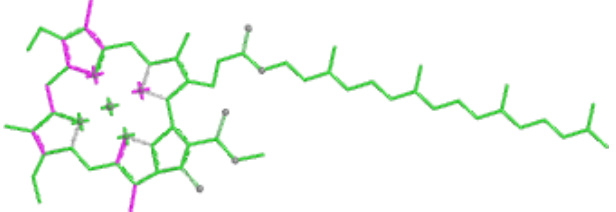
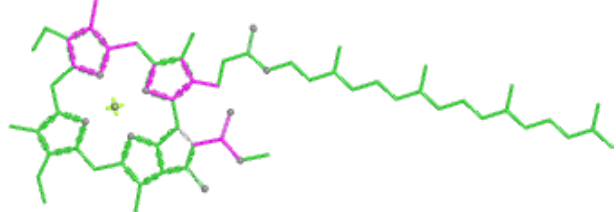
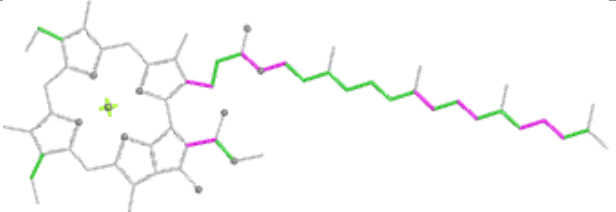
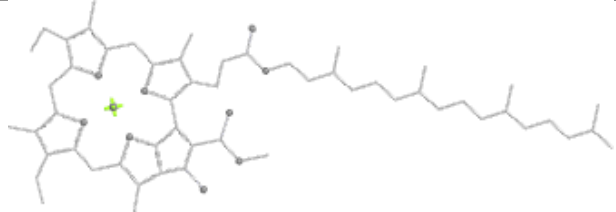
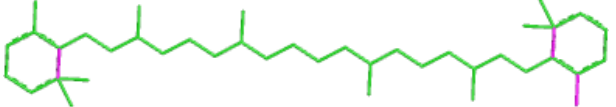
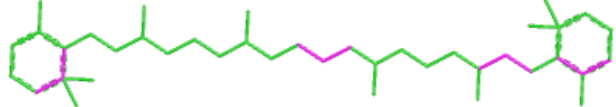
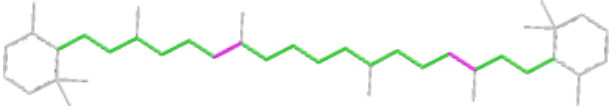
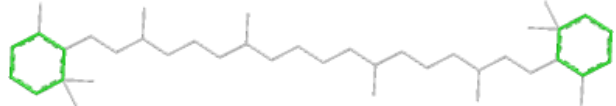
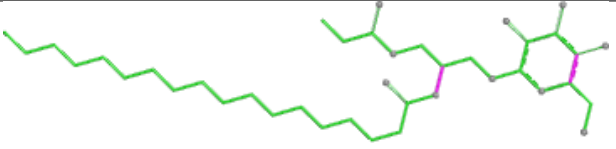
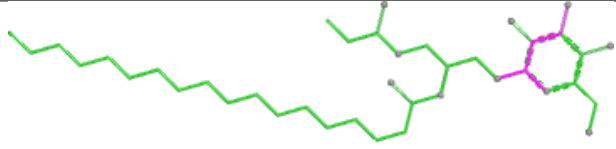
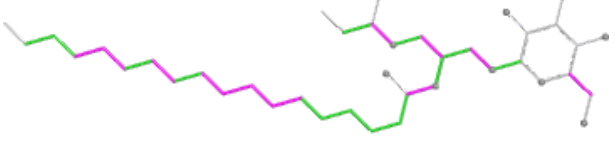
| Ligand BCR B 849                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

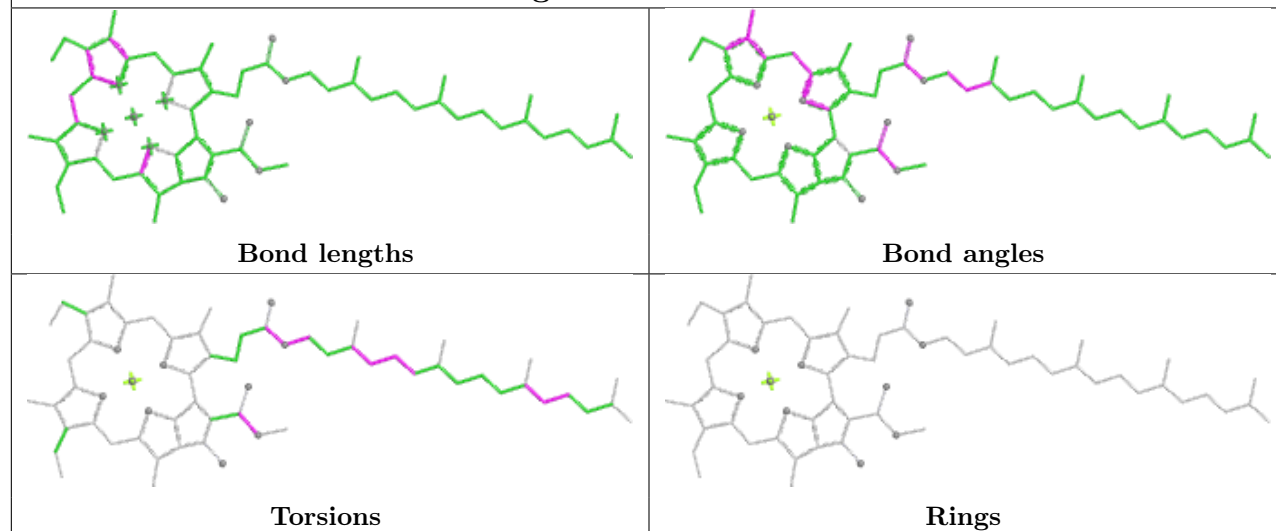
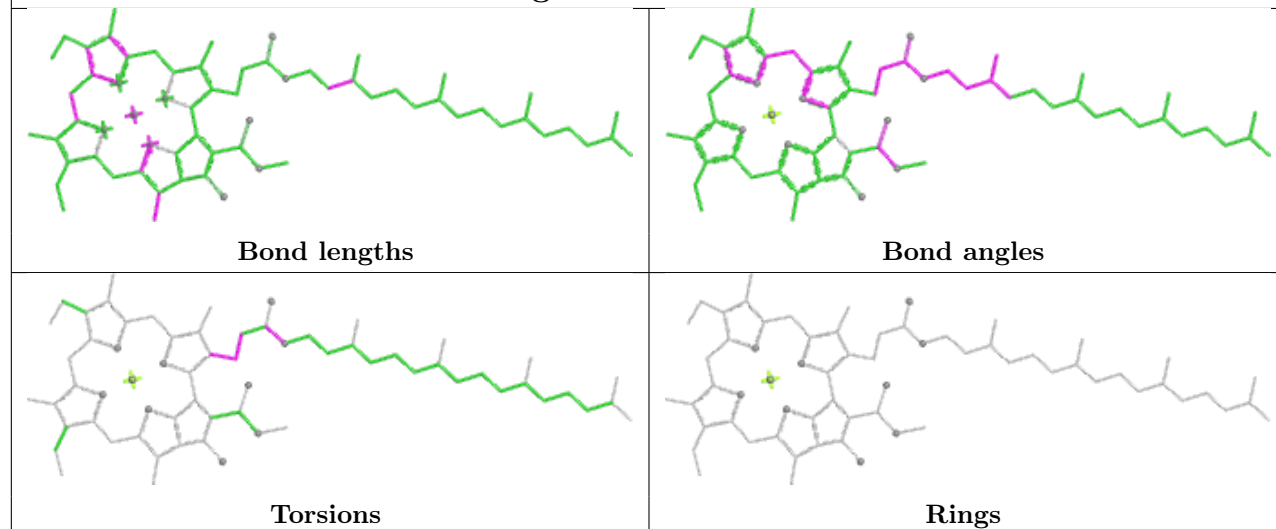
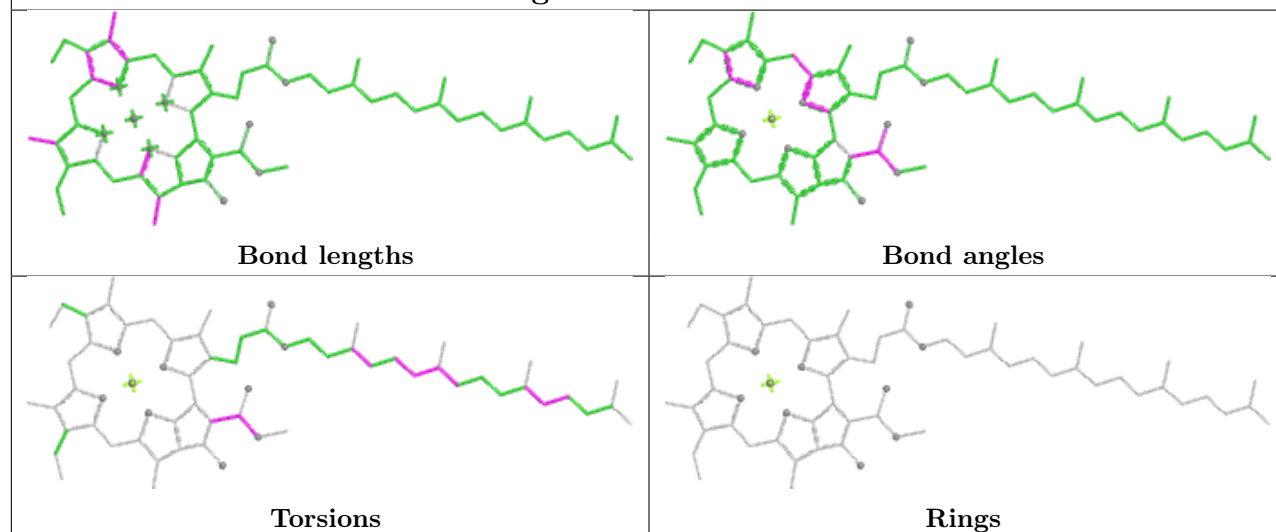
| Ligand BCR G 106                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



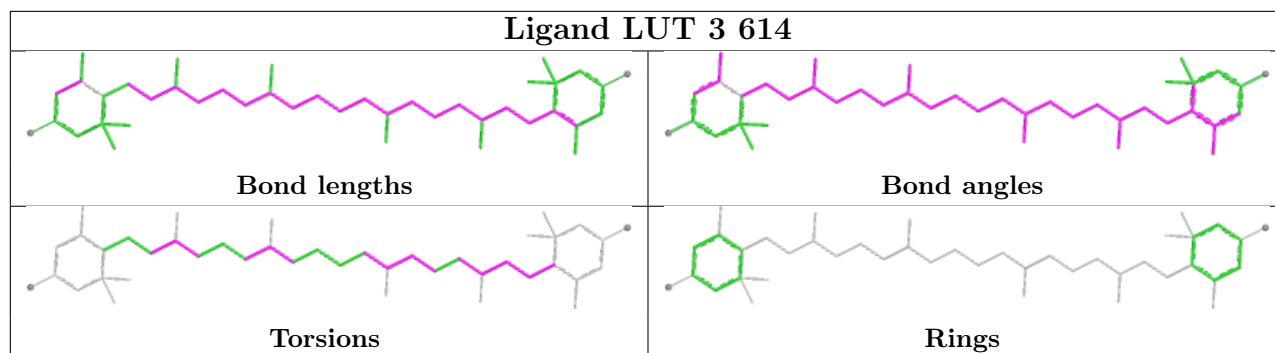
**Ligand CLA A 803****Ligand CLA B 808**



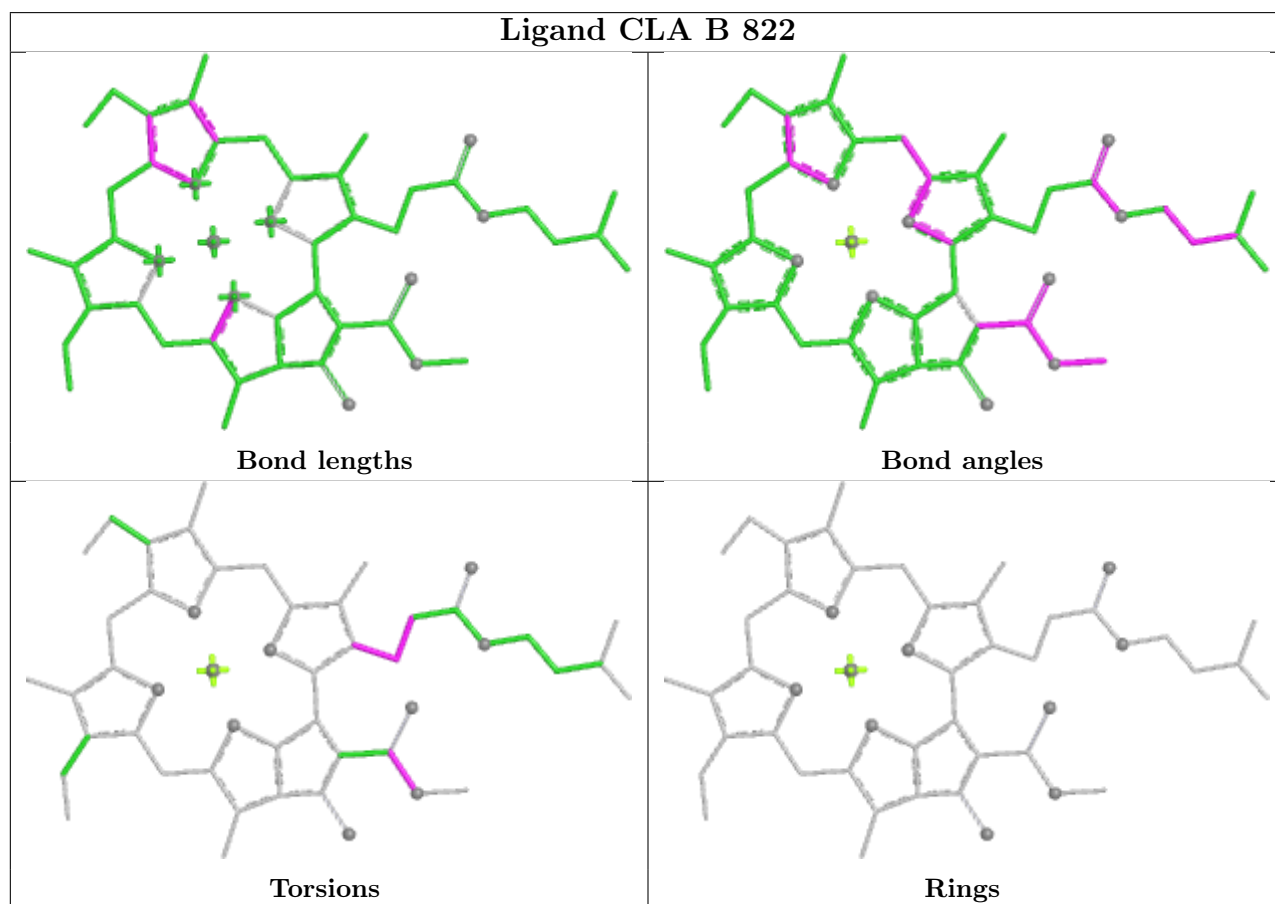
| Ligand CLA B 807                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR J 104                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand LMG G 101                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

**Ligand CLA B 823****Ligand CLA B 830****Ligand CLA A 829**

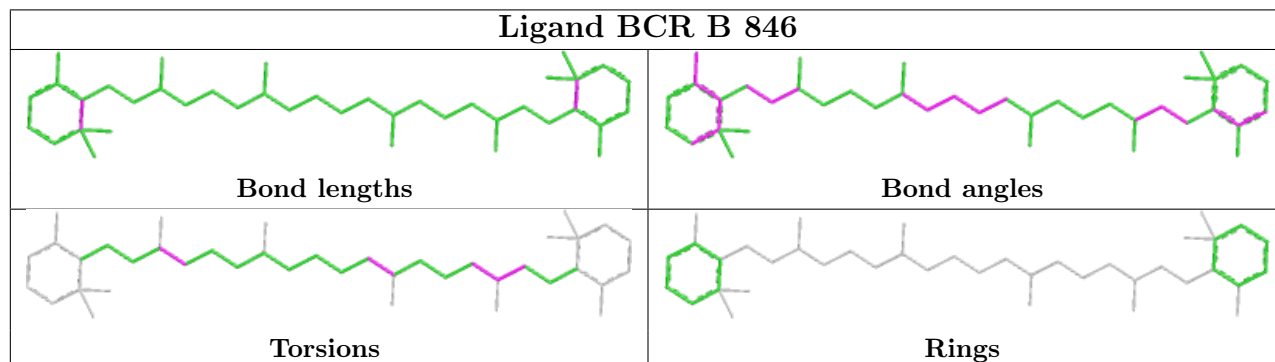
## Ligand LUT 3 614



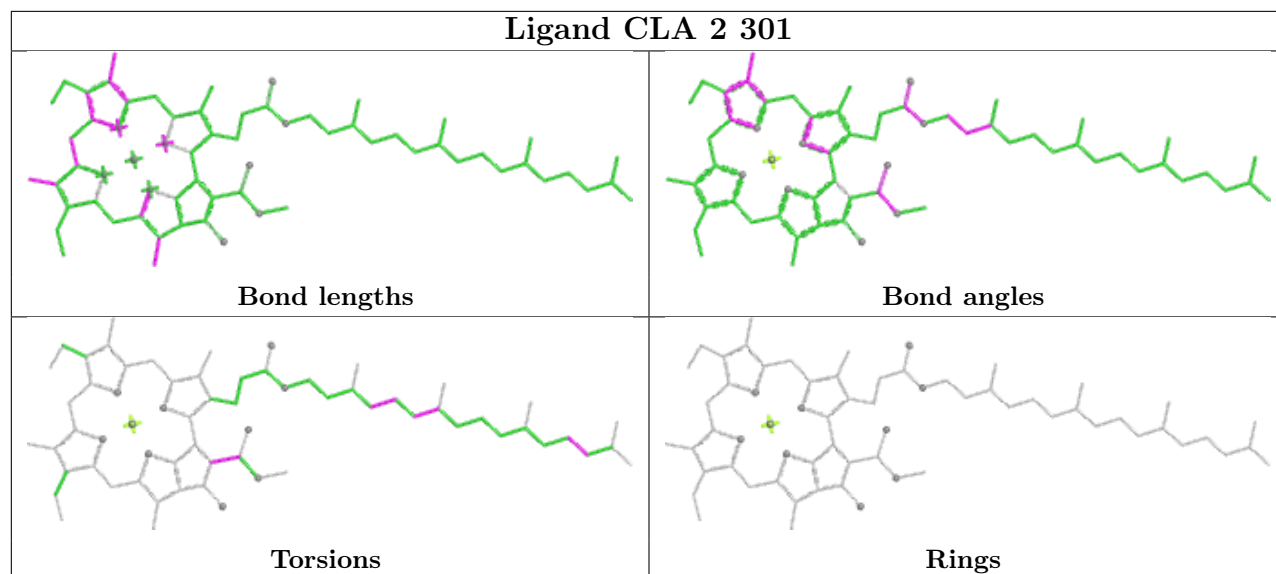
## Ligand CLA B 822



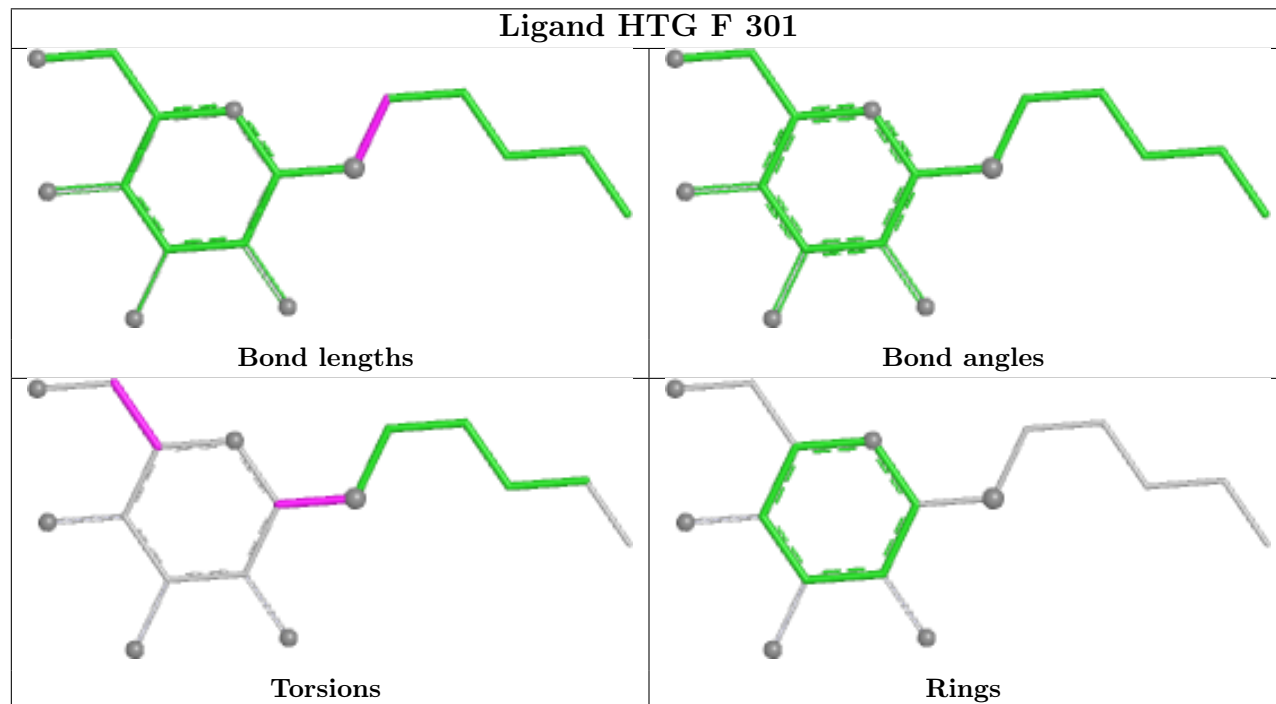
## Ligand BCR B 846

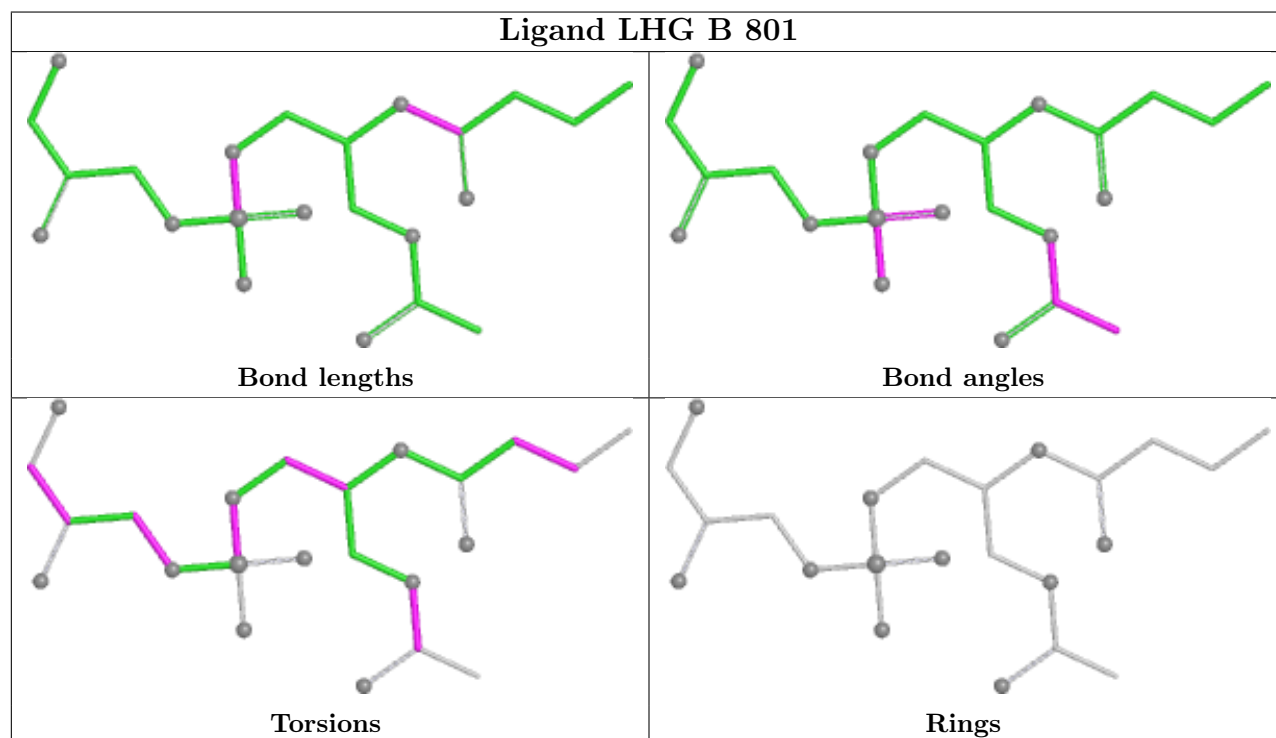
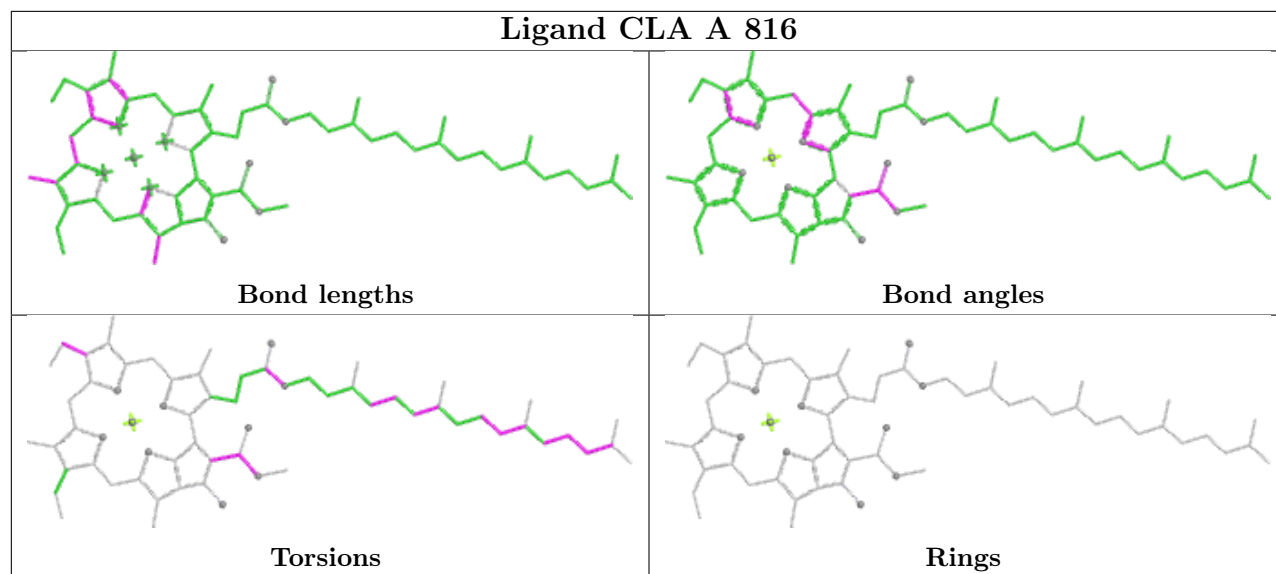


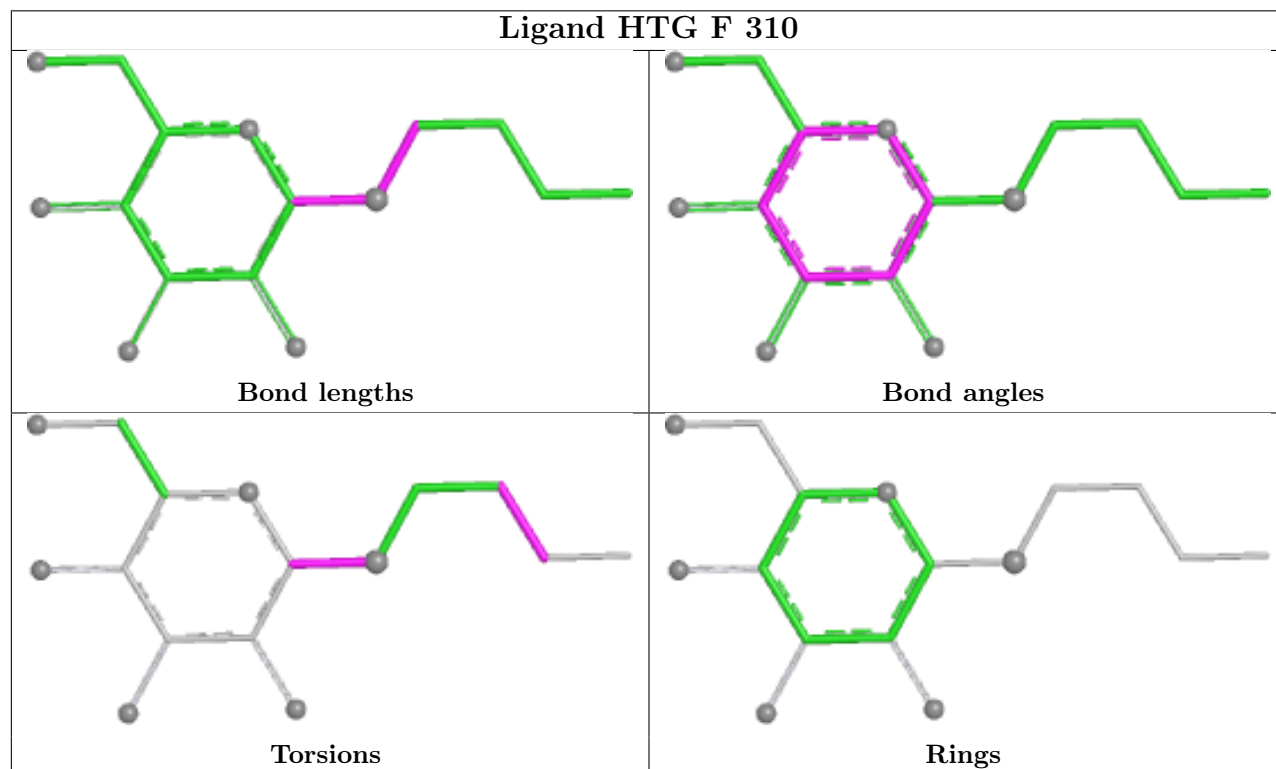
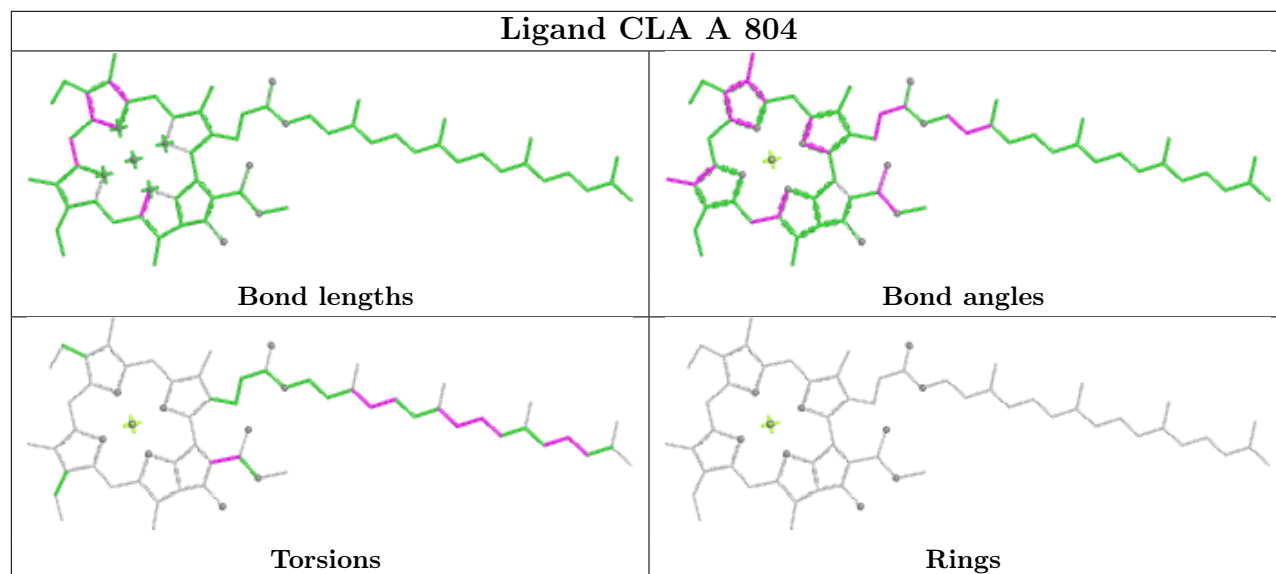
## Ligand CLA 2 301

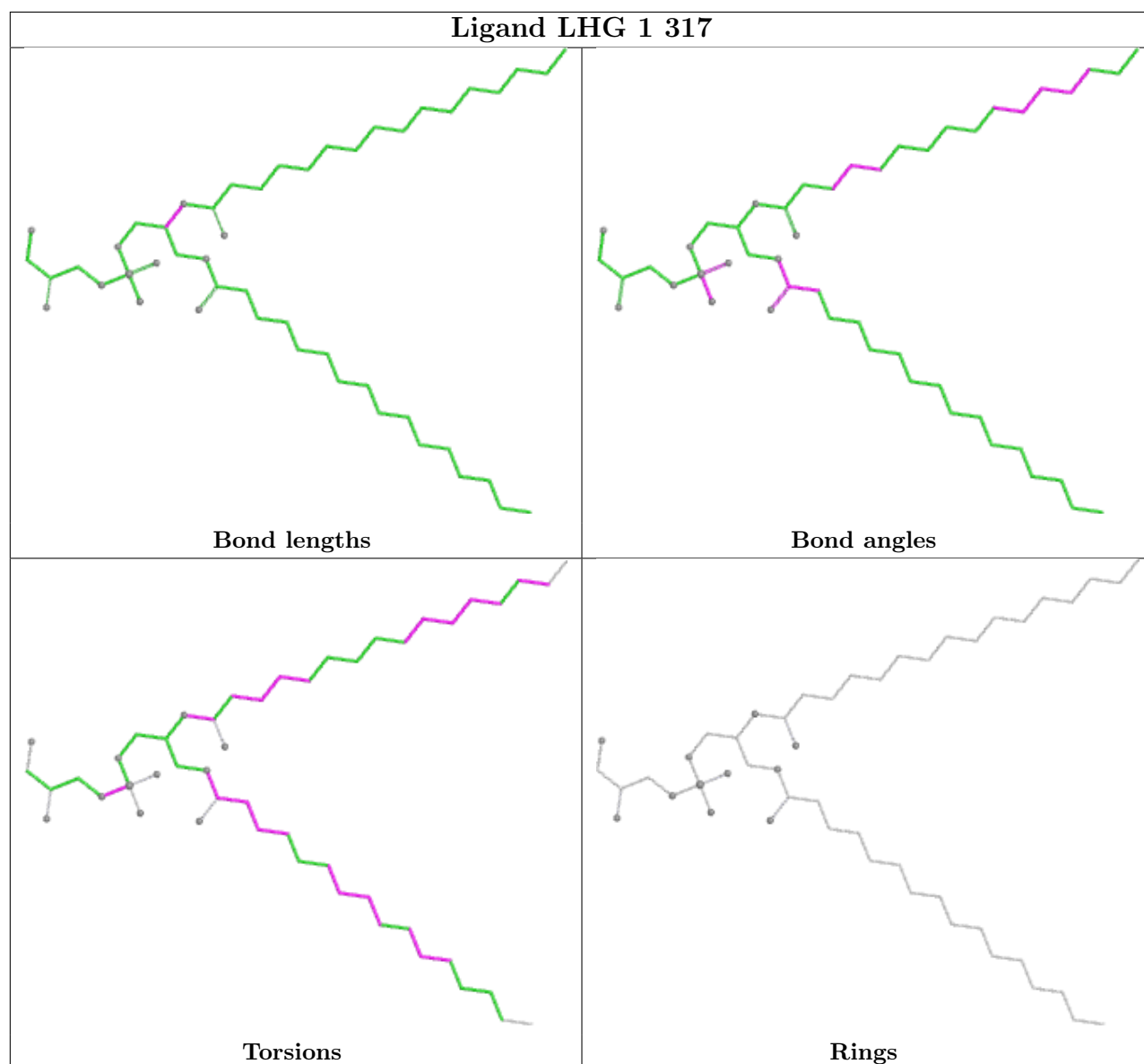
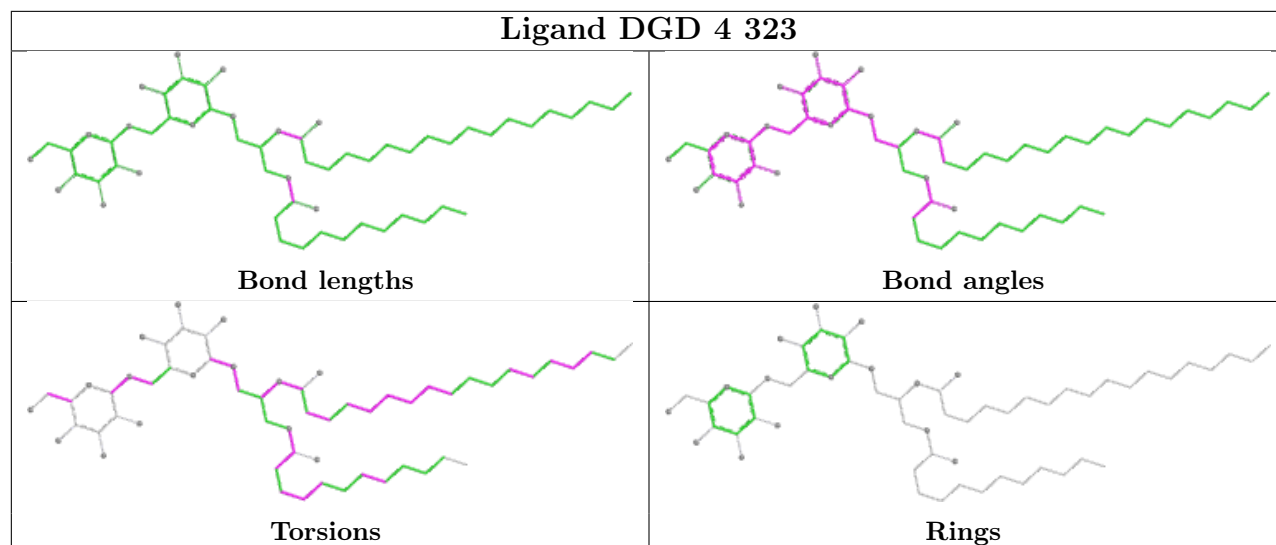


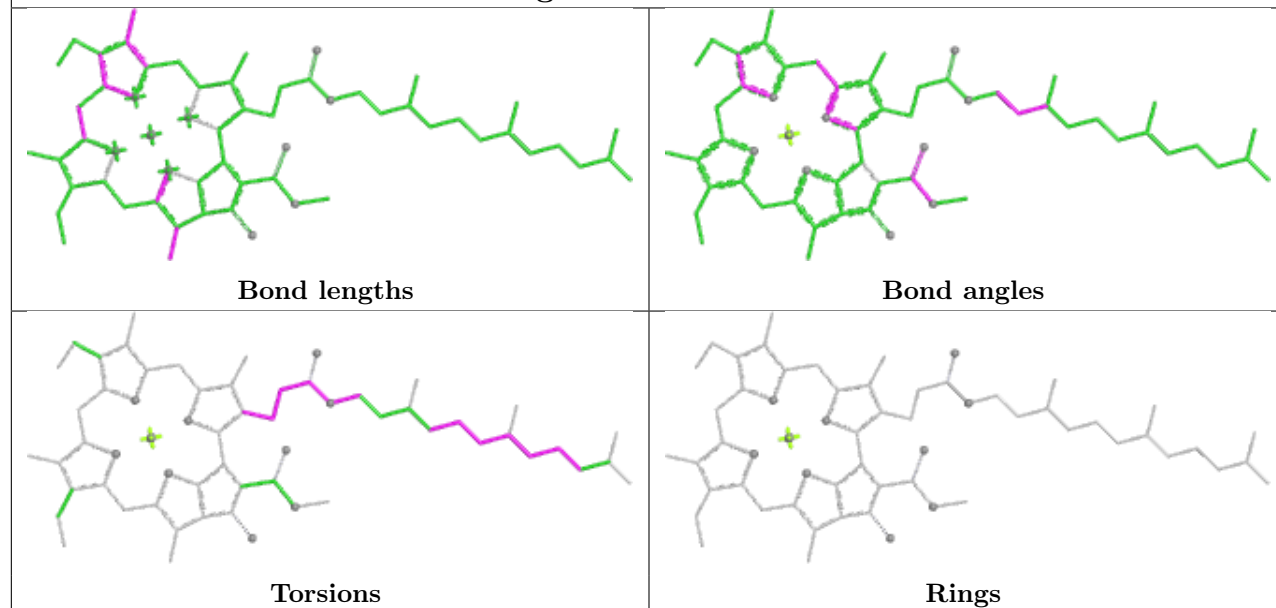
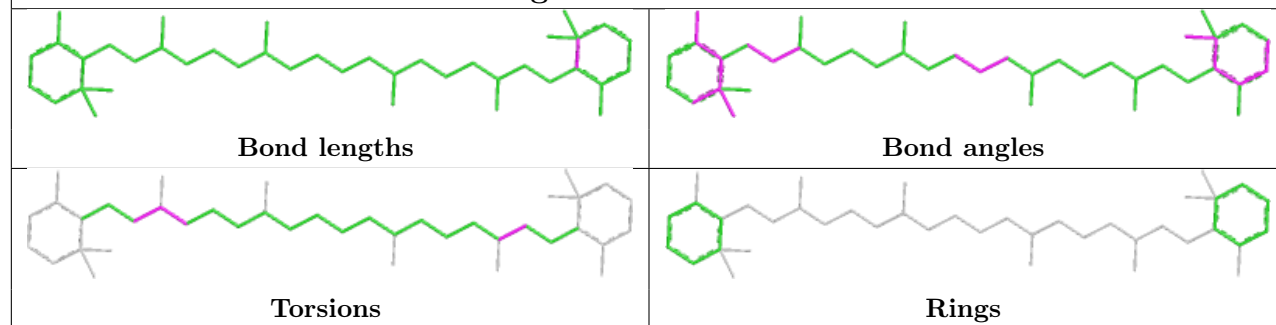
## Ligand HTG F 301





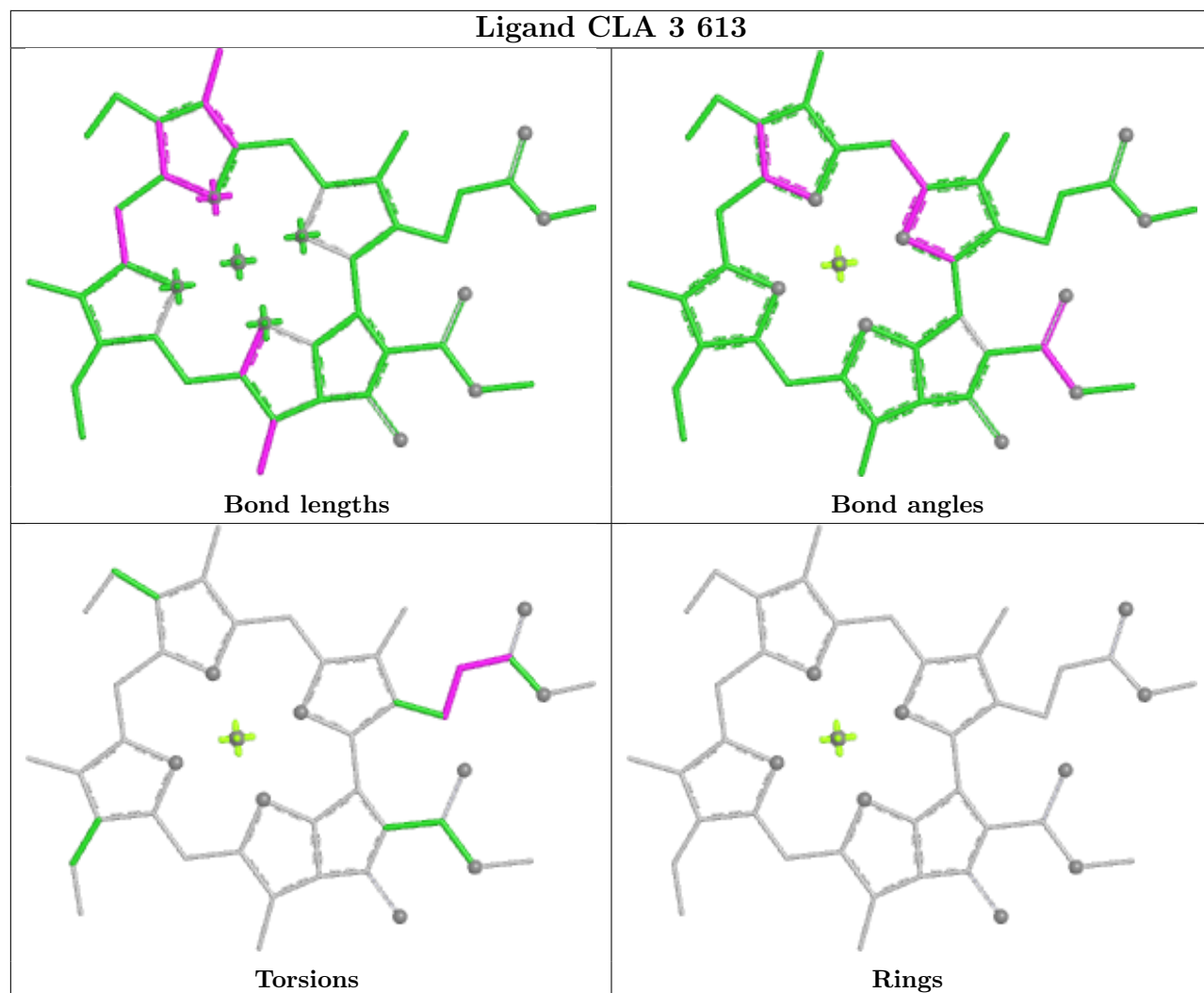




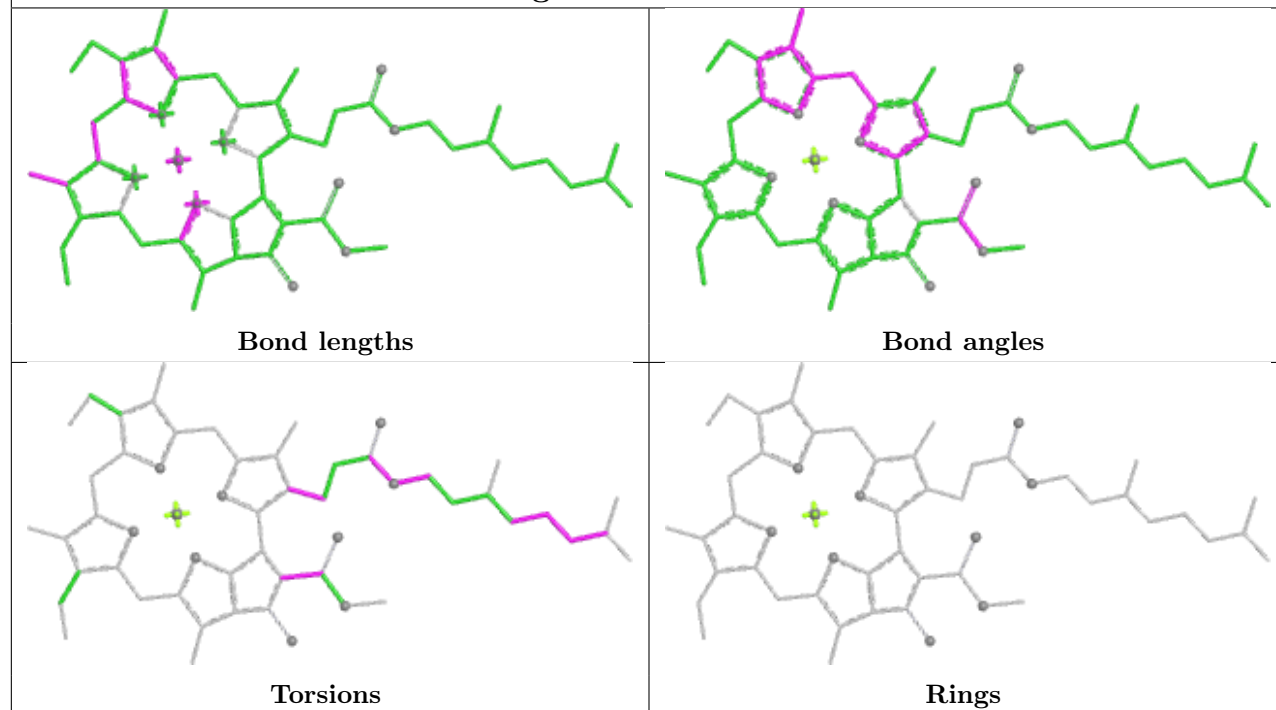
**Ligand CLA 2 303****Ligand BCR B 845**



