



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 11:00 AM JST

PDB ID : 5H2F / pdb\_00005h2f  
Title : Crystal structure of the PsbM-deletion mutant of photosystem II  
Authors : Uto, S.; Kawakami, K.; Umena, Y.; Iwai, M.; Ikeuchi, M.; Shen, J.R.; Kamiya, N.  
Deposited on : 2016-10-15  
Resolution : 2.20 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>.

---

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                          | : | 1.8.5 (274361), CSD as541be (2020)                               |
| 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                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

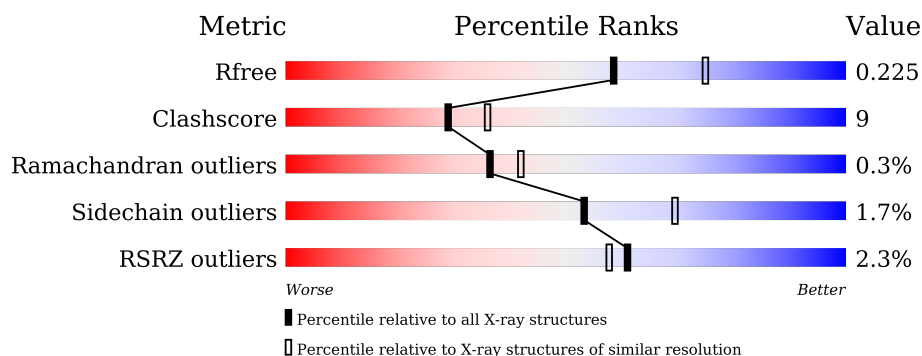
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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                      | 6164 (2.20-2.20)                                      |
| Clashscore            | 190562                      | 6851 (2.20-2.20)                                      |
| Ramachandran outliers | 187476                      | 6768 (2.20-2.20)                                      |
| Sidechain outliers    | 187428                      | 6769 (2.20-2.20)                                      |
| RSRZ outliers         | 180081                      | 6166 (2.20-2.20)                                      |

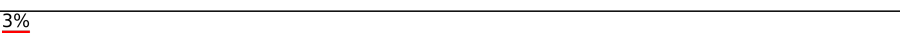
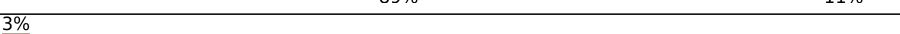
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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   | A     | 334    | <div> <div>2%</div> <div>87%</div> <div>13%</div> <div>.</div> </div> |
| 1   | a     | 334    | <div> <div>10%</div> <div>84%</div> <div>16%</div> </div>             |
| 2   | B     | 505    | <div> <div>3%</div> <div>86%</div> <div>14%</div> </div>              |
| 2   | b     | 505    | <div> <div>%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>  |
| 3   | C     | 455    | <div> <div>%</div> <div>85%</div> <div>15%</div> <div>.</div> </div>  |
| 3   | c     | 455    | <div> <div>84%</div> <div>16%</div> </div>                            |

Continued on next page...



Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D     | 342    |    |
| 4   | d     | 342    |    |
| 5   | E     | 80     |    |
| 5   | e     | 80     |    |
| 6   | F     | 33     |    |
| 6   | f     | 33     |    |
| 7   | H     | 63     |    |
| 7   | h     | 63     |    |
| 8   | I     | 36     |    |
| 8   | i     | 36     |    |
| 9   | J     | 40     |    |
| 9   | j     | 40     |    |
| 10  | K     | 37     |  |
| 10  | k     | 37     |  |
| 11  | L     | 35     |  |
| 11  | l     | 35     |  |
| 12  | O     | 243    |  |
| 12  | o     | 243    |  |
| 13  | T     | 30     |  |
| 13  | t     | 30     |  |
| 14  | U     | 97     |  |
| 14  | u     | 97     |  |
| 15  | V     | 137    |  |
| 15  | v     | 137    |  |
| 16  | Y     | 29     |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 16  | y     | 29     |                  |
| 17  | X     | 37     |                  |
| 17  | x     | 37     |                  |
| 18  | Z     | 62     |                  |
| 18  | z     | 62     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | DMS  | B     | 631 | -         | -        | X       | -                |
| 31  | DMS  | B     | 638 | -         | -        | X       | -                |
| 31  | DMS  | O     | 303 | -         | -        | X       | -                |
| 31  | DMS  | O     | 304 | -         | -        | X       | -                |
| 31  | DMS  | O     | 312 | -         | -        | X       | -                |
| 31  | DMS  | V     | 212 | -         | -        | X       | -                |
| 31  | DMS  | a     | 425 | -         | -        | X       | -                |
| 31  | DMS  | b     | 638 | -         | -        | X       | -                |
| 31  | DMS  | c     | 924 | -         | -        | X       | -                |
| 31  | DMS  | d     | 415 | -         | -        | X       | -                |
| 31  | DMS  | f     | 103 | -         | -        | X       | -                |
| 31  | DMS  | o     | 304 | -         | -        | X       | -                |
| 31  | DMS  | o     | 308 | -         | -        | X       | -                |
| 31  | DMS  | u     | 205 | -         | -        | X       | -                |
| 34  | HTG  | D     | 415 | -         | -        | X       | -                |
| 39  | HEC  | V     | 202 | X         | -        | -       | -                |
| 39  | HEC  | v     | 202 | X         | -        | -       | -                |

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 51892 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 Photosystem II protein D1 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 334      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2598  | 1706 | 428 | 449 | 15 |         |         |       |
| 1   | a     | 334      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2555  | 1675 | 427 | 438 | 15 |         |         |       |

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 505      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 3950  | 2596 | 661 | 680 | 13 |         |         |       |
| 2   | b     | 483      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3780  | 2484 | 631 | 652 | 13 |         |         |       |

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 451      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3470  | 2274 | 580 | 603 | 13 |         |         |       |
| 3   | c     | 455      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3521  | 2305 | 589 | 614 | 13 |         |         |       |

- Molecule 4 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 342      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2732  | 1814 | 442 | 464 | 12 |         |         |       |
| 4   | d     | 341      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 2717  | 1805 | 441 | 459 | 12 |         |         |       |

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5   | E     | 79       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 635   | 417 | 101 | 117 |         |         |       |
| 5   | e     | 79       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 636   | 418 | 101 | 117 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | F     | 33       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 269   | 184 | 44 | 40 | 1 |         |         |       |
| 6   | f     | 31       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 250   | 170 | 42 | 37 | 1 |         |         |       |

- Molecule 7 is a protein called Photosystem II reaction center protein H.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | H     | 63       | Total | C   | N  | O  | S | 0       | 3       | 0     |
|     |       |          | 522   | 347 | 87 | 86 | 2 |         |         |       |
| 7   | h     | 62       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 501   | 335 | 82 | 82 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | I     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 288   | 196 | 45 | 46 | 1 |         |         |       |
| 8   | i     | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 293   | 199 | 46 | 47 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | J     | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 251   | 171 | 37 | 42 | 1 |         |         |       |
| 9   | j     | 40       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 277   | 186 | 41 | 49 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10  | K     | 37       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 293   | 204 | 43 | 46 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10  | k     | 37       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 286   | 198 | 42 | 46 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 11  | L     | 35       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 287   | 192 | 46 | 49 |         |         |       |
| 11  | l     | 35       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 287   | 192 | 46 | 49 |         |         |       |

- Molecule 12 is a protein called Photosystem II manganese-stabilizing polypeptide.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 12  | O     | 243      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1853  | 1160 | 311 | 378 | 4 |         |         |       |
| 12  | o     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1833  | 1149 | 305 | 375 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 13  | T     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 253   | 177 | 36 | 38 | 2 |         |         |       |
| 13  | t     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 253   | 177 | 36 | 38 | 2 |         |         |       |

- Molecule 14 is a protein called Photosystem II 12 kDa extrinsic protein.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14  | U     | 97       | Total | C   | N   | O   | 0       | 1       | 0     |
|     |       |          | 782   | 496 | 132 | 154 |         |         |       |
| 14  | u     | 97       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 766   | 487 | 129 | 150 |         |         |       |

- Molecule 15 is a protein called Cytochrome c-550.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | V     | 137      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1066  | 677 | 177 | 208 | 4 |         |         |       |
| 15  | v     | 137      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1058  | 671 | 175 | 208 | 4 |         |         |       |

- Molecule 16 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 16  | Y     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 215   | 142 | 37 | 33 | 3 |         |         |       |
| 16  | y     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 207   | 134 | 37 | 33 | 3 |         |         |       |

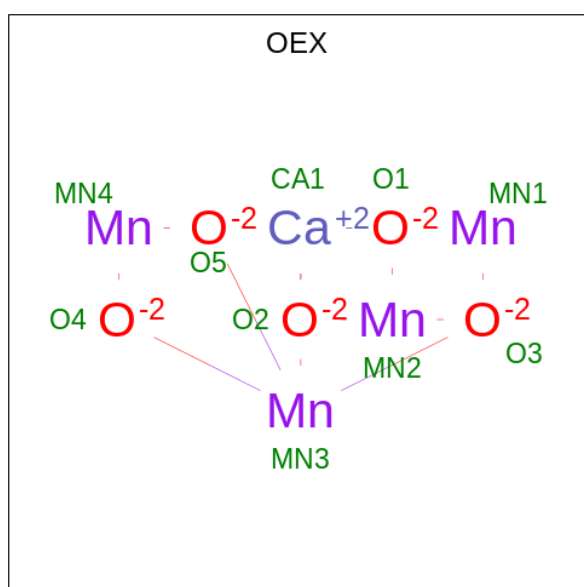
- Molecule 17 is a protein called Photosystem II reaction center X protein.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17  | X     | 37       | Total | C   | N  | O  | 0       | 1       | 0     |
|     |       |          | 269   | 183 | 40 | 46 |         |         |       |
| 17  | x     | 36       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 253   | 172 | 37 | 44 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 311 | 68 | 72 | 2 |         |         |       |
| 18  | z     | 61       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 436   | 299 | 67 | 69 | 1 |         |         |       |

- Molecule 19 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19  | A     | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |
| 19  | a     | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |

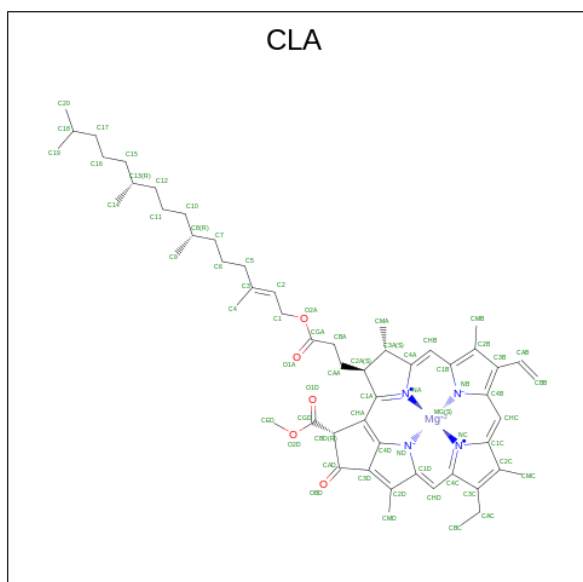
- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 20  | A     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 20  | a     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21  | A     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 21  | a     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 53    | 43 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 22  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

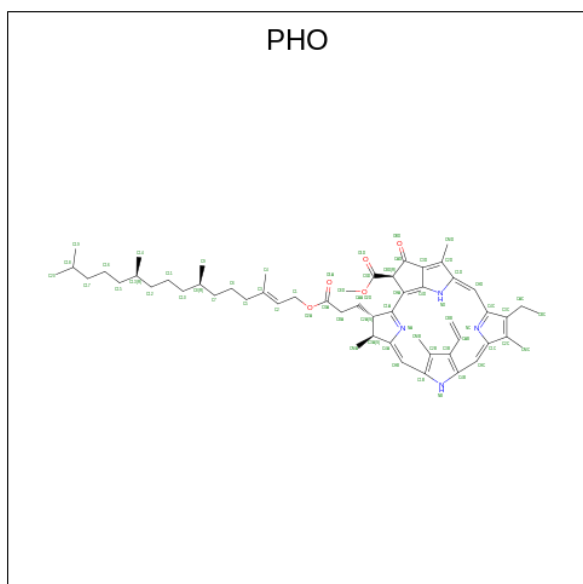
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

*Continued on next page...*

Continued from previous page...

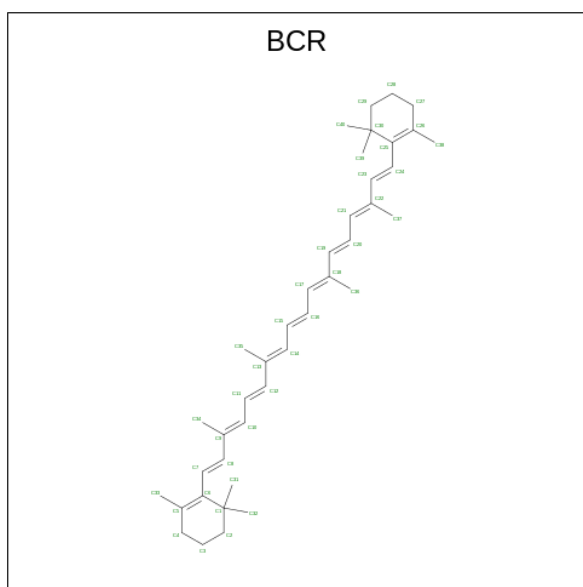
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |   |   |  | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|--|---------|---------|
| 23  | A     | 1        | Total | C  | N | O |  | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |  |         |         |
| 23  | D     | 1        | Total | C  | N | O |  | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |  |         |         |
| 23  | a     | 1        | Total | C  | N | O |  | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |  |         |         |
| 23  | a     | 1        | Total | C  | N | O |  | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |  |         |         |

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



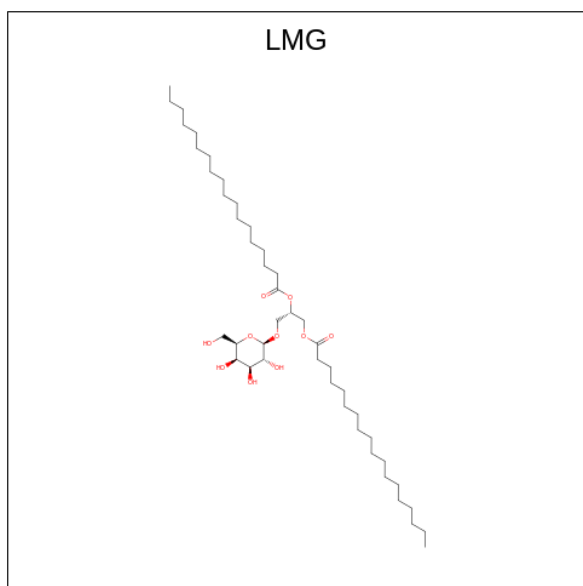
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 24  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | B     | 1        | Total C<br>19 19 | 0       | 0       |
| 24  | B     | 1        | Total C<br>30 30 | 0       | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | D     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | Y     | 1        | Total C<br>39 39 | 0       | 0       |
| 24  | a     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | b     | 1        | Total C<br>20 20 | 0       | 0       |
| 24  | b     | 1        | Total C<br>31 31 | 0       | 0       |
| 24  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | c     | 1        | Total C<br>40 40 | 0       | 0       |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 24  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | d     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | k     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | y     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



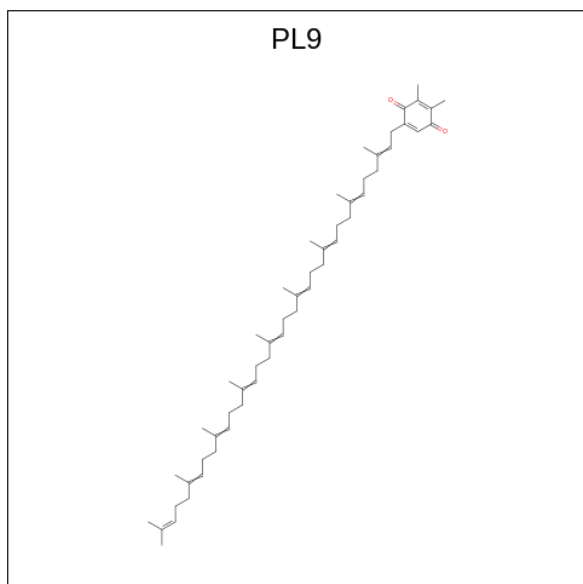
| Mol | Chain | Residues | Atoms                 | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 25  | A     | 1        | Total C O<br>51 41 10 | 0       | 0       |
| 25  | B     | 1        | Total C O<br>40 30 10 | 0       | 0       |
| 25  | C     | 1        | Total C O<br>51 41 10 | 0       | 0       |
| 25  | C     | 1        | Total C O<br>40 30 10 | 0       | 0       |
| 25  | D     | 1        | Total C O<br>46 36 10 | 0       | 0       |
| 25  | J     | 1        | Total C O<br>45 35 10 | 0       | 0       |
| 25  | b     | 1        | Total C O<br>43 33 10 | 0       | 0       |

Continued on next page...

Continued from previous page...

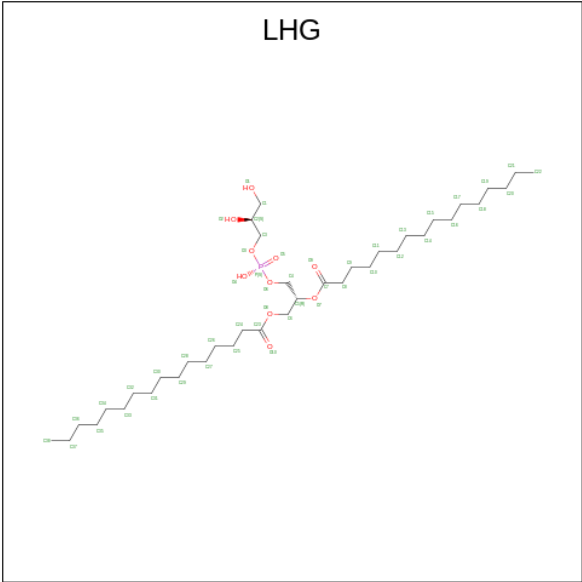
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 25  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 25  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 25  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 47    | 37 | 10 |         |         |
| 25  | i     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 25  | j     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 47    | 37 | 10 |         |         |

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



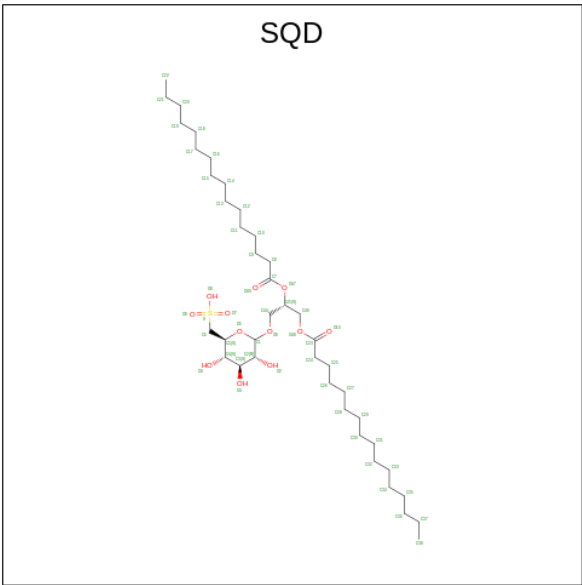
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 26  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 26  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 26  | a     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 26  | d     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 27  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 31    | 22 | 8  | 1 |         |         |
| 27  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 30    | 21 | 8  | 1 |         |         |
| 27  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 27  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 27  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 45    | 34 | 10 | 1 |         |         |
| 27  | L     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 40    | 29 | 10 | 1 |         |         |
| 27  | a     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 27  | a     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 45    | 34 | 10 | 1 |         |         |
| 27  | d     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 33    | 24 | 8  | 1 |         |         |
| 27  | d     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 27  | d     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 46    | 35 | 10 | 1 |         |         |
| 27  | l     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |

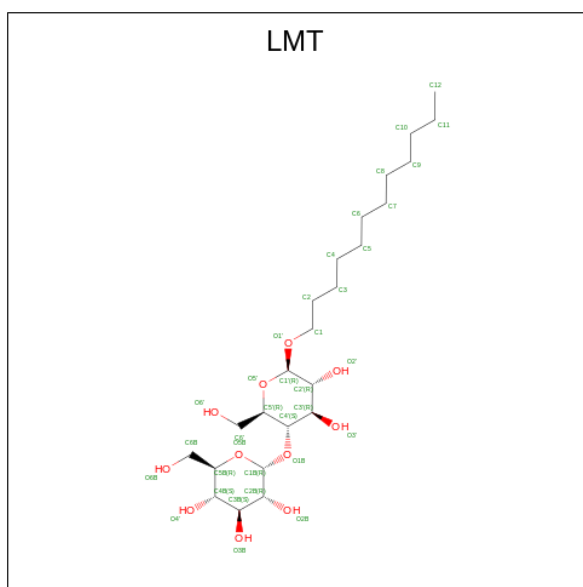
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 28  | A     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 49    | 36 | 12 | 1 |         |         |
| 28  | C     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 28  | D     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 20    | 9  | 10 | 1 |         |         |
| 28  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 28  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 51    | 38 | 12 | 1 |         |         |
| 28  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 38    | 26 | 11 | 1 |         |         |
| 28  | f     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 14    | 6  | 7  | 1 |         |         |
| 28  | l     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |

- Molecule 29 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 |
|-----|-------|----------|-------------|---------|---------|---------|---------|
| 29  | A     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 29  | B     | 1        | Total<br>24 | C<br>18 | O<br>6  | 0       | 0       |
| 29  | E     | 1        | Total<br>24 | C<br>18 | O<br>6  | 0       | 0       |
| 29  | I     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 29  | T     | 1        | Total<br>24 | C<br>18 | O<br>6  | 0       | 0       |
| 29  | Z     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 29  | a     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 29  | c     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 29  | c     | 1        | Total<br>24 | C<br>18 | O<br>6  | 0       | 0       |
| 29  | f     | 1        | Total<br>25 | C<br>19 | O<br>6  | 0       | 0       |
| 29  | t     | 1        | Total<br>24 | C<br>18 | O<br>6  | 0       | 0       |

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

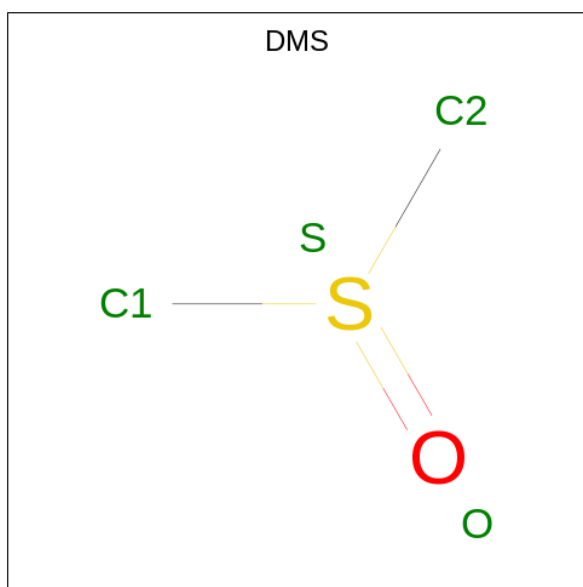
| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 30  | A     | 1        | Total C<br>5 5 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 30  | B     | 2        | Total C<br>23 23 | 0       | 0       |
| 30  | D     | 1        | Total C<br>16 16 | 0       | 0       |
| 30  | I     | 3        | Total C<br>45 45 | 0       | 0       |
| 30  | J     | 1        | Total C<br>16 16 | 0       | 0       |
| 30  | O     | 1        | Total C<br>16 16 | 0       | 0       |
| 30  | T     | 1        | Total C<br>13 13 | 0       | 0       |
| 30  | U     | 1        | Total C<br>14 14 | 0       | 0       |
| 30  | X     | 1        | Total C<br>16 16 | 0       | 0       |
| 30  | Z     | 1        | Total C<br>9 9   | 0       | 0       |
| 30  | a     | 2        | Total C<br>16 16 | 0       | 0       |
| 30  | b     | 2        | Total C<br>27 27 | 0       | 0       |
| 30  | c     | 1        | Total C<br>10 10 | 0       | 0       |
| 30  | d     | 1        | Total C<br>16 16 | 0       | 0       |
| 30  | i     | 4        | Total C<br>58 58 | 0       | 0       |
| 30  | j     | 1        | Total C<br>16 16 | 0       | 0       |
| 30  | t     | 1        | Total C<br>16 16 | 0       | 0       |
| 30  | u     | 1        | Total C<br>11 11 | 0       | 0       |
| 30  | x     | 1        | Total C<br>15 15 | 0       | 0       |

- Molecule 31 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 31  | A     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | A     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | A     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | A     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | A     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | B     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | B     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | B     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | B     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | B     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 31  | B     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 31  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 31  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | F     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | H     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | I     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | I     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | L     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | U     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 31  | U     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 31  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | f     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | i     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | l     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | l     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | l     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | t     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | t     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

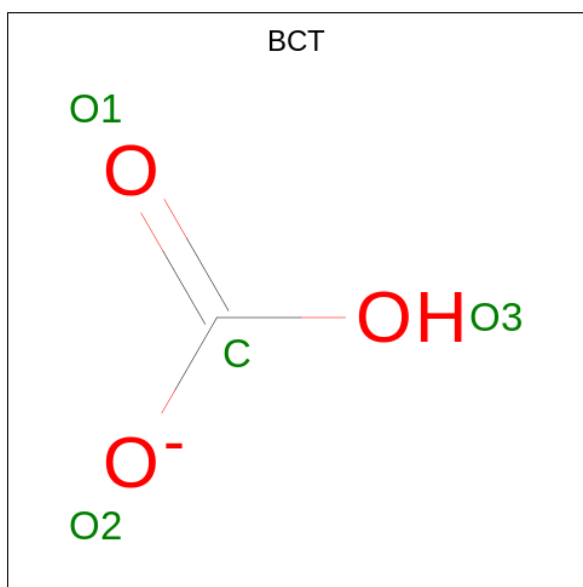
*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 31  | t     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | u     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | u     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | u     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | u     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 31  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).

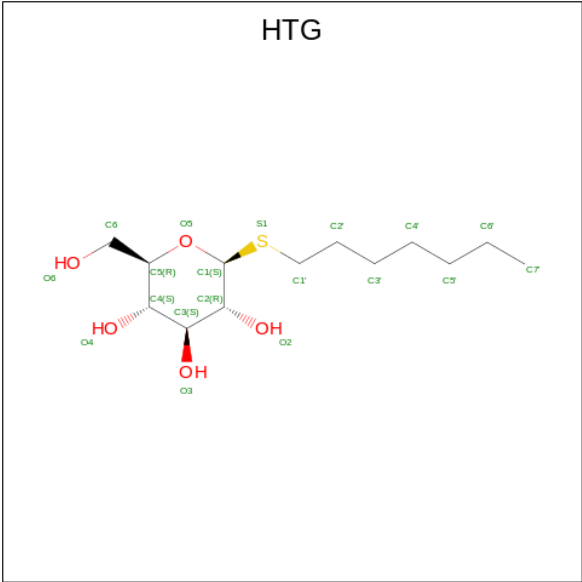


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 32  | A     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 8     | 2 | 6 |         |         |
| 32  | a     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 33  | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 33  | O     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 33  | b     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 33  | c     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 33  | o     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



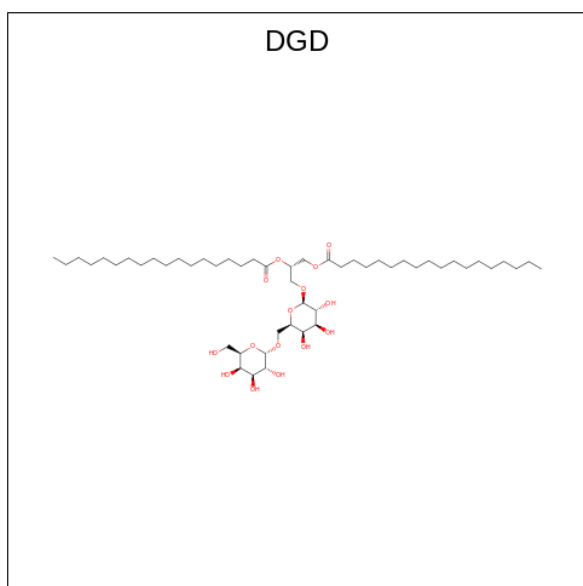
| Mol | Chain | Residues | Atoms                    | ZeroOcc | AltConf |
|-----|-------|----------|--------------------------|---------|---------|
| 34  | B     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | B     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | B     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | C     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | C     | 1        | Total C S<br>9 8 1       | 0       | 0       |
| 34  | C     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | D     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | D     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | V     | 1        | Total C O S<br>14 8 5 1  | 0       | 0       |
| 34  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 34  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 34  | c     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 34  | l     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 34  | v     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 16    | 10 | 5 | 1 |         |         |

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



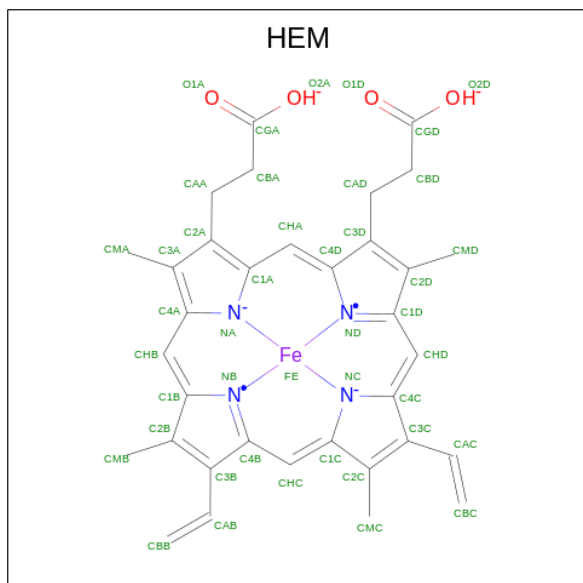
| Mol | Chain | Residues | Atoms |    |    |  | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|--|---------|---------|
| 35  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 35  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 35  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 35  | D     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 50    | 41 | 9  |  |         |         |
| 35  | H     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 35  | c     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 35  | c     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 35  | c     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |

*Continued on next page...*

Continued from previous page...

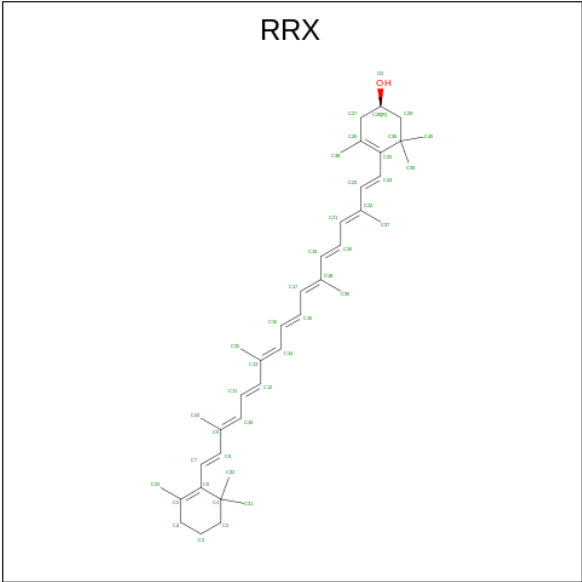
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 35  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 43    | 37 | 6  |         |         |
| 35  | h     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 36  | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 36  | e     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).

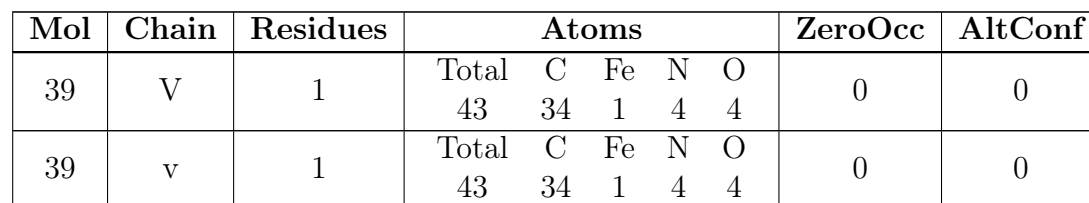


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 37  | H     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 41    | 40 | 1 |         |         |
| 37  | h     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 41    | 40 | 1 |         |         |

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 38  | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 38  | K     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 38  | j     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 38  | k     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 39 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>36</sub>FeN<sub>4</sub>O<sub>4</sub>).



- | Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 40  | A     | 132      | Total O<br>132 132 | 0       | 0       |
| 40  | B     | 256      | Total O<br>262 262 | 0       | 6       |
| 40  | C     | 174      | Total O<br>178 178 | 0       | 4       |
| 40  | D     | 130      | Total O<br>131 131 | 0       | 1       |
| 40  | E     | 33       | Total O<br>35 35   | 0       | 2       |
| 40  | F     | 4        | Total O<br>4 4     | 0       | 0       |
| 40  | H     | 39       | Total O<br>39 39   | 0       | 0       |
| 40  | I     | 5        | Total O<br>5 5     | 0       | 0       |
| 40  | J     | 15       | Total O<br>16 16   | 0       | 1       |
| 40  | K     | 7        | Total O<br>7 7     | 0       | 0       |



*Continued from previous page...*

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 40  | L     | 18       | Total O<br>19 19   | 0       | 1       |
| 40  | O     | 161      | Total O<br>166 166 | 0       | 5       |
| 40  | T     | 12       | Total O<br>12 12   | 0       | 0       |
| 40  | U     | 72       | Total O<br>74 74   | 0       | 2       |
| 40  | V     | 110      | Total O<br>113 113 | 0       | 3       |
| 40  | Y     | 7        | Total O<br>8 8     | 0       | 1       |
| 40  | X     | 15       | Total O<br>16 16   | 0       | 1       |
| 40  | Z     | 5        | Total O<br>5 5     | 0       | 0       |
| 40  | a     | 122      | Total O<br>123 123 | 0       | 1       |
| 40  | b     | 251      | Total O<br>261 261 | 0       | 10      |
| 40  | c     | 216      | Total O<br>220 220 | 0       | 4       |
| 40  | d     | 115      | Total O<br>115 115 | 0       | 0       |
| 40  | e     | 16       | Total O<br>17 17   | 0       | 1       |
| 40  | f     | 4        | Total O<br>4 4     | 0       | 0       |
| 40  | h     | 31       | Total O<br>31 31   | 0       | 0       |
| 40  | i     | 5        | Total O<br>5 5     | 0       | 0       |
| 40  | j     | 10       | Total O<br>10 10   | 0       | 0       |
| 40  | k     | 9        | Total O<br>10 10   | 0       | 1       |
| 40  | l     | 14       | Total O<br>15 15   | 0       | 1       |
| 40  | o     | 153      | Total O<br>156 156 | 0       | 3       |
| 40  | t     | 10       | Total O<br>10 10   | 0       | 0       |

*Continued on next page...*



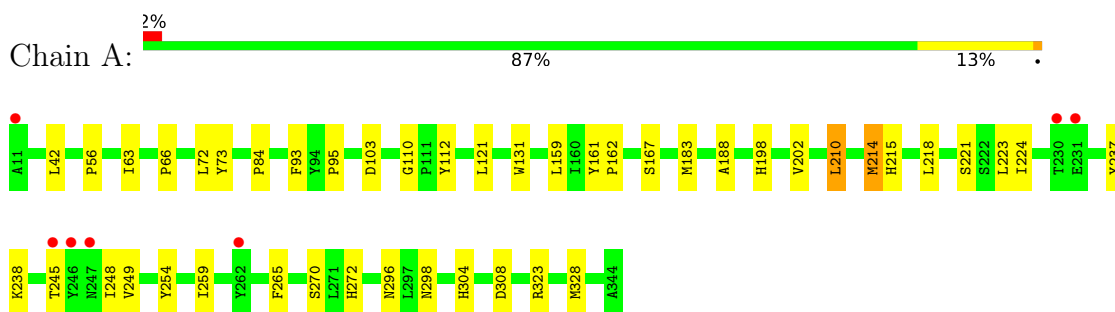
*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 40  | u     | 75       | Total<br>75 | O<br>75 | 0       | 0       |
| 40  | v     | 77       | Total<br>82 | O<br>82 | 0       | 5       |
| 40  | y     | 1        | Total<br>1  | O<br>1  | 0       | 0       |
| 40  | x     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 40  | z     | 8        | Total<br>8  | O<br>8  | 0       | 0       |

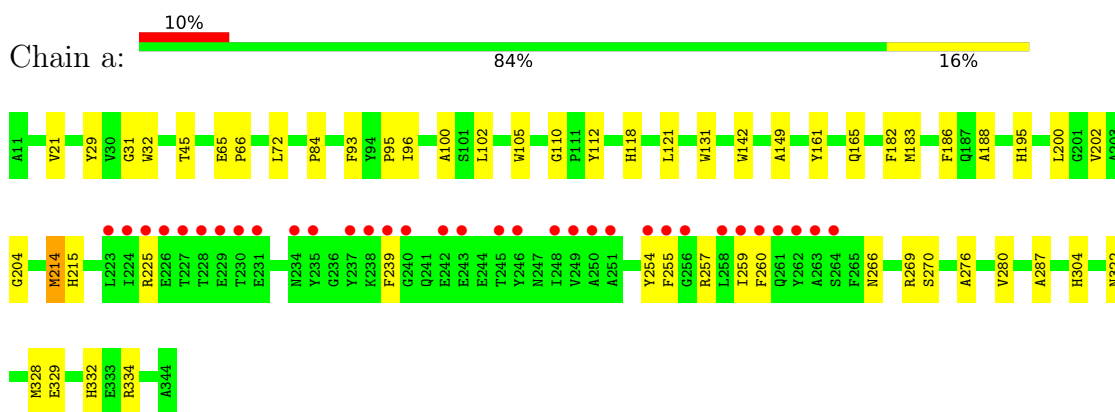
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

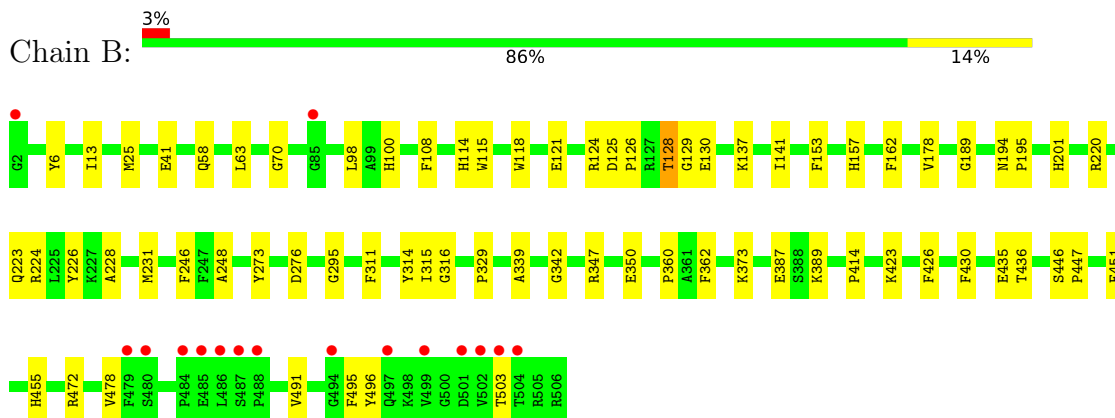
#### • Molecule 1: Photosystem II protein D1 1



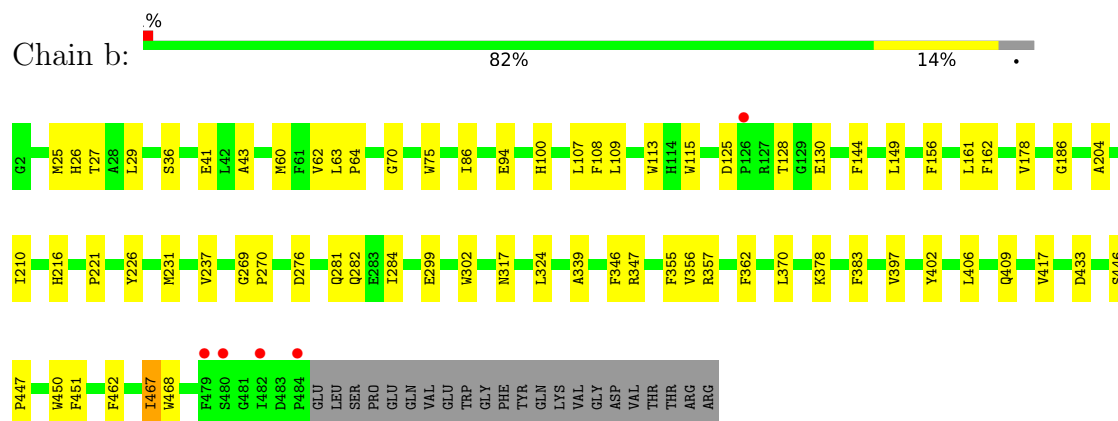
#### • Molecule 1: Photosystem II protein D1 1



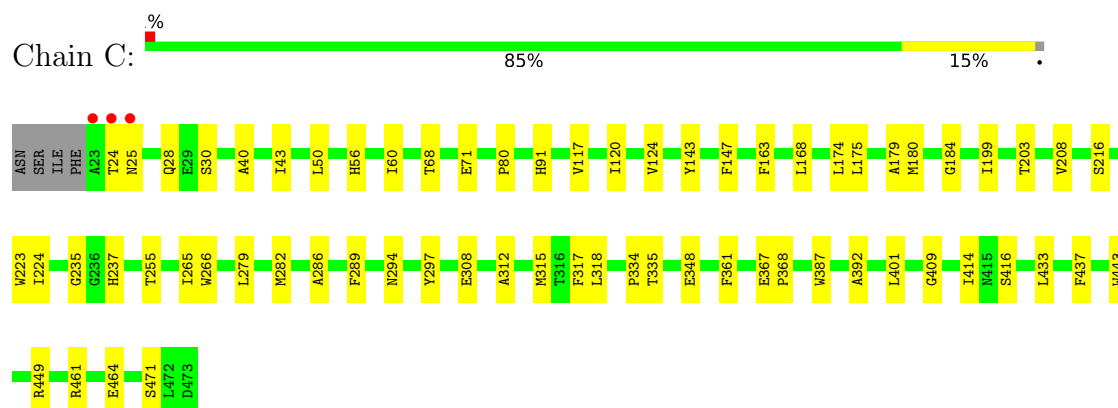
#### • Molecule 2: Photosystem II CP47 reaction center protein



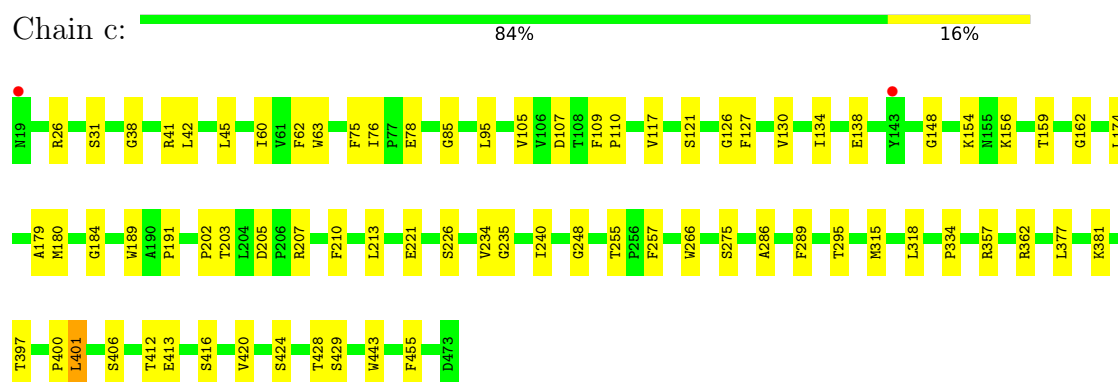
- Molecule 2: Photosystem II CP47 reaction center protein



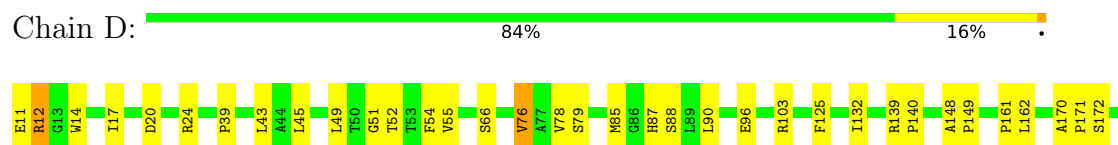
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein

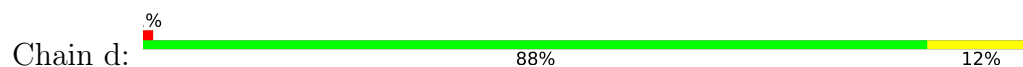


- Molecule 4: Photosystem II D2 protein

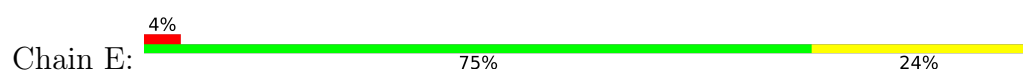




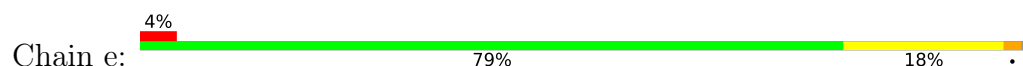
- Molecule 4: Photosystem II D2 protein



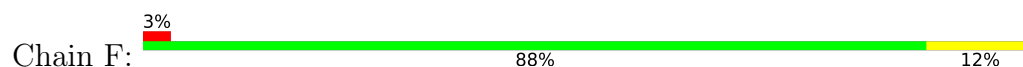
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



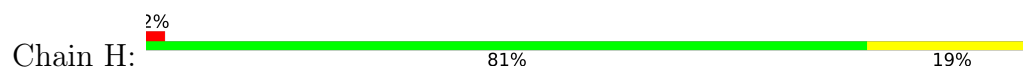
- Molecule 6: Cytochrome b559 subunit beta



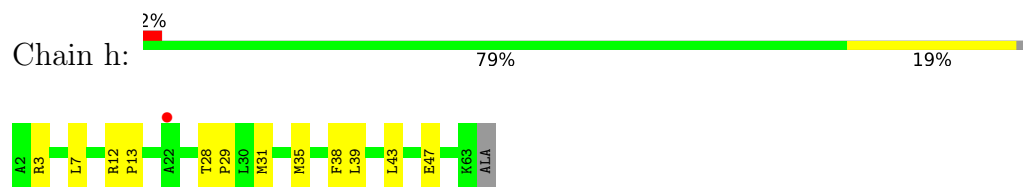
- Molecule 6: Cytochrome b559 subunit beta



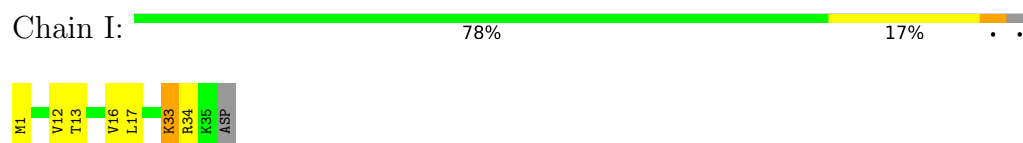
- Molecule 7: Photosystem II reaction center protein H



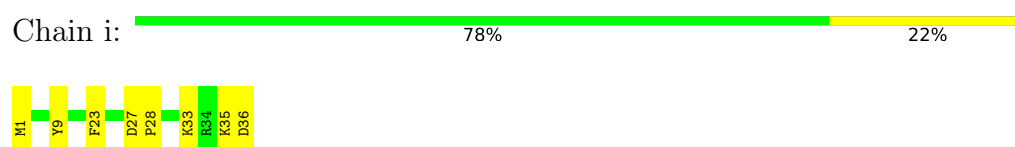
- Molecule 7: Photosystem II reaction center protein H