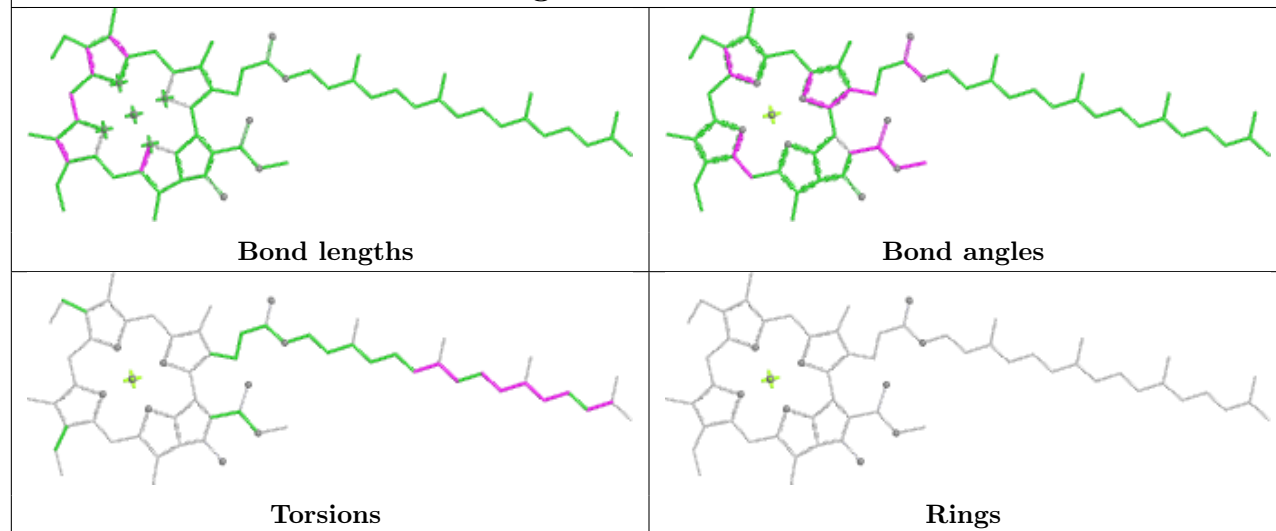
## Ligand CLA 3 613



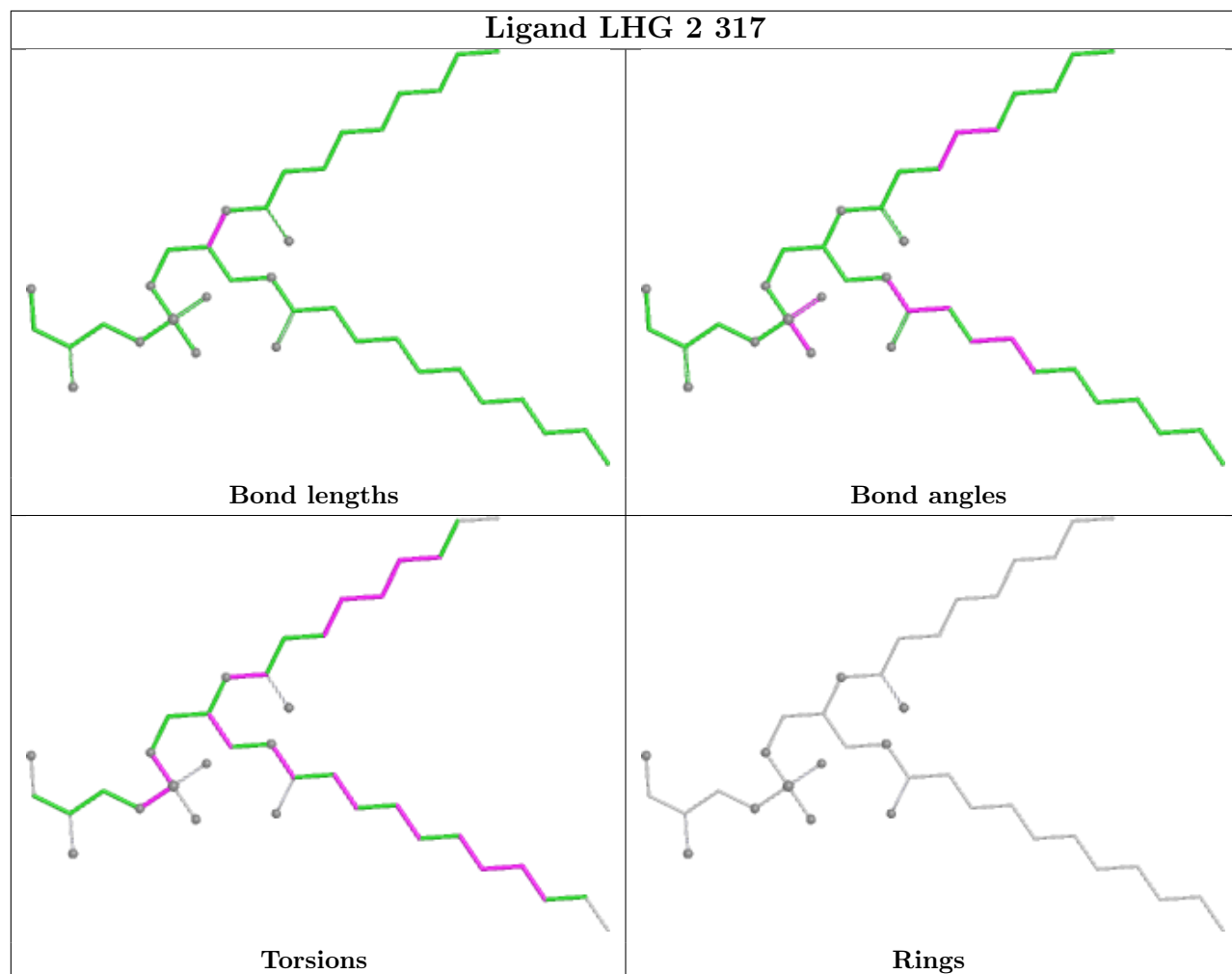
## Ligand CLA B 817



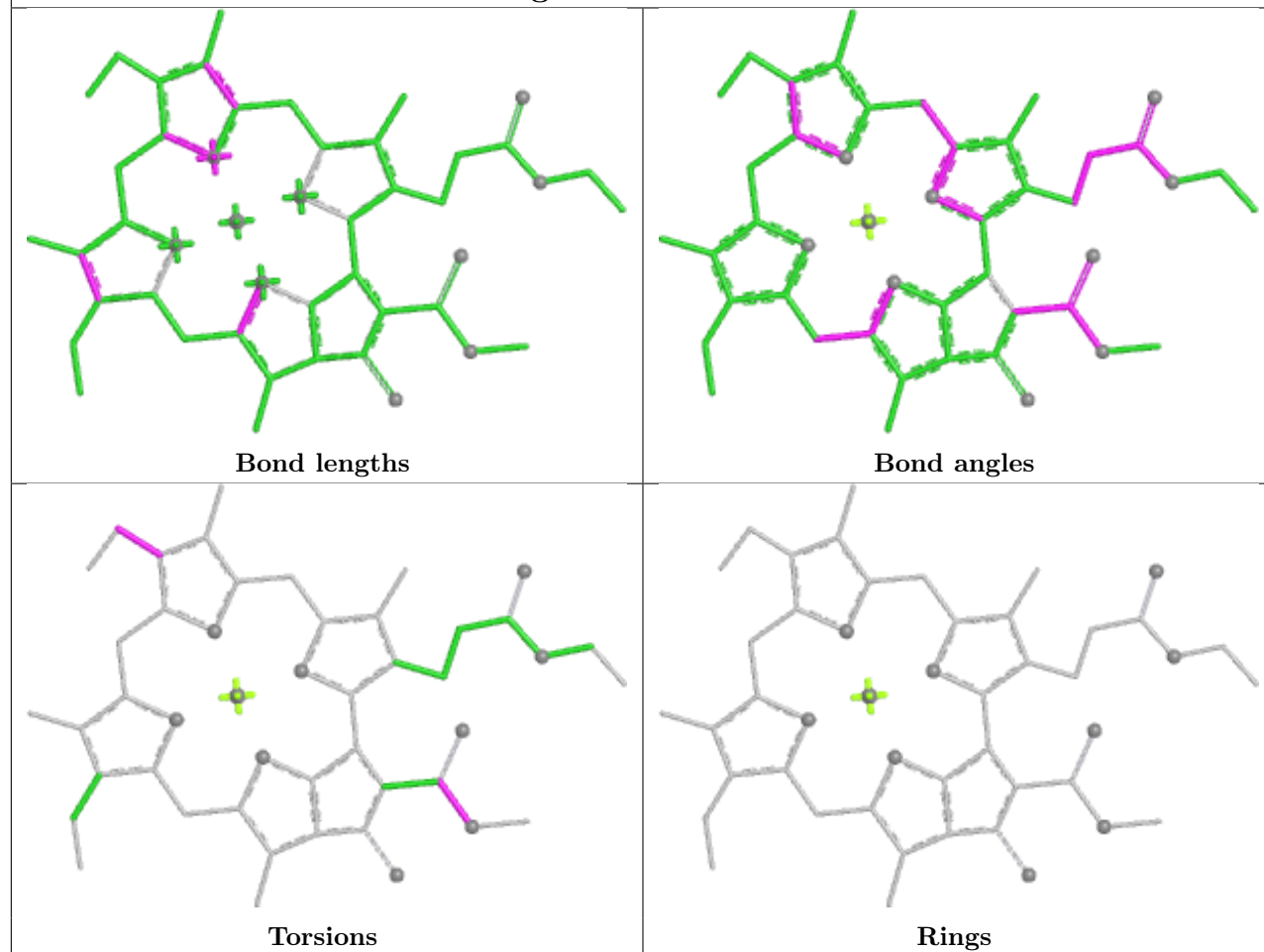
## Ligand CLA B 827



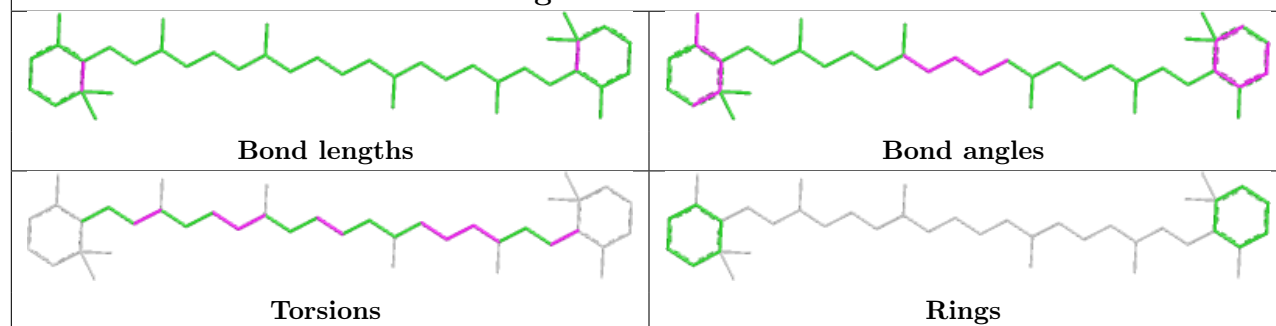
## Ligand LHG 2 317



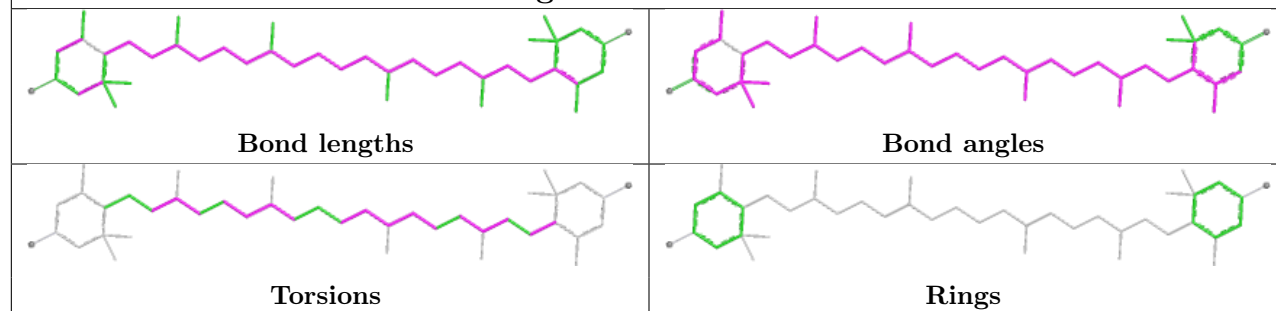
## Ligand CLA 4 314



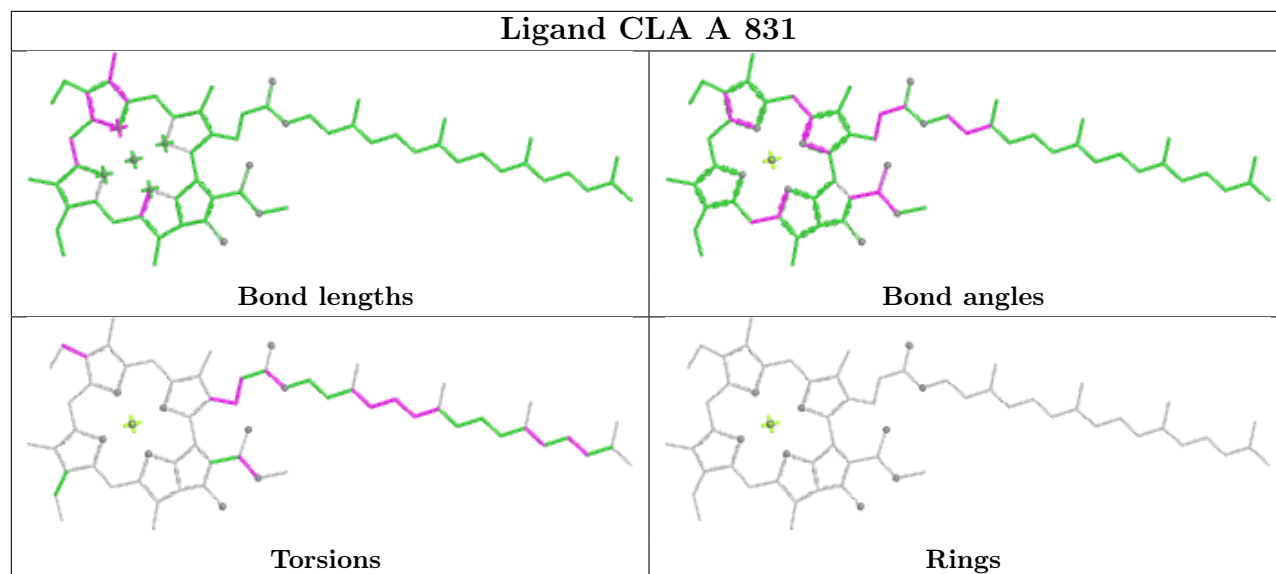
## Ligand BCR 1 316



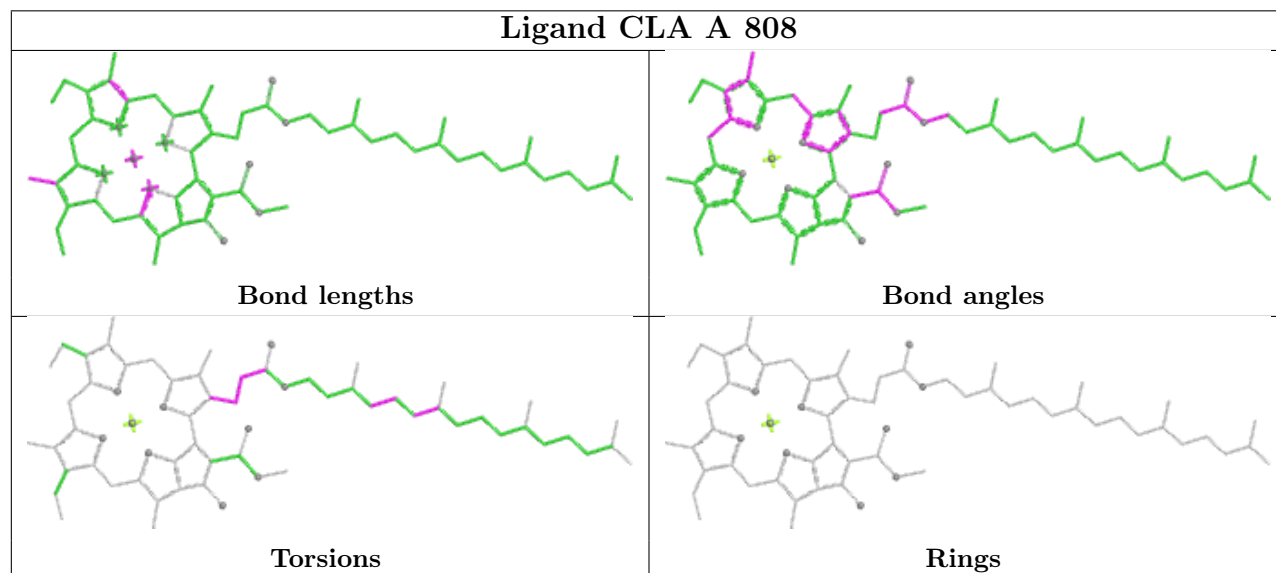
## Ligand LUT 4 316



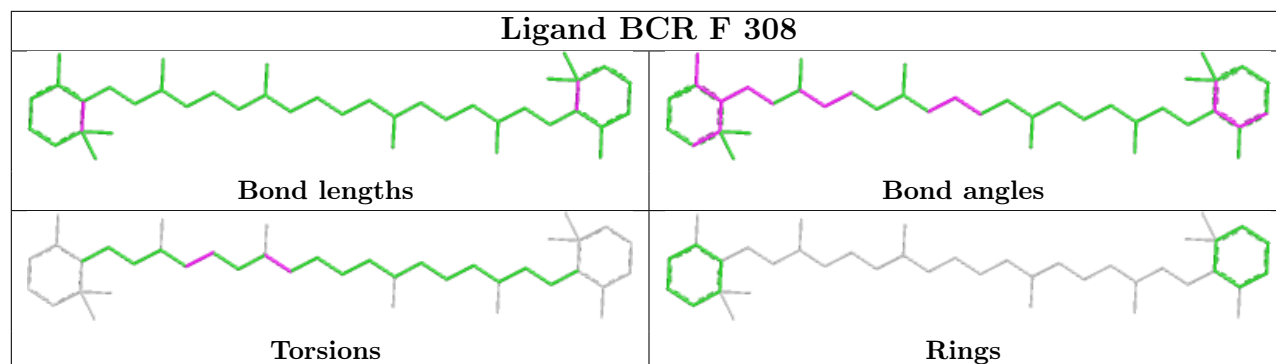
## Ligand CLA A 831



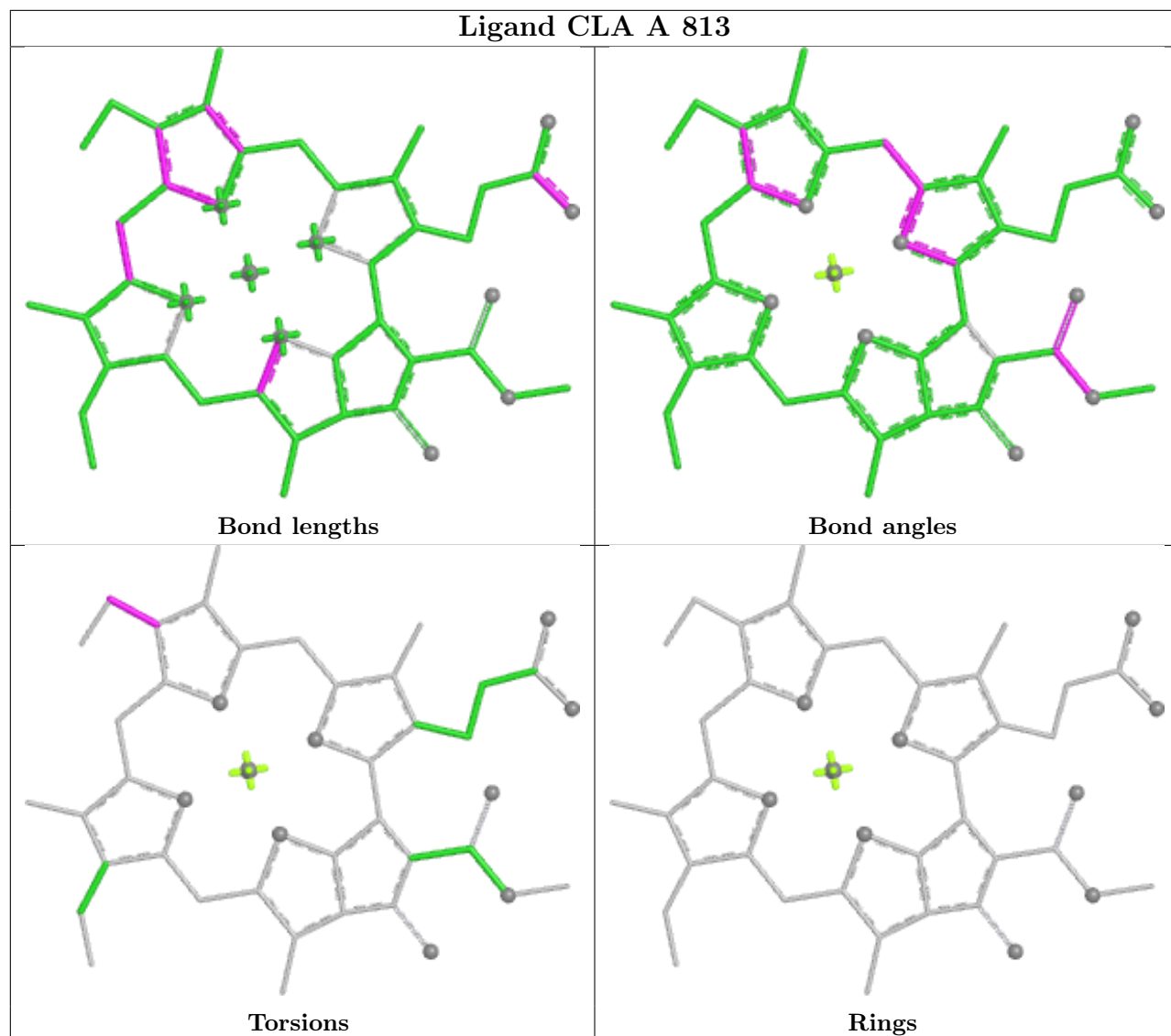
## Ligand CLA A 808

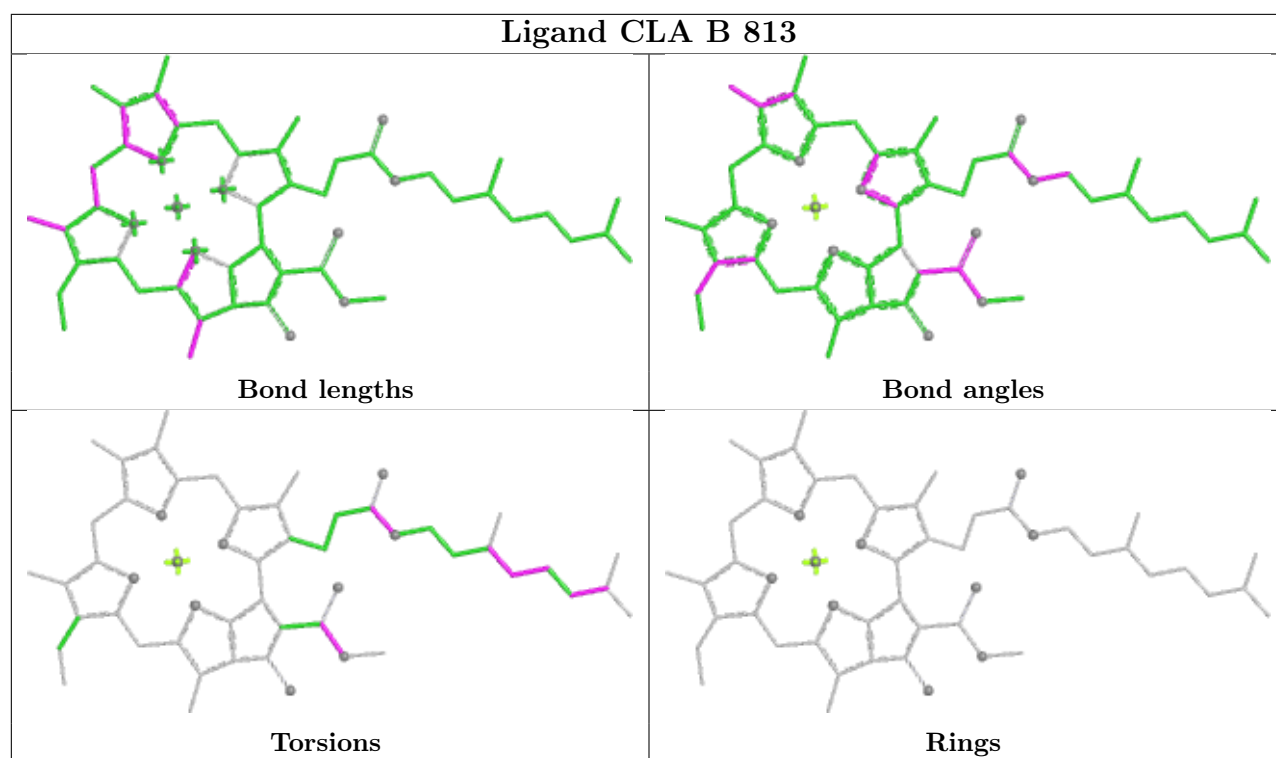


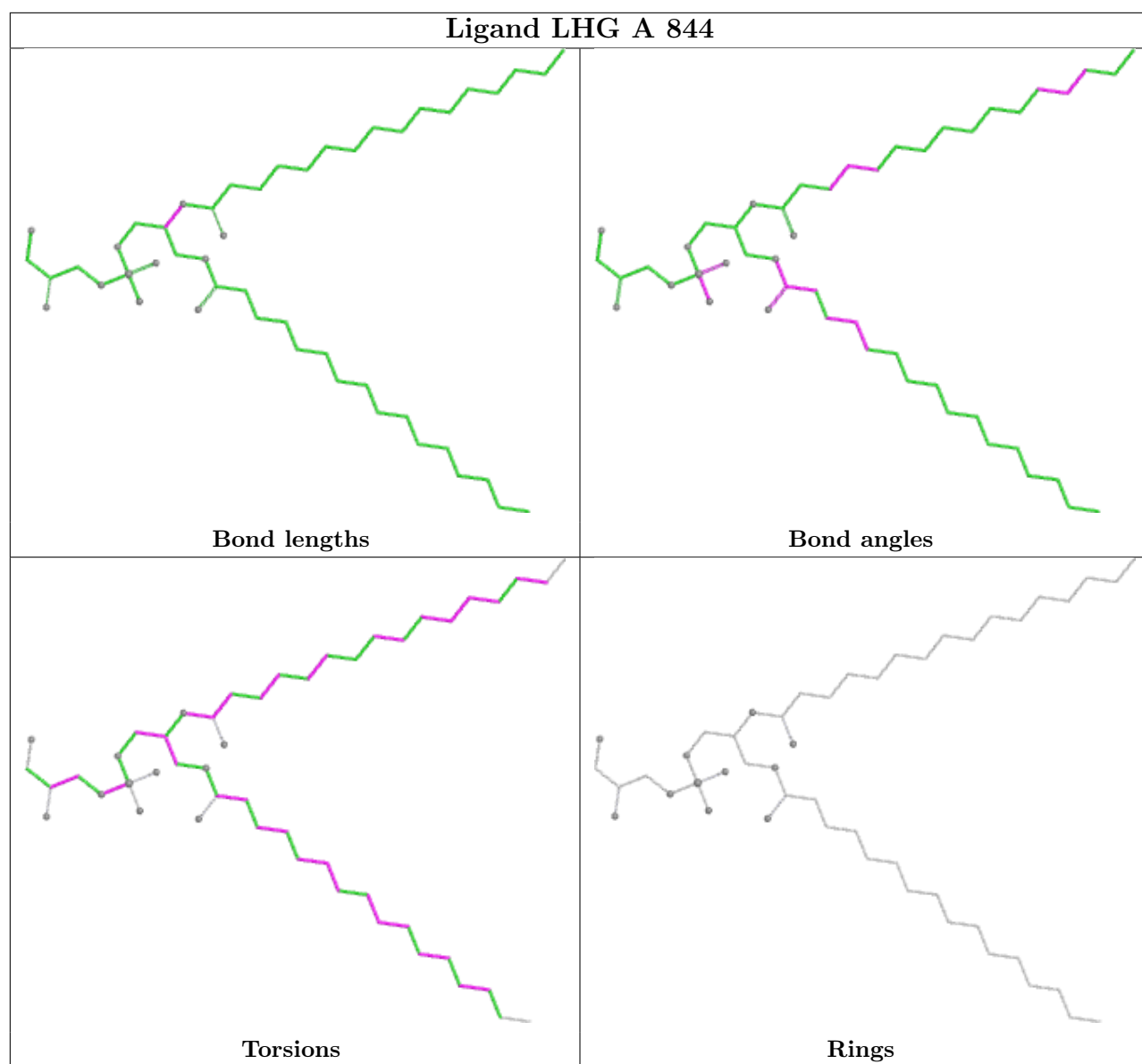
## Ligand BCR F 308



## Ligand CLA A 813

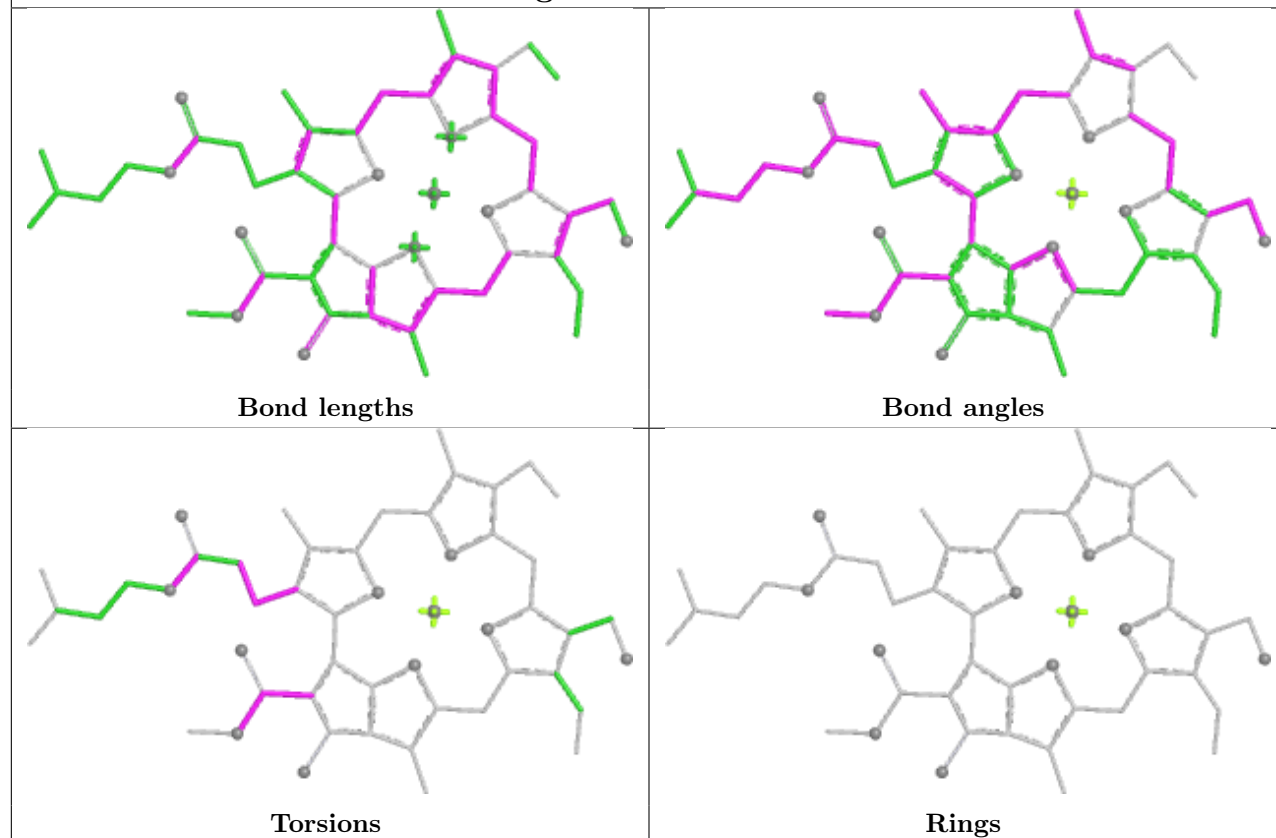




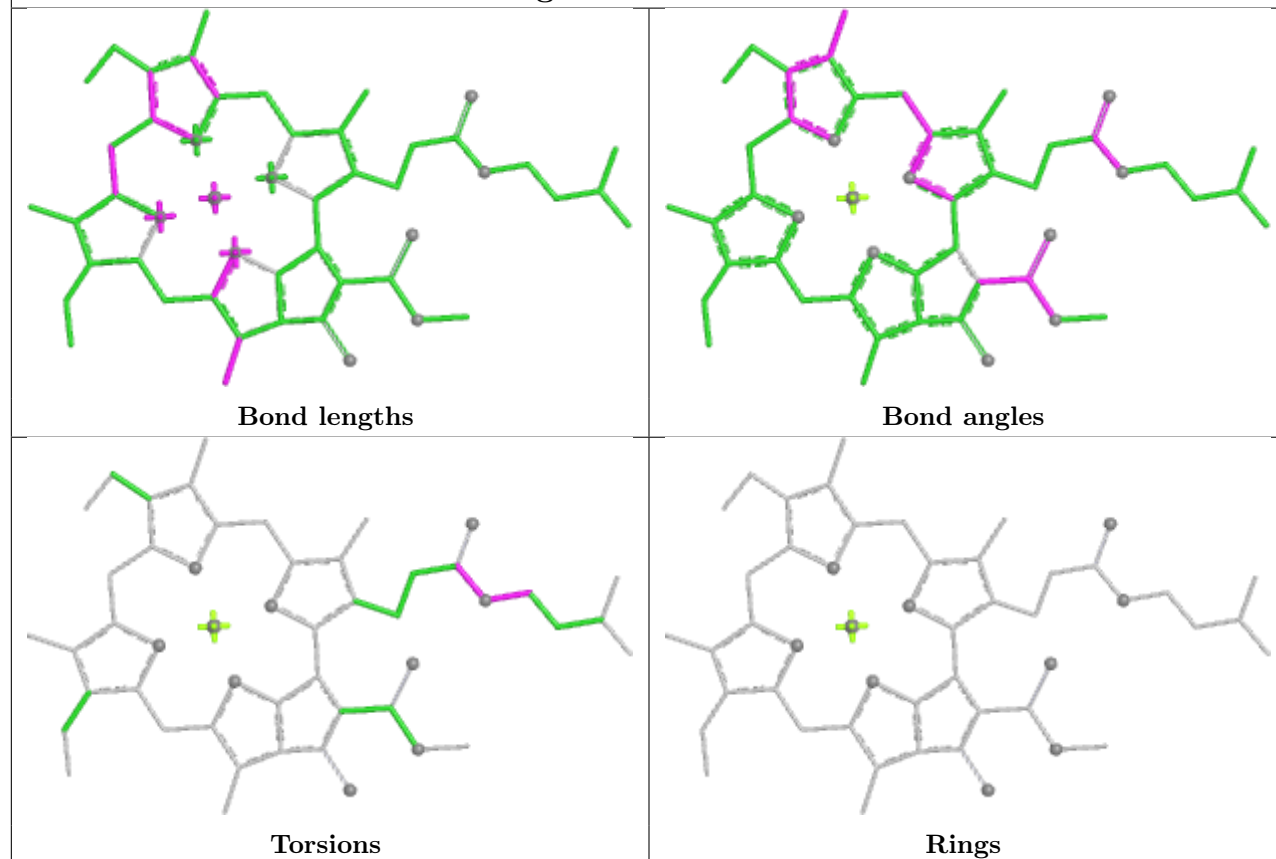


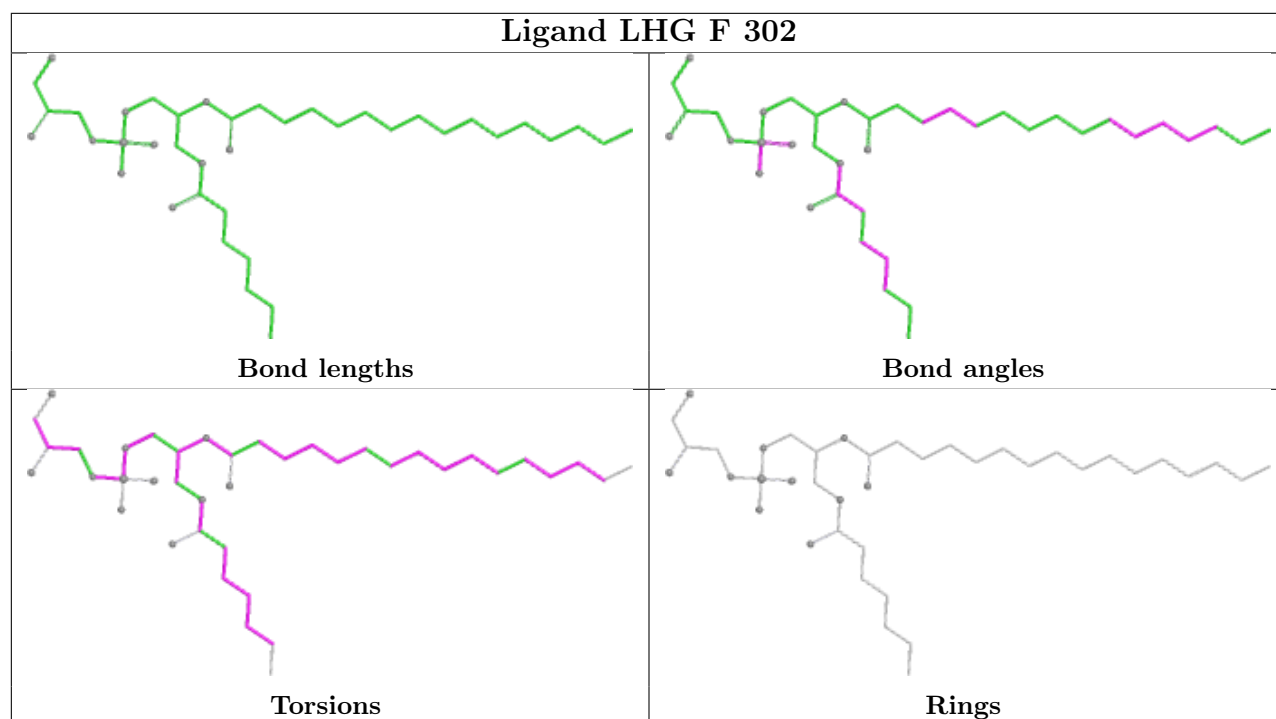
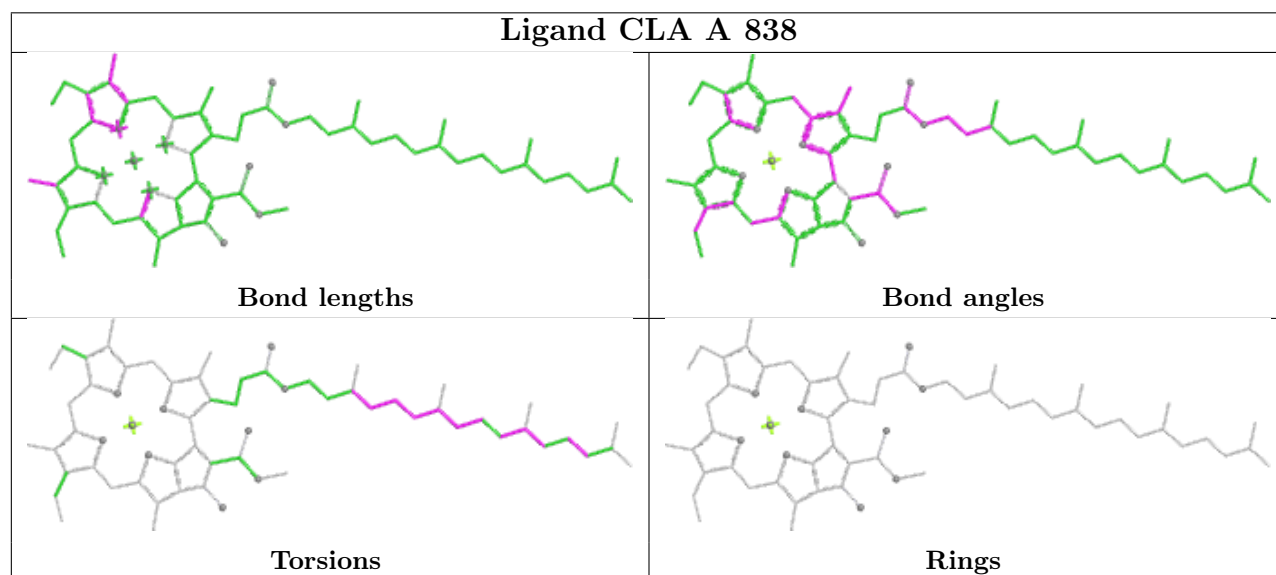
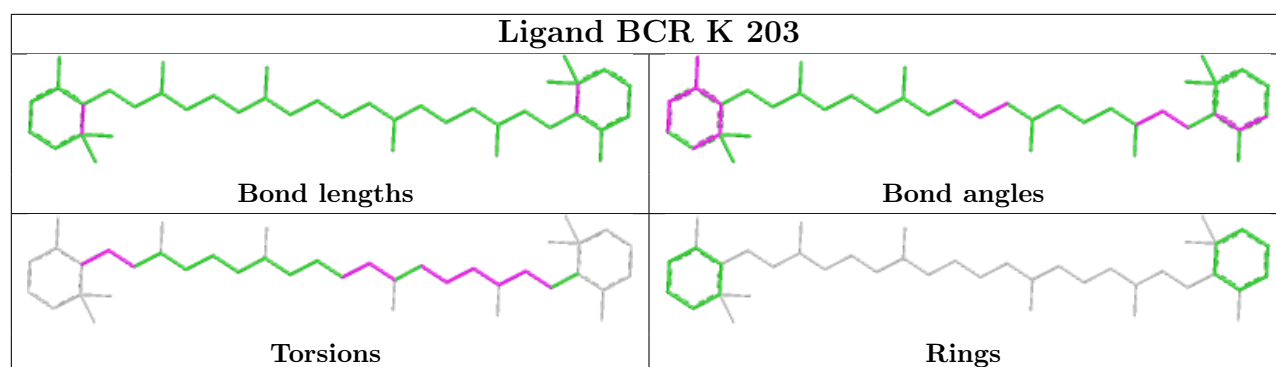


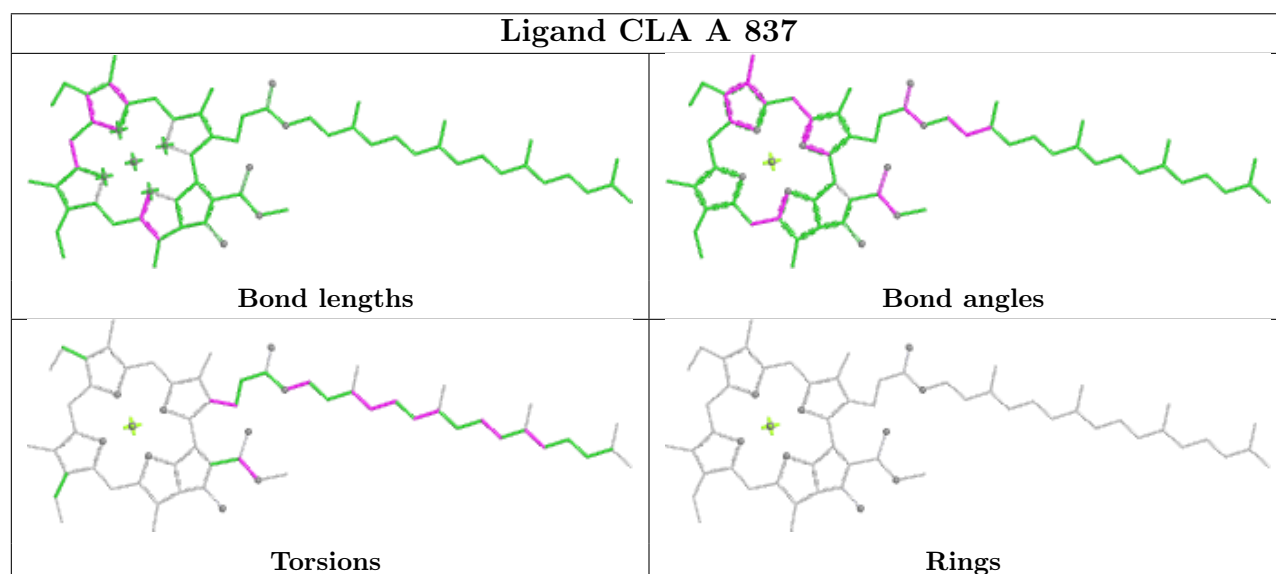
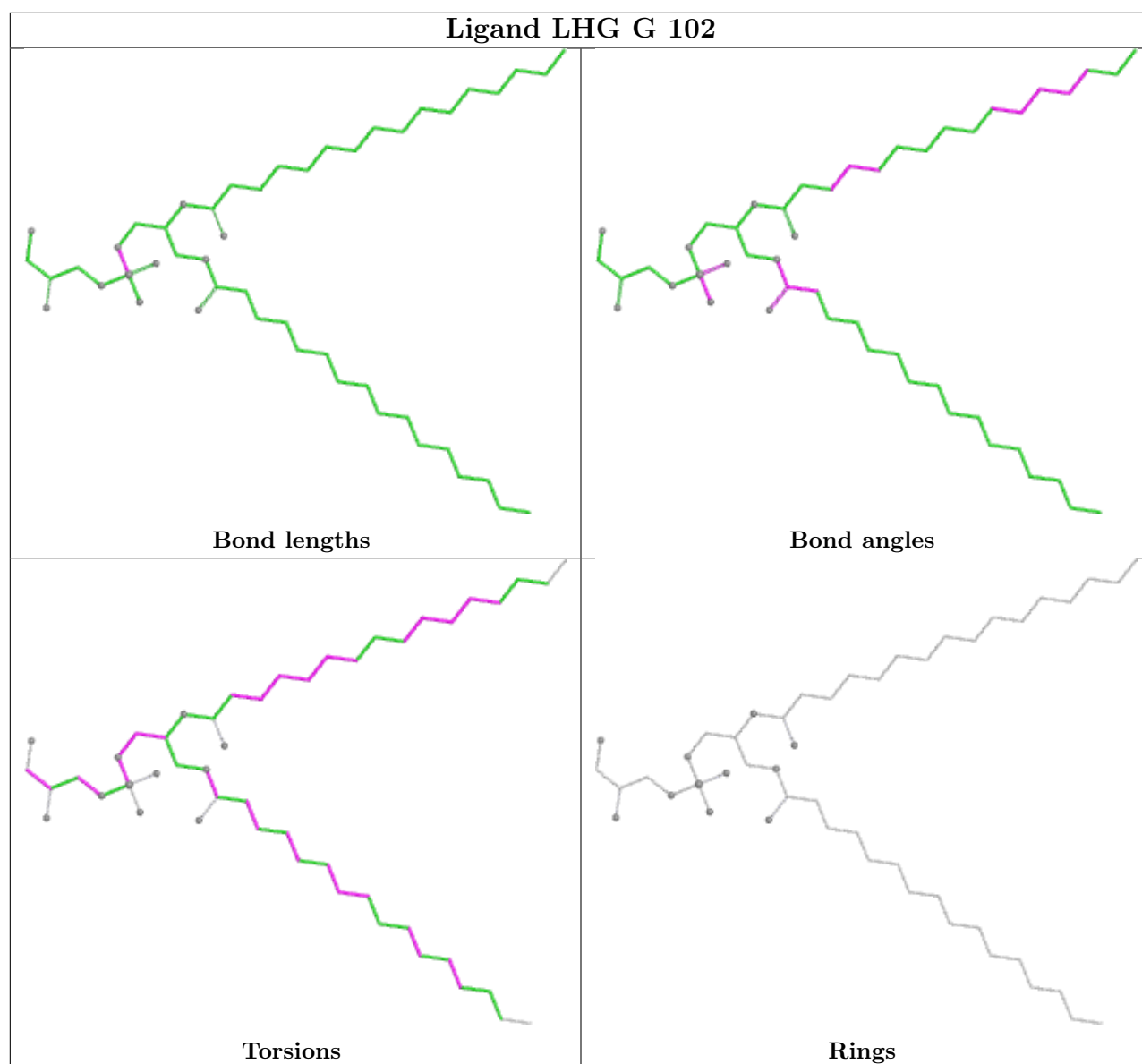
## Ligand CHL 4 306

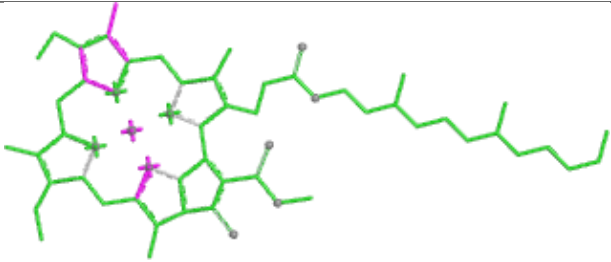
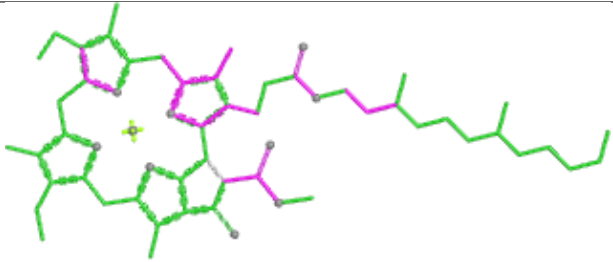
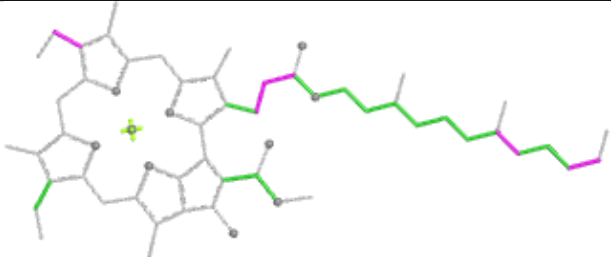
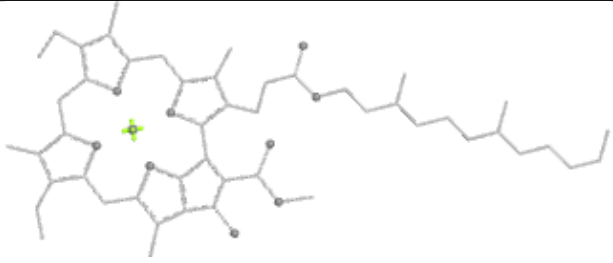


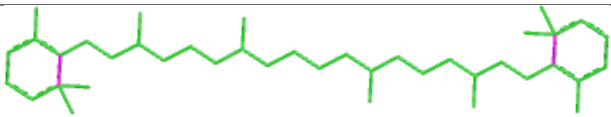
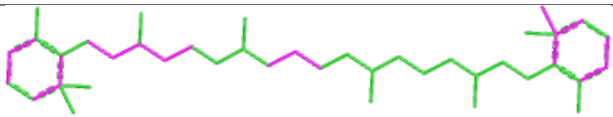
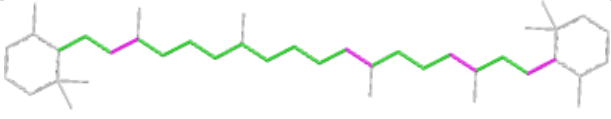
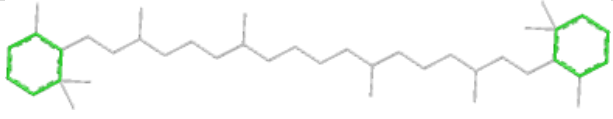
## Ligand CLA 4 308

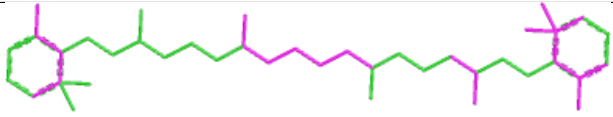
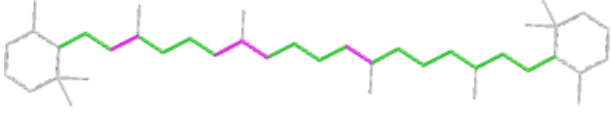
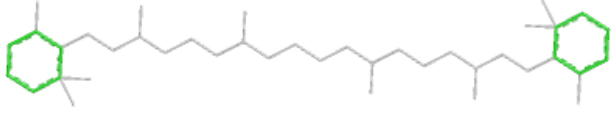


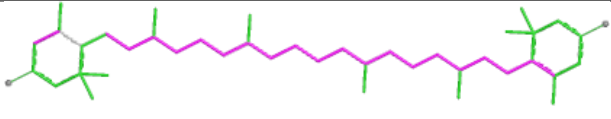
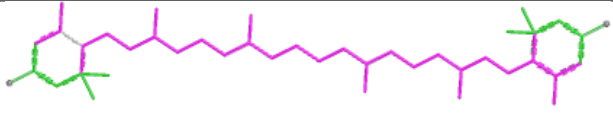
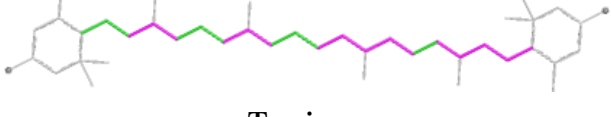
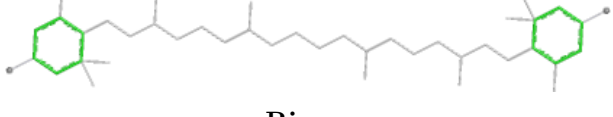




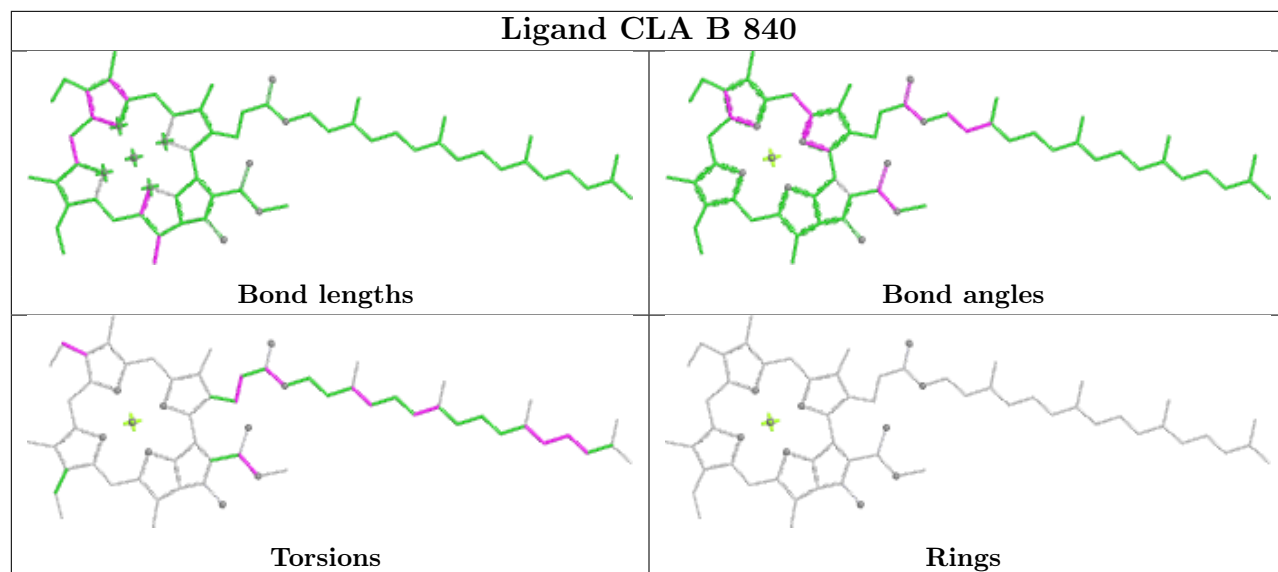
| Ligand CLA B 819                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR 4 318                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

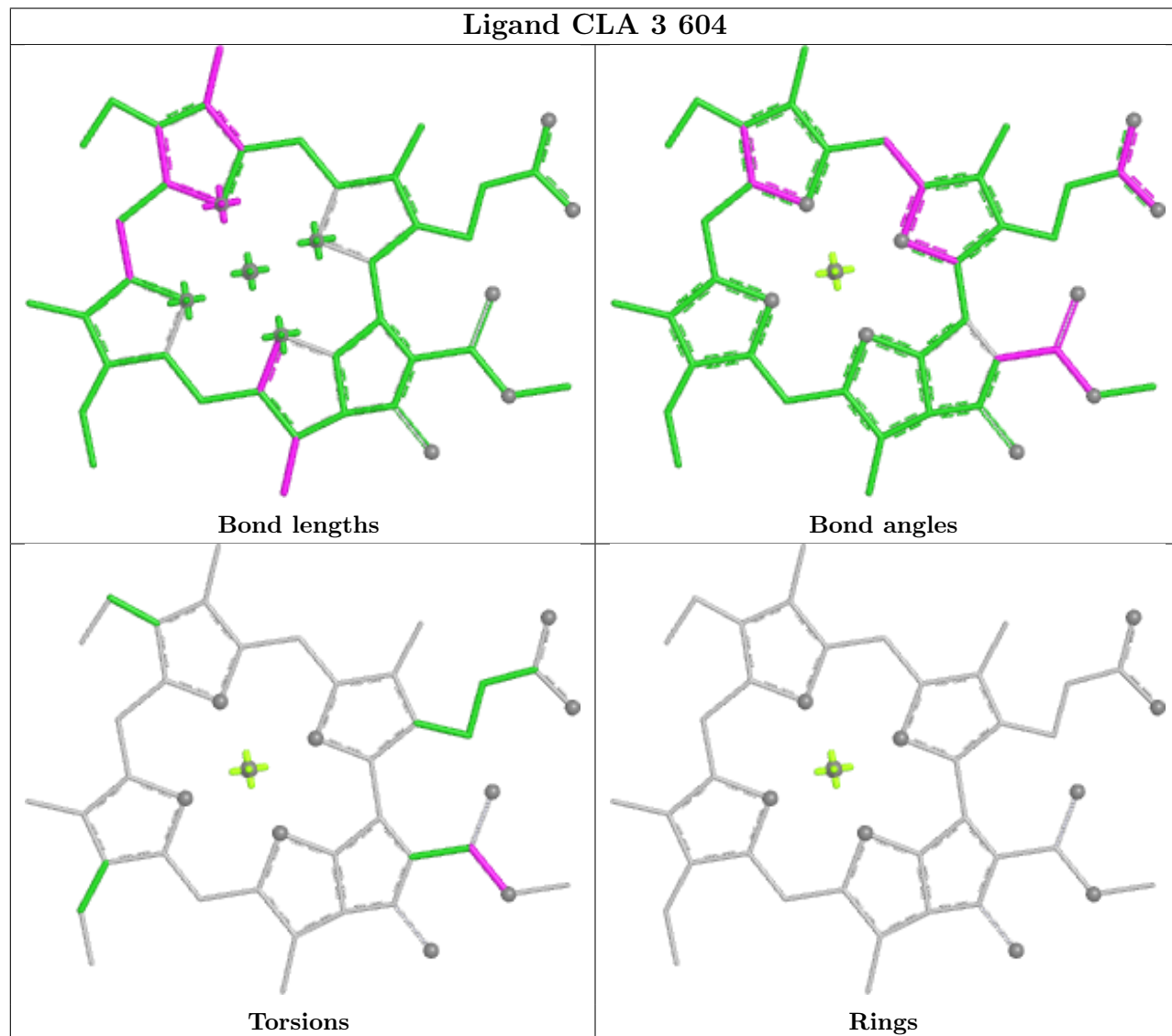
| Ligand BCR F 303                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

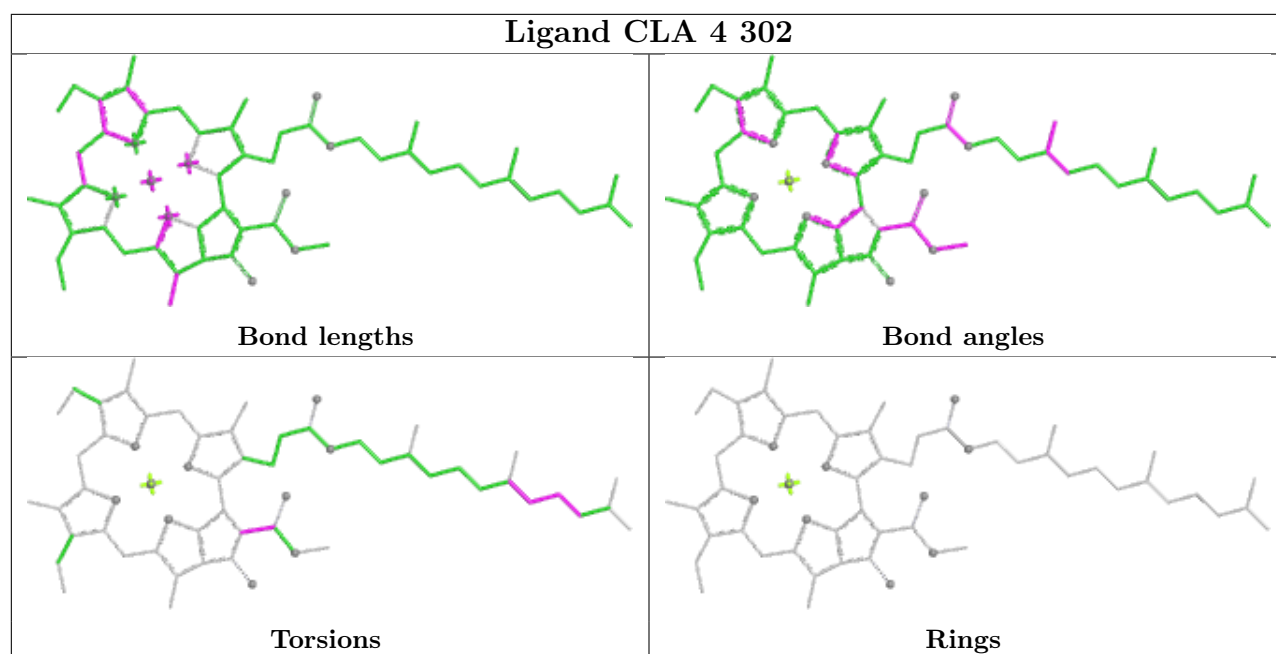
| Ligand LUT 2 314                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

## Ligand CLA B 840



## Ligand CLA 3 604





## 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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | 1     | 195/195 (100%)  | 0.58   | 15 (7%) 19 16  | 66, 95, 152, 193      | 0     |
| 2   | 2     | 204/269 (75%)   | 0.68   | 17 (8%) 17 14  | 87, 121, 159, 212     | 0     |
| 3   | 3     | 216/275 (78%)   | 0.76   | 23 (10%) 11 8  | 114, 161, 229, 257    | 0     |
| 4   | 4     | 195/198 (98%)   | 0.12   | 4 (2%) 63 59   | 60, 74, 111, 143      | 0     |
| 5   | A     | 742/758 (97%)   | 0.30   | 26 (3%) 47 43  | 52, 94, 150, 233      | 0     |
| 6   | B     | 733/734 (99%)   | 0.03   | 18 (2%) 58 54  | 30, 69, 98, 132       | 0     |
| 7   | C     | 80/81 (98%)     | 0.33   | 4 (5%) 34 30   | 30, 78, 94, 120       | 0     |
| 8   | D     | 140/143 (97%)   | 0.32   | 6 (4%) 40 36   | 66, 101, 137, 158     | 0     |
| 9   | E     | 63/66 (95%)     | -0.03  | 1 (1%) 70 66   | 65, 84, 111, 129      | 0     |
| 10  | F     | 152/154 (98%)   | 0.11   | 6 (3%) 43 39   | 30, 70, 96, 138       | 0     |
| 11  | G     | 95/97 (97%)     | 0.41   | 8 (8%) 17 14   | 30, 91, 125, 156      | 0     |
| 12  | H     | 88/88 (100%)    | 0.76   | 10 (11%) 10 7  | 96, 132, 182, 259     | 0     |
| 13  | I     | 30/40 (75%)     | 0.60   | 2 (6%) 24 20   | 92, 108, 146, 208     | 0     |
| 14  | J     | 39/42 (92%)     | 0.23   | 4 (10%) 12 9   | 60, 73, 101, 112      | 0     |
| 15  | L     | 151/157 (96%)   | 0.41   | 4 (2%) 57 53   | 102, 137, 165, 192    | 0     |
| 16  | K     | 77/80 (96%)     | 1.33   | 18 (23%) 2 1   | 137, 198, 248, 302    | 0     |
| All | All   | 3200/3377 (94%) | 0.33   | 166 (5%) 33 29 | 30, 91, 178, 302      | 0     |