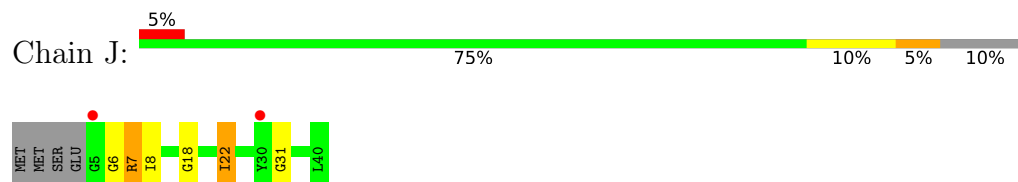
- Molecule 8: Photosystem II reaction center protein I



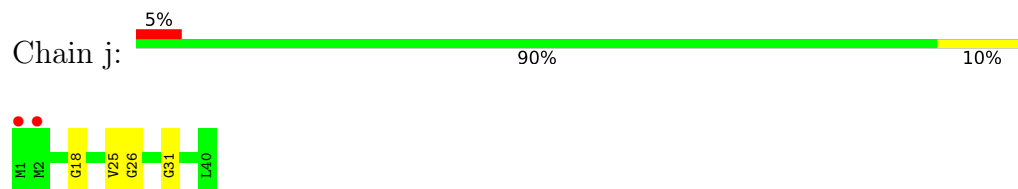
- Molecule 8: Photosystem II reaction center protein I



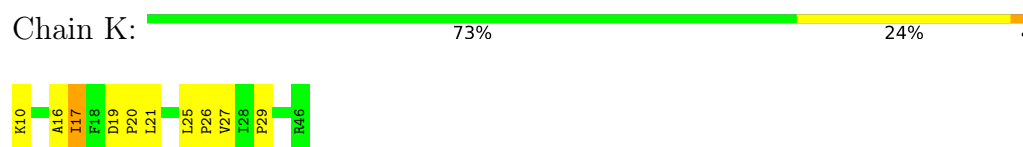
- Molecule 9: Photosystem II reaction center protein J



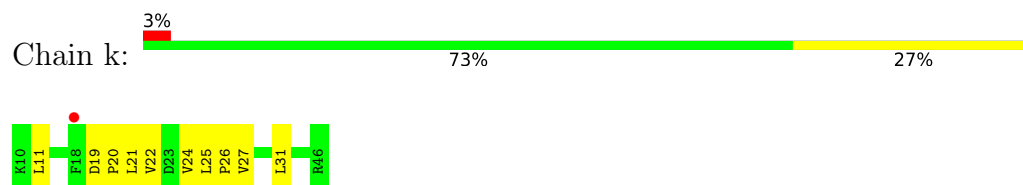
- Molecule 9: Photosystem II reaction center protein J



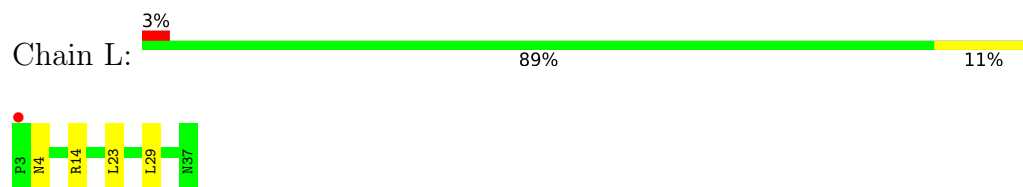
- Molecule 10: Photosystem II reaction center protein K



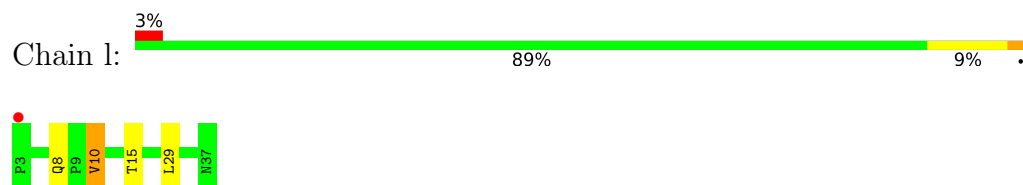
- Molecule 10: Photosystem II reaction center protein K



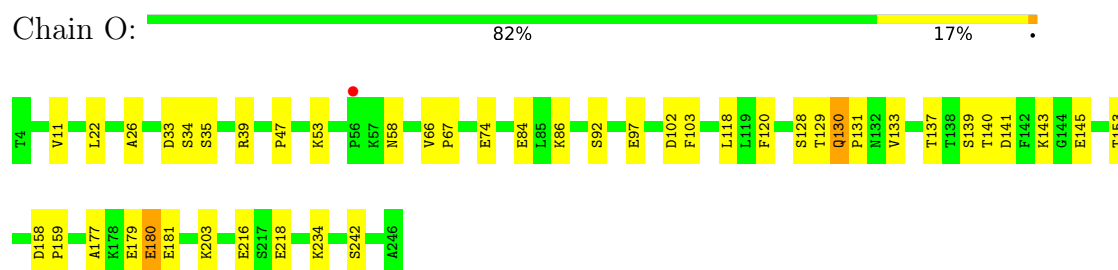
- Molecule 11: Photosystem II reaction center protein L



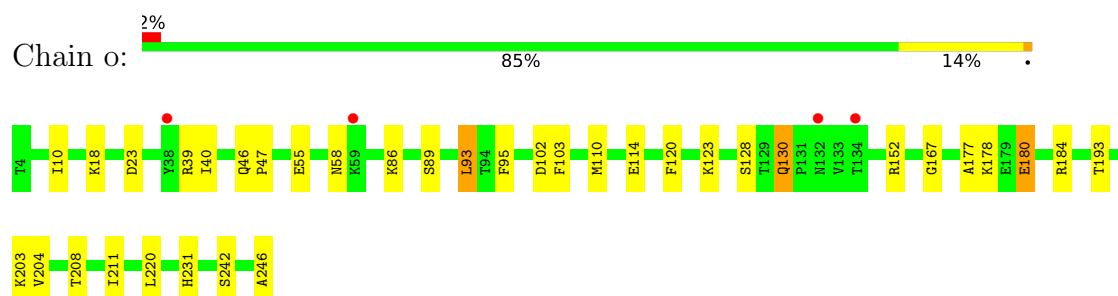
- Molecule 11: Photosystem II reaction center protein L



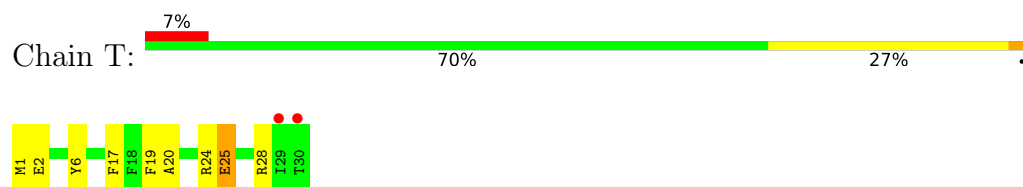
- Molecule 12: Photosystem II manganese-stabilizing polypeptide



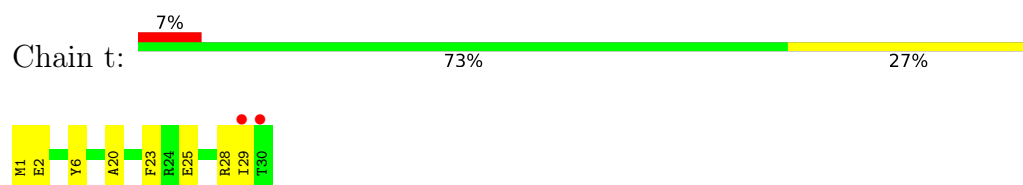
- Molecule 12: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II reaction center protein T



- Molecule 13: Photosystem II reaction center protein T



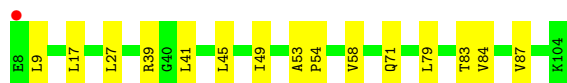
- Molecule 14: Photosystem II 12 kDa extrinsic protein

Chain U:  88% 12%



- Molecule 14: Photosystem II 12 kDa extrinsic protein

Chain u:  % 85% 15%



- Molecule 15: Cytochrome c-550

Chain V:  87% 12% .



- Molecule 15: Cytochrome c-550

Chain v:  82% 17% .



- Molecule 16: Photosystem II reaction center protein Ycf12

Chain Y:  3% 76% 24%



- Molecule 16: Photosystem II reaction center protein Ycf12

Chain y:  3% 72% 28%

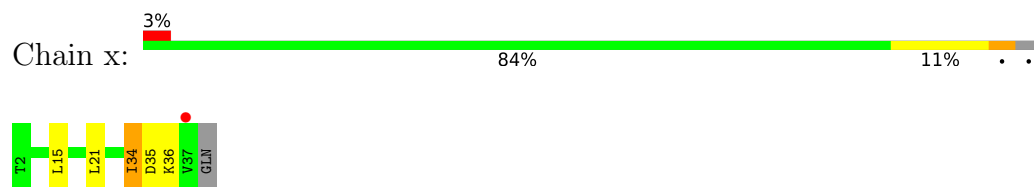


- Molecule 17: Photosystem II reaction center X protein

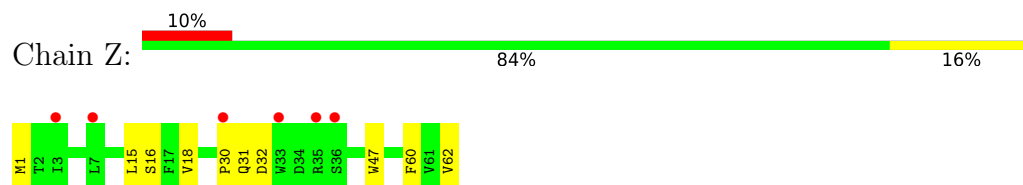
Chain X:  3% 81% 16%



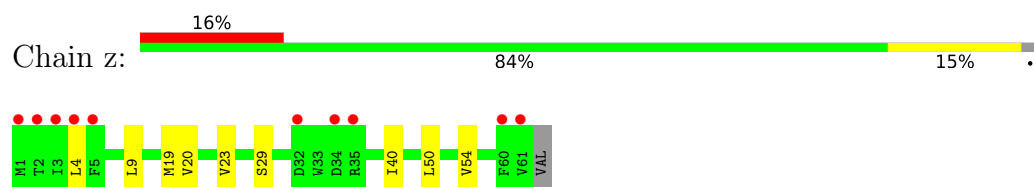
## • Molecule 17: Photosystem II reaction center X protein



## • Molecule 18: Photosystem II reaction center protein Z



## • Molecule 18: Photosystem II reaction center protein Z





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 121.95Å 226.99Å 285.89Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 50.00 – 2.20<br>50.00 – 2.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.2 (50.00-2.20)<br>96.3 (50.00-2.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.24 (at 2.20Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0117                                             | Depositor        |
| R, $R_{free}$                                                           | 0.174 , 0.226<br>0.174 , 0.225                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 19357 reflections (3.10%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 35.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.519                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 54.7                                                 | 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                                                   | 51892                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 42.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: HTG, HEC, RRX, BCT, MG, FME, OEX, HEM, LMT, PL9, CL, SQD, CA, DGD, LHG, LMG, FE2, UNL, PHO, DMS, BCR, CLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 1   | A     | 1.09         | 3/2686 (0.1%) | 1.03        | 6/3666 (0.2%) |
| 1   | a     | 1.13         | 8/2640 (0.3%) | 1.05        | 3/3604 (0.1%) |
| 2   | B     | 1.07         | 3/4099 (0.1%) | 1.03        | 4/5591 (0.1%) |
| 2   | b     | 1.06         | 2/3917 (0.1%) | 1.02        | 3/5342 (0.1%) |
| 3   | C     | 1.03         | 5/3583 (0.1%) | 1.00        | 2/4880 (0.0%) |
| 3   | c     | 1.01         | 2/3638 (0.1%) | 1.04        | 3/4953 (0.1%) |
| 4   | D     | 1.10         | 2/2836 (0.1%) | 0.99        | 1/3866 (0.0%) |
| 4   | d     | 1.04         | 0/2818        | 1.00        | 4/3842 (0.1%) |
| 5   | E     | 0.91         | 0/654         | 1.04        | 1/895 (0.1%)  |
| 5   | e     | 0.89         | 0/655         | 1.05        | 3/896 (0.3%)  |
| 6   | F     | 0.99         | 0/278         | 0.87        | 0/379         |
| 6   | f     | 0.90         | 0/257         | 0.94        | 0/349         |
| 7   | H     | 0.90         | 0/541         | 0.94        | 1/737 (0.1%)  |
| 7   | h     | 0.90         | 0/517         | 0.93        | 0/704         |
| 8   | I     | 0.89         | 0/285         | 1.00        | 0/385         |
| 8   | i     | 0.82         | 0/290         | 0.93        | 0/392         |
| 9   | J     | 0.94         | 0/257         | 1.08        | 1/349 (0.3%)  |
| 9   | j     | 0.88         | 0/283         | 1.01        | 0/384         |
| 10  | K     | 0.90         | 0/303         | 1.13        | 2/416 (0.5%)  |
| 10  | k     | 0.85         | 0/296         | 1.05        | 0/408         |
| 11  | L     | 0.97         | 0/294         | 1.03        | 1/399 (0.3%)  |
| 11  | l     | 0.93         | 0/294         | 1.08        | 0/399         |
| 12  | O     | 0.95         | 0/1887        | 1.02        | 1/2561 (0.0%) |
| 12  | o     | 0.86         | 0/1864        | 1.03        | 5/2535 (0.2%) |
| 13  | T     | 0.92         | 0/252         | 1.04        | 2/342 (0.6%)  |
| 13  | t     | 0.89         | 0/252         | 1.02        | 1/342 (0.3%)  |
| 14  | U     | 0.96         | 0/796         | 1.01        | 1/1078 (0.1%) |
| 14  | u     | 0.94         | 0/777         | 1.07        | 1/1054 (0.1%) |
| 15  | V     | 1.05         | 1/1090 (0.1%) | 1.04        | 0/1480        |
| 15  | v     | 0.95         | 0/1082        | 1.03        | 2/1472 (0.1%) |
| 16  | Y     | 0.80         | 0/216         | 1.04        | 0/289         |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 16  | y     | 0.69         | 0/208           | 1.05        | 0/278           |
| 17  | X     | 0.73         | 0/275           | 1.10        | 0/373           |
| 17  | x     | 0.77         | 0/256           | 1.05        | 0/349           |
| 18  | Z     | 0.83         | 0/463           | 1.04        | 0/636           |
| 18  | z     | 0.75         | 0/447           | 1.06        | 0/614           |
| All | All   | 1.01         | 26/41286 (0.1%) | 1.02        | 48/56239 (0.1%) |

The worst 5 of 26 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4   | D     | 87  | HIS  | CG-CD2  | 8.02 | 1.44        | 1.35     |
| 1   | A     | 56  | PRO  | CA-C    | 6.77 | 1.58        | 1.52     |
| 1   | a     | 195 | HIS  | ND1-CE1 | 6.00 | 1.38        | 1.32     |
| 1   | A     | 159 | LEU  | CA-C    | 5.80 | 1.58        | 1.52     |
| 1   | a     | 195 | HIS  | CG-CD2  | 5.78 | 1.42        | 1.35     |

The worst 5 of 48 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | a     | 142 | TRP  | N-CA-C | 7.31  | 121.91      | 112.92   |
| 2   | B     | 342 | GLY  | N-CA-C | -7.27 | 104.63      | 112.04   |
| 2   | b     | 269 | GLY  | CA-C-N | 6.76  | 127.15      | 119.92   |
| 2   | b     | 269 | GLY  | C-N-CA | 6.76  | 127.15      | 119.92   |
| 5   | E     | 76  | VAL  | N-CA-C | -6.39 | 104.11      | 110.62   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2598  | 0        | 2484     | 42      | 0            |
| 1   | a     | 2555  | 0        | 2420     | 41      | 0            |
| 2   | B     | 3950  | 0        | 3776     | 54      | 0            |
| 2   | b     | 3780  | 0        | 3636     | 70      | 0            |
| 3   | C     | 3470  | 0        | 3380     | 46      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | c     | 3521  | 0        | 3439     | 60      | 0            |
| 4   | D     | 2732  | 0        | 2640     | 57      | 0            |
| 4   | d     | 2717  | 0        | 2628     | 37      | 0            |
| 5   | E     | 635   | 0        | 613      | 12      | 0            |
| 5   | e     | 636   | 0        | 609      | 9       | 0            |
| 6   | F     | 269   | 0        | 277      | 3       | 0            |
| 6   | f     | 250   | 0        | 261      | 12      | 0            |
| 7   | H     | 522   | 0        | 547      | 13      | 0            |
| 7   | h     | 501   | 0        | 526      | 12      | 0            |
| 8   | I     | 288   | 0        | 307      | 3       | 0            |
| 8   | i     | 293   | 0        | 309      | 7       | 0            |
| 9   | J     | 251   | 0        | 257      | 8       | 0            |
| 9   | j     | 277   | 0        | 277      | 4       | 0            |
| 10  | K     | 293   | 0        | 305      | 9       | 0            |
| 10  | k     | 286   | 0        | 285      | 9       | 0            |
| 11  | L     | 287   | 0        | 299      | 3       | 0            |
| 11  | l     | 287   | 0        | 299      | 6       | 0            |
| 12  | O     | 1853  | 0        | 1819     | 36      | 0            |
| 12  | o     | 1833  | 0        | 1783     | 29      | 0            |
| 13  | T     | 253   | 0        | 247      | 5       | 0            |
| 13  | t     | 253   | 0        | 247      | 3       | 0            |
| 14  | U     | 782   | 0        | 786      | 7       | 0            |
| 14  | u     | 766   | 0        | 765      | 12      | 0            |
| 15  | V     | 1066  | 0        | 1075     | 22      | 0            |
| 15  | v     | 1058  | 0        | 1053     | 18      | 0            |
| 16  | Y     | 215   | 0        | 246      | 3       | 0            |
| 16  | y     | 207   | 0        | 221      | 9       | 0            |
| 17  | X     | 269   | 0        | 297      | 6       | 0            |
| 17  | x     | 253   | 0        | 274      | 4       | 0            |
| 18  | Z     | 453   | 0        | 471      | 5       | 0            |
| 18  | z     | 436   | 0        | 431      | 5       | 0            |
| 19  | A     | 10    | 0        | 0        | 0       | 0            |
| 19  | a     | 10    | 0        | 0        | 0       | 0            |
| 20  | A     | 1     | 0        | 0        | 0       | 0            |
| 20  | a     | 1     | 0        | 0        | 0       | 0            |
| 21  | A     | 2     | 0        | 0        | 0       | 0            |
| 21  | a     | 2     | 0        | 0        | 0       | 0            |
| 22  | A     | 185   | 0        | 193      | 10      | 0            |
| 22  | B     | 1014  | 0        | 1091     | 25      | 0            |
| 22  | C     | 836   | 0        | 915      | 32      | 0            |
| 22  | D     | 195   | 0        | 216      | 5       | 0            |
| 22  | a     | 256   | 0        | 277      | 11      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | b     | 1016  | 0        | 1096     | 47      | 0            |
| 22  | c     | 845   | 0        | 936      | 32      | 0            |
| 22  | d     | 130   | 0        | 144      | 3       | 0            |
| 23  | A     | 64    | 0        | 74       | 0       | 0            |
| 23  | D     | 64    | 0        | 74       | 5       | 0            |
| 23  | a     | 128   | 0        | 148      | 10      | 0            |
| 24  | A     | 40    | 0        | 56       | 1       | 0            |
| 24  | B     | 89    | 0        | 121      | 4       | 0            |
| 24  | C     | 80    | 0        | 112      | 5       | 0            |
| 24  | D     | 40    | 0        | 56       | 1       | 0            |
| 24  | K     | 40    | 0        | 56       | 0       | 0            |
| 24  | Y     | 39    | 0        | 53       | 2       | 0            |
| 24  | a     | 40    | 0        | 56       | 1       | 0            |
| 24  | b     | 91    | 0        | 123      | 11      | 0            |
| 24  | c     | 80    | 0        | 112      | 8       | 0            |
| 24  | d     | 40    | 0        | 56       | 2       | 0            |
| 24  | k     | 40    | 0        | 56       | 2       | 0            |
| 24  | y     | 40    | 0        | 56       | 3       | 0            |
| 25  | A     | 51    | 0        | 72       | 2       | 0            |
| 25  | B     | 40    | 0        | 50       | 3       | 0            |
| 25  | C     | 91    | 0        | 122      | 3       | 0            |
| 25  | D     | 46    | 0        | 62       | 5       | 0            |
| 25  | J     | 45    | 0        | 60       | 1       | 0            |
| 25  | b     | 43    | 0        | 56       | 1       | 0            |
| 25  | c     | 100   | 0        | 140      | 4       | 0            |
| 25  | d     | 47    | 0        | 64       | 4       | 0            |
| 25  | i     | 51    | 0        | 72       | 3       | 0            |
| 25  | j     | 47    | 0        | 64       | 2       | 0            |
| 26  | A     | 55    | 0        | 80       | 10      | 0            |
| 26  | D     | 55    | 0        | 80       | 5       | 0            |
| 26  | a     | 55    | 0        | 80       | 10      | 0            |
| 26  | d     | 55    | 0        | 80       | 5       | 0            |
| 27  | A     | 31    | 0        | 36       | 1       | 0            |
| 27  | C     | 30    | 0        | 33       | 1       | 0            |
| 27  | D     | 143   | 0        | 211      | 18      | 0            |
| 27  | L     | 40    | 0        | 53       | 7       | 0            |
| 27  | a     | 94    | 0        | 137      | 7       | 0            |
| 27  | d     | 128   | 0        | 178      | 6       | 0            |
| 27  | l     | 49    | 0        | 74       | 3       | 0            |
| 28  | A     | 49    | 0        | 64       | 2       | 0            |
| 28  | C     | 54    | 0        | 78       | 6       | 0            |
| 28  | D     | 20    | 0        | 16       | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | a     | 105   | 0        | 147      | 6       | 0            |
| 28  | b     | 38    | 0        | 47       | 2       | 0            |
| 28  | f     | 14    | 0        | 8        | 1       | 0            |
| 28  | l     | 54    | 0        | 78       | 1       | 0            |
| 29  | A     | 35    | 0        | 46       | 6       | 0            |
| 29  | B     | 24    | 0        | 35       | 3       | 0            |
| 29  | E     | 24    | 0        | 35       | 1       | 0            |
| 29  | I     | 35    | 0        | 46       | 0       | 0            |
| 29  | T     | 24    | 0        | 35       | 1       | 0            |
| 29  | Z     | 35    | 0        | 46       | 1       | 0            |
| 29  | a     | 35    | 0        | 46       | 7       | 0            |
| 29  | c     | 59    | 0        | 81       | 1       | 0            |
| 29  | f     | 25    | 0        | 35       | 0       | 0            |
| 29  | t     | 24    | 0        | 35       | 2       | 0            |
| 30  | A     | 5     | 0        | 0        | 0       | 0            |
| 30  | B     | 23    | 0        | 0        | 0       | 0            |
| 30  | D     | 16    | 0        | 0        | 0       | 0            |
| 30  | I     | 45    | 0        | 0        | 1       | 0            |
| 30  | J     | 16    | 0        | 0        | 0       | 0            |
| 30  | O     | 16    | 0        | 0        | 0       | 0            |
| 30  | T     | 13    | 0        | 0        | 0       | 0            |
| 30  | U     | 14    | 0        | 0        | 1       | 0            |
| 30  | X     | 16    | 0        | 0        | 1       | 0            |
| 30  | Z     | 9     | 0        | 0        | 0       | 0            |
| 30  | a     | 16    | 0        | 0        | 0       | 0            |
| 30  | b     | 27    | 0        | 0        | 0       | 0            |
| 30  | c     | 10    | 0        | 0        | 0       | 0            |
| 30  | d     | 16    | 0        | 0        | 0       | 0            |
| 30  | i     | 58    | 0        | 0        | 0       | 0            |
| 30  | j     | 16    | 0        | 0        | 1       | 0            |
| 30  | t     | 16    | 0        | 0        | 0       | 0            |
| 30  | u     | 11    | 0        | 0        | 0       | 0            |
| 30  | x     | 15    | 0        | 0        | 0       | 0            |
| 31  | A     | 20    | 0        | 30       | 4       | 0            |
| 31  | B     | 60    | 0        | 90       | 20      | 0            |
| 31  | C     | 60    | 0        | 90       | 6       | 0            |
| 31  | D     | 12    | 0        | 18       | 3       | 0            |
| 31  | F     | 4     | 0        | 6        | 0       | 0            |
| 31  | H     | 4     | 0        | 6        | 1       | 0            |
| 31  | I     | 8     | 0        | 12       | 0       | 0            |
| 31  | L     | 4     | 0        | 6        | 0       | 0            |
| 31  | O     | 48    | 0        | 72       | 22      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31  | U     | 8     | 0        | 12       | 1       | 0            |
| 31  | V     | 40    | 0        | 60       | 20      | 0            |
| 31  | a     | 20    | 0        | 30       | 8       | 0            |
| 31  | b     | 36    | 0        | 54       | 14      | 0            |
| 31  | c     | 76    | 0        | 114      | 23      | 0            |
| 31  | d     | 20    | 0        | 30       | 8       | 0            |
| 31  | f     | 4     | 0        | 6        | 4       | 0            |
| 31  | i     | 4     | 0        | 6        | 1       | 0            |
| 31  | l     | 12    | 0        | 18       | 1       | 0            |
| 31  | o     | 28    | 0        | 42       | 15      | 0            |
| 31  | t     | 12    | 0        | 18       | 0       | 0            |
| 31  | u     | 16    | 0        | 24       | 6       | 0            |
| 31  | v     | 36    | 0        | 54       | 8       | 0            |
| 32  | A     | 8     | 0        | 0        | 1       | 0            |
| 32  | a     | 4     | 0        | 0        | 0       | 0            |
| 33  | B     | 1     | 0        | 0        | 0       | 0            |
| 33  | O     | 1     | 0        | 0        | 0       | 0            |
| 33  | b     | 1     | 0        | 0        | 0       | 0            |
| 33  | c     | 1     | 0        | 0        | 0       | 0            |
| 33  | o     | 1     | 0        | 0        | 0       | 0            |
| 34  | B     | 57    | 0        | 78       | 3       | 0            |
| 34  | C     | 47    | 0        | 67       | 2       | 0            |
| 34  | D     | 38    | 0        | 52       | 11      | 0            |
| 34  | V     | 14    | 0        | 13       | 0       | 0            |
| 34  | b     | 95    | 0        | 130      | 7       | 0            |
| 34  | c     | 19    | 0        | 26       | 0       | 0            |
| 34  | l     | 19    | 0        | 26       | 3       | 0            |
| 34  | v     | 16    | 0        | 17       | 0       | 0            |
| 35  | C     | 186   | 0        | 246      | 3       | 0            |
| 35  | D     | 50    | 0        | 69       | 0       | 0            |
| 35  | H     | 62    | 0        | 82       | 2       | 0            |
| 35  | c     | 186   | 0        | 246      | 9       | 0            |
| 35  | d     | 43    | 0        | 62       | 0       | 0            |
| 35  | h     | 62    | 0        | 82       | 2       | 0            |
| 36  | E     | 43    | 0        | 30       | 1       | 0            |
| 36  | e     | 43    | 0        | 30       | 6       | 0            |
| 37  | H     | 41    | 0        | 56       | 4       | 0            |
| 37  | h     | 41    | 0        | 56       | 8       | 0            |
| 38  | J     | 1     | 0        | 0        | 0       | 0            |
| 38  | K     | 1     | 0        | 0        | 0       | 0            |
| 38  | j     | 1     | 0        | 0        | 0       | 0            |
| 38  | k     | 1     | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 39  | V     | 43    | 0        | 30       | 0       | 0            |
| 39  | v     | 43    | 0        | 30       | 1       | 0            |
| 40  | A     | 132   | 0        | 0        | 1       | 0            |
| 40  | B     | 262   | 0        | 0        | 6       | 0            |
| 40  | C     | 178   | 0        | 0        | 1       | 0            |
| 40  | D     | 131   | 0        | 0        | 5       | 0            |
| 40  | E     | 35    | 0        | 0        | 0       | 0            |
| 40  | F     | 4     | 0        | 0        | 0       | 0            |
| 40  | H     | 39    | 0        | 0        | 1       | 0            |
| 40  | I     | 5     | 0        | 0        | 0       | 0            |
| 40  | J     | 16    | 0        | 0        | 0       | 0            |
| 40  | K     | 7     | 0        | 0        | 0       | 0            |
| 40  | L     | 19    | 0        | 0        | 0       | 0            |
| 40  | O     | 166   | 0        | 0        | 10      | 0            |
| 40  | T     | 12    | 0        | 0        | 0       | 0            |
| 40  | U     | 74    | 0        | 0        | 2       | 0            |
| 40  | V     | 113   | 0        | 0        | 4       | 0            |
| 40  | X     | 16    | 0        | 0        | 0       | 0            |
| 40  | Y     | 8     | 0        | 0        | 0       | 0            |
| 40  | Z     | 5     | 0        | 0        | 1       | 0            |
| 40  | a     | 123   | 0        | 0        | 1       | 0            |
| 40  | b     | 261   | 0        | 0        | 11      | 0            |
| 40  | c     | 220   | 0        | 0        | 7       | 0            |
| 40  | d     | 115   | 0        | 0        | 0       | 0            |
| 40  | e     | 17    | 0        | 0        | 1       | 0            |
| 40  | f     | 4     | 0        | 0        | 0       | 0            |
| 40  | h     | 31    | 0        | 0        | 0       | 0            |
| 40  | i     | 5     | 0        | 0        | 0       | 0            |
| 40  | j     | 10    | 0        | 0        | 0       | 0            |
| 40  | k     | 10    | 0        | 0        | 0       | 0            |
| 40  | l     | 15    | 0        | 0        | 0       | 0            |
| 40  | o     | 156   | 0        | 0        | 5       | 0            |
| 40  | t     | 10    | 0        | 0        | 0       | 0            |
| 40  | u     | 75    | 0        | 0        | 3       | 0            |
| 40  | v     | 82    | 0        | 0        | 4       | 0            |
| 40  | x     | 5     | 0        | 0        | 0       | 0            |
| 40  | y     | 1     | 0        | 0        | 0       | 0            |
| 40  | z     | 8     | 0        | 0        | 0       | 0            |
| All | All   | 51892 | 0        | 50274    | 868     | 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 9.



The worst 5 of 868 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:c:362:ARG:HD3    | 31:c:924:DMS:H22  | 1.29                     | 1.13              |
| 1:a:214:MET:HG2    | 26:a:415:PL9:H102 | 1.31                     | 1.12              |
| 22:b:608:CLA:H92   | 22:b:608:CLA:H52  | 1.14                     | 1.10              |
| 2:b:347[B]:ARG:NH2 | 40:b:845[B]:HOH:O | 1.79                     | 1.07              |
| 3:c:362:ARG:HH11   | 31:c:924:DMS:H23  | 1.19                     | 1.07              |

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   | A     | 333/334 (100%) | 326 (98%) | 6 (2%)  | 1 (0%)   | 36          | 42  |
| 1   | a     | 333/334 (100%) | 321 (96%) | 11 (3%) | 1 (0%)   | 36          | 42  |
| 2   | B     | 506/505 (100%) | 495 (98%) | 11 (2%) | 0        | 100         | 100 |
| 2   | b     | 482/505 (95%)  | 465 (96%) | 17 (4%) | 0        | 100         | 100 |
| 3   | C     | 449/455 (99%)  | 434 (97%) | 13 (3%) | 2 (0%)   | 30          | 34  |
| 3   | c     | 454/455 (100%) | 435 (96%) | 18 (4%) | 1 (0%)   | 43          | 51  |
| 4   | D     | 343/342 (100%) | 336 (98%) | 6 (2%)  | 1 (0%)   | 36          | 42  |
| 4   | d     | 341/342 (100%) | 333 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 5   | E     | 77/80 (96%)    | 75 (97%)  | 1 (1%)  | 1 (1%)   | 9           | 8   |
| 5   | e     | 77/80 (96%)    | 75 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 6   | F     | 31/33 (94%)    | 31 (100%) | 0       | 0        | 100         | 100 |
| 6   | f     | 29/33 (88%)    | 29 (100%) | 0       | 0        | 100         | 100 |
| 7   | H     | 64/63 (102%)   | 60 (94%)  | 4 (6%)  | 0        | 100         | 100 |
| 7   | h     | 61/63 (97%)    | 58 (95%)  | 3 (5%)  | 0        | 100         | 100 |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 8   | I     | 33/36 (92%)     | 31 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 8   | i     | 34/36 (94%)     | 30 (88%)   | 4 (12%)  | 0        | 100         | 100 |
| 9   | J     | 34/40 (85%)     | 33 (97%)   | 0        | 1 (3%)   | 3           | 2   |
| 9   | j     | 38/40 (95%)     | 37 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 10  | K     | 35/37 (95%)     | 34 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 10  | k     | 35/37 (95%)     | 34 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 11  | L     | 33/35 (94%)     | 33 (100%)  | 0        | 0        | 100         | 100 |
| 11  | l     | 33/35 (94%)     | 33 (100%)  | 0        | 0        | 100         | 100 |
| 12  | O     | 242/243 (100%)  | 228 (94%)  | 12 (5%)  | 2 (1%)   | 16          | 16  |
| 12  | o     | 241/243 (99%)   | 231 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 13  | T     | 28/30 (93%)     | 28 (100%)  | 0        | 0        | 100         | 100 |
| 13  | t     | 28/30 (93%)     | 27 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 14  | U     | 96/97 (99%)     | 92 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 14  | u     | 95/97 (98%)     | 91 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 15  | V     | 136/137 (99%)   | 131 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 15  | v     | 136/137 (99%)   | 126 (93%)  | 9 (7%)   | 1 (1%)   | 18          | 19  |
| 16  | Y     | 27/29 (93%)     | 26 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 16  | y     | 27/29 (93%)     | 26 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 17  | X     | 36/37 (97%)     | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 17  | x     | 34/37 (92%)     | 31 (91%)   | 1 (3%)   | 2 (6%)   | 1           | 0   |
| 18  | Z     | 60/62 (97%)     | 56 (93%)   | 1 (2%)   | 3 (5%)   | 1           | 0   |
| 18  | z     | 59/62 (95%)     | 55 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| All | All   | 5100/5190 (98%) | 4921 (96%) | 163 (3%) | 16 (0%)  | 36          | 42  |

5 of 16 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 12  | ARG  |
| 3   | C     | 24  | THR  |
| 3   | C     | 416 | SER  |
| 5   | E     | 6   | GLY  |
| 18  | Z     | 31  | GLN  |

### 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   | A     | 263/270 (97%)  | 259 (98%)  | 4 (2%)   | 57          | 73  |
| 1   | a     | 252/270 (93%)  | 251 (100%) | 1 (0%)   | 84          | 92  |
| 2   | B     | 391/403 (97%)  | 385 (98%)  | 6 (2%)   | 57          | 73  |
| 2   | b     | 378/403 (94%)  | 375 (99%)  | 3 (1%)   | 73          | 85  |
| 3   | C     | 347/356 (98%)  | 343 (99%)  | 4 (1%)   | 63          | 78  |
| 3   | c     | 356/356 (100%) | 350 (98%)  | 6 (2%)   | 53          | 69  |
| 4   | D     | 278/277 (100%) | 278 (100%) | 0        | 100         | 100 |
| 4   | d     | 276/277 (100%) | 275 (100%) | 1 (0%)   | 84          | 92  |
| 5   | E     | 68/71 (96%)    | 66 (97%)   | 2 (3%)   | 37          | 51  |
| 5   | e     | 67/71 (94%)    | 65 (97%)   | 2 (3%)   | 36          | 49  |
| 6   | F     | 27/27 (100%)   | 27 (100%)  | 0        | 100         | 100 |
| 6   | f     | 25/27 (93%)    | 24 (96%)   | 1 (4%)   | 28          | 38  |
| 7   | H     | 56/53 (106%)   | 56 (100%)  | 0        | 100         | 100 |
| 7   | h     | 54/53 (102%)   | 54 (100%)  | 0        | 100         | 100 |
| 8   | I     | 31/32 (97%)    | 30 (97%)   | 1 (3%)   | 34          | 47  |
| 8   | i     | 31/32 (97%)    | 31 (100%)  | 0        | 100         | 100 |
| 9   | J     | 23/28 (82%)    | 22 (96%)   | 1 (4%)   | 26          | 35  |
| 9   | j     | 25/28 (89%)    | 25 (100%)  | 0        | 100         | 100 |
| 10  | K     | 30/30 (100%)   | 27 (90%)   | 3 (10%)  | 7           | 7   |
| 10  | k     | 28/30 (93%)    | 27 (96%)   | 1 (4%)   | 31          | 42  |
| 11  | L     | 33/33 (100%)   | 33 (100%)  | 0        | 100         | 100 |
| 11  | l     | 33/33 (100%)   | 32 (97%)   | 1 (3%)   | 36          | 49  |
| 12  | O     | 203/206 (98%)  | 196 (97%)  | 7 (3%)   | 32          | 44  |
| 12  | o     | 199/206 (97%)  | 194 (98%)  | 5 (2%)   | 42          | 56  |
| 13  | T     | 24/26 (92%)    | 23 (96%)   | 1 (4%)   | 26          | 36  |
| 13  | t     | 24/26 (92%)    | 22 (92%)   | 2 (8%)   | 10          | 11  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 14  | U     | 85/84 (101%)    | 84 (99%)   | 1 (1%)   | 63          | 78  |
| 14  | u     | 82/84 (98%)     | 81 (99%)   | 1 (1%)   | 63          | 78  |
| 15  | V     | 117/117 (100%)  | 114 (97%)  | 3 (3%)   | 40          | 55  |
| 15  | v     | 115/117 (98%)   | 111 (96%)  | 4 (4%)   | 32          | 43  |
| 16  | Y     | 22/22 (100%)    | 18 (82%)   | 4 (18%)  | 2           | 1   |
| 16  | y     | 19/22 (86%)     | 19 (100%)  | 0        | 100         | 100 |
| 17  | X     | 29/30 (97%)     | 27 (93%)   | 2 (7%)   | 14          | 16  |
| 17  | x     | 27/30 (90%)     | 26 (96%)   | 1 (4%)   | 30          | 41  |
| 18  | Z     | 45/52 (86%)     | 45 (100%)  | 0        | 100         | 100 |
| 18  | z     | 40/52 (77%)     | 38 (95%)   | 2 (5%)   | 22          | 28  |
| All | All   | 4103/4234 (97%) | 4033 (98%) | 70 (2%)  | 53          | 69  |

5 of 70 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | o     | 93  | LEU  |
| 12  | o     | 242 | SER  |
| 15  | v     | 28  | GLU  |
| 12  | O     | 130 | GLN  |
| 12  | O     | 118 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 179 | GLN  |
| 11  | l     | 6   | ASN  |
| 2   | b     | 281 | GLN  |
| 4   | d     | 186 | GLN  |
| 12  | o     | 104 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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 |
| 8   | FME  | I     | 1   | 8    | 8,9,10       | 0.99 | 0        | 7,9,11      | 1.42 | 1 (14%)  |
| 13  | FME  | T     | 1   | 13   | 8,9,10       | 0.63 | 0        | 7,9,11      | 1.38 | 2 (28%)  |
| 13  | FME  | t     | 1   | 13   | 8,9,10       | 0.61 | 0        | 7,9,11      | 1.72 | 1 (14%)  |
| 8   | FME  | i     | 1   | 8    | 8,9,10       | 0.53 | 0        | 7,9,11      | 1.35 | 1 (14%)  |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 8   | FME  | I     | 1   | 8    | -       | 1/7/9/11 | -     |
| 13  | FME  | T     | 1   | 13   | -       | 2/7/9/11 | -     |
| 13  | FME  | t     | 1   | 13   | -       | 2/7/9/11 | -     |
| 8   | FME  | i     | 1   | 8    | -       | 2/7/9/11 | -     |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 13  | t     | 1   | FME  | CE-SD-CG | 3.92  | 113.85      | 100.40   |
| 8   | i     | 1   | FME  | O-C-CA   | -2.32 | 118.69      | 124.78   |
| 8   | I     | 1   | FME  | CE-SD-CG | 2.26  | 108.15      | 100.40   |
| 13  | T     | 1   | FME  | CE-SD-CG | 2.24  | 108.08      | 100.40   |
| 13  | T     | 1   | FME  | C-CA-N   | 2.05  | 113.42      | 109.73   |

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | I     | 1   | FME  | O1-CN-N-CA  |
| 13  | T     | 1   | FME  | O1-CN-N-CA  |
| 13  | T     | 1   | FME  | CA-CB-CG-SD |
| 13  | t     | 1   | FME  | O1-CN-N-CA  |
| 13  | t     | 1   | FME  | CA-CB-CG-SD |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 352 ligands modelled in this entry, 15 are monoatomic and 27 are unknown - leaving 310 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 31  | DMS  | V     | 201 | -    | 3,3,3        | 2.64 | 1 (33%)     | 3,3,3       | 0.90 | 0           |
| 31  | DMS  | v     | 201 | -    | 3,3,3        | 2.59 | 1 (33%)     | 3,3,3       | 0.85 | 0           |
| 31  | DMS  | O     | 311 | -    | 3,3,3        | 2.97 | 1 (33%)     | 3,3,3       | 0.91 | 0           |
| 36  | HEM  | E     | 102 | 6,5  | 50,50,50     | 2.00 | 8 (16%)     | 66,82,82    | 1.65 | 12 (18%)    |
| 31  | DMS  | t     | 103 | -    | 3,3,3        | 2.70 | 1 (33%)     | 3,3,3       | 0.64 | 0           |
| 31  | DMS  | C     | 526 | -    | 3,3,3        | 2.59 | 1 (33%)     | 3,3,3       | 0.56 | 0           |
| 34  | HTG  | V     | 203 | -    | 14,14,19     | 0.69 | 0           | 18,19,24    | 3.11 | 7 (38%)     |
| 29  | LMT  | a     | 419 | -    | 36,36,36     | 0.78 | 0           | 47,47,47    | 1.36 | 5 (10%)     |
| 31  | DMS  | c     | 928 | -    | 3,3,3        | 2.70 | 1 (33%)     | 3,3,3       | 0.77 | 0           |
| 35  | DGD  | C     | 518 | -    | 63,63,67     | 0.96 | 3 (4%)      | 77,77,81    | 1.28 | 10 (12%)    |
| 31  | DMS  | B     | 630 | -    | 3,3,3        | 2.81 | 1 (33%)     | 3,3,3       | 0.91 | 0           |
| 22  | CLA  | c     | 910 | 3    | 69,73,73     | 2.18 | 19 (27%)    | 83,113,113  | 2.49 | 32 (38%)    |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | DMS  | c     | 923    | -    | 3,3,3        | 2.50 | 1 (33%)  | 3,3,3       | 0.40 | 0        |
| 31  | DMS  | v     | 204    | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.69 | 0        |
| 22  | CLA  | B     | 603    | 2    | 69,73,73     | 2.59 | 23 (33%) | 83,113,113  | 2.50 | 36 (43%) |
| 32  | BCT  | A     | 421[B] | 20   | 2,3,3        | 0.95 | 0        | 2,3,3       | 0.41 | 0        |
| 31  | DMS  | c     | 939    | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.65 | 0        |
| 31  | DMS  | l     | 105    | -    | 3,3,3        | 2.74 | 1 (33%)  | 3,3,3       | 0.72 | 0        |
| 24  | BCR  | b     | 620    | -    | 41,41,41     | 0.85 | 0        | 56,56,56    | 1.34 | 8 (14%)  |
| 22  | CLA  | B     | 602    | 40   | 69,73,73     | 2.79 | 23 (33%) | 83,113,113  | 2.45 | 28 (33%) |
| 22  | CLA  | C     | 504    | 3    | 69,73,73     | 2.68 | 23 (33%) | 83,113,113  | 2.44 | 30 (36%) |
| 25  | LMG  | J     | 101    | 38   | 45,45,55     | 0.99 | 2 (4%)   | 53,53,63    | 1.04 | 6 (11%)  |
| 29  | LMT  | A     | 414    | -    | 36,36,36     | 0.80 | 0        | 47,47,47    | 1.14 | 4 (8%)   |
| 31  | DMS  | c     | 944    | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 22  | CLA  | B     | 617    | 2    | 59,63,73     | 2.21 | 17 (28%) | 71,101,113  | 2.82 | 31 (43%) |
| 31  | DMS  | I     | 106    | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.75 | 0        |
| 22  | CLA  | B     | 611    | 40   | 69,73,73     | 2.91 | 19 (27%) | 83,113,113  | 2.44 | 24 (28%) |
| 35  | DGD  | D     | 407    | -    | 50,50,67     | 1.18 | 3 (6%)   | 58,58,81    | 1.31 | 6 (10%)  |
| 31  | DMS  | c     | 935    | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.89 | 0        |
| 24  | BCR  | D     | 405    | -    | 41,41,41     | 1.00 | 1 (2%)   | 56,56,56    | 1.97 | 15 (26%) |
| 31  | DMS  | A     | 419    | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.82 | 0        |
| 31  | DMS  | b     | 633    | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 31  | DMS  | c     | 936    | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 31  | DMS  | O     | 310    | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.86 | 0        |
| 36  | HEM  | e     | 101    | 6,5  | 50,50,50     | 2.03 | 9 (18%)  | 66,82,82    | 1.47 | 10 (15%) |
| 34  | HTG  | B     | 626    | -    | 19,19,19     | 0.73 | 0        | 23,24,24    | 1.83 | 5 (21%)  |
| 22  | CLA  | c     | 904    | 3    | 69,73,73     | 2.61 | 21 (30%) | 83,113,113  | 2.51 | 32 (38%) |
| 22  | CLA  | b     | 614    | 2    | 63,67,73     | 2.36 | 19 (30%) | 75,105,113  | 2.56 | 25 (33%) |
| 24  | BCR  | Y     | 101    | -    | 40,40,41     | 0.93 | 2 (5%)   | 52,54,56    | 1.70 | 15 (28%) |
| 31  | DMS  | B     | 635    | -    | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.69 | 0        |
| 22  | CLA  | c     | 905    | 40   | 69,73,73     | 2.65 | 21 (30%) | 83,113,113  | 2.40 | 27 (32%) |
| 34  | HTG  | v     | 203    | -    | 16,16,19     | 1.05 | 1 (6%)   | 20,21,24    | 3.06 | 7 (35%)  |
| 22  | CLA  | C     | 510    | 3    | 69,73,73     | 2.17 | 21 (30%) | 83,113,113  | 2.56 | 30 (36%) |
| 31  | DMS  | c     | 927    | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.42 | 0        |
| 28  | SQD  | A     | 413    | -    | 48,49,54     | 1.08 | 3 (6%)   | 57,60,65    | 1.74 | 9 (15%)  |
| 34  | HTG  | b     | 624    | -    | 19,19,19     | 1.06 | 1 (5%)   | 23,24,24    | 2.19 | 6 (26%)  |
| 28  | SQD  | a     | 414    | -    | 53,54,54     | 1.09 | 3 (5%)   | 62,65,65    | 2.00 | 12 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | DMS  | C     | 540 | -    | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.89 | 0        |
| 31  | DMS  | B     | 642 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 1.04 | 0        |
| 31  | DMS  | O     | 303 | -    | 3,3,3        | 2.74 | 1 (33%)  | 3,3,3       | 0.77 | 0        |
| 25  | LMG  | d     | 409 | -    | 47,47,55     | 1.09 | 3 (6%)   | 55,55,63    | 1.46 | 8 (14%)  |
| 31  | DMS  | v     | 209 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.63 | 0        |
| 31  | DMS  | b     | 636 | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.70 | 0        |
| 35  | DGD  | c     | 917 | -    | 63,63,67     | 0.97 | 3 (4%)   | 77,77,81    | 1.00 | 3 (3%)   |
| 31  | DMS  | F     | 101 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 35  | DGD  | h     | 102 | -    | 63,63,67     | 0.97 | 3 (4%)   | 77,77,81    | 1.14 | 5 (6%)   |
| 31  | DMS  | D     | 418 | -    | 3,3,3        | 2.40 | 1 (33%)  | 3,3,3       | 0.67 | 0        |
| 22  | CLA  | b     | 612 | 2    | 69,73,73     | 2.18 | 20 (28%) | 83,113,113  | 2.41 | 30 (36%) |
| 31  | DMS  | D     | 416 | -    | 3,3,3        | 2.50 | 1 (33%)  | 3,3,3       | 0.63 | 0        |
| 31  | DMS  | c     | 934 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.67 | 0        |
| 24  | BCR  | C     | 516 | -    | 41,41,41     | 0.91 | 0        | 56,56,56    | 1.36 | 7 (12%)  |
| 34  | HTG  | B     | 623 | -    | 19,19,19     | 1.16 | 1 (5%)   | 23,24,24    | 1.78 | 3 (13%)  |
| 31  | DMS  | d     | 412 | -    | 3,3,3        | 2.56 | 1 (33%)  | 3,3,3       | 0.83 | 0        |
| 31  | DMS  | A     | 416 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 1.06 | 0        |
| 24  | BCR  | y     | 101 | -    | 41,41,41     | 0.89 | 0        | 56,56,56    | 1.59 | 14 (25%) |
| 25  | LMG  | A     | 410 | -    | 51,51,55     | 0.95 | 2 (3%)   | 59,59,63    | 1.09 | 5 (8%)   |
| 31  | DMS  | C     | 524 | -    | 3,3,3        | 2.48 | 1 (33%)  | 3,3,3       | 0.86 | 0        |
| 31  | DMS  | v     | 205 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.83 | 0        |
| 22  | CLA  | b     | 617 | 2    | 64,68,73     | 2.90 | 22 (34%) | 77,107,113  | 2.64 | 30 (38%) |
| 31  | DMS  | O     | 305 | -    | 3,3,3        | 2.90 | 1 (33%)  | 3,3,3       | 0.84 | 0        |
| 22  | CLA  | B     | 604 | 2    | 69,73,73     | 2.25 | 18 (26%) | 83,113,113  | 2.46 | 32 (38%) |
| 29  | LMT  | B     | 622 | -    | 24,24,36     | 0.63 | 1 (4%)   | 29,29,47    | 0.84 | 1 (3%)   |
| 31  | DMS  | U     | 202 | -    | 3,3,3        | 2.77 | 1 (33%)  | 3,3,3       | 1.29 | 0        |
| 31  | DMS  | C     | 537 | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.70 | 0        |
| 23  | PHO  | a     | 411 | -    | 58,69,69     | 2.60 | 12 (20%) | 56,99,99    | 3.03 | 14 (25%) |
| 31  | DMS  | c     | 929 | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.84 | 0        |
| 22  | CLA  | B     | 605 | 2    | 69,73,73     | 2.08 | 19 (27%) | 83,113,113  | 2.50 | 34 (40%) |
| 23  | PHO  | A     | 407 | -    | 58,69,69     | 2.45 | 14 (24%) | 56,99,99    | 2.63 | 16 (28%) |
| 25  | LMG  | c     | 920 | -    | 51,51,55     | 0.99 | 2 (3%)   | 59,59,63    | 1.09 | 5 (8%)   |
| 31  | DMS  | O     | 308 | -    | 3,3,3        | 2.79 | 1 (33%)  | 3,3,3       | 0.62 | 0        |
| 31  | DMS  | V     | 211 | -    | 3,3,3        | 2.81 | 1 (33%)  | 3,3,3       | 0.77 | 0        |
| 22  | CLA  | B     | 613 | 2    | 69,73,73     | 2.64 | 22 (31%) | 83,113,113  | 2.25 | 31 (37%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | DMS  | t     | 105 | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.61 | 0        |
| 31  | DMS  | O     | 314 | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.76 | 0        |
| 31  | DMS  | o     | 305 | -    | 3,3,3        | 2.60 | 1 (33%)  | 3,3,3       | 0.66 | 0        |
| 27  | LHG  | L     | 101 | -    | 39,39,48     | 1.05 | 2 (5%)   | 42,45,54    | 1.19 | 4 (9%)   |
| 22  | CLA  | C     | 513 | 3    | 60,64,73     | 2.86 | 22 (36%) | 72,102,113  | 2.51 | 26 (36%) |
| 25  | LMG  | D     | 412 | -    | 46,46,55     | 1.14 | 3 (6%)   | 54,54,63    | 1.12 | 2 (3%)   |
| 22  | CLA  | C     | 514 | 3    | 69,73,73     | 2.66 | 21 (30%) | 83,113,113  | 2.39 | 28 (33%) |
| 24  | BCR  | K     | 101 | -    | 41,41,41     | 0.86 | 0        | 56,56,56    | 1.19 | 4 (7%)   |
| 31  | DMS  | C     | 528 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 31  | DMS  | o     | 304 | -    | 3,3,3        | 2.81 | 1 (33%)  | 3,3,3       | 1.15 | 0        |
| 24  | BCR  | c     | 916 | -    | 41,41,41     | 0.86 | 0        | 56,56,56    | 1.55 | 10 (17%) |
| 31  | DMS  | a     | 421 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 22  | CLA  | C     | 508 | 40   | 69,73,73     | 2.29 | 21 (30%) | 83,113,113  | 2.41 | 25 (30%) |
| 31  | DMS  | a     | 402 | -    | 3,3,3        | 2.38 | 1 (33%)  | 3,3,3       | 0.73 | 0        |
| 22  | CLA  | a     | 412 | 1    | 69,73,73     | 2.29 | 21 (30%) | 83,113,113  | 2.35 | 30 (36%) |
| 34  | HTG  | b     | 627 | -    | 19,19,19     | 1.03 | 2 (10%)  | 23,24,24    | 1.84 | 3 (13%)  |
| 31  | DMS  | B     | 639 | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.71 | 0        |
| 31  | DMS  | c     | 937 | -    | 3,3,3        | 2.88 | 1 (33%)  | 3,3,3       | 0.82 | 0        |
| 22  | CLA  | b     | 609 | 2    | 69,73,73     | 2.25 | 21 (30%) | 83,113,113  | 2.23 | 27 (32%) |
| 31  | DMS  | C     | 525 | -    | 3,3,3        | 2.45 | 1 (33%)  | 3,3,3       | 0.62 | 0        |
| 27  | LHG  | d     | 407 | -    | 48,48,48     | 0.75 | 2 (4%)   | 51,54,54    | 1.06 | 3 (5%)   |
| 22  | CLA  | C     | 505 | 40   | 69,73,73     | 3.02 | 22 (31%) | 83,113,113  | 2.23 | 21 (25%) |
| 28  | SQD  | a     | 418 | -    | 50,51,54     | 1.16 | 3 (6%)   | 59,62,65    | 1.47 | 8 (13%)  |
| 25  | LMG  | C     | 520 | -    | 51,51,55     | 1.08 | 2 (3%)   | 59,59,63    | 1.23 | 5 (8%)   |
| 35  | DGD  | H     | 102 | -    | 63,63,67     | 1.02 | 3 (4%)   | 77,77,81    | 1.16 | 6 (7%)   |
| 25  | LMG  | b     | 622 | -    | 43,43,55     | 1.35 | 4 (9%)   | 51,51,63    | 1.90 | 12 (23%) |
| 31  | DMS  | V     | 206 | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 22  | CLA  | c     | 911 | 3    | 69,73,73     | 2.25 | 20 (28%) | 83,113,113  | 2.36 | 27 (32%) |
| 31  | DMS  | c     | 933 | -    | 3,3,3        | 2.84 | 1 (33%)  | 3,3,3       | 0.92 | 0        |
| 31  | DMS  | u     | 203 | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.76 | 0        |
| 31  | DMS  | b     | 635 | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 31  | DMS  | V     | 208 | -    | 3,3,3        | 2.60 | 1 (33%)  | 3,3,3       | 0.40 | 0        |
| 34  | HTG  | b     | 632 | -    | 19,19,19     | 1.08 | 2 (10%)  | 23,24,24    | 2.54 | 7 (30%)  |
| 22  | CLA  | c     | 908 | 40   | 69,73,73     | 2.72 | 20 (28%) | 83,113,113  | 2.50 | 23 (27%) |
| 31  | DMS  | v     | 206 | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.73 | 0        |