The worst 5 of 166 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 16  | K     | 90  | LEU  | 6.2  |
| 3   | 3     | 128 | LEU  | 5.9  |
| 12  | H     | 142 | LEU  | 5.7  |
| 1   | 1     | 109 | ALA  | 5.5  |
| 16  | K     | 72  | PRO  | 5.5  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 17  | CLA  | A     | 843 | 52/65 | 0.66 | 0.14 | 173,188,196,199             | 0     |
| 25  | HTG  | 4     | 322 | 19/19 | 0.71 | 0.16 | 107,129,140,145             | 0     |
| 25  | HTG  | F     | 310 | 16/19 | 0.71 | 0.14 | 114,141,144,146             | 0     |
| 26  | DGD  | 4     | 323 | 60/66 | 0.72 | 0.17 | 90,115,130,138              | 0     |
| 22  | LHG  | G     | 102 | 49/49 | 0.74 | 0.20 | 92,119,171,174              | 0     |
| 25  | HTG  | F     | 301 | 17/19 | 0.75 | 0.16 | 124,149,155,159             | 0     |
| 25  | HTG  | B     | 851 | 19/19 | 0.77 | 0.16 | 107,134,142,143             | 0     |
| 22  | LHG  | F     | 302 | 40/49 | 0.77 | 0.21 | 111,140,164,167             | 0     |
| 17  | CLA  | 3     | 610 | 52/65 | 0.77 | 0.14 | 177,188,210,215             | 0     |
| 21  | BCR  | K     | 203 | 40/40 | 0.77 | 0.18 | 142,185,227,229             | 0     |
| 24  | LMG  | B     | 852 | 52/55 | 0.78 | 0.17 | 100,127,143,148             | 0     |
| 21  | BCR  | 2     | 316 | 40/40 | 0.78 | 0.19 | 148,157,172,173             | 0     |
| 20  | XAT  | 3     | 615 | 44/44 | 0.79 | 0.15 | 62,89,98,100                | 0     |
| 24  | LMG  | 4     | 320 | 49/55 | 0.80 | 0.16 | 96,119,174,176              | 0     |
| 24  | LMG  | F     | 309 | 55/55 | 0.81 | 0.14 | 91,108,120,124              | 0     |
| 17  | CLA  | L     | 204 | 50/65 | 0.82 | 0.12 | 122,147,157,163             | 0     |
| 17  | CLA  | J     | 103 | 42/65 | 0.82 | 0.12 | 83,101,120,125              | 0     |
| 24  | LMG  | G     | 101 | 40/55 | 0.83 | 0.15 | 110,157,180,181             | 0     |
| 23  | LMT  | 2     | 318 | 35/35 | 0.83 | 0.15 | 120,133,143,146             | 0     |
| 22  | LHG  | A     | 845 | 27/49 | 0.83 | 0.12 | 128,174,191,196             | 0     |
| 17  | CLA  | A     | 821 | 49/65 | 0.84 | 0.12 | 130,142,169,175             | 0     |
| 21  | BCR  | 3     | 616 | 40/40 | 0.85 | 0.14 | 156,164,187,189             | 0     |
| 17  | CLA  | L     | 202 | 65/65 | 0.85 | 0.12 | 142,154,170,175             | 0     |
| 17  | CLA  | 3     | 612 | 45/65 | 0.85 | 0.11 | 197,212,229,235             | 0     |
| 22  | LHG  | B     | 801 | 23/49 | 0.85 | 0.15 | 67,88,119,120               | 0     |
| 23  | LMT  | A     | 855 | 35/35 | 0.86 | 0.13 | 97,154,171,172              | 0     |
| 17  | CLA  | A     | 822 | 51/65 | 0.86 | 0.11 | 137,148,164,169             | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 18  | CHL  | 3     | 601 | 56/66 | 0.86 | 0.13 | 108,134,146,147             | 0     |
| 20  | XAT  | 2     | 315 | 44/44 | 0.86 | 0.14 | 62,89,98,100                | 0     |
| 17  | CLA  | 2     | 303 | 60/65 | 0.86 | 0.11 | 120,132,139,142             | 0     |
| 17  | CLA  | L     | 203 | 65/65 | 0.87 | 0.13 | 119,143,157,167             | 0     |
| 17  | CLA  | K     | 201 | 45/65 | 0.87 | 0.11 | 172,184,191,193             | 0     |
| 18  | CHL  | 2     | 305 | 48/66 | 0.87 | 0.13 | 105,129,162,162             | 0     |
| 24  | LMG  | 4     | 319 | 50/55 | 0.87 | 0.15 | 68,89,131,132               | 0     |
| 25  | HTG  | 4     | 321 | 19/19 | 0.87 | 0.16 | 125,139,147,147             | 0     |
| 17  | CLA  | 4     | 304 | 50/65 | 0.88 | 0.11 | 55,78,112,117               | 0     |
| 21  | BCR  | L     | 206 | 40/40 | 0.88 | 0.12 | 156,168,177,178             | 0     |
| 17  | CLA  | 3     | 609 | 50/65 | 0.88 | 0.10 | 147,163,173,175             | 0     |
| 22  | LHG  | 2     | 317 | 37/49 | 0.88 | 0.19 | 155,163,179,187             | 0     |
| 17  | CLA  | 1     | 304 | 42/65 | 0.88 | 0.12 | 80,107,125,133              | 0     |
| 17  | CLA  | A     | 837 | 65/65 | 0.88 | 0.13 | 92,103,174,177              | 0     |
| 17  | CLA  | 3     | 604 | 45/65 | 0.88 | 0.11 | 137,162,170,173             | 0     |
| 17  | CLA  | 3     | 605 | 42/65 | 0.89 | 0.11 | 125,135,143,147             | 0     |
| 17  | CLA  | G     | 103 | 41/65 | 0.89 | 0.14 | 105,122,131,136             | 0     |
| 17  | CLA  | 1     | 307 | 65/65 | 0.89 | 0.12 | 74,93,123,129               | 0     |
| 18  | CHL  | 4     | 301 | 61/66 | 0.89 | 0.12 | 66,78,116,118               | 0     |
| 26  | DGD  | B     | 850 | 66/66 | 0.89 | 0.14 | 80,94,119,120               | 0     |
| 17  | CLA  | 3     | 602 | 60/65 | 0.90 | 0.12 | 132,157,174,178             | 0     |
| 17  | CLA  | A     | 817 | 65/65 | 0.90 | 0.13 | 103,129,169,173             | 0     |
| 17  | CLA  | 2     | 310 | 52/65 | 0.90 | 0.09 | 106,113,156,164             | 0     |
| 19  | LUT  | 3     | 614 | 42/42 | 0.90 | 0.11 | 127,146,163,166             | 0     |
| 22  | LHG  | 1     | 317 | 49/49 | 0.90 | 0.16 | 85,100,127,130              | 0     |
| 17  | CLA  | 2     | 312 | 43/65 | 0.90 | 0.10 | 122,142,146,147             | 0     |
| 17  | CLA  | K     | 202 | 60/65 | 0.90 | 0.09 | 146,176,193,196             | 0     |
| 21  | BCR  | 1     | 316 | 40/40 | 0.90 | 0.12 | 98,125,149,151              | 0     |
| 17  | CLA  | 2     | 309 | 41/65 | 0.91 | 0.10 | 126,134,143,146             | 0     |
| 17  | CLA  | A     | 819 | 45/65 | 0.91 | 0.11 | 126,138,151,155             | 0     |
| 17  | CLA  | 1     | 303 | 51/65 | 0.91 | 0.12 | 112,124,138,143             | 0     |
| 17  | CLA  | 1     | 312 | 55/65 | 0.91 | 0.11 | 74,88,119,123               | 0     |
| 17  | CLA  | A     | 825 | 65/65 | 0.91 | 0.11 | 76,98,163,165               | 0     |
| 18  | CHL  | 1     | 305 | 48/66 | 0.91 | 0.13 | 102,114,132,134             | 0     |
| 17  | CLA  | A     | 833 | 50/65 | 0.91 | 0.11 | 120,135,146,157             | 0     |
| 17  | CLA  | A     | 834 | 45/65 | 0.91 | 0.09 | 156,170,177,185             | 0     |
| 17  | CLA  | A     | 835 | 51/65 | 0.91 | 0.11 | 78,102,129,135              | 0     |
| 17  | CLA  | 2     | 302 | 51/65 | 0.91 | 0.10 | 89,102,120,127              | 0     |
| 17  | CLA  | 1     | 306 | 46/65 | 0.91 | 0.11 | 91,101,117,120              | 0     |
| 17  | CLA  | B     | 803 | 65/65 | 0.91 | 0.11 | 106,119,153,161             | 0     |
| 17  | CLA  | B     | 814 | 55/65 | 0.91 | 0.11 | 61,75,121,123               | 0     |
| 17  | CLA  | B     | 817 | 55/65 | 0.91 | 0.11 | 72,86,123,134               | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 17  | CLA  | 4     | 310 | 60/65 | 0.91 | 0.10 | 68,89,116,121               | 0     |
| 21  | BCR  | 4     | 318 | 40/40 | 0.91 | 0.12 | 61,90,99,104                | 0     |
| 21  | BCR  | A     | 846 | 40/40 | 0.91 | 0.12 | 116,137,151,153             | 0     |
| 21  | BCR  | J     | 105 | 40/40 | 0.91 | 0.14 | 73,85,100,101               | 0     |
| 17  | CLA  | G     | 105 | 46/65 | 0.91 | 0.10 | 92,122,136,144              | 0     |
| 17  | CLA  | A     | 814 | 50/65 | 0.91 | 0.14 | 119,141,161,164             | 0     |
| 17  | CLA  | 4     | 311 | 52/65 | 0.92 | 0.10 | 72,83,118,119               | 0     |
| 17  | CLA  | B     | 824 | 55/65 | 0.92 | 0.12 | 63,74,104,112               | 0     |
| 21  | BCR  | A     | 849 | 40/40 | 0.92 | 0.14 | 100,137,196,199             | 0     |
| 21  | BCR  | B     | 845 | 40/40 | 0.92 | 0.11 | 62,73,118,122               | 0     |
| 21  | BCR  | B     | 847 | 40/40 | 0.92 | 0.12 | 49,65,85,92                 | 0     |
| 18  | CHL  | 2     | 313 | 43/66 | 0.92 | 0.08 | 99,119,137,139              | 0     |
| 17  | CLA  | A     | 830 | 50/65 | 0.92 | 0.12 | 102,117,152,156             | 0     |
| 17  | CLA  | A     | 809 | 65/65 | 0.92 | 0.13 | 100,120,149,151             | 0     |
| 17  | CLA  | 3     | 613 | 46/65 | 0.92 | 0.09 | 106,121,156,159             | 0     |
| 17  | CLA  | A     | 816 | 65/65 | 0.92 | 0.12 | 116,134,152,155             | 0     |
| 17  | CLA  | 4     | 303 | 60/65 | 0.92 | 0.10 | 52,67,108,113               | 0     |
| 17  | CLA  | 2     | 301 | 65/65 | 0.92 | 0.12 | 86,105,122,135              | 0     |
| 25  | HTG  | J     | 102 | 19/19 | 0.92 | 0.10 | 75,82,115,120               | 0     |
| 17  | CLA  | 4     | 309 | 60/65 | 0.92 | 0.11 | 61,72,98,100                | 0     |
| 17  | CLA  | 1     | 309 | 65/65 | 0.92 | 0.10 | 84,105,142,147              | 0     |
| 21  | BCR  | J     | 104 | 40/40 | 0.93 | 0.11 | 63,73,87,91                 | 0     |
| 17  | CLA  | B     | 812 | 65/65 | 0.93 | 0.13 | 76,107,137,144              | 0     |
| 21  | BCR  | L     | 201 | 40/40 | 0.93 | 0.10 | 95,107,120,123              | 0     |
| 18  | CHL  | 2     | 304 | 43/66 | 0.93 | 0.11 | 101,117,129,137             | 0     |
| 17  | CLA  | B     | 813 | 54/65 | 0.93 | 0.09 | 61,90,114,117               | 0     |
| 17  | CLA  | 3     | 606 | 47/65 | 0.93 | 0.09 | 113,124,135,138             | 0     |
| 17  | CLA  | 1     | 302 | 65/65 | 0.93 | 0.10 | 70,87,125,128               | 0     |
| 17  | CLA  | B     | 818 | 55/65 | 0.93 | 0.11 | 63,73,95,102                | 0     |
| 18  | CHL  | 4     | 305 | 56/66 | 0.93 | 0.10 | 68,77,116,118               | 0     |
| 18  | CHL  | 4     | 306 | 51/66 | 0.93 | 0.09 | 66,79,130,133               | 0     |
| 18  | CHL  | 4     | 315 | 43/66 | 0.93 | 0.09 | 67,88,102,117               | 0     |
| 19  | LUT  | 1     | 314 | 42/42 | 0.93 | 0.10 | 67,95,116,120               | 0     |
| 19  | LUT  | 2     | 314 | 42/42 | 0.93 | 0.10 | 97,114,124,130              | 0     |
| 17  | CLA  | B     | 820 | 60/65 | 0.93 | 0.10 | 46,66,85,87                 | 0     |
| 19  | LUT  | 4     | 316 | 42/42 | 0.93 | 0.10 | 63,72,86,91                 | 0     |
| 17  | CLA  | 1     | 313 | 46/65 | 0.93 | 0.08 | 73,84,105,117               | 0     |
| 17  | CLA  | 3     | 611 | 55/65 | 0.93 | 0.10 | 143,177,193,195             | 0     |
| 17  | CLA  | G     | 104 | 50/65 | 0.93 | 0.09 | 76,95,125,133               | 0     |
| 17  | CLA  | A     | 811 | 54/65 | 0.93 | 0.11 | 107,127,140,140             | 0     |
| 17  | CLA  | 2     | 307 | 50/65 | 0.93 | 0.10 | 90,95,110,113               | 0     |
| 25  | HTG  | A     | 854 | 19/19 | 0.93 | 0.07 | 63,78,85,96                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 17  | CLA  | A     | 815 | 45/65 | 0.93 | 0.09 | 114,125,135,140             | 0     |
| 17  | CLA  | A     | 836 | 65/65 | 0.93 | 0.11 | 86,106,146,154              | 0     |
| 25  | HTG  | F     | 305 | 19/19 | 0.93 | 0.14 | 62,83,100,104               | 0     |
| 17  | CLA  | 3     | 603 | 50/65 | 0.93 | 0.10 | 116,128,132,135             | 0     |
| 17  | CLA  | 2     | 308 | 60/65 | 0.93 | 0.12 | 111,122,145,151             | 0     |
| 17  | CLA  | 1     | 310 | 52/65 | 0.93 | 0.10 | 88,103,145,147              | 0     |
| 21  | BCR  | F     | 303 | 40/40 | 0.93 | 0.12 | 48,60,65,66                 | 0     |
| 17  | CLA  | 2     | 311 | 65/65 | 0.94 | 0.09 | 109,127,142,147             | 0     |
| 17  | CLA  | A     | 826 | 65/65 | 0.94 | 0.10 | 90,119,149,154              | 0     |
| 17  | CLA  | B     | 816 | 65/65 | 0.94 | 0.12 | 65,78,97,99                 | 0     |
| 17  | CLA  | 4     | 308 | 50/65 | 0.94 | 0.09 | 52,64,103,109               | 0     |
| 17  | CLA  | 1     | 301 | 65/65 | 0.94 | 0.10 | 60,72,107,115               | 0     |
| 17  | CLA  | 1     | 308 | 60/65 | 0.94 | 0.11 | 89,100,129,133              | 0     |
| 18  | CHL  | 2     | 306 | 51/66 | 0.94 | 0.12 | 84,101,141,144              | 0     |
| 17  | CLA  | B     | 822 | 50/65 | 0.94 | 0.10 | 70,80,109,113               | 0     |
| 21  | BCR  | A     | 847 | 40/40 | 0.94 | 0.12 | 87,120,171,173              | 0     |
| 21  | BCR  | A     | 848 | 40/40 | 0.94 | 0.12 | 92,116,163,164              | 0     |
| 17  | CLA  | 3     | 608 | 50/65 | 0.94 | 0.09 | 120,130,136,139             | 0     |
| 18  | CHL  | 3     | 607 | 47/66 | 0.94 | 0.10 | 124,135,160,166             | 0     |
| 21  | BCR  | B     | 846 | 40/40 | 0.94 | 0.10 | 62,77,125,126               | 0     |
| 17  | CLA  | B     | 834 | 58/65 | 0.94 | 0.10 | 46,59,102,105               | 0     |
| 17  | CLA  | 4     | 312 | 56/65 | 0.94 | 0.09 | 70,84,109,112               | 0     |
| 21  | BCR  | G     | 106 | 40/40 | 0.94 | 0.10 | 71,90,129,130               | 0     |
| 21  | BCR  | I     | 101 | 40/40 | 0.94 | 0.10 | 92,99,112,114               | 0     |
| 17  | CLA  | A     | 820 | 65/65 | 0.94 | 0.11 | 103,126,143,144             | 0     |
| 17  | CLA  | 4     | 314 | 47/65 | 0.94 | 0.08 | 57,70,104,106               | 0     |
| 17  | CLA  | 1     | 311 | 60/65 | 0.94 | 0.10 | 64,75,111,113               | 0     |
| 21  | BCR  | L     | 205 | 40/40 | 0.94 | 0.13 | 101,116,137,137             | 0     |
| 17  | CLA  | B     | 809 | 65/65 | 0.94 | 0.11 | 71,88,138,144               | 0     |
| 17  | CLA  | A     | 824 | 65/65 | 0.94 | 0.11 | 90,102,108,111              | 0     |
| 17  | CLA  | B     | 833 | 60/65 | 0.95 | 0.08 | 44,58,104,110               | 0     |
| 17  | CLA  | A     | 803 | 55/65 | 0.95 | 0.10 | 64,82,119,124               | 0     |
| 17  | CLA  | B     | 835 | 65/65 | 0.95 | 0.09 | 53,67,106,116               | 0     |
| 17  | CLA  | B     | 836 | 45/65 | 0.95 | 0.07 | 62,71,94,97                 | 0     |
| 17  | CLA  | B     | 839 | 47/65 | 0.95 | 0.08 | 52,58,84,93                 | 0     |
| 17  | CLA  | F     | 304 | 65/65 | 0.95 | 0.10 | 44,58,76,84                 | 0     |
| 21  | BCR  | A     | 850 | 40/40 | 0.95 | 0.11 | 72,108,147,148              | 0     |
| 21  | BCR  | A     | 851 | 40/40 | 0.95 | 0.09 | 45,63,77,79                 | 0     |
| 17  | CLA  | F     | 307 | 55/65 | 0.95 | 0.07 | 49,67,123,125               | 0     |
| 17  | CLA  | A     | 804 | 65/65 | 0.95 | 0.10 | 77,91,115,117               | 0     |
| 17  | CLA  | A     | 827 | 65/65 | 0.95 | 0.10 | 64,76,89,94                 | 0     |
| 17  | CLA  | A     | 829 | 65/65 | 0.95 | 0.09 | 68,82,94,98                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 21  | BCR  | F     | 308 | 40/40 | 0.95 | 0.09 | 53,62,72,78                 | 0     |
| 17  | CLA  | J     | 101 | 65/65 | 0.95 | 0.11 | 62,76,93,101                | 0     |
| 17  | CLA  | A     | 853 | 65/65 | 0.95 | 0.11 | 48,61,88,96                 | 0     |
| 17  | CLA  | A     | 806 | 65/65 | 0.95 | 0.10 | 72,81,131,134               | 0     |
| 17  | CLA  | 2     | 319 | 46/65 | 0.95 | 0.09 | 68,80,109,111               | 0     |
| 17  | CLA  | B     | 823 | 65/65 | 0.95 | 0.10 | 62,75,131,140               | 0     |
| 17  | CLA  | A     | 810 | 65/65 | 0.95 | 0.10 | 80,88,102,113               | 0     |
| 20  | XAT  | 4     | 317 | 44/44 | 0.95 | 0.09 | 58,67,81,88                 | 0     |
| 17  | CLA  | B     | 825 | 60/65 | 0.95 | 0.09 | 51,60,107,115               | 0     |
| 17  | CLA  | B     | 826 | 65/65 | 0.95 | 0.09 | 50,67,87,92                 | 0     |
| 17  | CLA  | A     | 812 | 65/65 | 0.96 | 0.09 | 88,112,121,122              | 0     |
| 21  | BCR  | B     | 848 | 40/40 | 0.96 | 0.07 | 48,58,74,79                 | 0     |
| 21  | BCR  | B     | 849 | 40/40 | 0.96 | 0.07 | 60,75,82,83                 | 0     |
| 17  | CLA  | A     | 823 | 55/65 | 0.96 | 0.09 | 105,121,137,143             | 0     |
| 17  | CLA  | A     | 805 | 65/65 | 0.96 | 0.10 | 69,82,91,93                 | 0     |
| 17  | CLA  | B     | 821 | 65/65 | 0.96 | 0.07 | 56,67,98,103                | 0     |
| 17  | CLA  | A     | 801 | 65/65 | 0.96 | 0.10 | 52,67,83,87                 | 0     |
| 17  | CLA  | A     | 838 | 65/65 | 0.96 | 0.09 | 45,55,71,78                 | 0     |
| 17  | CLA  | A     | 839 | 65/65 | 0.96 | 0.09 | 47,59,97,101                | 0     |
| 17  | CLA  | A     | 840 | 65/65 | 0.96 | 0.08 | 52,63,76,90                 | 0     |
| 17  | CLA  | A     | 841 | 65/65 | 0.96 | 0.10 | 82,100,138,149              | 0     |
| 17  | CLA  | B     | 827 | 65/65 | 0.96 | 0.08 | 43,58,106,109               | 0     |
| 17  | CLA  | B     | 829 | 65/65 | 0.96 | 0.10 | 54,65,124,133               | 0     |
| 17  | CLA  | B     | 830 | 65/65 | 0.96 | 0.09 | 48,68,83,97                 | 0     |
| 17  | CLA  | B     | 831 | 65/65 | 0.96 | 0.10 | 48,63,105,107               | 0     |
| 17  | CLA  | B     | 832 | 50/65 | 0.96 | 0.08 | 53,62,96,105                | 0     |
| 17  | CLA  | A     | 807 | 65/65 | 0.96 | 0.09 | 59,73,104,120               | 0     |
| 17  | CLA  | A     | 808 | 65/65 | 0.96 | 0.08 | 54,69,114,118               | 0     |
| 17  | CLA  | A     | 828 | 65/65 | 0.96 | 0.09 | 73,89,106,107               | 0     |
| 17  | CLA  | B     | 804 | 65/65 | 0.96 | 0.10 | 50,60,68,74                 | 0     |
| 17  | CLA  | B     | 837 | 60/65 | 0.96 | 0.09 | 46,57,105,106               | 0     |
| 17  | CLA  | B     | 838 | 65/65 | 0.96 | 0.08 | 43,58,72,81                 | 0     |
| 17  | CLA  | B     | 805 | 65/65 | 0.96 | 0.09 | 62,78,101,112               | 0     |
| 17  | CLA  | B     | 840 | 65/65 | 0.96 | 0.08 | 70,91,118,124               | 0     |
| 17  | CLA  | B     | 841 | 65/65 | 0.96 | 0.09 | 57,72,127,136               | 0     |
| 17  | CLA  | B     | 842 | 65/65 | 0.96 | 0.09 | 57,69,84,94                 | 0     |
| 17  | CLA  | B     | 806 | 45/65 | 0.96 | 0.07 | 62,71,90,114                | 0     |
| 17  | CLA  | B     | 808 | 65/65 | 0.96 | 0.08 | 49,70,88,92                 | 0     |
| 17  | CLA  | A     | 802 | 65/65 | 0.96 | 0.09 | 59,73,82,90                 | 0     |
| 17  | CLA  | B     | 811 | 65/65 | 0.96 | 0.09 | 70,83,118,125               | 0     |
| 17  | CLA  | 4     | 313 | 45/65 | 0.96 | 0.07 | 73,98,120,127               | 0     |
| 17  | CLA  | A     | 831 | 65/65 | 0.96 | 0.08 | 84,103,108,110              | 0     |

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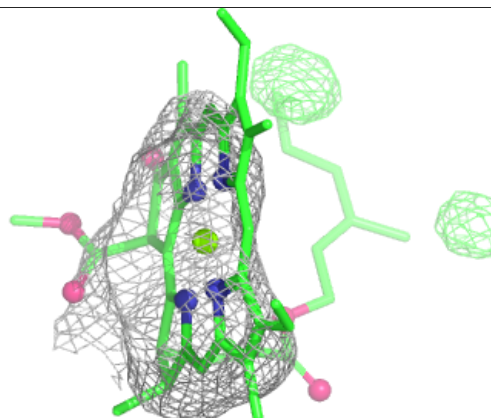
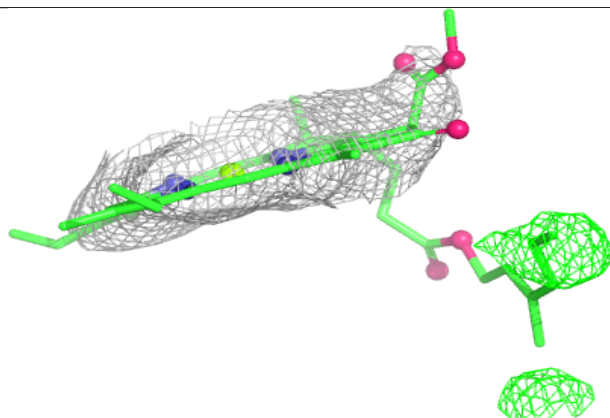
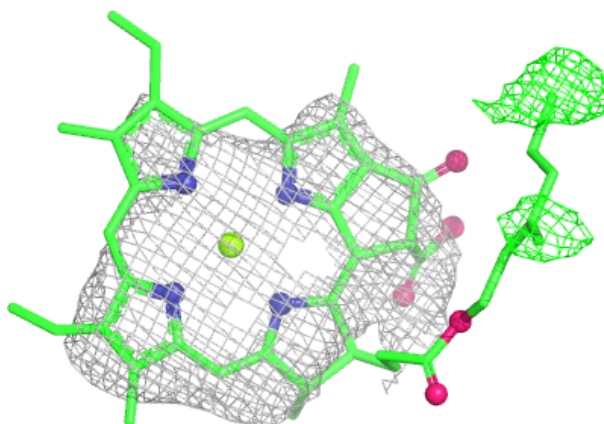
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 17  | CLA  | A     | 832 | 65/65 | 0.96 | 0.10 | 89,101,142,149              | 0     |
| 21  | BCR  | B     | 844 | 40/40 | 0.96 | 0.11 | 69,83,97,102                | 0     |
| 17  | CLA  | B     | 815 | 65/65 | 0.96 | 0.08 | 57,67,75,77                 | 0     |
| 17  | CLA  | 4     | 302 | 60/65 | 0.96 | 0.08 | 50,62,94,97                 | 0     |
| 27  | PQN  | A     | 842 | 33/33 | 0.96 | 0.10 | 49,61,85,91                 | 0     |
| 27  | PQN  | B     | 843 | 33/33 | 0.96 | 0.10 | 65,84,91,97                 | 0     |
| 17  | CLA  | B     | 810 | 65/65 | 0.97 | 0.09 | 63,73,95,101                | 0     |
| 18  | CHL  | 4     | 307 | 51/66 | 0.97 | 0.07 | 60,73,90,101                | 0     |
| 17  | CLA  | B     | 828 | 65/65 | 0.97 | 0.07 | 45,58,72,78                 | 0     |
| 17  | CLA  | A     | 818 | 65/65 | 0.97 | 0.10 | 91,103,125,130              | 0     |
| 17  | CLA  | F     | 306 | 45/65 | 0.97 | 0.06 | 55,66,75,85                 | 0     |
| 17  | CLA  | B     | 807 | 65/65 | 0.97 | 0.10 | 57,69,79,82                 | 0     |
| 17  | CLA  | A     | 813 | 45/65 | 0.97 | 0.08 | 89,111,120,126              | 0     |
| 20  | XAT  | 1     | 315 | 44/44 | 0.97 | 0.09 | 62,89,98,100                | 0     |
| 17  | CLA  | B     | 819 | 59/65 | 0.97 | 0.09 | 55,66,81,85                 | 0     |
| 22  | LHG  | A     | 844 | 49/49 | 0.97 | 0.09 | 69,83,92,96                 | 0     |
| 17  | CLA  | B     | 802 | 65/65 | 0.97 | 0.07 | 48,60,81,93                 | 0     |
| 28  | SF4  | A     | 852 | 8/8   | 0.99 | 0.04 | 55,67,73,74                 | 0     |
| 28  | SF4  | C     | 101 | 8/8   | 0.99 | 0.03 | 69,76,84,85                 | 0     |
| 28  | SF4  | C     | 102 | 8/8   | 0.99 | 0.03 | 75,76,85,89                 | 0     |

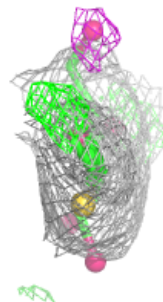
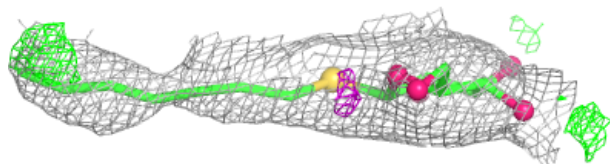
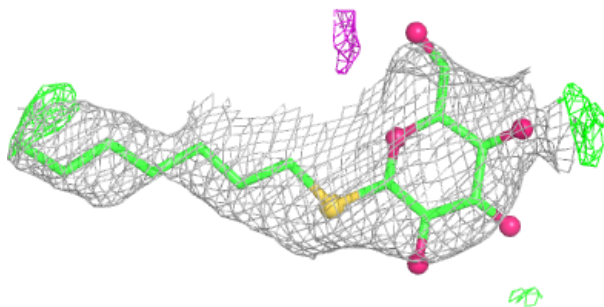
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around CLA A 843:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

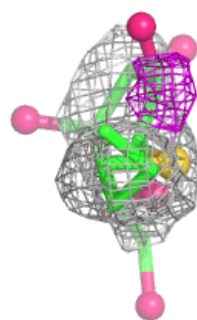
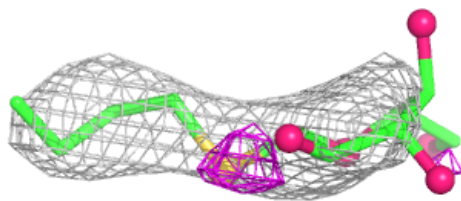
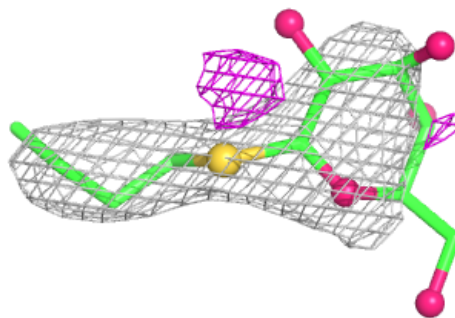
**Electron density around HTG 4 322:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HTG F 310:**

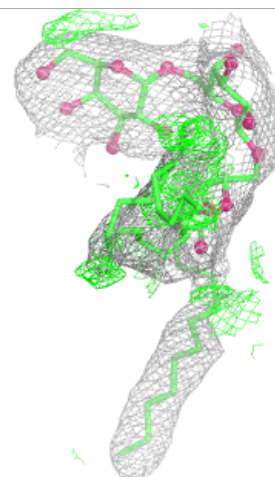
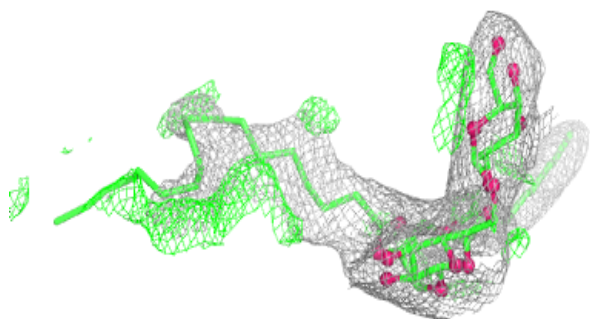
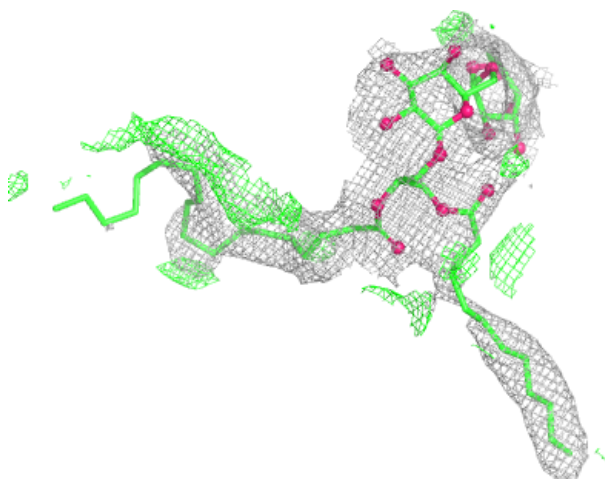
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around DGD 4 323:**

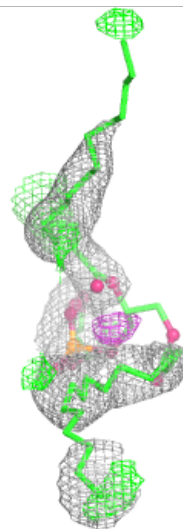
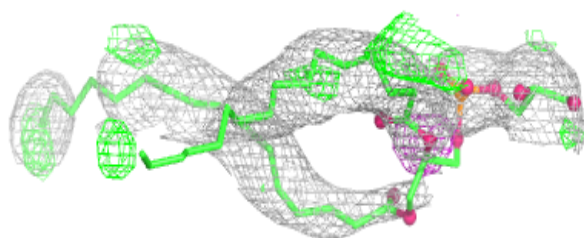
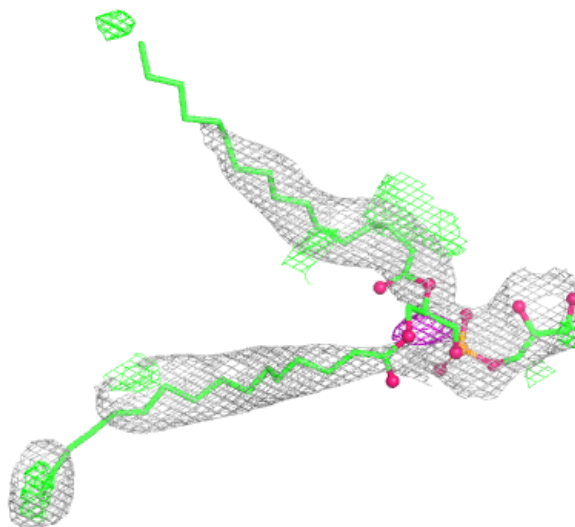
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





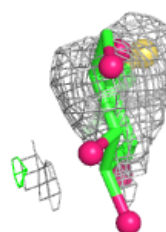
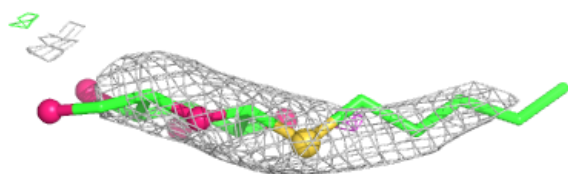
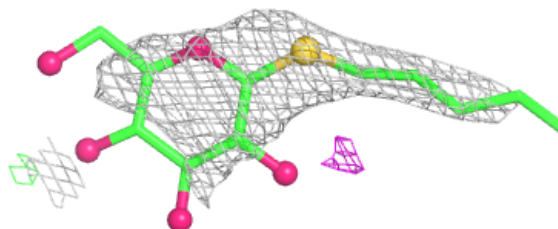
**Electron density around LHG G 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

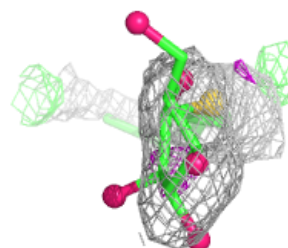
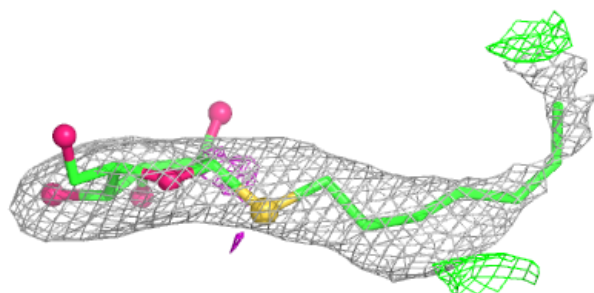
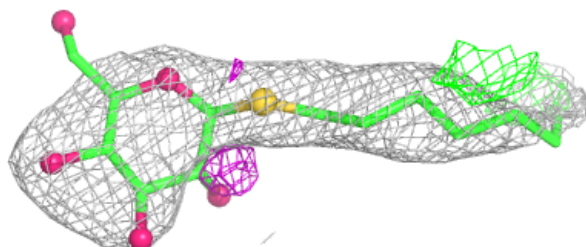


**Electron density around HTG F 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

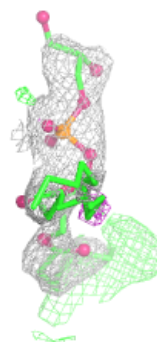
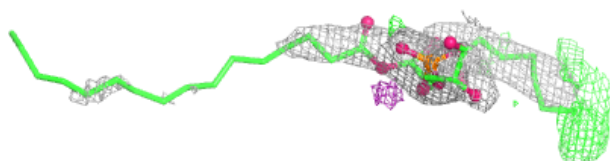
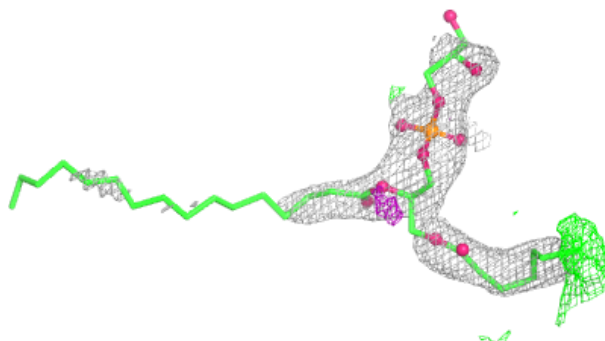
**Electron density around HTG B 851:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

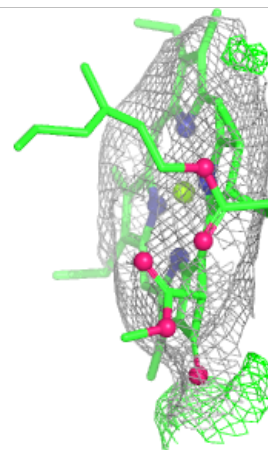
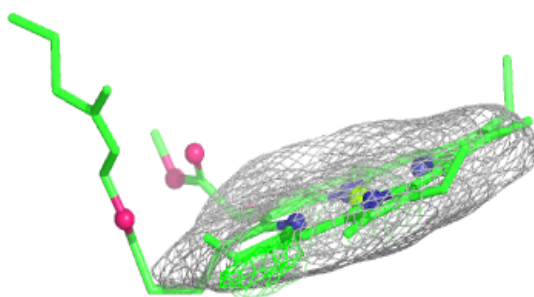
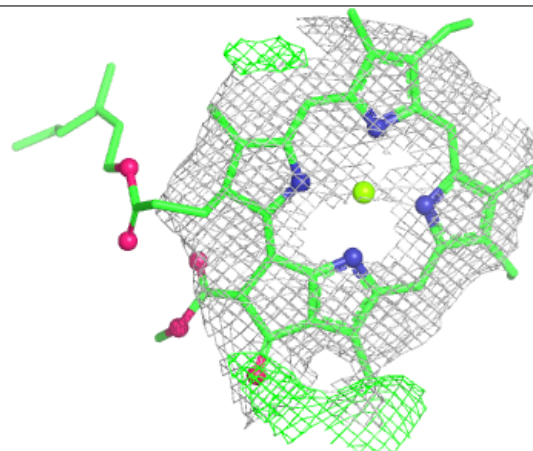


**Electron density around LHG F 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

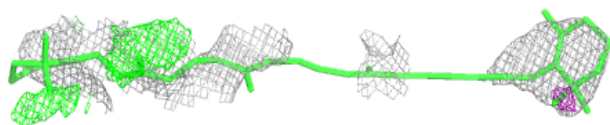
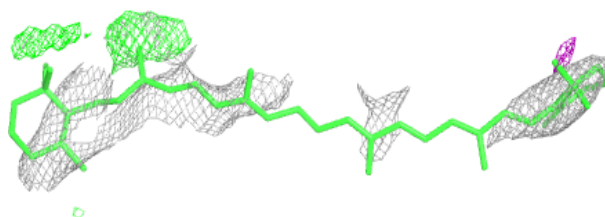
**Electron density around CLA 3 610:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

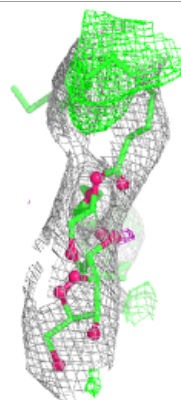
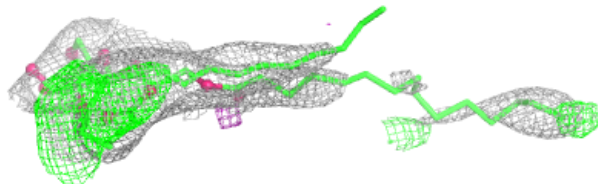
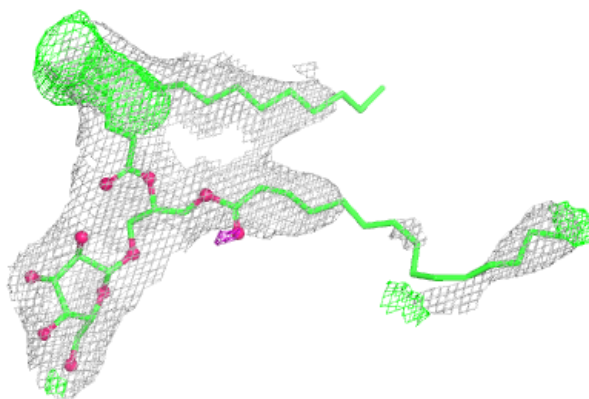


**Electron density around BCR K 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

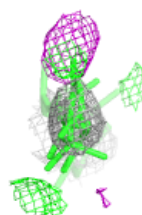
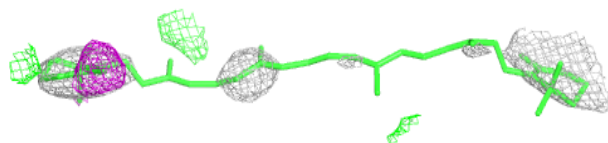
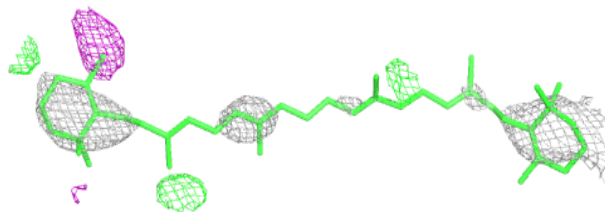
**Electron density around LMG B 852:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

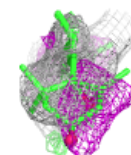
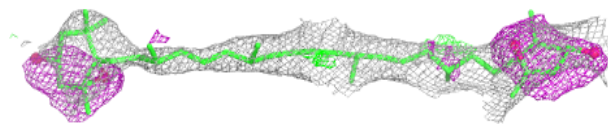
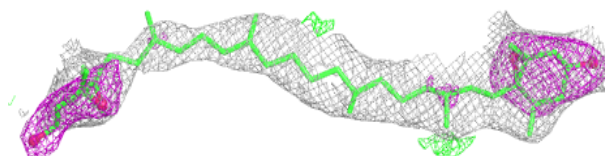


**Electron density around BCR 2 316:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

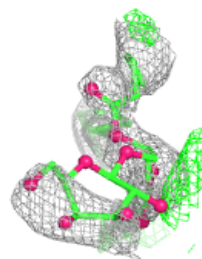
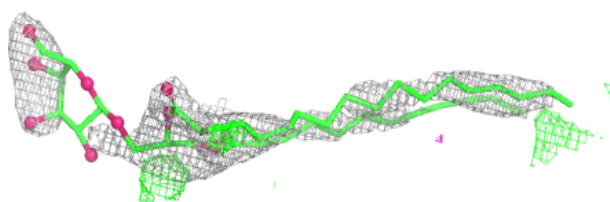
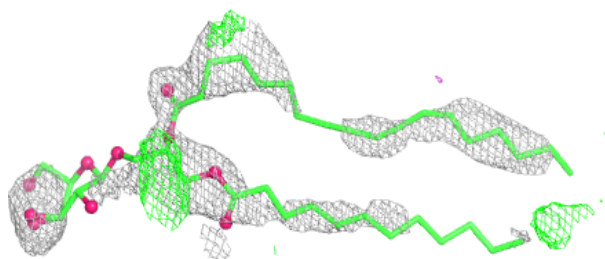
**Electron density around XAT 3 615:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



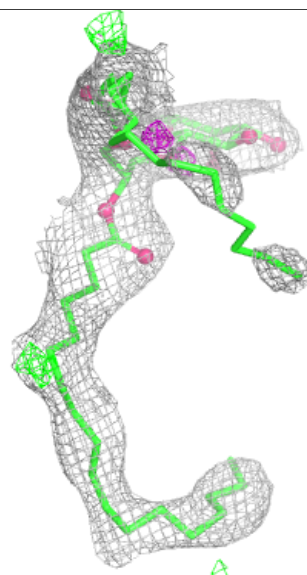
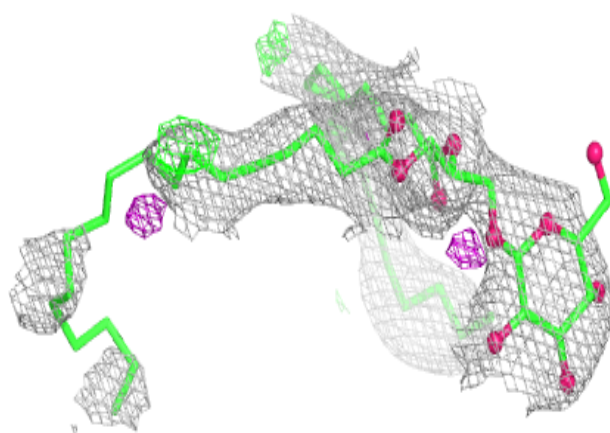
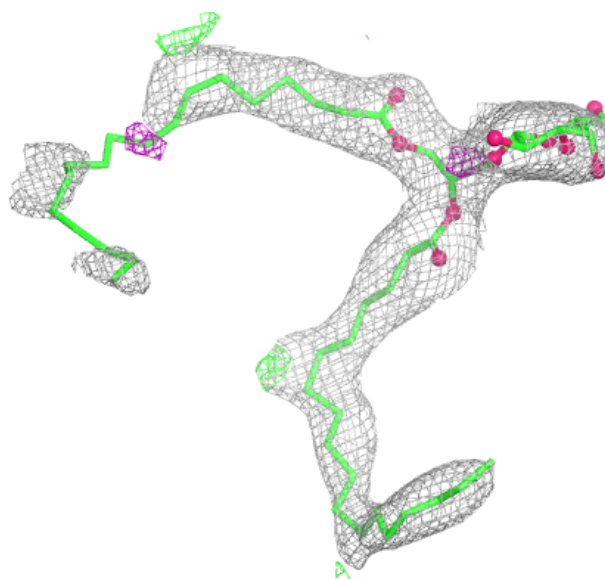
**Electron density around LMG 4 320:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LMG F 309:**

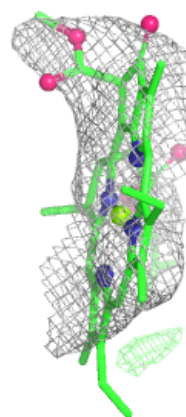
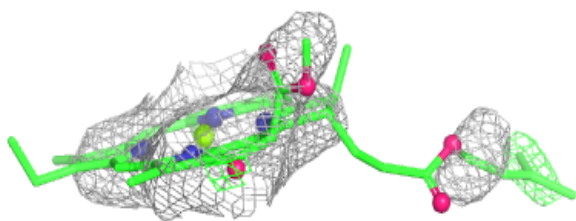
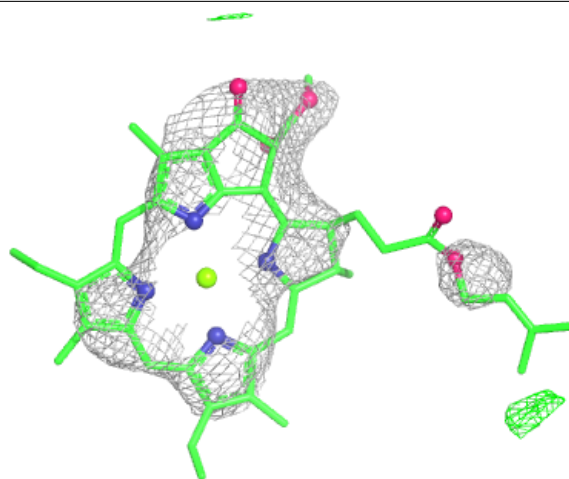
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA L 204:**

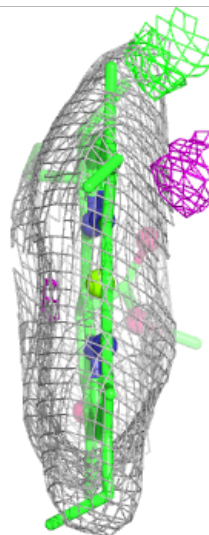
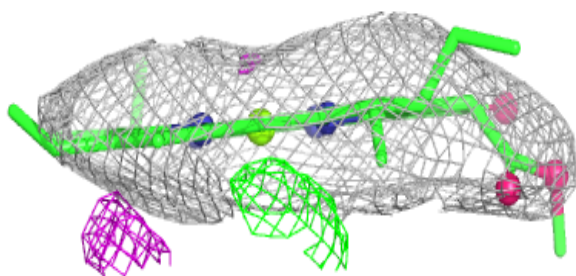
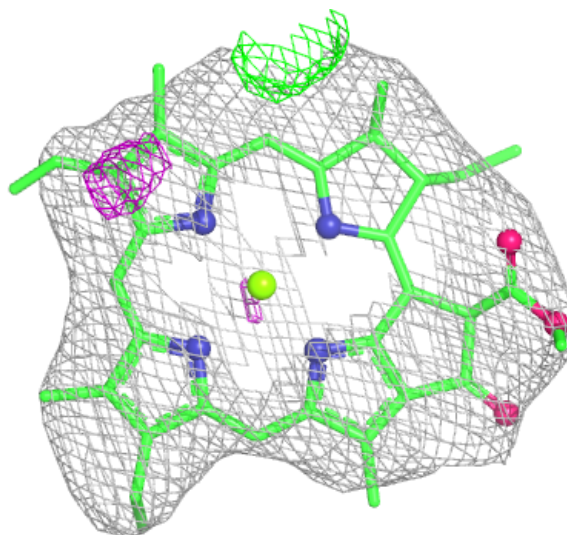
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





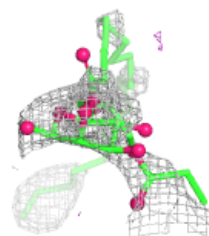
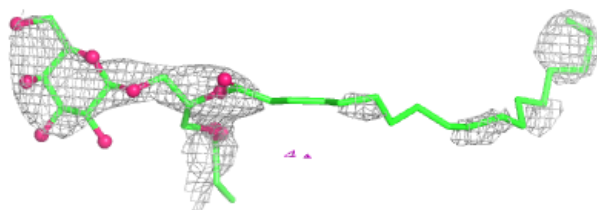
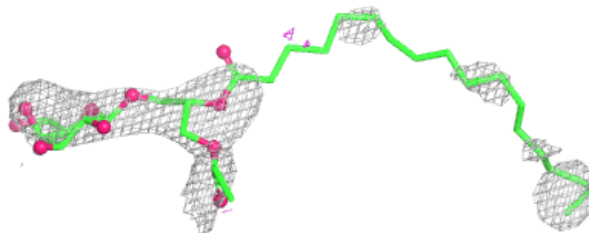
**Electron density around CLA J 103:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

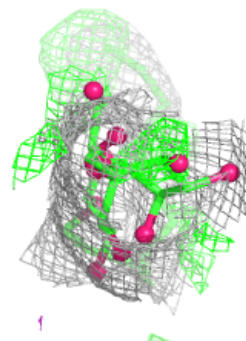
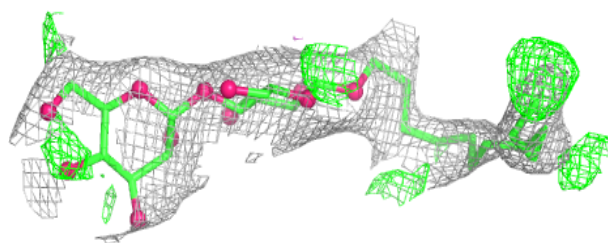
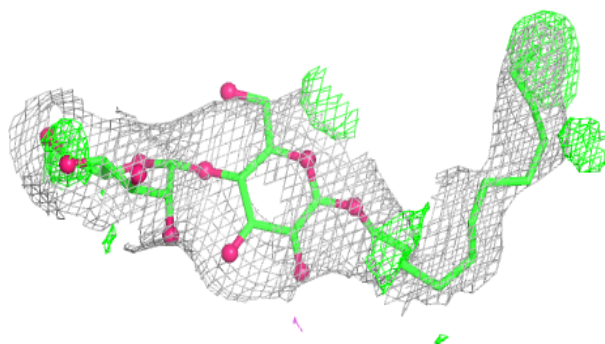


**Electron density around LMG G 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

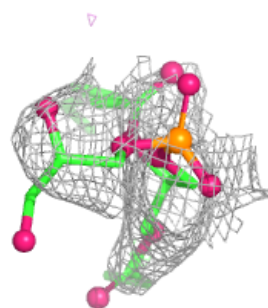
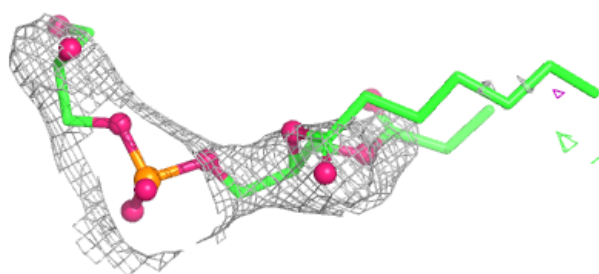
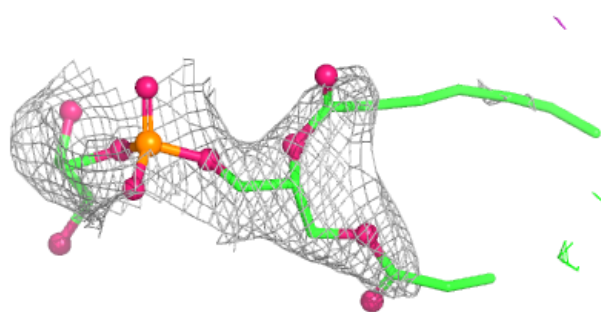
**Electron density around LMT 2 318:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

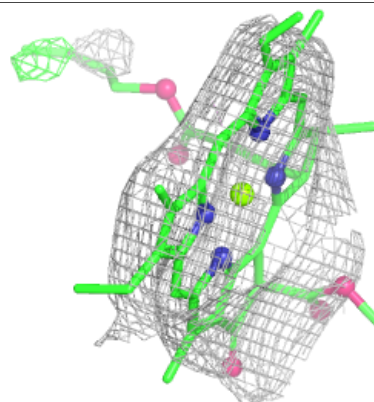
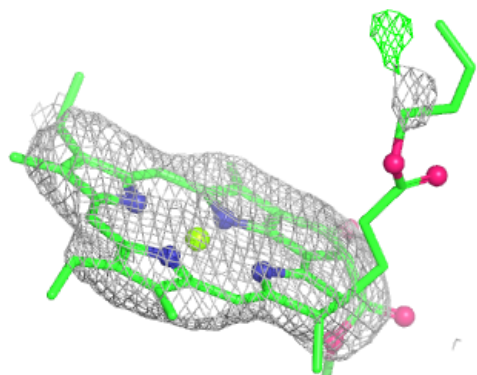
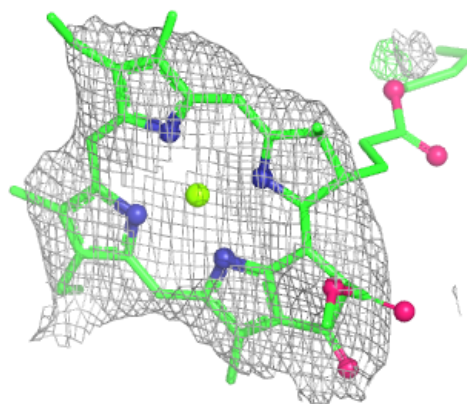


**Electron density around LHG A 845:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

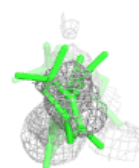
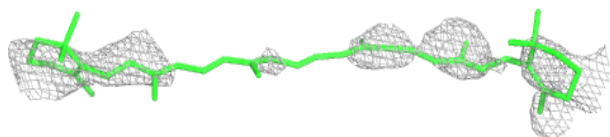
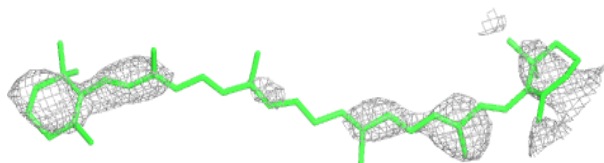
**Electron density around CLA A 821:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

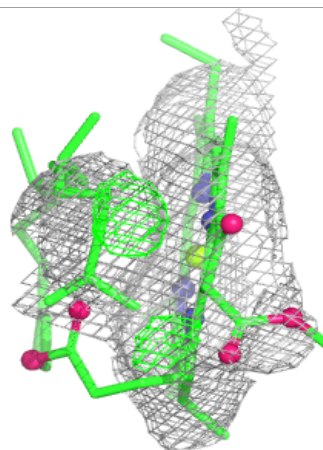
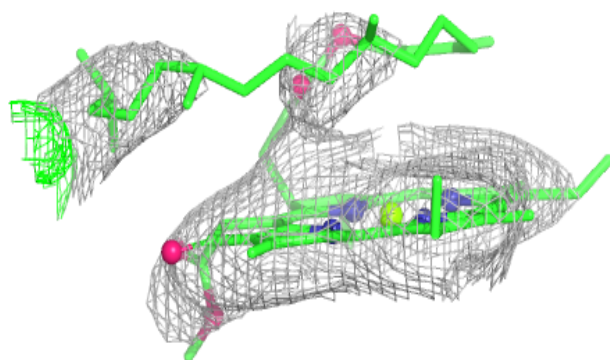
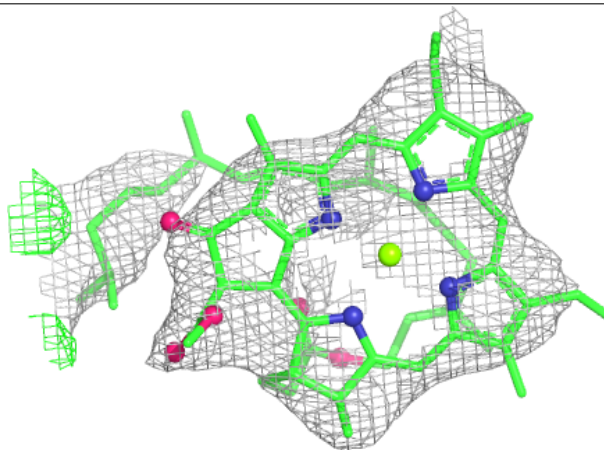


**Electron density around BCR 3 616:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

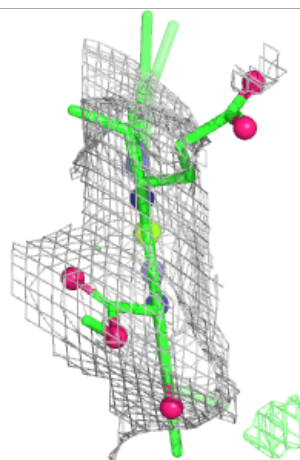
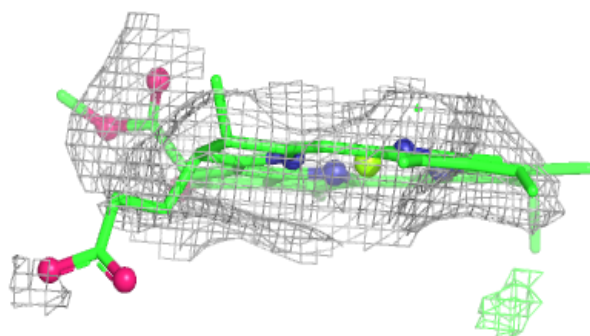
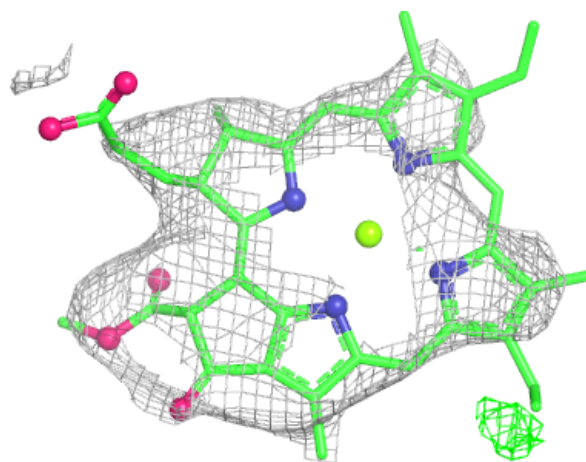
**Electron density around CLA L 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 3 612:**

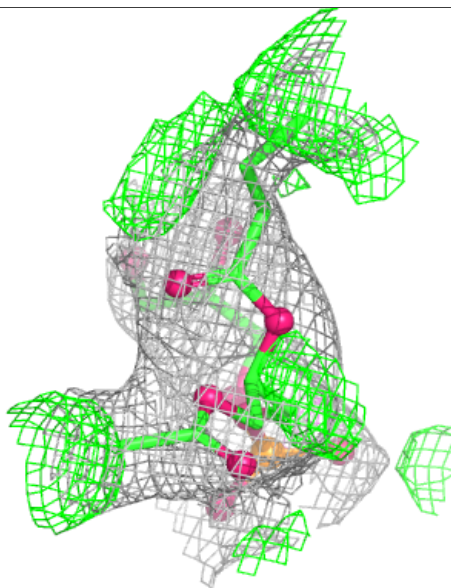
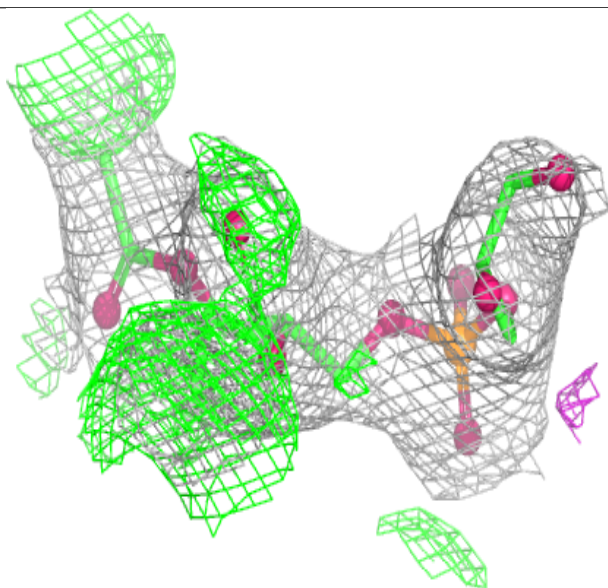
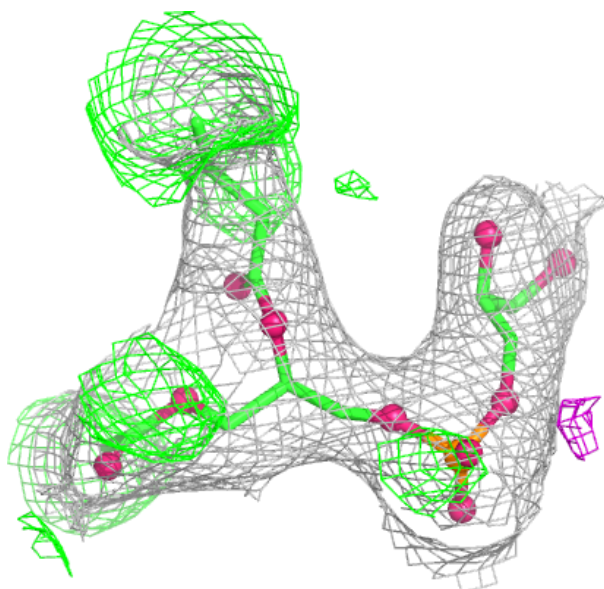
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





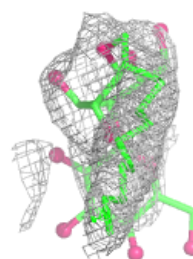
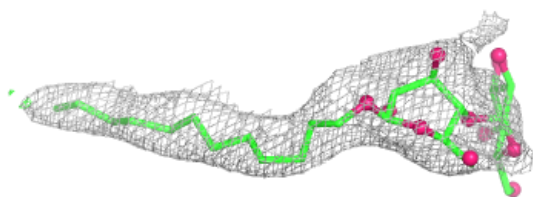
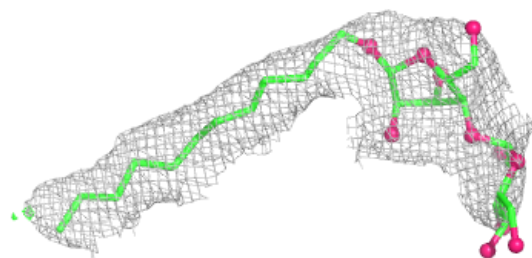
**Electron density around LHG B 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



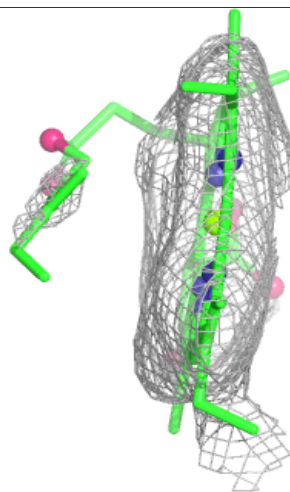
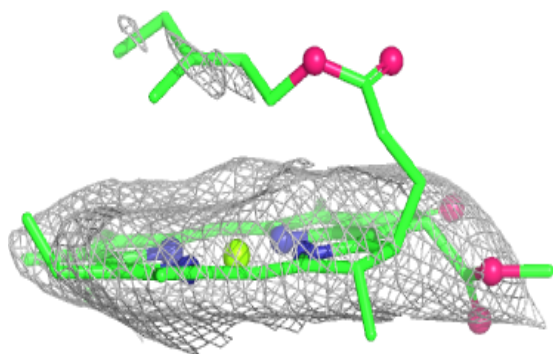
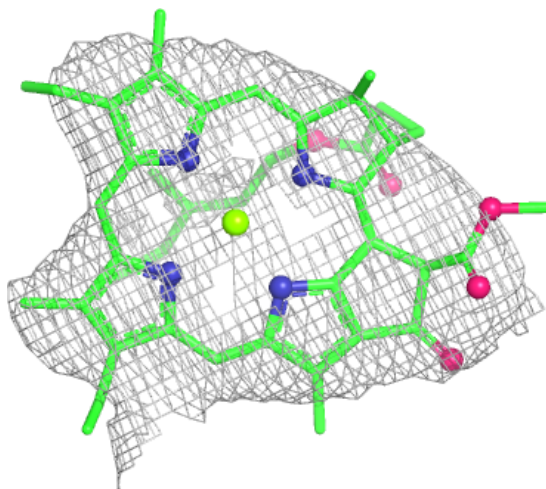
**Electron density around LMT A 855:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 822:**