| Mol | Type | Chain | Res | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | DMS  | o     | 302 | -      | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.95 | 0        |
| 22  | CLA  | B     | 612 | 2      | 69,73,73     | 2.17 | 17 (24%) | 83,113,113  | 2.42 | 30 (36%) |
| 26  | PL9  | d     | 405 | -      | 55,55,55     | 1.03 | 5 (9%)   | 68,69,69    | 1.48 | 9 (13%)  |
| 25  | LMG  | c     | 930 | -      | 49,49,55     | 1.10 | 3 (6%)   | 57,57,63    | 1.06 | 4 (7%)   |
| 22  | CLA  | B     | 615 | 2      | 57,61,73     | 2.63 | 20 (35%) | 68,98,113   | 3.03 | 30 (44%) |
| 24  | BCR  | A     | 409 | -      | 41,41,41     | 1.08 | 2 (4%)   | 56,56,56    | 1.27 | 5 (8%)   |
| 31  | DMS  | t     | 104 | -      | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 31  | DMS  | U     | 203 | -      | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 1.24 | 0        |
| 31  | DMS  | b     | 638 | -      | 3,3,3        | 2.98 | 1 (33%)  | 3,3,3       | 0.69 | 0        |
| 24  | BCR  | B     | 619 | -      | 30,30,41     | 0.92 | 0        | 39,39,56    | 1.32 | 7 (17%)  |
| 27  | LHG  | a     | 416 | -      | 48,48,48     | 1.13 | 2 (4%)   | 51,54,54    | 1.18 | 4 (7%)   |
| 31  | DMS  | C     | 529 | -      | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 22  | CLA  | B     | 616 | 2      | 69,73,73     | 2.66 | 21 (30%) | 83,113,113  | 2.34 | 25 (30%) |
| 28  | SQD  | D     | 408 | -      | 19,20,54     | 0.97 | 2 (10%)  | 26,29,65    | 1.93 | 7 (26%)  |
| 34  | HTG  | b     | 623 | -      | 19,19,19     | 1.10 | 1 (5%)   | 23,24,24    | 1.32 | 4 (17%)  |
| 31  | DMS  | V     | 212 | -      | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 1.18 | 0        |
| 31  | DMS  | v     | 210 | -      | 3,3,3        | 2.84 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 31  | DMS  | u     | 205 | -      | 3,3,3        | 3.07 | 1 (33%)  | 3,3,3       | 1.19 | 0        |
| 31  | DMS  | A     | 418 | -      | 3,3,3        | 2.41 | 1 (33%)  | 3,3,3       | 1.25 | 0        |
| 22  | CLA  | b     | 610 | 2      | 69,73,73     | 2.60 | 21 (30%) | 83,113,113  | 2.22 | 28 (33%) |
| 31  | DMS  | V     | 210 | -      | 3,3,3        | 2.77 | 1 (33%)  | 3,3,3       | 0.89 | 0        |
| 22  | CLA  | D     | 404 | 4      | 69,73,73     | 2.43 | 18 (26%) | 83,113,113  | 2.22 | 24 (28%) |
| 19  | OEX  | A     | 401 | 3,40,1 | 0,14,14      | -    | -        | -           | -    | -        |
| 22  | CLA  | d     | 402 | 4      | 69,73,73     | 2.08 | 22 (31%) | 83,113,113  | 2.54 | 29 (34%) |
| 22  | CLA  | A     | 405 | 1      | 69,73,73     | 2.40 | 18 (26%) | 83,113,113  | 2.27 | 26 (31%) |
| 22  | CLA  | C     | 502 | 3      | 69,73,73     | 2.12 | 20 (28%) | 83,113,113  | 2.41 | 25 (30%) |
| 29  | LMT  | t     | 101 | -      | 24,24,36     | 0.45 | 0        | 29,29,47    | 1.34 | 4 (13%)  |
| 22  | CLA  | b     | 608 | 40     | 69,73,73     | 2.44 | 22 (31%) | 83,113,113  | 2.29 | 26 (31%) |
| 31  | DMS  | C     | 538 | -      | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 27  | LHG  | d     | 401 | -      | 32,32,48     | 1.24 | 2 (6%)   | 36,37,54    | 1.18 | 4 (11%)  |
| 34  | HTG  | D     | 415 | -      | 19,19,19     | 1.16 | 1 (5%)   | 23,24,24    | 2.71 | 7 (30%)  |
| 25  | LMG  | j     | 101 | 38     | 47,47,55     | 1.01 | 2 (4%)   | 55,55,63    | 1.18 | 9 (16%)  |
| 28  | SQD  | C     | 501 | -      | 53,54,54     | 1.04 | 3 (5%)   | 62,65,65    | 1.95 | 14 (22%) |
| 22  | CLA  | b     | 603 | 2      | 69,73,73     | 2.83 | 20 (28%) | 83,113,113  | 2.46 | 30 (36%) |
| 28  | SQD  | l     | 101 | -      | 53,54,54     | 1.12 | 4 (7%)   | 62,65,65    | 1.47 | 8 (12%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | DMS  | A     | 417 | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 31  | DMS  | I     | 101 | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.69 | 0        |
| 31  | DMS  | C     | 539 | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.61 | 0        |
| 22  | CLA  | c     | 907 | 3    | 69,73,73     | 2.37 | 20 (28%) | 83,113,113  | 2.36 | 28 (33%) |
| 25  | LMG  | i     | 101 | -    | 51,51,55     | 0.99 | 2 (3%)   | 59,59,63    | 1.18 | 7 (11%)  |
| 31  | DMS  | C     | 536 | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.45 | 0        |
| 24  | BCR  | b     | 618 | -    | 20,20,41     | 0.89 | 1 (5%)   | 27,27,56    | 1.73 | 5 (18%)  |
| 31  | DMS  | C     | 535 | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 24  | BCR  | d     | 404 | -    | 41,41,41     | 1.05 | 3 (7%)   | 56,56,56    | 1.77 | 13 (23%) |
| 31  | DMS  | b     | 634 | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 31  | DMS  | B     | 641 | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.84 | 0        |
| 27  | LHG  | d     | 408 | -    | 45,45,48     | 1.04 | 2 (4%)   | 48,51,54    | 0.73 | 0        |
| 22  | CLA  | D     | 403 | 4    | 69,73,73     | 2.07 | 19 (27%) | 83,113,113  | 2.55 | 27 (32%) |
| 31  | DMS  | B     | 629 | -    | 3,3,3        | 2.54 | 1 (33%)  | 3,3,3       | 1.19 | 0        |
| 22  | CLA  | B     | 607 | 2    | 69,73,73     | 2.37 | 20 (28%) | 83,113,113  | 2.50 | 33 (39%) |
| 22  | CLA  | a     | 408 | 40   | 69,73,73     | 2.57 | 23 (33%) | 83,113,113  | 2.64 | 33 (39%) |
| 29  | LMT  | I     | 102 | -    | 36,36,36     | 0.68 | 1 (2%)   | 47,47,47    | 1.36 | 4 (8%)   |
| 22  | CLA  | b     | 606 | 2    | 69,73,73     | 2.25 | 19 (27%) | 83,113,113  | 2.46 | 26 (31%) |
| 28  | SQD  | b     | 621 | -    | 37,38,54     | 1.04 | 2 (5%)   | 45,48,65    | 1.50 | 8 (17%)  |
| 22  | CLA  | b     | 604 | 2    | 69,73,73     | 2.61 | 20 (28%) | 83,113,113  | 2.43 | 26 (31%) |
| 34  | HTG  | C     | 523 | -    | 8,8,19       | 0.38 | 0        | 7,7,24      | 1.42 | 1 (14%)  |
| 29  | LMT  | c     | 931 | -    | 24,24,36     | 0.79 | 1 (4%)   | 29,29,47    | 0.86 | 2 (6%)   |
| 22  | CLA  | c     | 902 | 3    | 69,73,73     | 2.45 | 18 (26%) | 83,113,113  | 2.54 | 23 (27%) |
| 31  | DMS  | b     | 637 | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.61 | 0        |
| 31  | DMS  | b     | 631 | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 24  | BCR  | c     | 915 | -    | 41,41,41     | 0.84 | 1 (2%)   | 56,56,56    | 1.39 | 8 (14%)  |
| 31  | DMS  | u     | 202 | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 1.05 | 0        |
| 31  | DMS  | O     | 309 | -    | 3,3,3        | 2.54 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 27  | LHG  | a     | 423 | -    | 44,44,48     | 1.02 | 2 (4%)   | 47,50,54    | 1.08 | 4 (8%)   |
| 31  | DMS  | O     | 306 | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.75 | 0        |
| 25  | LMG  | B     | 621 | -    | 40,40,55     | 1.26 | 3 (7%)   | 48,48,63    | 1.39 | 8 (16%)  |
| 35  | DGD  | c     | 919 | -    | 63,63,67     | 0.98 | 4 (6%)   | 77,77,81    | 1.15 | 6 (7%)   |
| 31  | DMS  | B     | 634 | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.65 | 0        |
| 31  | DMS  | O     | 313 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 31  | DMS  | i     | 106 | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.55 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | D     | 401 | 40   | 69,73,73     | 1.92 | 17 (24%) | 83,113,113  | 2.65 | 31 (37%) |
| 31  | DMS  | f     | 103 | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.91 | 0        |
| 31  | DMS  | o     | 307 | -    | 3,3,3        | 2.60 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 22  | CLA  | A     | 408 | 1    | 69,73,73     | 2.16 | 19 (27%) | 83,113,113  | 2.43 | 31 (37%) |
| 22  | CLA  | a     | 409 | 40   | 65,69,73     | 2.15 | 20 (30%) | 78,108,113  | 2.79 | 33 (42%) |
| 31  | DMS  | v     | 211 | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.76 | 0        |
| 35  | DGD  | c     | 918 | -    | 63,63,67     | 0.94 | 4 (6%)   | 77,77,81    | 1.03 | 4 (5%)   |
| 22  | CLA  | b     | 605 | 2    | 69,73,73     | 2.51 | 22 (31%) | 83,113,113  | 2.35 | 22 (26%) |
| 34  | HTG  | C     | 532 | -    | 19,19,19     | 1.15 | 2 (10%)  | 23,24,24    | 1.90 | 1 (4%)   |
| 22  | CLA  | c     | 906 | 3    | 69,73,73     | 2.40 | 21 (30%) | 83,113,113  | 2.23 | 23 (27%) |
| 22  | CLA  | c     | 912 | 3    | 69,73,73     | 2.89 | 20 (28%) | 83,113,113  | 2.25 | 29 (34%) |
| 25  | LMG  | C     | 531 | -    | 40,40,55     | 1.19 | 3 (7%)   | 48,48,63    | 1.13 | 3 (6%)   |
| 31  | DMS  | c     | 926 | -    | 3,3,3        | 2.60 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 31  | DMS  | A     | 420 | -    | 3,3,3        | 2.74 | 1 (33%)  | 3,3,3       | 1.35 | 0        |
| 22  | CLA  | b     | 615 | 2    | 56,60,73     | 2.75 | 22 (39%) | 67,97,113   | 2.53 | 31 (46%) |
| 31  | DMS  | c     | 925 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 1.11 | 0        |
| 31  | DMS  | B     | 638 | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.40 | 0        |
| 22  | CLA  | C     | 512 | 3    | 69,73,73     | 2.56 | 22 (31%) | 83,113,113  | 2.46 | 29 (34%) |
| 34  | HTG  | C     | 521 | -    | 19,19,19     | 0.94 | 2 (10%)  | 23,24,24    | 1.64 | 2 (8%)   |
| 31  | DMS  | c     | 942 | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.72 | 0        |
| 31  | DMS  | o     | 306 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 31  | DMS  | V     | 204 | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.82 | 0        |
| 22  | CLA  | b     | 616 | 2    | 69,73,73     | 2.38 | 20 (28%) | 83,113,113  | 2.30 | 28 (33%) |
| 22  | CLA  | d     | 403 | 4    | 69,73,73     | 2.92 | 22 (31%) | 83,113,113  | 2.24 | 26 (31%) |
| 31  | DMS  | b     | 630 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.29 | 0        |
| 29  | LMT  | Z     | 101 | -    | 36,36,36     | 0.67 | 1 (2%)   | 47,47,47    | 1.15 | 3 (6%)   |
| 22  | CLA  | a     | 407 | 1    | 69,73,73     | 2.32 | 20 (28%) | 83,113,113  | 2.25 | 29 (34%) |
| 31  | DMS  | c     | 943 | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 27  | LHG  | D     | 409 | -    | 48,48,48     | 1.02 | 2 (4%)   | 51,54,54    | 1.37 | 5 (9%)   |
| 34  | HTG  | l     | 106 | -    | 19,19,19     | 1.01 | 2 (10%)  | 23,24,24    | 2.09 | 3 (13%)  |
| 31  | DMS  | c     | 924 | -    | 3,3,3        | 2.82 | 1 (33%)  | 3,3,3       | 1.32 | 1 (33%)  |
| 27  | LHG  | D     | 411 | -    | 44,44,48     | 0.98 | 2 (4%)   | 47,50,54    | 1.03 | 3 (6%)   |
| 22  | CLA  | b     | 602 | 40   | 69,73,73     | 3.34 | 20 (28%) | 83,113,113  | 2.47 | 23 (27%) |
| 37  | RRX  | H     | 101 | -    | 42,42,42     | 0.82 | 0        | 57,58,58    | 1.47 | 8 (14%)  |
| 31  | DMS  | V     | 209 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.49 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | DMS  | a     | 401 | -    | 3,3,3        | 2.74 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 31  | DMS  | O     | 307 | -    | 3,3,3        | 2.79 | 1 (33%)  | 3,3,3       | 0.91 | 0        |
| 31  | DMS  | d     | 411 | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.94 | 0        |
| 24  | BCR  | b     | 619 | -    | 31,31,41     | 1.10 | 2 (6%)   | 40,40,56    | 1.34 | 8 (20%)  |
| 31  | DMS  | B     | 633 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.46 | 0        |
| 31  | DMS  | C     | 533 | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.75 | 0        |
| 27  | LHG  | l     | 102 | -    | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.08 | 2 (3%)   |
| 24  | BCR  | a     | 413 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.16 | 8 (14%)  |
| 31  | DMS  | V     | 205 | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 34  | HTG  | b     | 626 | -    | 19,19,19     | 0.84 | 1 (5%)   | 23,24,24    | 1.61 | 5 (21%)  |
| 29  | LMT  | c     | 921 | -    | 36,36,36     | 0.67 | 1 (2%)   | 47,47,47    | 1.03 | 4 (8%)   |
| 31  | DMS  | o     | 303 | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 26  | PL9  | D     | 406 | -    | 55,55,55     | 0.94 | 3 (5%)   | 68,69,69    | 1.56 | 14 (20%) |
| 31  | DMS  | a     | 424 | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 1.02 | 0        |
| 31  | DMS  | D     | 417 | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 29  | LMT  | T     | 102 | -    | 24,24,36     | 0.73 | 1 (4%)   | 29,29,47    | 1.27 | 3 (10%)  |
| 31  | DMS  | C     | 534 | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 23  | PHO  | D     | 402 | -    | 58,69,69     | 2.79 | 11 (18%) | 56,99,99    | 2.60 | 16 (28%) |
| 31  | DMS  | v     | 208 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 31  | DMS  | B     | 637 | -    | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.71 | 0        |
| 31  | DMS  | O     | 312 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.96 | 0        |
| 31  | DMS  | V     | 207 | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.89 | 0        |
| 31  | DMS  | v     | 207 | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.65 | 0        |
| 22  | CLA  | C     | 511 | 3    | 69,73,73     | 2.36 | 20 (28%) | 83,113,113  | 2.17 | 26 (31%) |
| 31  | DMS  | B     | 631 | -    | 3,3,3        | 2.56 | 1 (33%)  | 3,3,3       | 0.62 | 0        |
| 35  | DGD  | C     | 517 | -    | 63,63,67     | 0.85 | 3 (4%)   | 77,77,81    | 1.33 | 12 (15%) |
| 22  | CLA  | C     | 509 | 3    | 69,73,73     | 2.43 | 20 (28%) | 83,113,113  | 2.30 | 24 (28%) |
| 24  | BCR  | B     | 620 | -    | 41,41,41     | 0.97 | 2 (4%)   | 56,56,56    | 1.48 | 11 (19%) |
| 32  | BCT  | a     | 422 | 20   | 2,3,3        | 0.87 | 0        | 2,3,3       | 1.11 | 0        |
| 35  | DGD  | C     | 519 | -    | 63,63,67     | 0.82 | 2 (3%)   | 77,77,81    | 1.20 | 9 (11%)  |
| 31  | DMS  | b     | 629 | -    | 3,3,3        | 2.28 | 1 (33%)  | 3,3,3       | 1.10 | 0        |
| 27  | LHG  | A     | 412 | -    | 30,30,48     | 1.38 | 2 (6%)   | 33,35,54    | 1.44 | 4 (12%)  |
| 31  | DMS  | B     | 628 | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.77 | 0        |
| 31  | DMS  | u     | 204 | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 31  | DMS  | c     | 938 | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.83 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | SQD  | f     | 101 | -    | 12,13,54     | 2.23 | 1 (8%)   | 15,16,65    | 1.26 | 2 (13%)  |
| 24  | BCR  | B     | 618 | -    | 19,19,41     | 0.91 | 1 (5%)   | 26,26,56    | 1.42 | 5 (19%)  |
| 22  | CLA  | B     | 614 | 2    | 65,69,73     | 2.31 | 18 (27%) | 78,108,113  | 2.25 | 28 (35%) |
| 29  | LMT  | E     | 101 | -    | 24,24,36     | 0.64 | 0        | 29,29,47    | 0.99 | 1 (3%)   |
| 31  | DMS  | O     | 304 | -    | 3,3,3        | 2.57 | 1 (33%)  | 3,3,3       | 0.42 | 0        |
| 22  | CLA  | B     | 610 | 2    | 69,73,73     | 2.41 | 22 (31%) | 83,113,113  | 2.22 | 23 (27%) |
| 22  | CLA  | c     | 913 | 3    | 69,73,73     | 2.50 | 24 (34%) | 83,113,113  | 2.31 | 27 (32%) |
| 22  | CLA  | b     | 613 | 2    | 69,73,73     | 2.57 | 21 (30%) | 83,113,113  | 2.34 | 28 (33%) |
| 29  | LMT  | f     | 102 | -    | 25,25,36     | 1.01 | 1 (4%)   | 30,30,47    | 1.22 | 5 (16%)  |
| 22  | CLA  | c     | 909 | 3    | 69,73,73     | 3.21 | 23 (33%) | 83,113,113  | 2.36 | 26 (31%) |
| 34  | HTG  | c     | 922 | -    | 19,19,19     | 0.84 | 1 (5%)   | 23,24,24    | 1.70 | 2 (8%)   |
| 39  | HEC  | v     | 202 | 15   | 50,50,50     | 1.95 | 10 (20%) | 68,82,82    | 1.66 | 10 (14%) |
| 31  | DMS  | C     | 530 | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.85 | 0        |
| 31  | DMS  | l     | 103 | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.66 | 0        |
| 31  | DMS  | o     | 308 | -    | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.83 | 0        |
| 22  | CLA  | c     | 914 | 3    | 69,73,73     | 2.36 | 20 (28%) | 83,113,113  | 2.34 | 28 (33%) |
| 22  | CLA  | b     | 611 | 40   | 69,73,73     | 2.55 | 21 (30%) | 83,113,113  | 2.37 | 26 (31%) |
| 22  | CLA  | B     | 609 | 2    | 69,73,73     | 2.58 | 22 (31%) | 83,113,113  | 2.40 | 26 (31%) |
| 31  | DMS  | B     | 636 | -    | 3,3,3        | 2.60 | 1 (33%)  | 3,3,3       | 0.63 | 0        |
| 24  | BCR  | C     | 515 | -    | 41,41,41     | 0.81 | 1 (2%)   | 56,56,56    | 1.48 | 9 (16%)  |
| 31  | DMS  | d     | 413 | -    | 3,3,3        | 2.54 | 1 (33%)  | 3,3,3       | 0.39 | 0        |
| 31  | DMS  | c     | 940 | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 31  | DMS  | H     | 103 | -    | 3,3,3        | 2.91 | 1 (33%)  | 3,3,3       | 1.19 | 0        |
| 31  | DMS  | B     | 632 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 22  | CLA  | B     | 606 | 2    | 69,73,73     | 2.81 | 19 (27%) | 83,113,113  | 2.49 | 30 (36%) |
| 31  | DMS  | l     | 104 | -    | 3,3,3        | 2.77 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 22  | CLA  | C     | 503 | 3    | 69,73,73     | 2.41 | 20 (28%) | 83,113,113  | 2.37 | 22 (26%) |
| 22  | CLA  | C     | 507 | 3    | 69,73,73     | 2.28 | 21 (30%) | 83,113,113  | 2.37 | 23 (27%) |
| 22  | CLA  | A     | 406 | 40   | 59,63,73     | 2.34 | 21 (35%) | 71,101,113  | 2.83 | 31 (43%) |
| 27  | LHG  | D     | 410 | -    | 48,48,48     | 0.79 | 2 (4%)   | 51,54,54    | 1.08 | 4 (7%)   |
| 23  | PHO  | a     | 410 | -    | 58,69,69     | 2.60 | 13 (22%) | 56,99,99    | 2.35 | 12 (21%) |
| 31  | DMS  | B     | 640 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.61 | 0        |
| 34  | HTG  | D     | 414 | -    | 19,19,19     | 0.86 | 1 (5%)   | 23,24,24    | 1.84 | 1 (4%)   |
| 31  | DMS  | d     | 414 | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 31  | DMS  | a     | 425 | -    | 3,3,3        | 3.01 | 1 (33%)  | 3,3,3       | 0.88 | 0        |



| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | BCR  | k     | 101    | -      | 41,41,41     | 0.91 | 0        | 56,56,56    | 1.23 | 6 (10%)  |
| 26  | PL9  | a     | 415    | -      | 55,55,55     | 0.96 | 3 (5%)   | 68,69,69    | 1.49 | 12 (17%) |
| 31  | DMS  | d     | 415    | -      | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.61 | 0        |
| 32  | BCT  | A     | 421[A] | 20     | 2,3,3        | 0.79 | 0        | 2,3,3       | 0.11 | 0        |
| 31  | DMS  | L     | 102    | -      | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.95 | 0        |
| 39  | HEC  | V     | 202    | 15     | 50,50,50     | 1.90 | 10 (20%) | 68,82,82    | 1.48 | 10 (14%) |
| 22  | CLA  | c     | 903    | 3      | 69,73,73     | 2.03 | 18 (26%) | 83,113,113  | 2.45 | 27 (32%) |
| 34  | HTG  | B     | 627    | -      | 19,19,19     | 1.01 | 1 (5%)   | 23,24,24    | 2.02 | 4 (17%)  |
| 27  | LHG  | C     | 522    | -      | 29,29,48     | 1.31 | 2 (6%)   | 33,34,54    | 1.38 | 4 (12%)  |
| 37  | RRX  | h     | 101    | -      | 42,42,42     | 0.97 | 0        | 57,58,58    | 1.19 | 5 (8%)   |
| 31  | DMS  | c     | 941    | -      | 3,3,3        | 2.60 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 22  | CLA  | C     | 506    | 3      | 69,73,73     | 2.59 | 19 (27%) | 83,113,113  | 2.25 | 23 (27%) |
| 31  | DMS  | C     | 527    | -      | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 22  | CLA  | b     | 607    | 2      | 69,73,73     | 2.25 | 22 (31%) | 83,113,113  | 2.64 | 28 (33%) |
| 35  | DGD  | d     | 406    | -      | 42,42,67     | 1.24 | 3 (7%)   | 44,45,81    | 1.09 | 3 (6%)   |
| 19  | OEX  | a     | 403    | 3,40,1 | 0,14,14      | -    | -        | -           | -    | -        |
| 22  | CLA  | B     | 608    | 40     | 69,73,73     | 2.18 | 19 (27%) | 83,113,113  | 2.40 | 33 (39%) |
| 26  | PL9  | A     | 411    | -      | 55,55,55     | 0.97 | 3 (5%)   | 68,69,69    | 1.72 | 14 (20%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 24  | BCR  | d     | 404 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 34  | HTG  | b     | 626 | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 36  | HEM  | E     | 102 | 6,5  | -       | 1/14/54/54    | -       |
| 29  | LMT  | c     | 921 | -    | -       | 11/21/61/61   | 0/2/2/2 |
| 26  | PL9  | D     | 406 | -    | -       | 8/53/73/73    | 0/1/1/1 |
| 27  | LHG  | L     | 101 | -    | -       | 20/44/44/53   | -       |
| 34  | HTG  | V     | 203 | -    | -       | 0/5/25/30     | 0/1/1/1 |
| 22  | CLA  | C     | 513 | 3    | -       | 11/29/105/115 | -       |
| 29  | LMT  | a     | 419 | -    | -       | 14/21/61/61   | 0/2/2/2 |
| 25  | LMG  | D     | 412 | -    | -       | 14/41/61/70   | 0/1/1/1 |
| 29  | LMT  | T     | 102 | -    | -       | 10/15/35/61   | 0/1/1/2 |
| 22  | CLA  | C     | 514 | 3    | -       | 18/39/115/115 | -       |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 24  | BCR  | K     | 101 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 35  | DGD  | C     | 518 | -    | -       | 23/51/91/95   | 0/2/2/2 |
| 27  | LHG  | d     | 408 | -    | -       | 17/50/50/53   | -       |
| 22  | CLA  | c     | 910 | 3    | -       | 15/39/115/115 | -       |
| 23  | PHO  | D     | 402 | -    | -       | 6/37/103/103  | 0/5/6/6 |
| 24  | BCR  | c     | 916 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 603 | 2    | -       | 8/39/115/115  | -       |
| 22  | CLA  | C     | 508 | 40   | -       | 11/39/115/115 | -       |
| 22  | CLA  | C     | 511 | 3    | -       | 14/39/115/115 | -       |
| 22  | CLA  | D     | 403 | 4    | -       | 0/39/115/115  | -       |
| 35  | DGD  | C     | 517 | -    | -       | 19/51/91/95   | 0/2/2/2 |
| 22  | CLA  | C     | 509 | 3    | -       | 11/39/115/115 | -       |
| 24  | BCR  | B     | 620 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 607 | 2    | -       | 14/39/115/115 | -       |
| 22  | CLA  | a     | 412 | 1    | -       | 12/39/115/115 | -       |
| 35  | DGD  | C     | 519 | -    | -       | 29/51/91/95   | 0/2/2/2 |
| 22  | CLA  | a     | 408 | 40   | -       | 6/39/115/115  | -       |
| 29  | LMT  | I     | 102 | -    | -       | 11/21/61/61   | 0/2/2/2 |
| 22  | CLA  | b     | 606 | 2    | -       | 3/39/115/115  | -       |
| 24  | BCR  | b     | 620 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 602 | 40   | -       | 25/39/115/115 | -       |
| 27  | LHG  | A     | 412 | -    | -       | 14/33/33/53   | -       |
| 28  | SQD  | b     | 621 | -    | -       | 16/32/52/69   | 0/1/1/1 |
| 34  | HTG  | b     | 627 | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 22  | CLA  | b     | 604 | 2    | -       | 10/39/115/115 | -       |
| 34  | HTG  | C     | 523 | -    | -       | 1/6/6/30      | -       |
| 22  | CLA  | b     | 609 | 2    | -       | 7/39/115/115  | -       |
| 22  | CLA  | C     | 504 | 3    | -       | 3/39/115/115  | -       |
| 25  | LMG  | J     | 101 | 38   | -       | 9/40/60/70    | 0/1/1/1 |
| 29  | LMT  | c     | 931 | -    | -       | 11/15/35/61   | 0/1/1/2 |
| 29  | LMT  | A     | 414 | -    | -       | 14/21/61/61   | 0/2/2/2 |
| 22  | CLA  | c     | 902 | 3    | -       | 4/39/115/115  | -       |
| 28  | SQD  | f     | 101 | -    | -       | 4/12/12/69    | -       |
| 24  | BCR  | c     | 915 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 617 | 2    | -       | 5/27/103/115  | -       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 22  | CLA  | B     | 611 | 40   | -       | 9/39/115/115  | -       |
| 27  | LHG  | d     | 407 | -    | -       | 20/53/53/53   | -       |
| 35  | DGD  | D     | 407 | -    | -       | 29/44/64/95   | 0/1/1/2 |
| 27  | LHG  | a     | 423 | -    | -       | 22/49/49/53   | -       |
| 24  | BCR  | B     | 618 | -    | -       | 0/11/28/63    | 0/1/1/2 |
| 24  | BCR  | D     | 405 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 22  | CLA  | C     | 505 | 40   | -       | 6/39/115/115  | -       |
| 28  | SQD  | a     | 418 | -    | -       | 24/46/66/69   | 0/1/1/1 |
| 25  | LMG  | C     | 520 | -    | -       | 19/46/66/70   | 0/1/1/1 |
| 22  | CLA  | B     | 614 | 2    | -       | 6/35/111/115  | -       |
| 25  | LMG  | B     | 621 | -    | -       | 23/35/55/70   | 0/1/1/1 |
| 29  | LMT  | E     | 101 | -    | -       | 9/15/35/61    | 0/1/1/2 |
| 35  | DGD  | H     | 102 | -    | -       | 17/51/91/95   | 0/2/2/2 |
| 35  | DGD  | c     | 919 | -    | -       | 20/51/91/95   | 0/2/2/2 |
| 25  | LMG  | b     | 622 | -    | -       | 20/38/58/70   | 0/1/1/1 |
| 22  | CLA  | B     | 610 | 2    | -       | 4/39/115/115  | -       |
| 22  | CLA  | c     | 913 | 3    | -       | 21/39/115/115 | -       |
| 22  | CLA  | b     | 613 | 2    | -       | 6/39/115/115  | -       |
| 36  | HEM  | e     | 101 | 6,5  | -       | 7/14/54/54    | -       |
| 34  | HTG  | B     | 626 | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 29  | LMT  | f     | 102 | -    | -       | 10/17/37/61   | 0/1/1/2 |
| 22  | CLA  | c     | 909 | 3    | -       | 12/39/115/115 | -       |
| 34  | HTG  | c     | 922 | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 22  | CLA  | c     | 904 | 3    | -       | 7/39/115/115  | -       |
| 22  | CLA  | b     | 614 | 2    | -       | 6/32/108/115  | -       |
| 24  | BCR  | Y     | 101 | -    | -       | 6/29/60/63    | 0/2/2/2 |
| 22  | CLA  | c     | 911 | 3    | -       | 7/39/115/115  | -       |
| 22  | CLA  | c     | 905 | 40   | -       | 15/39/115/115 | -       |
| 34  | HTG  | v     | 203 | -    | -       | 5/7/27/30     | 0/1/1/1 |
| 39  | HEC  | v     | 202 | 15   | 1/1/3/7 | 5/14/54/54    | -       |
| 22  | CLA  | C     | 510 | 3    | -       | 13/39/115/115 | -       |
| 22  | CLA  | D     | 401 | 40   | -       | 6/39/115/115  | -       |
| 28  | SQD  | A     | 413 | -    | -       | 26/44/64/69   | 0/1/1/1 |
| 34  | HTG  | b     | 624 | -    | -       | 4/10/30/30    | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 22  | CLA  | c     | 914 | 3    | -       | 16/39/115/115 | -       |
| 28  | SQD  | a     | 414 | -    | -       | 27/49/69/69   | 0/1/1/1 |
| 34  | HTG  | b     | 632 | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 22  | CLA  | A     | 408 | 1    | -       | 13/39/115/115 | -       |
| 22  | CLA  | b     | 611 | 40   | -       | 7/39/115/115  | -       |
| 22  | CLA  | c     | 908 | 40   | -       | 11/39/115/115 | -       |
| 22  | CLA  | a     | 409 | 40   | -       | 10/35/111/115 | -       |
| 22  | CLA  | B     | 609 | 2    | -       | 2/39/115/115  | -       |
| 25  | LMG  | d     | 409 | -    | -       | 28/42/62/70   | 0/1/1/1 |
| 24  | BCR  | C     | 515 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 612 | 2    | -       | 11/39/115/115 | -       |
| 26  | PL9  | d     | 405 | -    | -       | 6/53/73/73    | 0/1/1/1 |
| 25  | LMG  | c     | 930 | -    | -       | 12/44/64/70   | 0/1/1/1 |
| 22  | CLA  | B     | 606 | 2    | -       | 11/39/115/115 | -       |
| 22  | CLA  | C     | 503 | 3    | -       | 9/39/115/115  | -       |
| 22  | CLA  | C     | 507 | 3    | -       | 11/39/115/115 | -       |
| 35  | DGD  | c     | 917 | -    | -       | 21/51/91/95   | 0/2/2/2 |
| 35  | DGD  | c     | 918 | -    | -       | 22/51/91/95   | 0/2/2/2 |
| 22  | CLA  | B     | 615 | 2    | -       | 11/25/101/115 | -       |
| 24  | BCR  | A     | 409 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 22  | CLA  | A     | 406 | 40   | -       | 5/27/103/115  | -       |
| 22  | CLA  | b     | 605 | 2    | -       | 11/39/115/115 | -       |
| 27  | LHG  | D     | 410 | -    | -       | 12/53/53/53   | -       |
| 22  | CLA  | c     | 906 | 3    | -       | 10/39/115/115 | -       |
| 34  | HTG  | C     | 532 | -    | -       | 7/10/30/30    | 0/1/1/1 |
| 35  | DGD  | h     | 102 | -    | -       | 18/51/91/95   | 0/2/2/2 |
| 22  | CLA  | c     | 912 | 3    | -       | 4/39/115/115  | -       |
| 22  | CLA  | b     | 612 | 2    | -       | 10/39/115/115 | -       |
| 25  | LMG  | C     | 531 | -    | -       | 14/35/55/70   | 0/1/1/1 |
| 24  | BCR  | C     | 516 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 34  | HTG  | B     | 623 | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 24  | BCR  | B     | 619 | -    | -       | 1/24/41/63    | 0/1/1/2 |
| 22  | CLA  | b     | 615 | 2    | -       | 6/24/100/115  | -       |
| 27  | LHG  | a     | 416 | -    | -       | 28/53/53/53   | -       |
| 23  | PHO  | a     | 410 | -    | -       | 1/37/103/103  | 0/5/6/6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 22  | CLA  | B     | 616 | 2    | -       | 12/39/115/115 | -       |
| 22  | CLA  | C     | 512 | 3    | -       | 1/39/115/115  | -       |
| 28  | SQD  | D     | 408 | -    | -       | 3/12/32/69    | 0/1/1/1 |
| 34  | HTG  | b     | 623 | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 34  | HTG  | C     | 521 | -    | -       | 4/10/30/30    | 0/1/1/1 |
| 24  | BCR  | y     | 101 | -    | -       | 5/29/63/63    | 0/2/2/2 |
| 25  | LMG  | A     | 410 | -    | -       | 28/46/66/70   | 0/1/1/1 |
| 34  | HTG  | D     | 414 | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 22  | CLA  | b     | 610 | 2    | -       | 3/39/115/115  | -       |
| 22  | CLA  | D     | 404 | 4    | -       | 13/39/115/115 | -       |
| 22  | CLA  | b     | 616 | 2    | -       | 9/39/115/115  | -       |
| 22  | CLA  | d     | 403 | 4    | -       | 10/39/115/115 | -       |
| 22  | CLA  | b     | 617 | 2    | -       | 8/33/109/115  | -       |
| 29  | LMT  | Z     | 101 | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 22  | CLA  | a     | 407 | 1    | -       | 7/39/115/115  | -       |
| 22  | CLA  | d     | 402 | 4    | -       | 10/39/115/115 | -       |
| 22  | CLA  | B     | 604 | 2    | -       | 7/39/115/115  | -       |
| 22  | CLA  | A     | 405 | 1    | -       | 7/39/115/115  | -       |
| 24  | BCR  | k     | 101 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 26  | PL9  | a     | 415 | -    | -       | 15/53/73/73   | 0/1/1/1 |
| 29  | LMT  | B     | 622 | -    | -       | 8/15/35/61    | 0/1/1/2 |
| 39  | HEC  | V     | 202 | 15   | 1/1/3/7 | 4/14/54/54    | -       |
| 22  | CLA  | C     | 502 | 3    | -       | 7/39/115/115  | -       |
| 22  | CLA  | c     | 903 | 3    | -       | 10/39/115/115 | -       |
| 27  | LHG  | D     | 409 | -    | -       | 15/53/53/53   | -       |
| 22  | CLA  | b     | 608 | 40   | -       | 16/39/115/115 | -       |
| 29  | LMT  | t     | 101 | -    | -       | 10/15/35/61   | 0/1/1/2 |
| 34  | HTG  | l     | 106 | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 34  | HTG  | B     | 627 | -    | -       | 7/10/30/30    | 0/1/1/1 |
| 27  | LHG  | d     | 401 | -    | -       | 15/34/34/53   | -       |
| 27  | LHG  | C     | 522 | -    | -       | 15/31/31/53   | -       |
| 25  | LMG  | j     | 101 | 38   | -       | 13/42/62/70   | 0/1/1/1 |
| 34  | HTG  | D     | 415 | -    | -       | 8/10/30/30    | 0/1/1/1 |
| 28  | SQD  | C     | 501 | -    | -       | 27/49/69/69   | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 23  | PHO  | a     | 411 | -    | -       | 6/37/103/103  | 0/5/6/6 |
| 27  | LHG  | D     | 411 | -    | -       | 12/49/49/53   | -       |
| 22  | CLA  | b     | 603 | 2    | -       | 3/39/115/115  | -       |
| 27  | LHG  | l     | 102 | -    | -       | 26/53/53/53   | -       |
| 28  | SQD  | l     | 101 | -    | -       | 32/49/69/69   | 0/1/1/1 |
| 22  | CLA  | b     | 602 | 40   | -       | 23/39/115/115 | -       |
| 37  | RRX  | H     | 101 | -    | -       | 1/29/65/65    | 0/2/2/2 |
| 37  | RRX  | h     | 101 | -    | -       | 8/29/65/65    | 0/2/2/2 |
| 22  | CLA  | B     | 605 | 2    | -       | 9/39/115/115  | -       |
| 23  | PHO  | A     | 407 | -    | -       | 2/37/103/103  | 0/5/6/6 |
| 22  | CLA  | C     | 506 | 3    | -       | 5/39/115/115  | -       |
| 22  | CLA  | b     | 607 | 2    | -       | 7/39/115/115  | -       |
| 25  | LMG  | c     | 920 | -    | -       | 21/46/66/70   | 0/1/1/1 |
| 35  | DGD  | d     | 406 | -    | -       | 30/44/44/95   | -       |
| 22  | CLA  | B     | 613 | 2    | -       | 4/39/115/115  | -       |
| 22  | CLA  | c     | 907 | 3    | -       | 11/39/115/115 | -       |
| 24  | BCR  | b     | 619 | -    | -       | 4/26/43/63    | 0/1/1/2 |
| 25  | LMG  | i     | 101 | -    | -       | 26/46/66/70   | 0/1/1/1 |
| 24  | BCR  | b     | 618 | -    | -       | 7/13/30/63    | 0/1/1/2 |
| 22  | CLA  | B     | 608 | 40   | -       | 7/39/115/115  | -       |
| 24  | BCR  | a     | 413 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | PL9  | A     | 411 | -    | -       | 12/53/73/73   | 0/1/1/1 |

The worst 5 of 1813 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 22  | b     | 602 | CLA  | MG-NA | 19.40 | 2.52        | 2.06     |
| 22  | B     | 606 | CLA  | MG-NA | 15.87 | 2.44        | 2.06     |
| 22  | b     | 617 | CLA  | MG-NA | 15.18 | 2.42        | 2.06     |
| 22  | c     | 912 | CLA  | MG-NA | 14.71 | 2.41        | 2.06     |
| 22  | B     | 602 | CLA  | MG-NA | 14.39 | 2.40        | 2.06     |

The worst 5 of 2614 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 22  | b     | 602 | CLA  | C4A-NA-C1A | 11.72 | 111.97      | 106.71   |
| 22  | C     | 506 | CLA  | C4A-NA-C1A | 11.20 | 111.74      | 106.71   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 22  | B     | 602 | CLA  | C4A-NA-C1A | 10.95 | 111.63      | 106.71   |
| 22  | c     | 912 | CLA  | C4A-NA-C1A | 10.35 | 111.36      | 106.71   |
| 22  | D     | 401 | CLA  | C2B-C1B-NB | 10.01 | 116.94      | 110.23   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 39  | V     | 202 | HEC  | NA   |
| 39  | v     | 202 | HEC  | NA   |

5 of 1800 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 408 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 602 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 602 | CLA  | O2A-C1-C2-C3    |
| 22  | B     | 602 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 606 | CLA  | C4B-C3B-CAB-CBB |

There are no ring outliers.