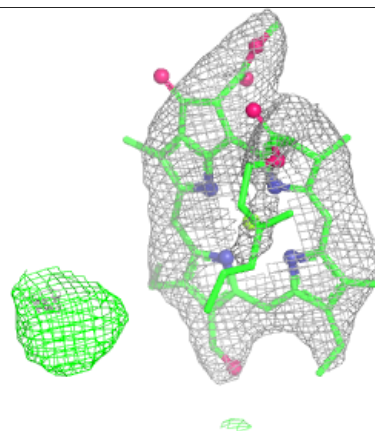
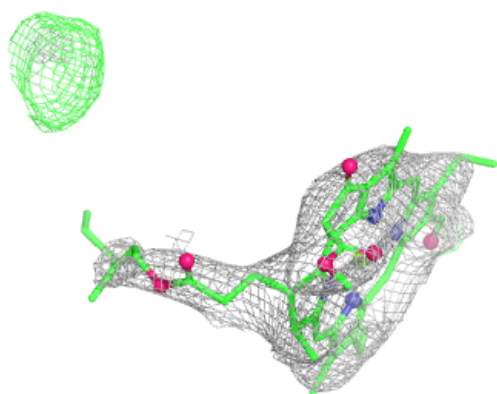
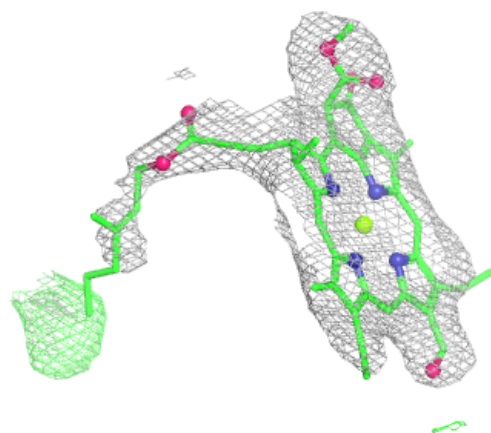
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



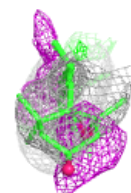
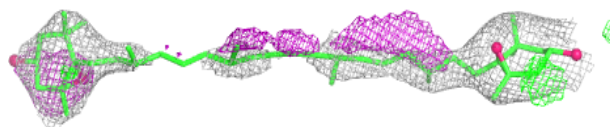
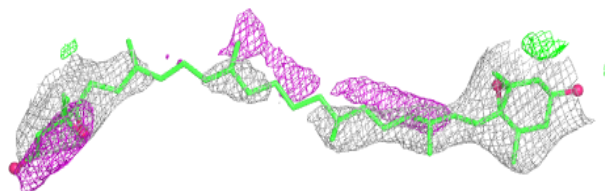


**Electron density around CHL 3 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

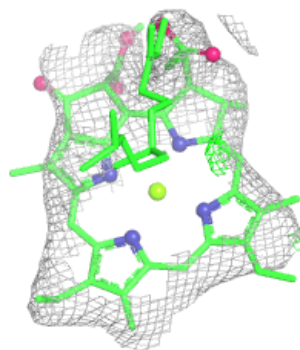
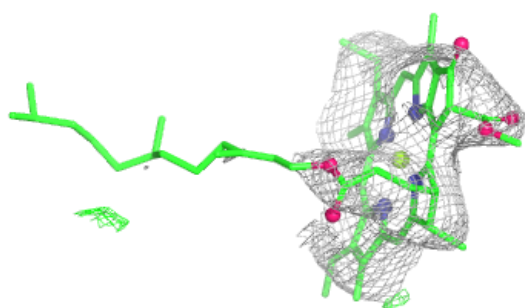
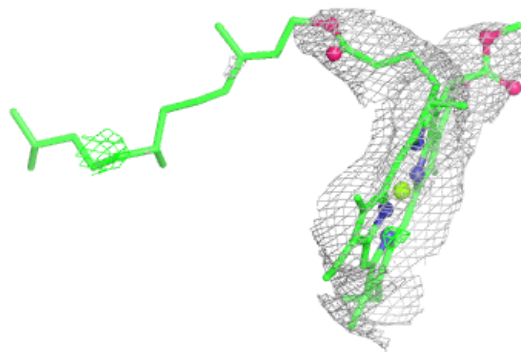
**Electron density around XAT 2 315:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

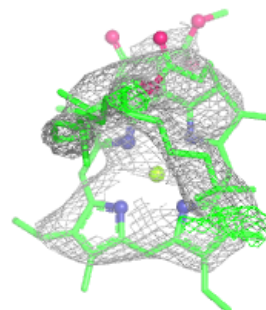
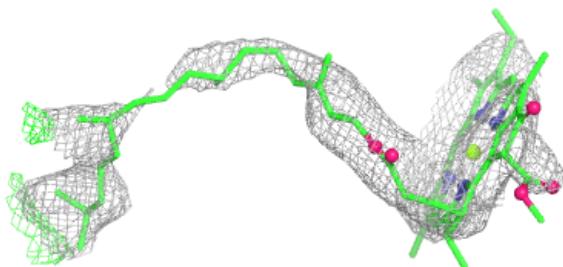
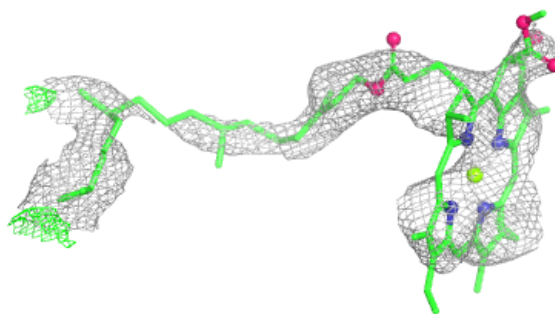


**Electron density around CLA 2 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

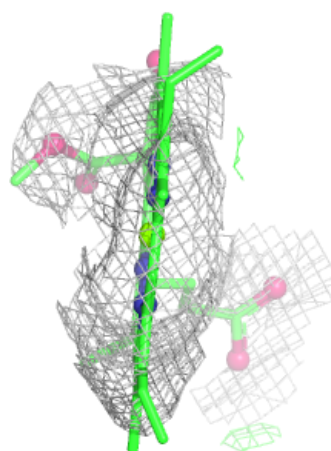
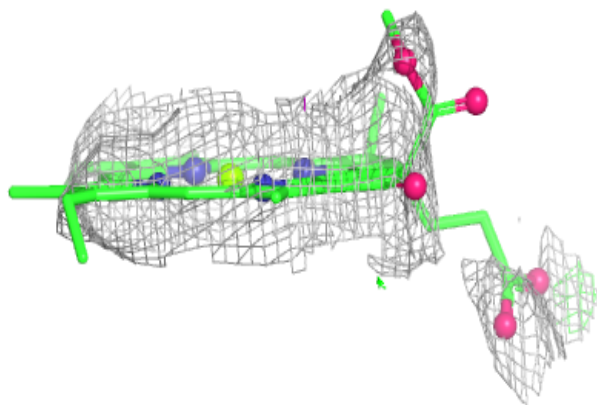
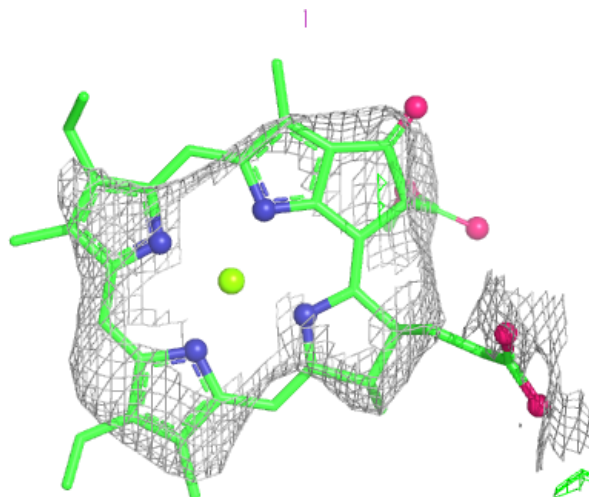
**Electron density around CLA L 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



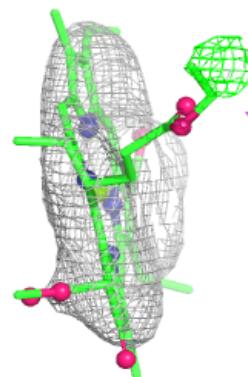
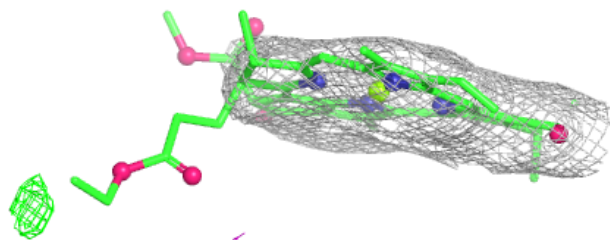
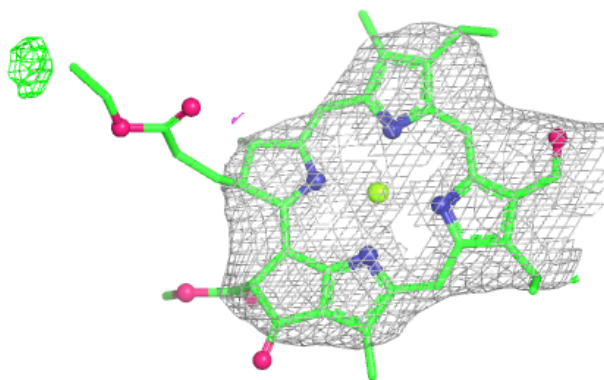
**Electron density around CLA K 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

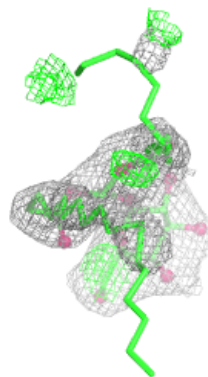
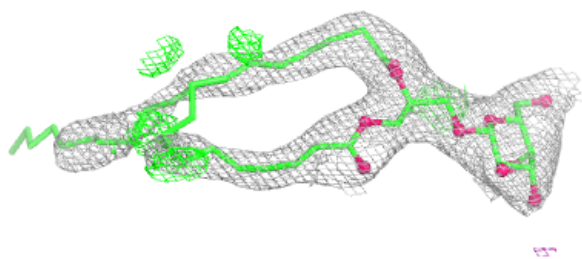
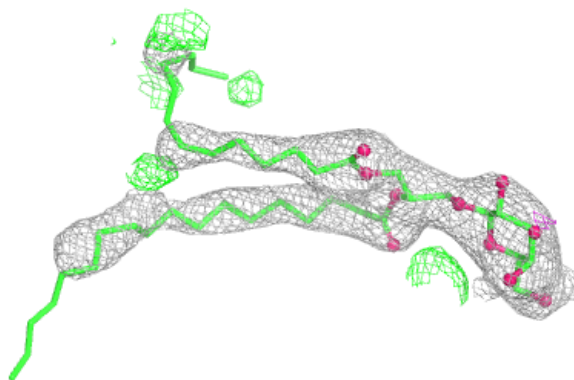


**Electron density around CHL 2 305:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

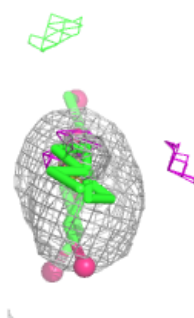
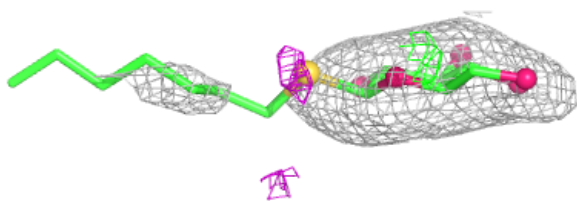
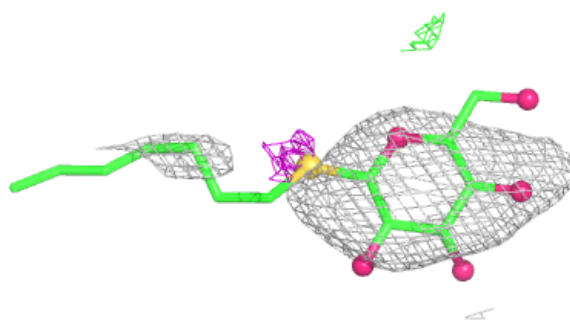
**Electron density around LMG 4 319:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



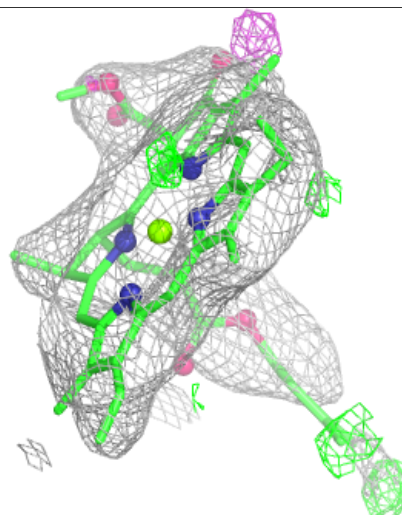
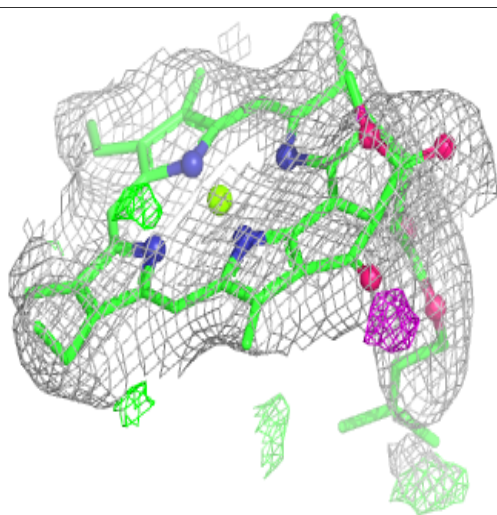
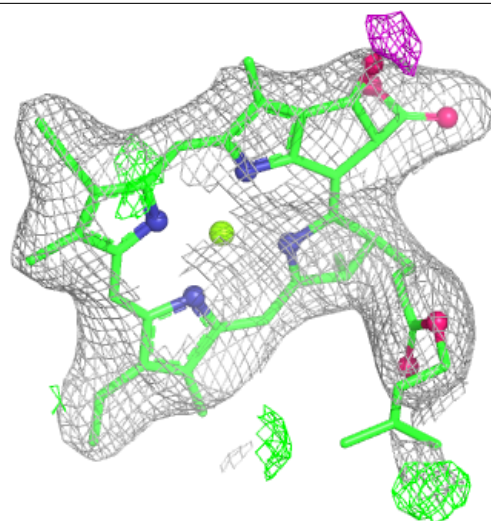
**Electron density around HTG 4 321:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 4 304:**

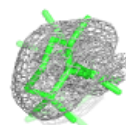
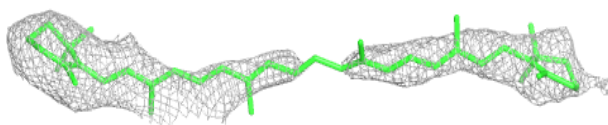
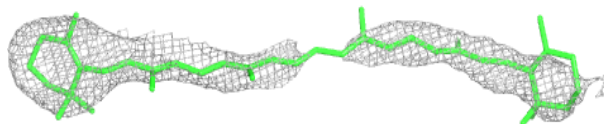
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





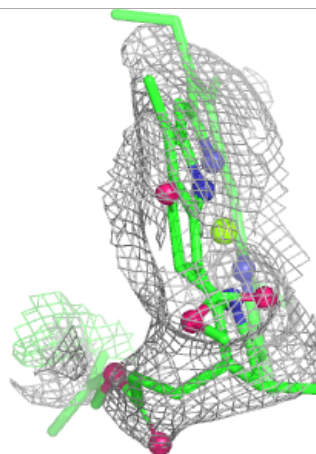
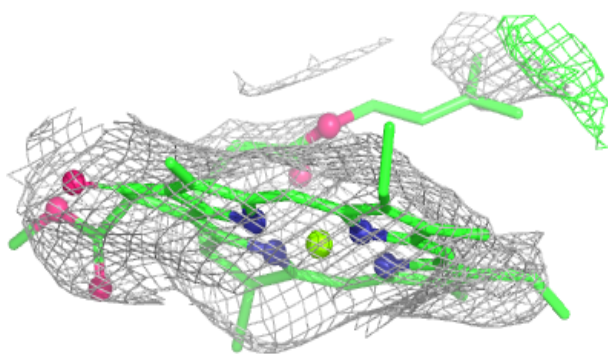
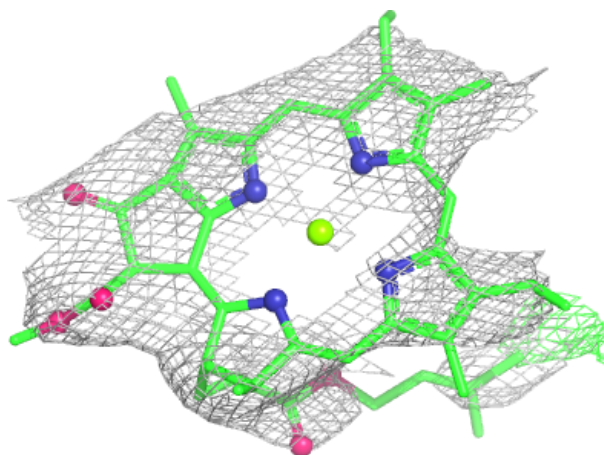
**Electron density around BCR L 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 3 609:**

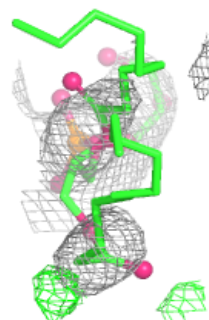
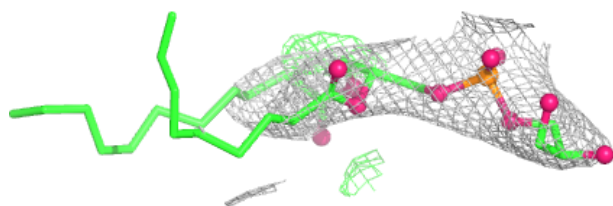
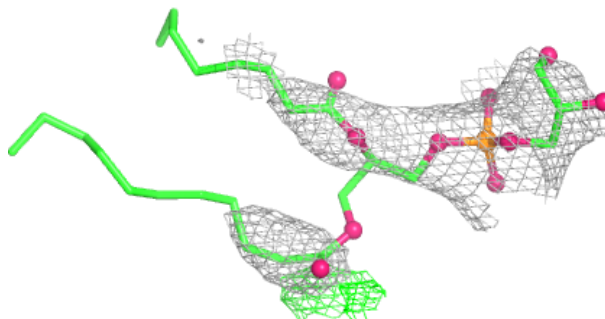
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





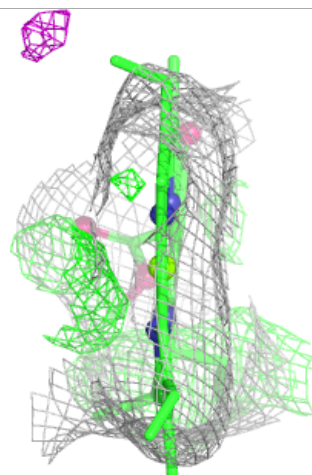
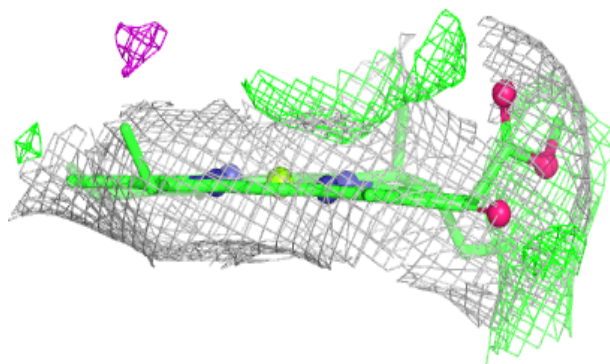
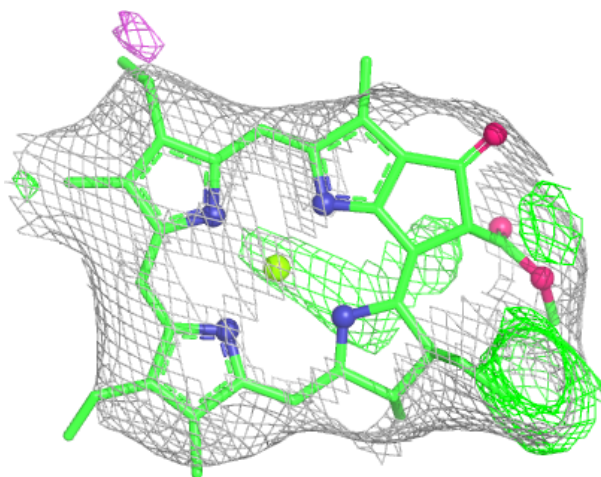
**Electron density around LHG 2 317:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



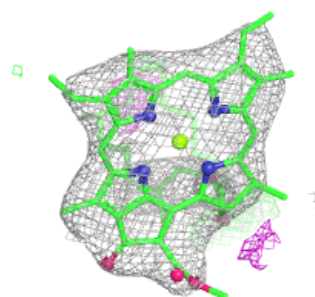
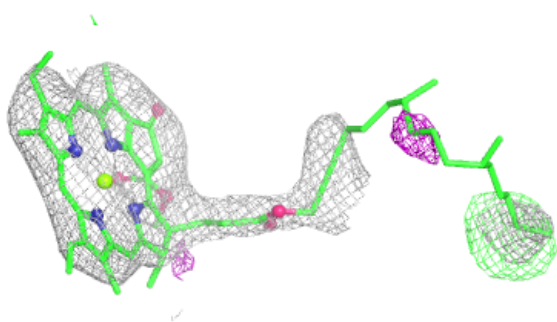
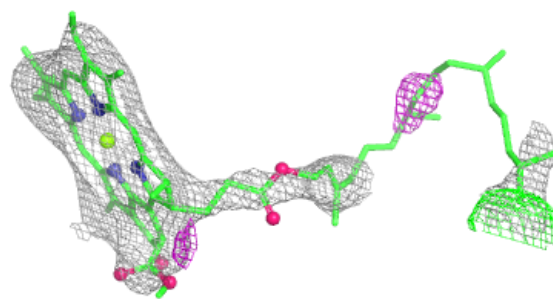
**Electron density around CLA 1 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



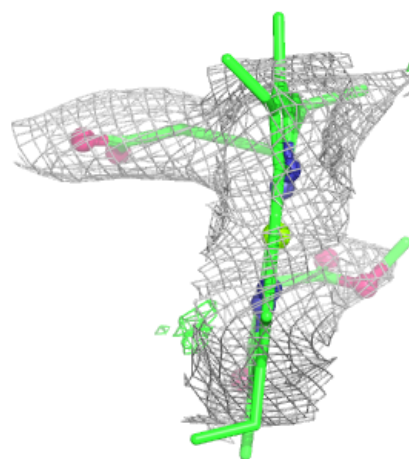
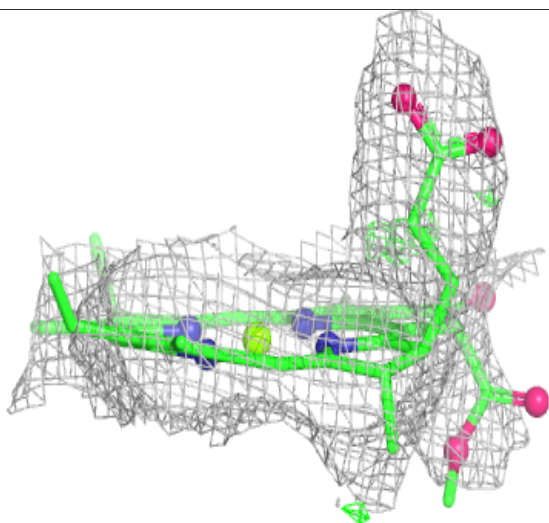
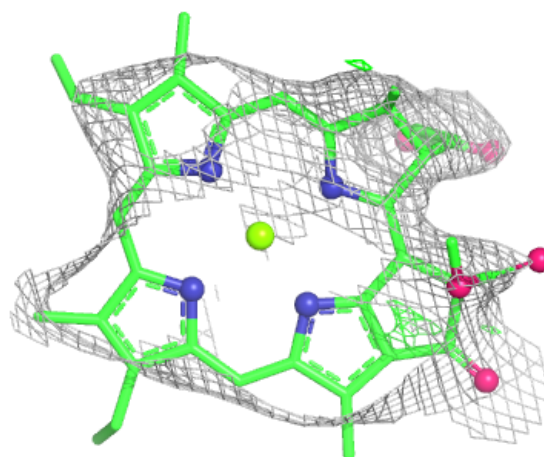
**Electron density around CLA A 837:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



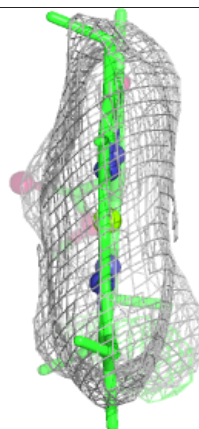
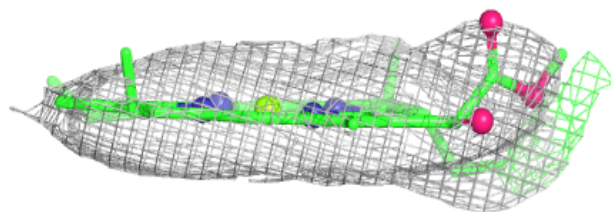
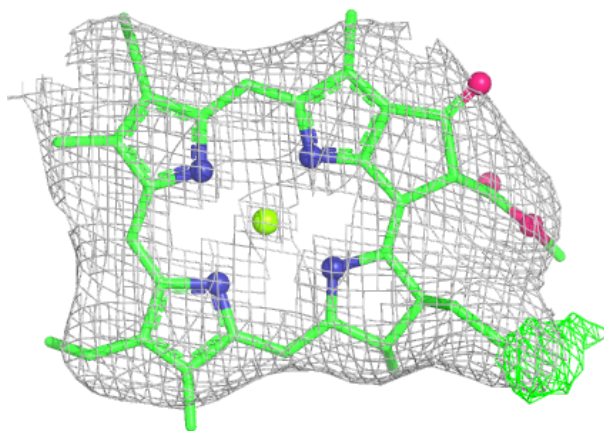
**Electron density around CLA 3 604:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



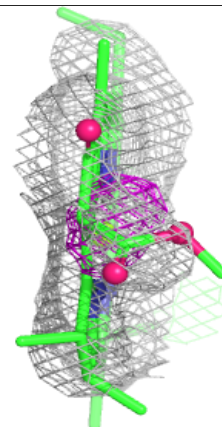
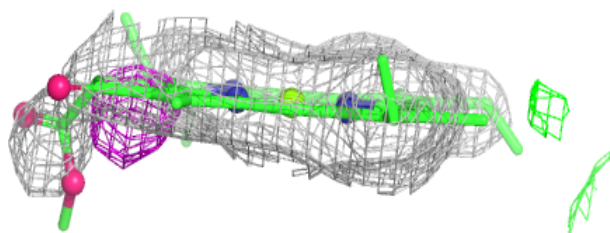
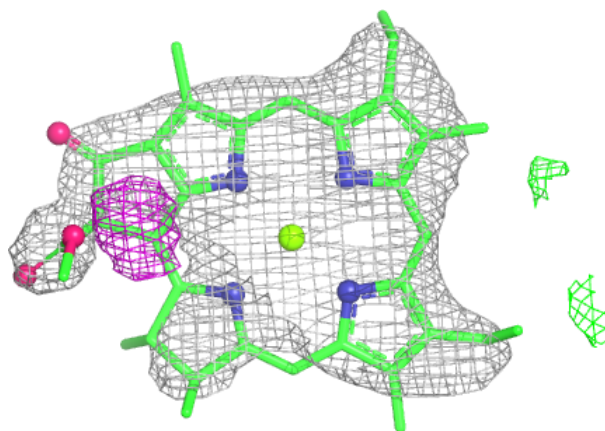
**Electron density around CLA 3 605:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

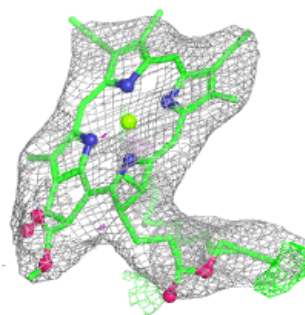
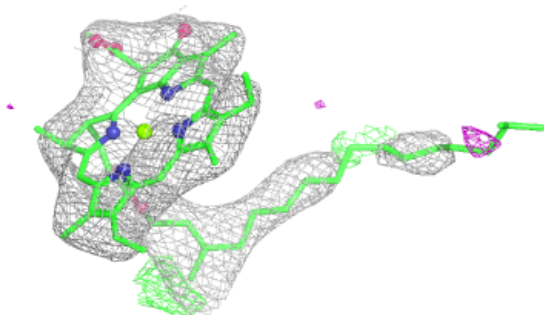
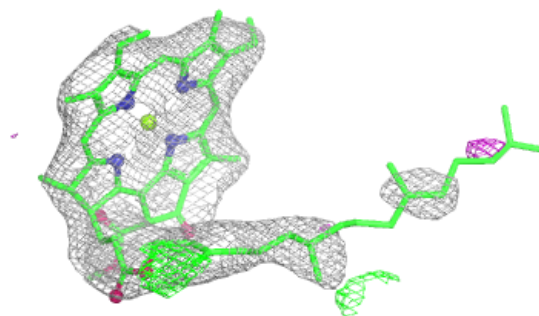


**Electron density around CLA G 103:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA 1 307:**

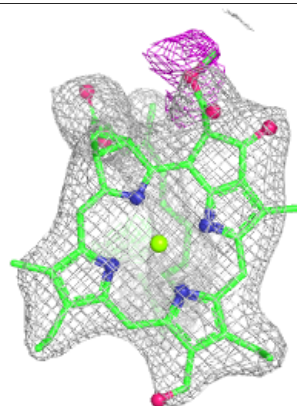
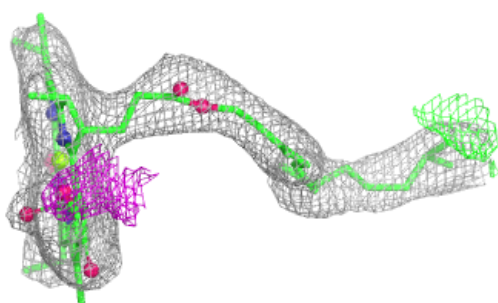
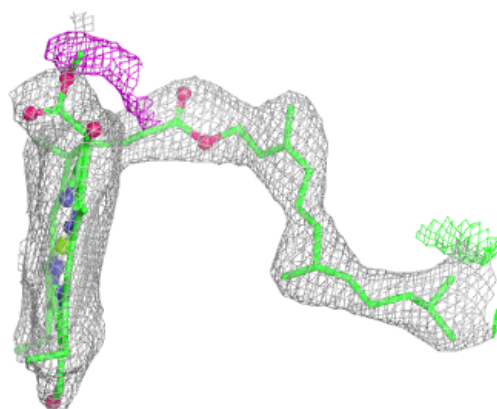
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



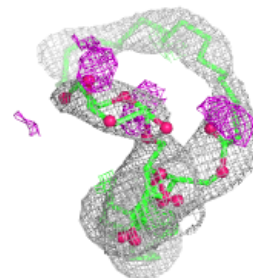
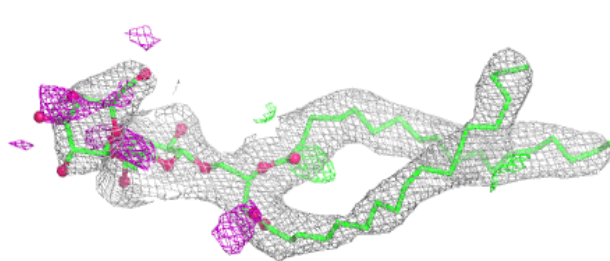
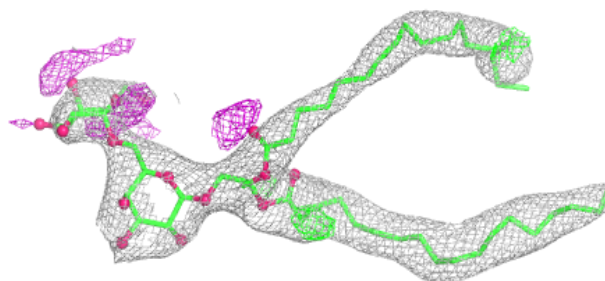


**Electron density around CHL 4 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

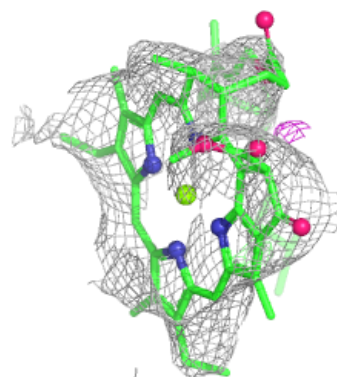
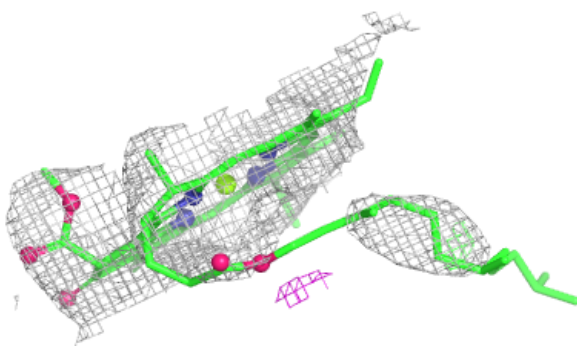
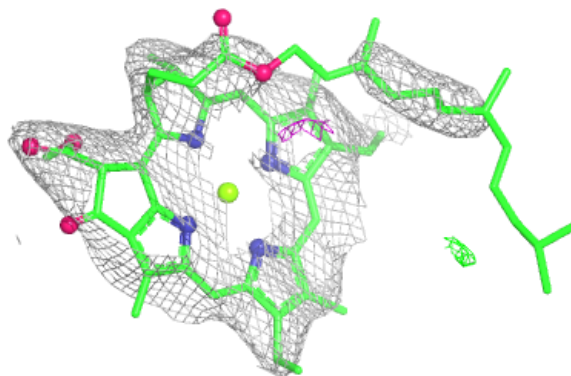
**Electron density around DGD B 850:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

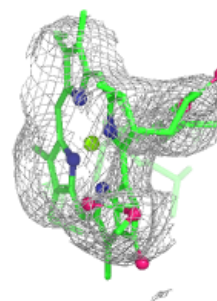
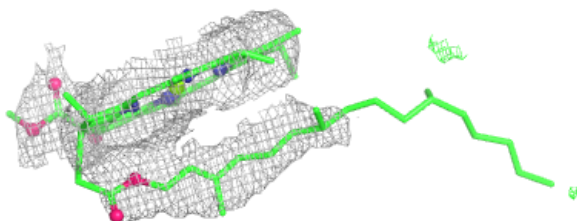
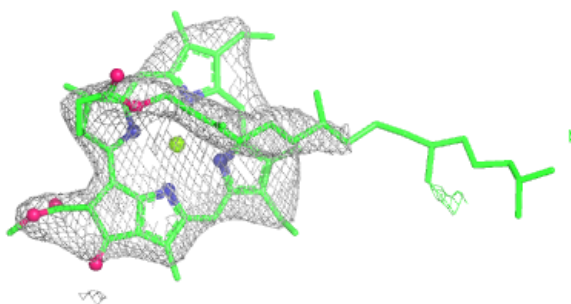


**Electron density around CLA 3 602:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 817:**

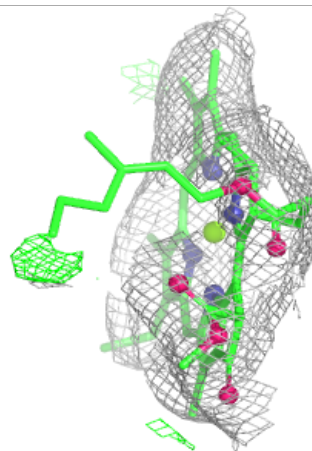
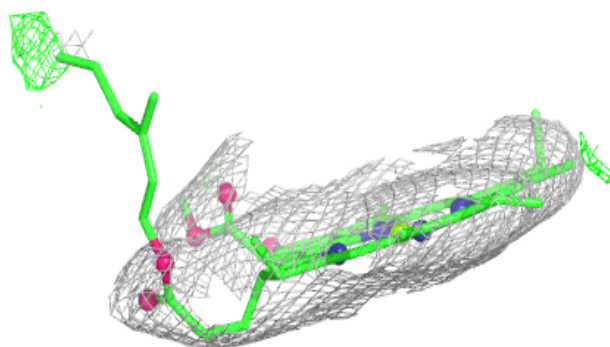
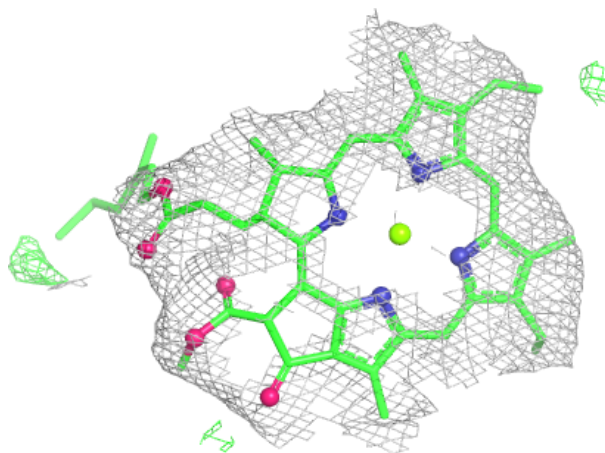
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





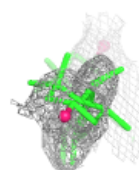
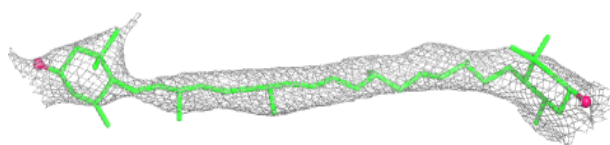
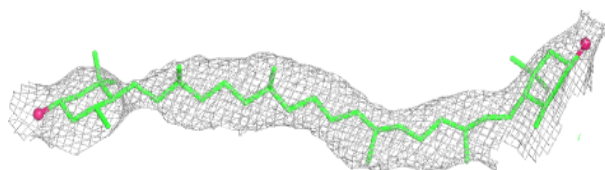
**Electron density around CLA 2 310:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

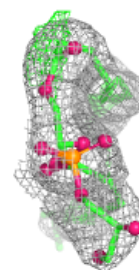
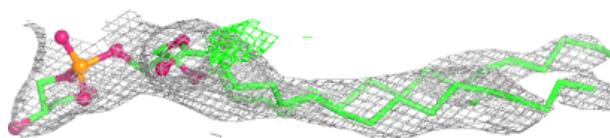
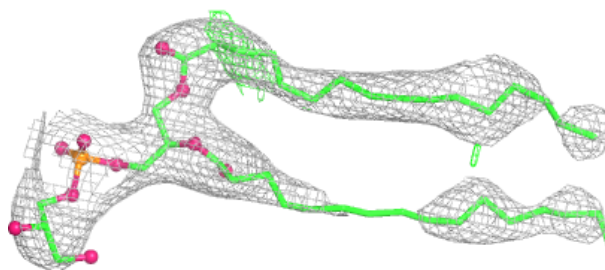


**Electron density around LUT 3 614:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

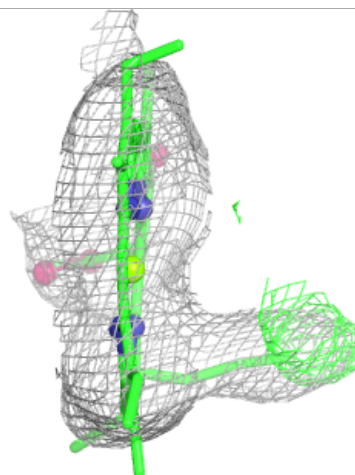
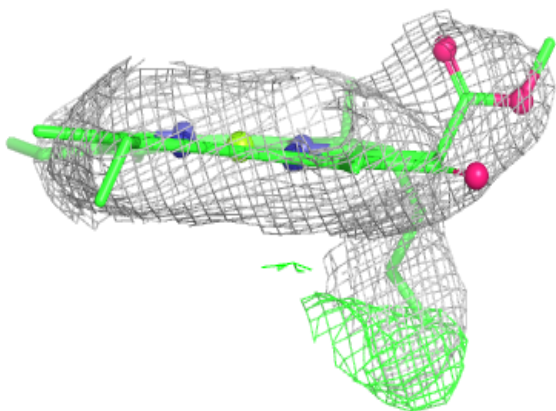
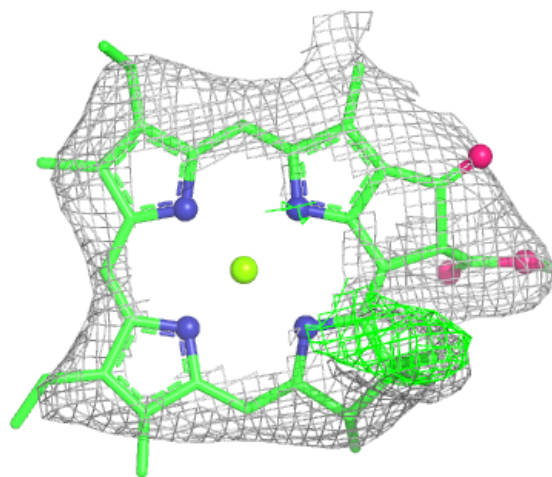
**Electron density around LHG 1 317:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



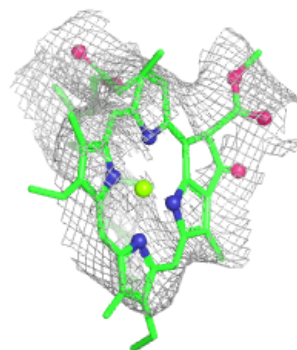
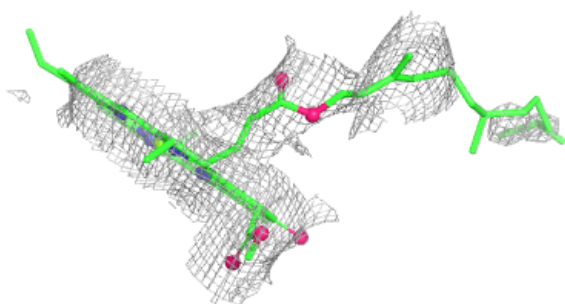
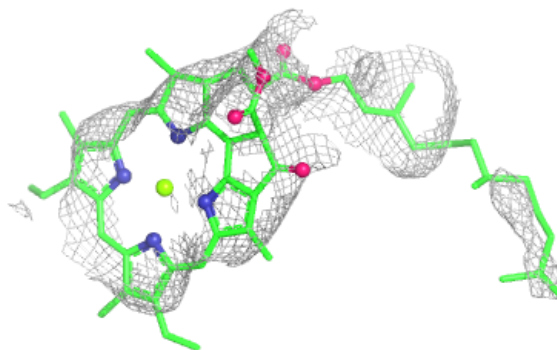
**Electron density around CLA 2 312:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

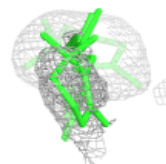
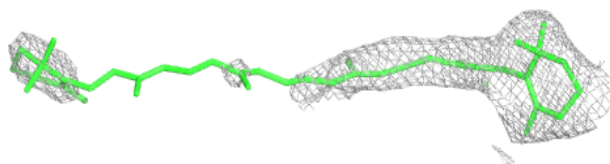
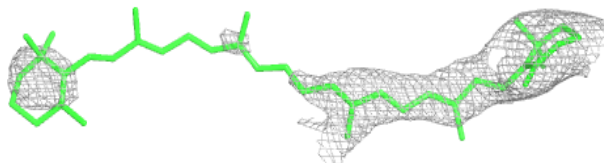


**Electron density around CLA K 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

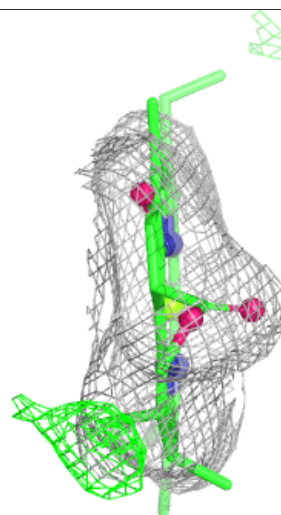
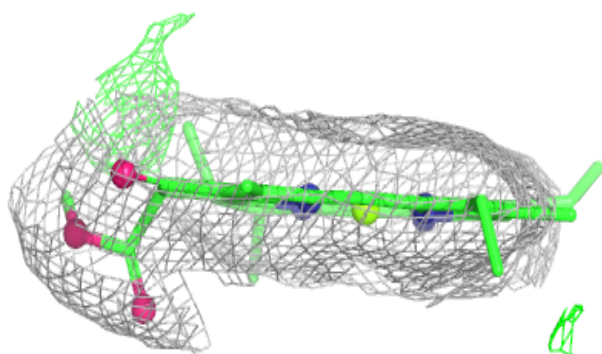
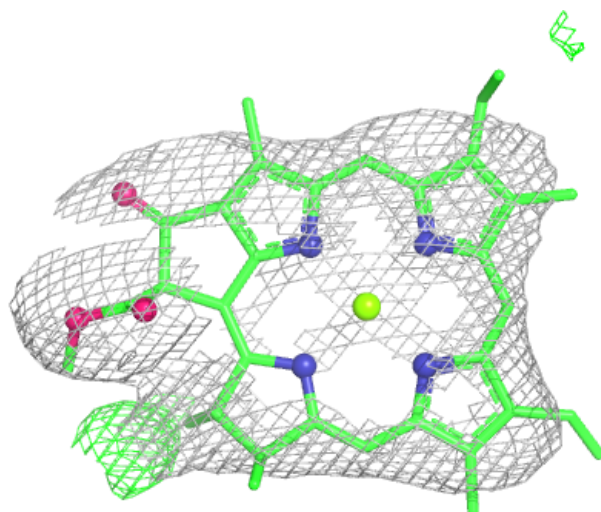
**Electron density around BCR 1 316:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



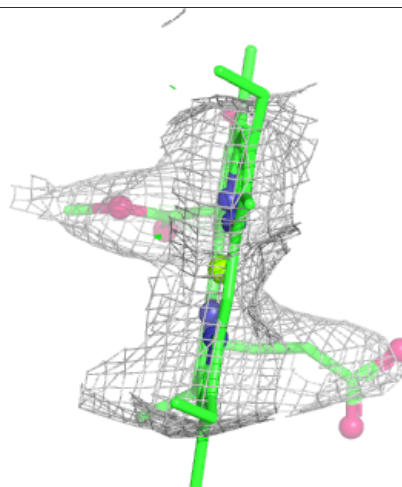
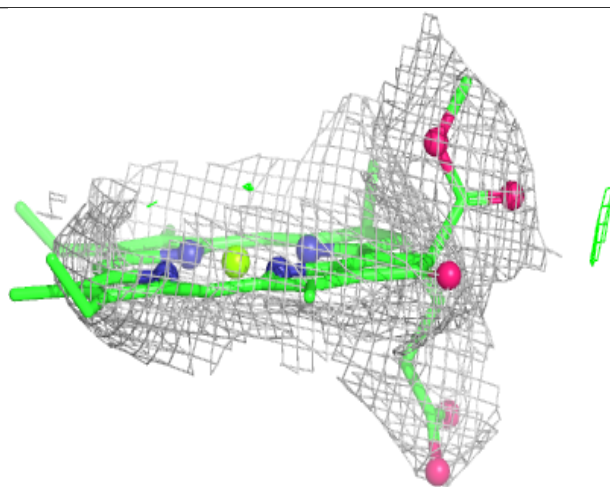
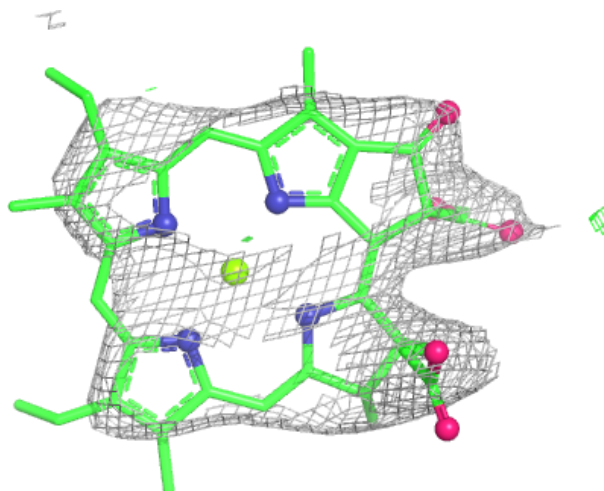
**Electron density around CLA 2 309:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 819:**

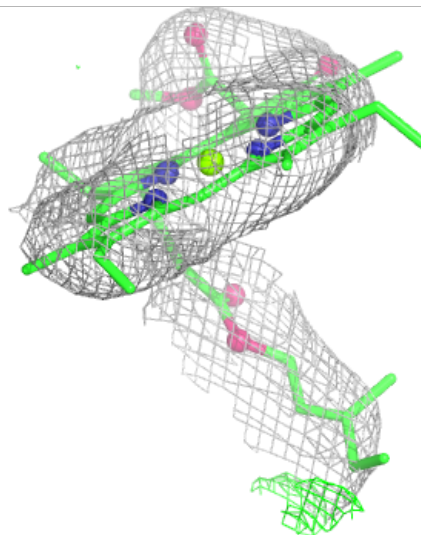
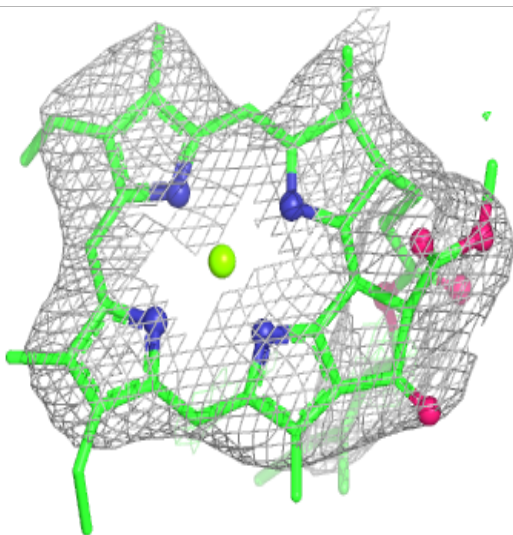
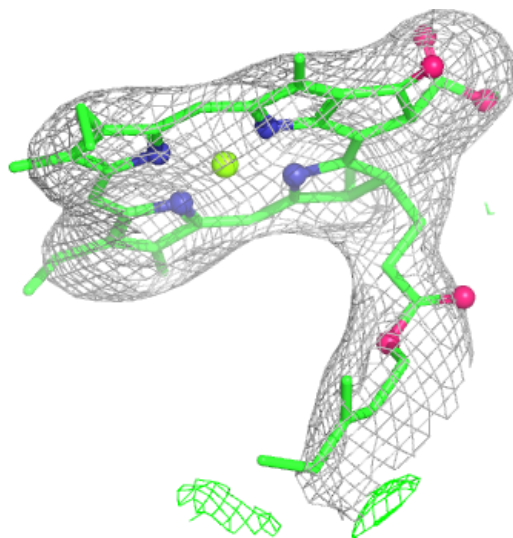
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





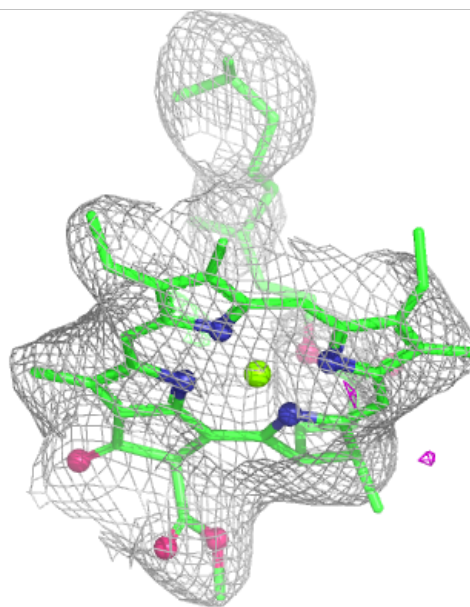
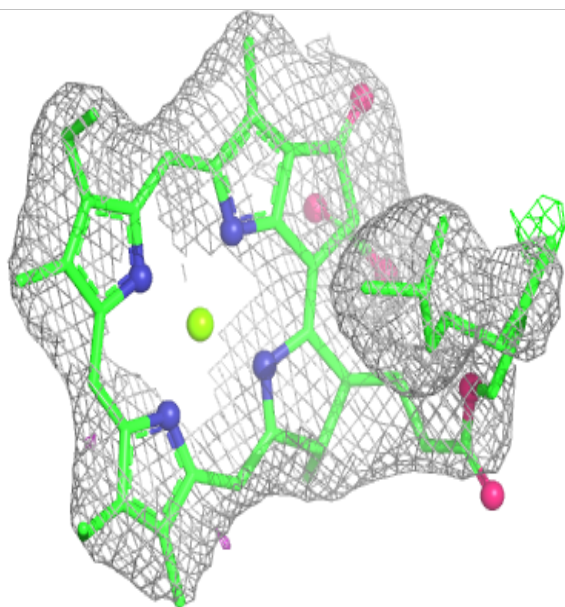
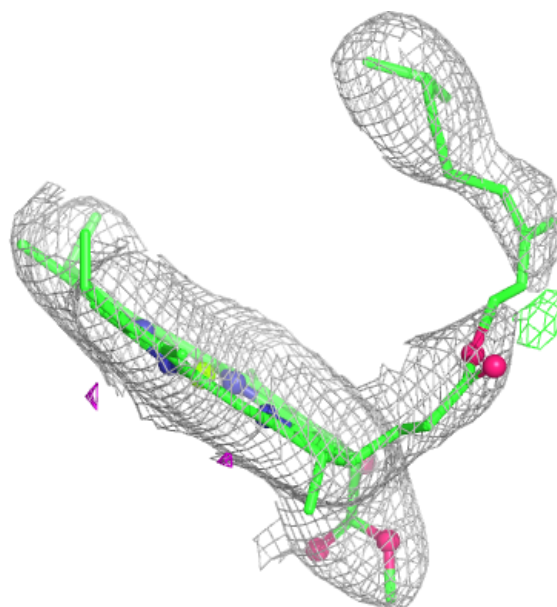
**Electron density around CLA 1 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 1 312:**

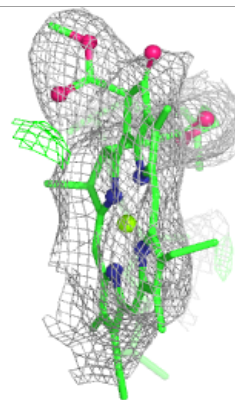
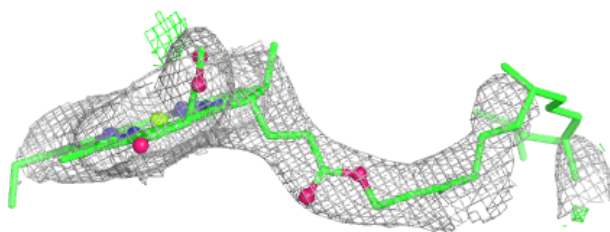
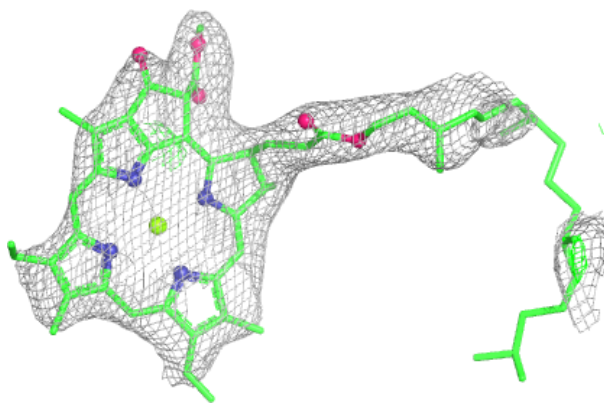
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



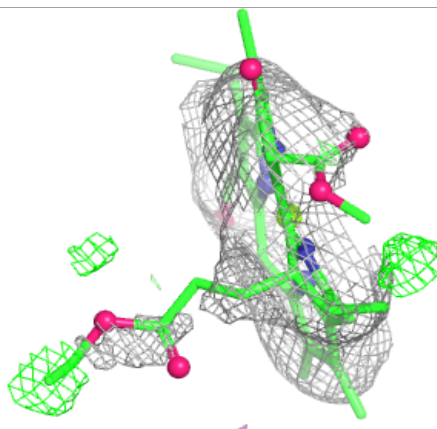
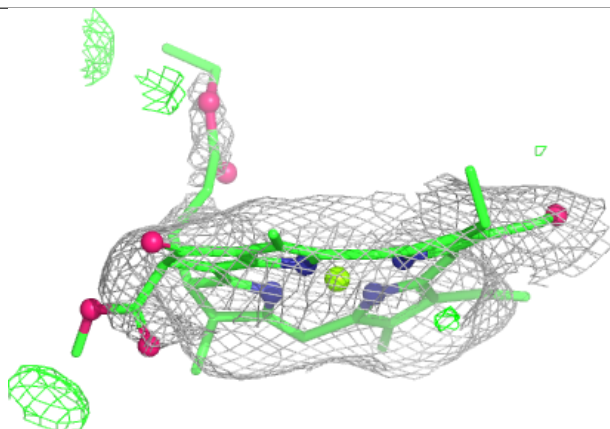
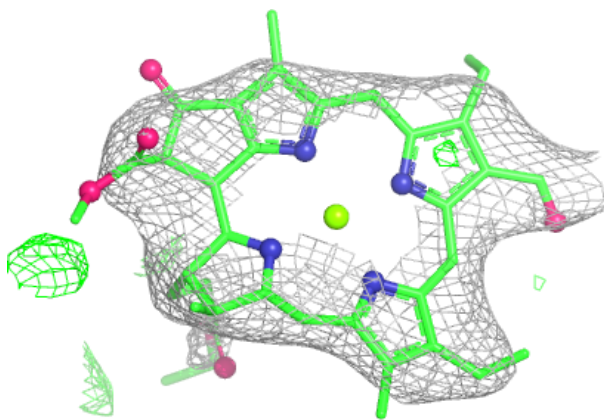


**Electron density around CLA A 825:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

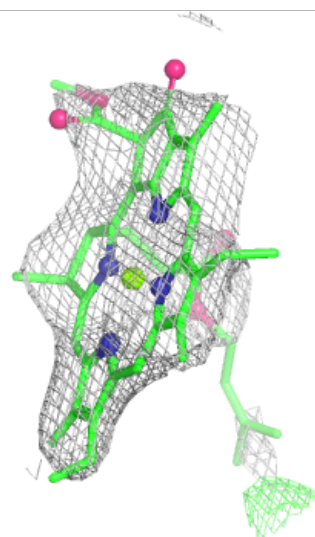
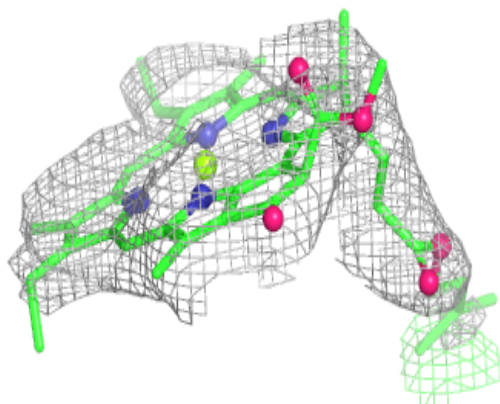
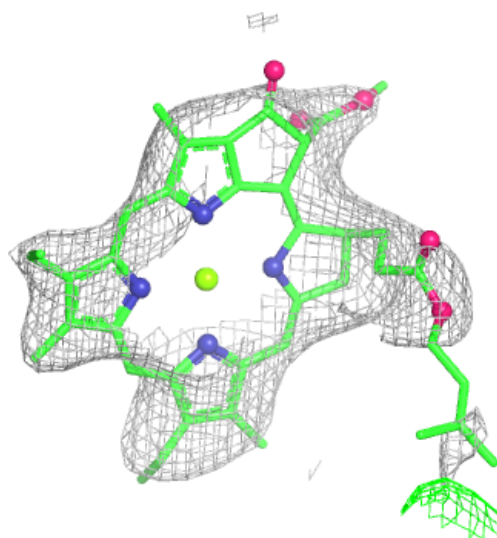
**Electron density around CHL 1 305:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



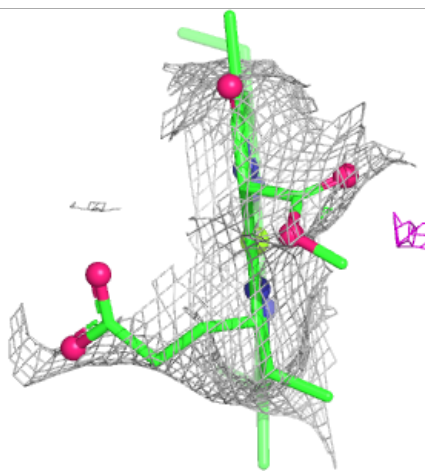
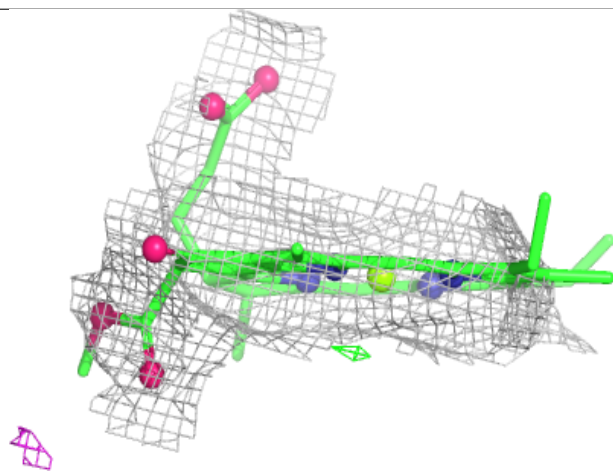
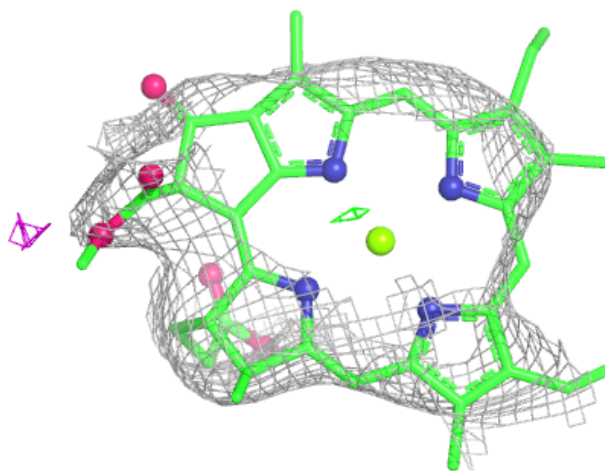
**Electron density around CLA A 833:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



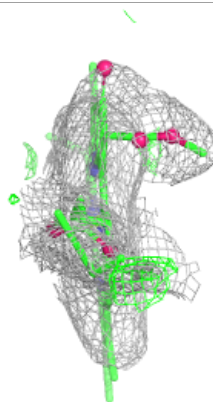
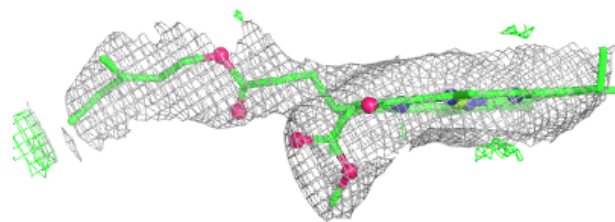
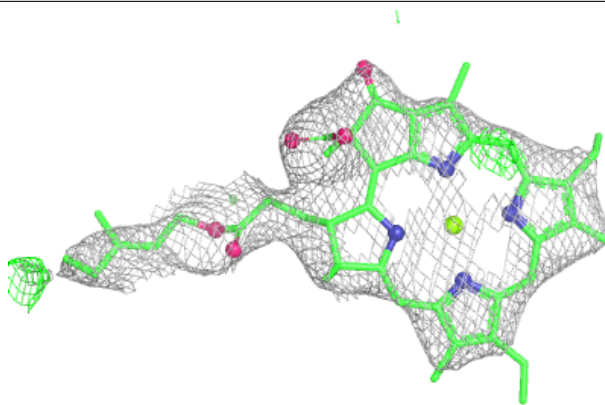
**Electron density around CLA A 834:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



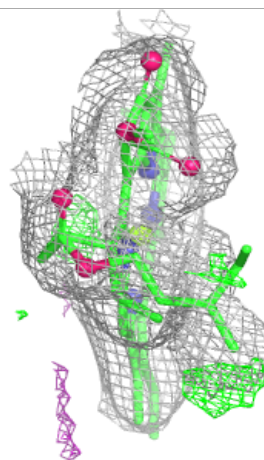
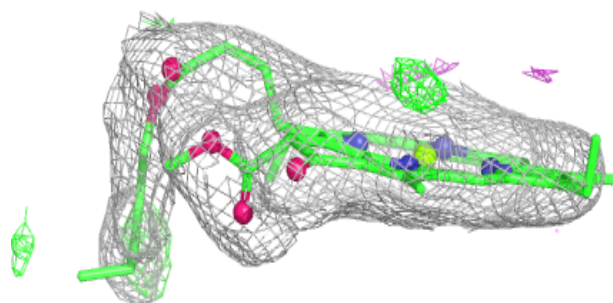
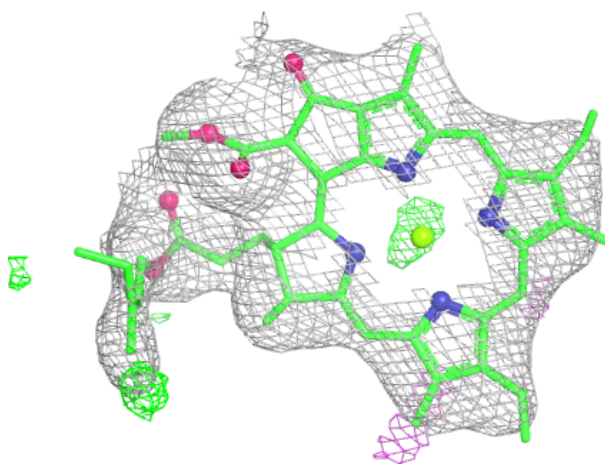
**Electron density around CLA A 835:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



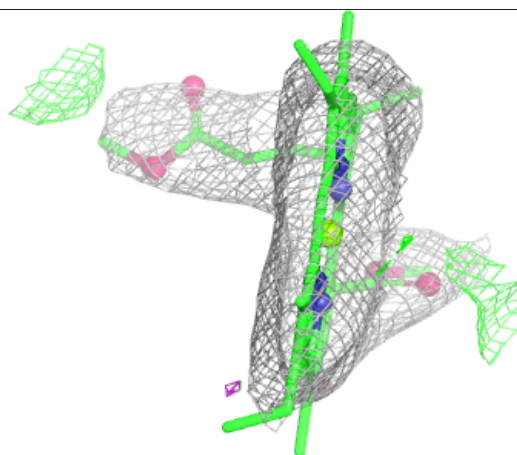
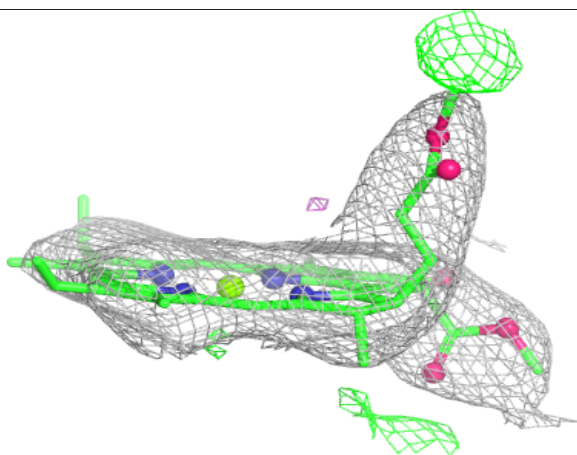
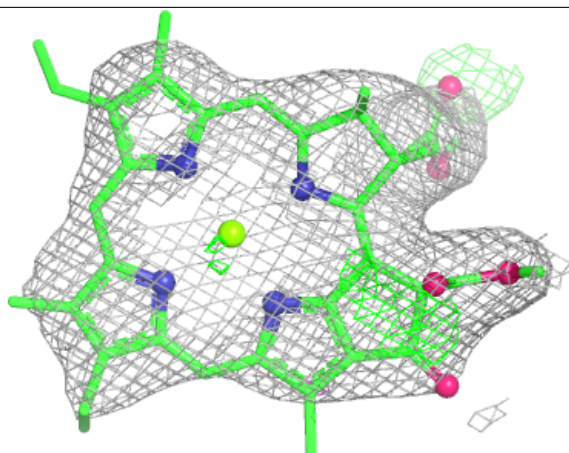
**Electron density around CLA 2 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 1 306:**

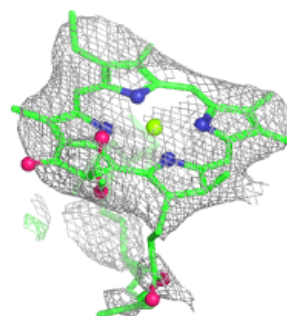
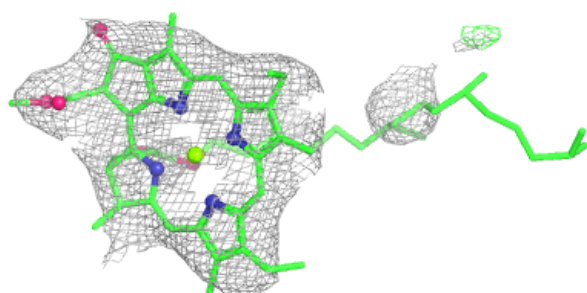
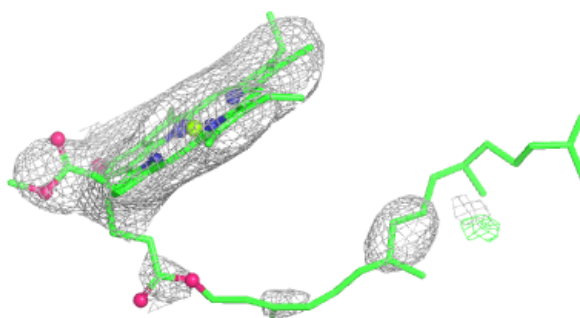
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



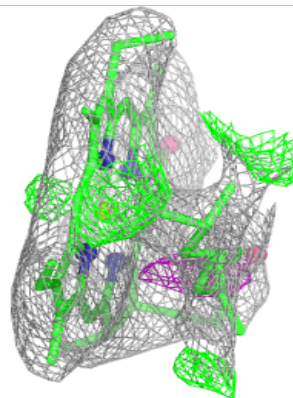
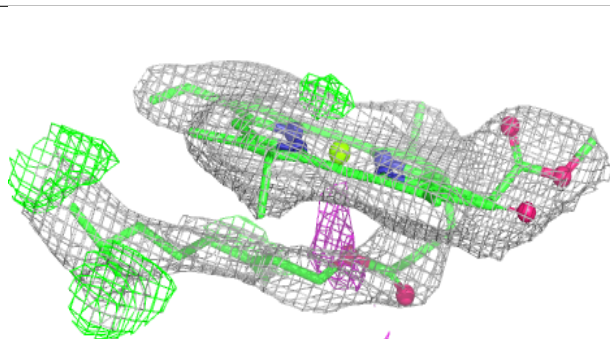
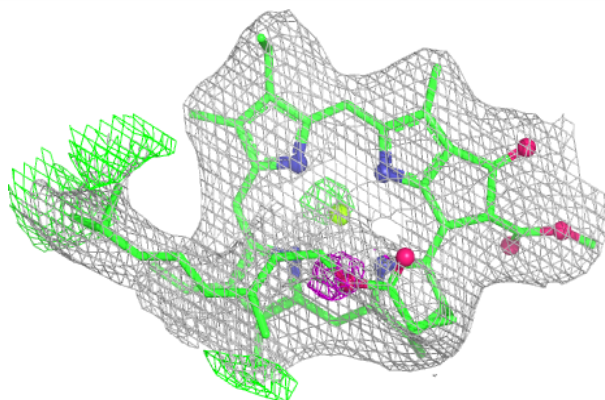


**Electron density around CLA B 803:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

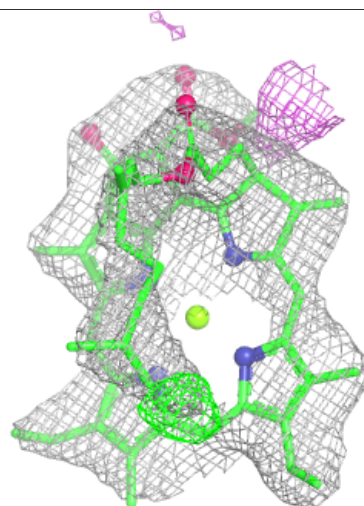
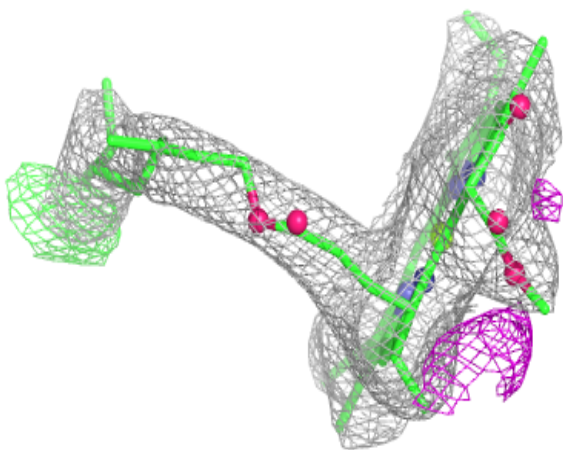
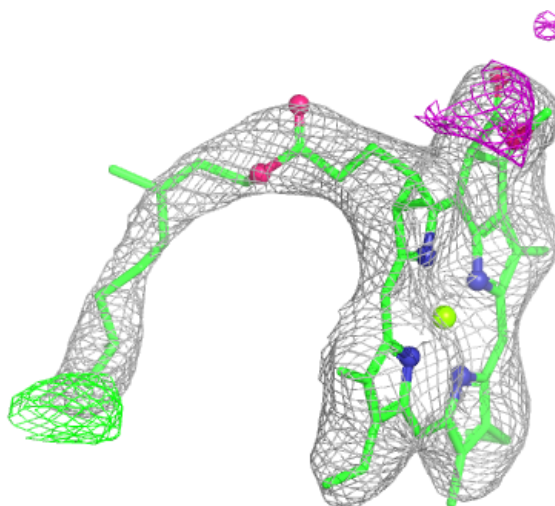
**Electron density around CLA B 814:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 817:**

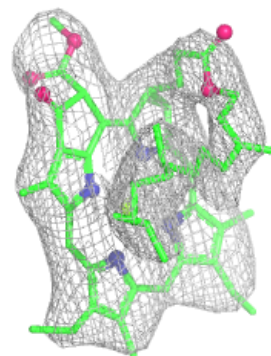
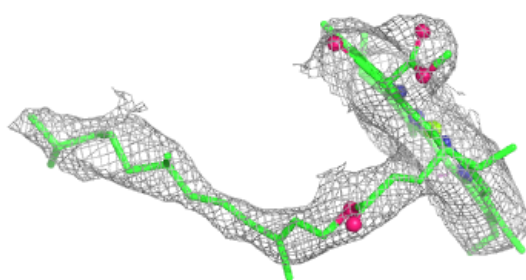
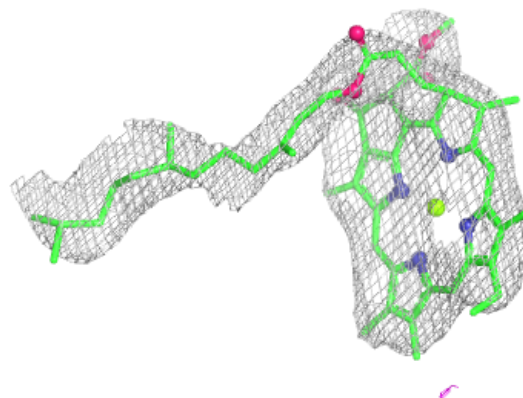
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



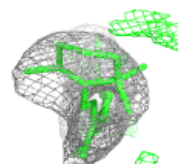
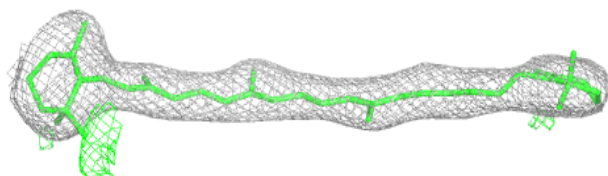
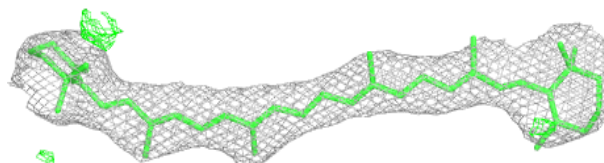


**Electron density around CLA 4 310:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

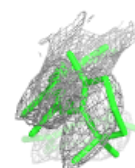
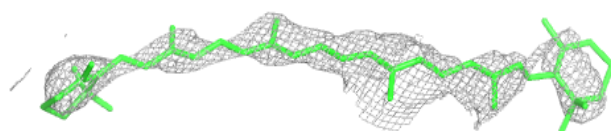
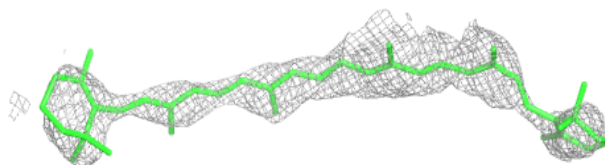
**Electron density around BCR 4 318:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

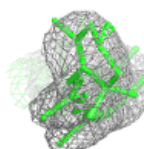
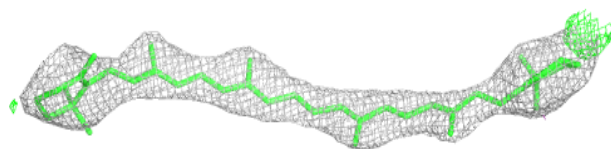
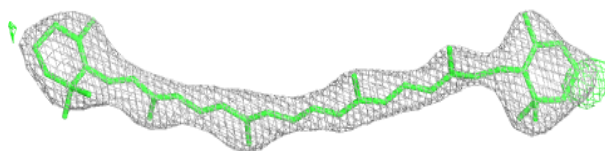


**Electron density around BCR A 846:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

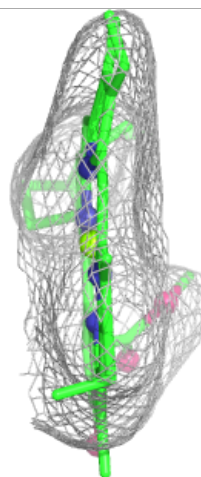
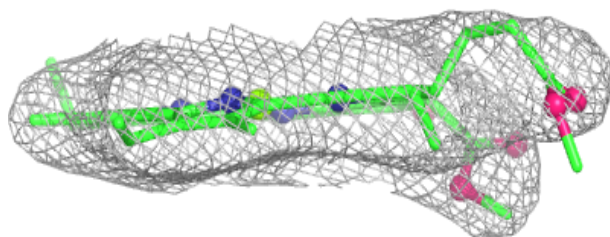
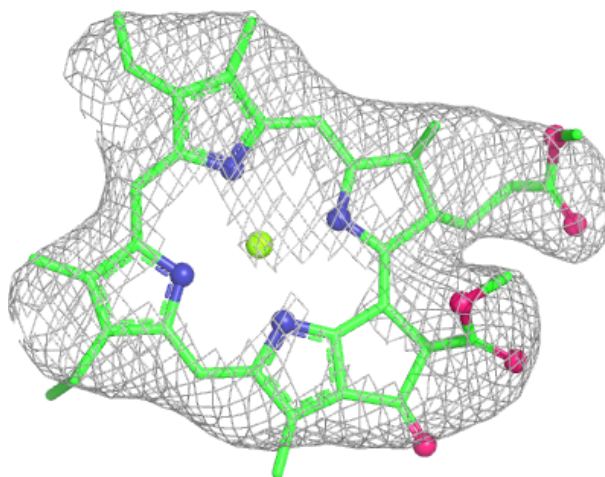
**Electron density around BCR J 105:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



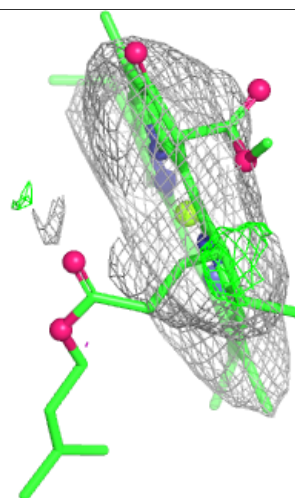
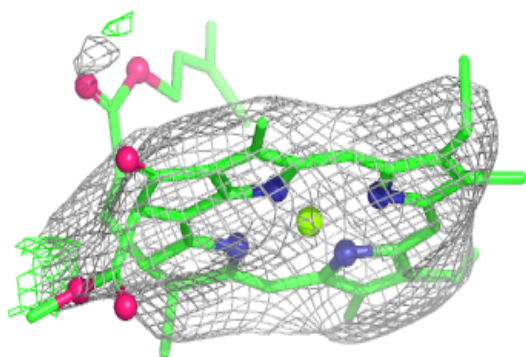
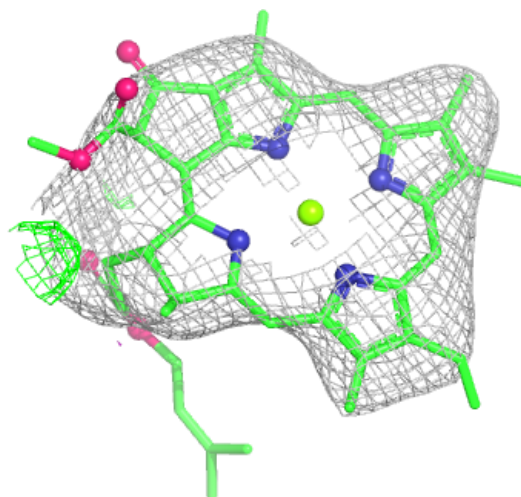
**Electron density around CLA G 105:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



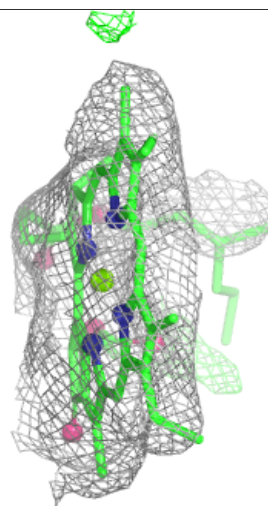
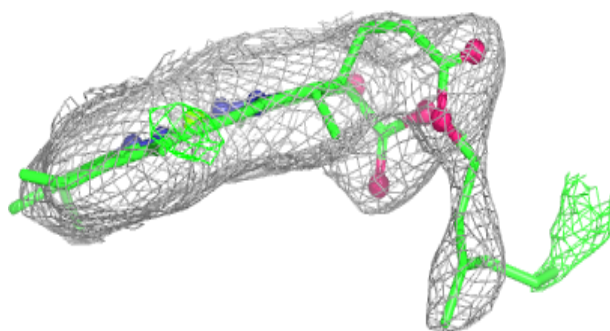
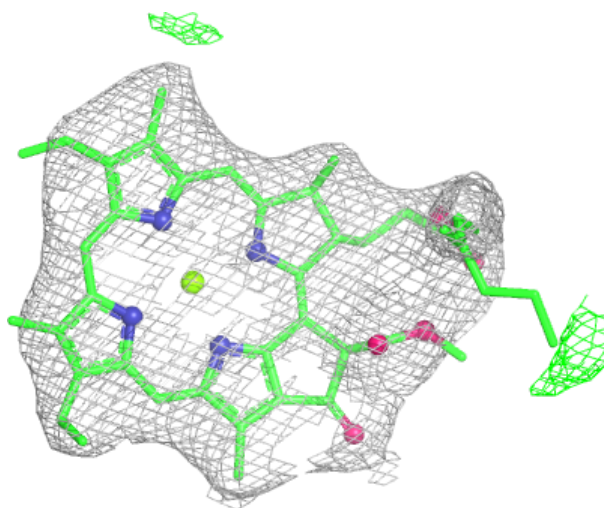
**Electron density around CLA A 814:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



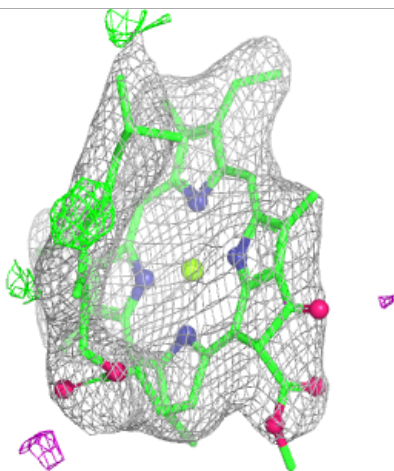
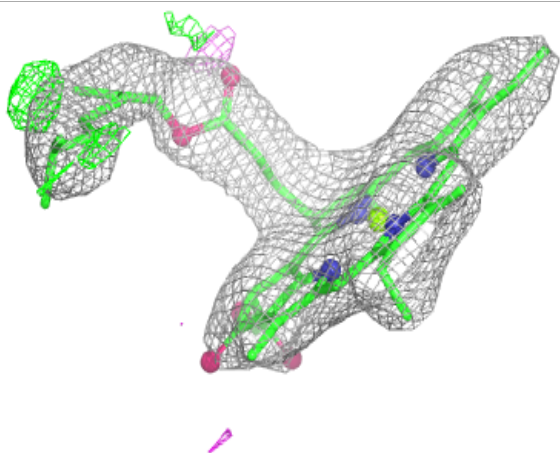
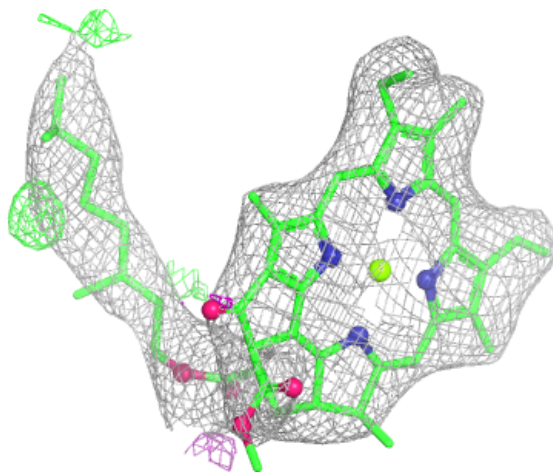
**Electron density around CLA 4 311:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 824:**

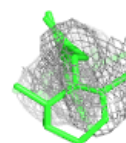
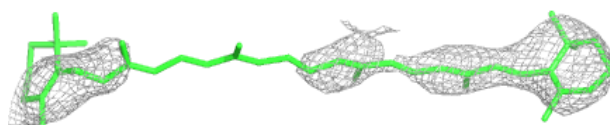
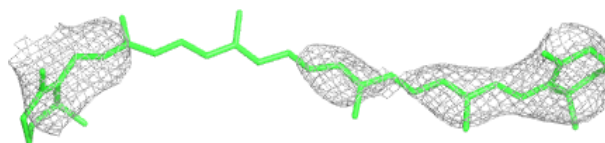
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



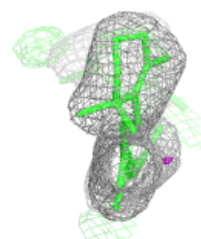
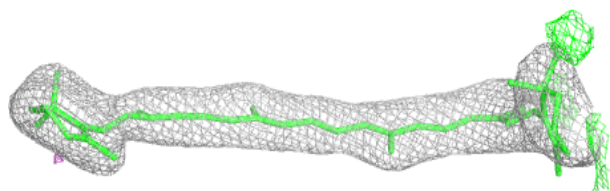
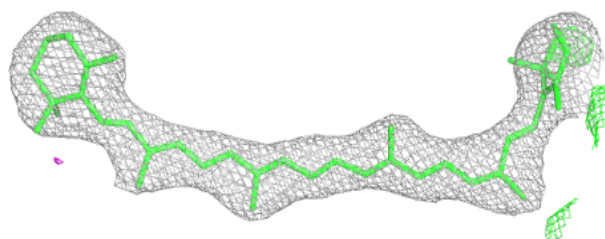


**Electron density around BCR A 849:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

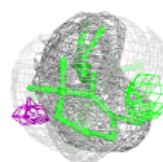
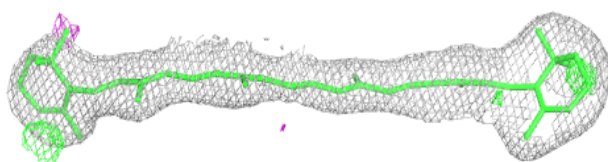
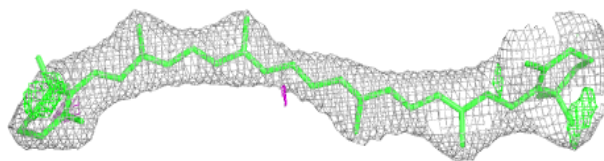
**Electron density around BCR B 845:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BCR B 847:**

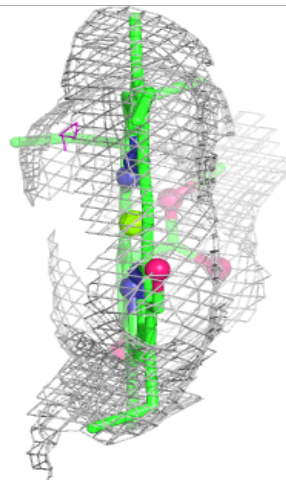
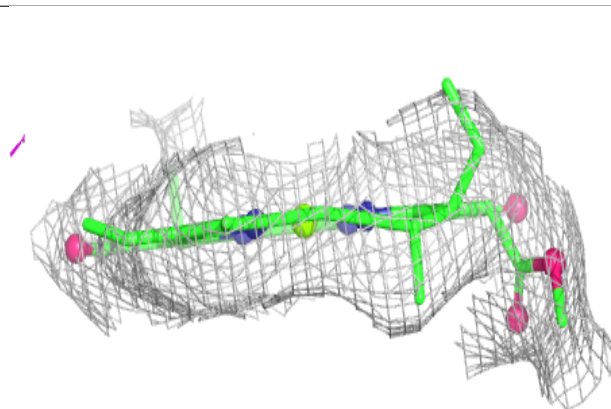
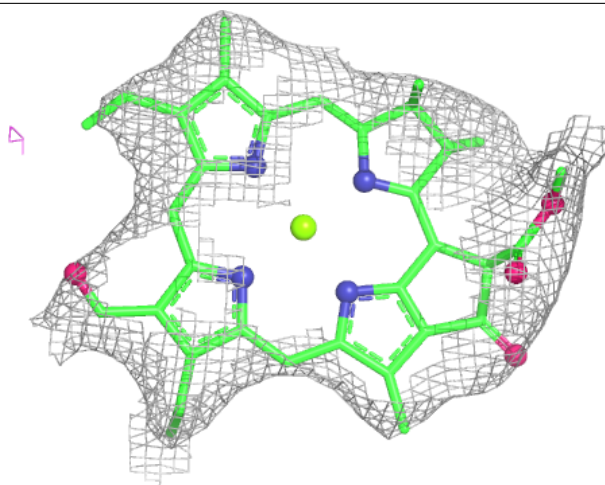
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





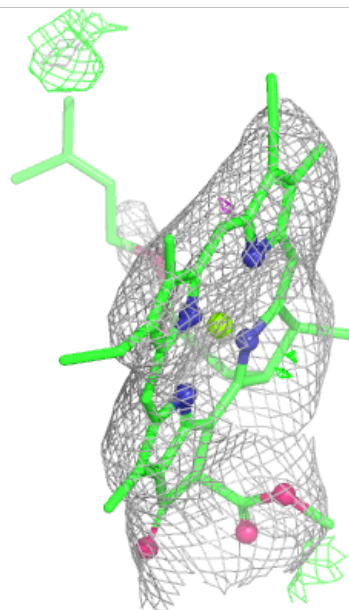
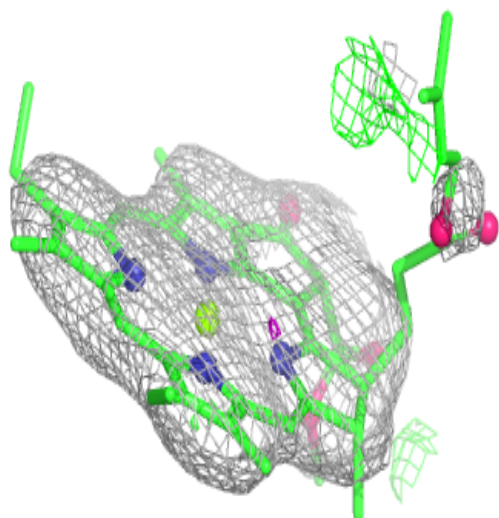
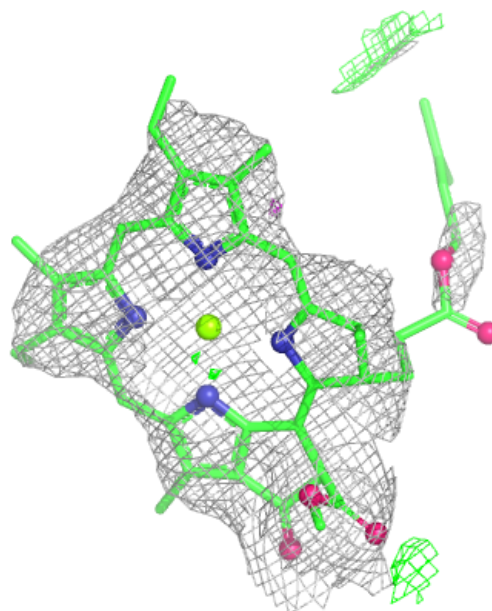
**Electron density around CHL 2 313:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



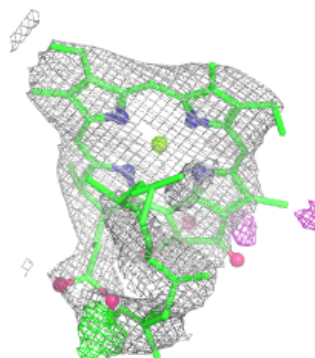
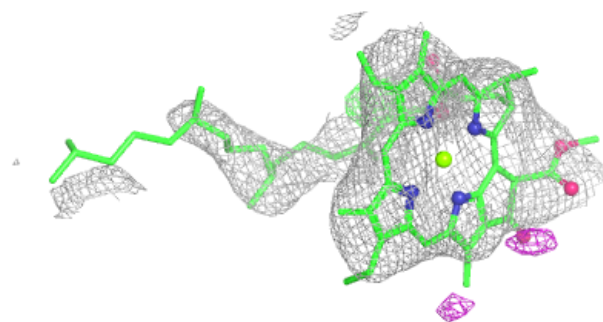
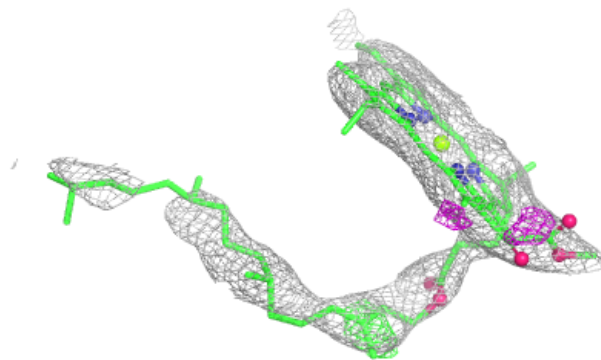
**Electron density around CLA A 830:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

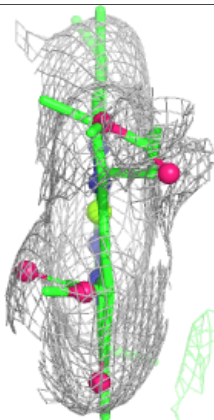
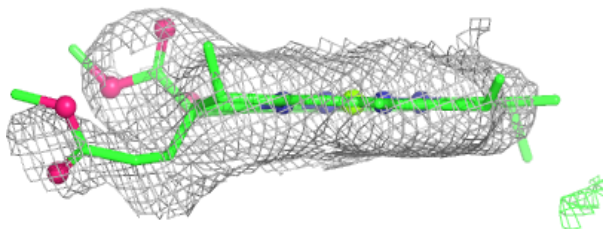
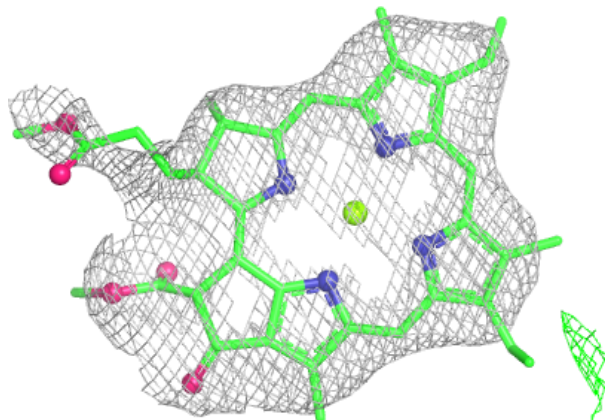


**Electron density around CLA A 809:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

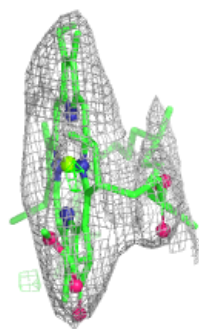
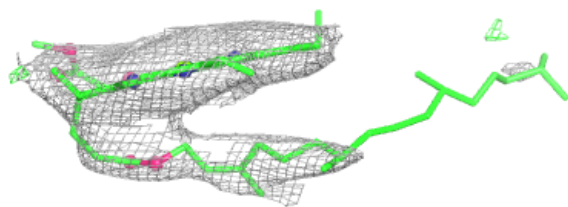
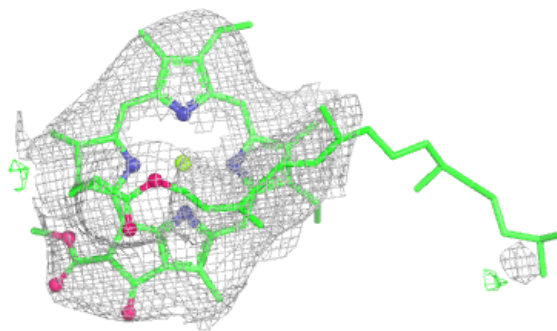
**Electron density around CLA 3 613:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



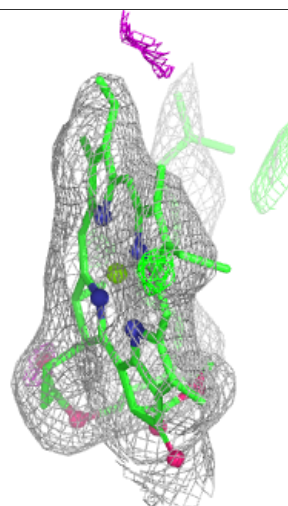
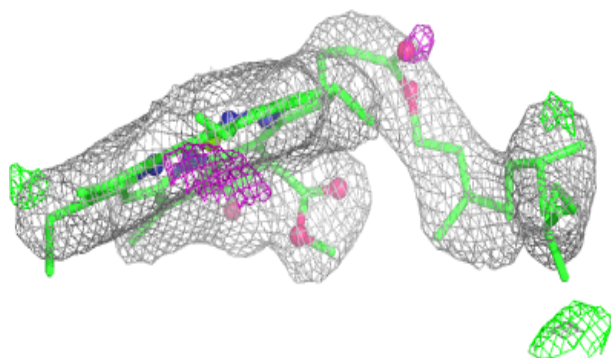
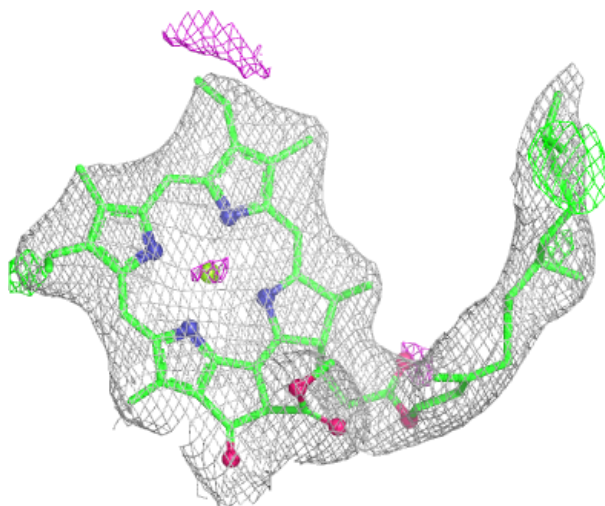
**Electron density around CLA A 816:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 4 303:**

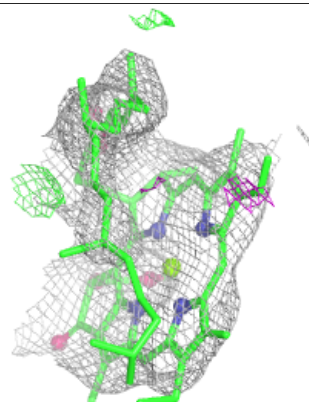
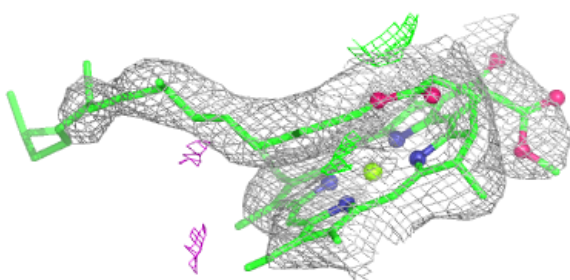
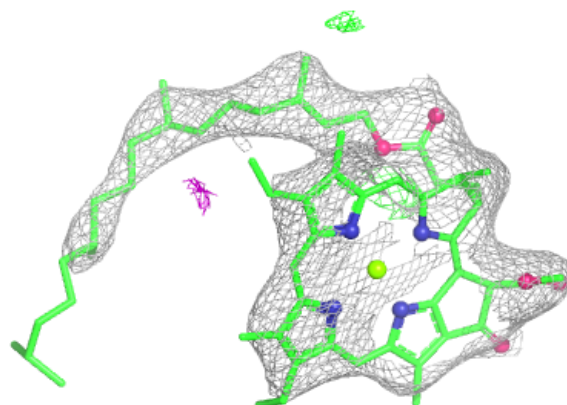
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



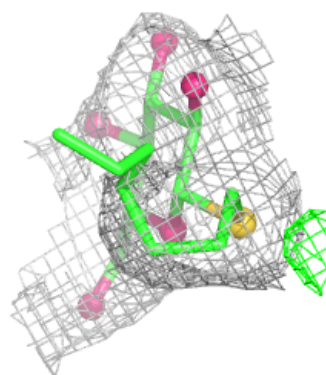
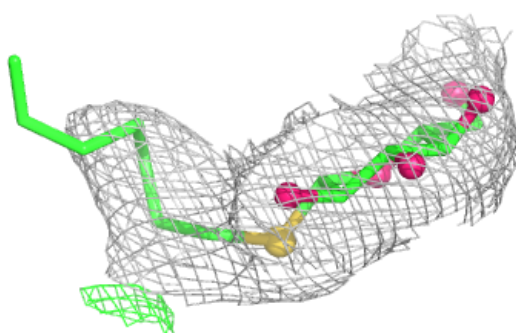
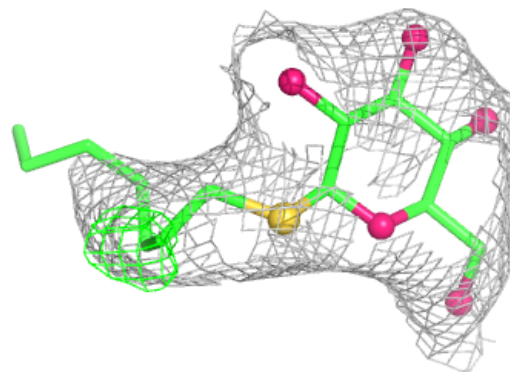


**Electron density around CLA 2 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

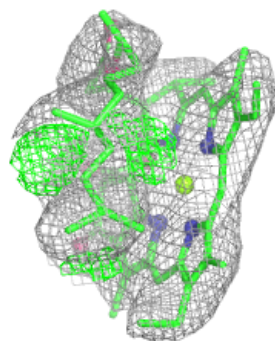
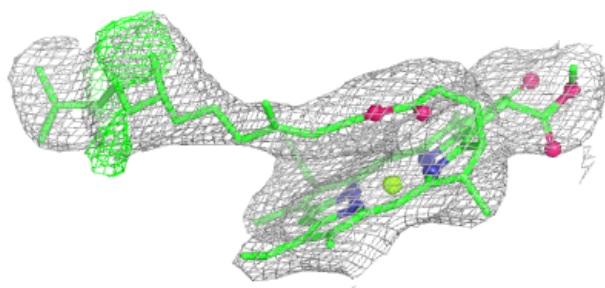
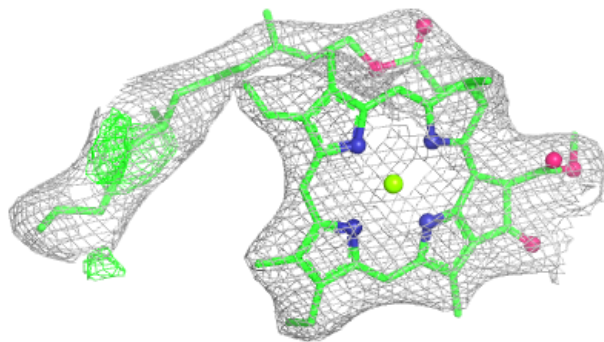
**Electron density around HTG J 102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

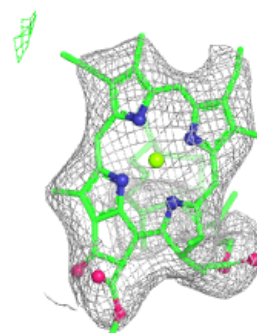
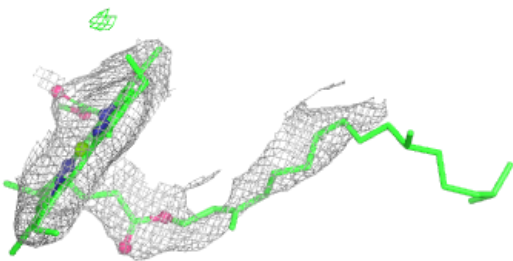
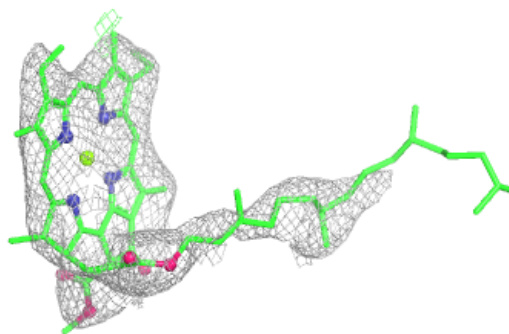


**Electron density around CLA 4 309:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

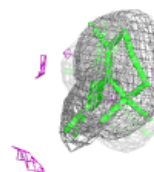
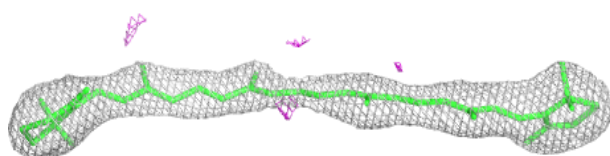
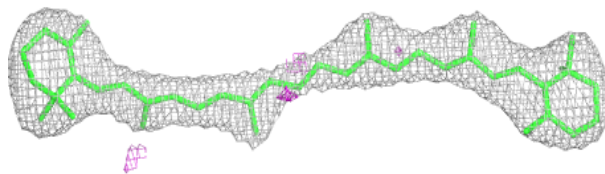
**Electron density around CLA 1 309:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BCR J 104:**

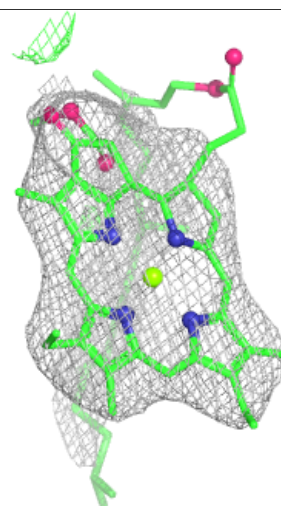
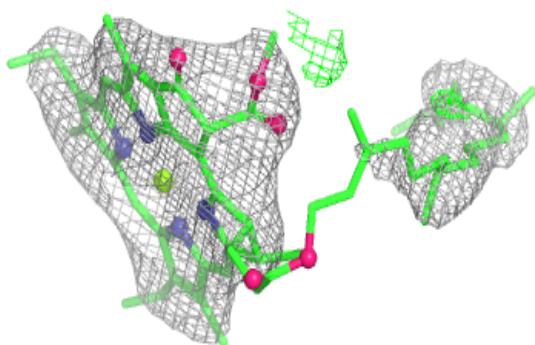
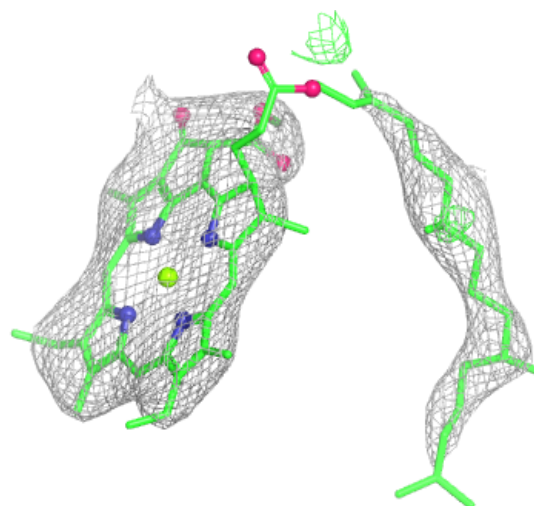
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





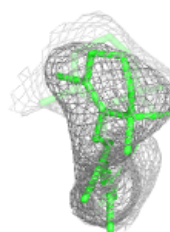
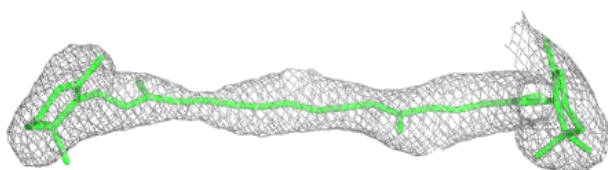
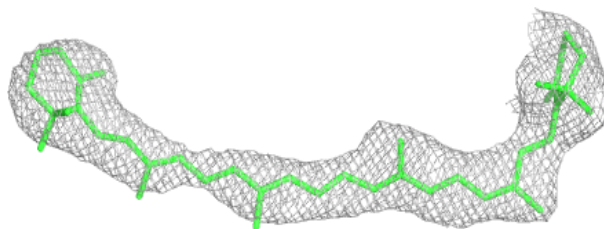
**Electron density around CLA B 812:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

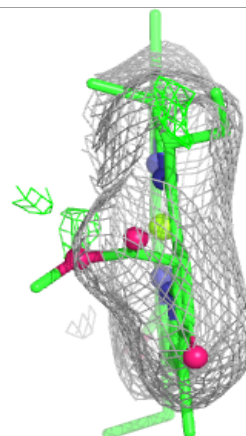
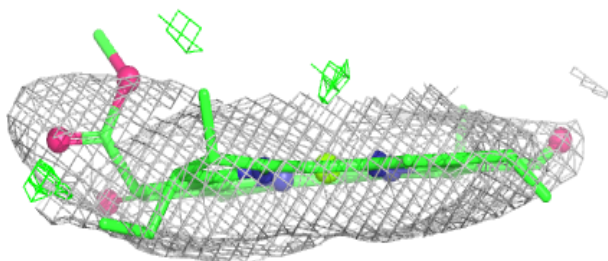
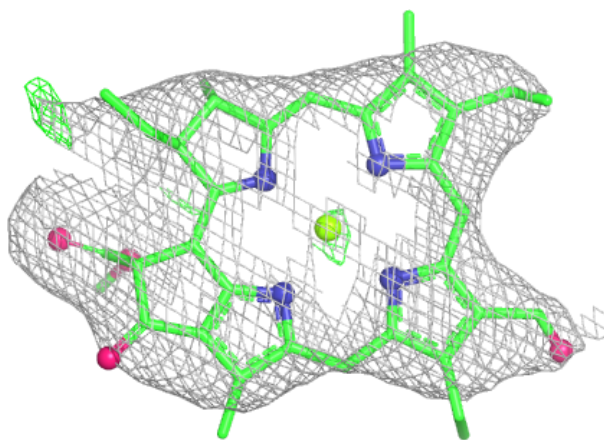


**Electron density around BCR L 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

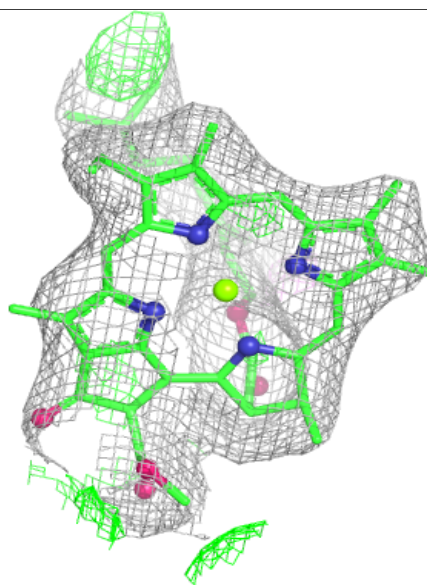
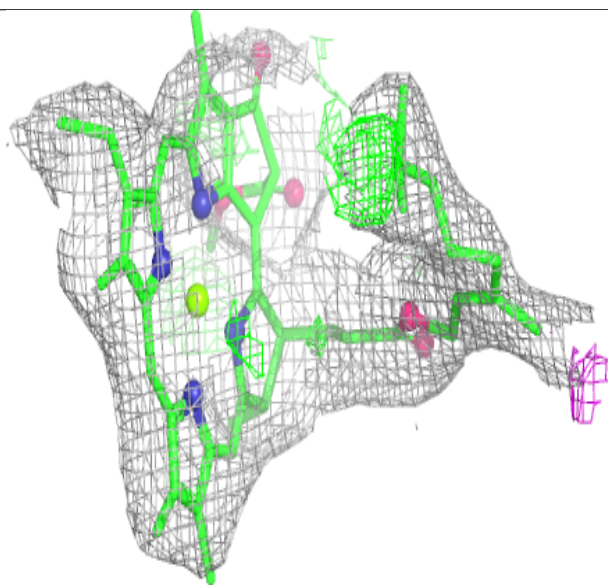
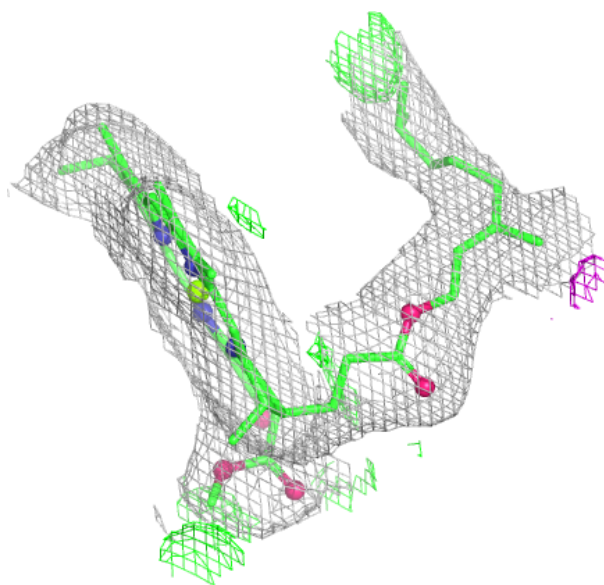
**Electron density around CHL 2 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



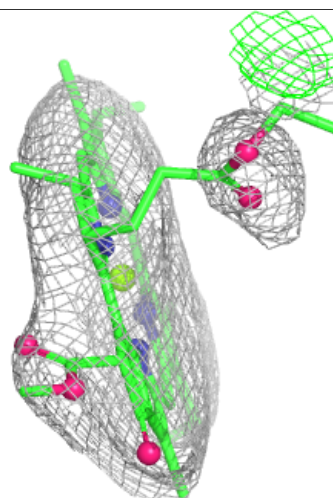
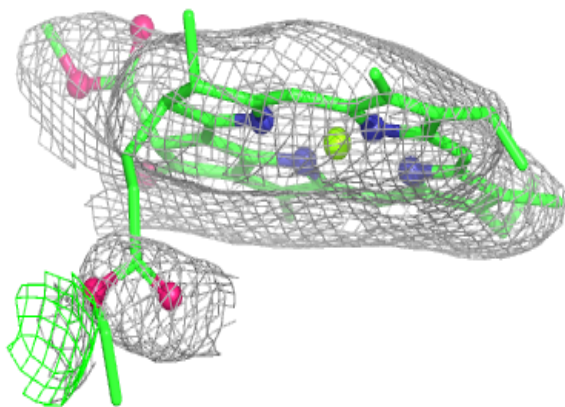
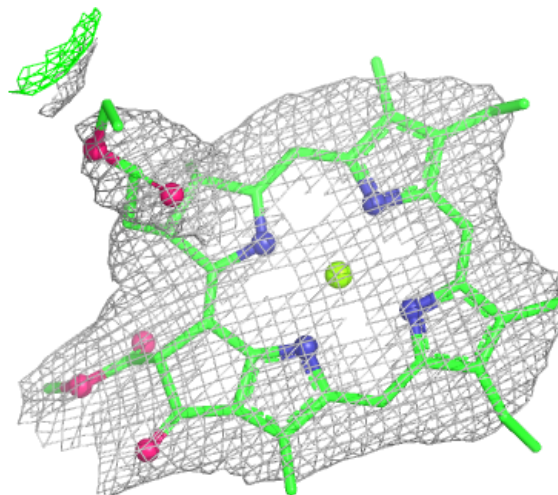
**Electron density around CLA B 813:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



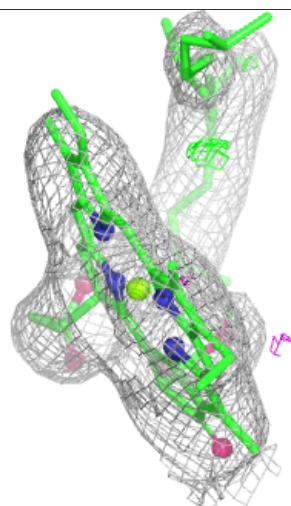
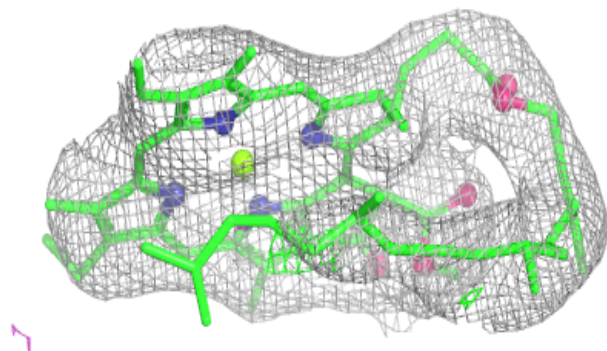
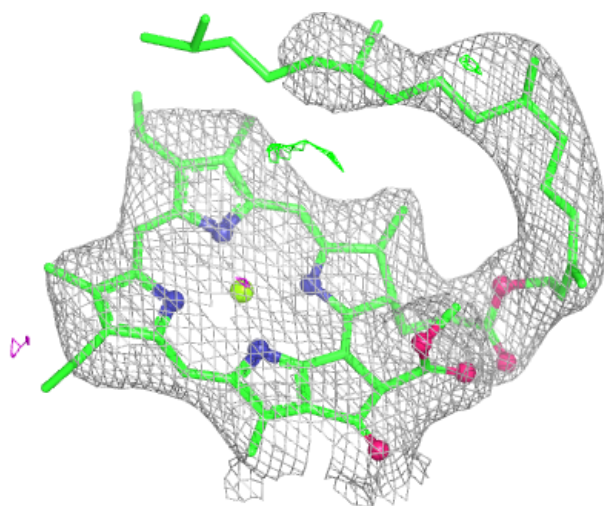
**Electron density around CLA 3 606:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 1 302:**