211 monomers are involved in 519 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 31  | V     | 201    | DMS  | 1       | 0            |
| 31  | v     | 201    | DMS  | 1       | 0            |
| 31  | O     | 311    | DMS  | 3       | 0            |
| 36  | E     | 102    | HEM  | 1       | 0            |
| 29  | a     | 419    | LMT  | 7       | 0            |
| 35  | C     | 518    | DGD  | 1       | 0            |
| 31  | B     | 630    | DMS  | 1       | 0            |
| 22  | c     | 910    | CLA  | 3       | 0            |
| 22  | B     | 603    | CLA  | 1       | 0            |
| 32  | A     | 421[B] | BCT  | 1       | 0            |
| 31  | c     | 939    | DMS  | 2       | 0            |
| 24  | b     | 620    | BCR  | 3       | 0            |
| 22  | C     | 504    | CLA  | 2       | 0            |
| 25  | J     | 101    | LMG  | 1       | 0            |
| 29  | A     | 414    | LMT  | 6       | 0            |
| 22  | B     | 611    | CLA  | 6       | 0            |
| 31  | c     | 935    | DMS  | 2       | 0            |
| 24  | D     | 405    | BCR  | 1       | 0            |
| 31  | A     | 419    | DMS  | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | b     | 633 | DMS  | 1       | 0            |
| 31  | O     | 310 | DMS  | 3       | 0            |
| 36  | e     | 101 | HEM  | 6       | 0            |
| 22  | c     | 904 | CLA  | 8       | 0            |
| 22  | b     | 614 | CLA  | 4       | 0            |
| 24  | Y     | 101 | BCR  | 2       | 0            |
| 31  | B     | 635 | DMS  | 1       | 0            |
| 22  | c     | 905 | CLA  | 2       | 0            |
| 22  | C     | 510 | CLA  | 2       | 0            |
| 31  | c     | 927 | DMS  | 1       | 0            |
| 28  | A     | 413 | SQD  | 2       | 0            |
| 28  | a     | 414 | SQD  | 6       | 0            |
| 31  | C     | 540 | DMS  | 1       | 0            |
| 31  | B     | 642 | DMS  | 1       | 0            |
| 31  | O     | 303 | DMS  | 4       | 0            |
| 25  | d     | 409 | LMG  | 4       | 0            |
| 31  | b     | 636 | DMS  | 1       | 0            |
| 35  | c     | 917 | DGD  | 3       | 0            |
| 35  | h     | 102 | DGD  | 2       | 0            |
| 22  | b     | 612 | CLA  | 2       | 0            |
| 31  | D     | 416 | DMS  | 3       | 0            |
| 31  | c     | 934 | DMS  | 2       | 0            |
| 24  | C     | 516 | BCR  | 1       | 0            |
| 34  | B     | 623 | HTG  | 3       | 0            |
| 24  | y     | 101 | BCR  | 3       | 0            |
| 25  | A     | 410 | LMG  | 2       | 0            |
| 31  | v     | 205 | DMS  | 2       | 0            |
| 22  | b     | 617 | CLA  | 2       | 0            |
| 22  | B     | 604 | CLA  | 1       | 0            |
| 29  | B     | 622 | LMT  | 3       | 0            |
| 23  | a     | 411 | PHO  | 8       | 0            |
| 31  | c     | 929 | DMS  | 2       | 0            |
| 22  | B     | 605 | CLA  | 1       | 0            |
| 25  | c     | 920 | LMG  | 1       | 0            |
| 22  | B     | 613 | CLA  | 1       | 0            |
| 31  | o     | 305 | DMS  | 3       | 0            |
| 27  | L     | 101 | LHG  | 7       | 0            |
| 22  | C     | 513 | CLA  | 5       | 0            |
| 25  | D     | 412 | LMG  | 5       | 0            |
| 22  | C     | 514 | CLA  | 5       | 0            |
| 31  | o     | 304 | DMS  | 4       | 0            |
| 24  | c     | 916 | BCR  | 6       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | C     | 508 | CLA  | 2       | 0            |
| 22  | a     | 412 | CLA  | 2       | 0            |
| 34  | b     | 627 | HTG  | 1       | 0            |
| 31  | c     | 937 | DMS  | 1       | 0            |
| 22  | b     | 609 | CLA  | 5       | 0            |
| 27  | d     | 407 | LHG  | 1       | 0            |
| 22  | C     | 505 | CLA  | 4       | 0            |
| 25  | C     | 520 | LMG  | 1       | 0            |
| 35  | H     | 102 | DGD  | 2       | 0            |
| 25  | b     | 622 | LMG  | 1       | 0            |
| 31  | V     | 206 | DMS  | 3       | 0            |
| 22  | c     | 911 | CLA  | 2       | 0            |
| 31  | c     | 933 | DMS  | 2       | 0            |
| 31  | u     | 203 | DMS  | 2       | 0            |
| 34  | b     | 632 | HTG  | 2       | 0            |
| 22  | c     | 908 | CLA  | 2       | 0            |
| 31  | v     | 206 | DMS  | 3       | 0            |
| 31  | o     | 302 | DMS  | 1       | 0            |
| 22  | B     | 612 | CLA  | 1       | 0            |
| 26  | d     | 405 | PL9  | 5       | 0            |
| 25  | c     | 930 | LMG  | 3       | 0            |
| 24  | A     | 409 | BCR  | 1       | 0            |
| 31  | U     | 203 | DMS  | 1       | 0            |
| 31  | b     | 638 | DMS  | 9       | 0            |
| 27  | a     | 416 | LHG  | 1       | 0            |
| 34  | b     | 623 | HTG  | 3       | 0            |
| 31  | V     | 212 | DMS  | 11      | 0            |
| 31  | v     | 210 | DMS  | 2       | 0            |
| 31  | u     | 205 | DMS  | 5       | 0            |
| 22  | b     | 610 | CLA  | 4       | 0            |
| 22  | d     | 402 | CLA  | 2       | 0            |
| 22  | A     | 405 | CLA  | 4       | 0            |
| 29  | t     | 101 | LMT  | 2       | 0            |
| 22  | b     | 608 | CLA  | 7       | 0            |
| 34  | D     | 415 | HTG  | 9       | 0            |
| 25  | j     | 101 | LMG  | 2       | 0            |
| 28  | C     | 501 | SQD  | 6       | 0            |
| 22  | b     | 603 | CLA  | 2       | 0            |
| 28  | l     | 101 | SQD  | 1       | 0            |
| 25  | i     | 101 | LMG  | 3       | 0            |
| 31  | C     | 536 | DMS  | 1       | 0            |
| 24  | b     | 618 | BCR  | 7       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | d     | 404 | BCR  | 2       | 0            |
| 31  | B     | 641 | DMS  | 1       | 0            |
| 27  | d     | 408 | LHG  | 5       | 0            |
| 22  | D     | 403 | CLA  | 1       | 0            |
| 31  | B     | 629 | DMS  | 1       | 0            |
| 22  | B     | 607 | CLA  | 5       | 0            |
| 22  | a     | 408 | CLA  | 4       | 0            |
| 22  | b     | 606 | CLA  | 5       | 0            |
| 28  | b     | 621 | SQD  | 2       | 0            |
| 22  | b     | 604 | CLA  | 1       | 0            |
| 29  | c     | 931 | LMT  | 1       | 0            |
| 22  | c     | 902 | CLA  | 4       | 0            |
| 24  | c     | 915 | BCR  | 2       | 0            |
| 31  | u     | 202 | DMS  | 2       | 0            |
| 27  | a     | 423 | LHG  | 6       | 0            |
| 31  | O     | 306 | DMS  | 2       | 0            |
| 25  | B     | 621 | LMG  | 3       | 0            |
| 35  | c     | 919 | DGD  | 4       | 0            |
| 31  | i     | 106 | DMS  | 1       | 0            |
| 22  | D     | 401 | CLA  | 4       | 0            |
| 31  | f     | 103 | DMS  | 4       | 0            |
| 31  | o     | 307 | DMS  | 1       | 0            |
| 22  | A     | 408 | CLA  | 3       | 0            |
| 22  | a     | 409 | CLA  | 3       | 0            |
| 35  | c     | 918 | DGD  | 3       | 0            |
| 22  | b     | 605 | CLA  | 2       | 0            |
| 34  | C     | 532 | HTG  | 1       | 0            |
| 22  | c     | 906 | CLA  | 2       | 0            |
| 22  | c     | 912 | CLA  | 4       | 0            |
| 25  | C     | 531 | LMG  | 2       | 0            |
| 31  | A     | 420 | DMS  | 2       | 0            |
| 22  | b     | 615 | CLA  | 5       | 0            |
| 31  | c     | 925 | DMS  | 2       | 0            |
| 31  | B     | 638 | DMS  | 5       | 0            |
| 34  | C     | 521 | HTG  | 1       | 0            |
| 31  | c     | 942 | DMS  | 1       | 0            |
| 22  | b     | 616 | CLA  | 2       | 0            |
| 22  | d     | 403 | CLA  | 1       | 0            |
| 31  | b     | 630 | DMS  | 2       | 0            |
| 29  | Z     | 101 | LMT  | 1       | 0            |
| 22  | a     | 407 | CLA  | 2       | 0            |
| 27  | D     | 409 | LHG  | 7       | 0            |

*Continued on next page...*



*Continued from previous page...*

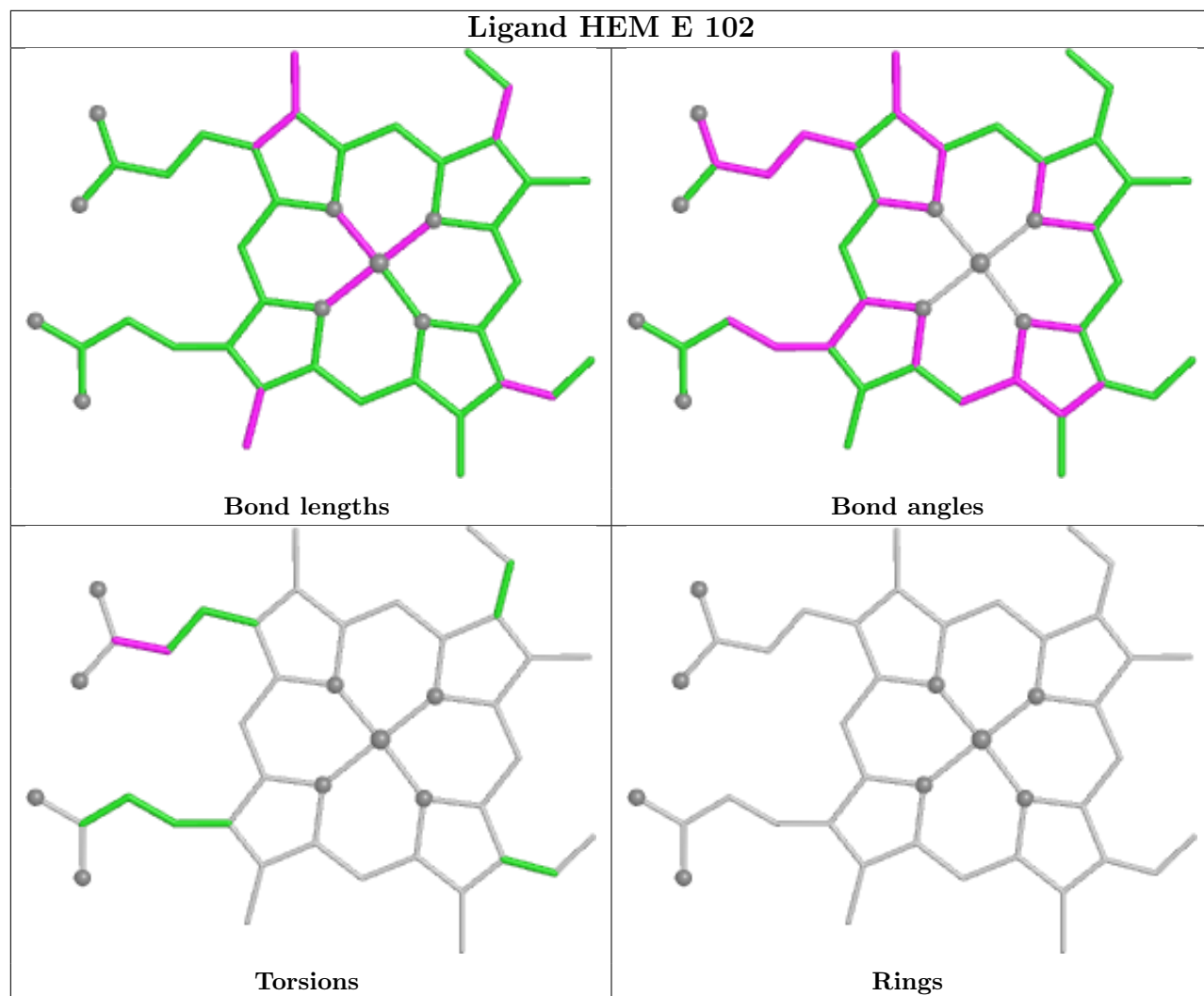
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 34  | l     | 106 | HTG  | 3       | 0            |
| 31  | c     | 924 | DMS  | 7       | 0            |
| 27  | D     | 411 | LHG  | 8       | 0            |
| 22  | b     | 602 | CLA  | 5       | 0            |
| 37  | H     | 101 | RRX  | 4       | 0            |
| 31  | a     | 401 | DMS  | 1       | 0            |
| 31  | d     | 411 | DMS  | 3       | 0            |
| 24  | b     | 619 | BCR  | 1       | 0            |
| 31  | B     | 633 | DMS  | 1       | 0            |
| 27  | l     | 102 | LHG  | 3       | 0            |
| 24  | a     | 413 | BCR  | 1       | 0            |
| 31  | V     | 205 | DMS  | 2       | 0            |
| 34  | b     | 626 | HTG  | 2       | 0            |
| 31  | o     | 303 | DMS  | 2       | 0            |
| 26  | D     | 406 | PL9  | 5       | 0            |
| 29  | T     | 102 | LMT  | 1       | 0            |
| 23  | D     | 402 | PHO  | 5       | 0            |
| 31  | O     | 312 | DMS  | 4       | 0            |
| 31  | V     | 207 | DMS  | 3       | 0            |
| 22  | C     | 511 | CLA  | 3       | 0            |
| 31  | B     | 631 | DMS  | 4       | 0            |
| 22  | C     | 509 | CLA  | 3       | 0            |
| 24  | B     | 620 | BCR  | 1       | 0            |
| 35  | C     | 519 | DGD  | 2       | 0            |
| 31  | b     | 629 | DMS  | 1       | 0            |
| 27  | A     | 412 | LHG  | 1       | 0            |
| 31  | B     | 628 | DMS  | 3       | 0            |
| 28  | f     | 101 | SQD  | 1       | 0            |
| 24  | B     | 618 | BCR  | 3       | 0            |
| 22  | B     | 614 | CLA  | 2       | 0            |
| 29  | E     | 101 | LMT  | 1       | 0            |
| 31  | O     | 304 | DMS  | 6       | 0            |
| 22  | B     | 610 | CLA  | 1       | 0            |
| 22  | c     | 913 | CLA  | 3       | 0            |
| 22  | c     | 909 | CLA  | 2       | 0            |
| 39  | v     | 202 | HEC  | 1       | 0            |
| 31  | C     | 530 | DMS  | 2       | 0            |
| 31  | o     | 308 | DMS  | 4       | 0            |
| 22  | c     | 914 | CLA  | 2       | 0            |
| 22  | b     | 611 | CLA  | 4       | 0            |
| 31  | B     | 636 | DMS  | 1       | 0            |
| 24  | C     | 515 | BCR  | 4       | 0            |

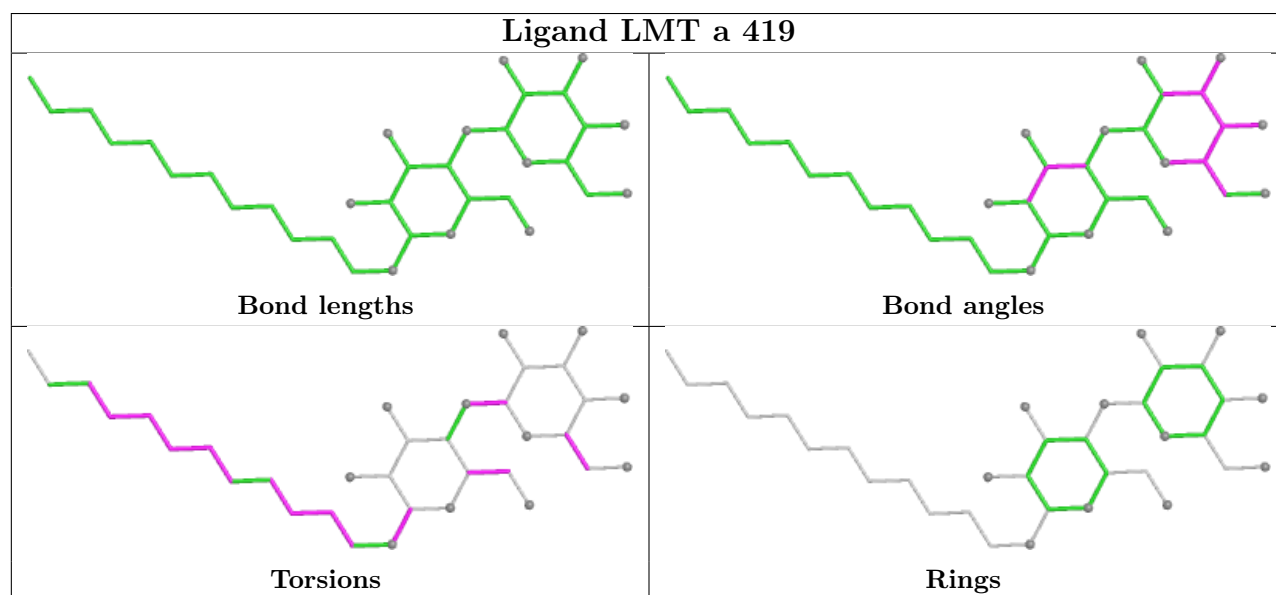
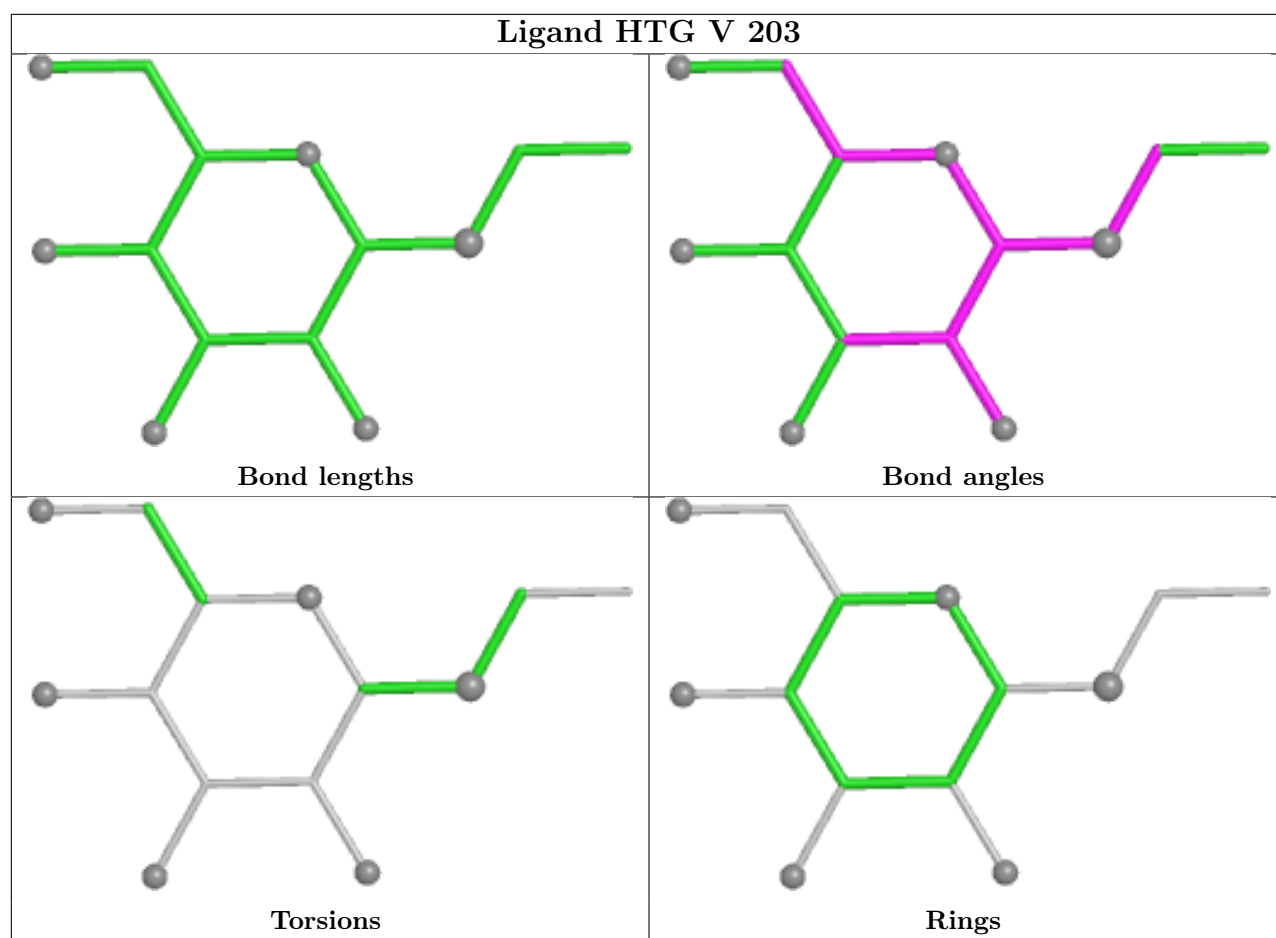
*Continued on next page...*

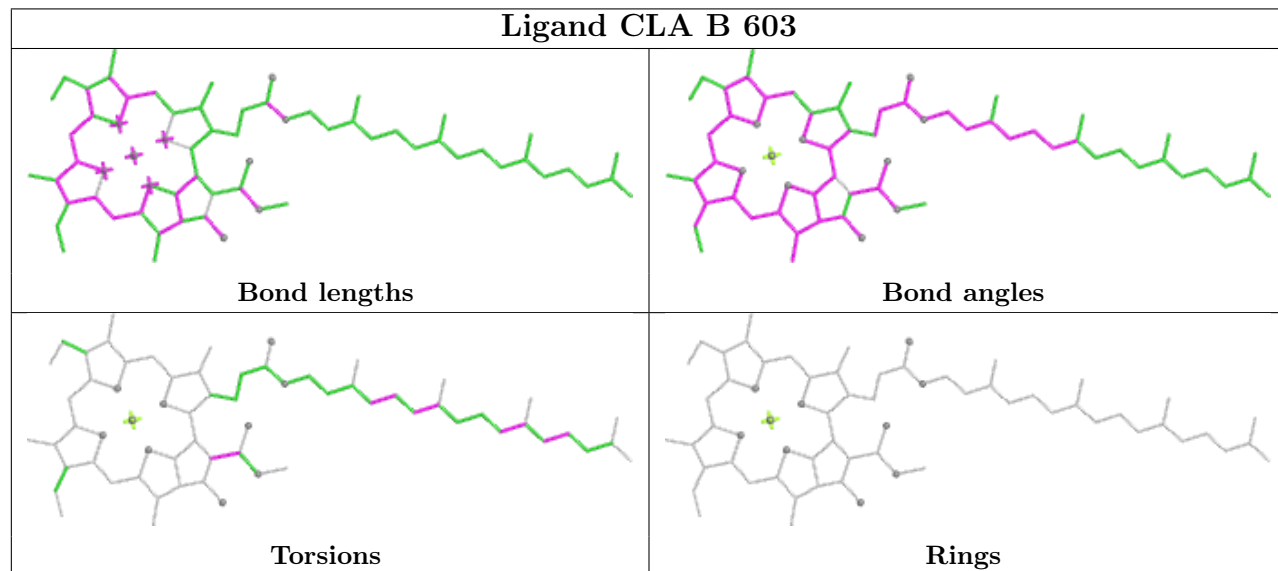
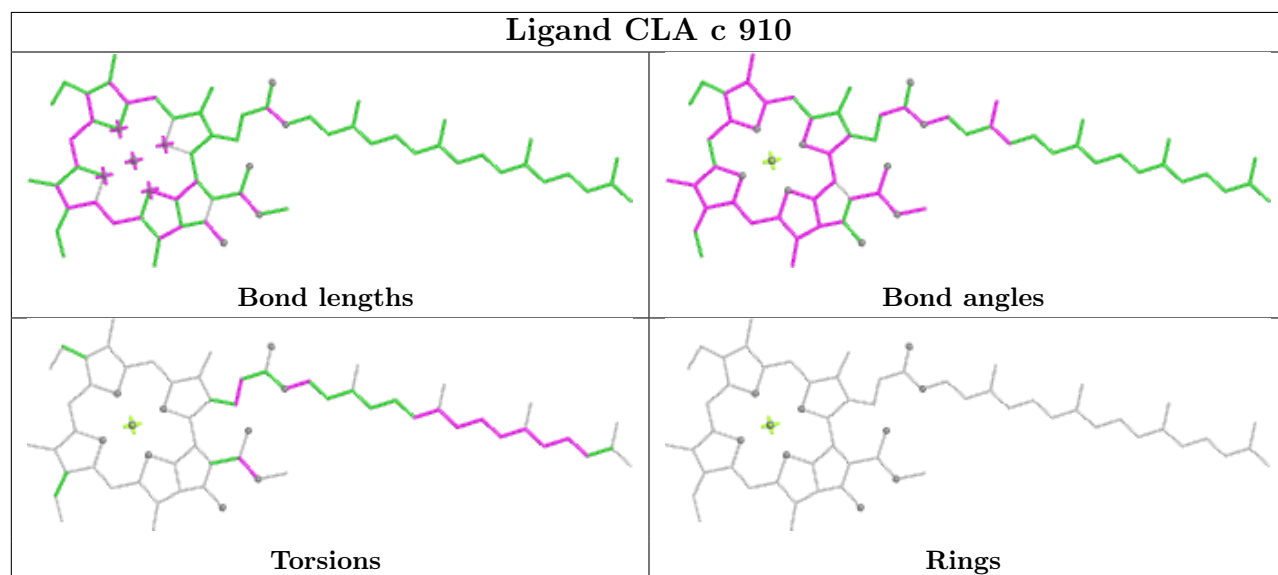
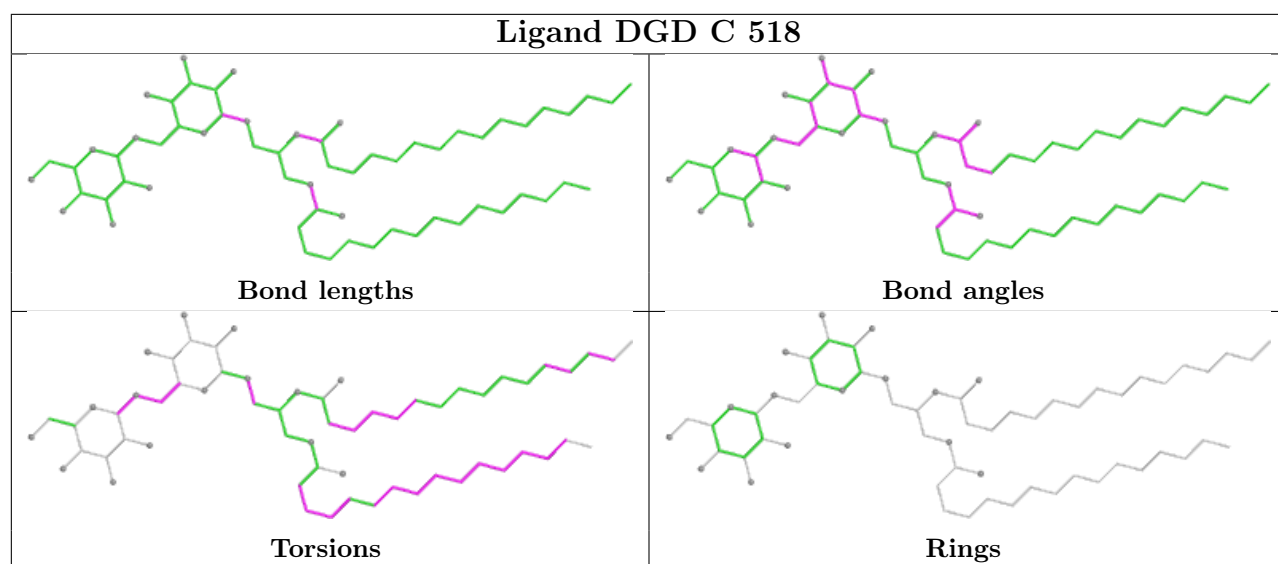
*Continued from previous page...*

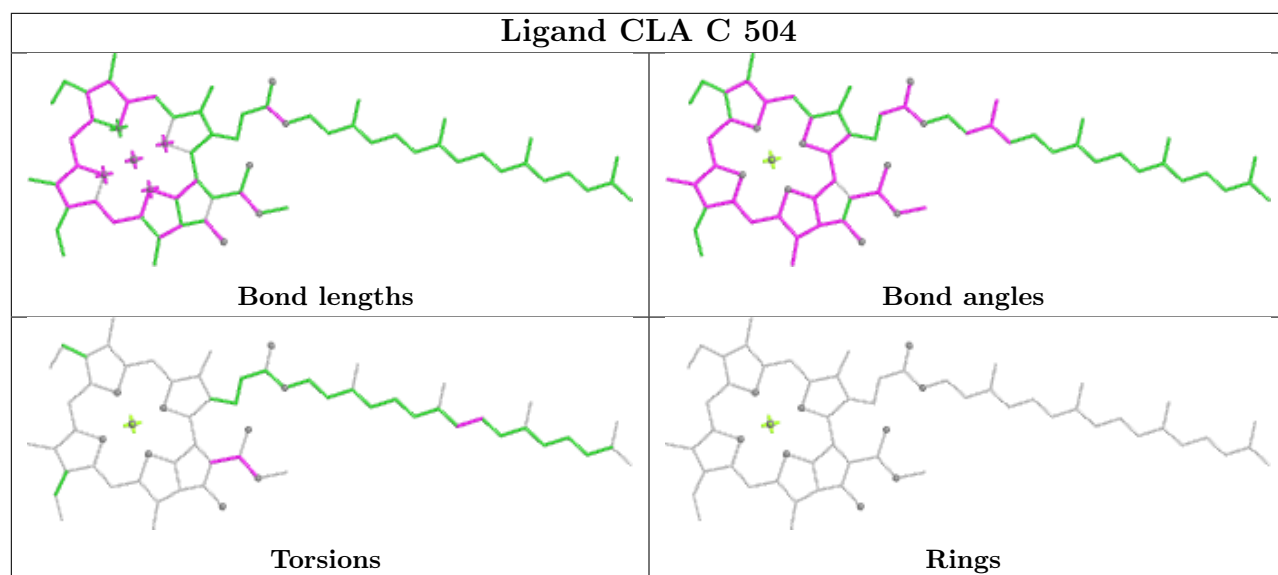
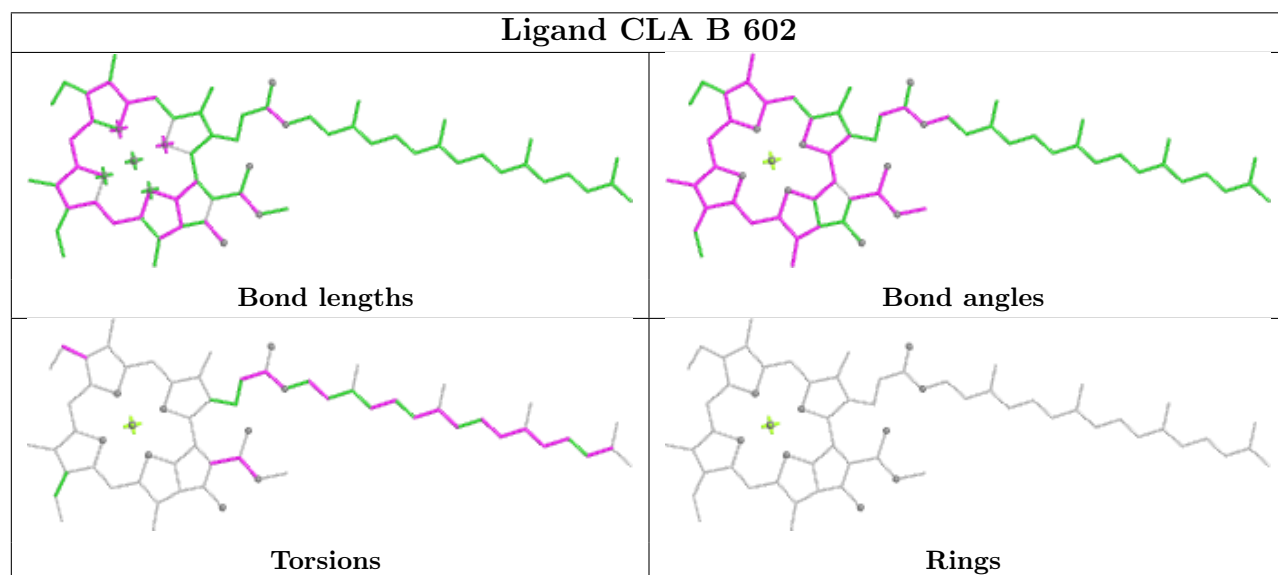
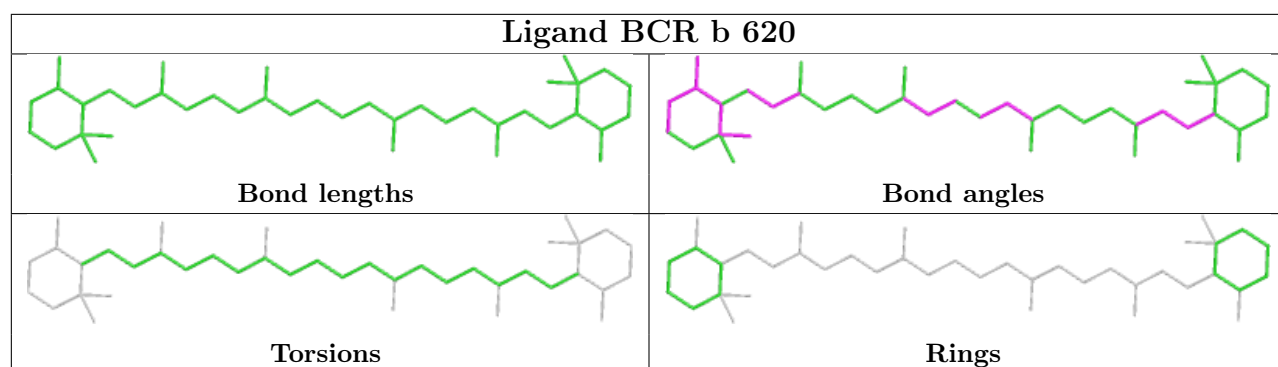
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | c     | 940 | DMS  | 2       | 0            |
| 31  | H     | 103 | DMS  | 1       | 0            |
| 31  | B     | 632 | DMS  | 1       | 0            |
| 22  | B     | 606 | CLA  | 7       | 0            |
| 31  | l     | 104 | DMS  | 1       | 0            |
| 22  | C     | 503 | CLA  | 5       | 0            |
| 22  | C     | 507 | CLA  | 5       | 0            |
| 22  | A     | 406 | CLA  | 3       | 0            |
| 27  | D     | 410 | LHG  | 3       | 0            |
| 23  | a     | 410 | PHO  | 2       | 0            |
| 31  | B     | 640 | DMS  | 1       | 0            |
| 34  | D     | 414 | HTG  | 2       | 0            |
| 31  | a     | 425 | DMS  | 7       | 0            |
| 24  | k     | 101 | BCR  | 2       | 0            |
| 26  | a     | 415 | PL9  | 10      | 0            |
| 31  | d     | 415 | DMS  | 5       | 0            |
| 22  | c     | 903 | CLA  | 3       | 0            |
| 27  | C     | 522 | LHG  | 1       | 0            |
| 37  | h     | 101 | RRX  | 8       | 0            |
| 22  | C     | 506 | CLA  | 1       | 0            |
| 31  | C     | 527 | DMS  | 2       | 0            |
| 22  | b     | 607 | CLA  | 1       | 0            |
| 22  | B     | 608 | CLA  | 6       | 0            |
| 26  | A     | 411 | PL9  | 10      | 0            |

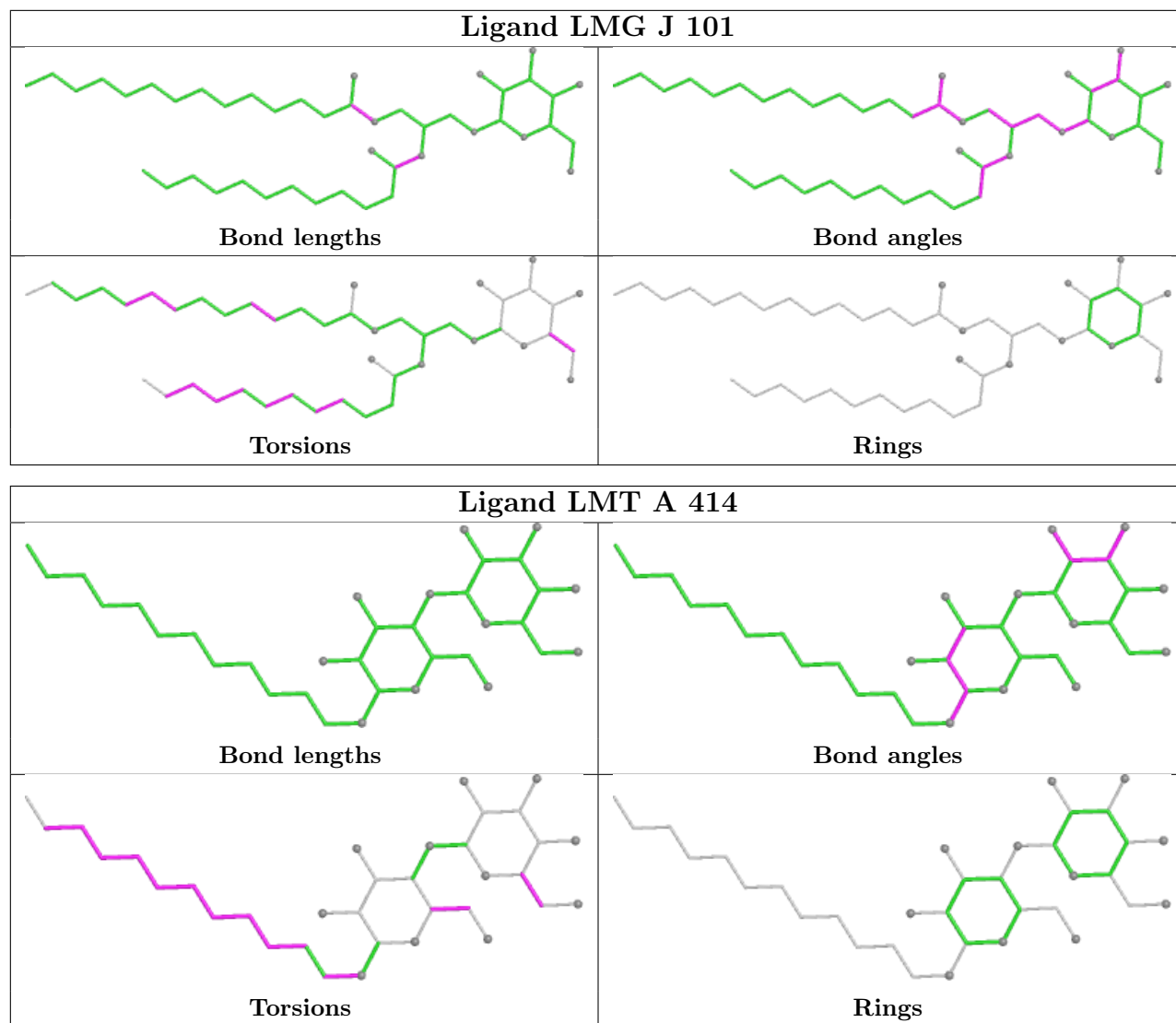
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