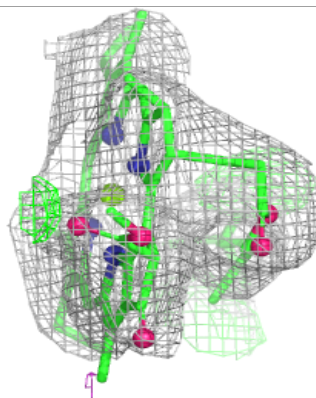
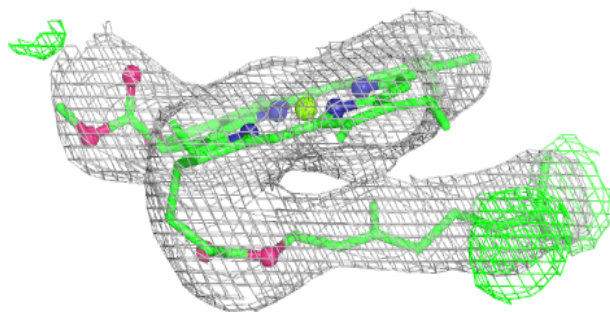
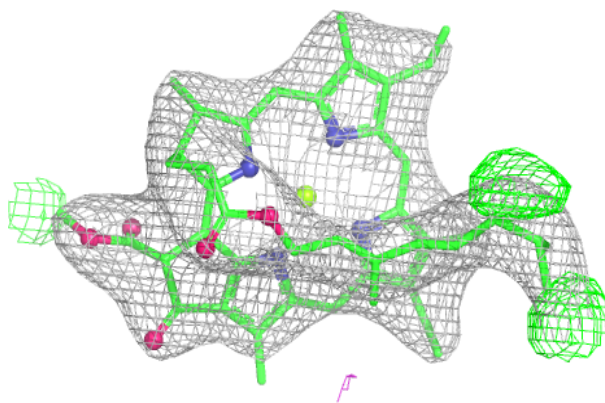
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



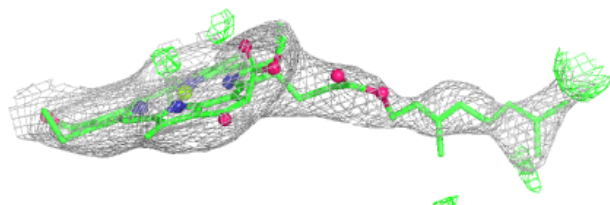
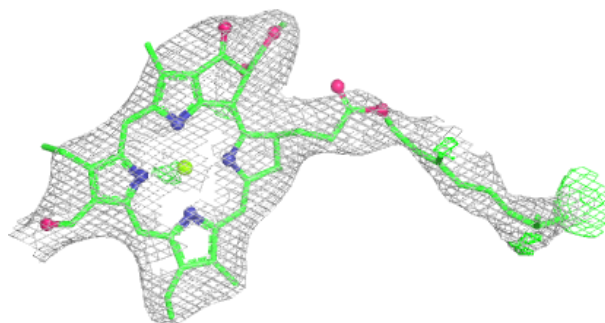


**Electron density around CLA B 818:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

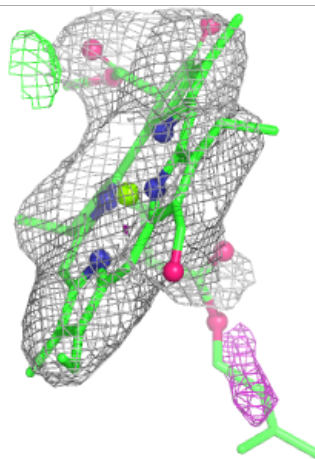
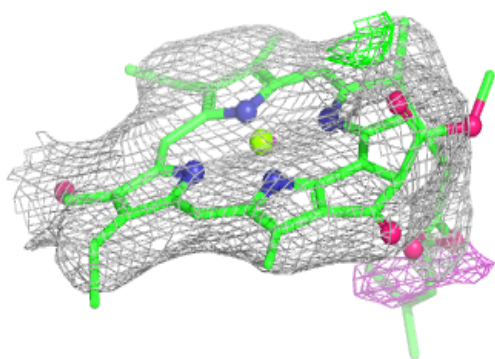
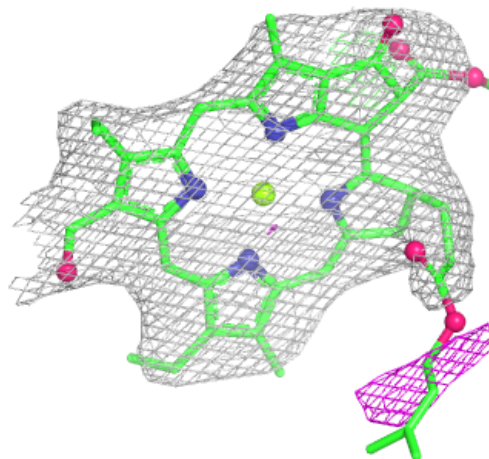
**Electron density around CHL 4 305:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



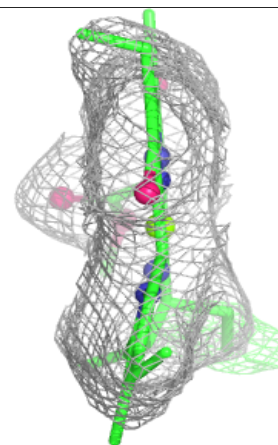
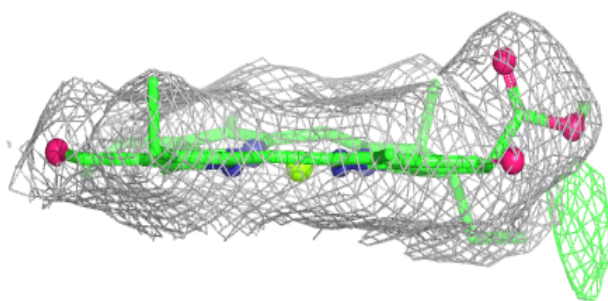
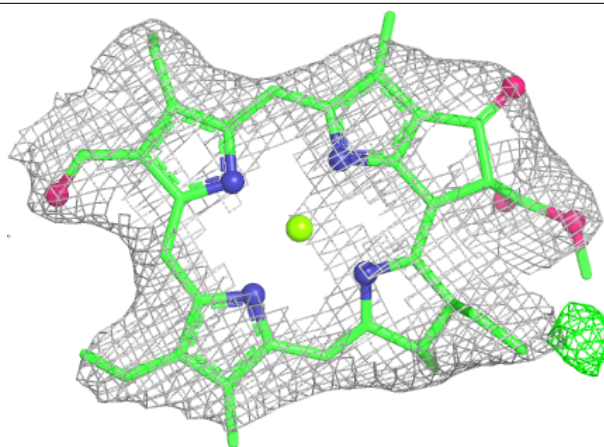
**Electron density around CHL 4 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

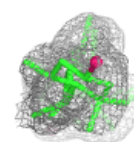
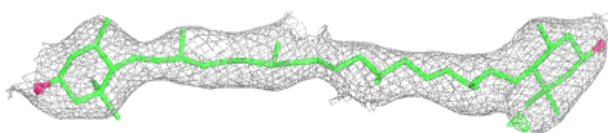
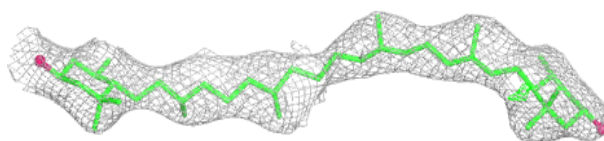


**Electron density around CHL 4 315:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LUT 1 314:**

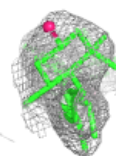
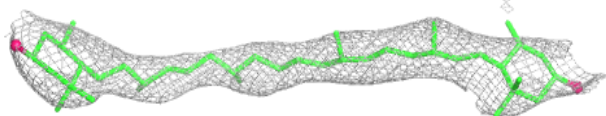
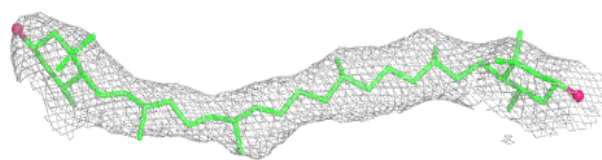
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



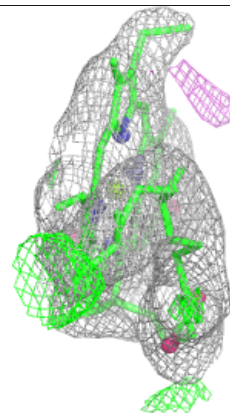
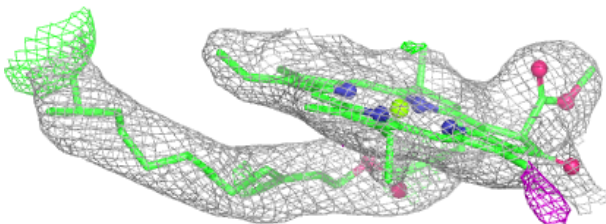
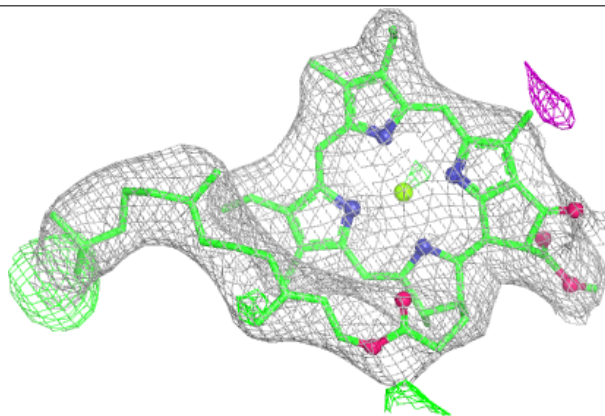


**Electron density around LUT 2 314:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

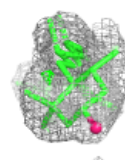
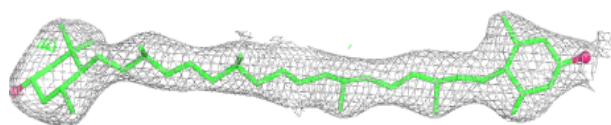
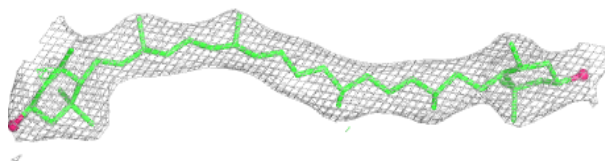
**Electron density around CLA B 820:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

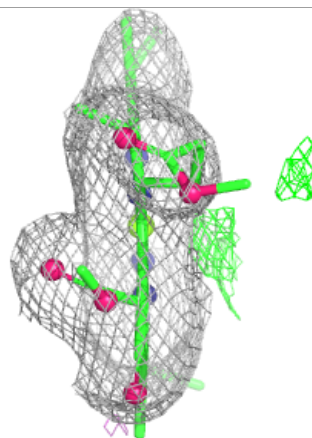
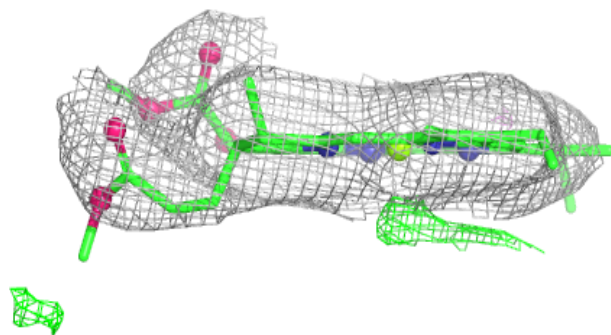
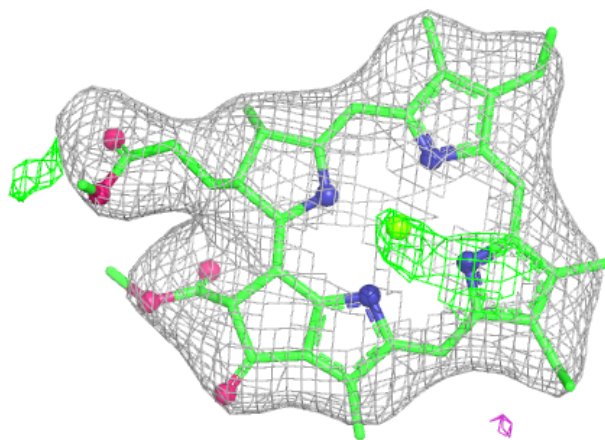


**Electron density around LUT 4 316:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

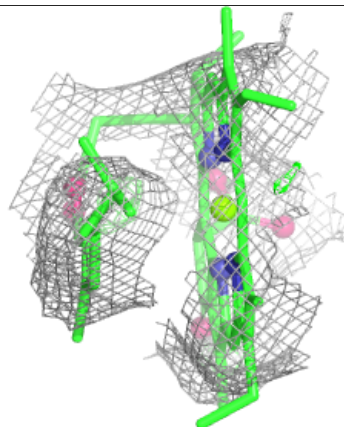
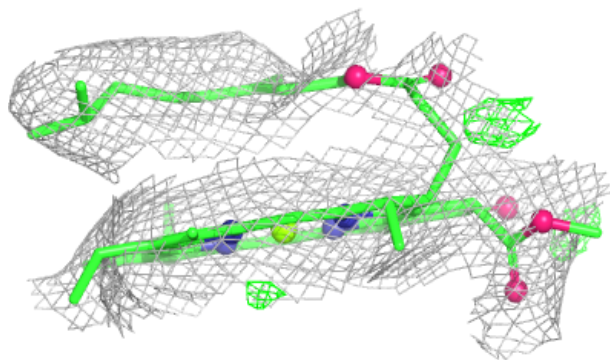
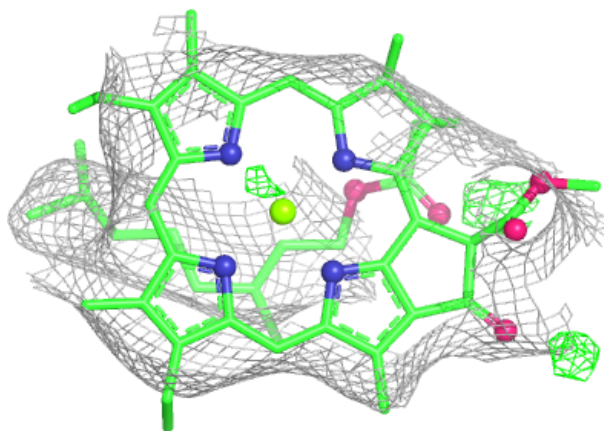
**Electron density around CLA 1 313:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

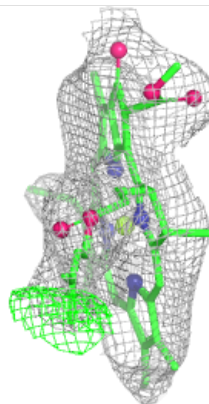
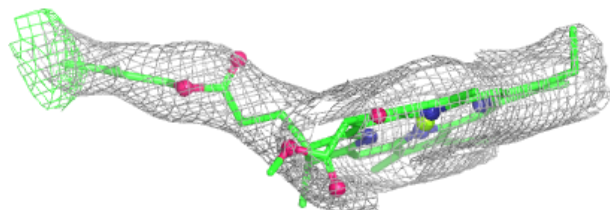
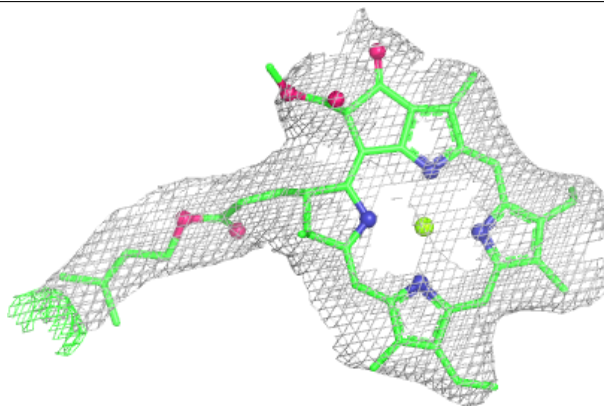


**Electron density around CLA 3 611:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

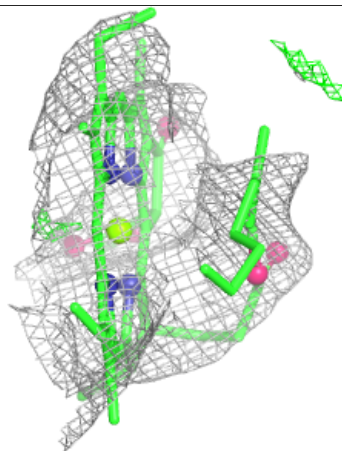
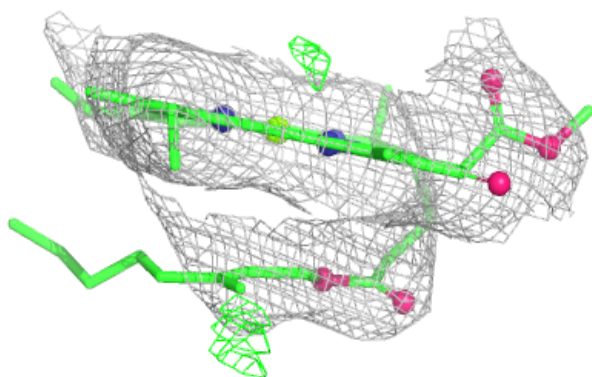
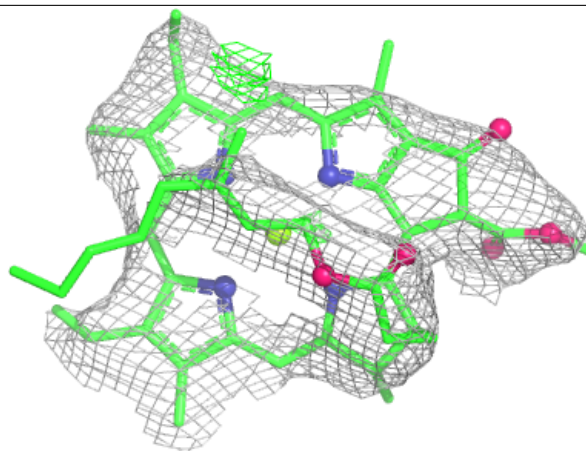
**Electron density around CLA G 104:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 811:**

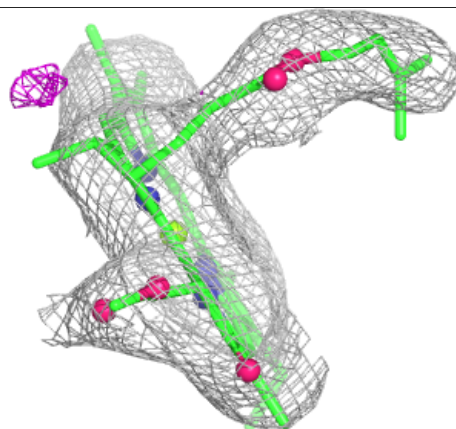
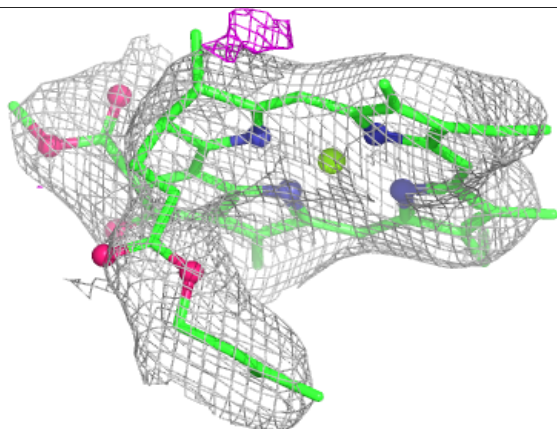
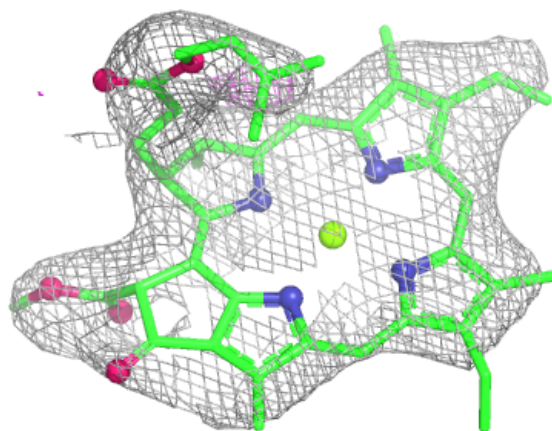
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



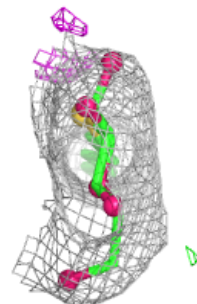
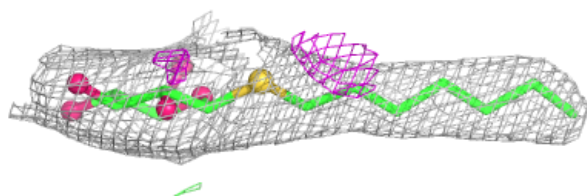
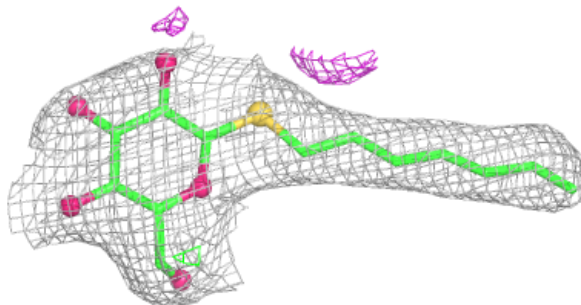


**Electron density around CLA 2 307:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

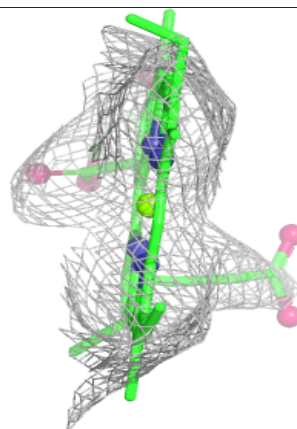
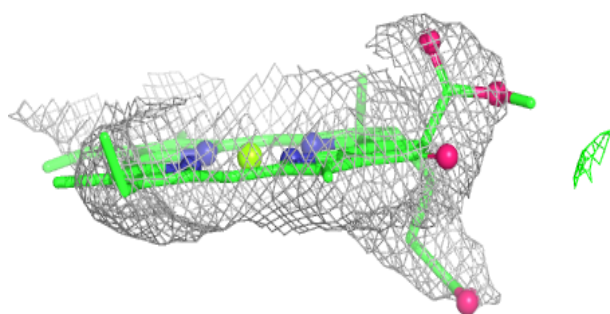
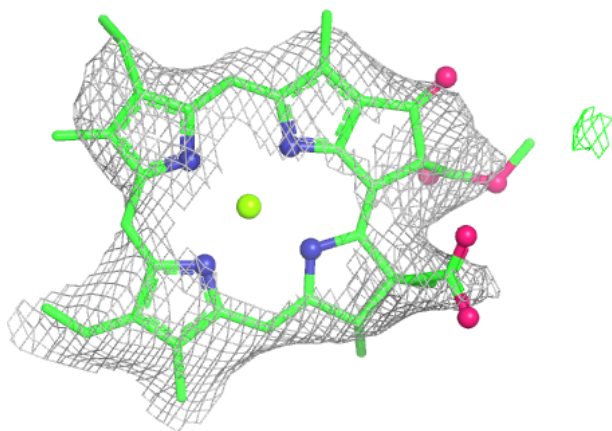
**Electron density around HTG A 854:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

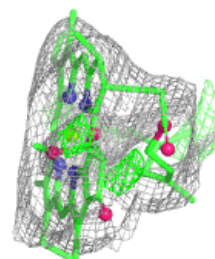
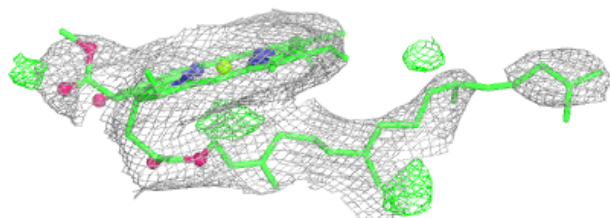
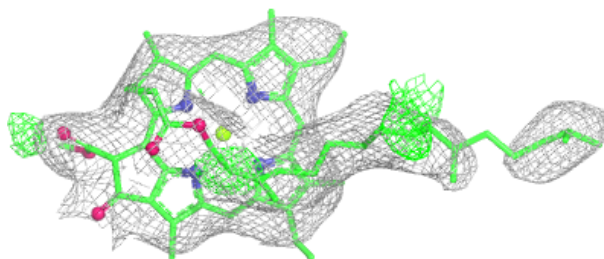


**Electron density around CLA A 815:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

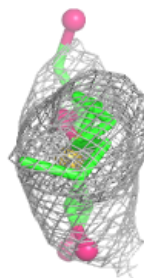
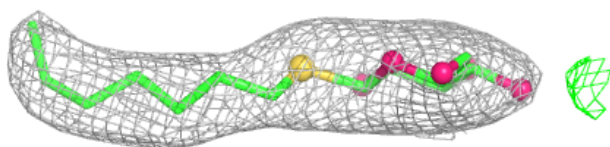
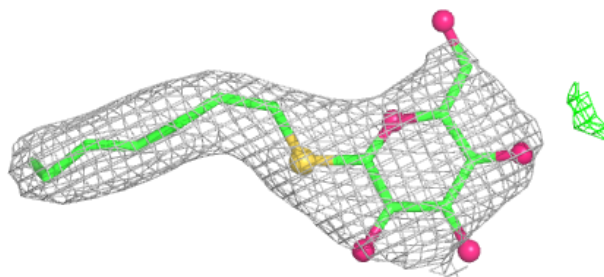
**Electron density around CLA A 836:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



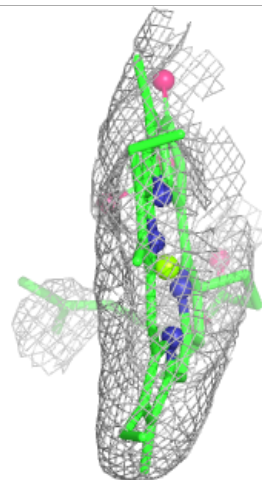
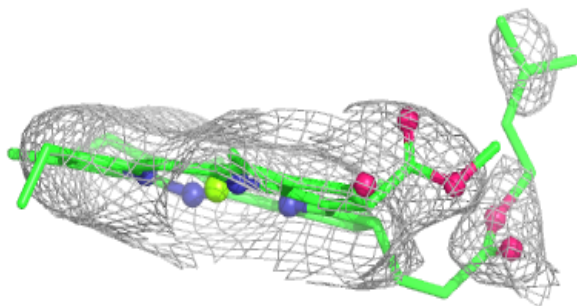
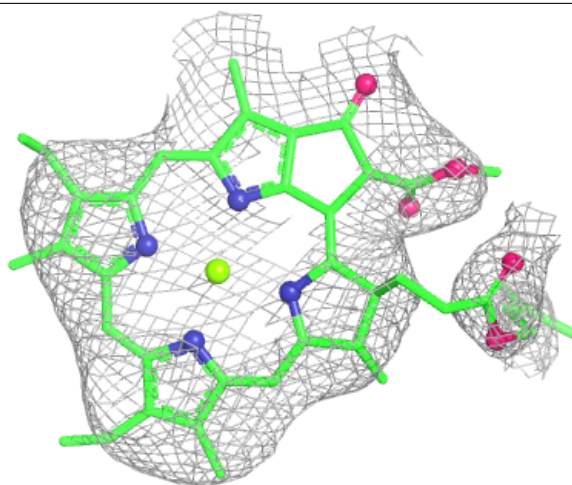
**Electron density around HTG F 305:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 3 603:**

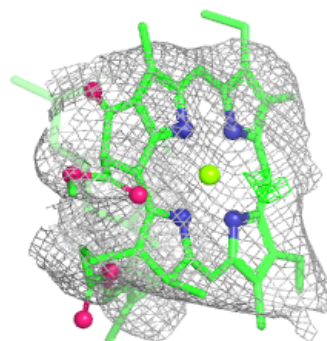
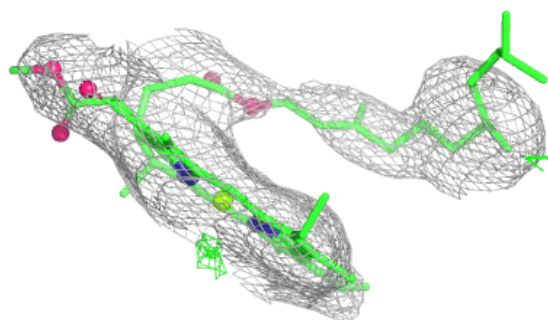
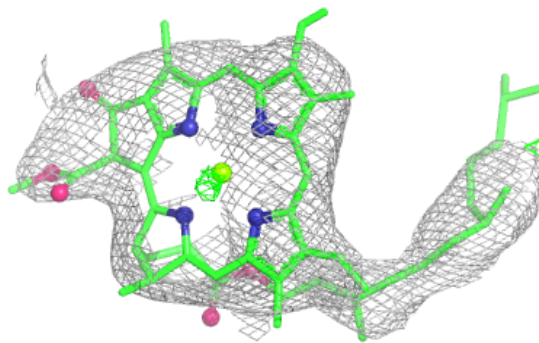
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





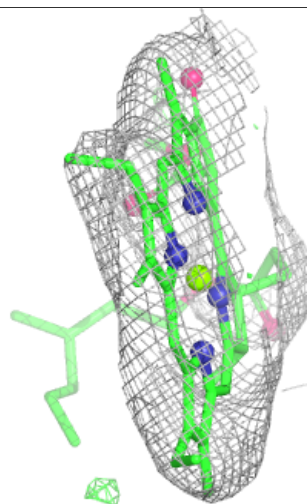
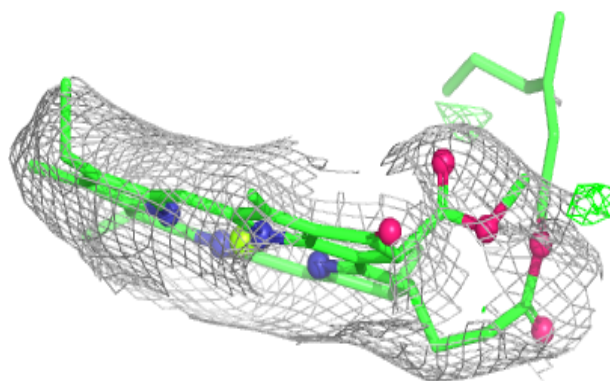
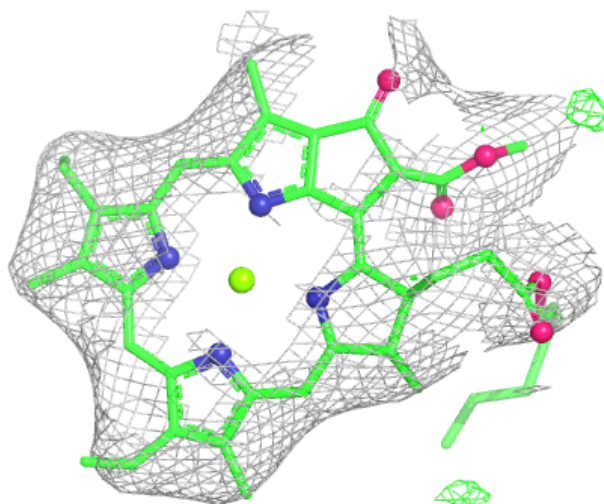
**Electron density around CLA 2 308:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



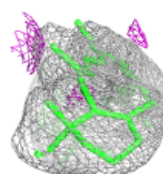
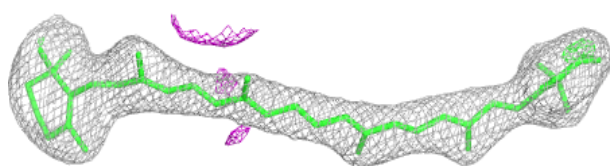
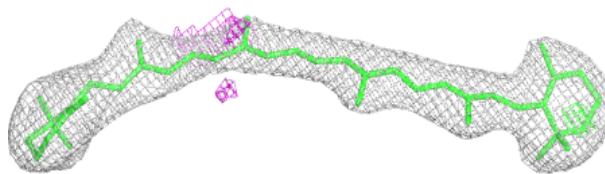
**Electron density around CLA 1 310:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

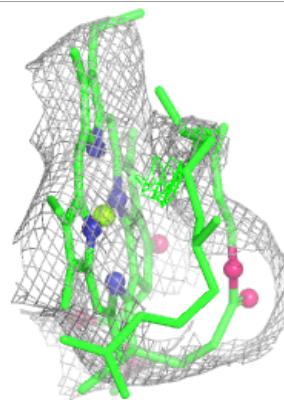
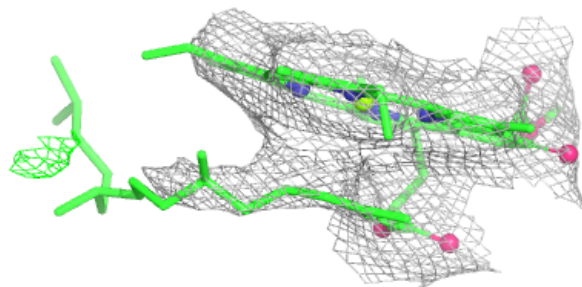
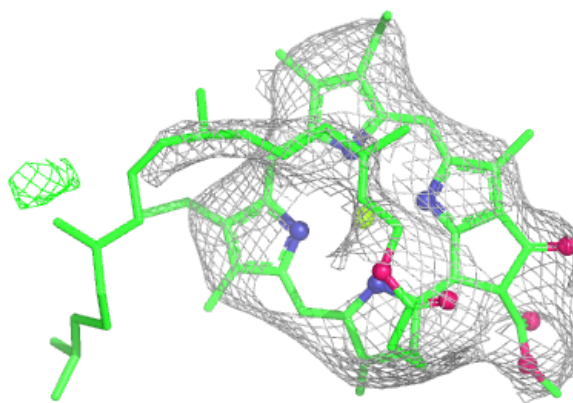


**Electron density around BCR F 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

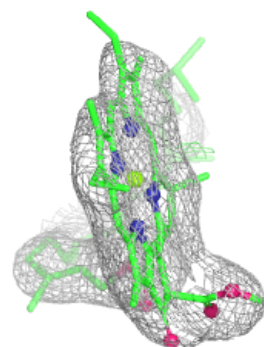
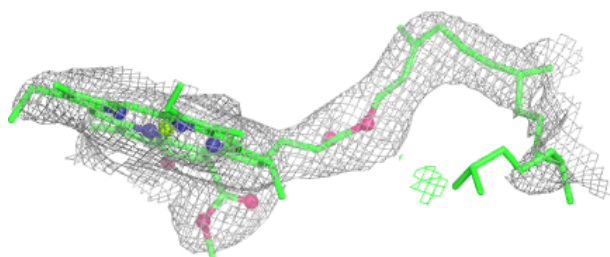
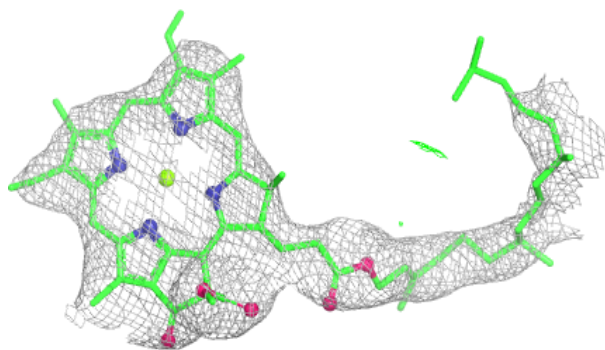
**Electron density around CLA 2 311:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

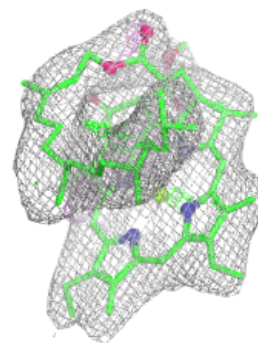
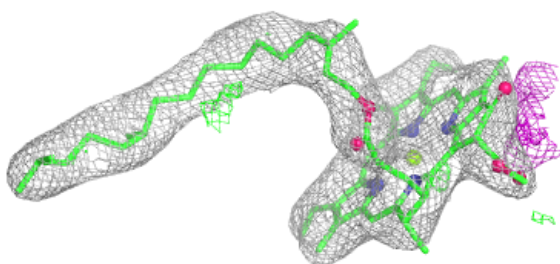
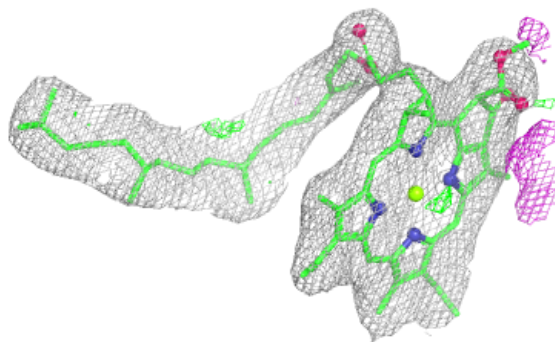


**Electron density around CLA A 826:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 816:**

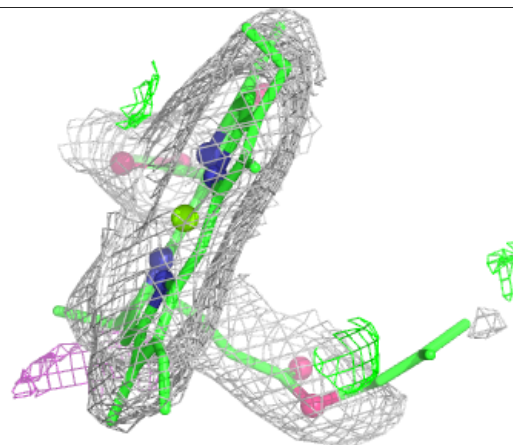
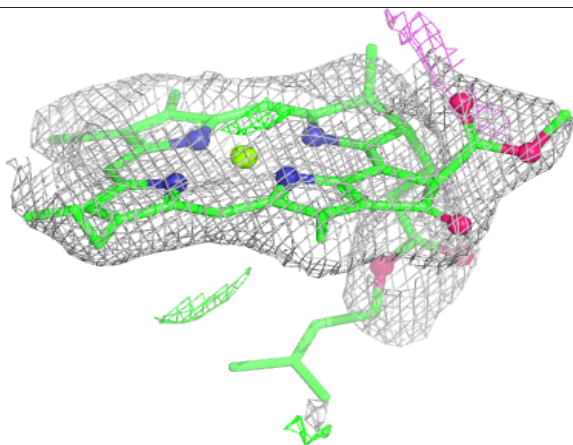
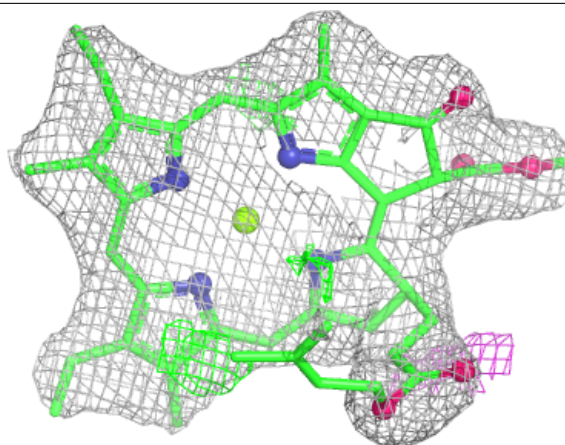
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



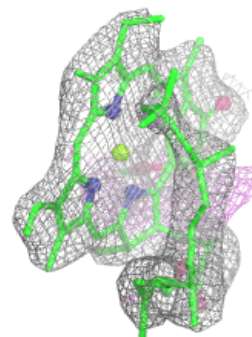
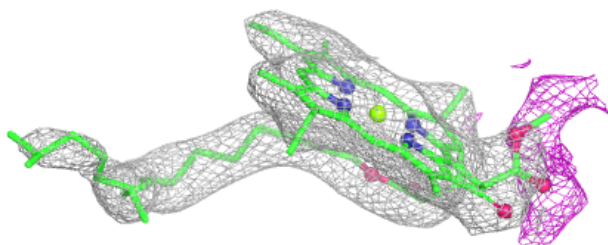
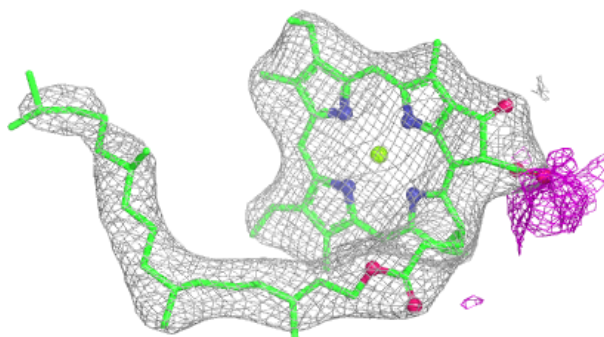


**Electron density around CLA 4 308:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

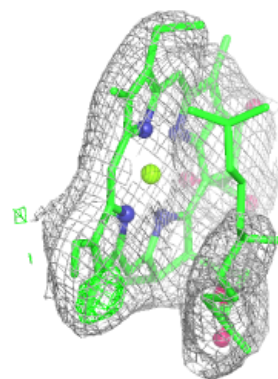
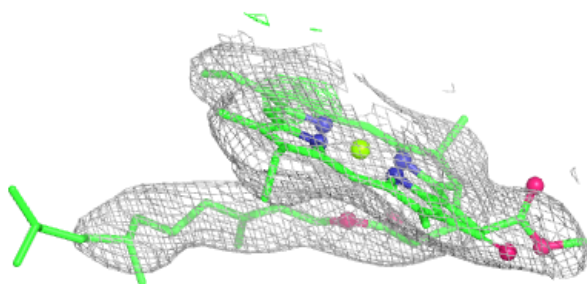
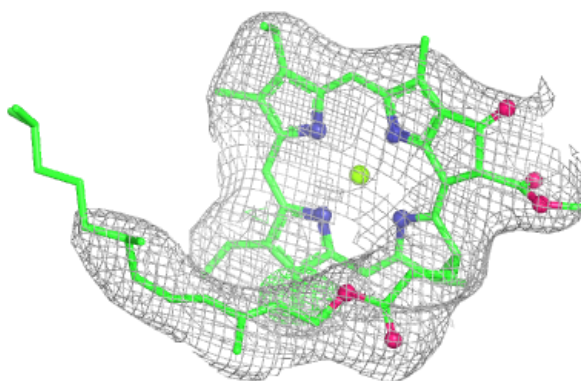
**Electron density around CLA 1 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

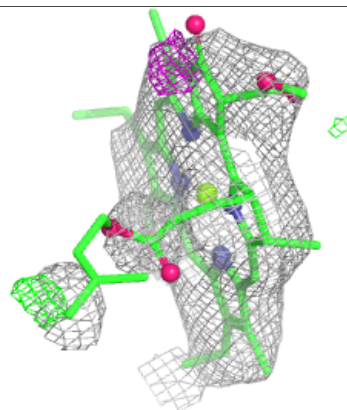
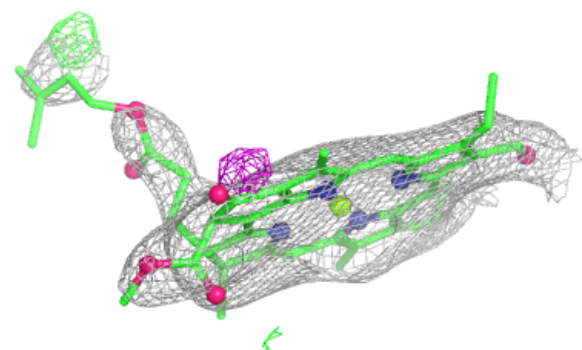
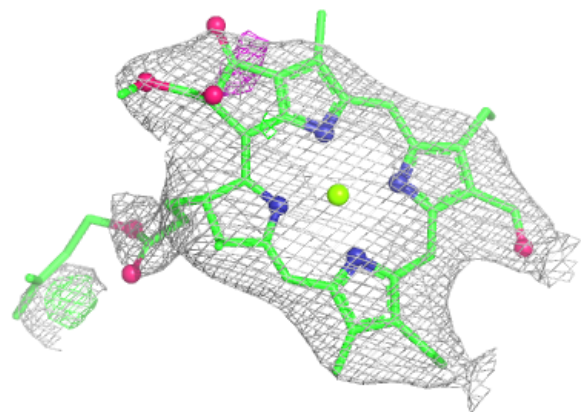


**Electron density around CLA 1 308:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

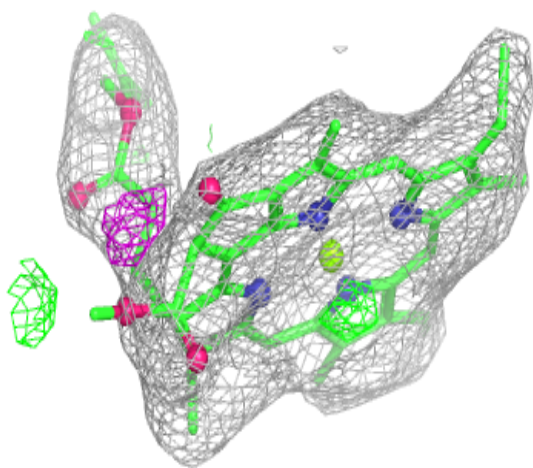
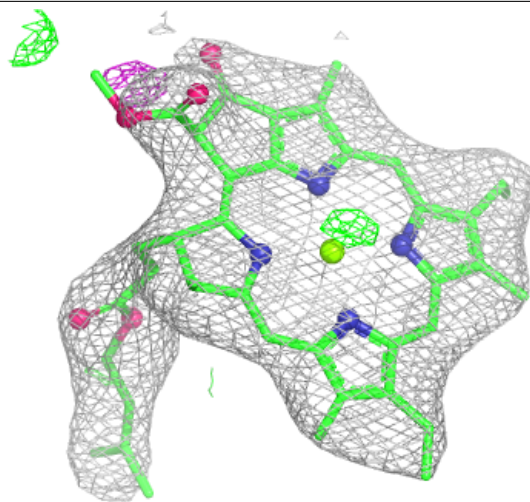
**Electron density around CHL 2 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



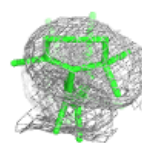
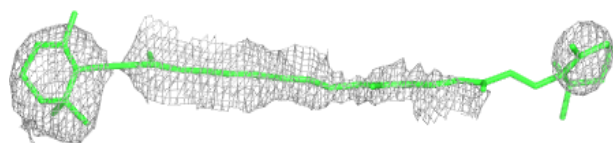
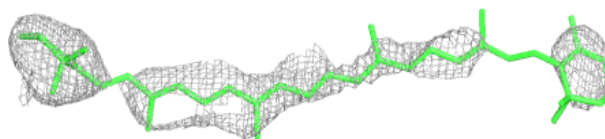
**Electron density around CLA B 822:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

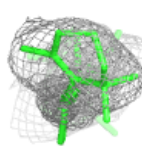
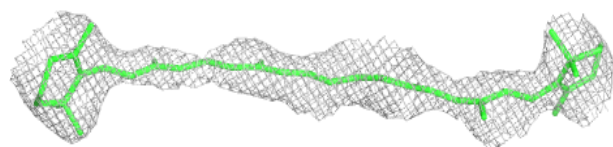
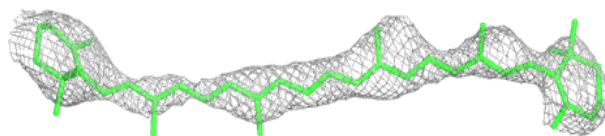


**Electron density around BCR A 847:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR A 848:**

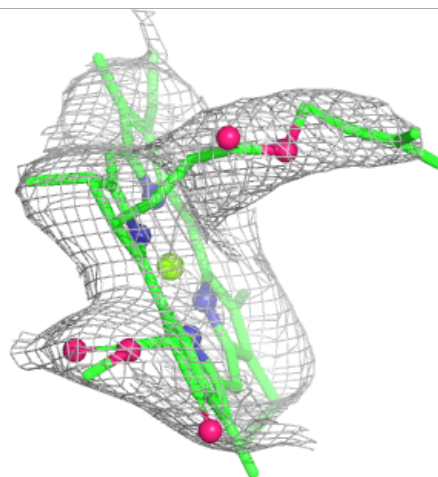
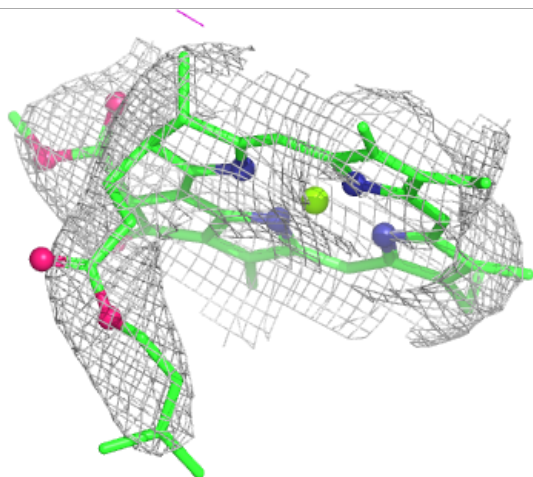
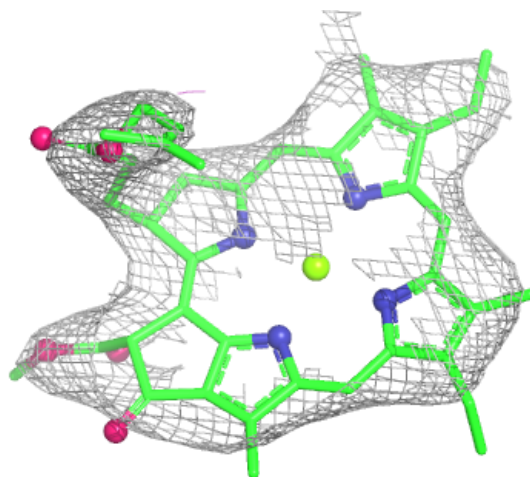
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





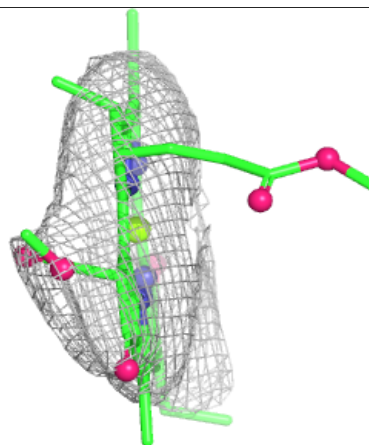
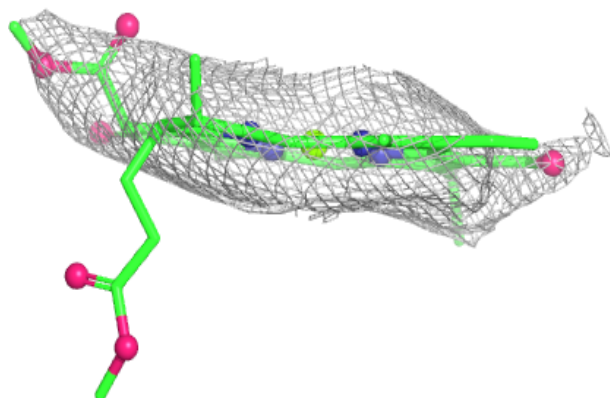
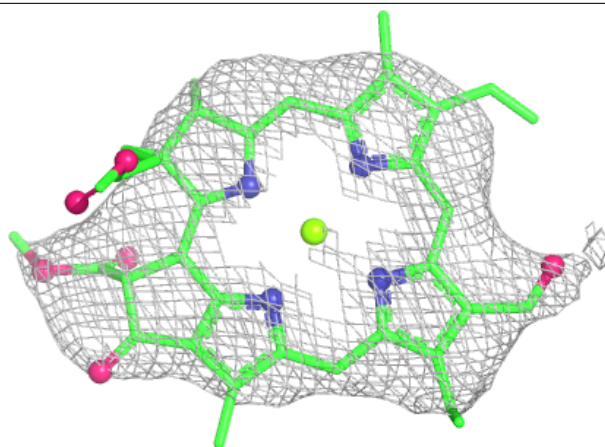
**Electron density around CLA 3 608:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

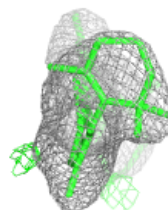
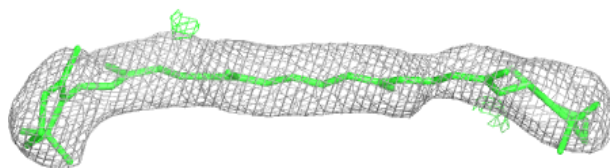
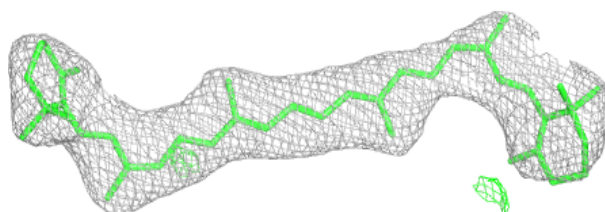


**Electron density around CHL 3 607:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

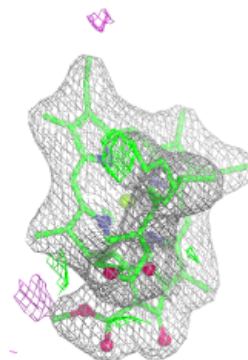
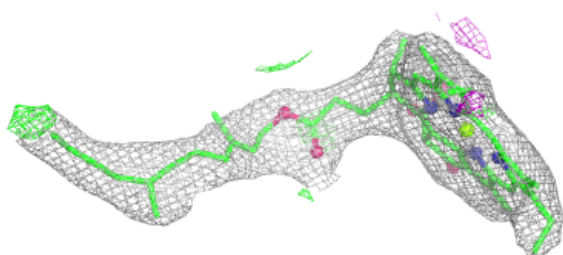
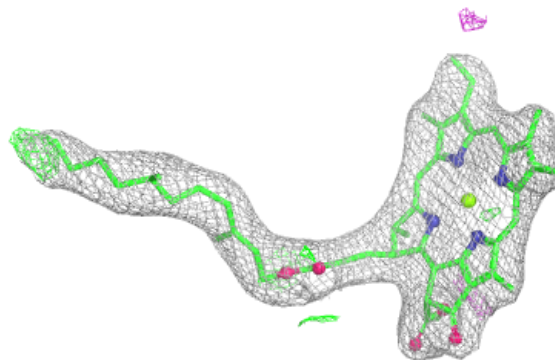
**Electron density around BCR B 846:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



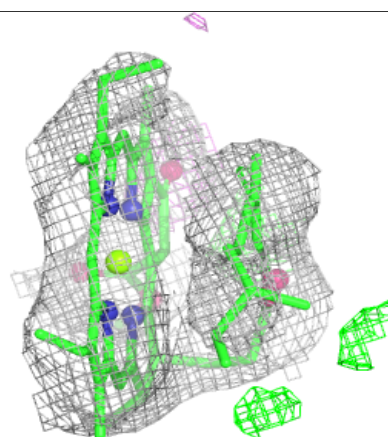
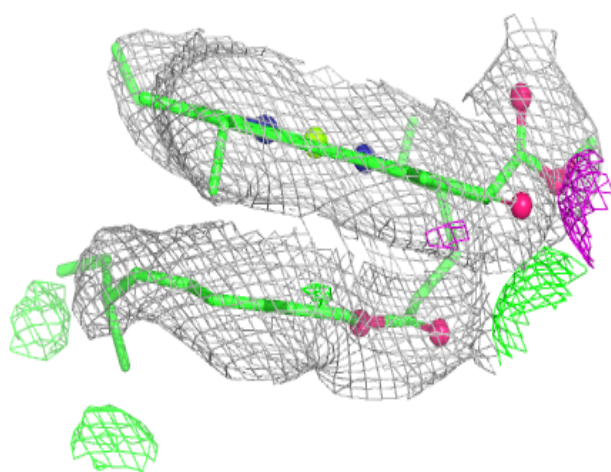
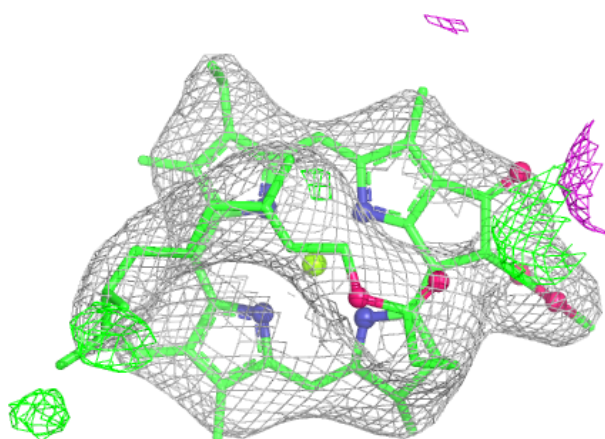
**Electron density around CLA B 834:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



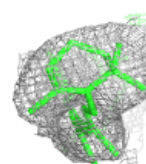
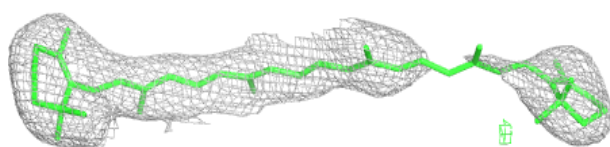
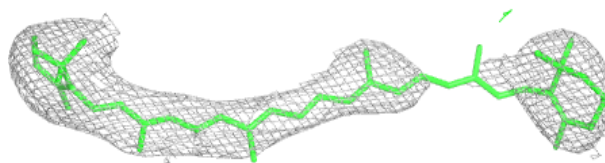
**Electron density around CLA 4 312:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

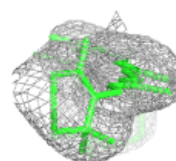
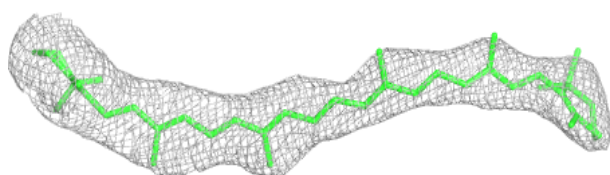
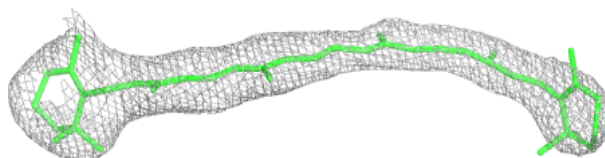


**Electron density around BCR G 106:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

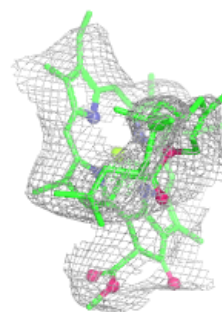
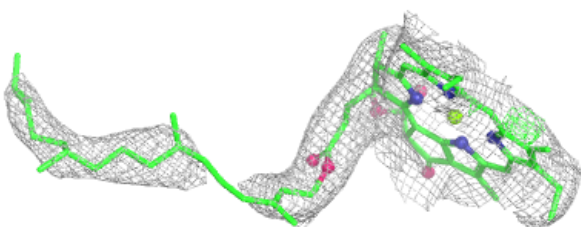
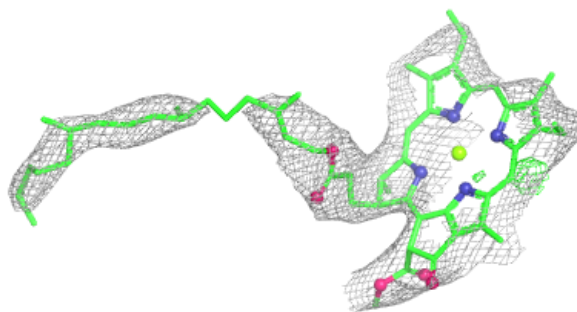
**Electron density around BCR I 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 820:**