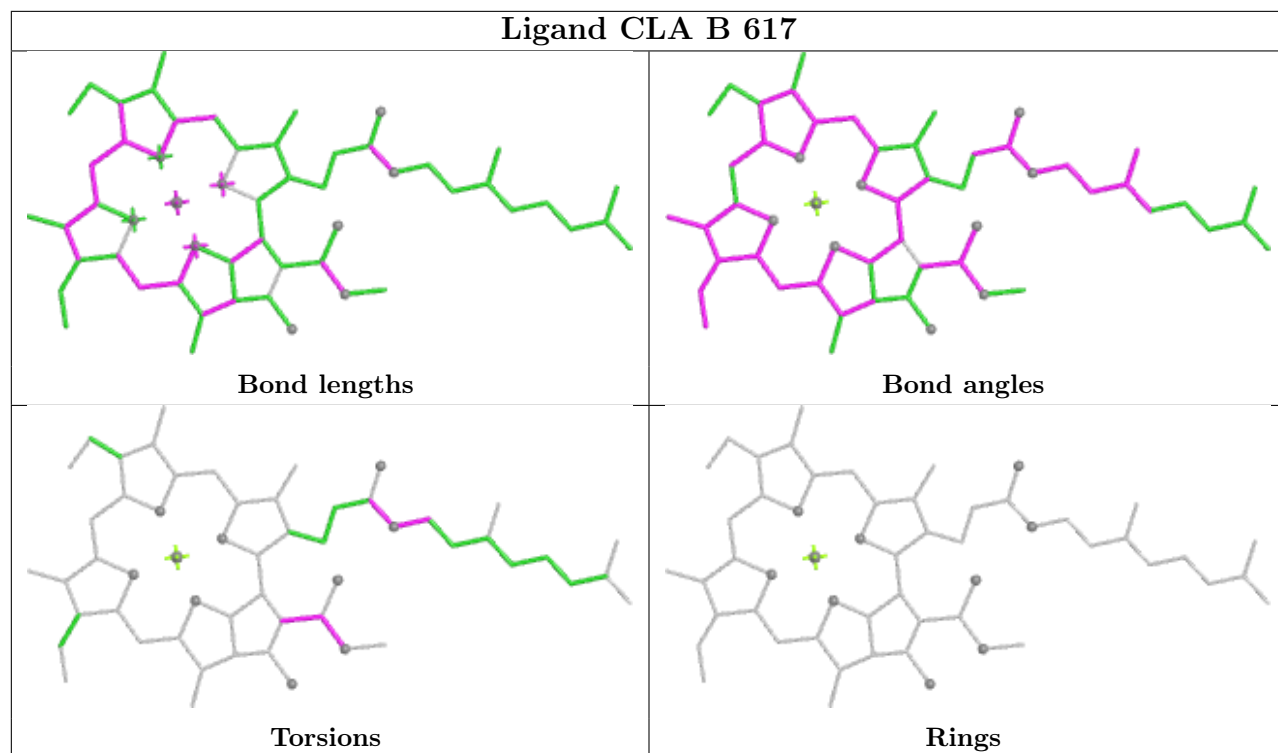




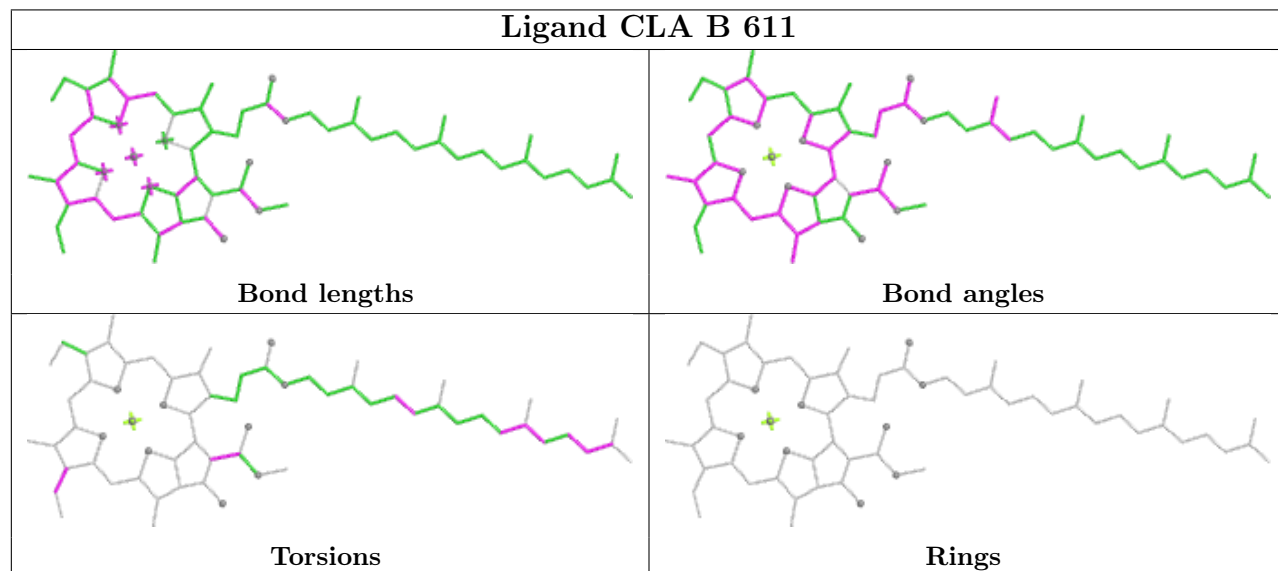




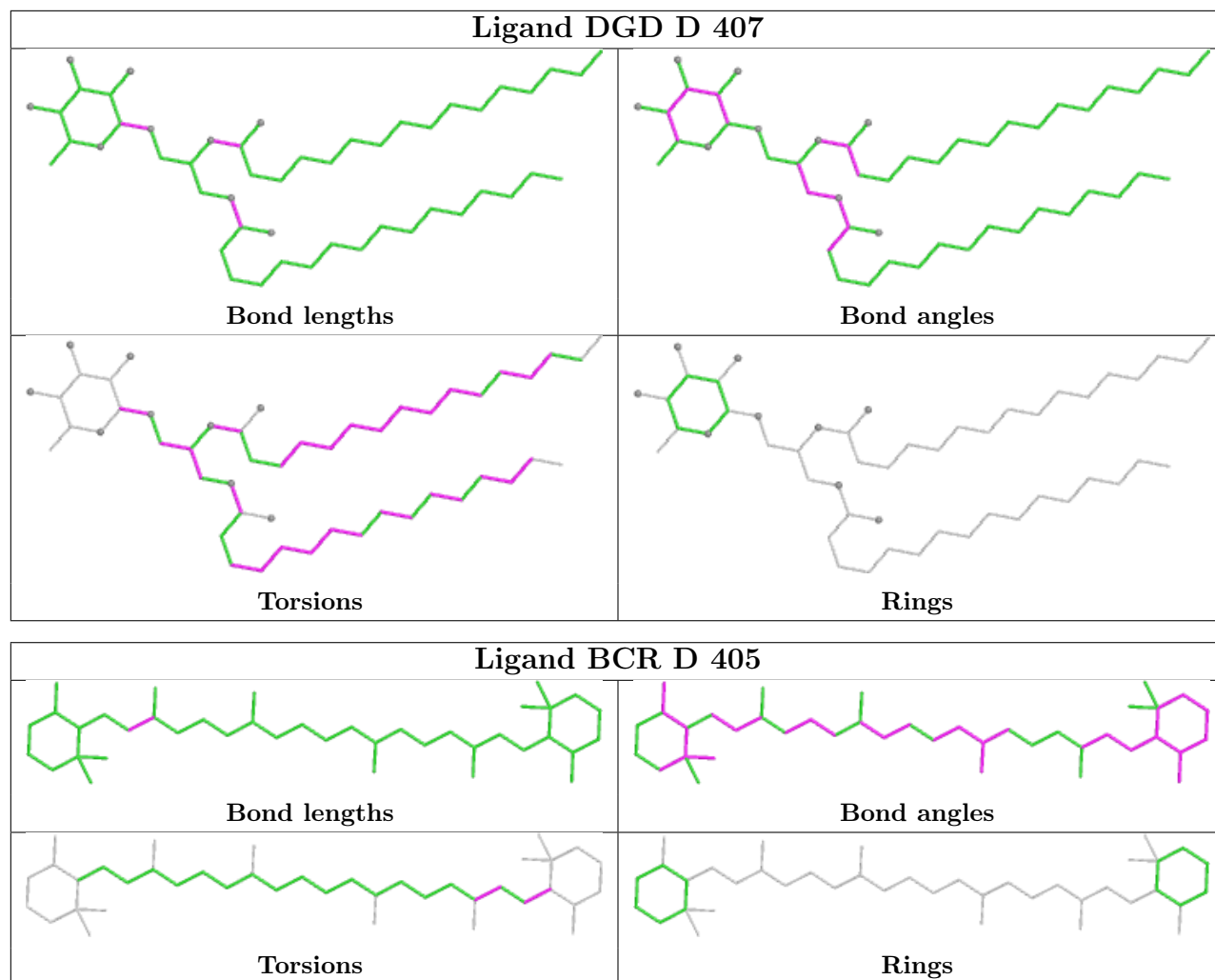
## Ligand CLA B 617



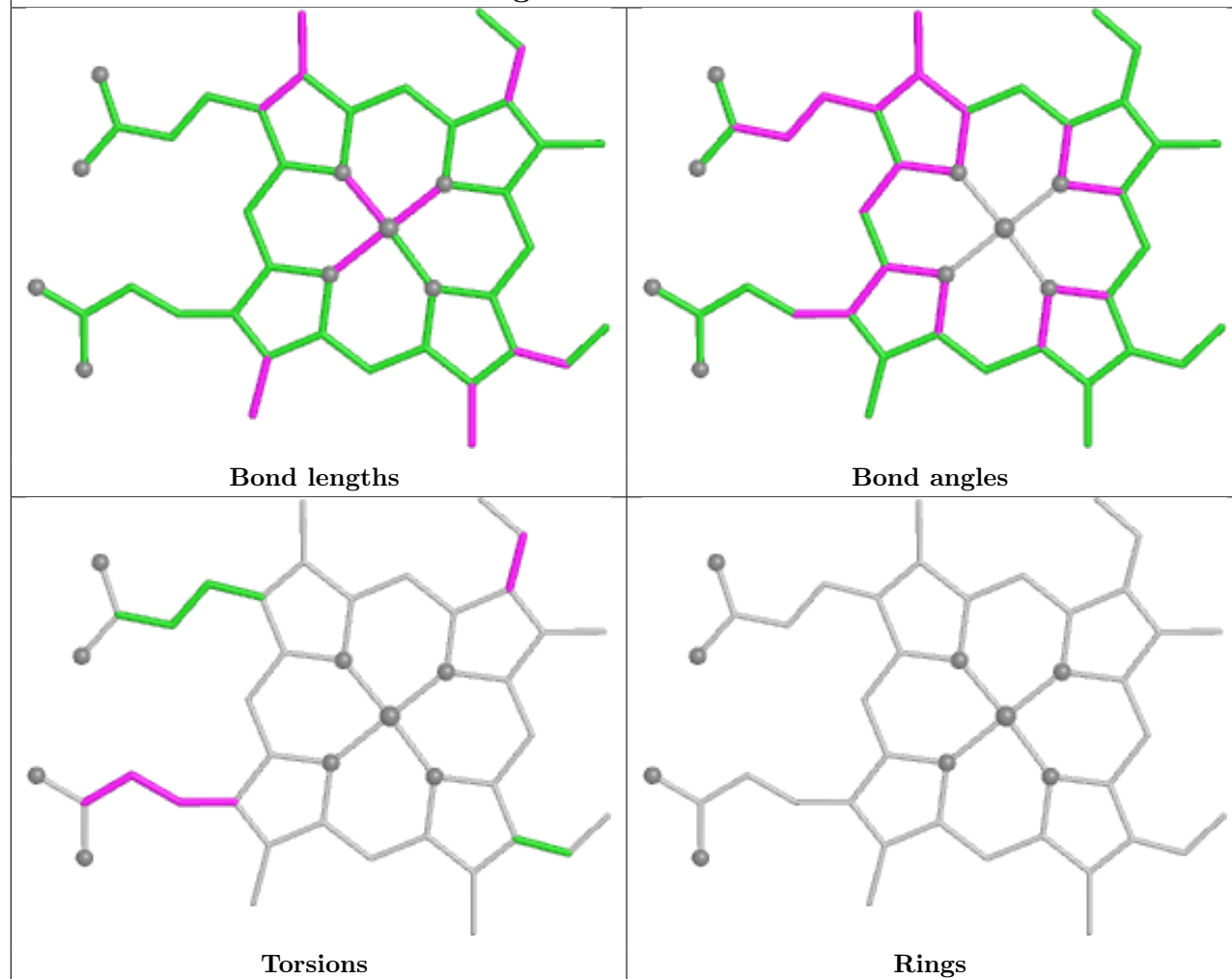
## Ligand CLA B 611



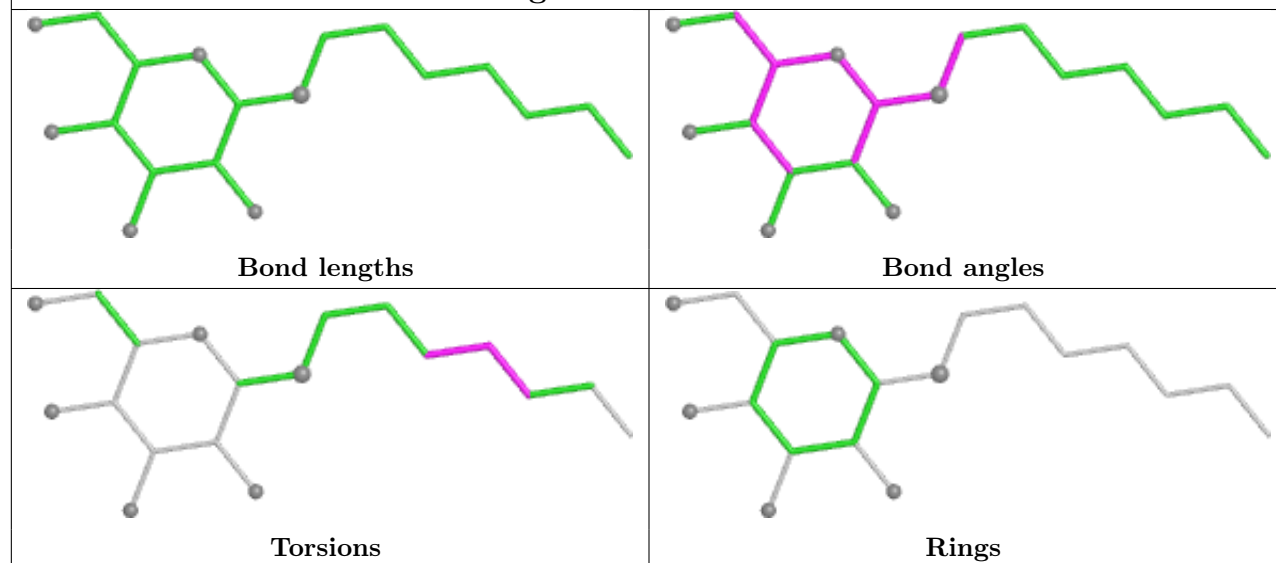


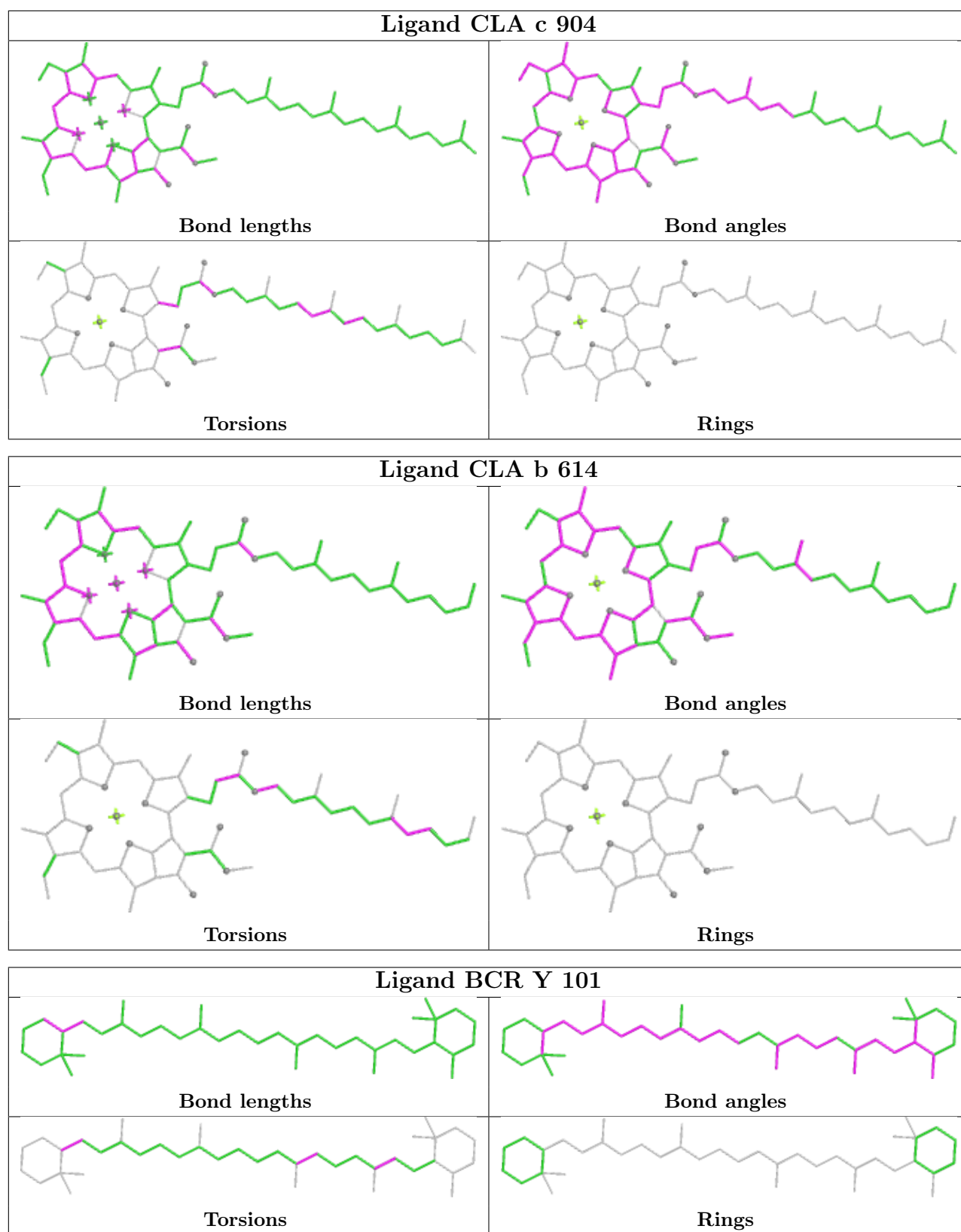


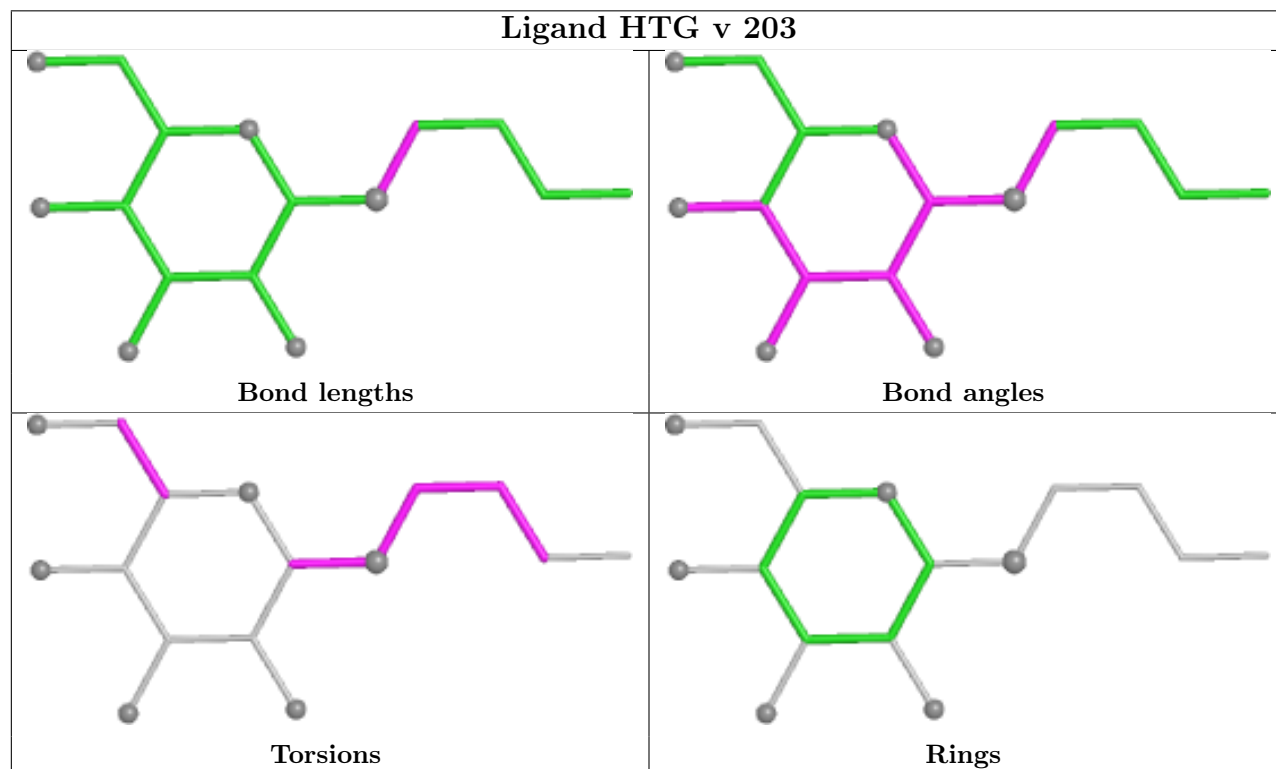
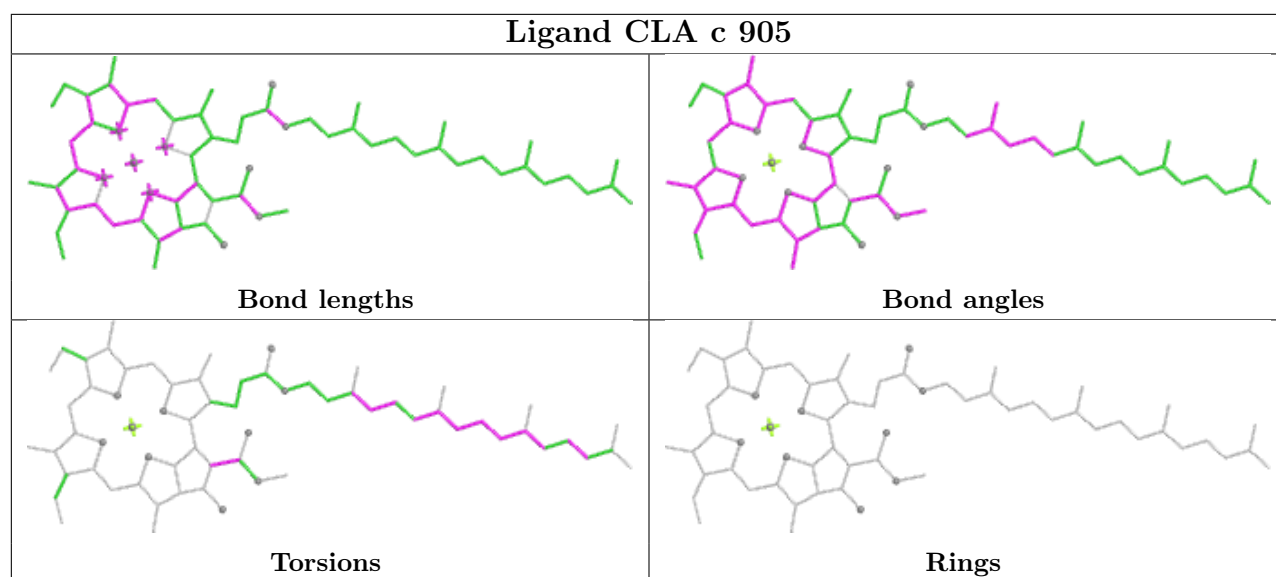
## Ligand HEM e 101

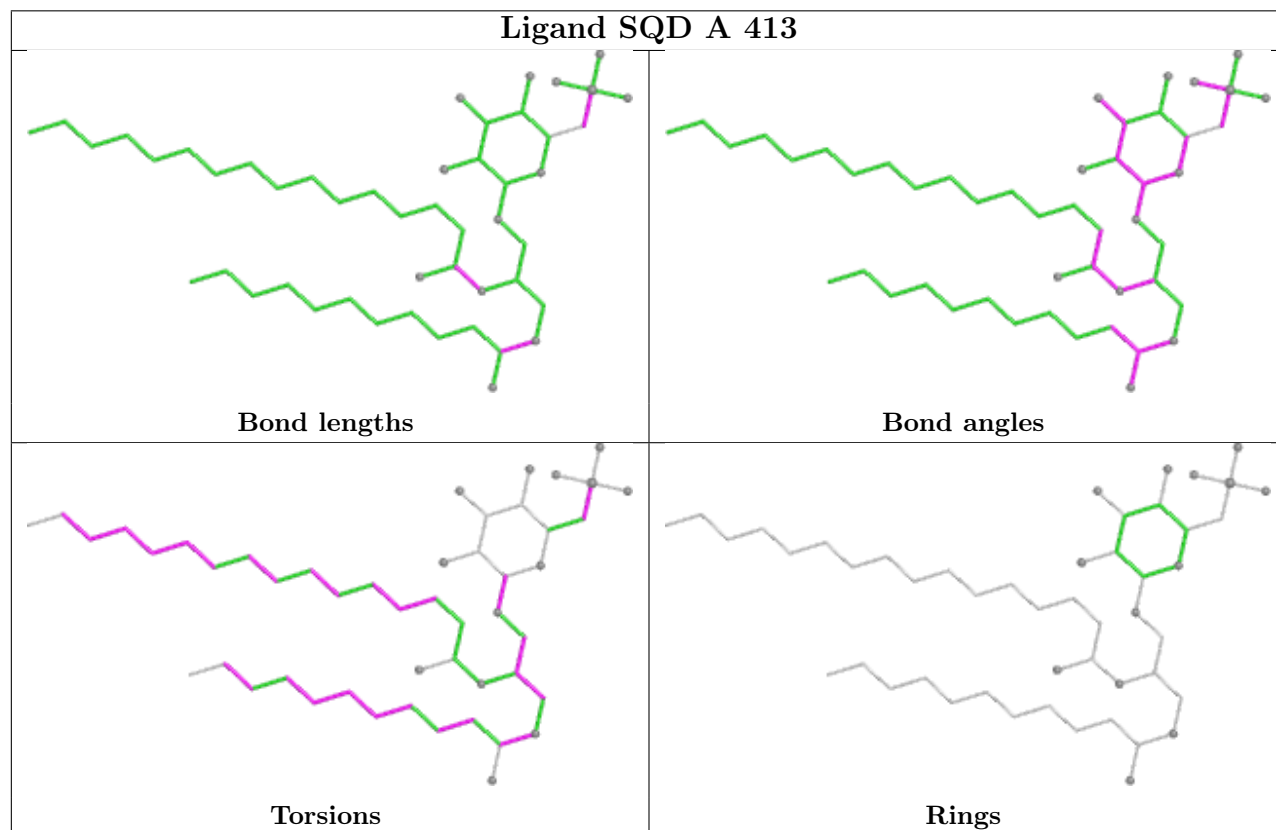
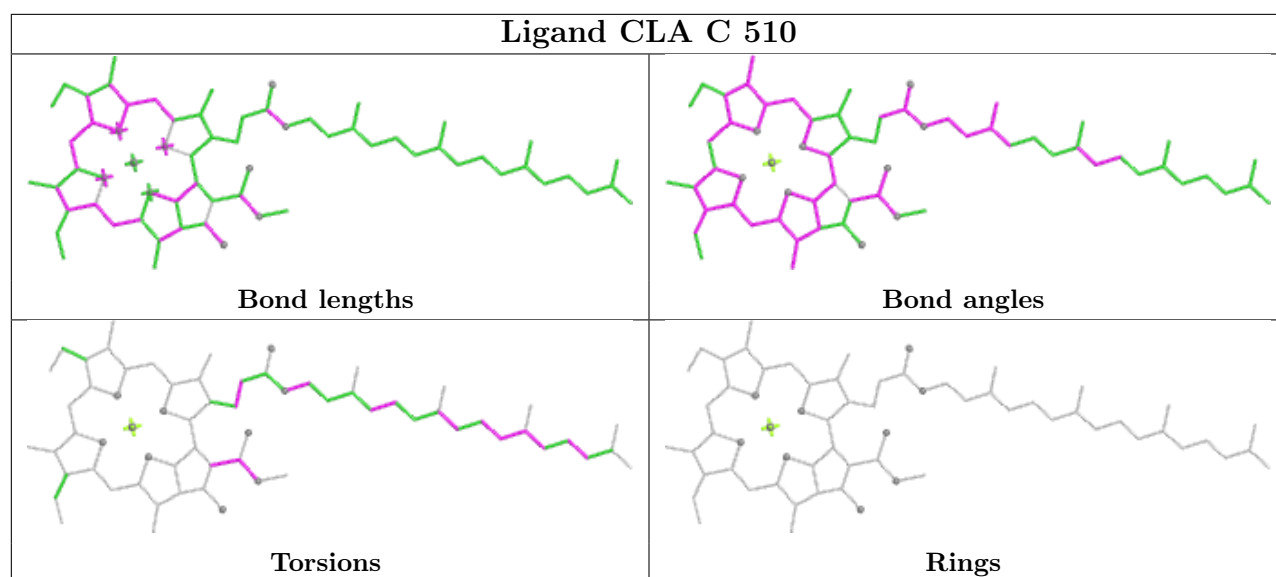


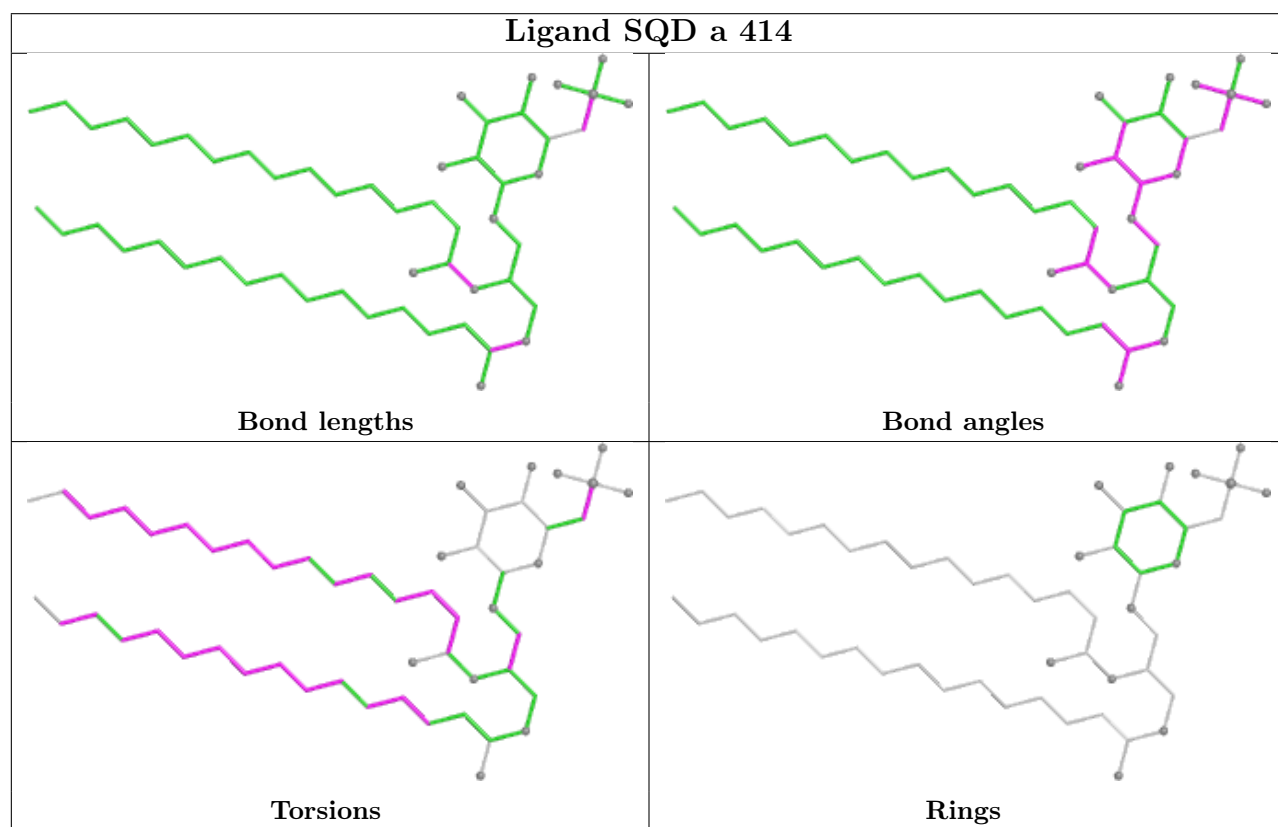
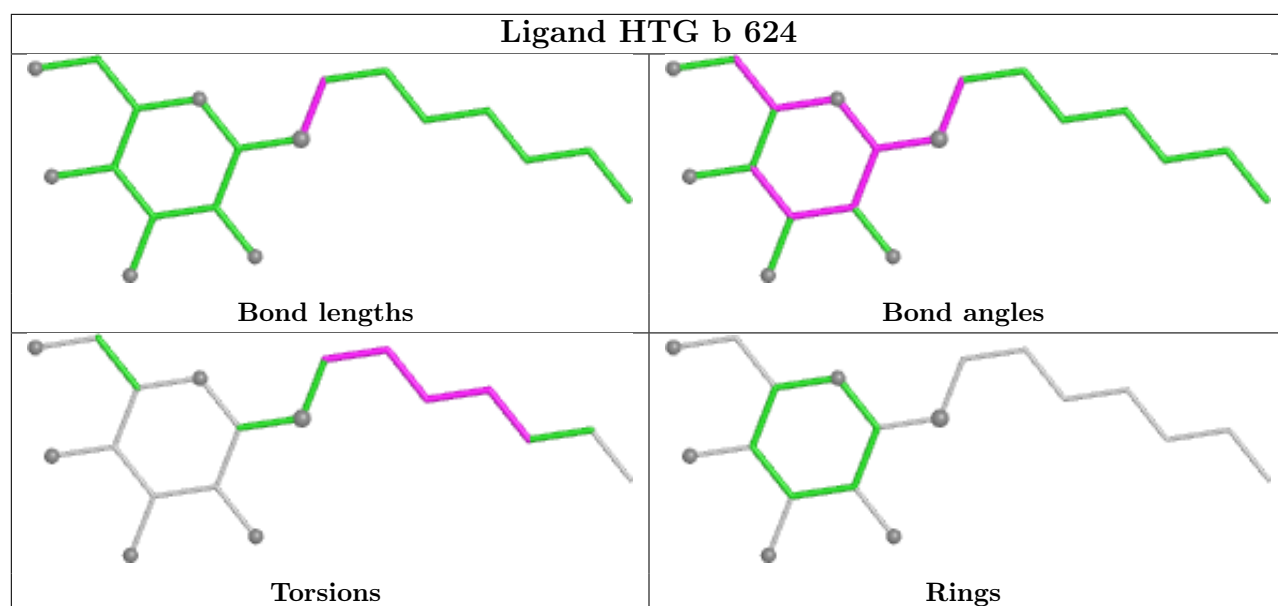
## Ligand HTG B 626

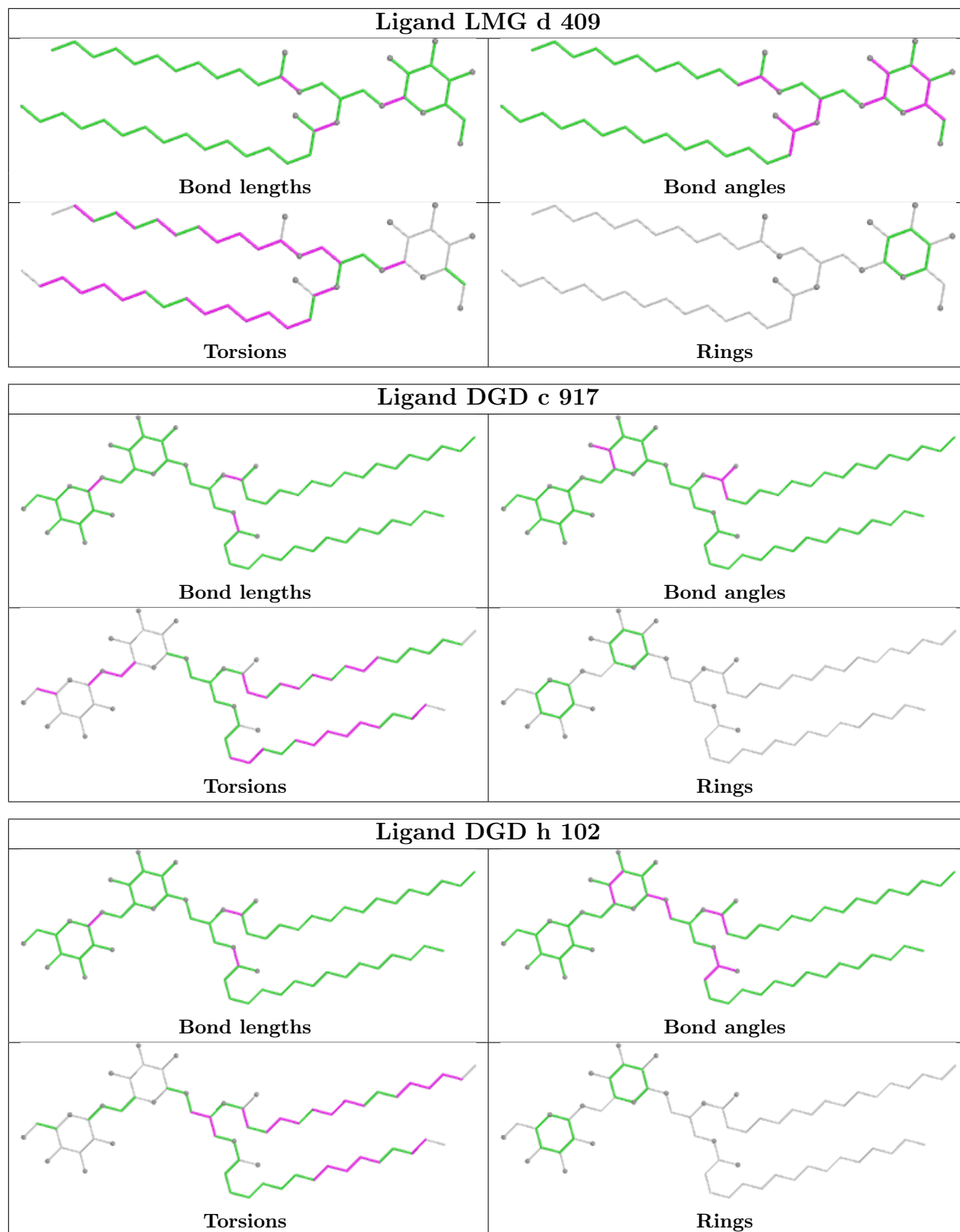


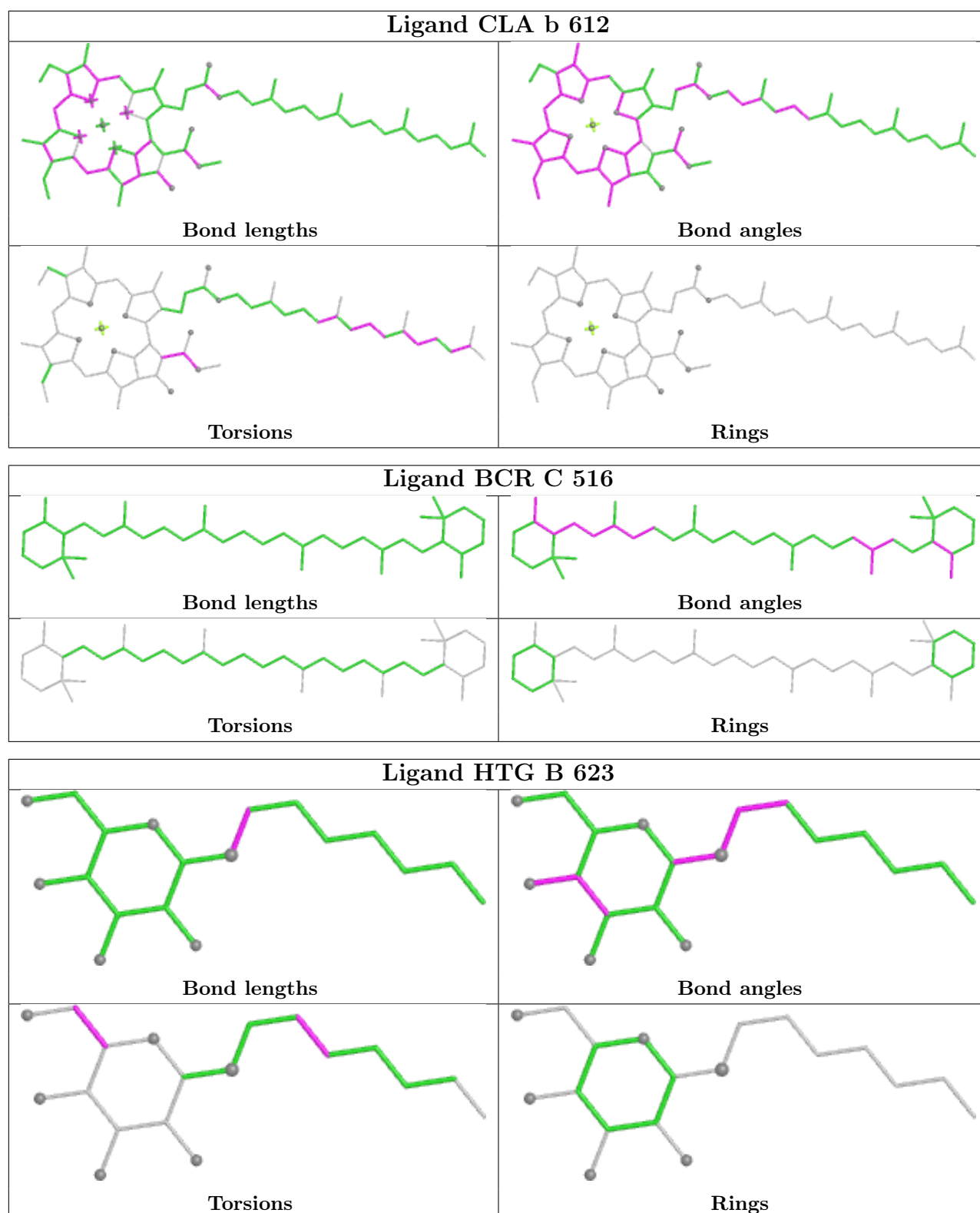




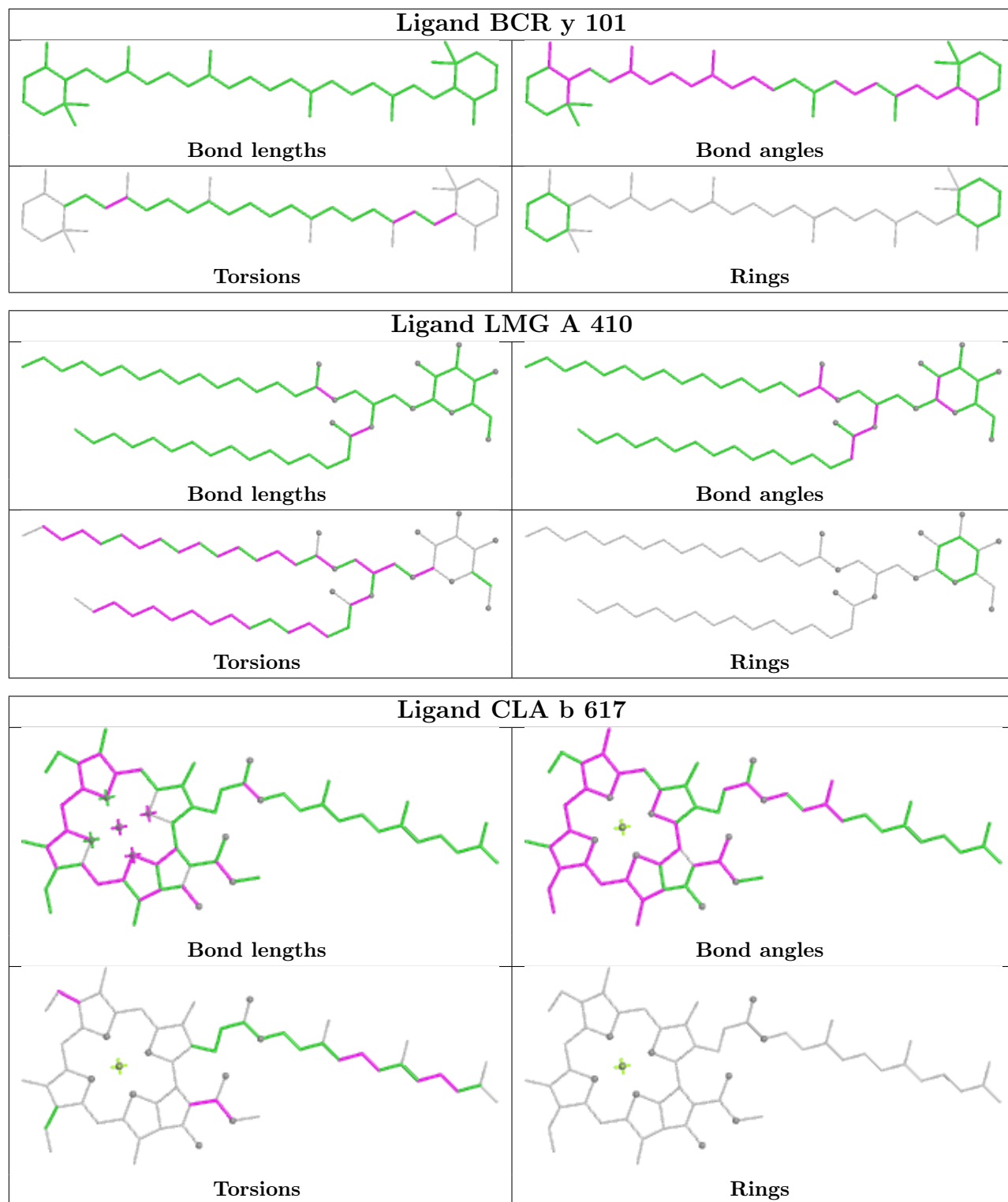


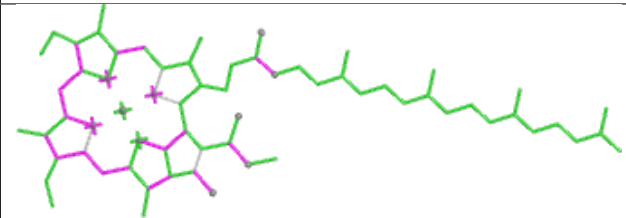
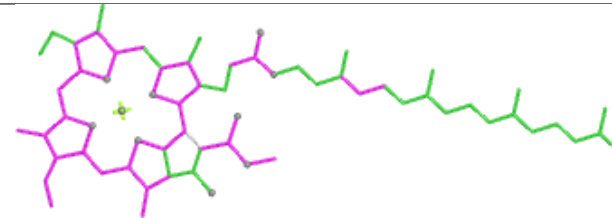
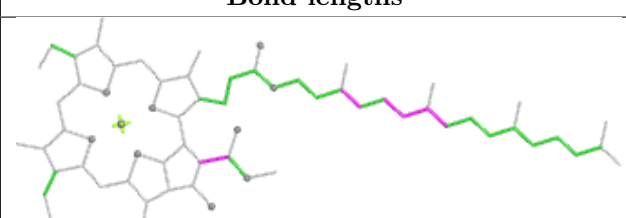
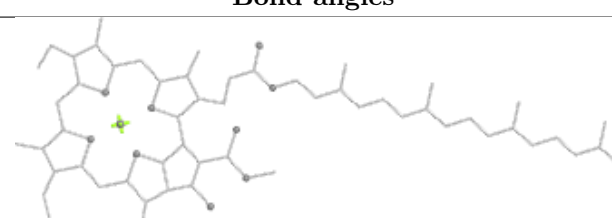


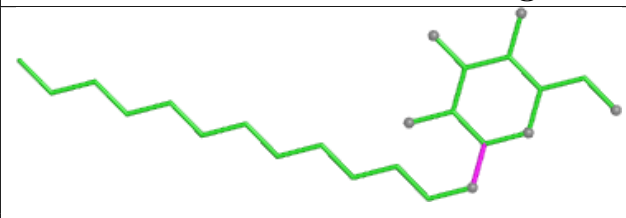
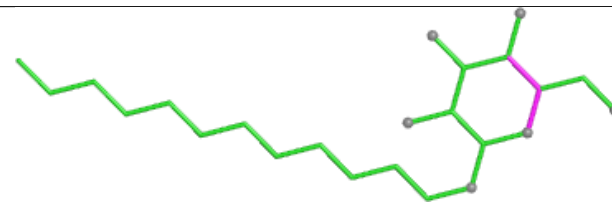
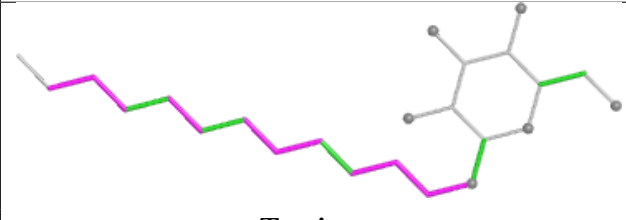
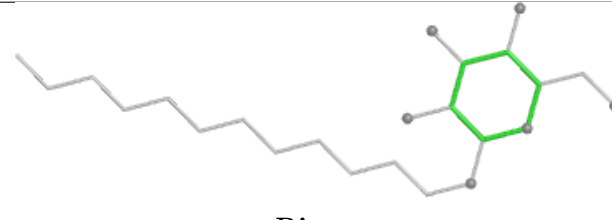


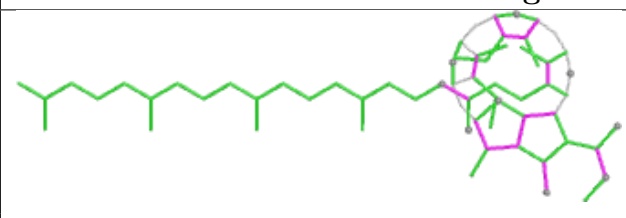
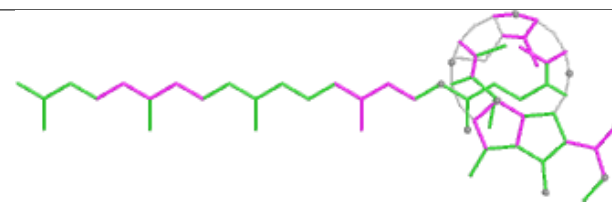
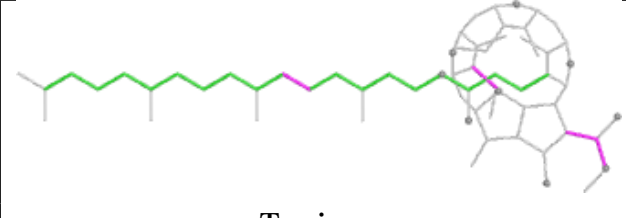
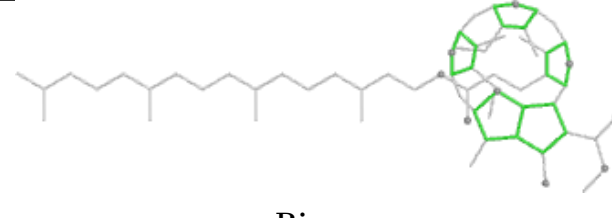


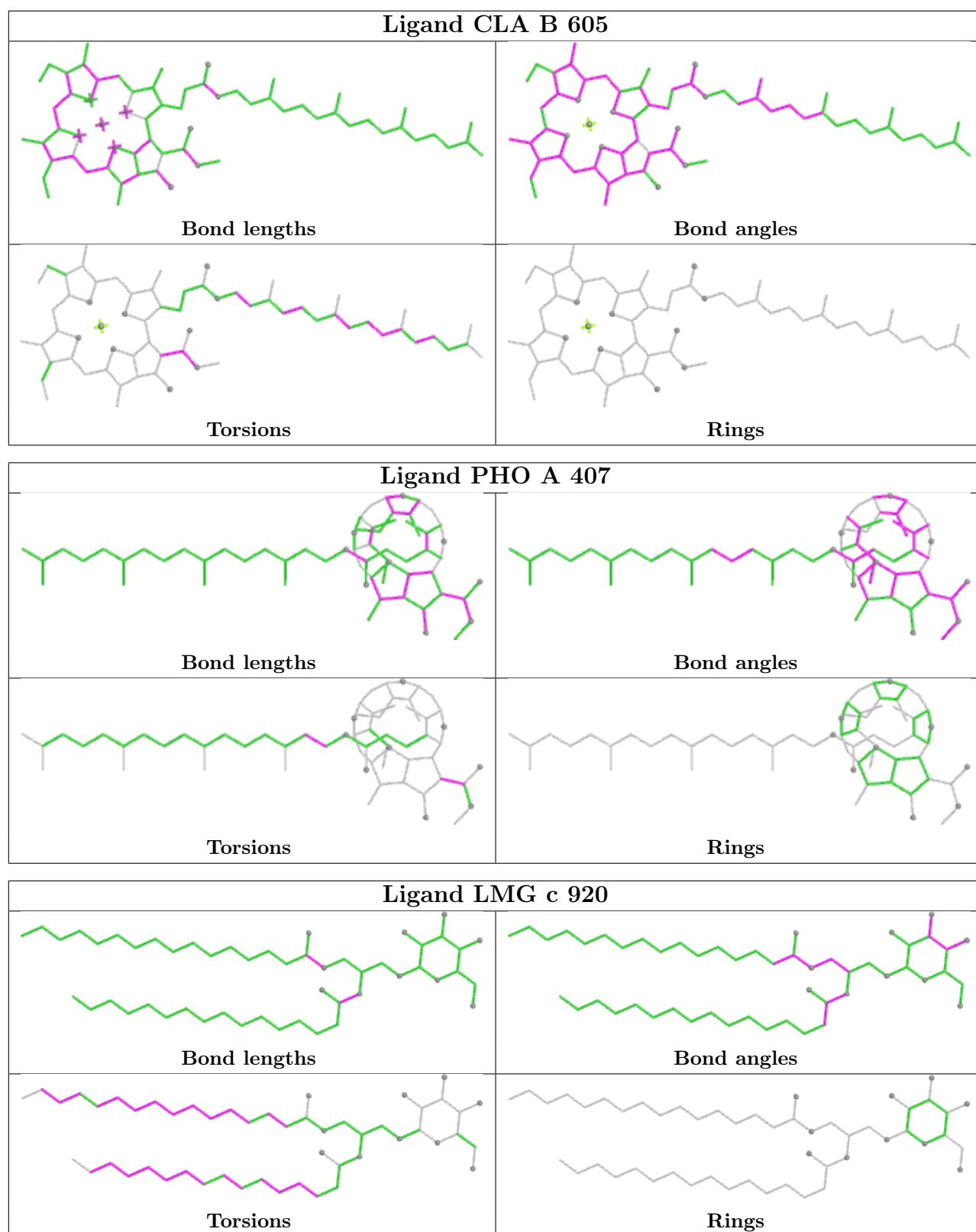


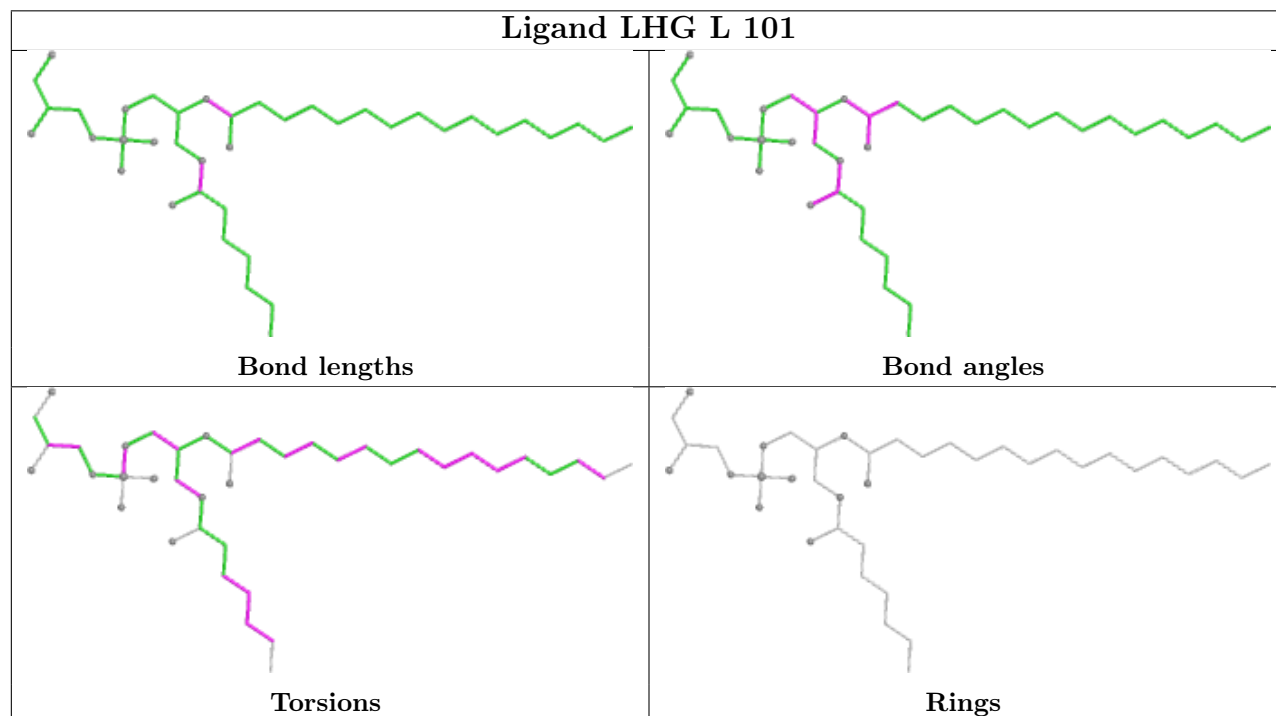
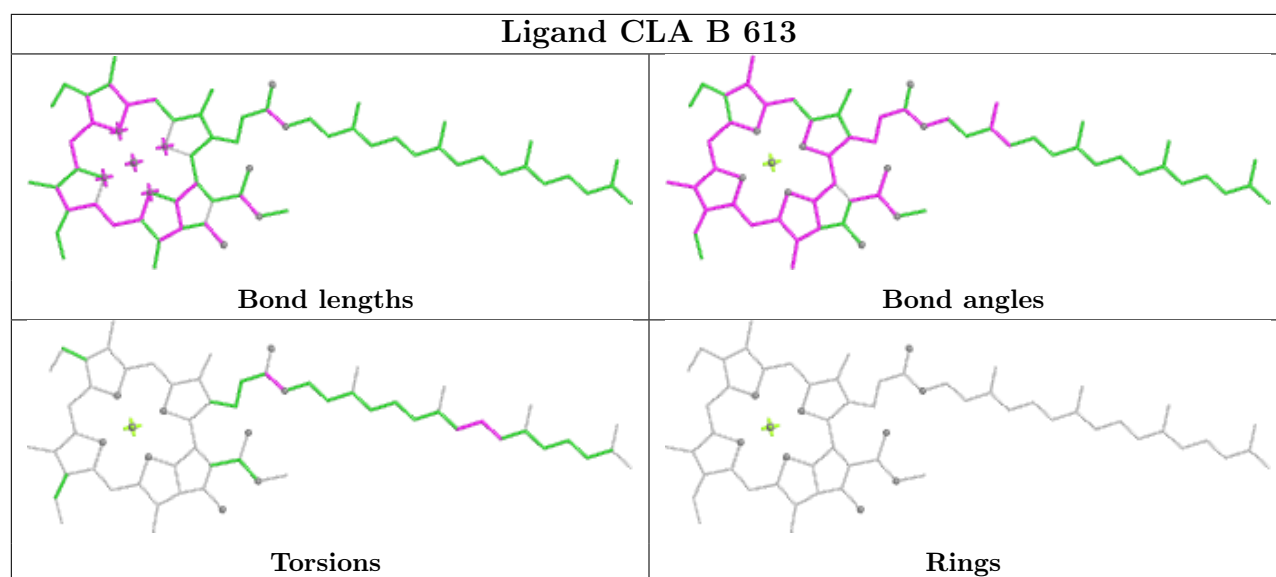


| Ligand CLA B 604                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

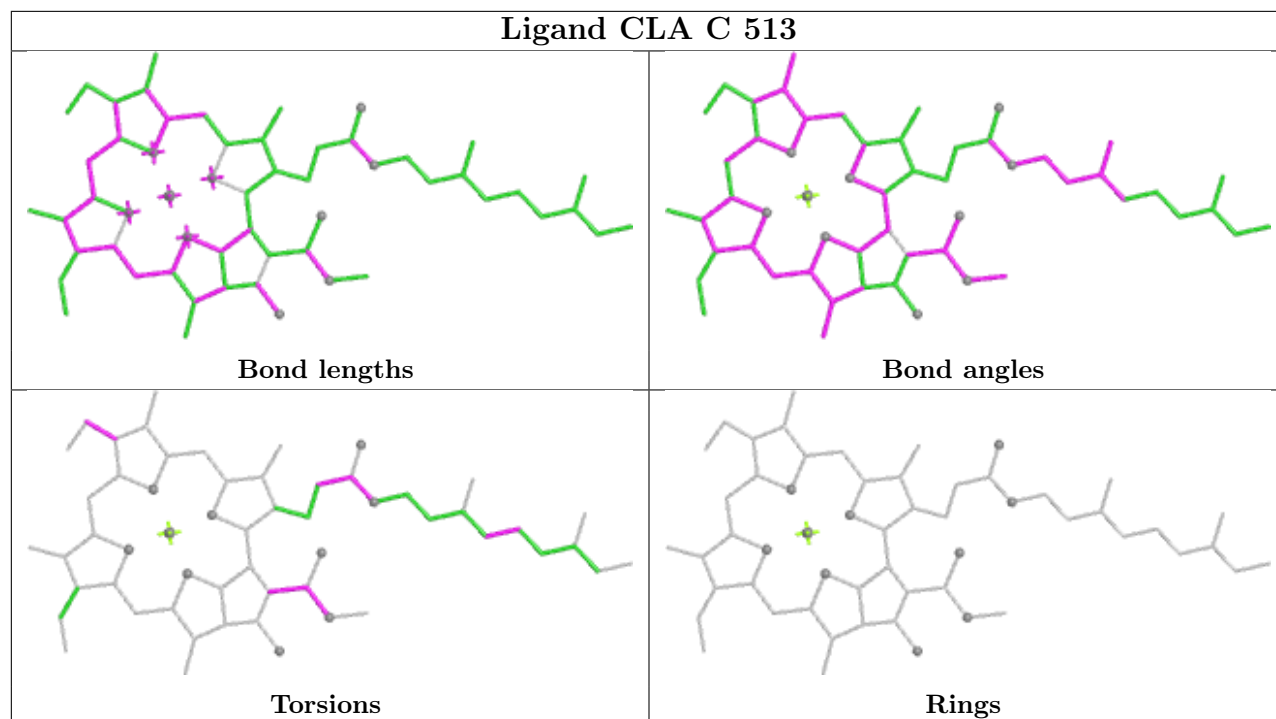
| Ligand LMT B 622                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand PHO a 411                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

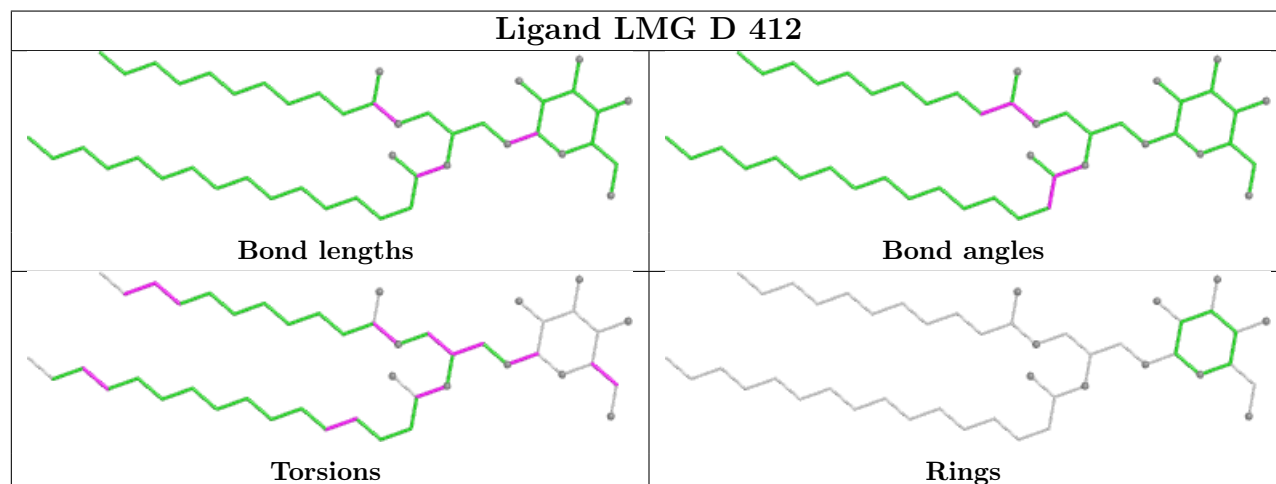




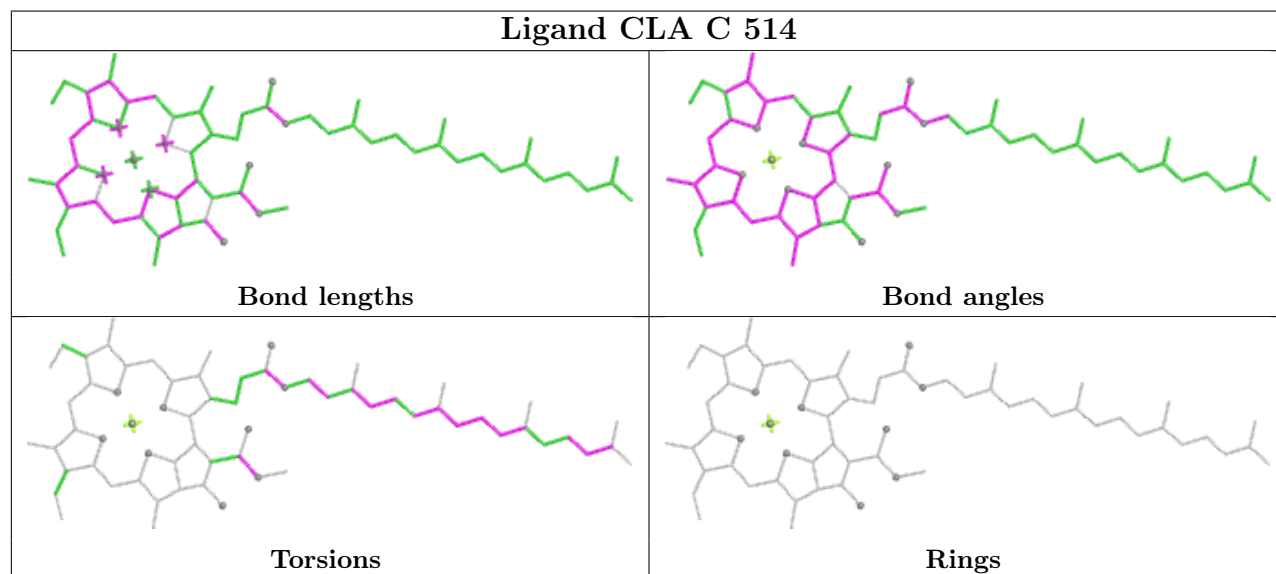
## Ligand CLA C 513

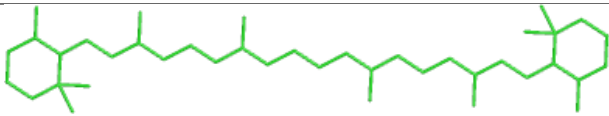
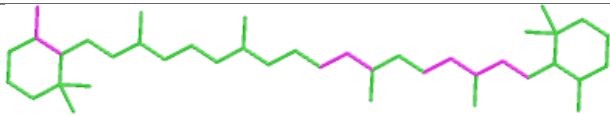
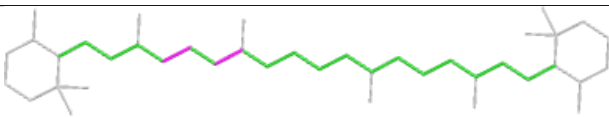
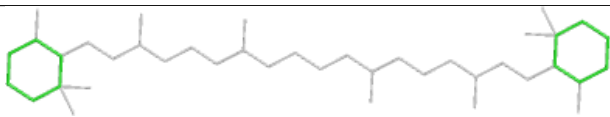


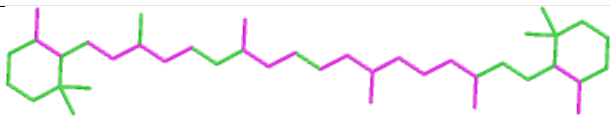
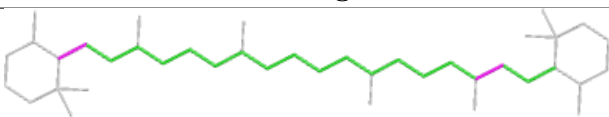
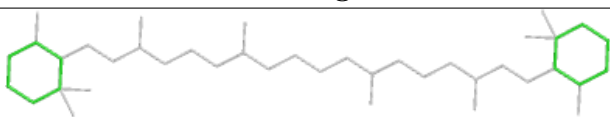
## Ligand LMG D 412

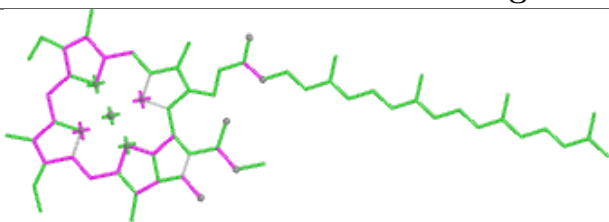
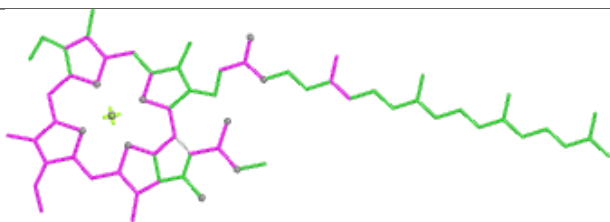
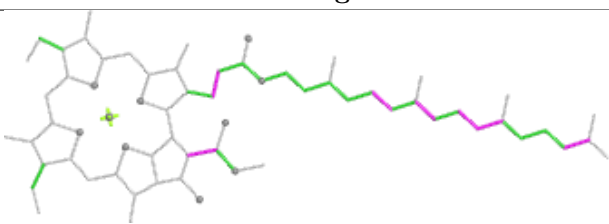
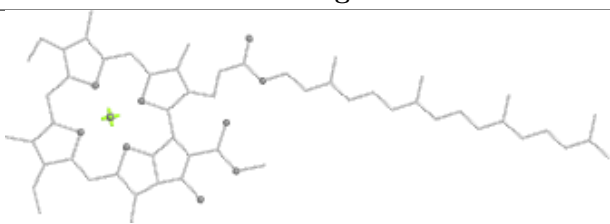


## Ligand CLA C 514

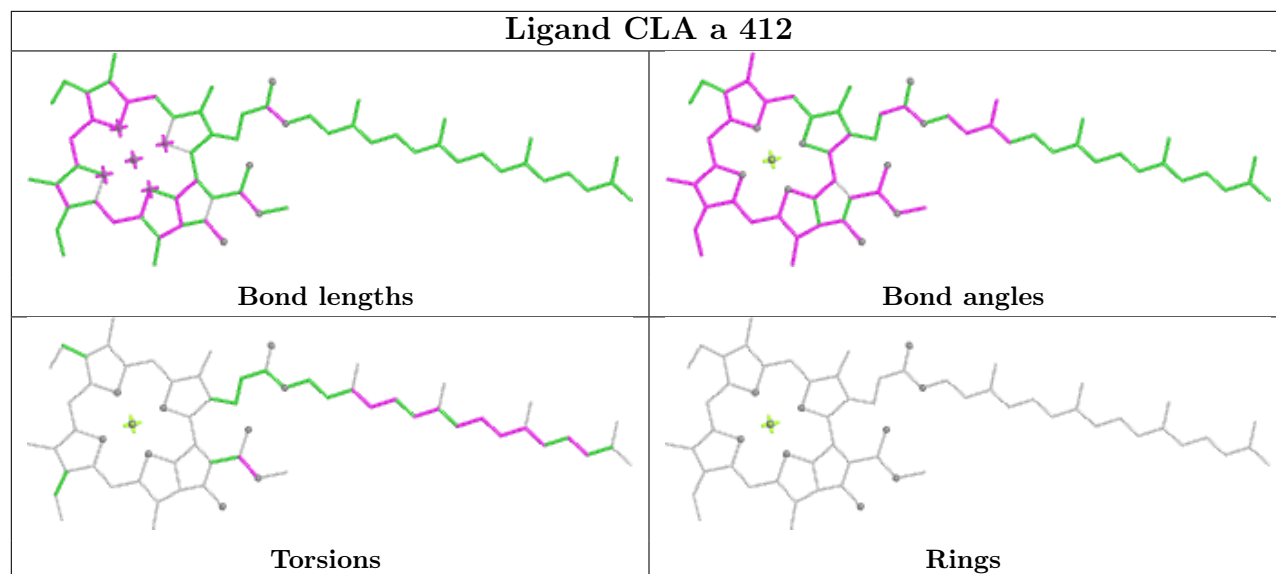


| Ligand BCR K 101                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|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

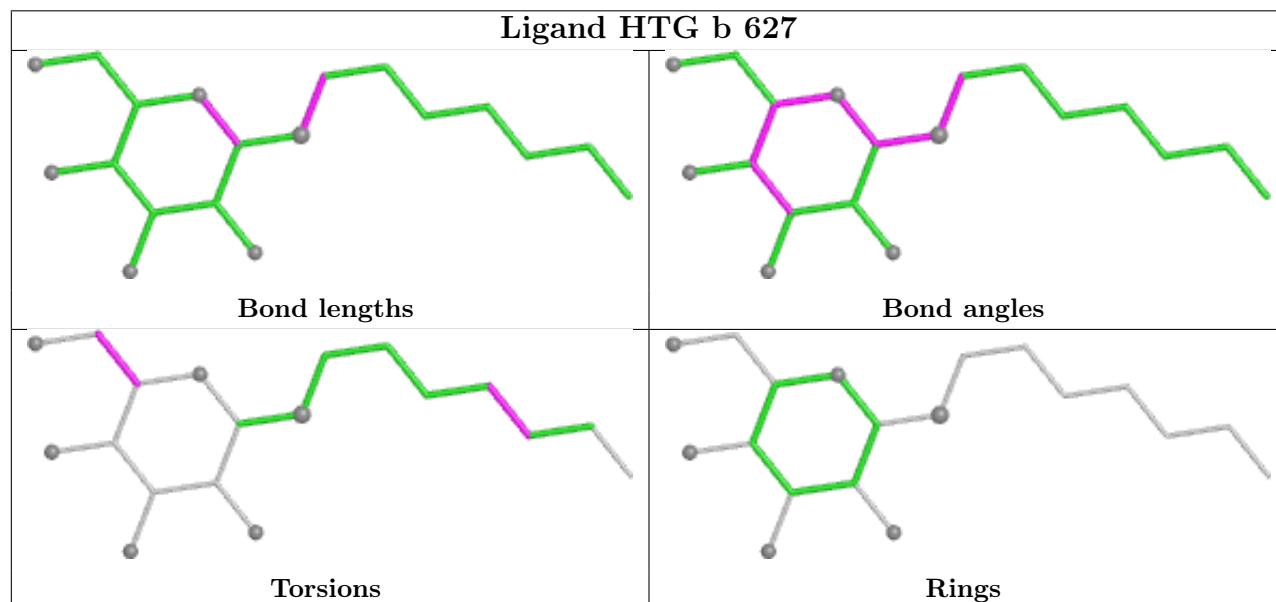
| Ligand BCR c 916                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA C 508                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

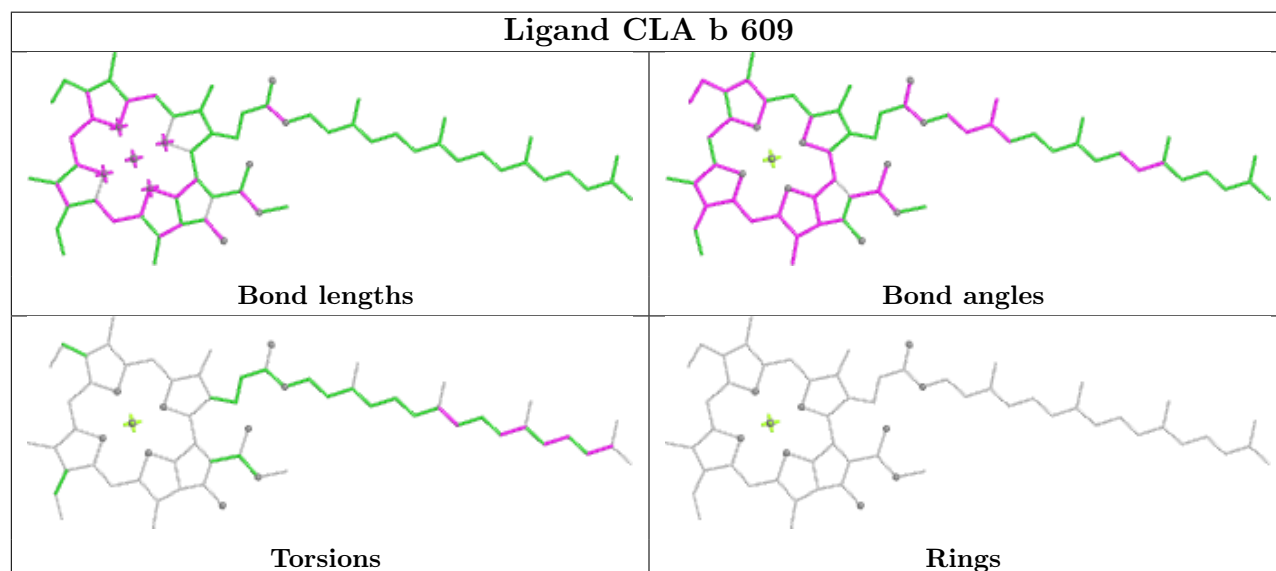
## Ligand CLA a 412

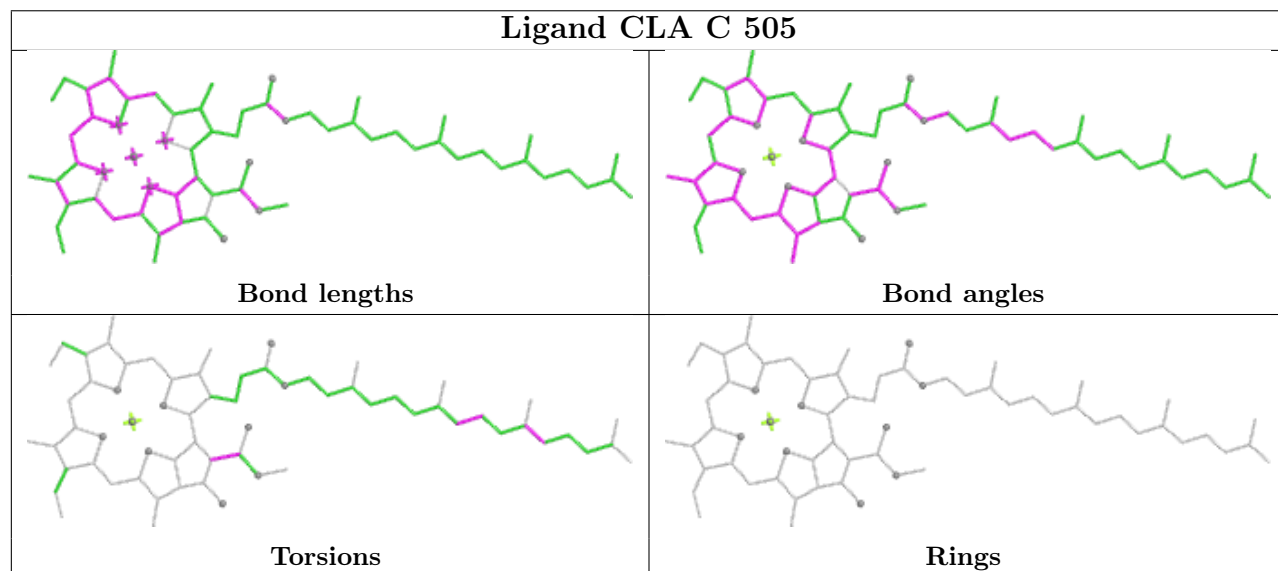
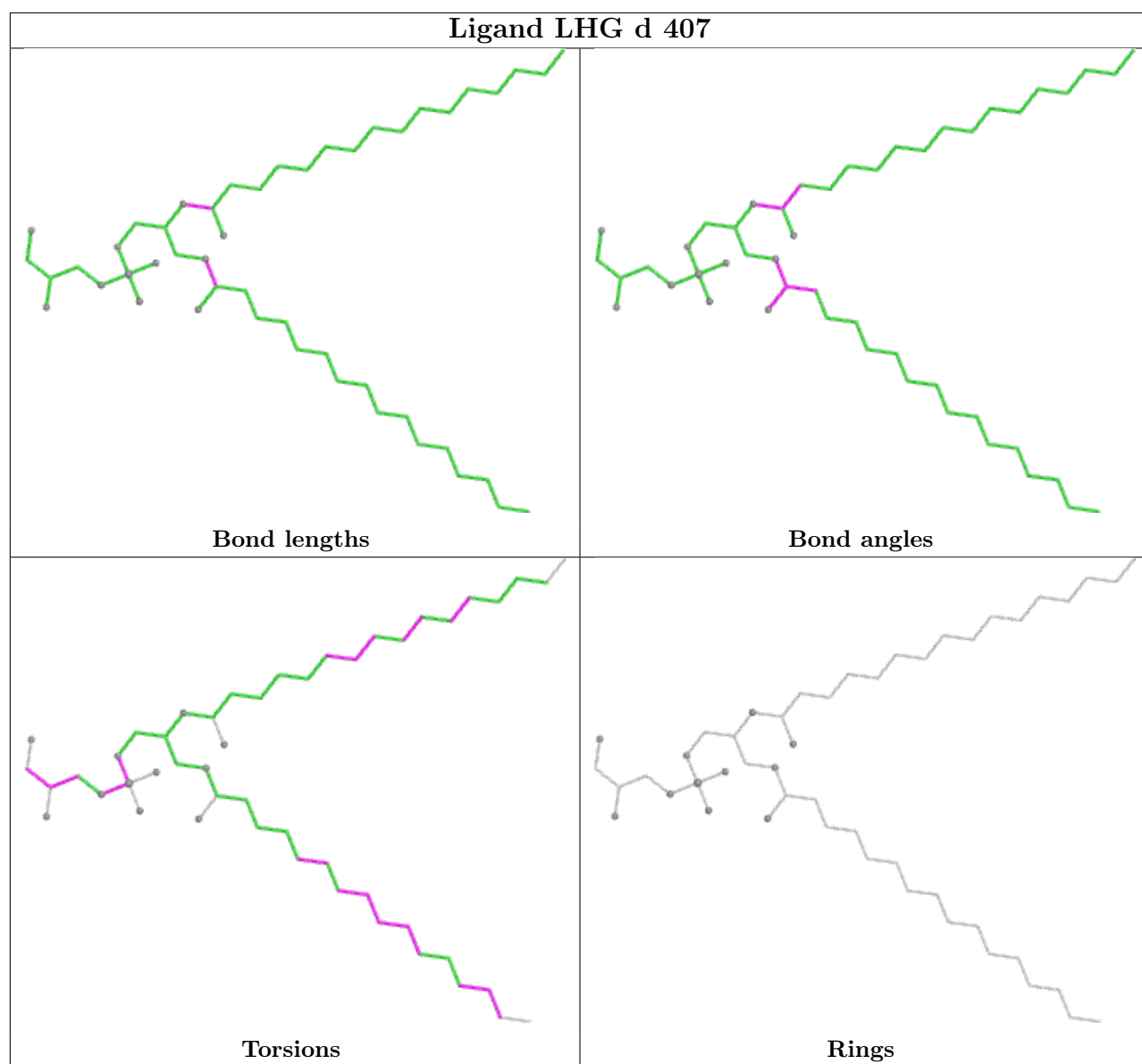


## Ligand HTG b 627

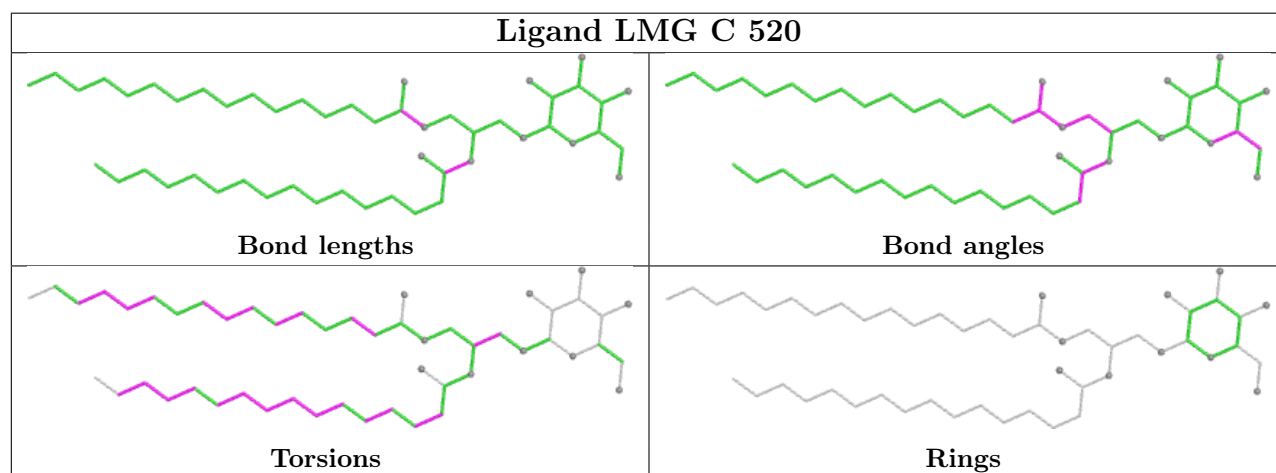
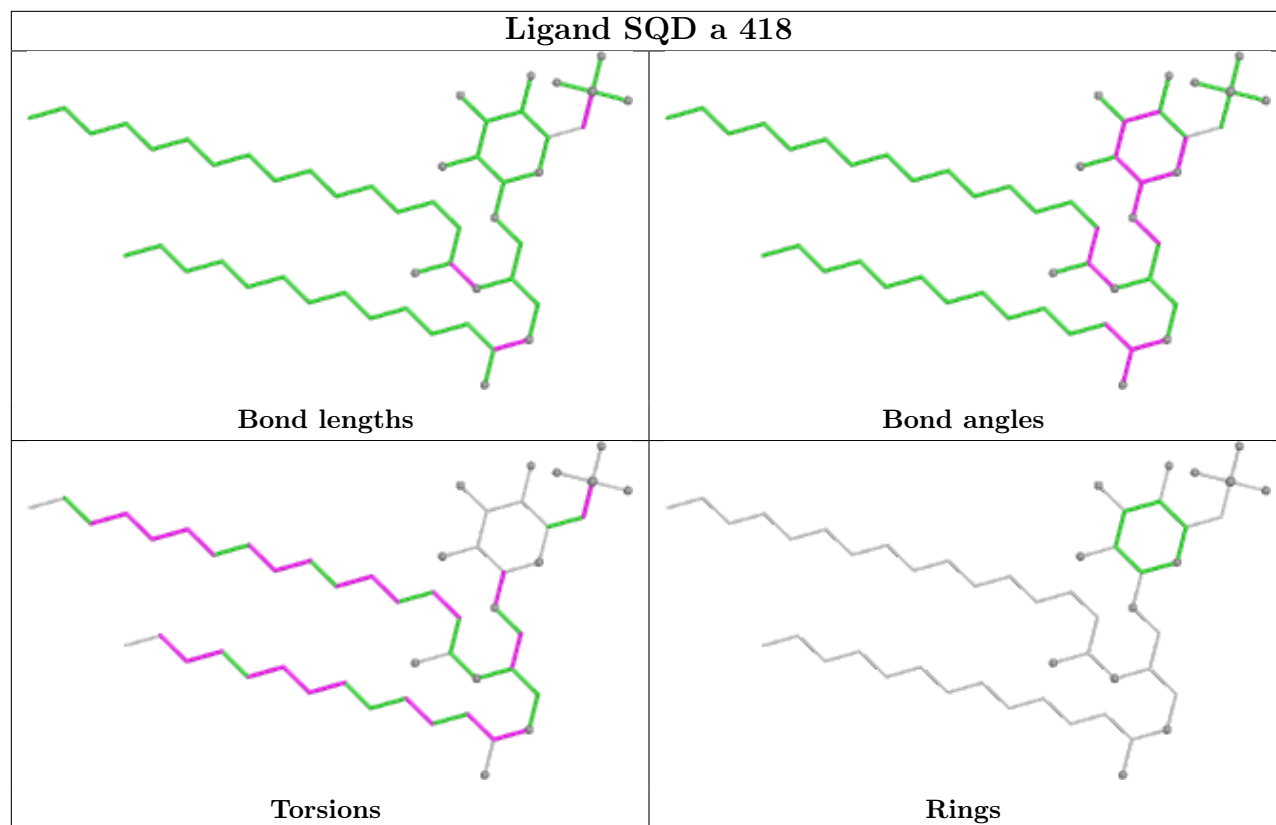


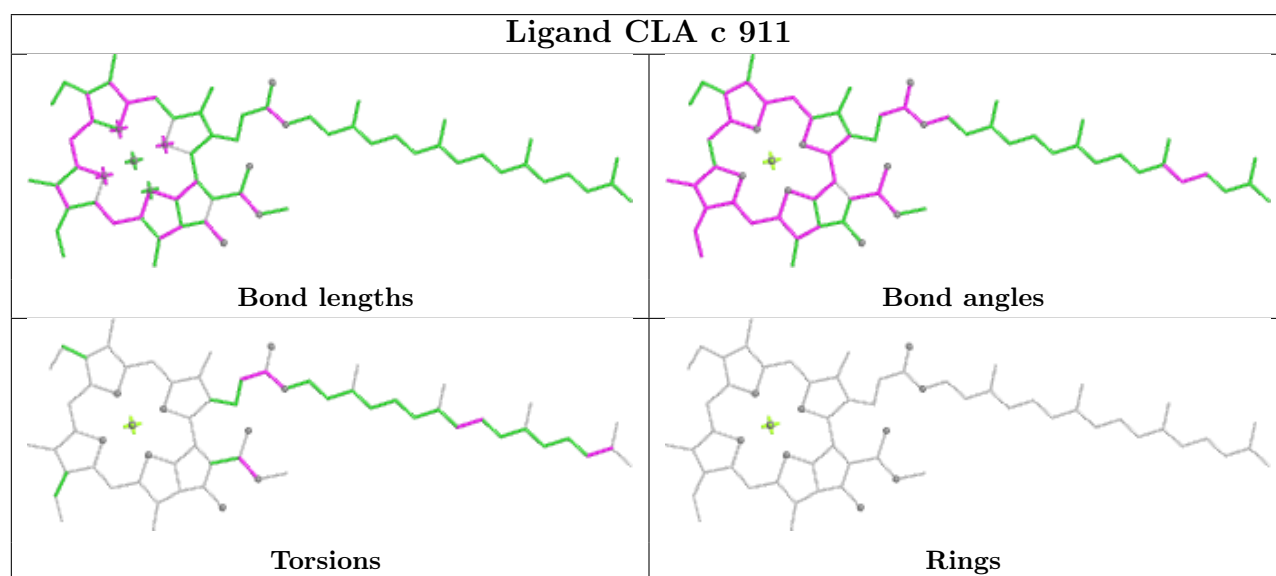
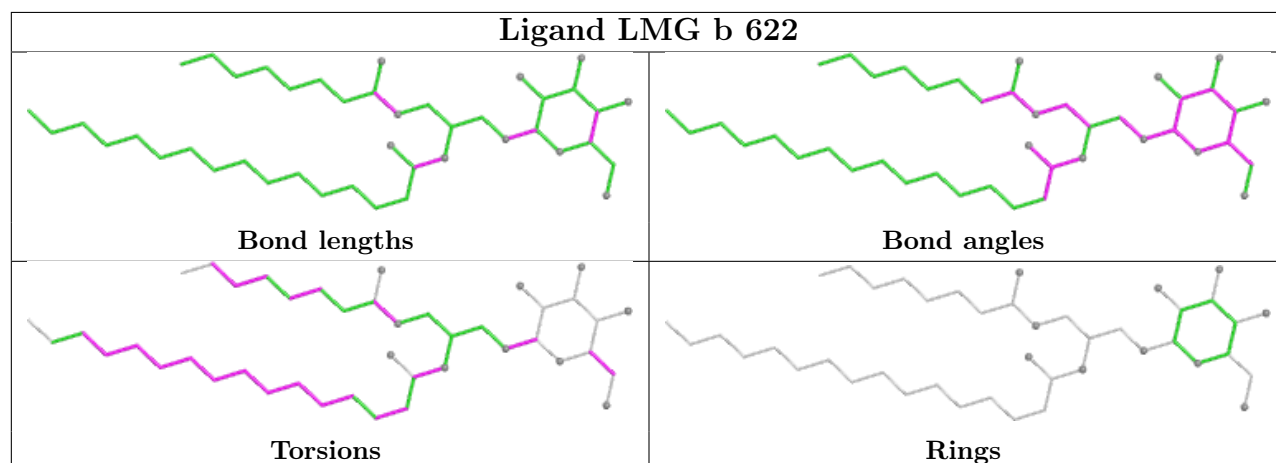
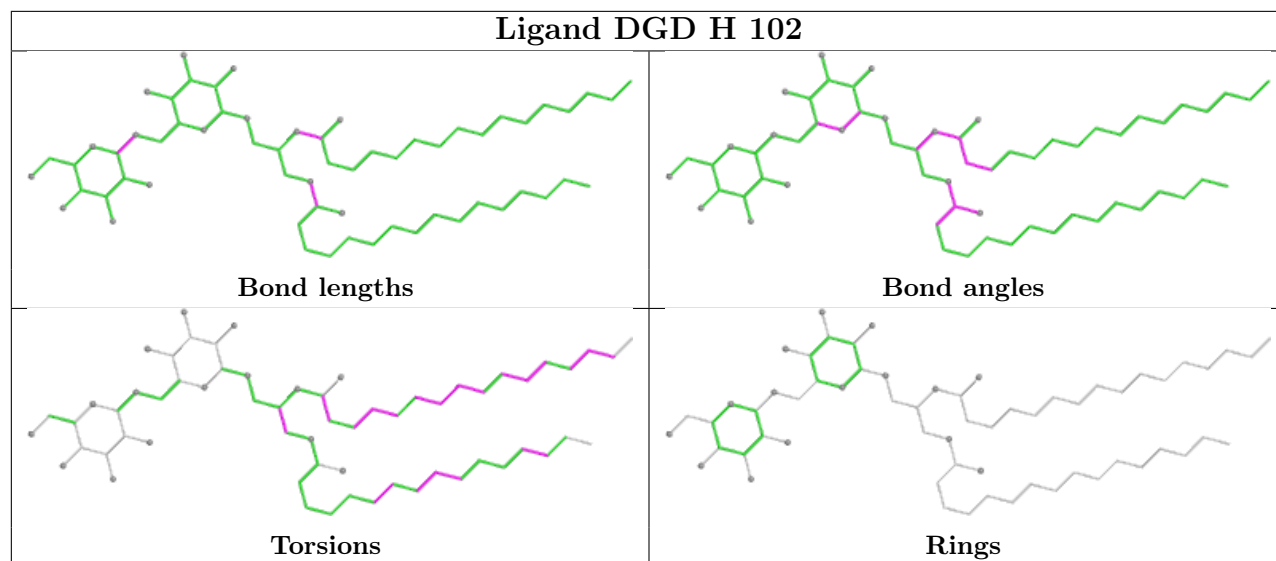
## Ligand CLA b 609

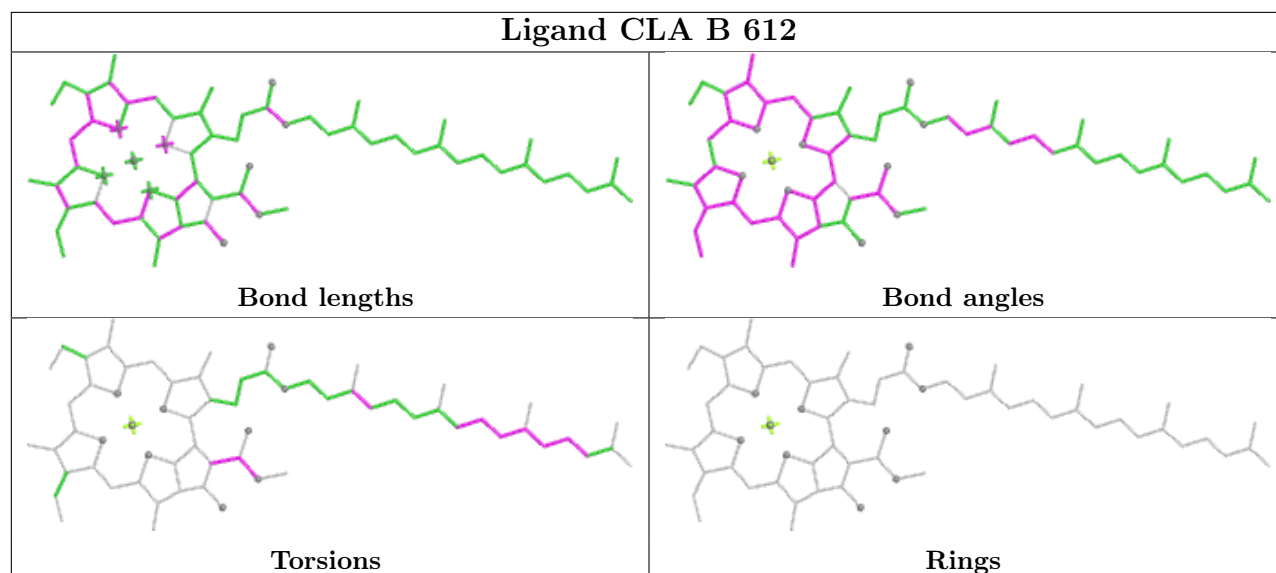
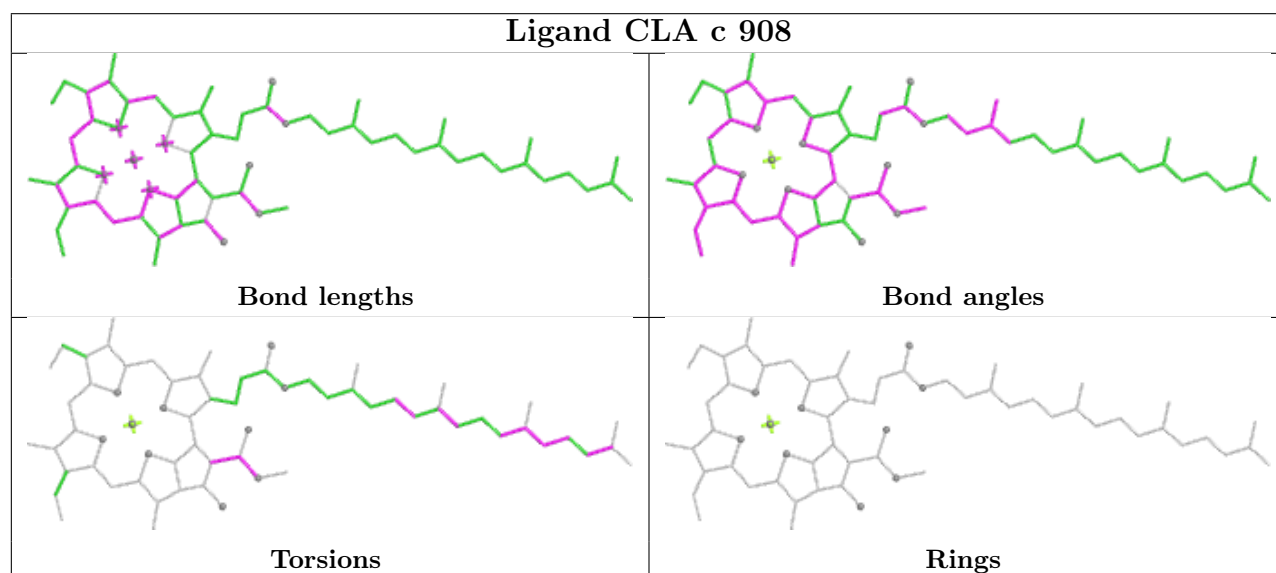
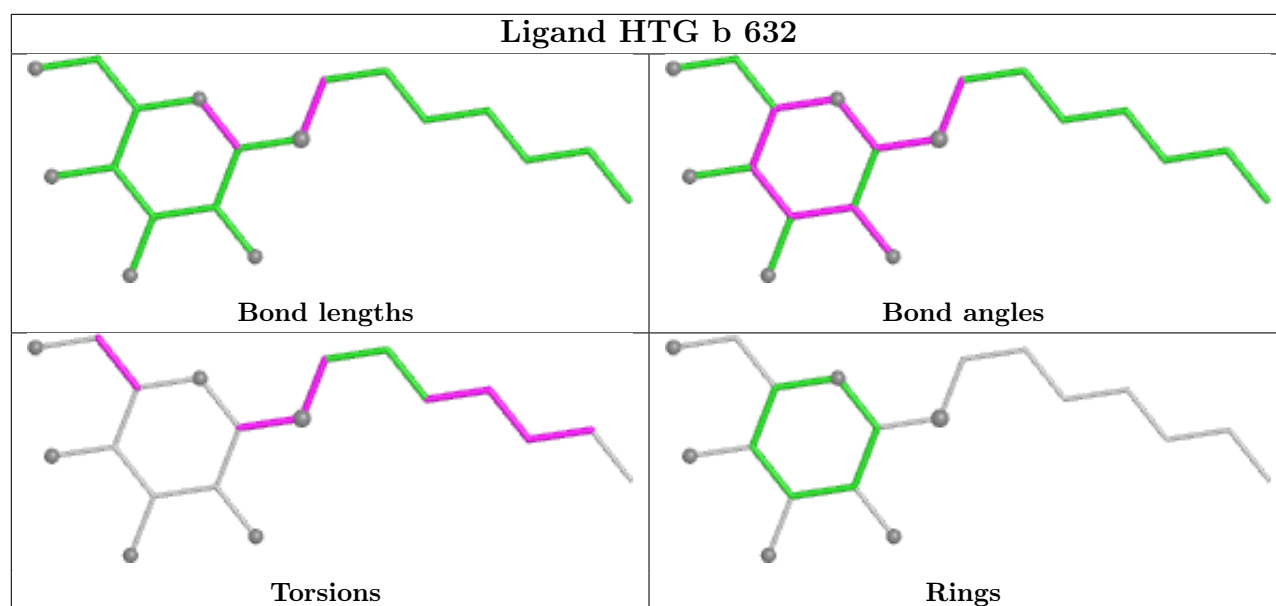