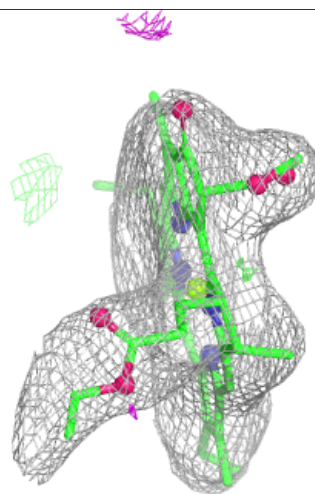
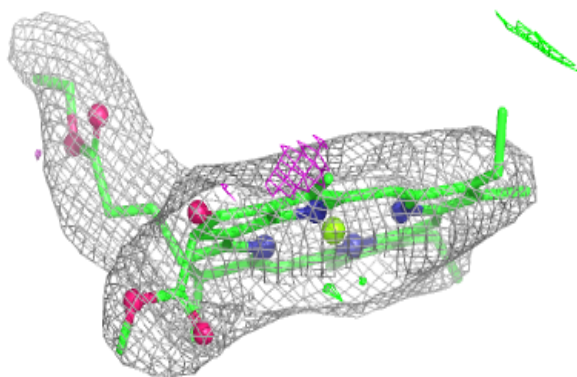
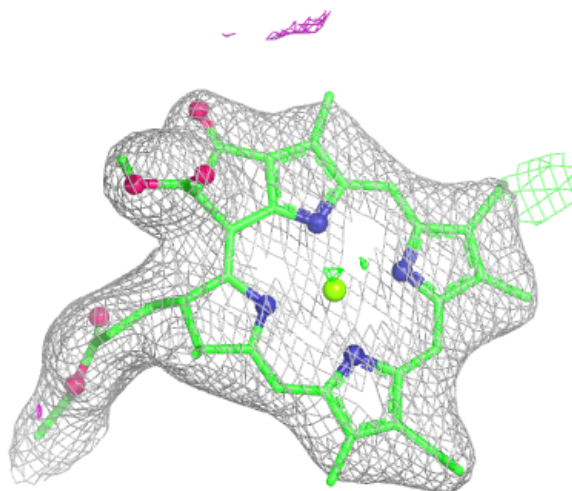
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





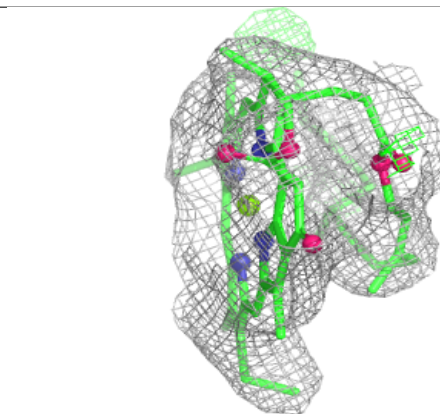
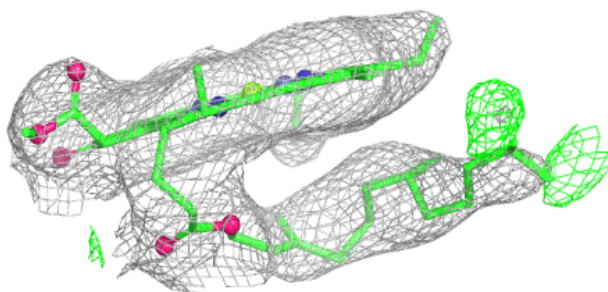
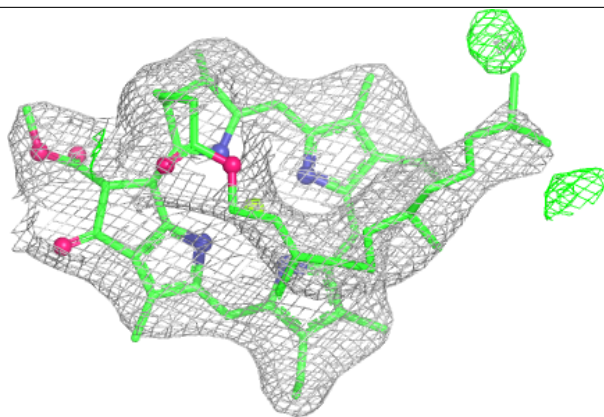
**Electron density around CLA 4 314:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

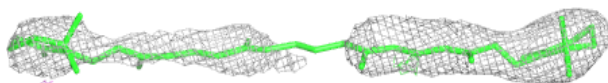
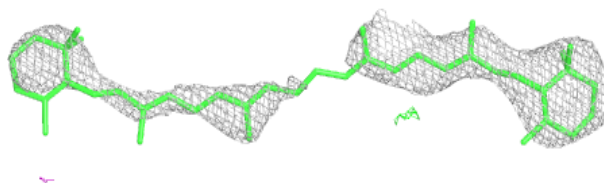


**Electron density around CLA 1 311:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR L 205:**

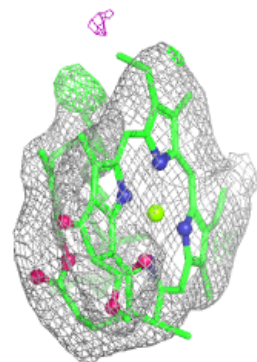
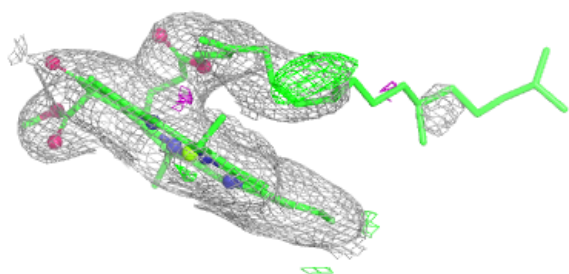
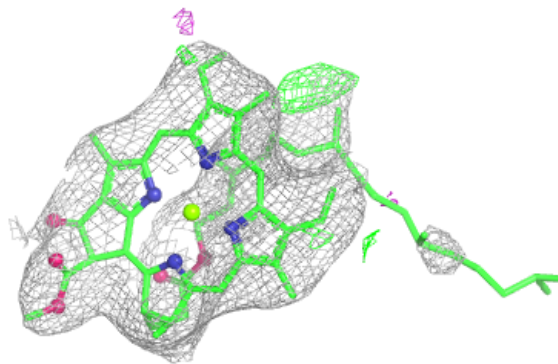
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





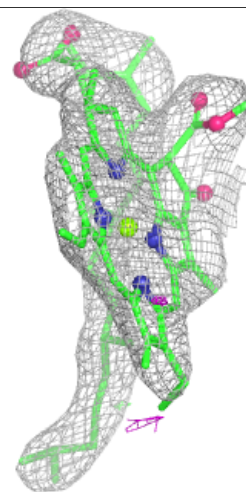
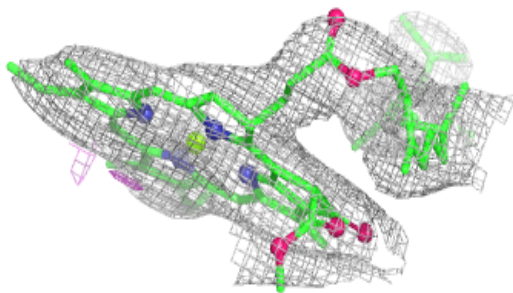
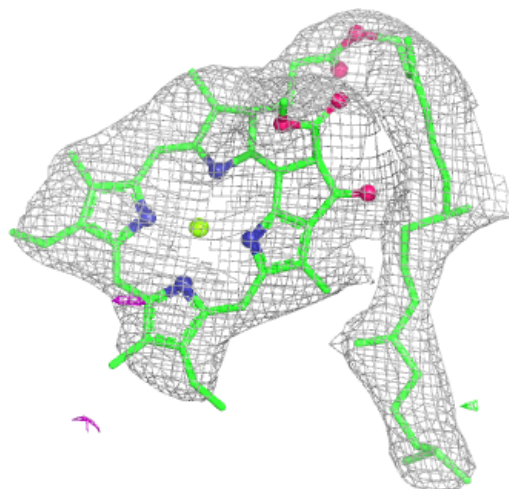
**Electron density around CLA B 809:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



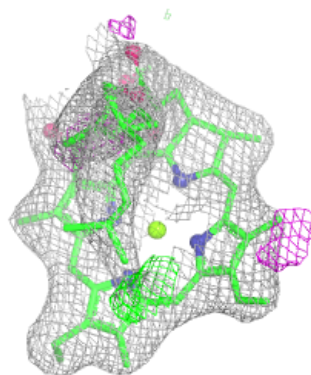
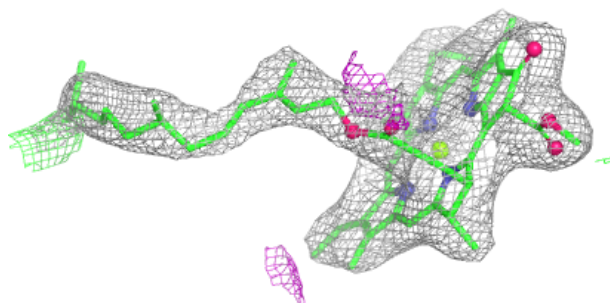
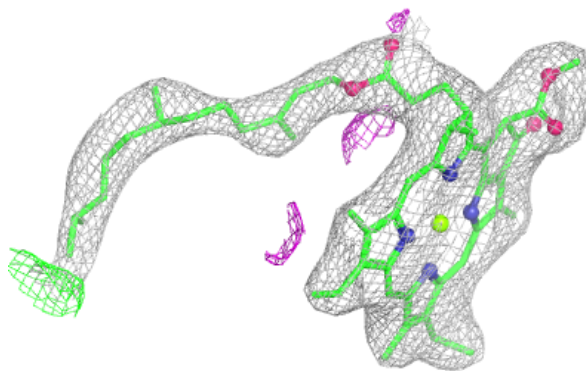
**Electron density around CLA A 824:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



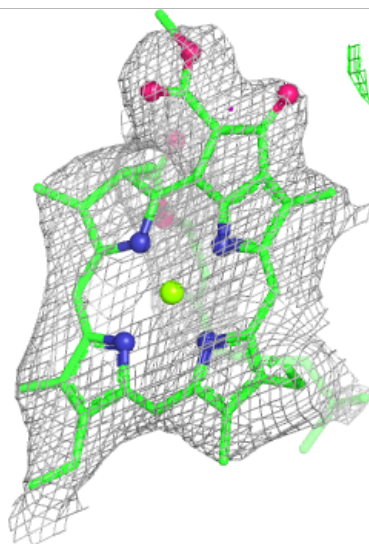
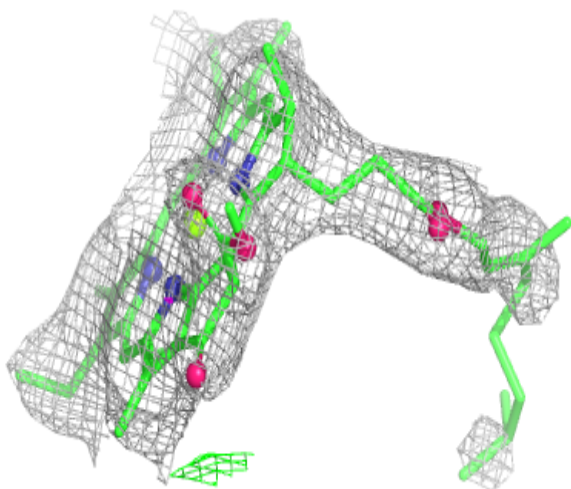
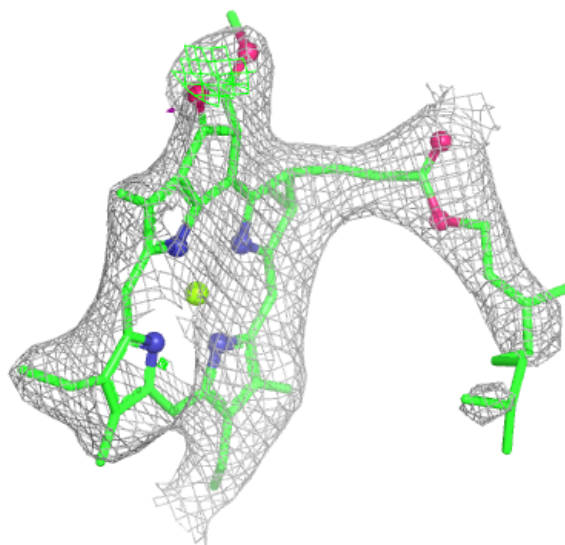
**Electron density around CLA B 833:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



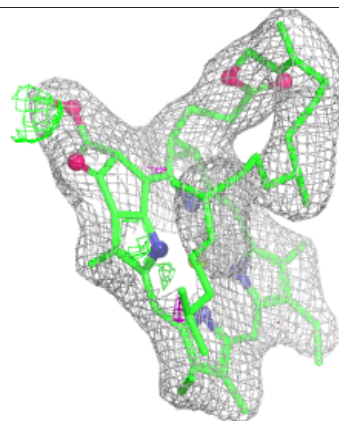
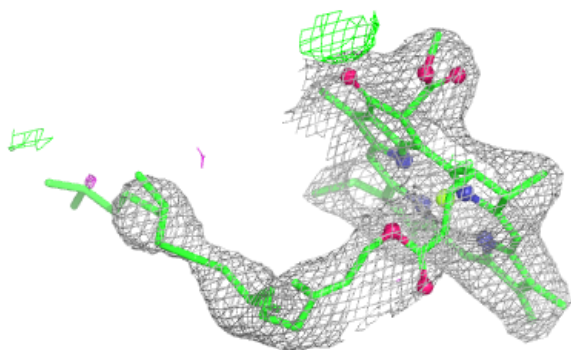
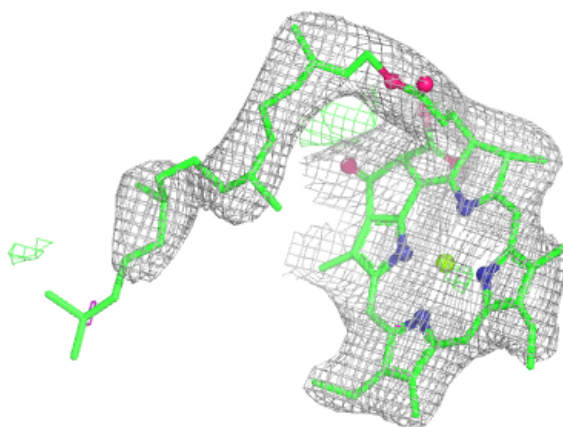
**Electron density around CLA A 803:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



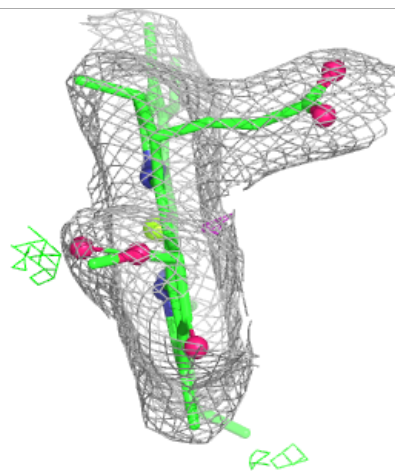
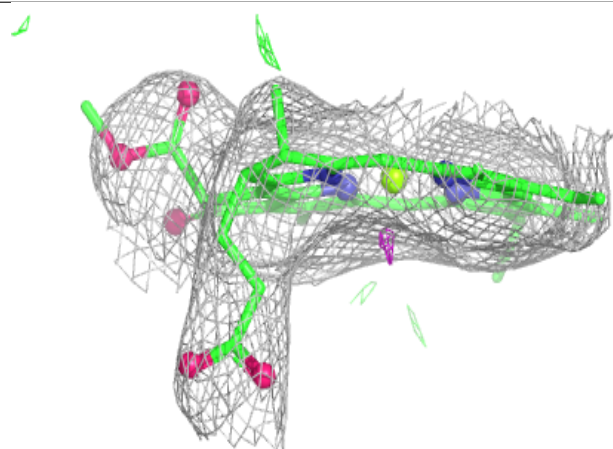
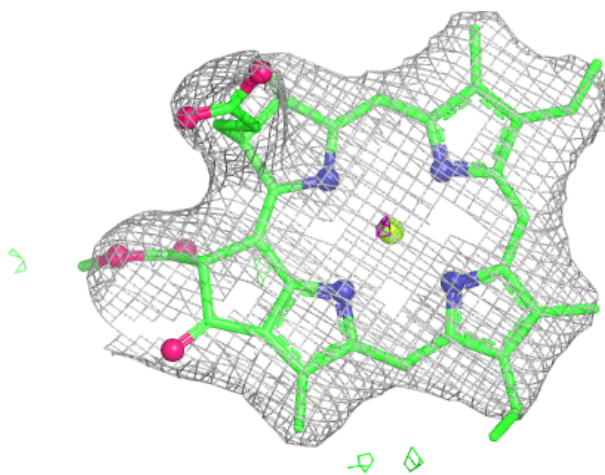
**Electron density around CLA B 835:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 836:**

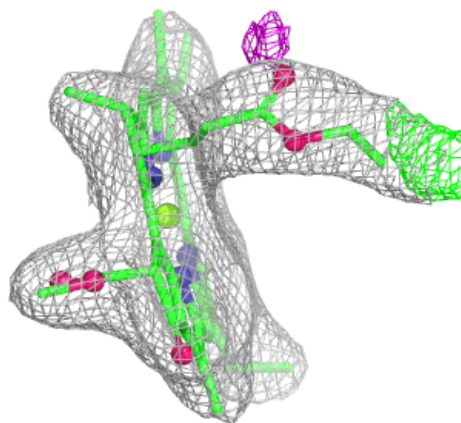
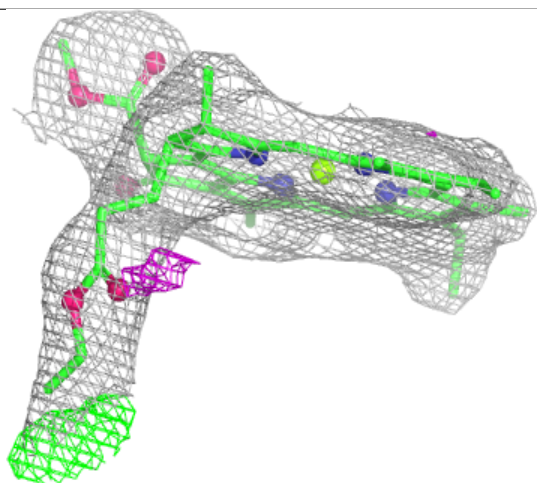
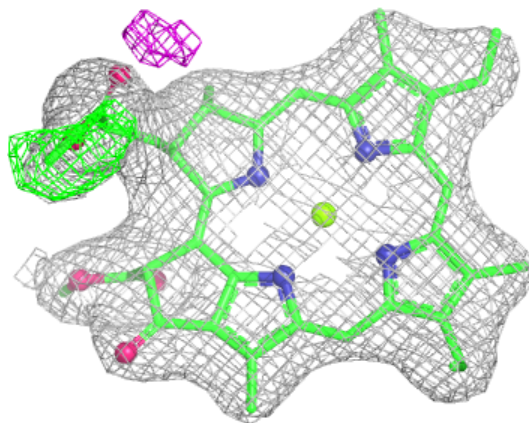
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





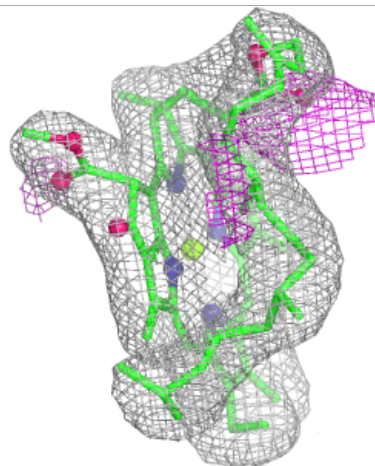
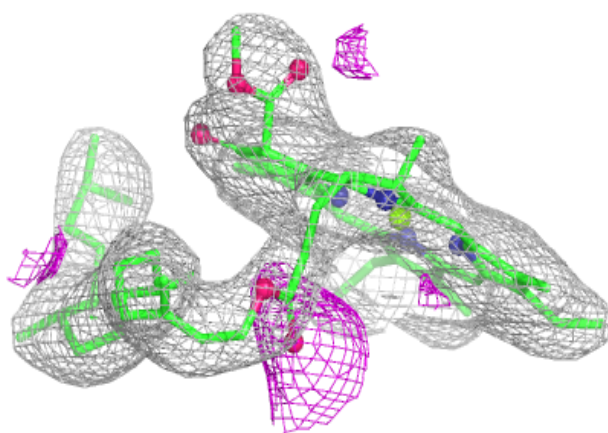
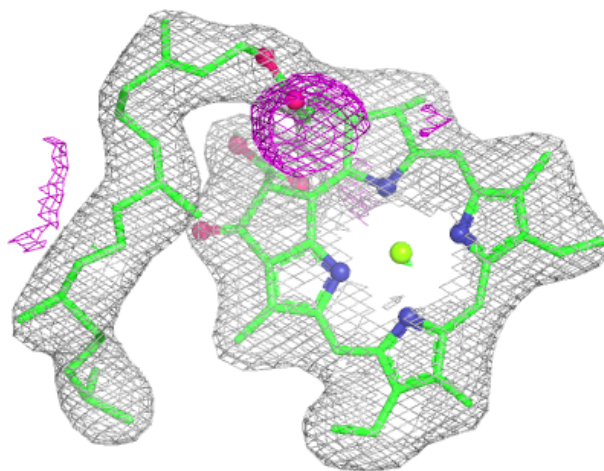
**Electron density around CLA B 839:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA F 304:**

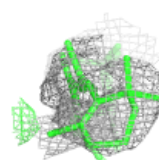
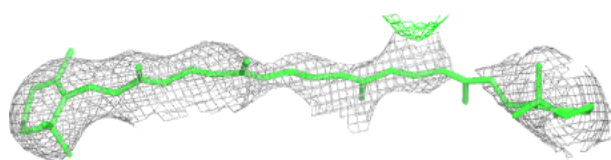
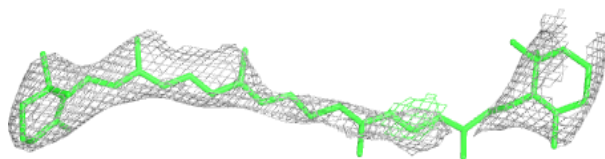
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



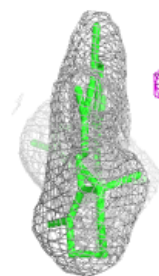
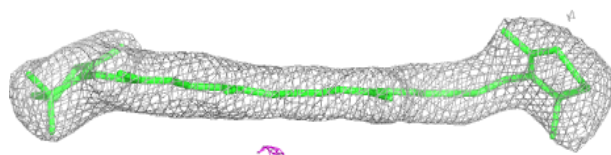
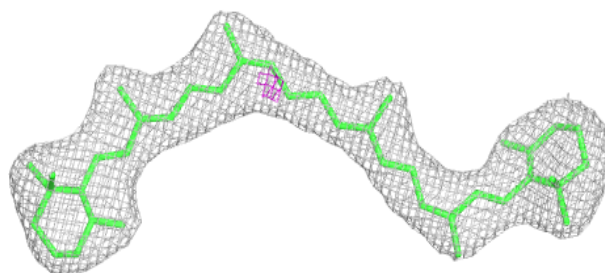


**Electron density around BCR A 850:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

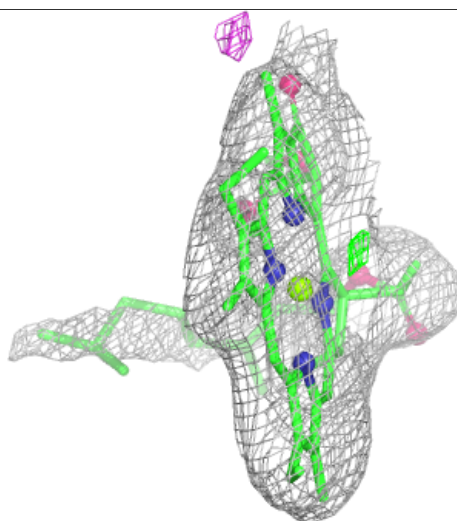
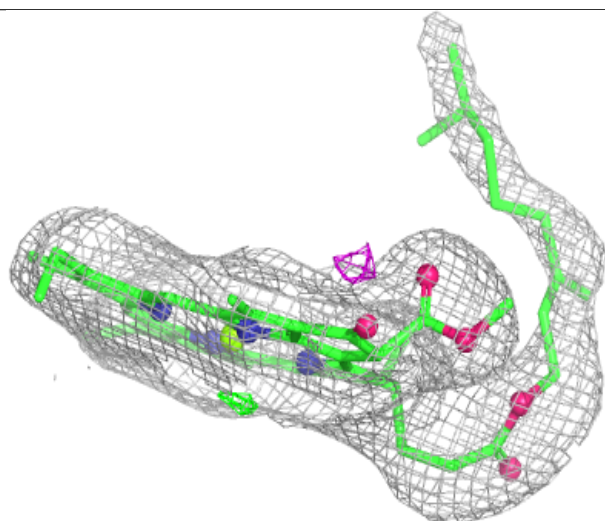
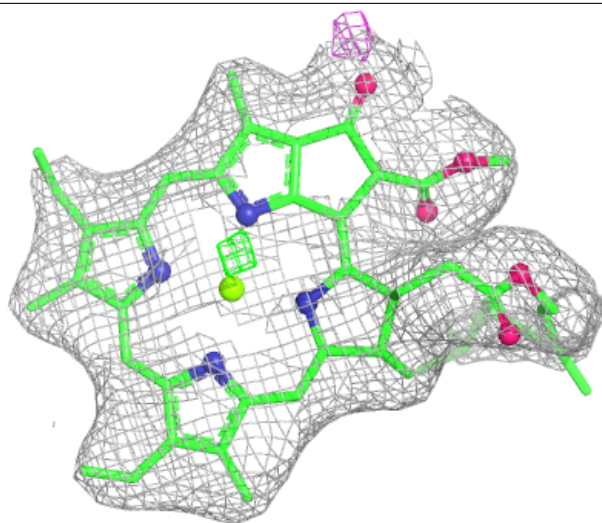
**Electron density around BCR A 851:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



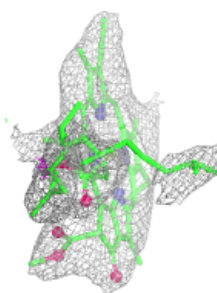
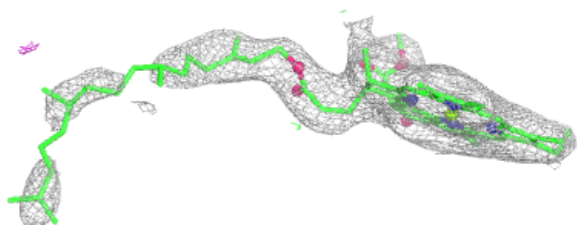
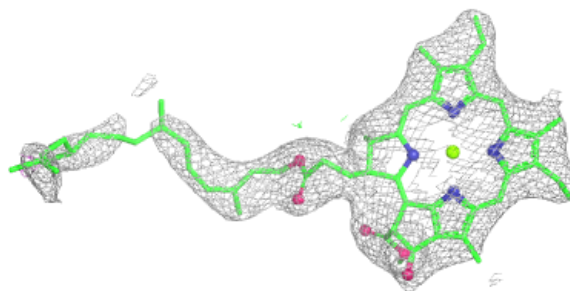
**Electron density around CLA F 307:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

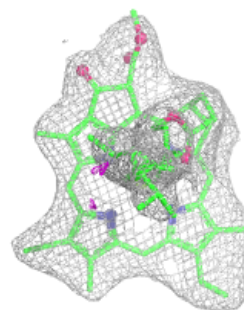
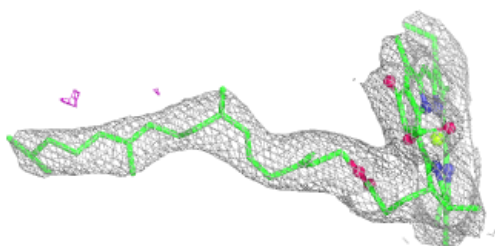
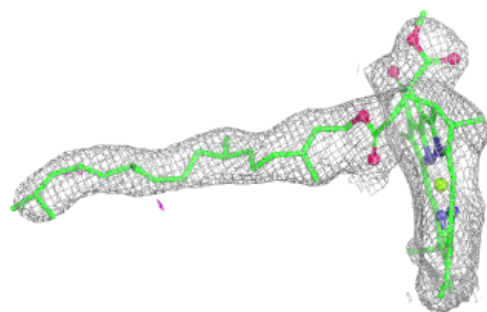


**Electron density around CLA A 804:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

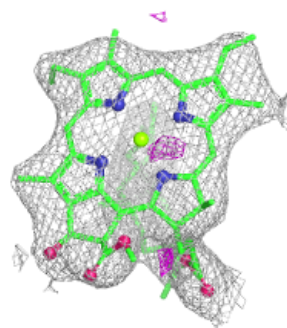
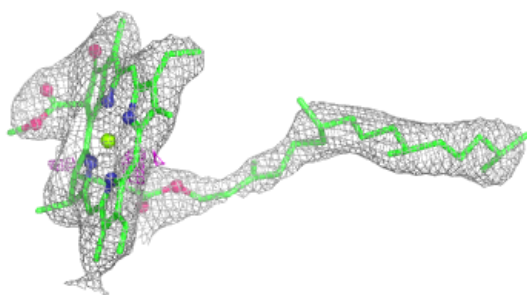
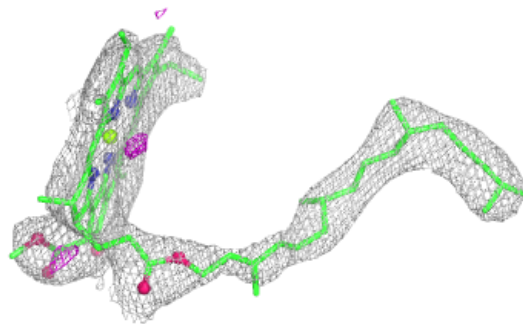
**Electron density around CLA A 827:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

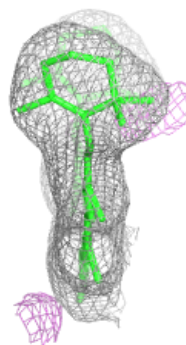
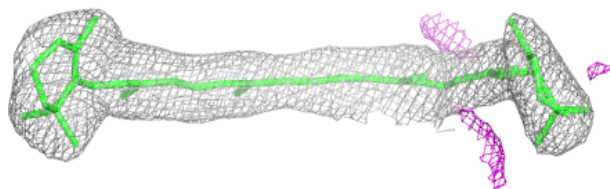
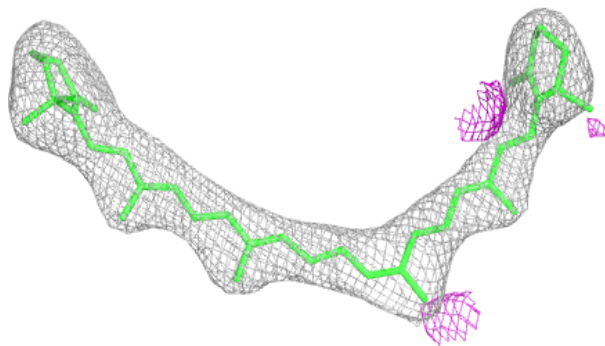


**Electron density around CLA A 829:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

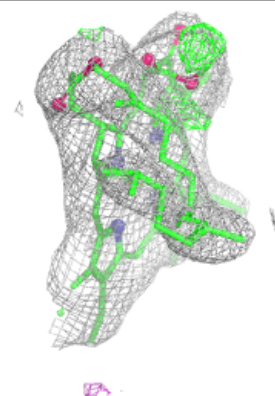
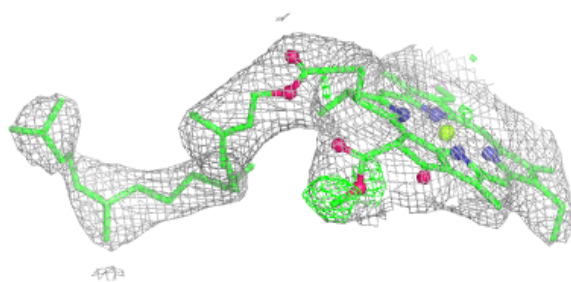
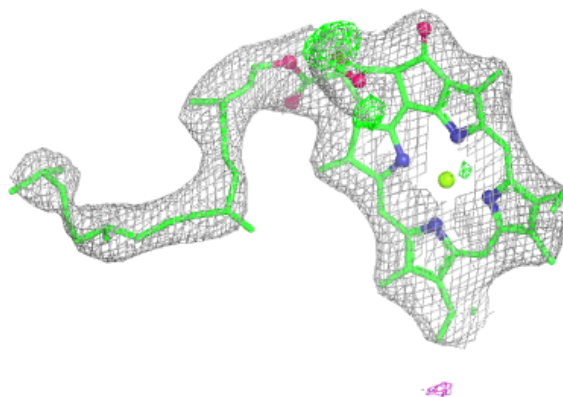
**Electron density around BCR F 308:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

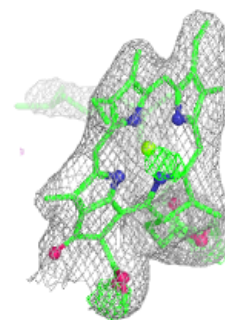
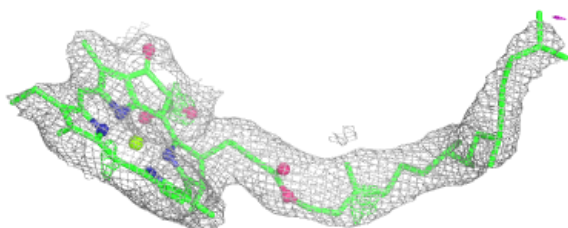
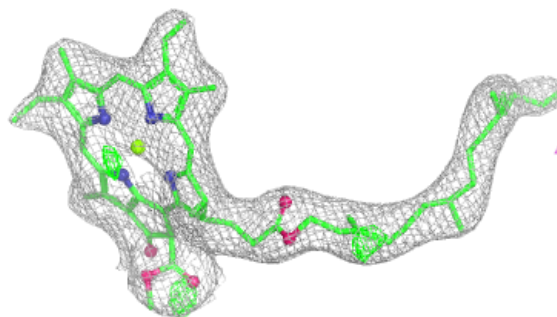


**Electron density around CLA J 101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 853:**

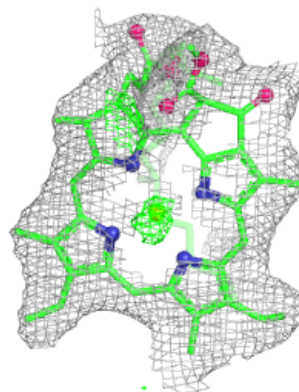
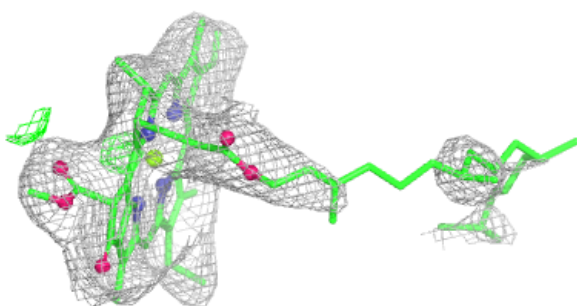
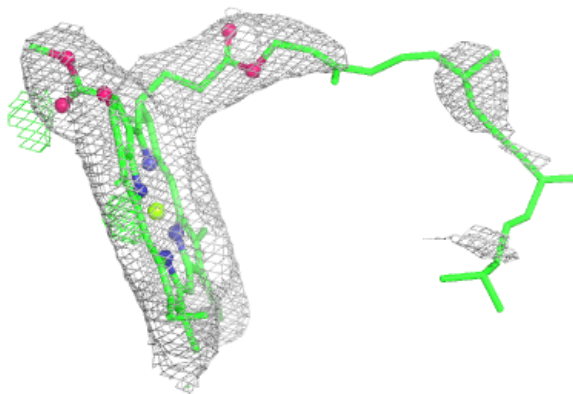
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





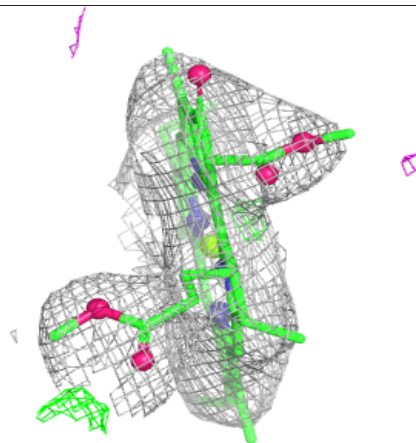
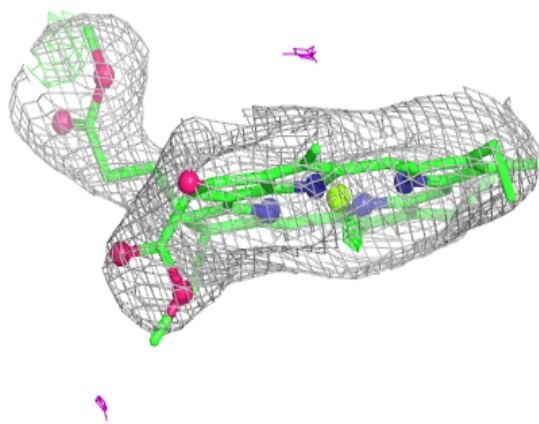
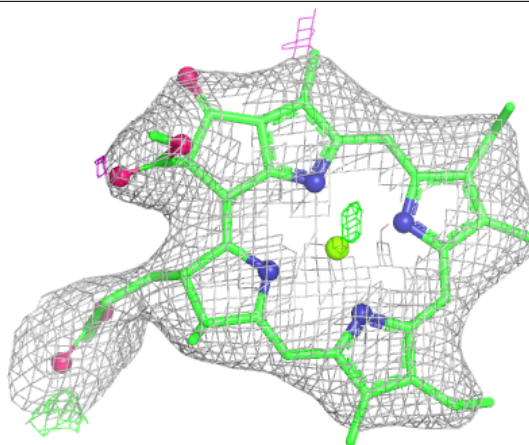
**Electron density around CLA A 806:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



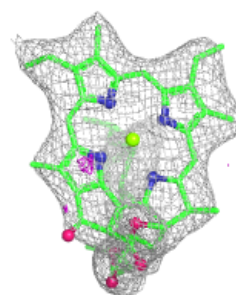
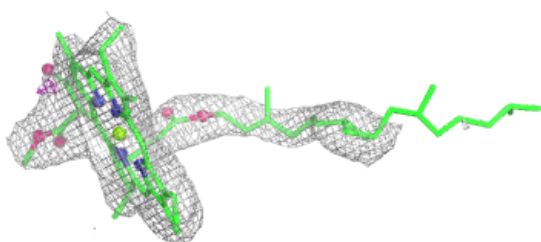
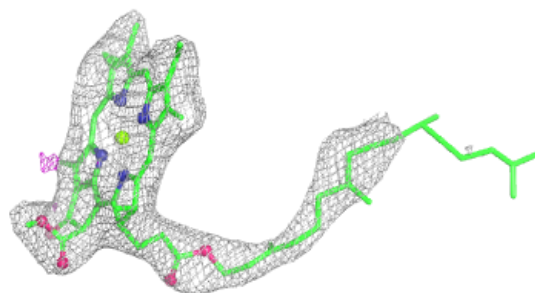
**Electron density around CLA 2 319:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

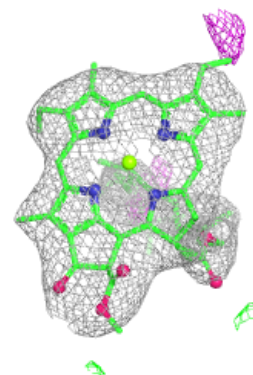
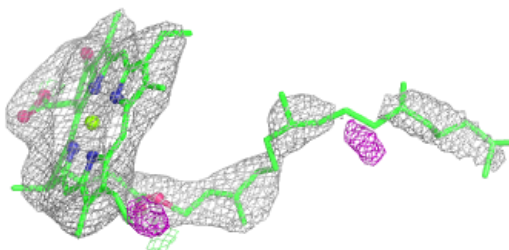
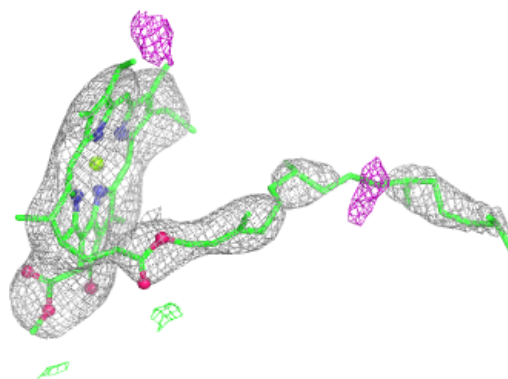


**Electron density around CLA B 823:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 810:**

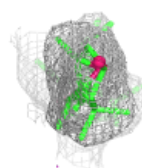
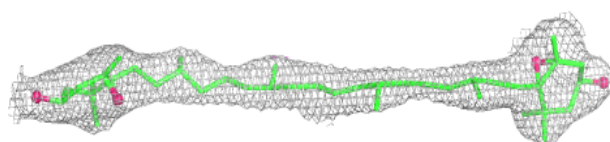
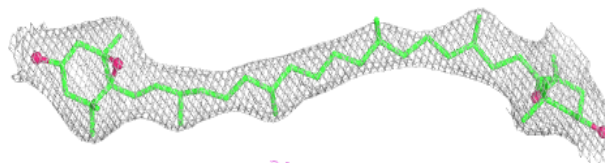
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



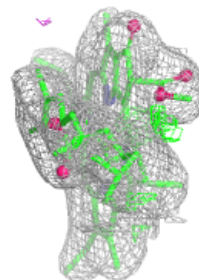
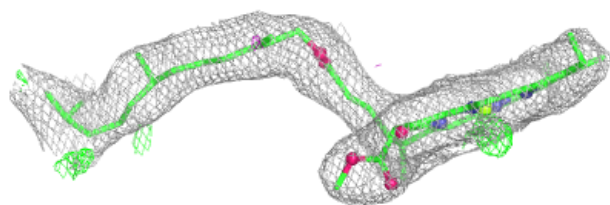
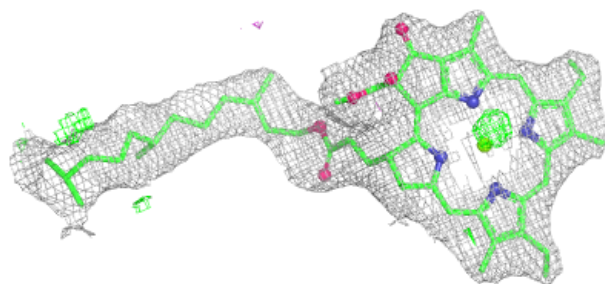


**Electron density around XAT 4 317:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

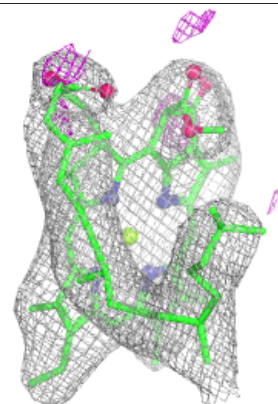
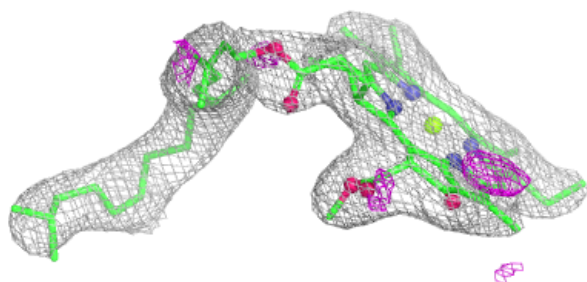
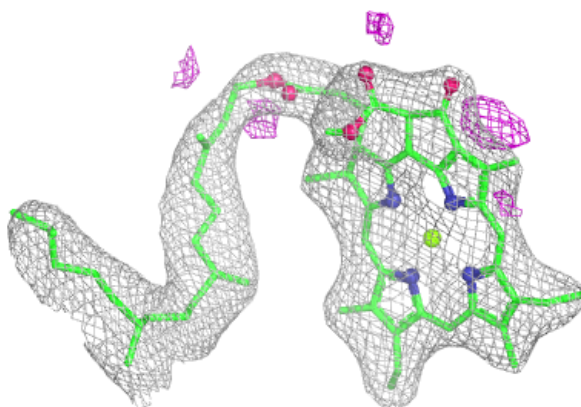
**Electron density around CLA B 825:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



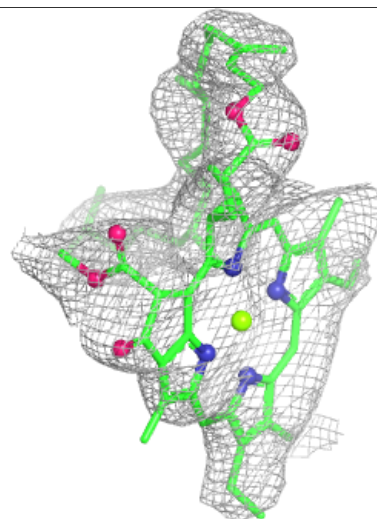
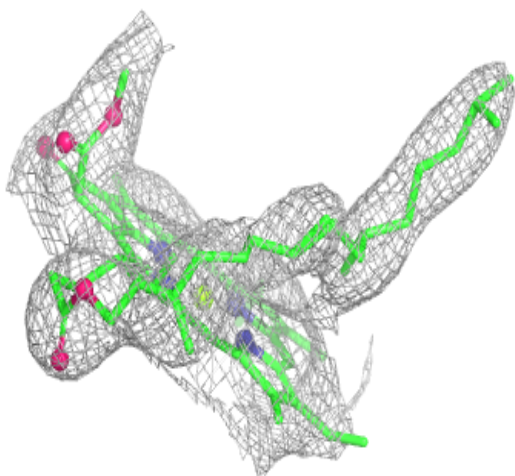
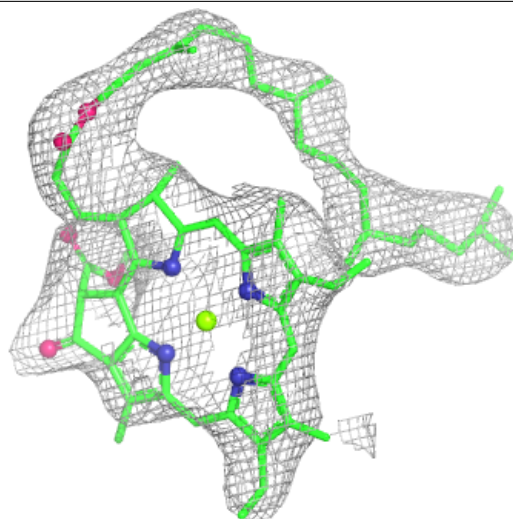
**Electron density around CLA B 826:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



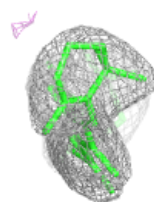
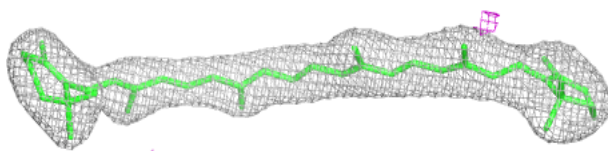
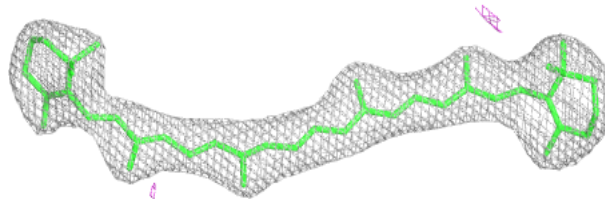
**Electron density around CLA A 812:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

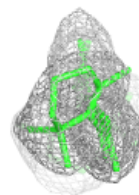
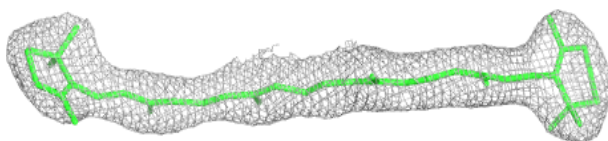
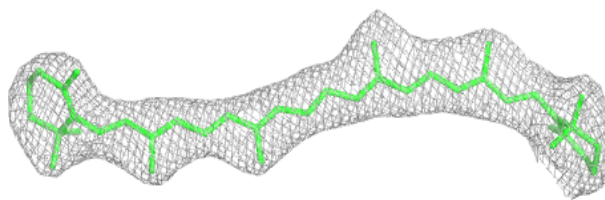


**Electron density around BCR B 848:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

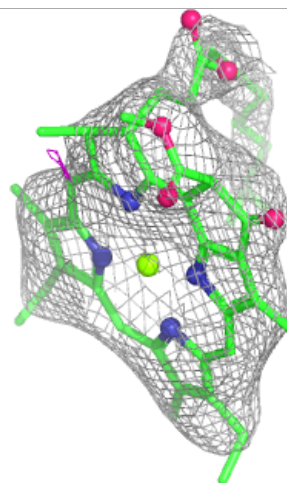
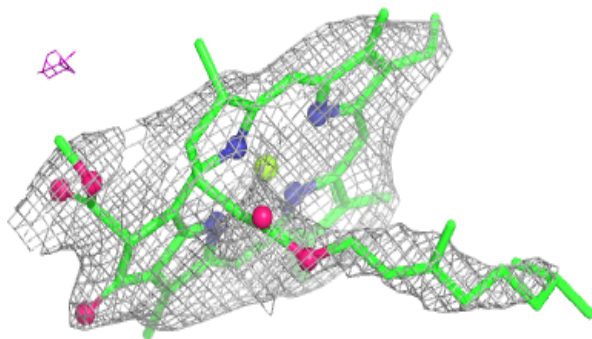
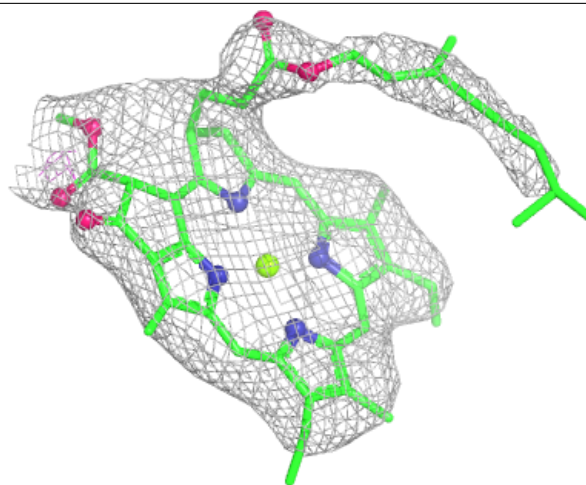
**Electron density around BCR B 849:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 823:**

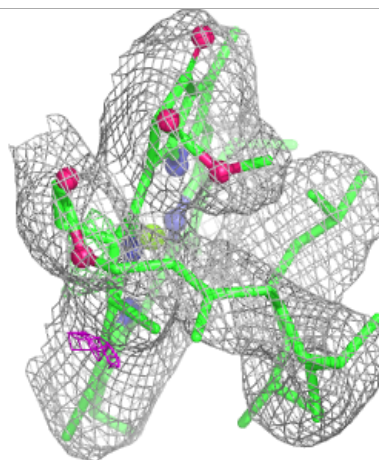
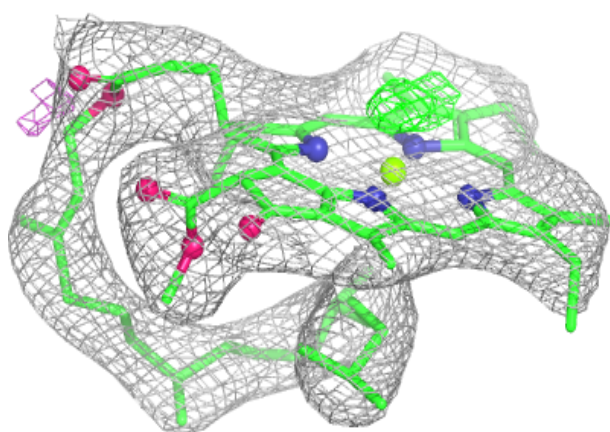
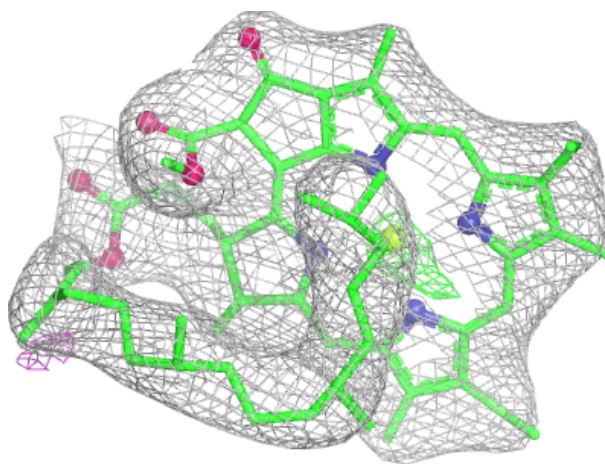
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





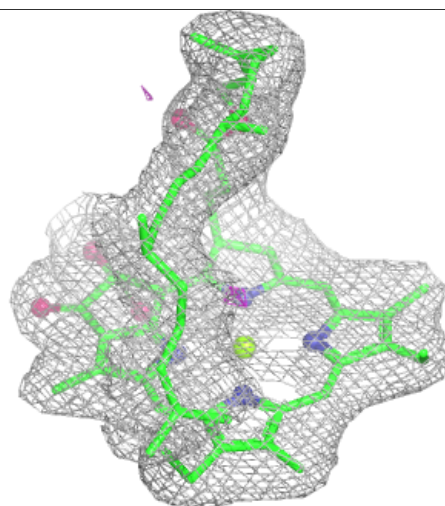
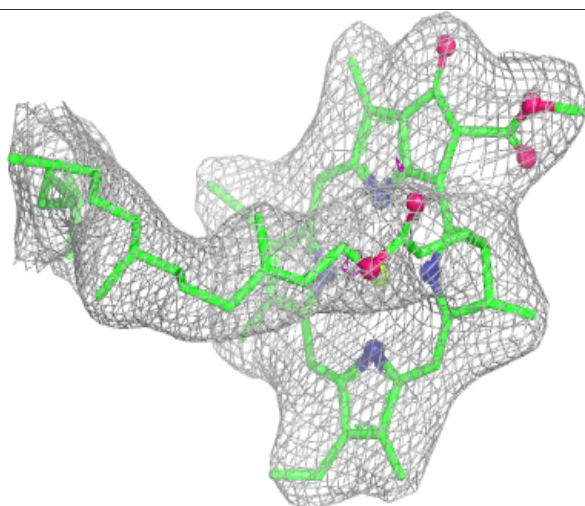
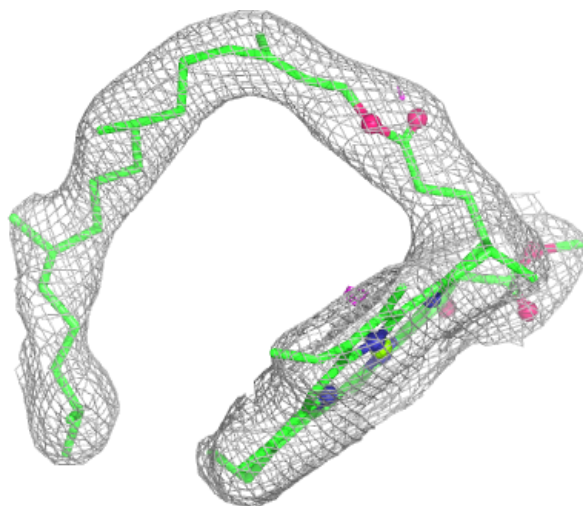
**Electron density around CLA A 805:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



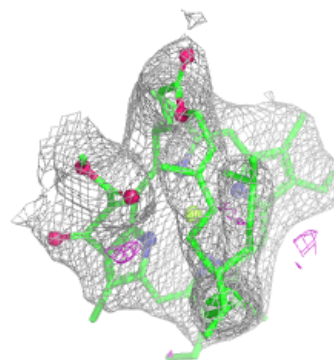
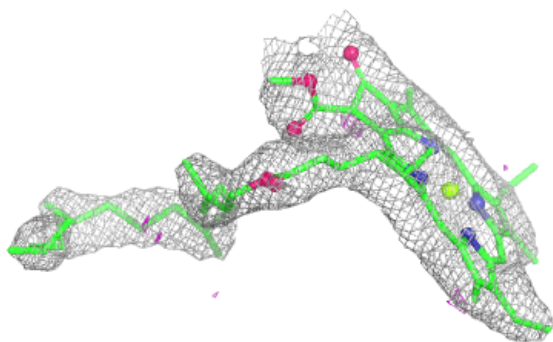
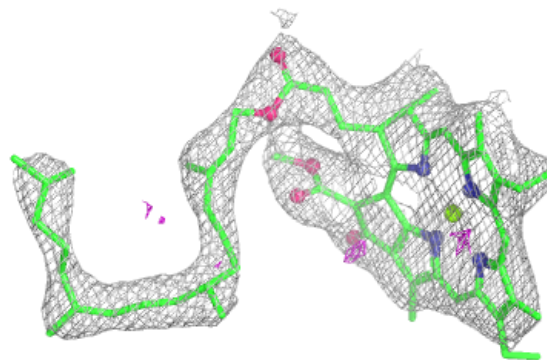
**Electron density around CLA B 821:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

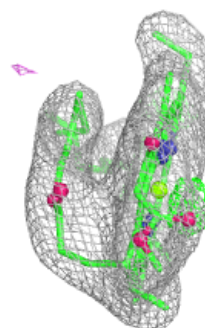
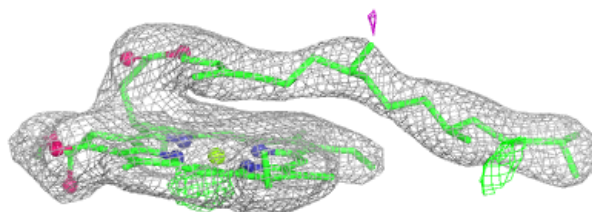
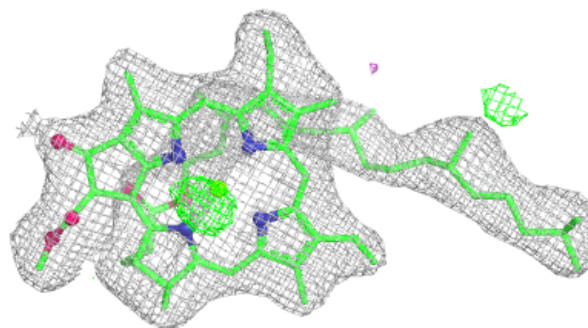


**Electron density around CLA A 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 838:**

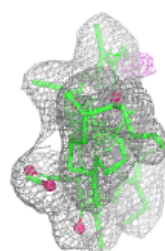
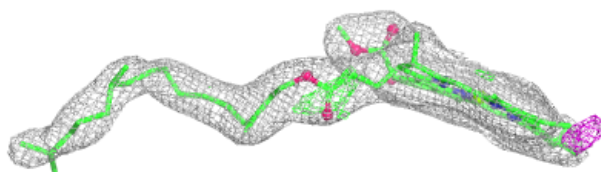
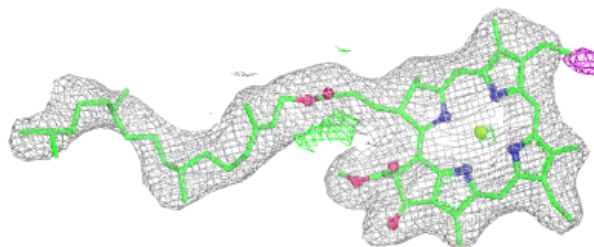
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