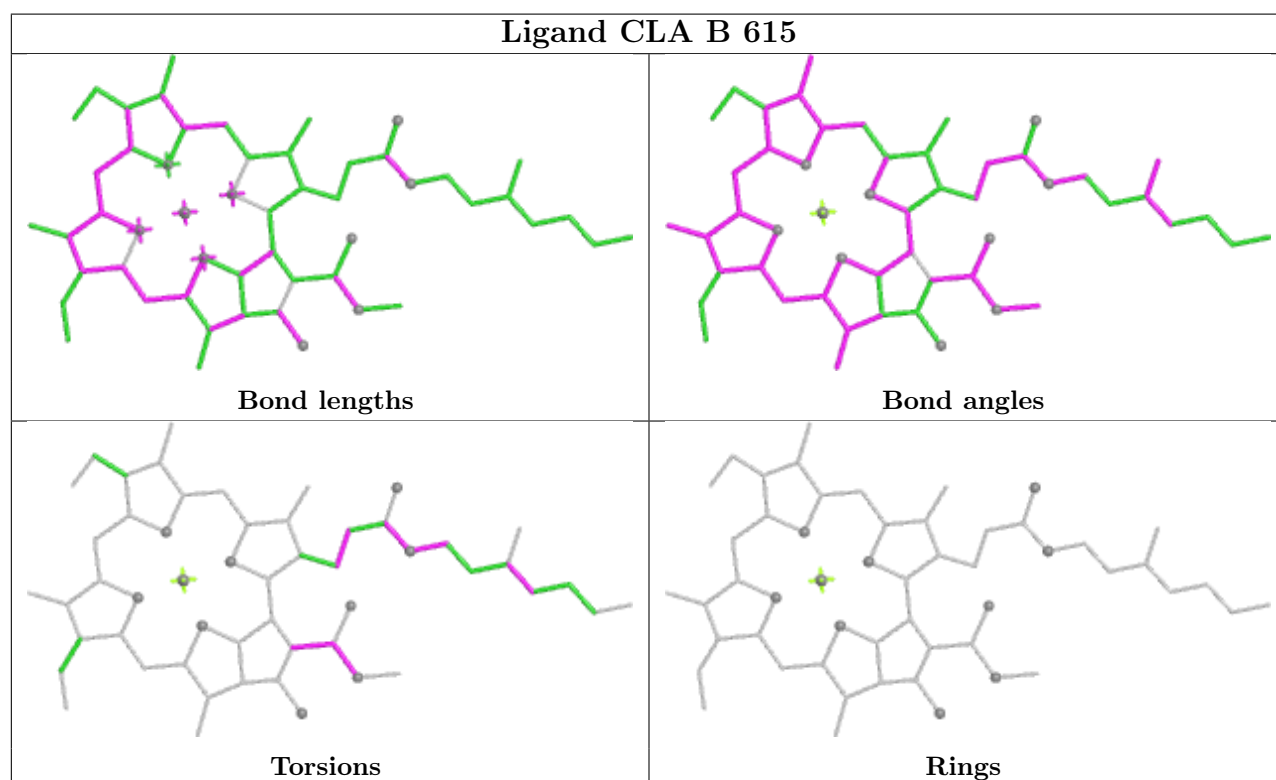
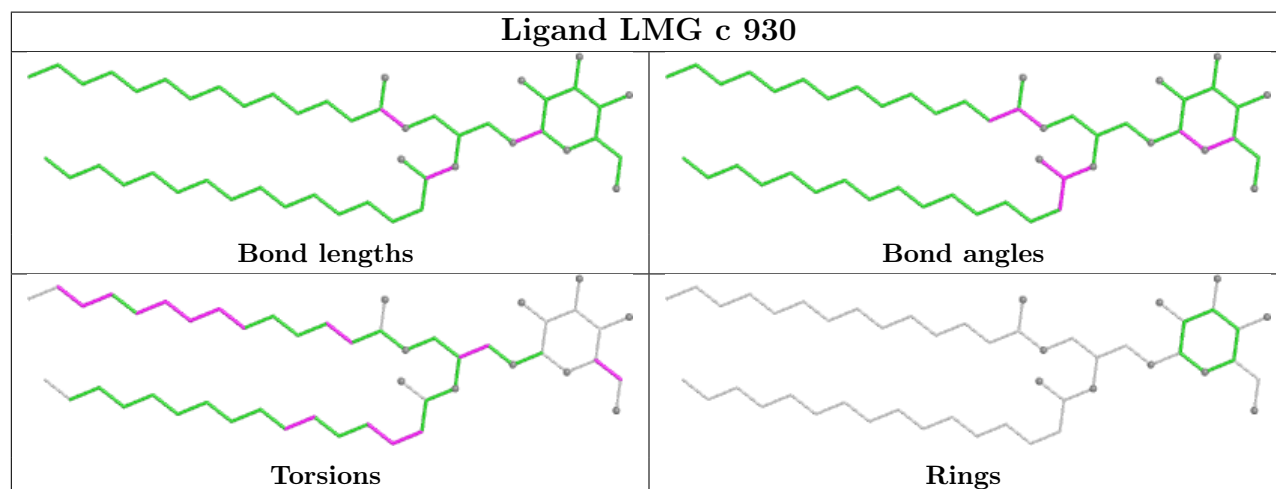
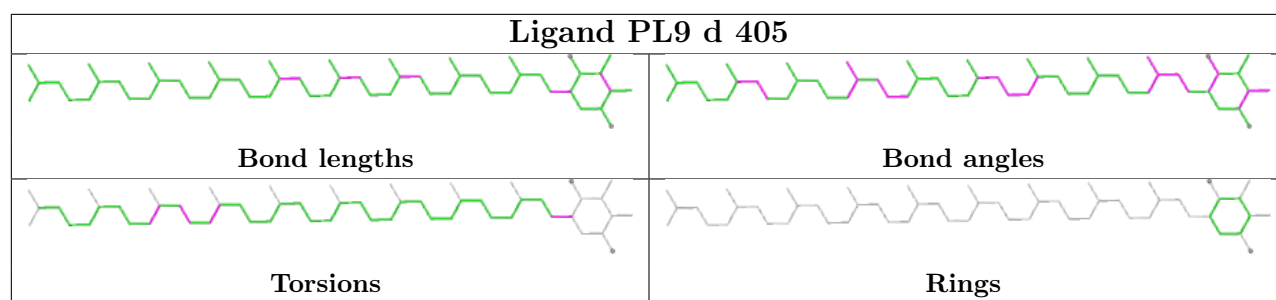


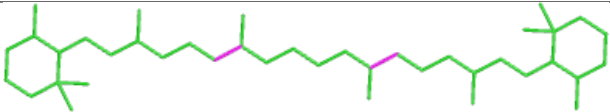
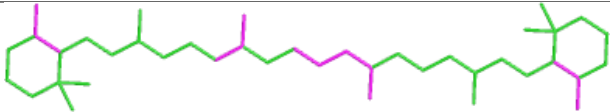
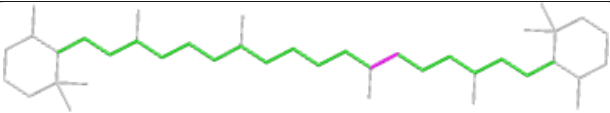
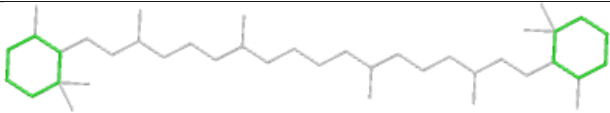




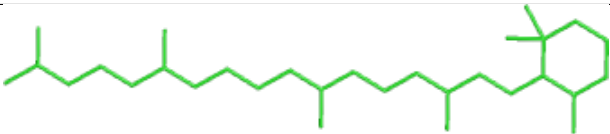
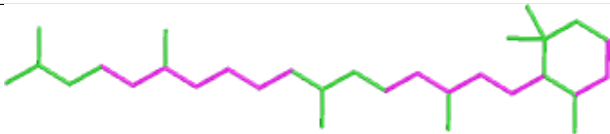
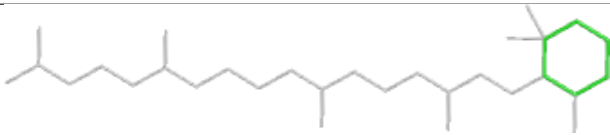


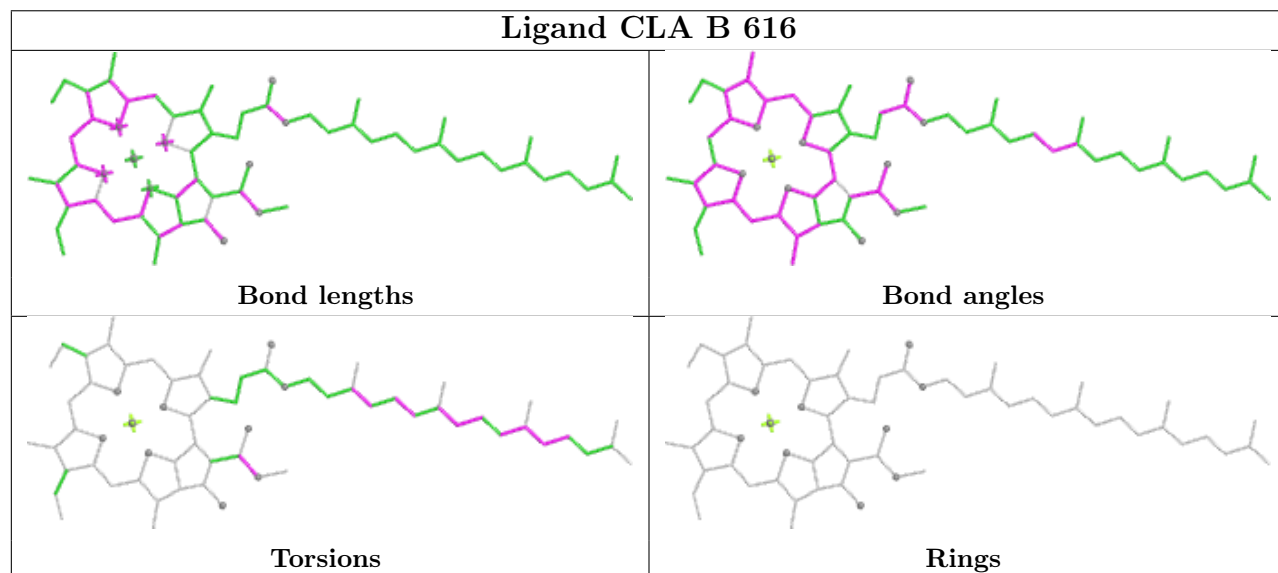
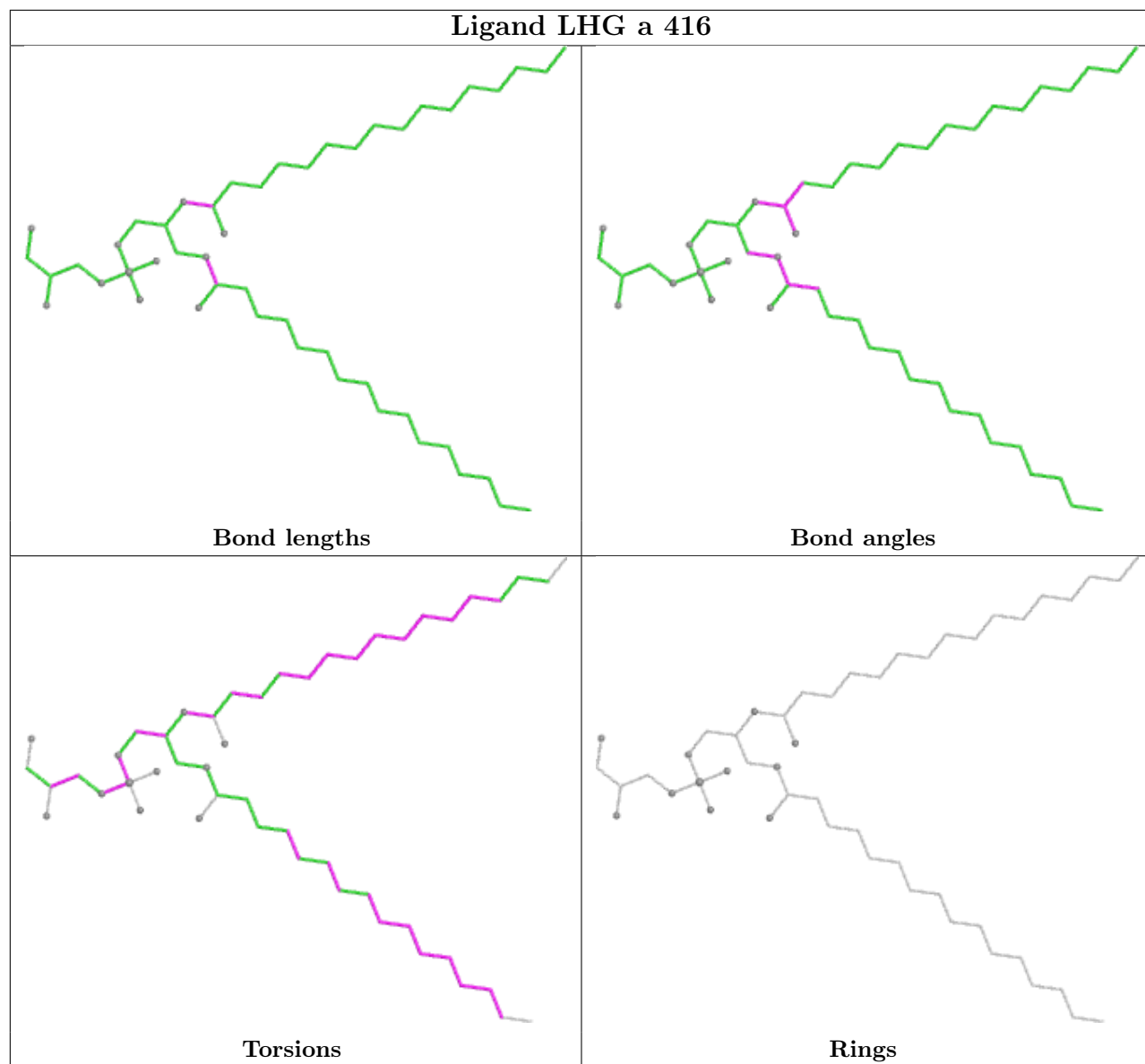


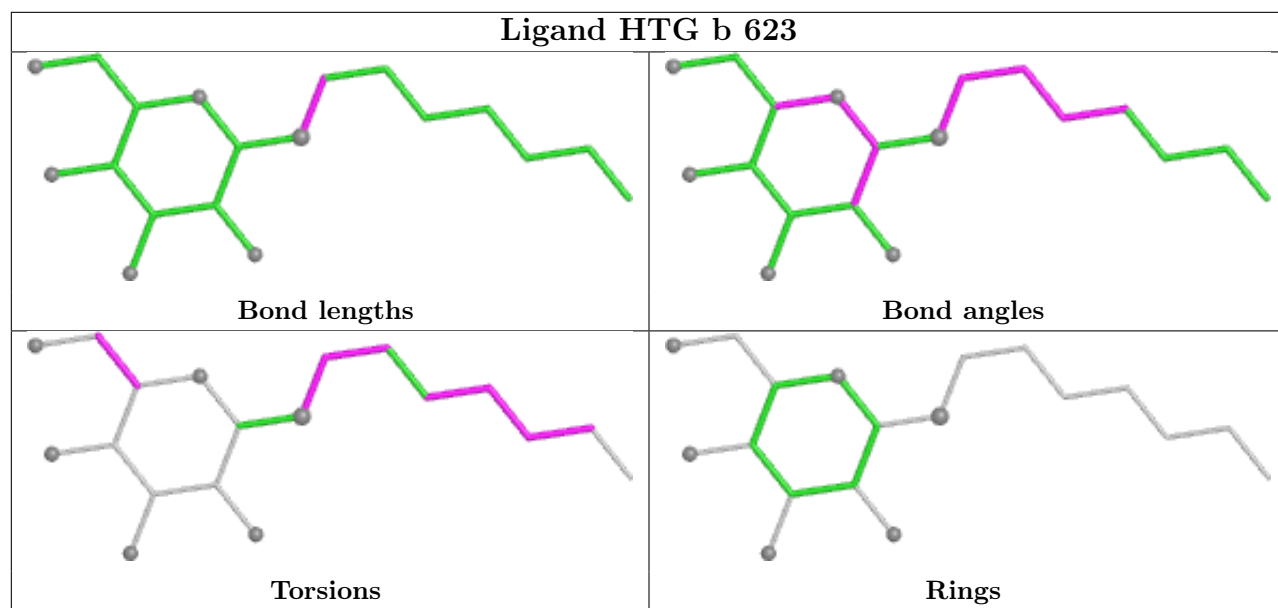
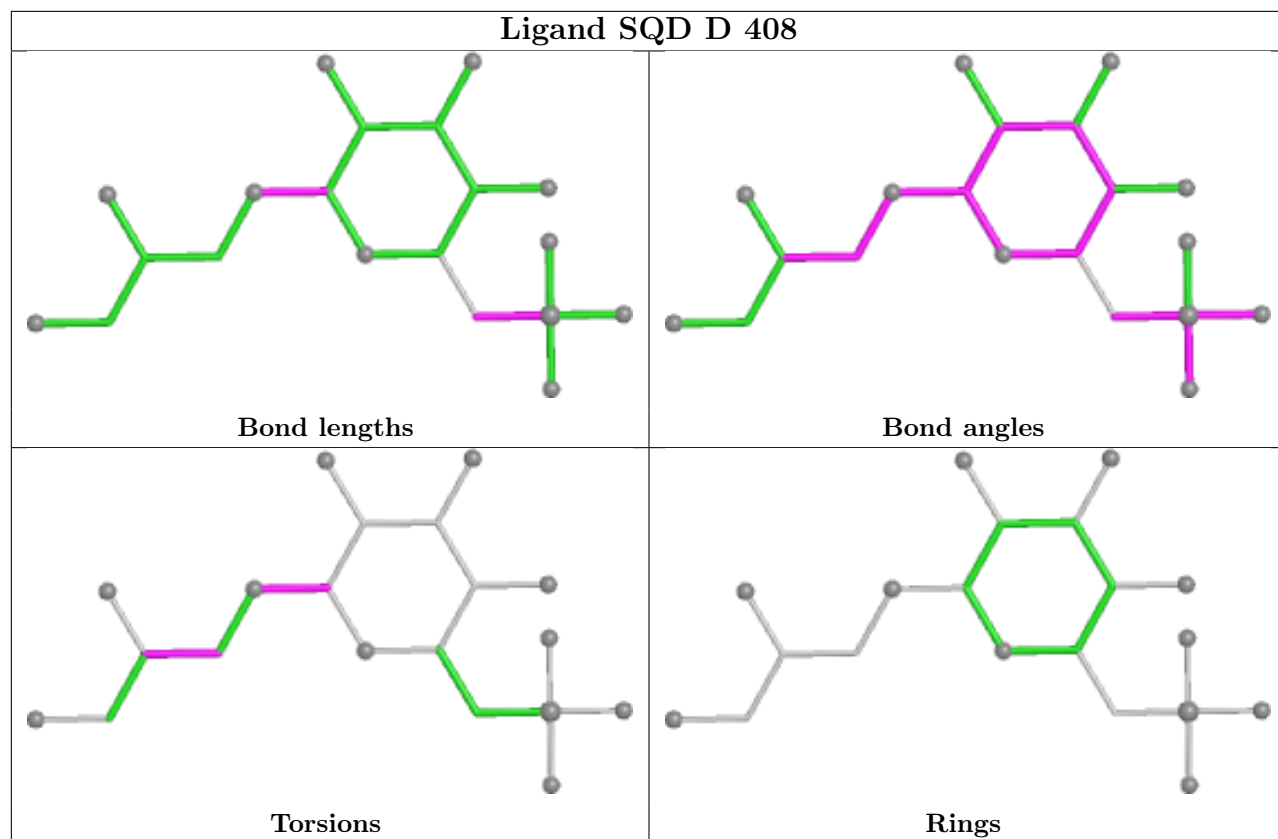


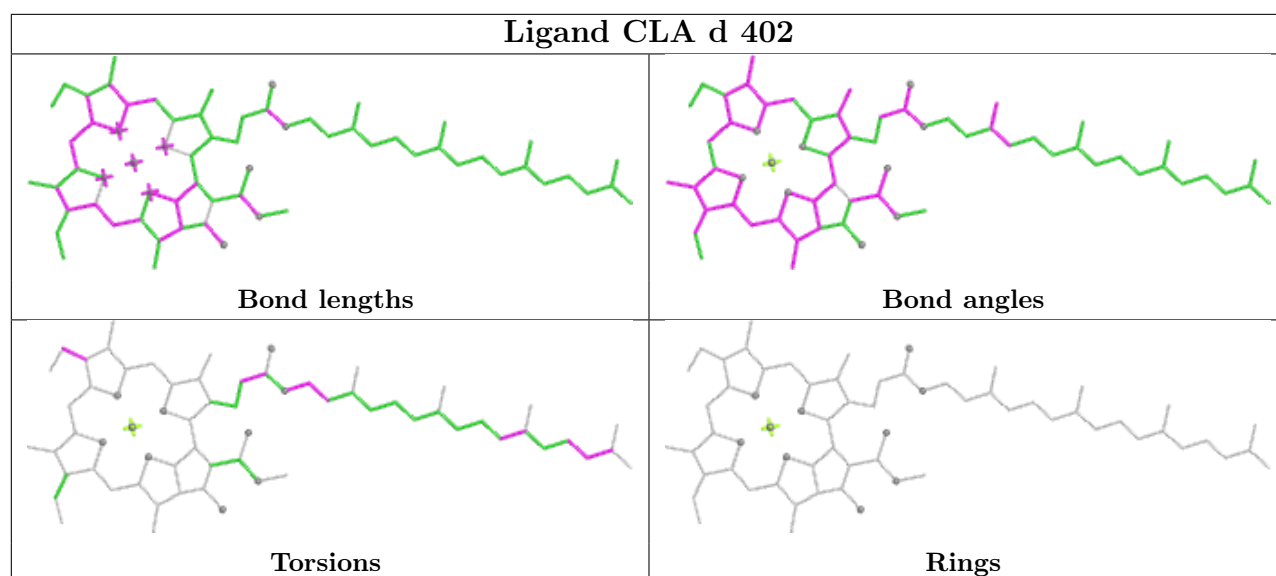
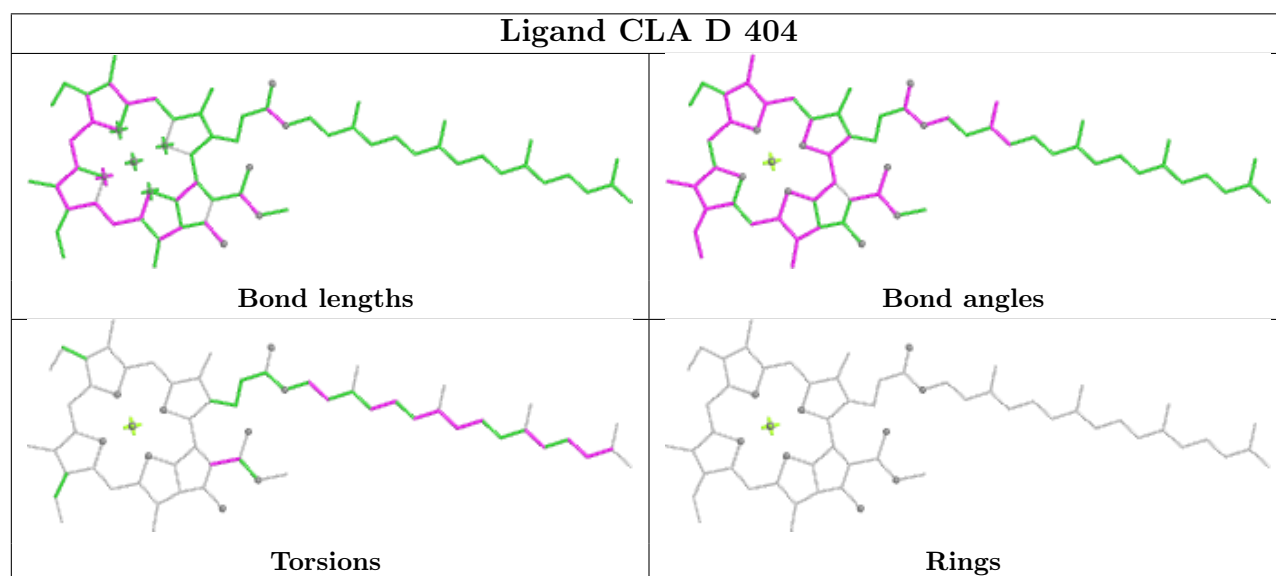
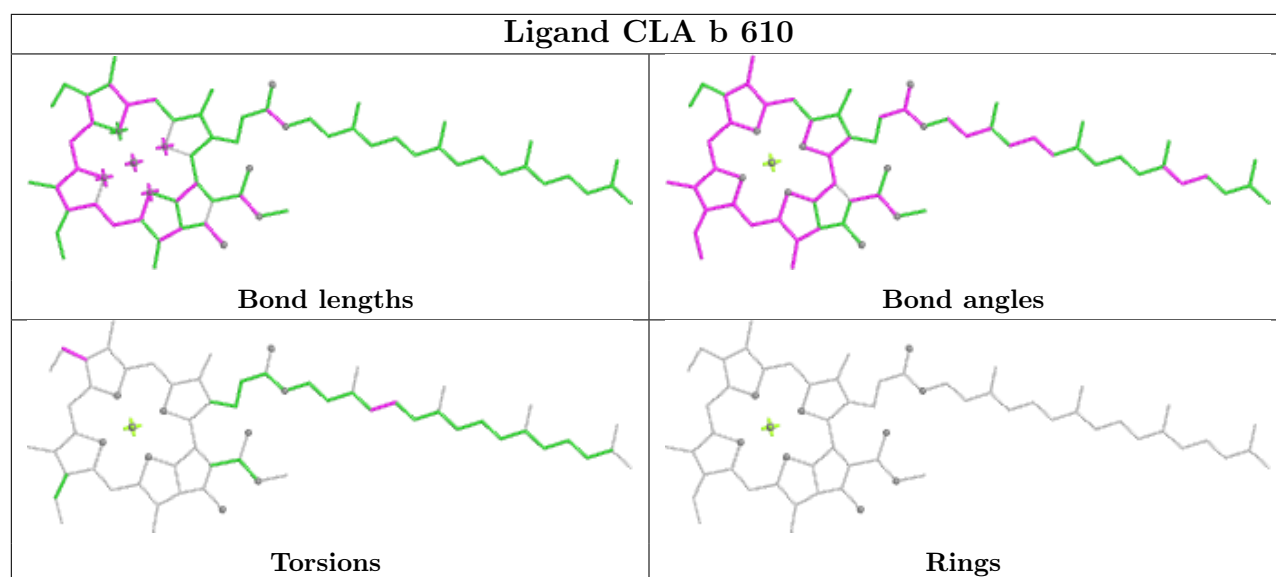
| Ligand BCR A 409                                                                  |  |                                                                                    |  |
|-----------------------------------------------------------------------------------|--|------------------------------------------------------------------------------------|--|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

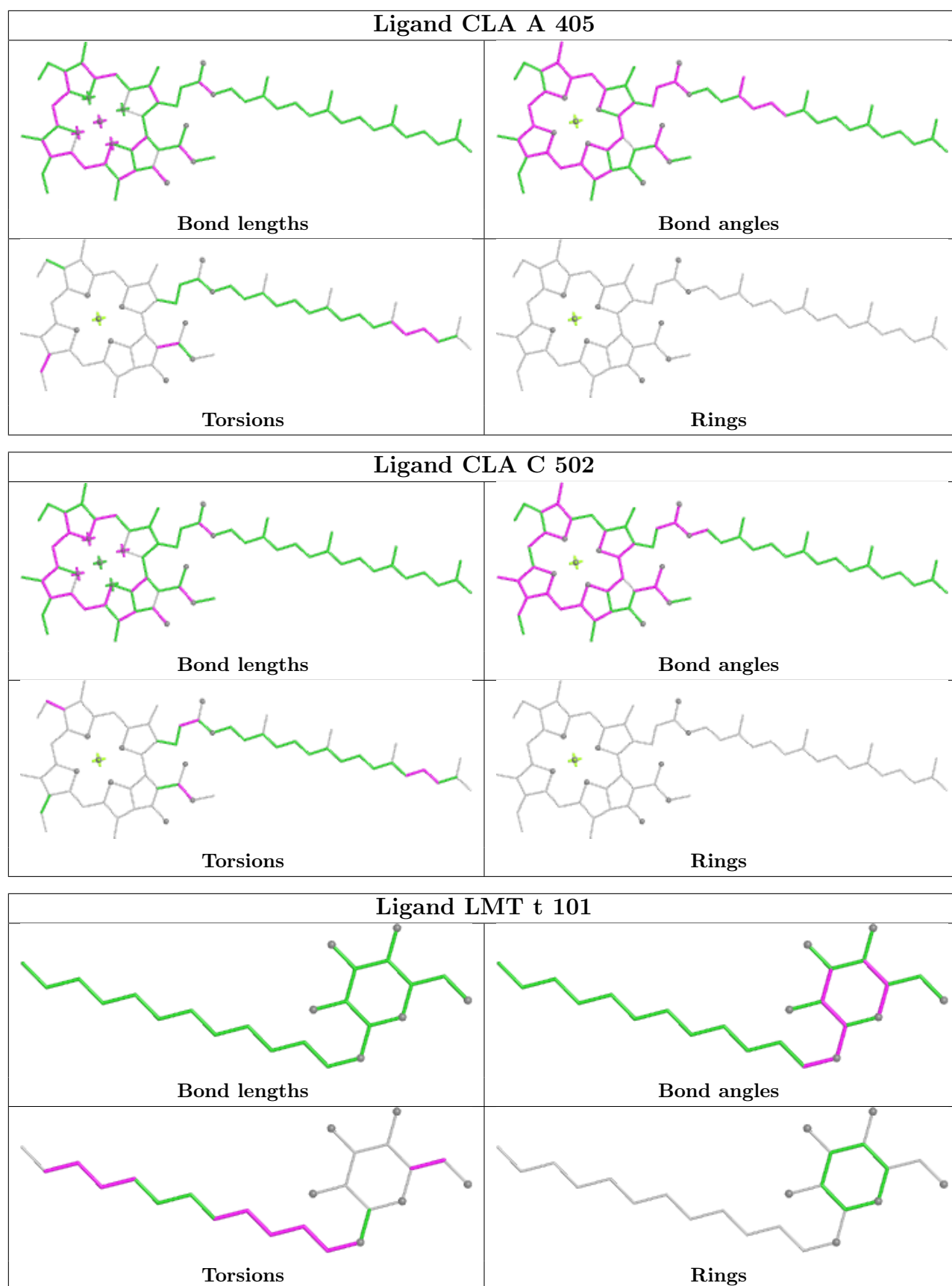
| Ligand BCR B 619                                                                  |  |                                                                                    |  |
|-----------------------------------------------------------------------------------|--|------------------------------------------------------------------------------------|--|
|  |  |  |  |
| Bond lengths                                                                      |  | Bond angles                                                                        |  |
|  |  |  |  |
| Torsions                                                                          |  | Rings                                                                              |  |



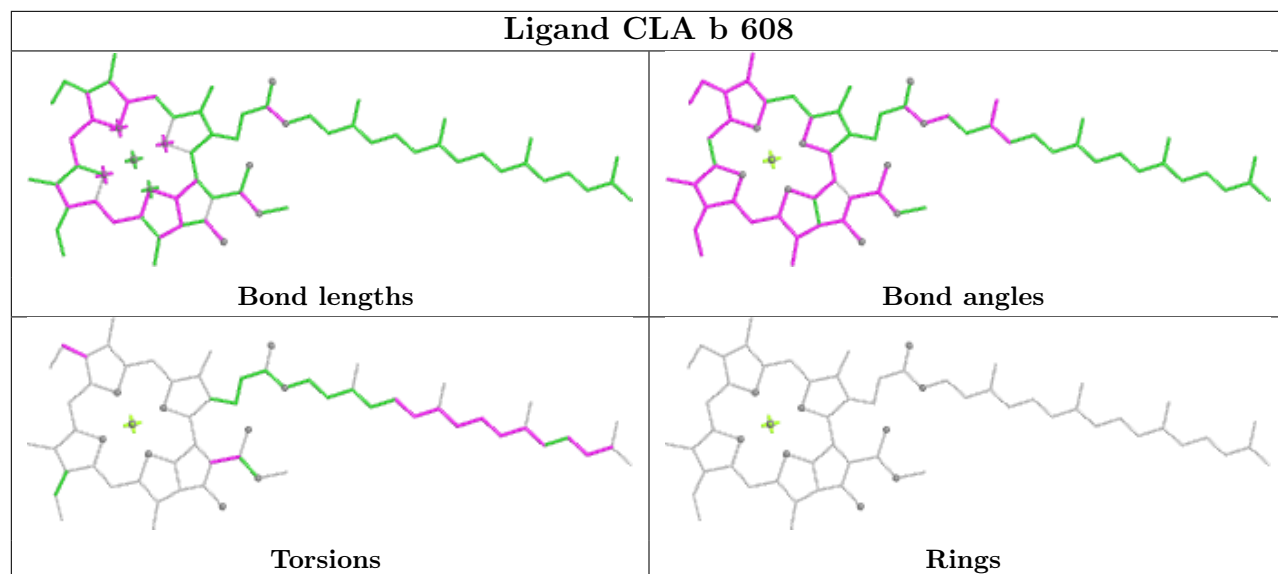




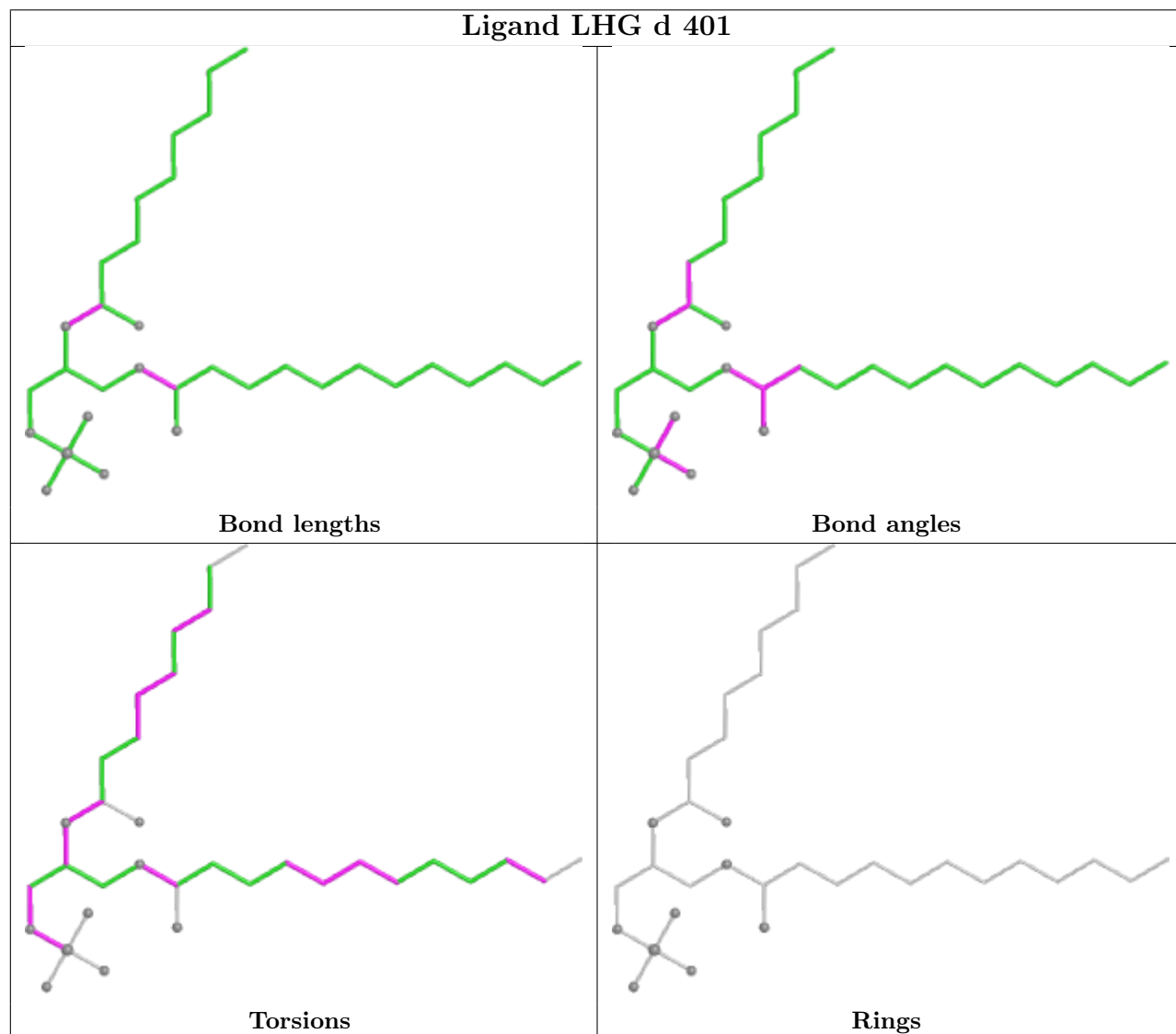


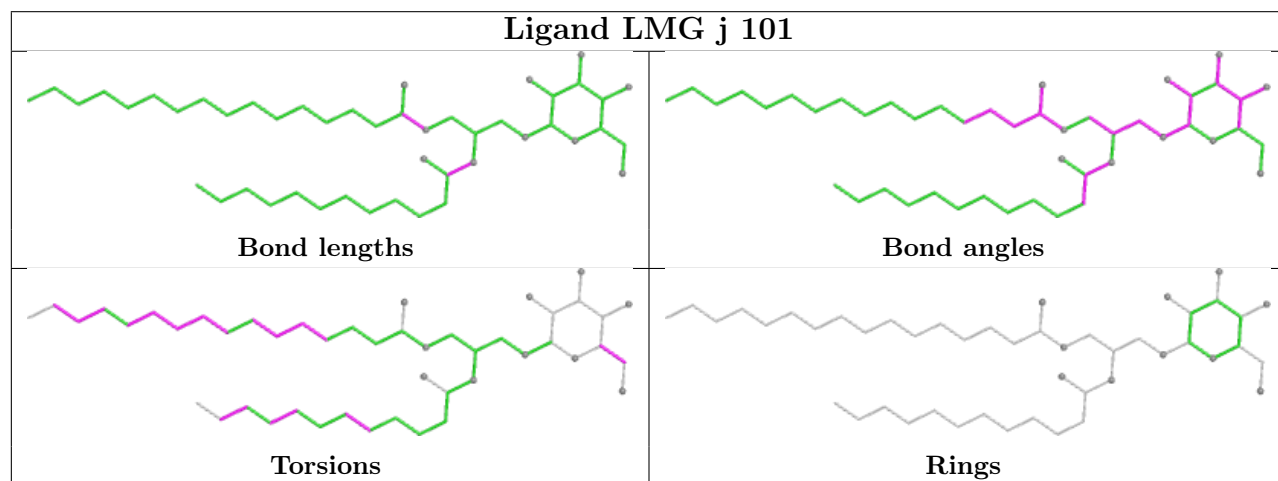
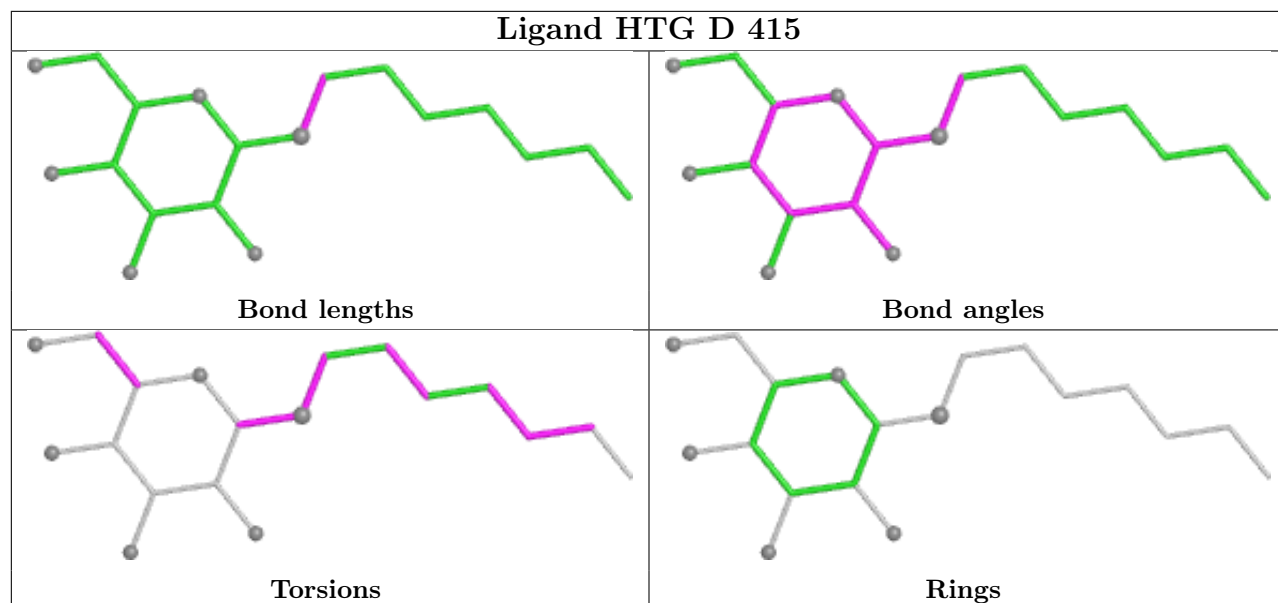


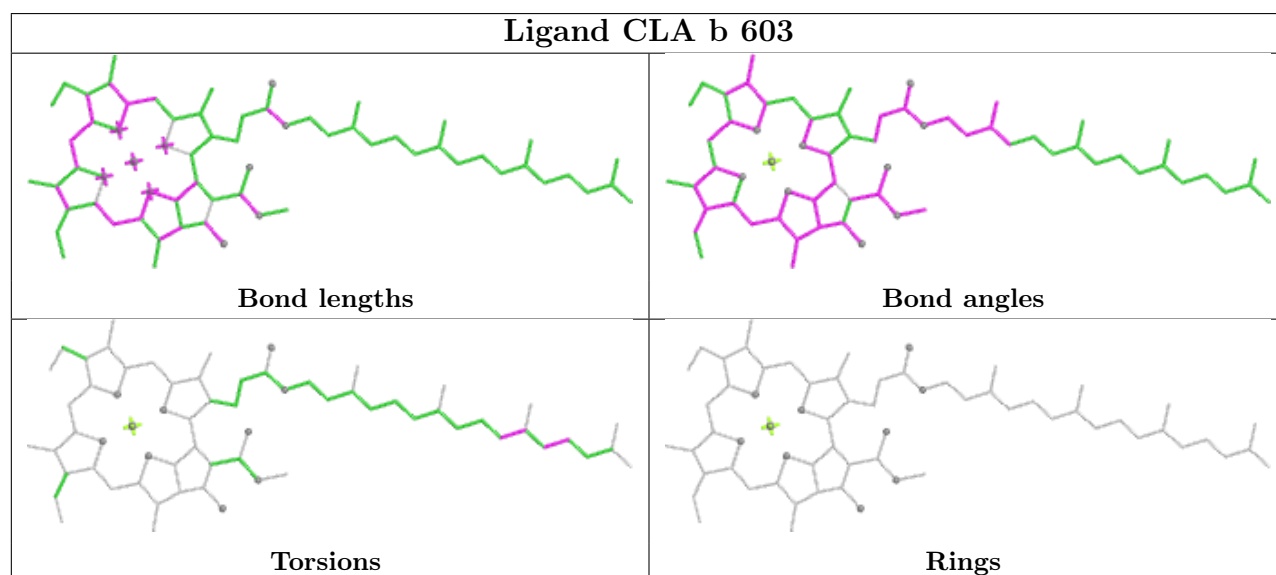
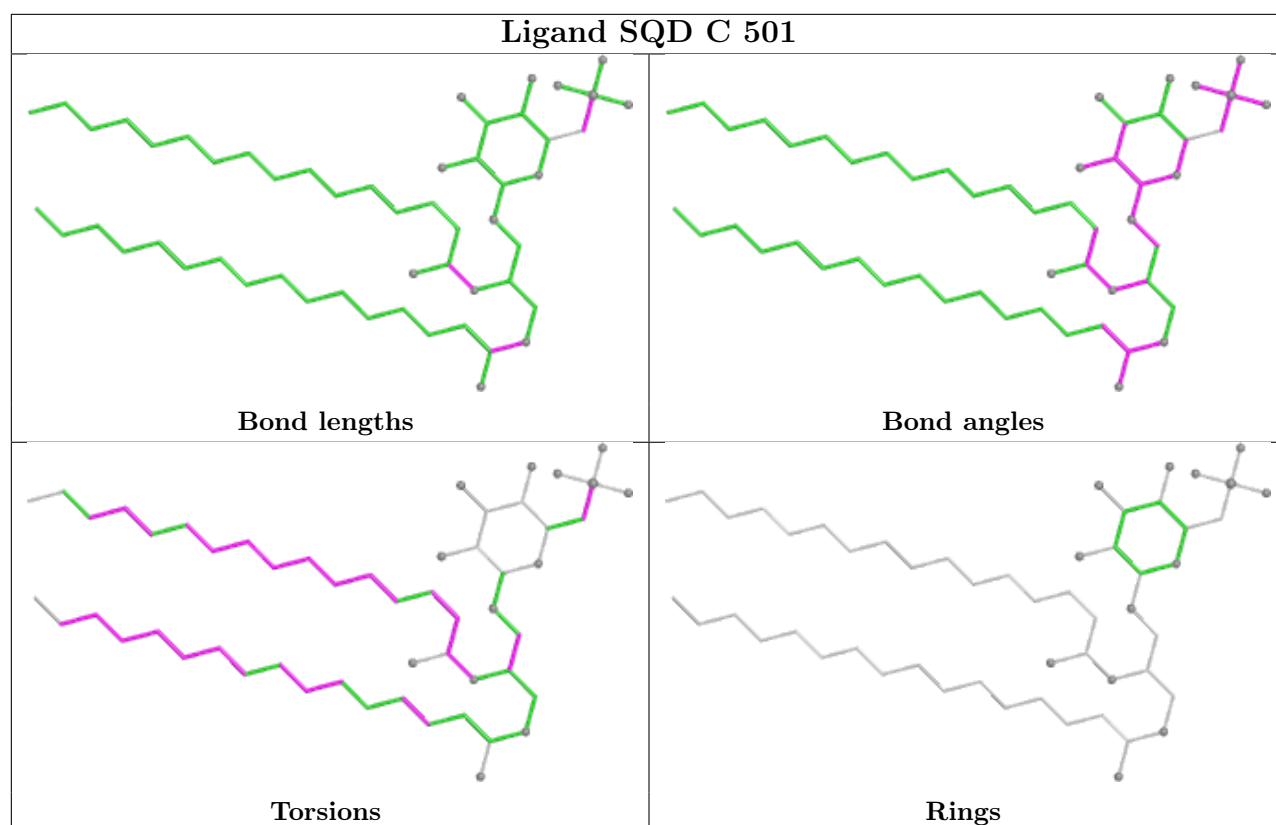
## Ligand CLA b 608