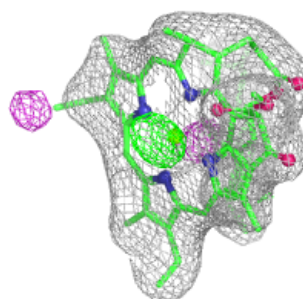
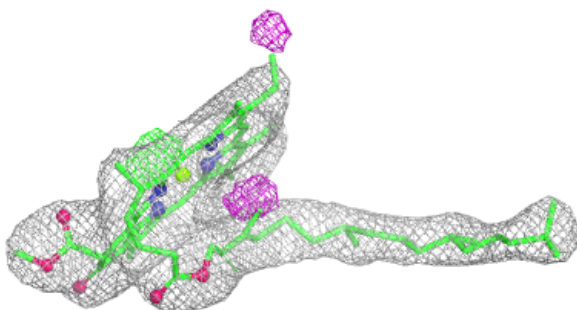
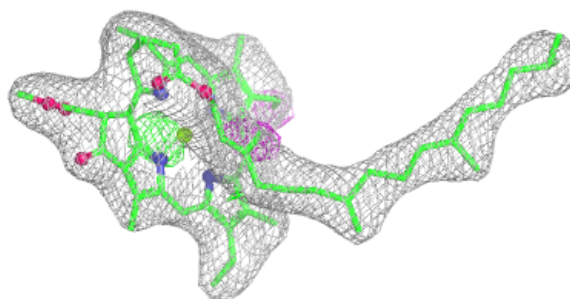


**Electron density around CLA A 839:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

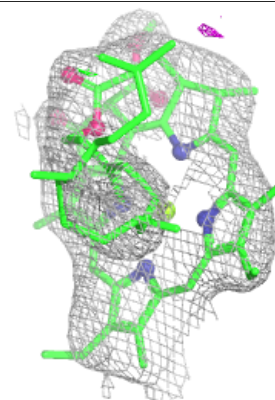
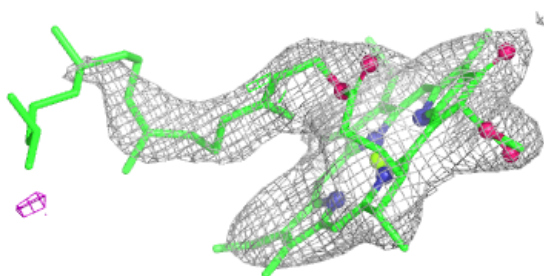
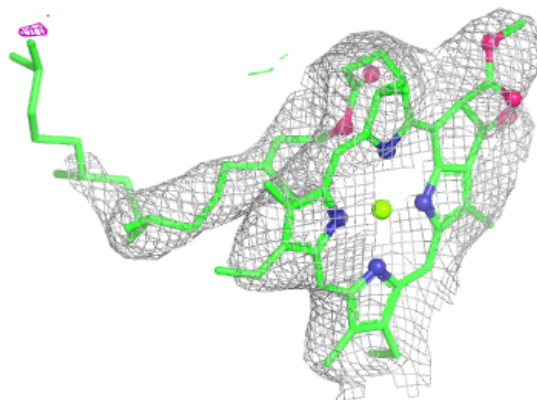
**Electron density around CLA A 840:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

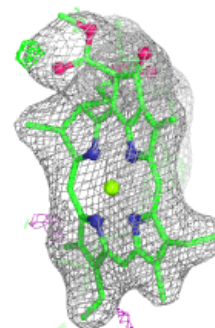
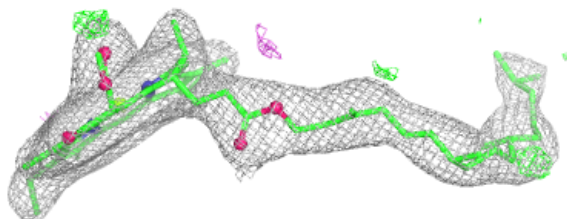
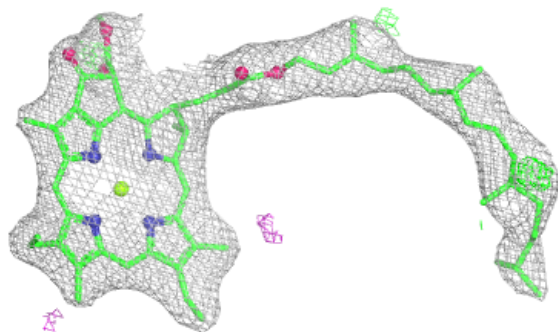


**Electron density around CLA A 841:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

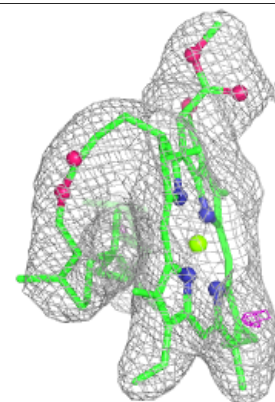
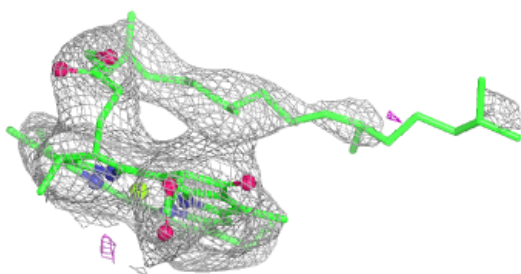
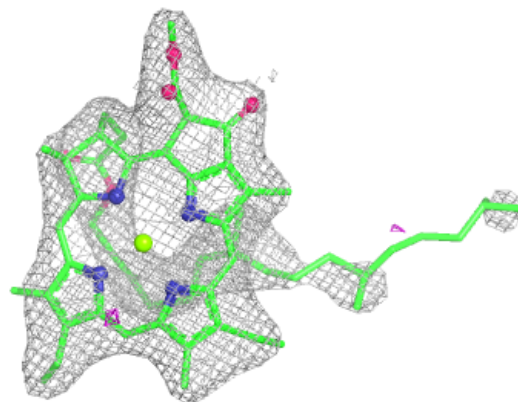
**Electron density around CLA B 827:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

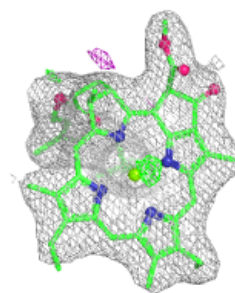
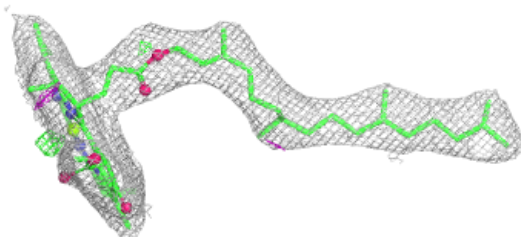
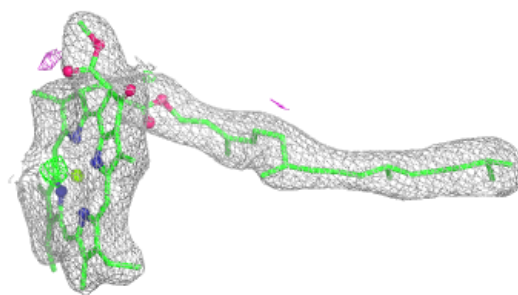


**Electron density around CLA B 829:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

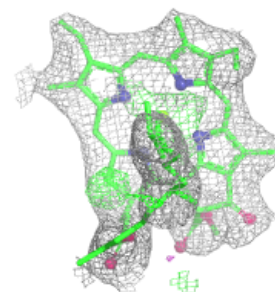
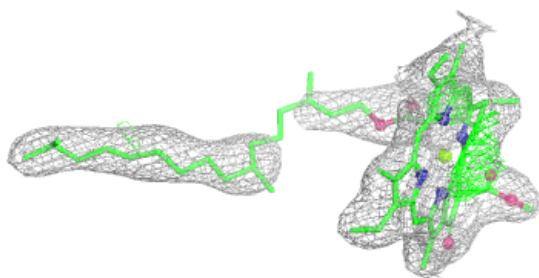
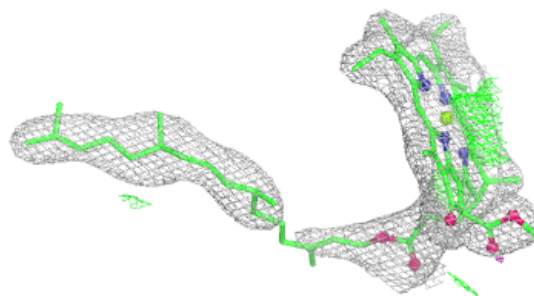
**Electron density around CLA B 830:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



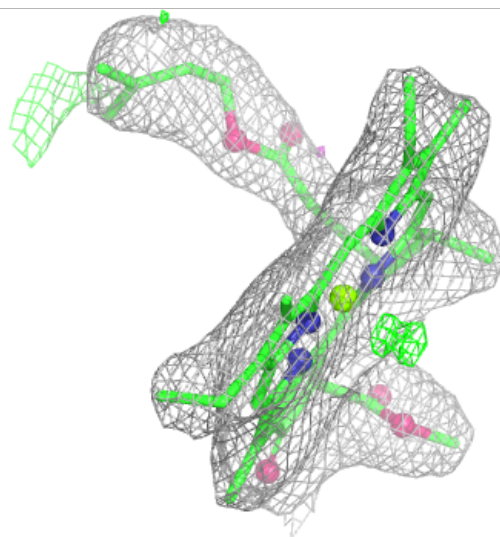
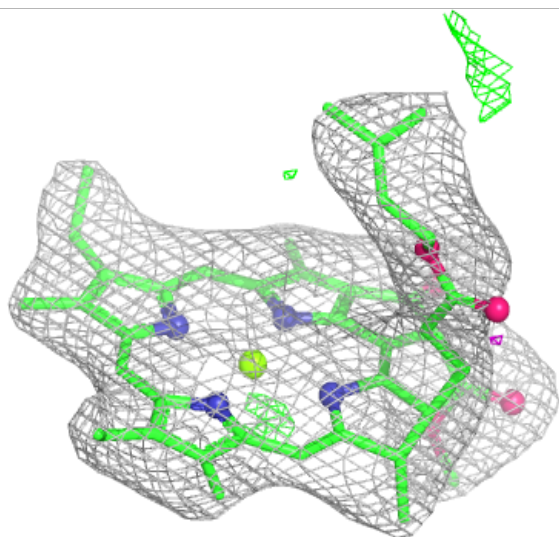
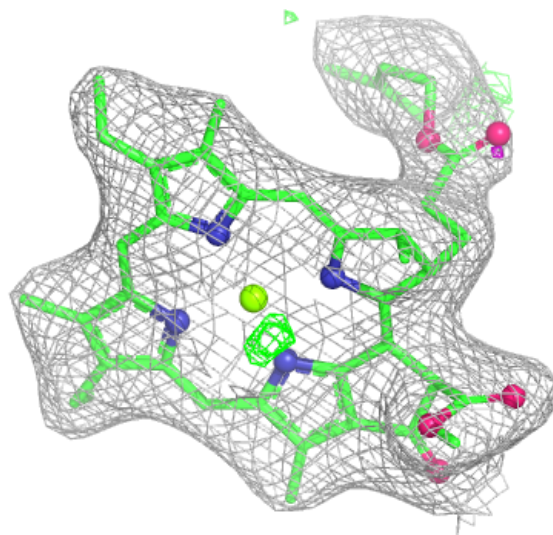
**Electron density around CLA B 831:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 832:**

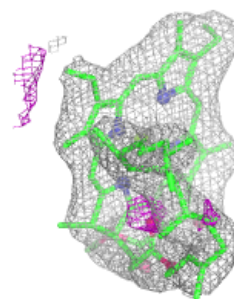
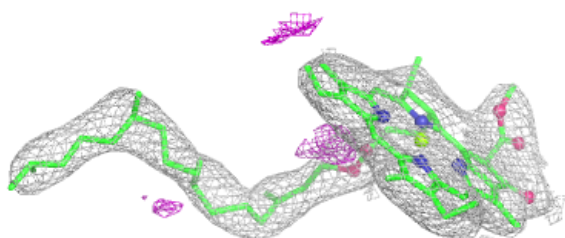
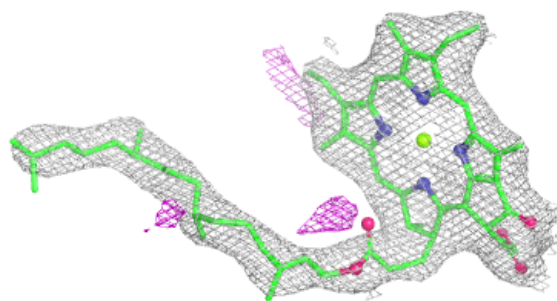
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



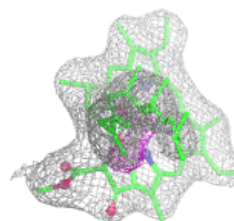
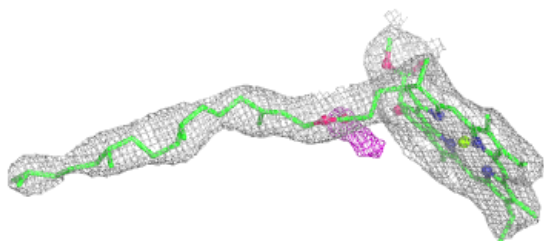
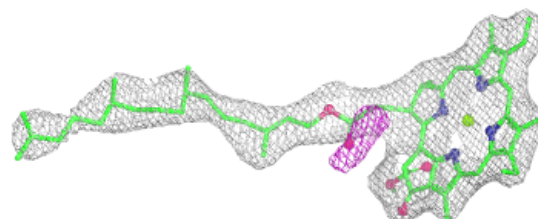


**Electron density around CLA A 807:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

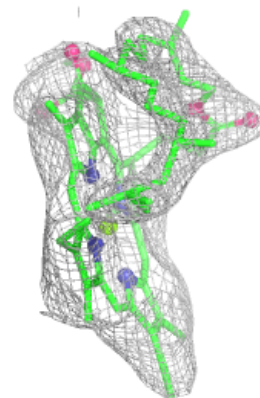
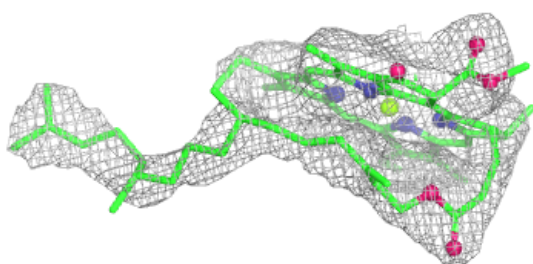
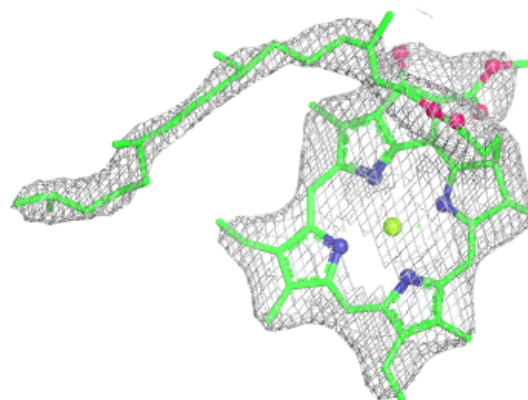
**Electron density around CLA A 808:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

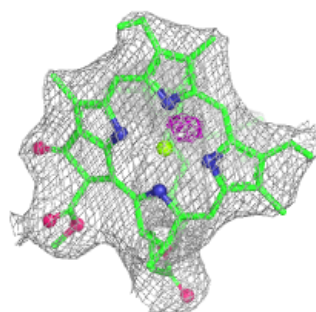
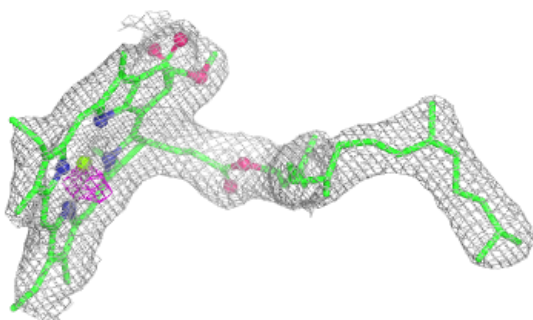
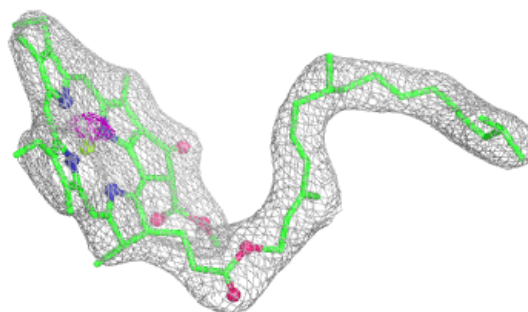


**Electron density around CLA A 828:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

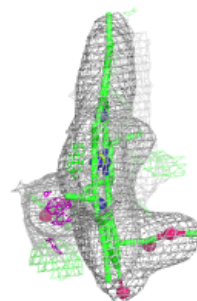
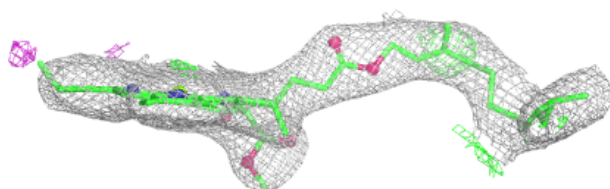
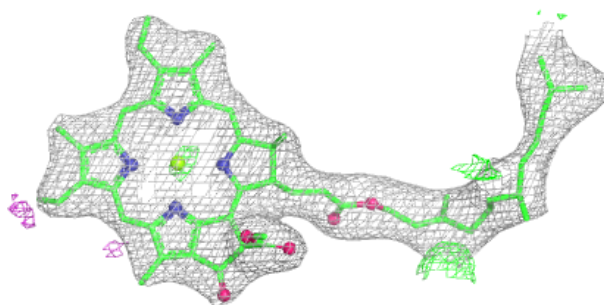
**Electron density around CLA B 804:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

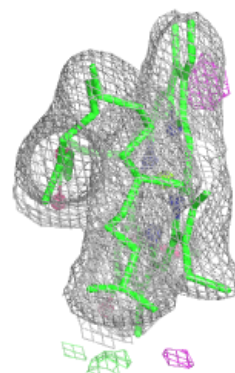
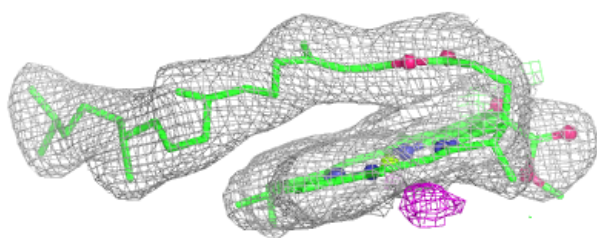
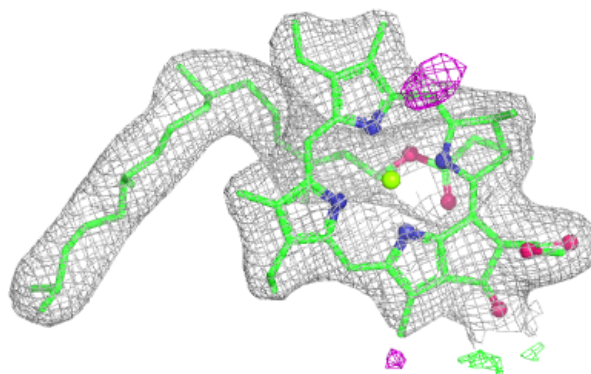


**Electron density around CLA B 837:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 838:**

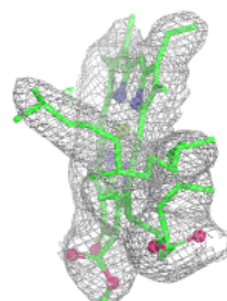
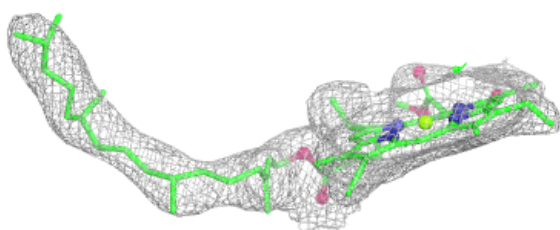
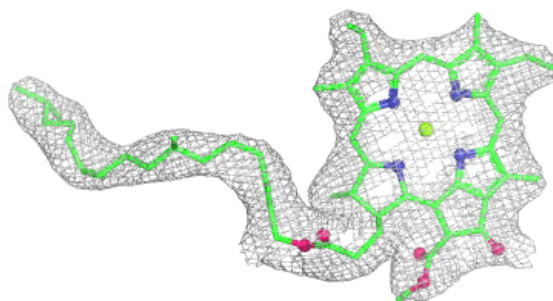
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



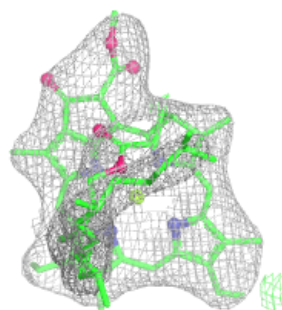
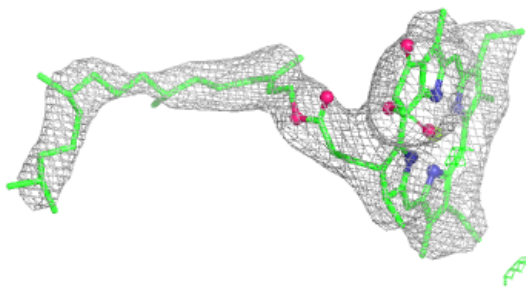
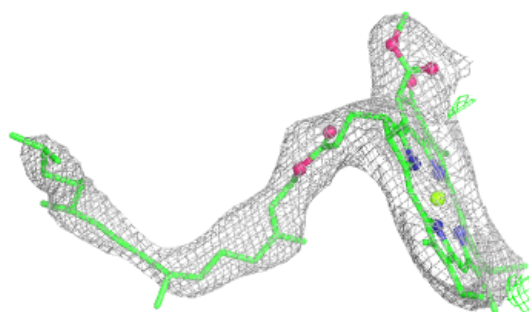


**Electron density around CLA B 805:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

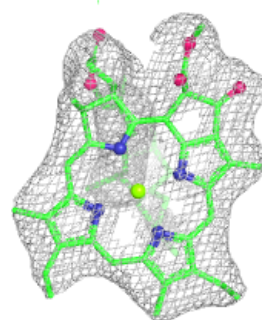
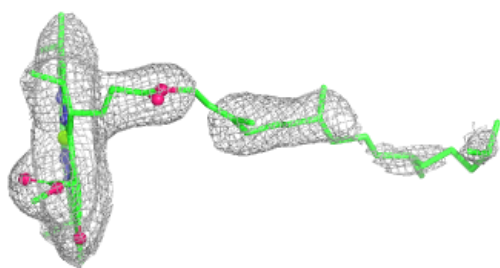
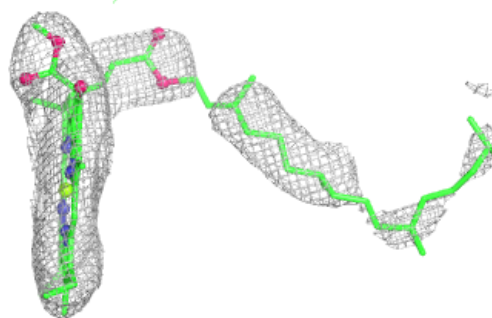
**Electron density around CLA B 840:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

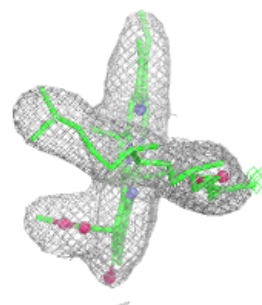
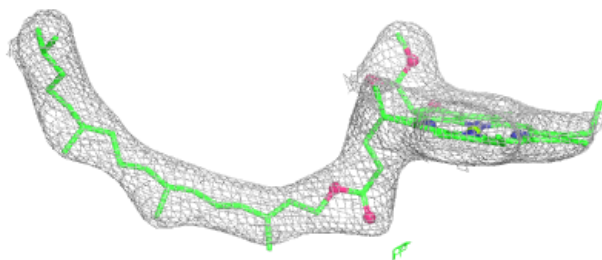
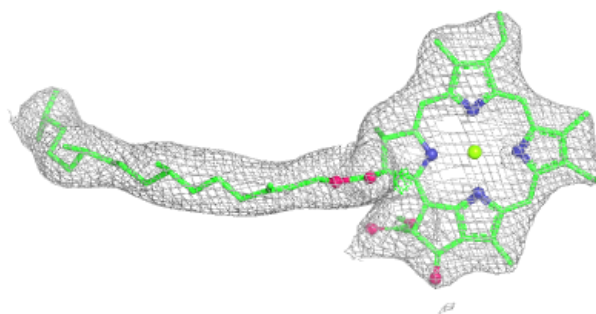


**Electron density around CLA B 841:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

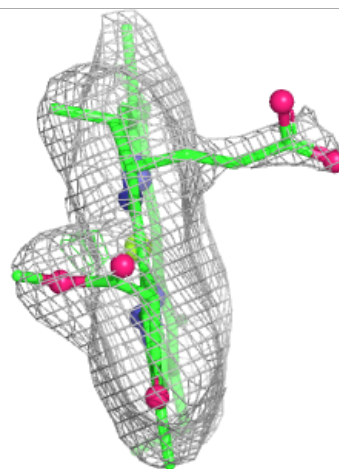
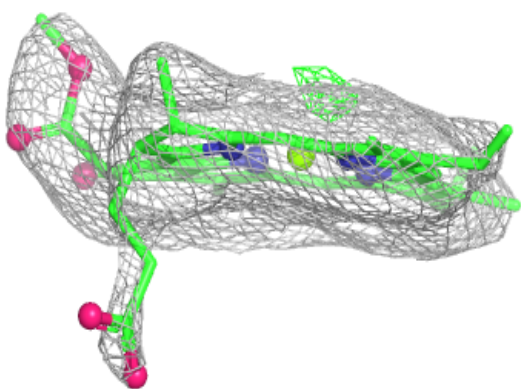
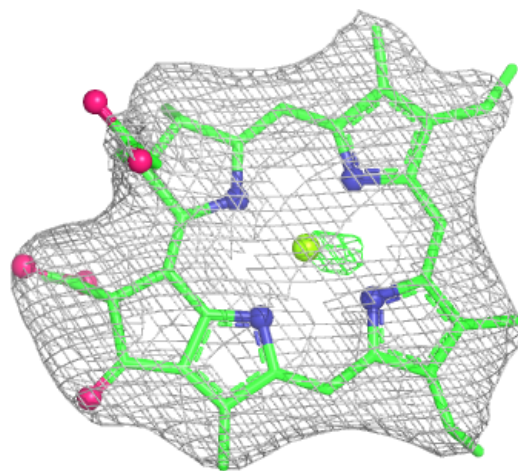
**Electron density around CLA B 842:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



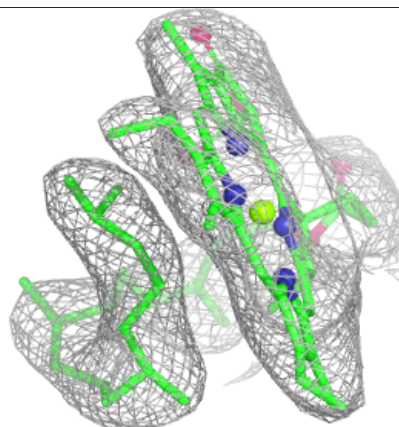
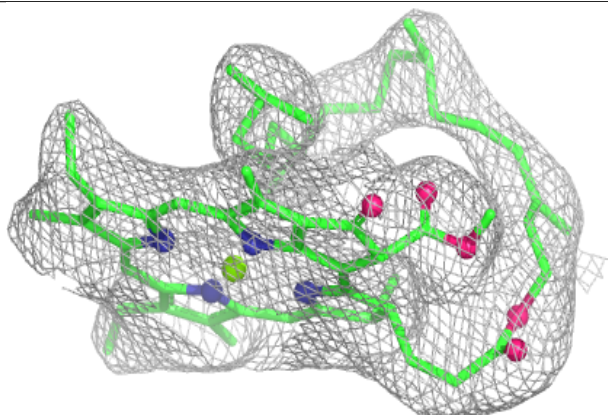
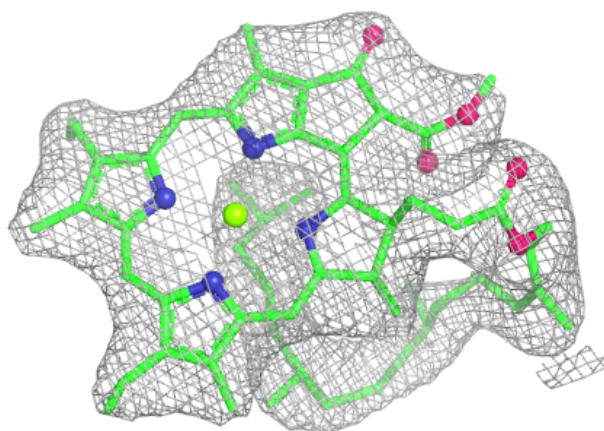
**Electron density around CLA B 806:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

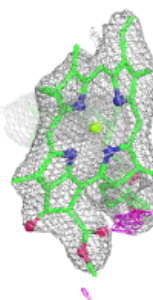
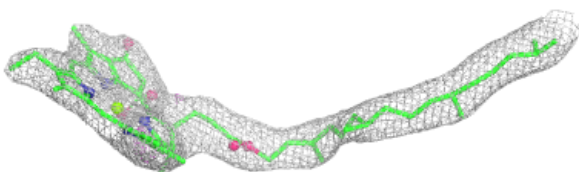
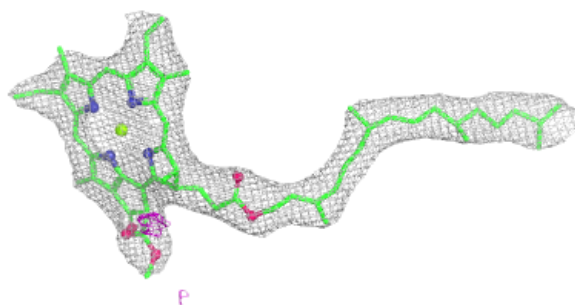


**Electron density around CLA B 808:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

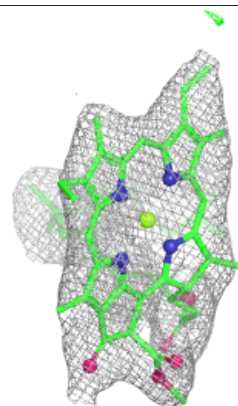
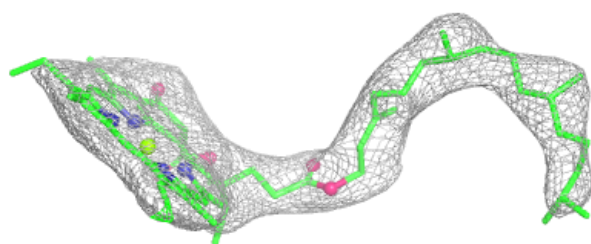
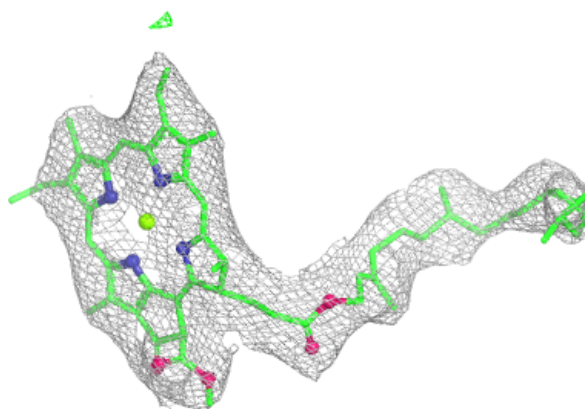
**Electron density around CLA A 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 811:**

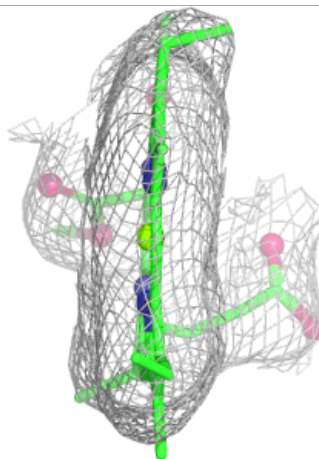
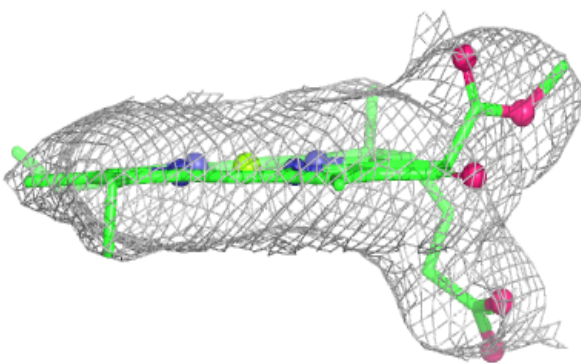
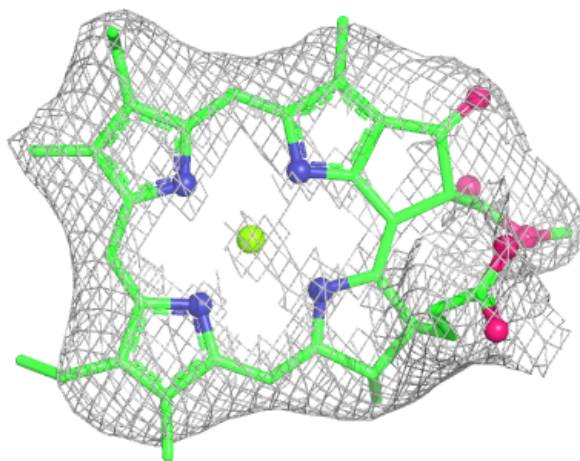
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





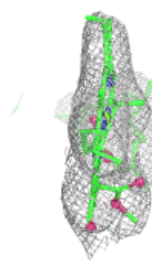
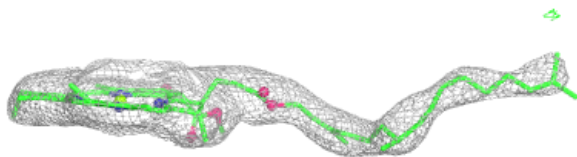
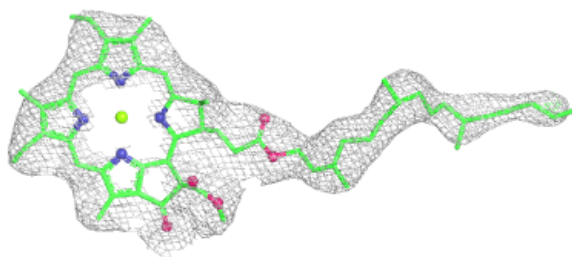
**Electron density around CLA 4 313:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

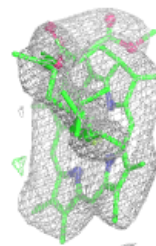
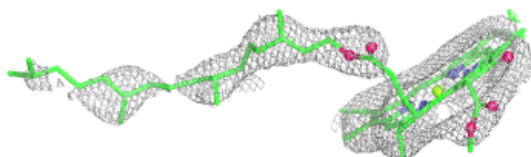


**Electron density around CLA A 831:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 832:**

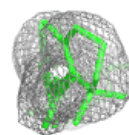
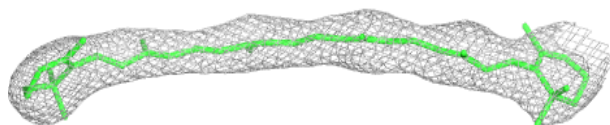
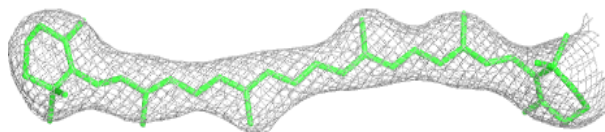
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



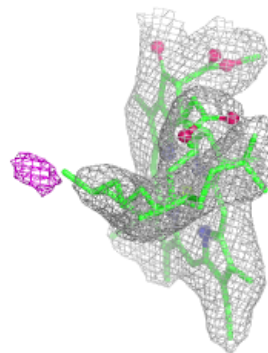
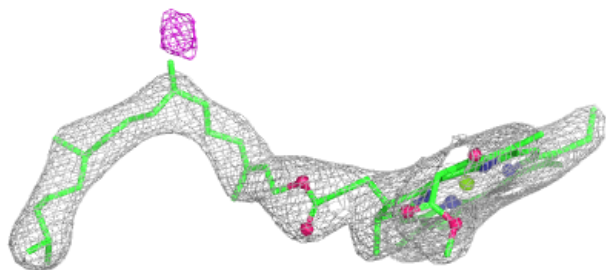
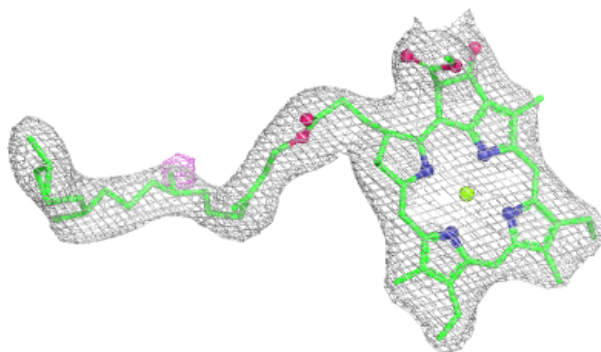


**Electron density around BCR B 844:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

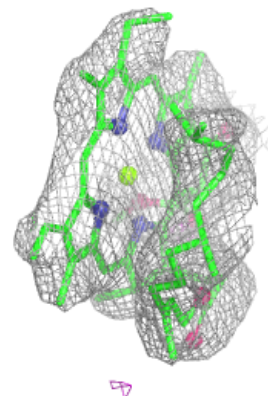
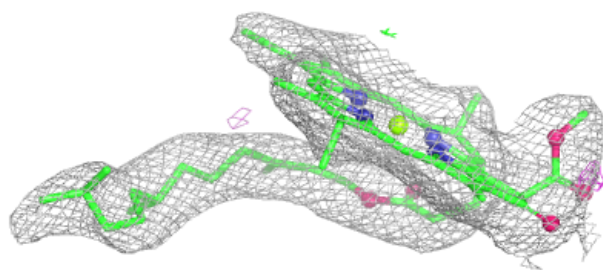
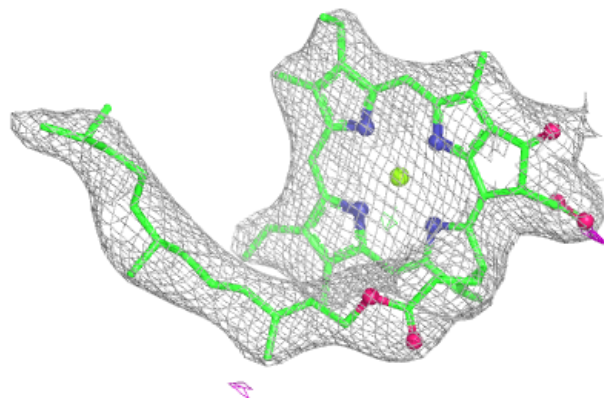
**Electron density around CLA B 815:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

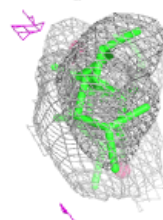
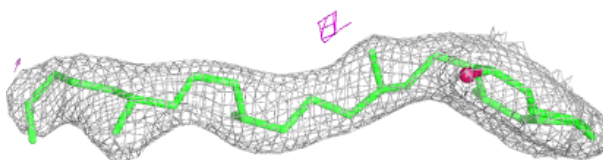
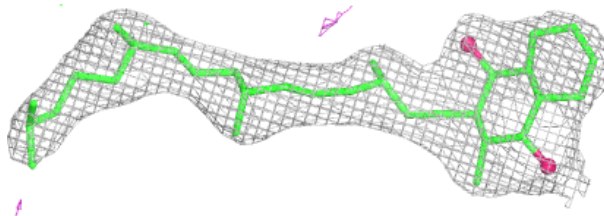


**Electron density around CLA 4 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

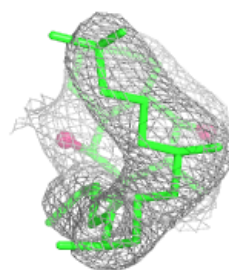
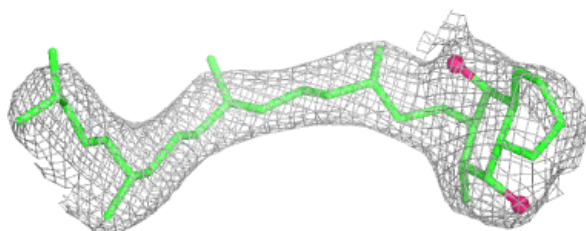
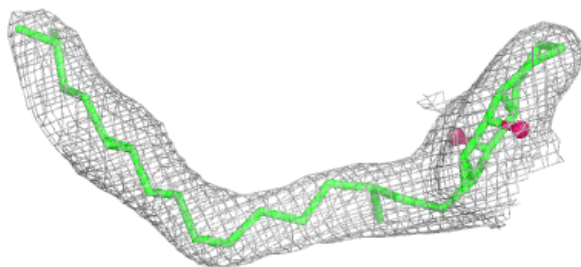
**Electron density around PQN A 842:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



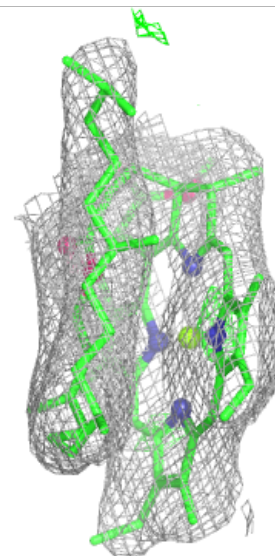
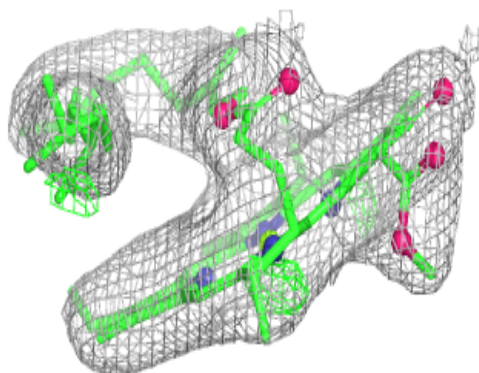
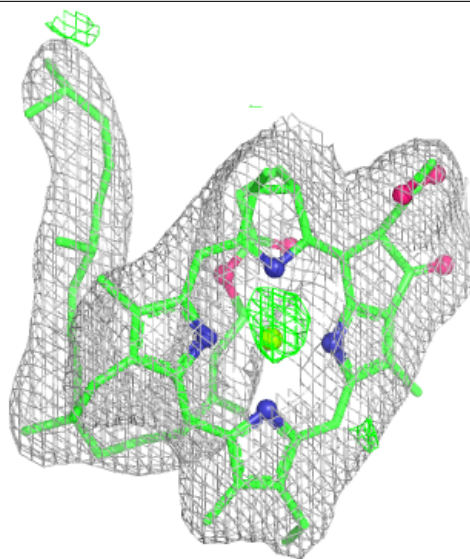
**Electron density around PQN B 843:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



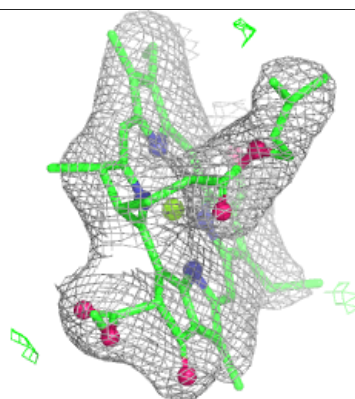
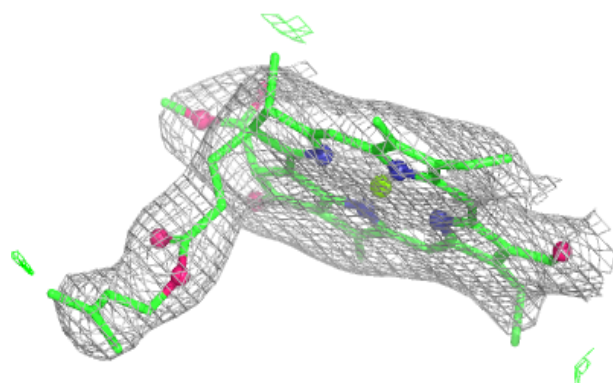
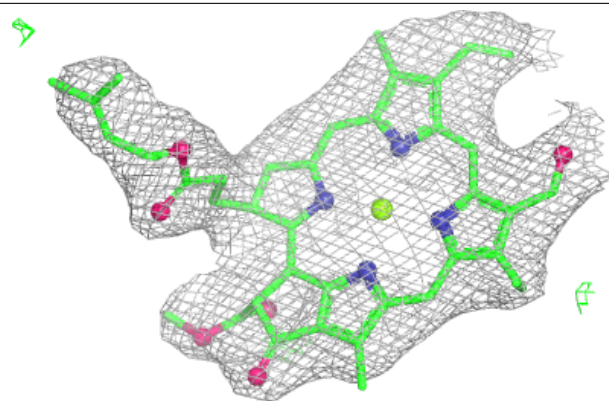
**Electron density around CLA B 810:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

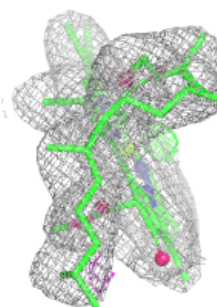
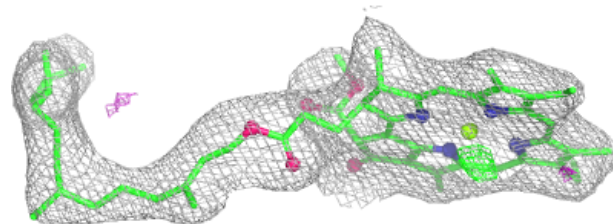
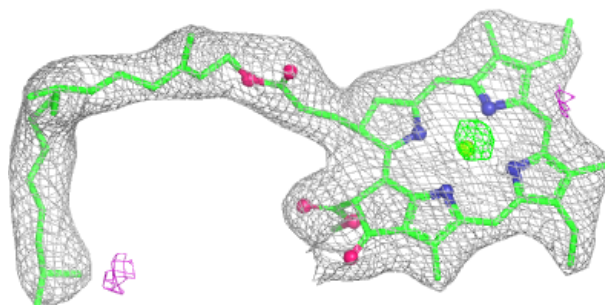


**Electron density around CHL 4 307:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 828:**

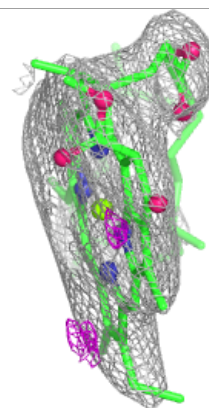
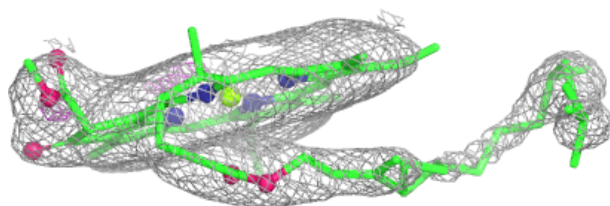
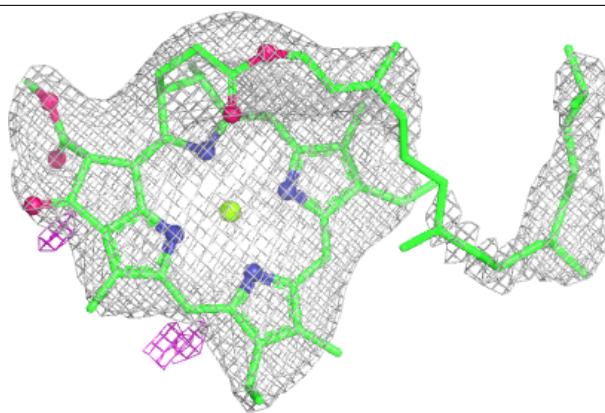
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



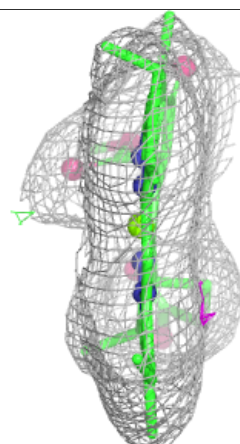
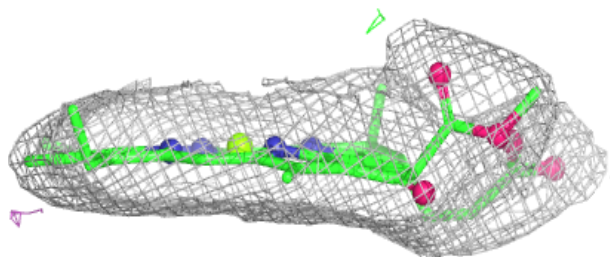
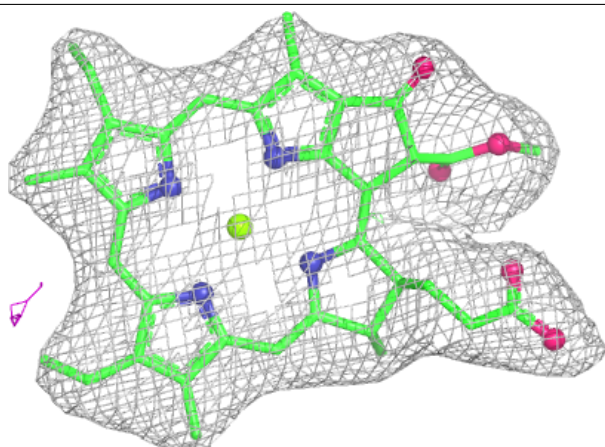


**Electron density around CLA A 818:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

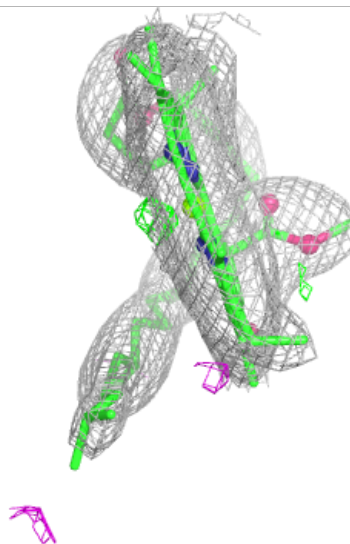
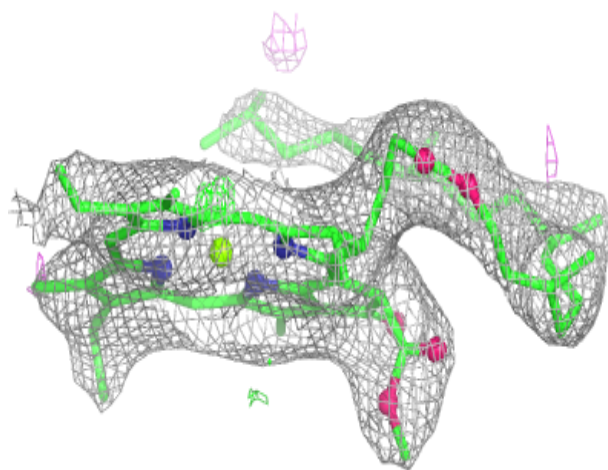
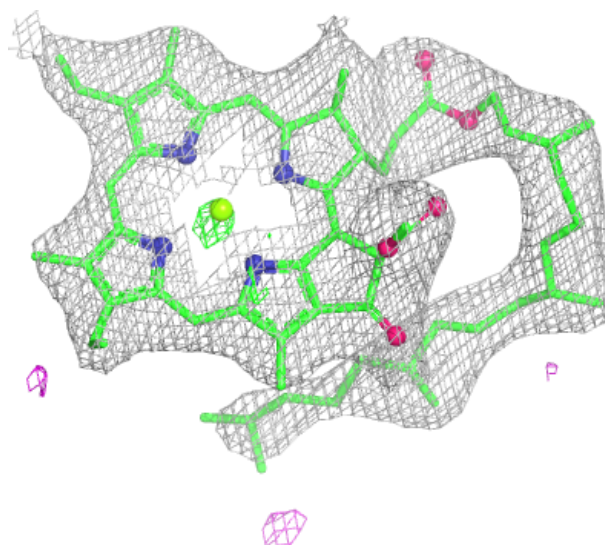
**Electron density around CLA F 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 807:**

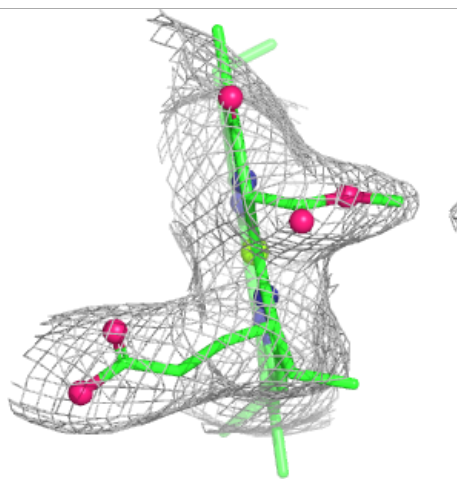
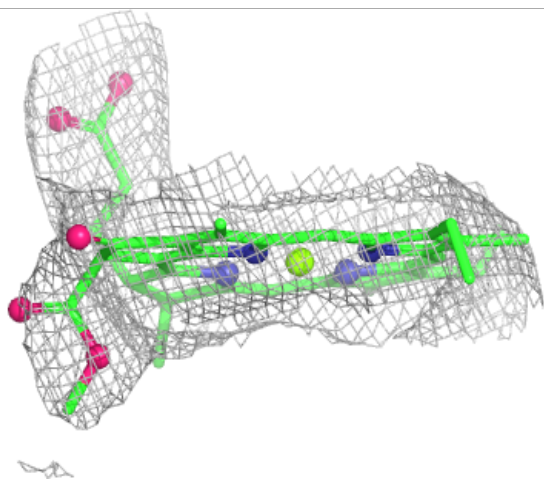
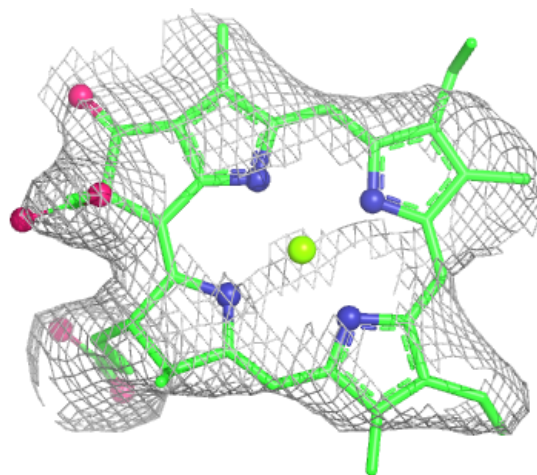
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





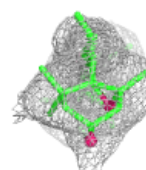
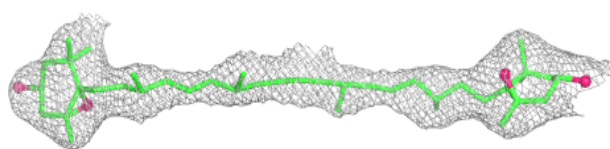
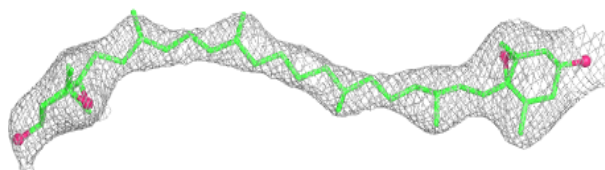
**Electron density around CLA A 813:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

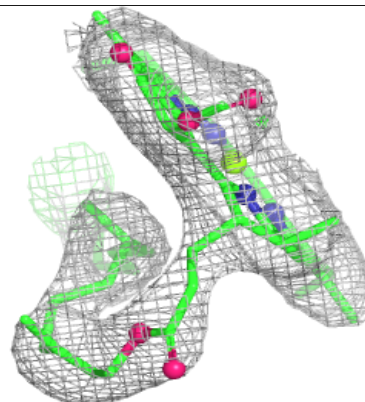
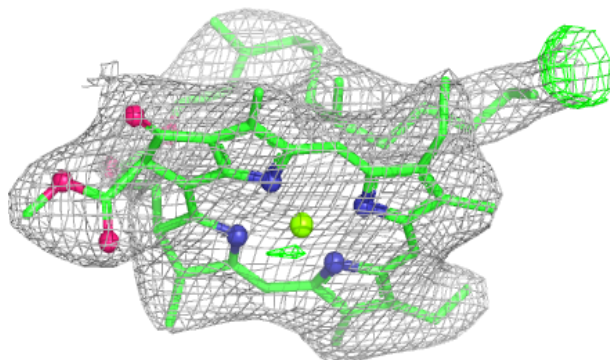
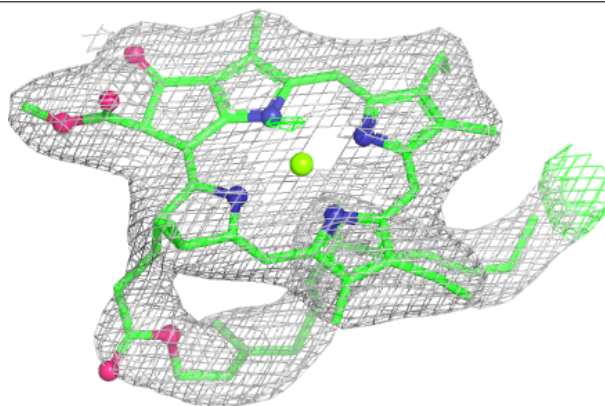


**Electron density around XAT 1 315:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

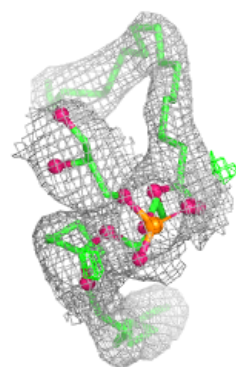
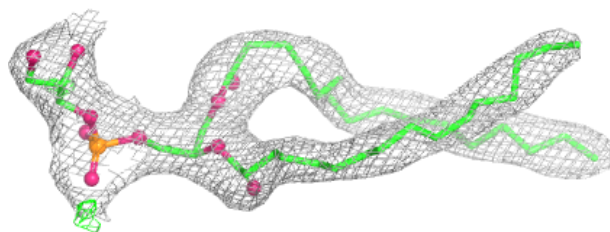
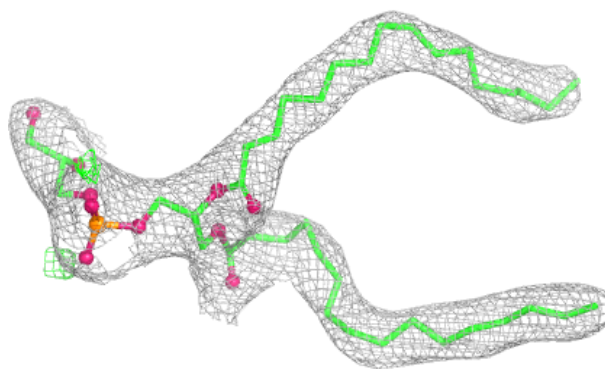
**Electron density around CLA B 819:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

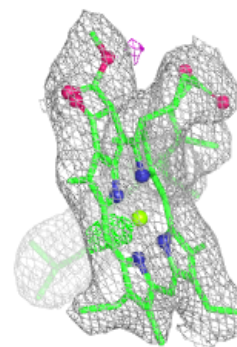
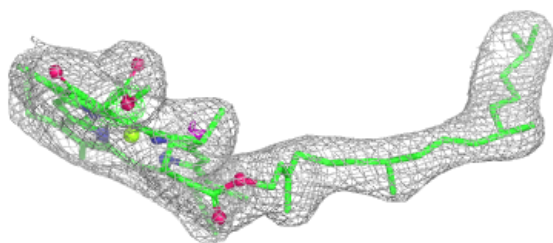
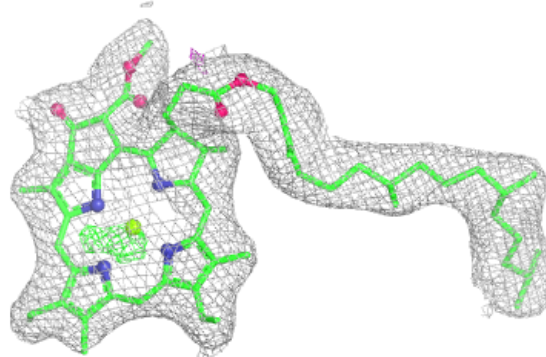


**Electron density around LHG A 844:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.