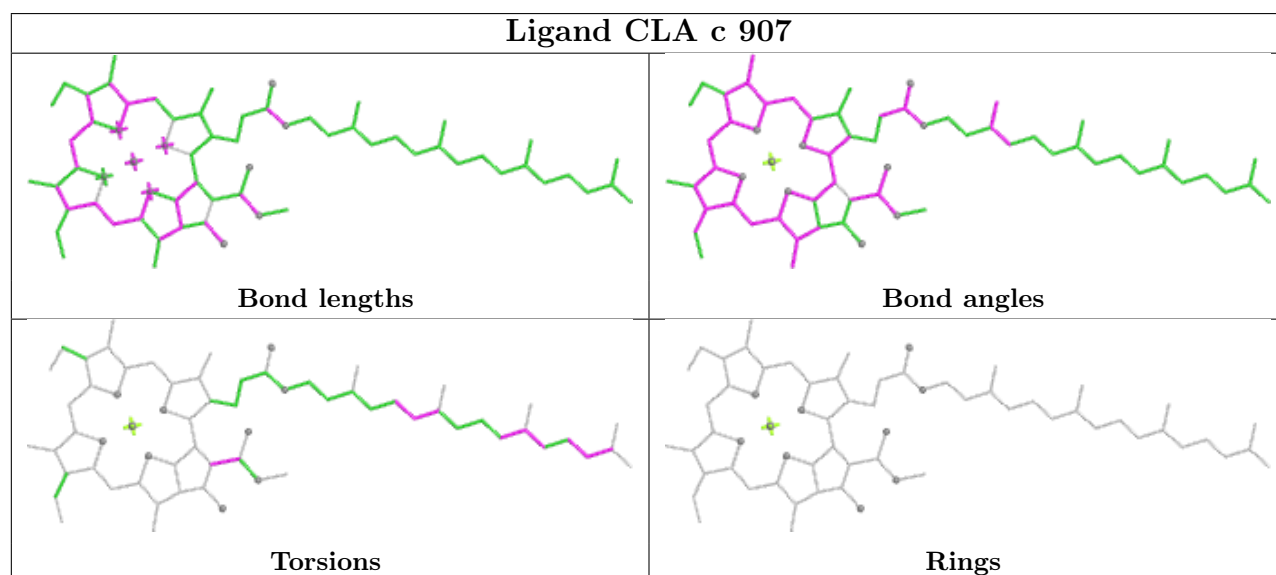
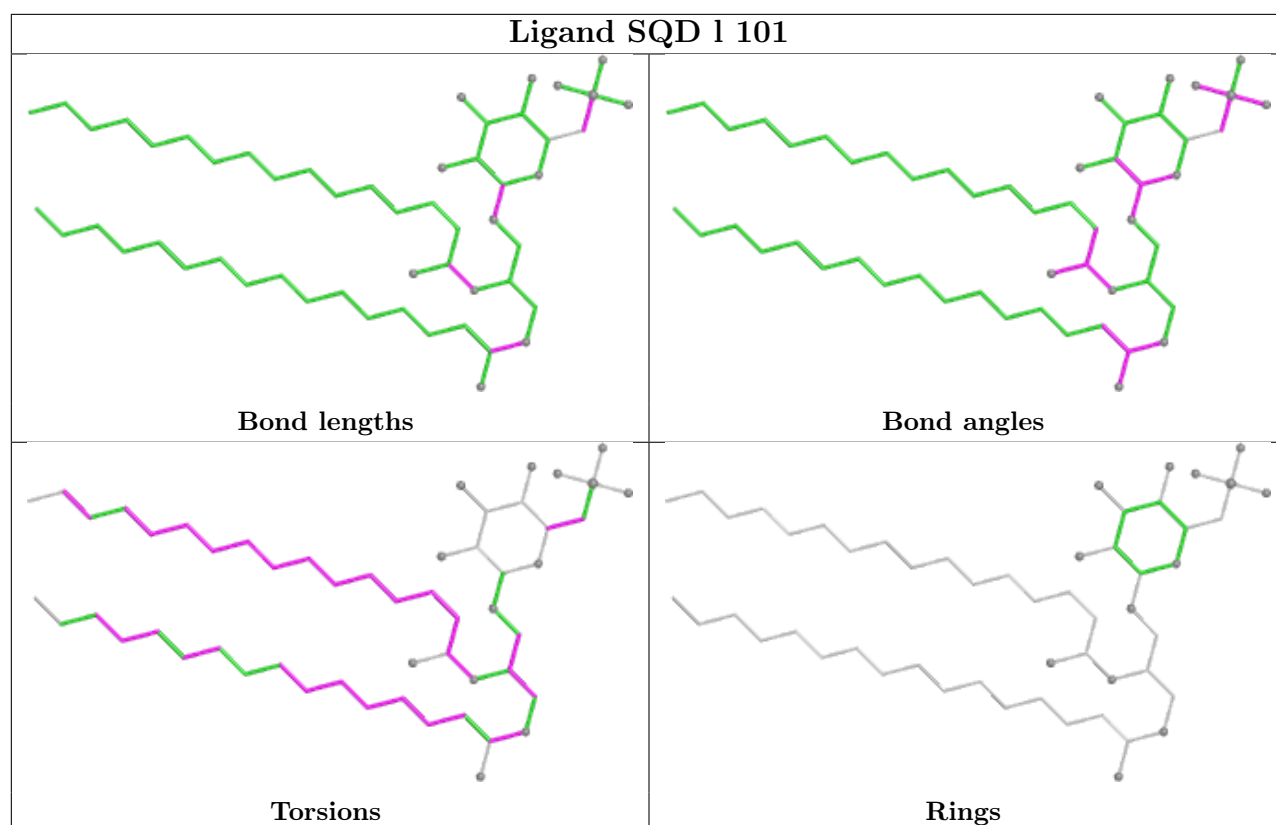


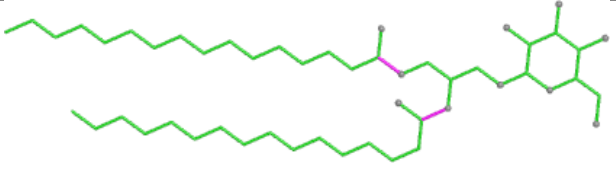
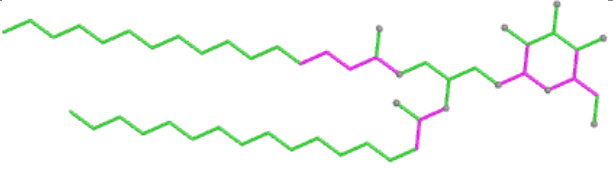
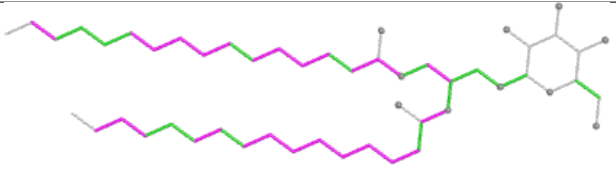
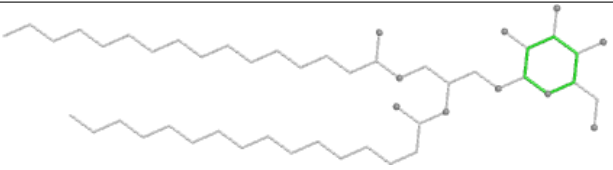
## Ligand LHG d 401

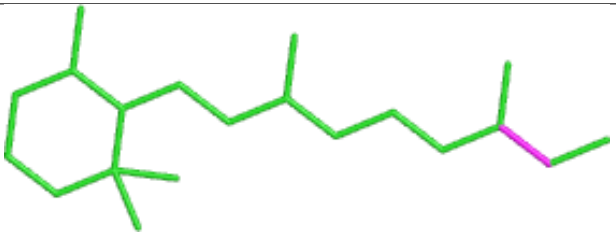
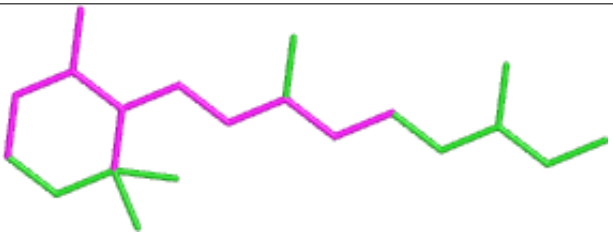
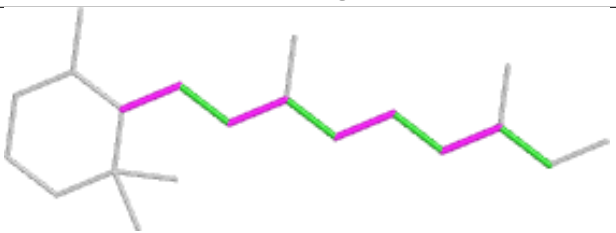
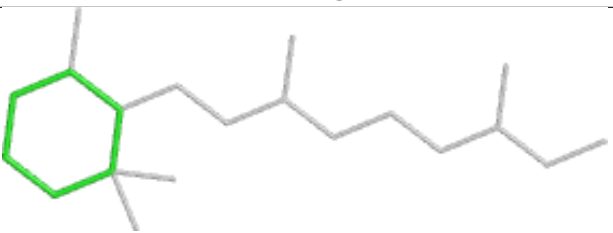


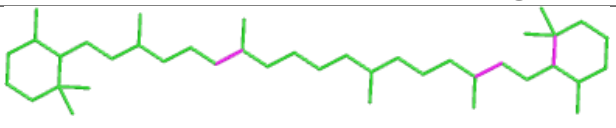
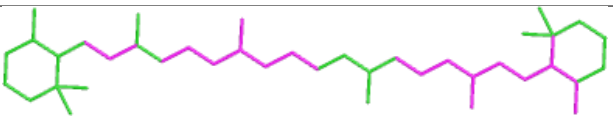
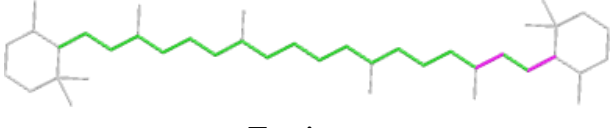
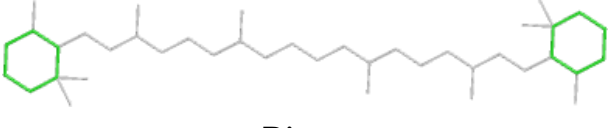


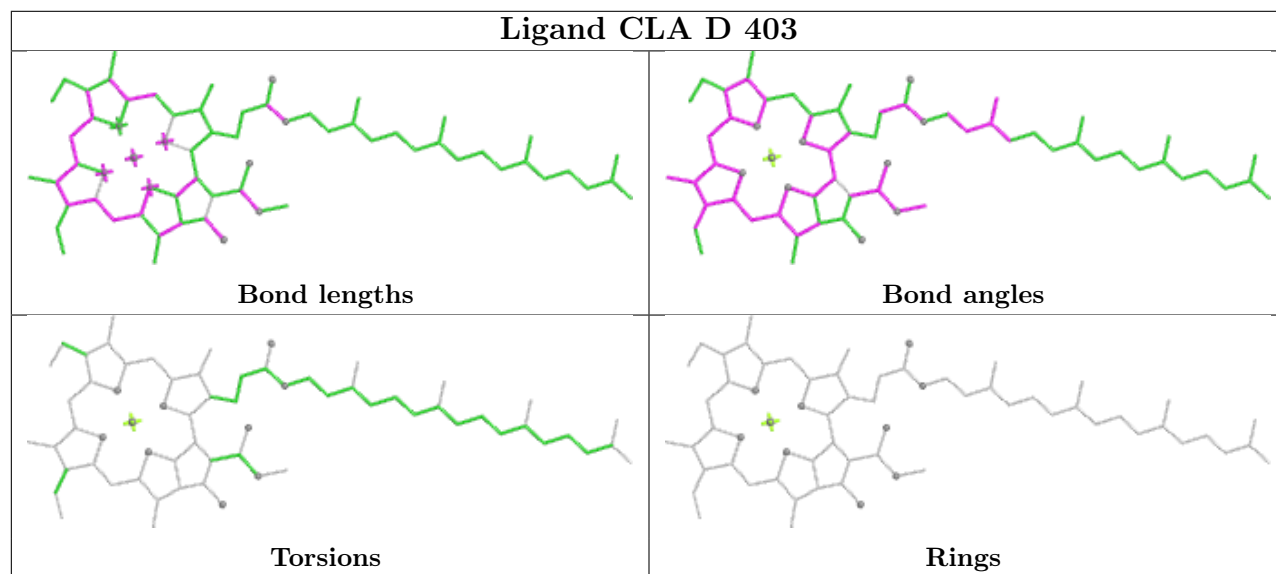
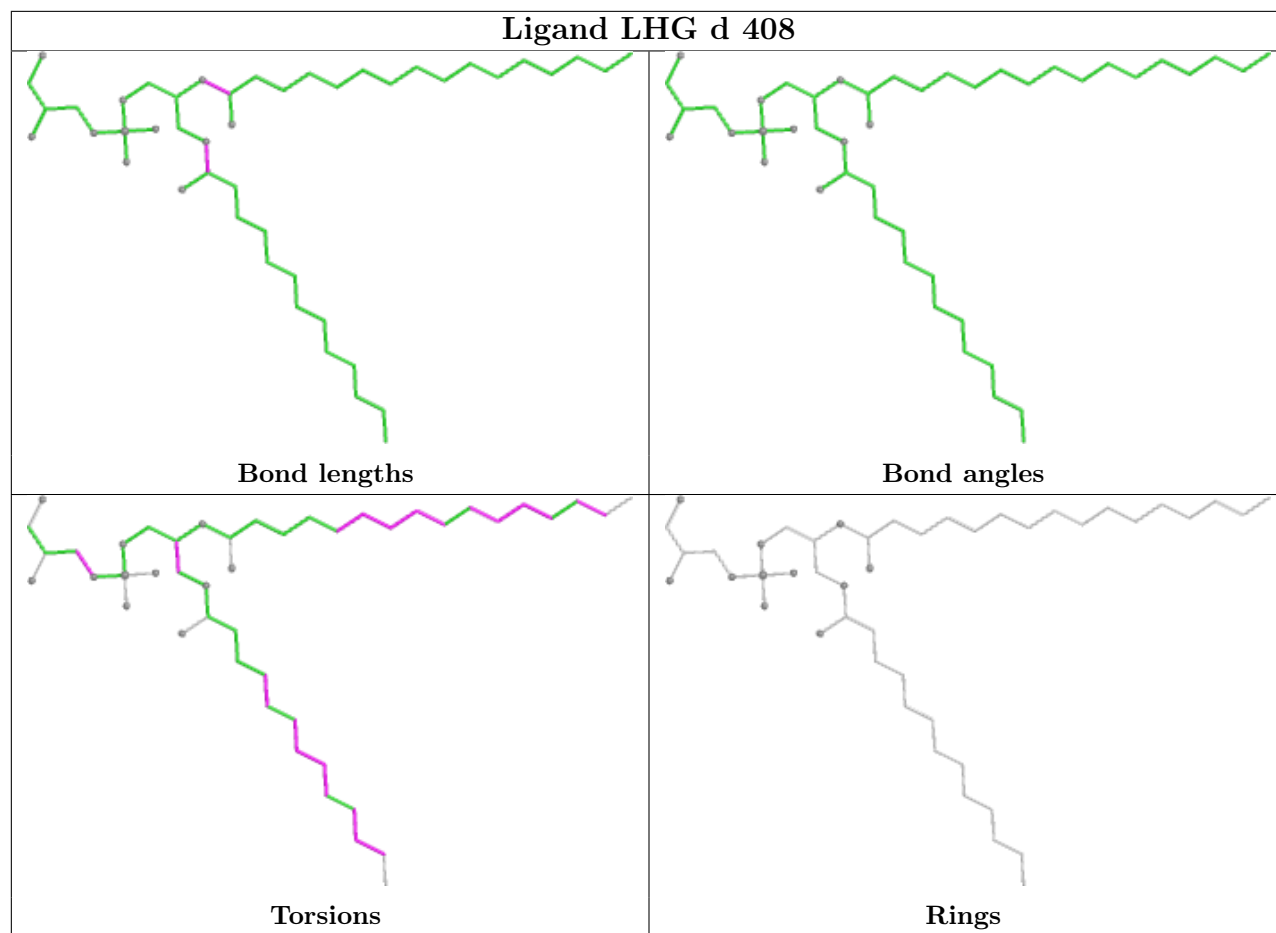


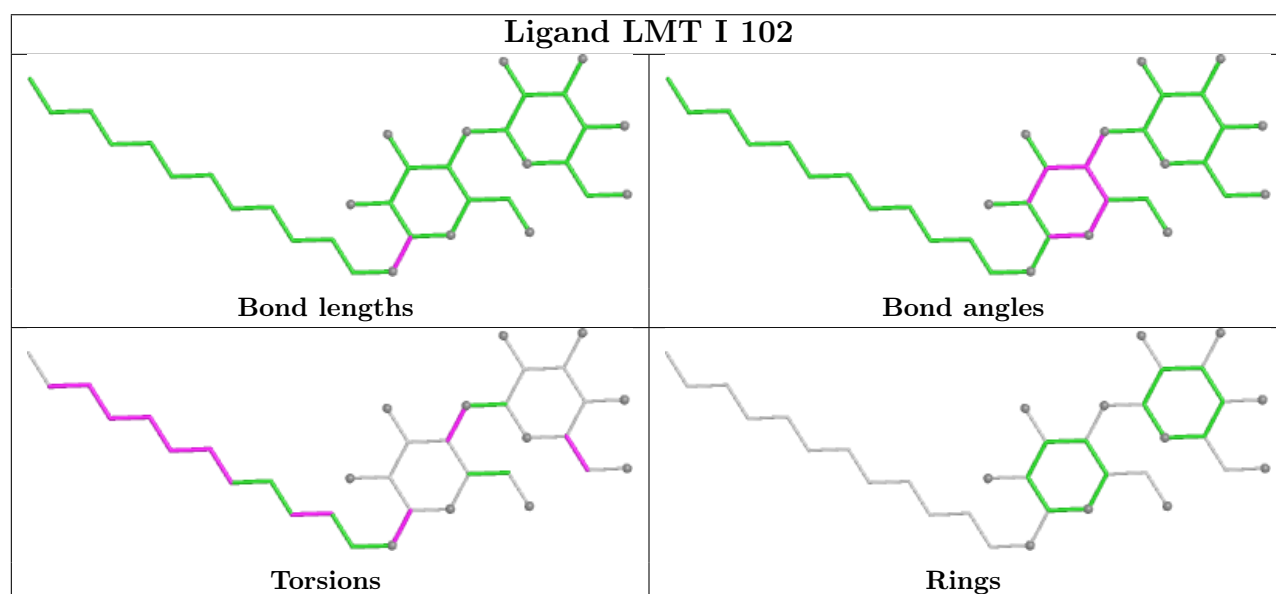
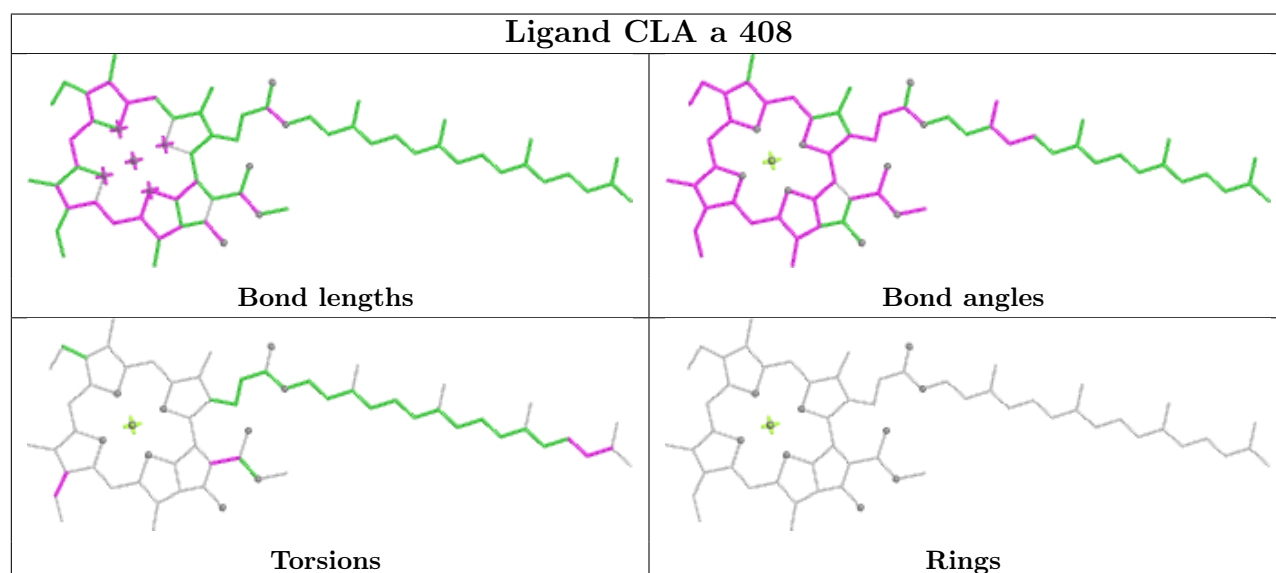
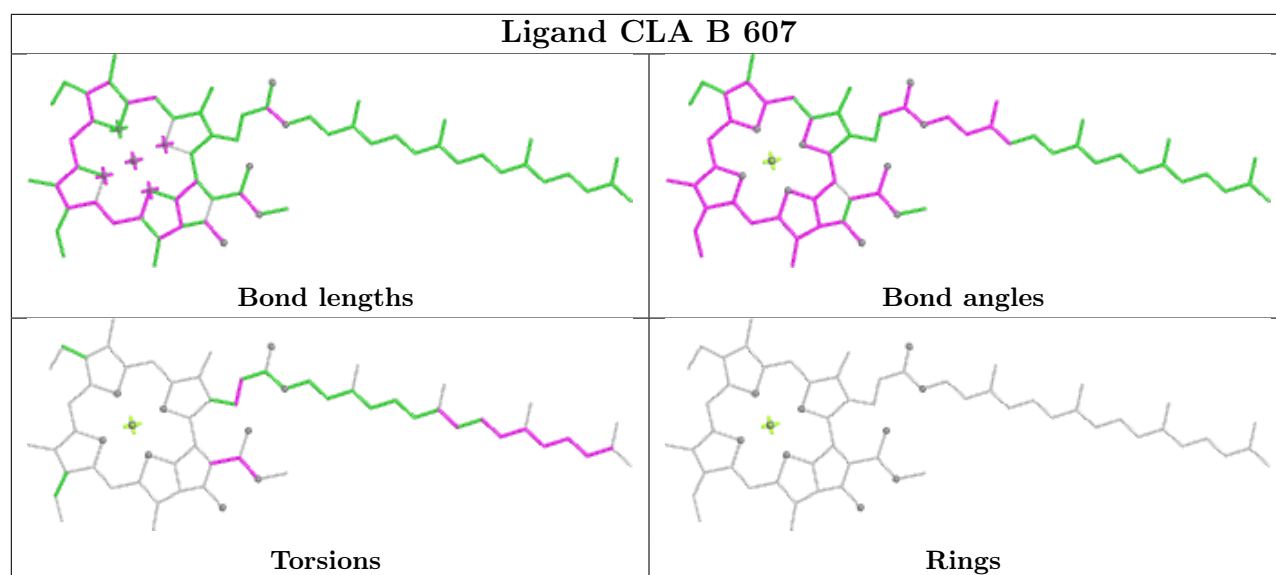


| Ligand LMG i 101                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

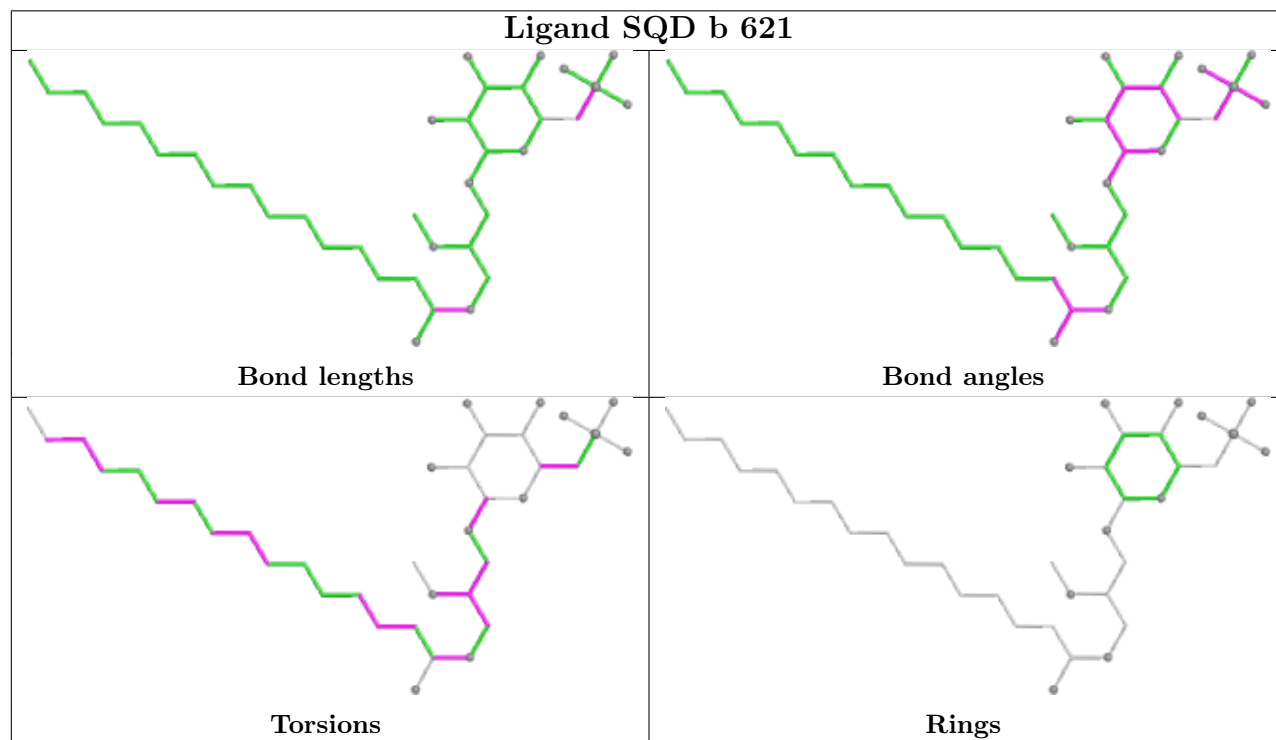
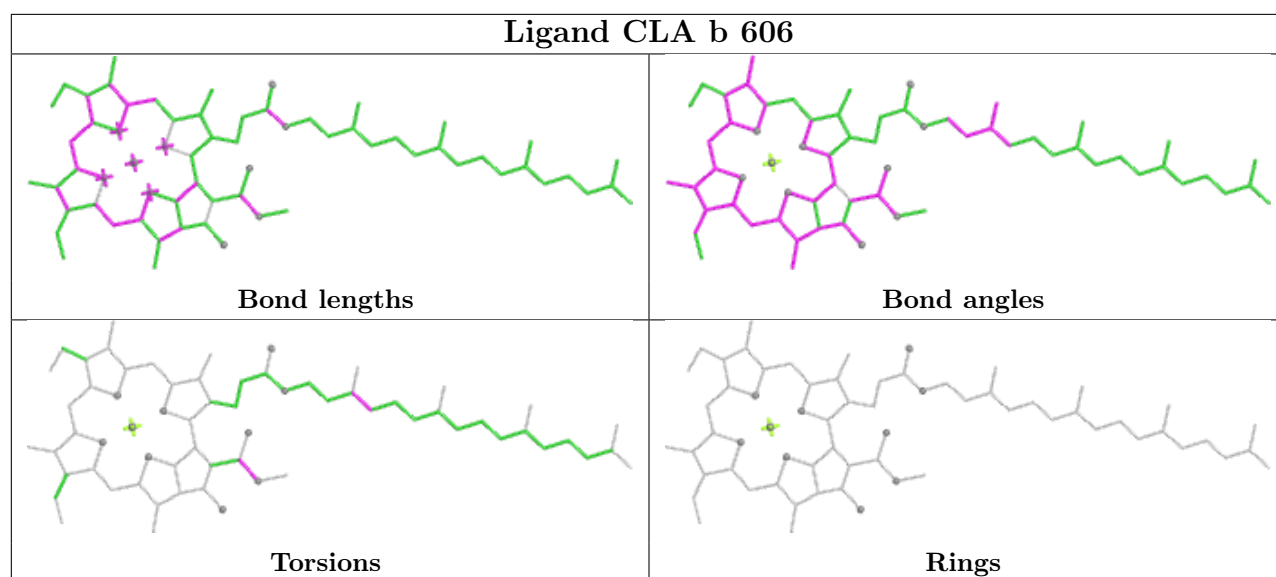
| Ligand BCR b 618                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

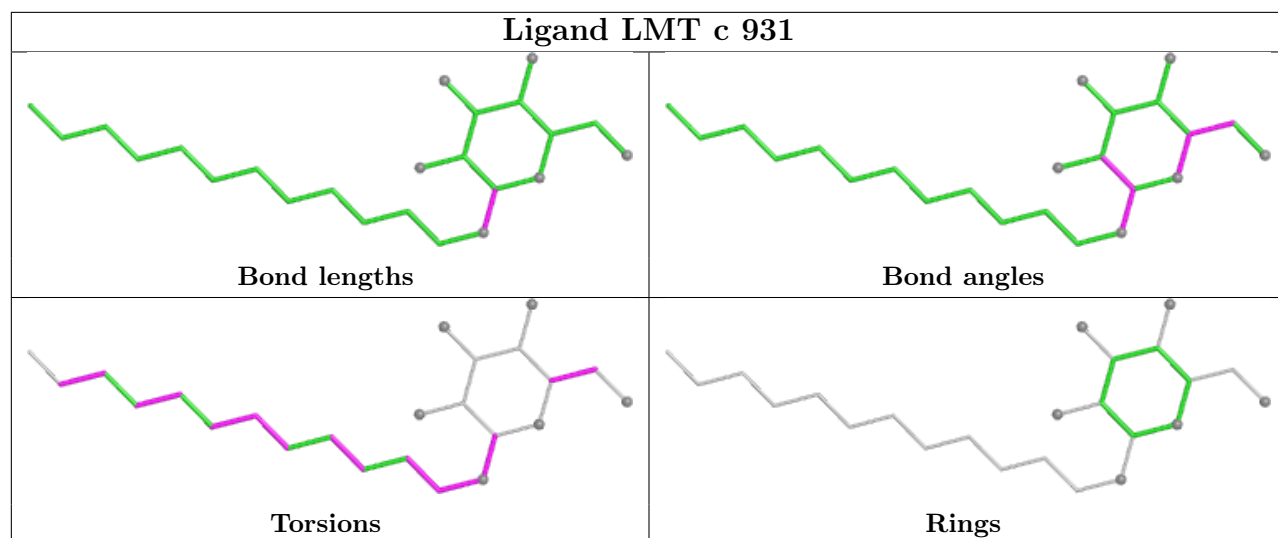
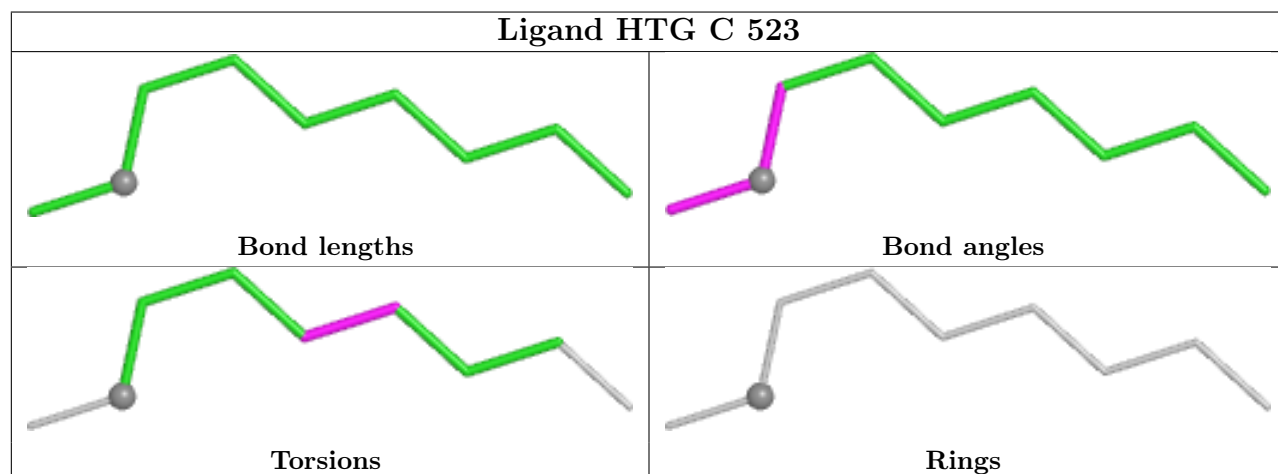
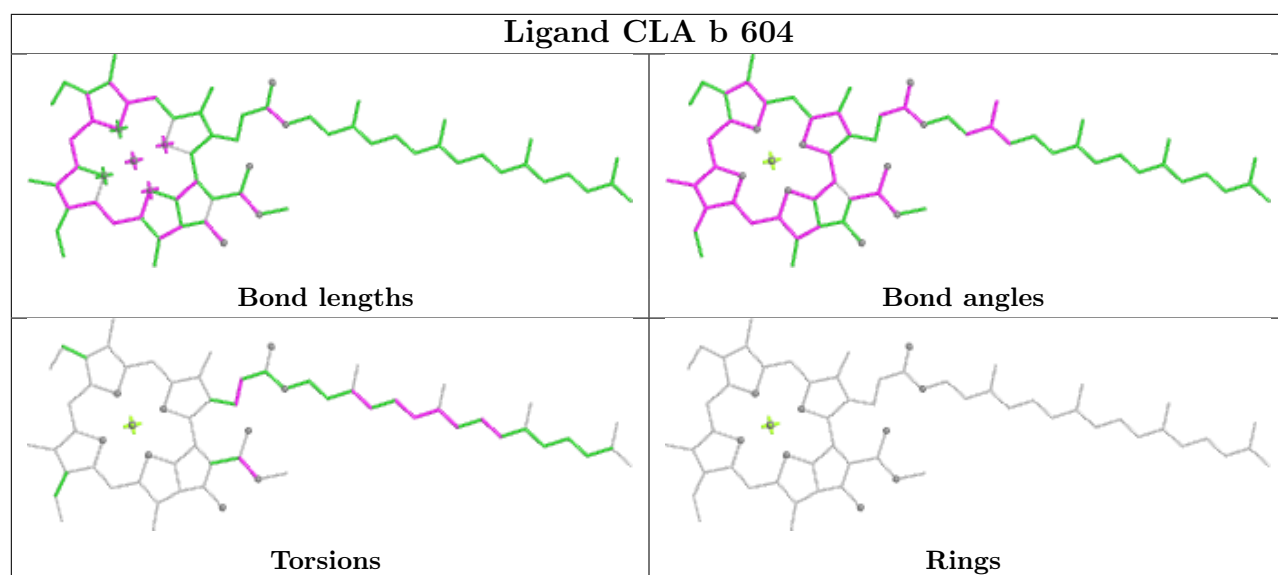
| Ligand BCR d 404                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

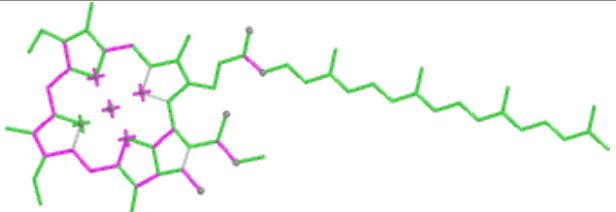
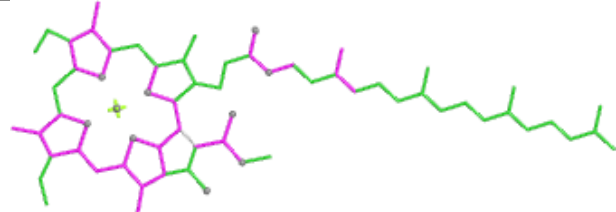
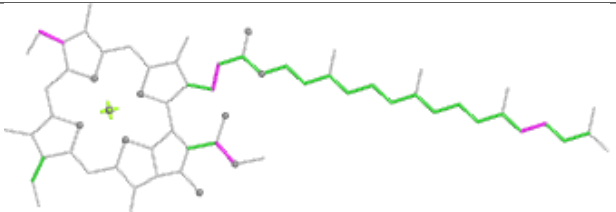
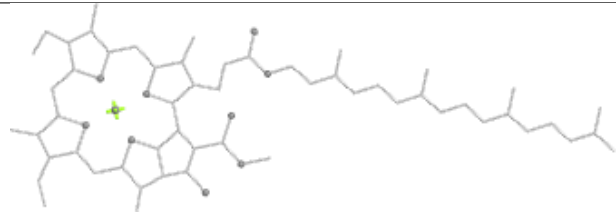


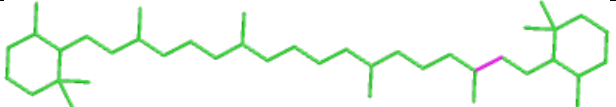
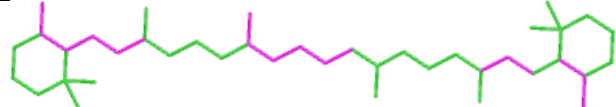
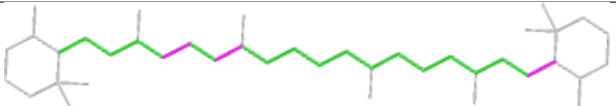
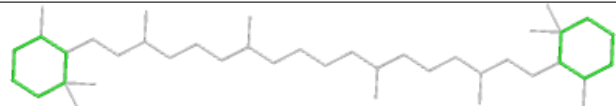


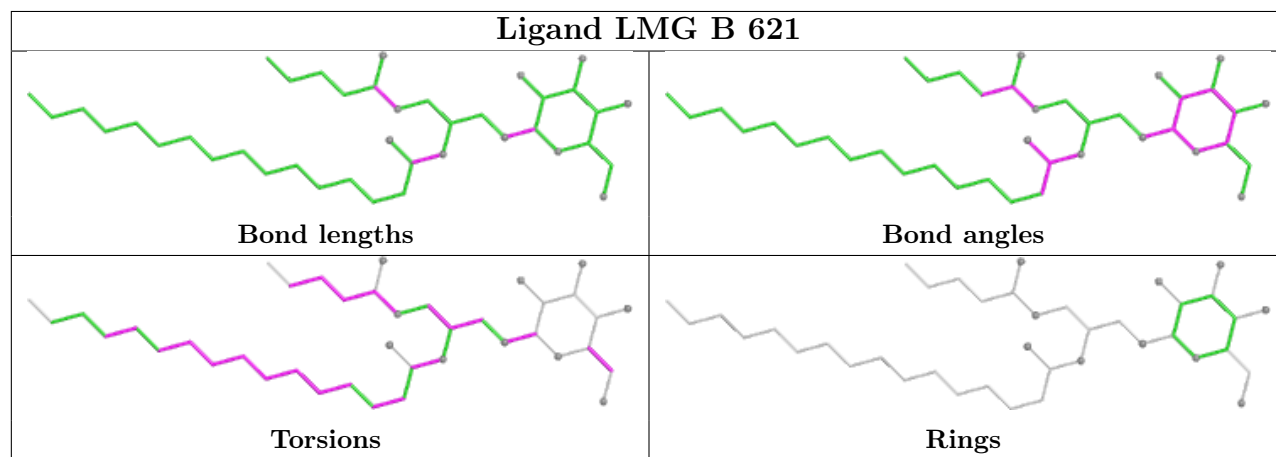
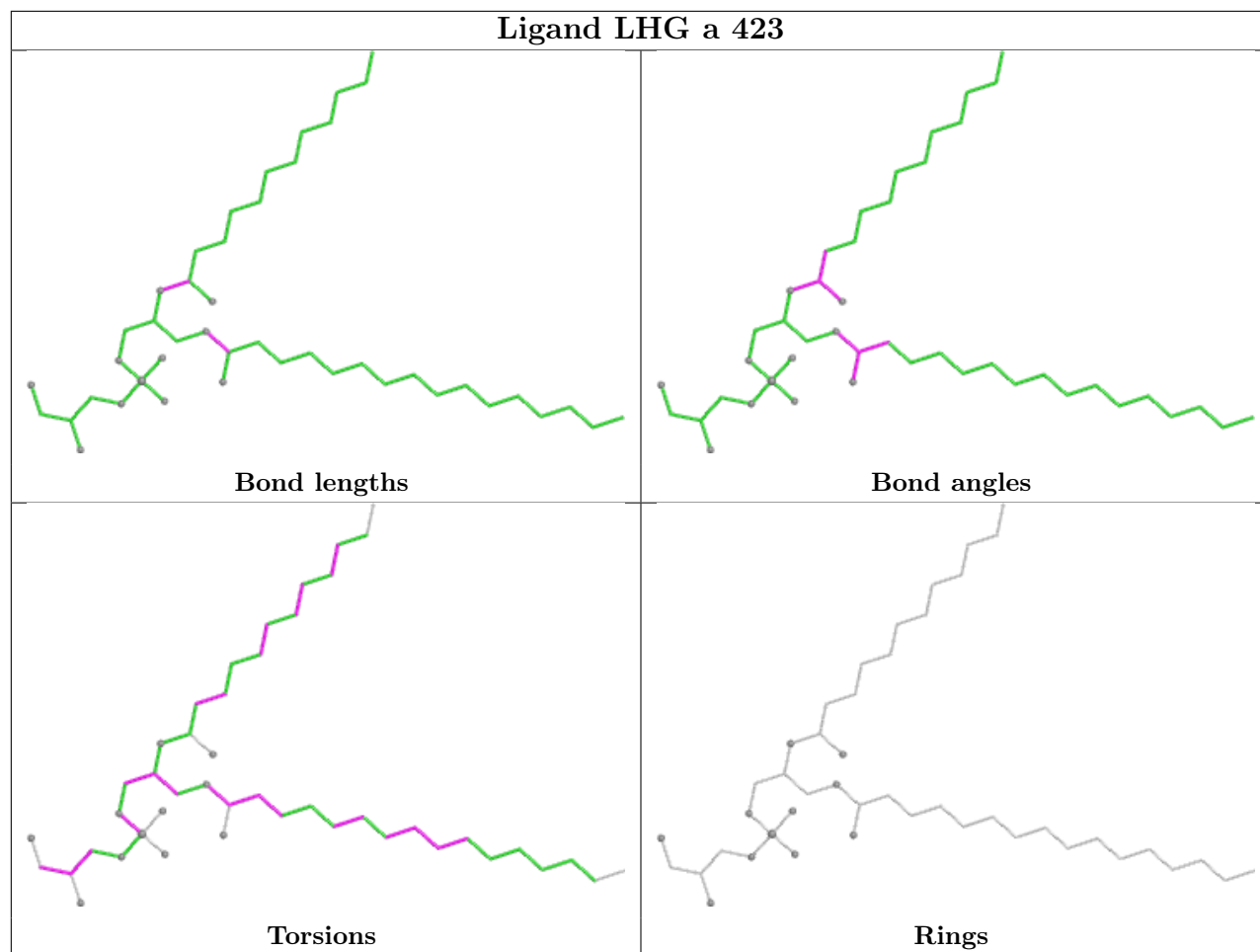


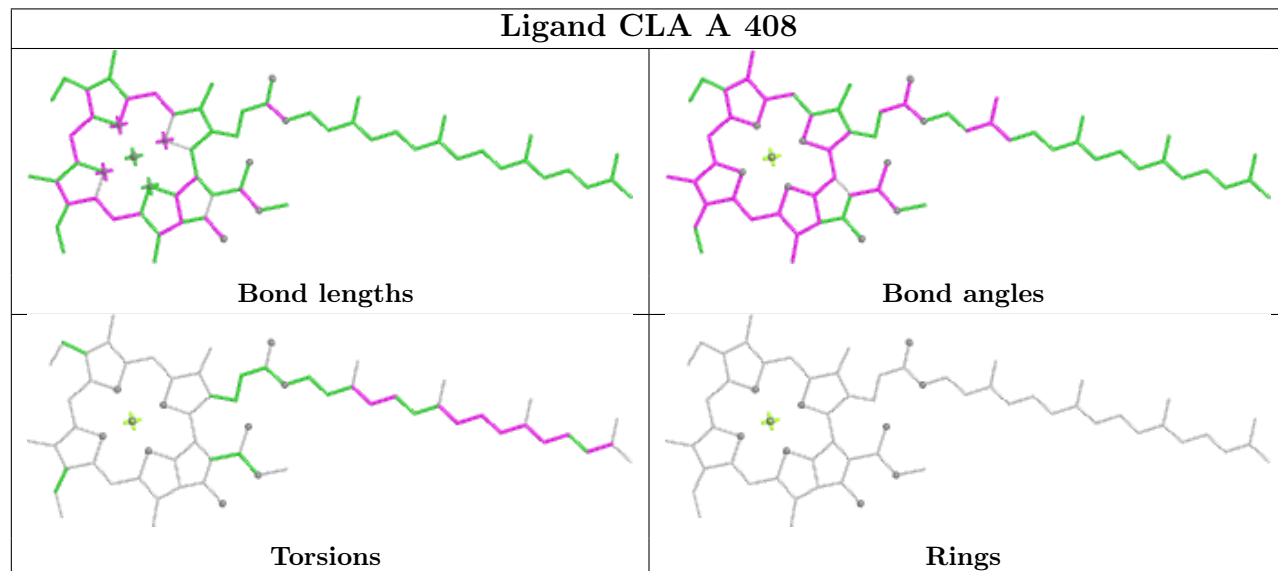
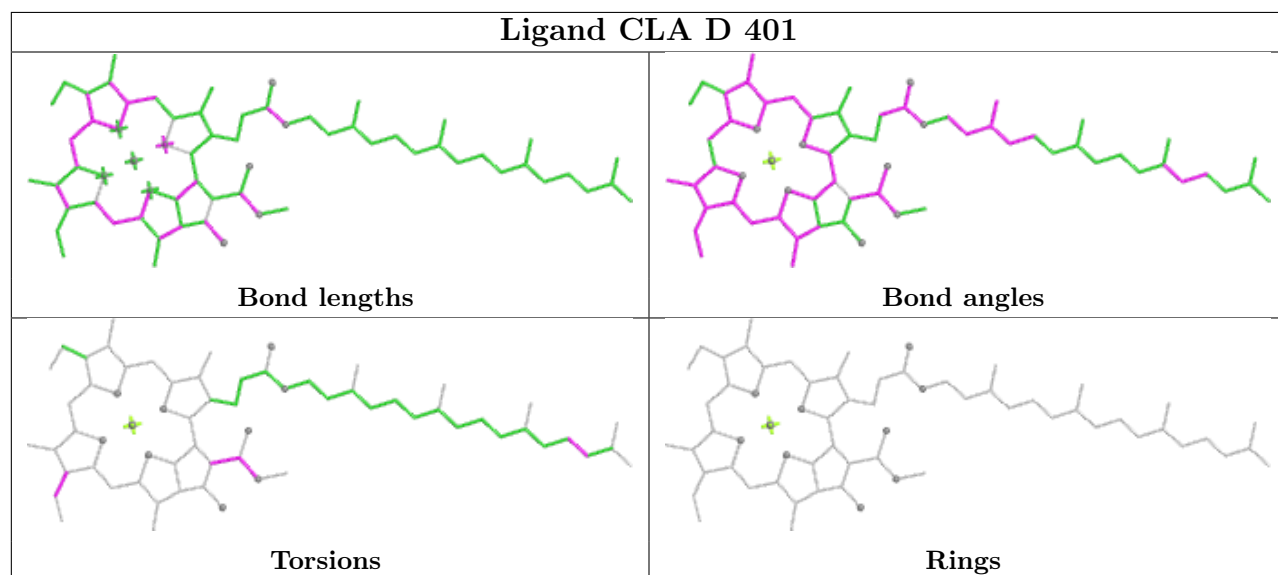
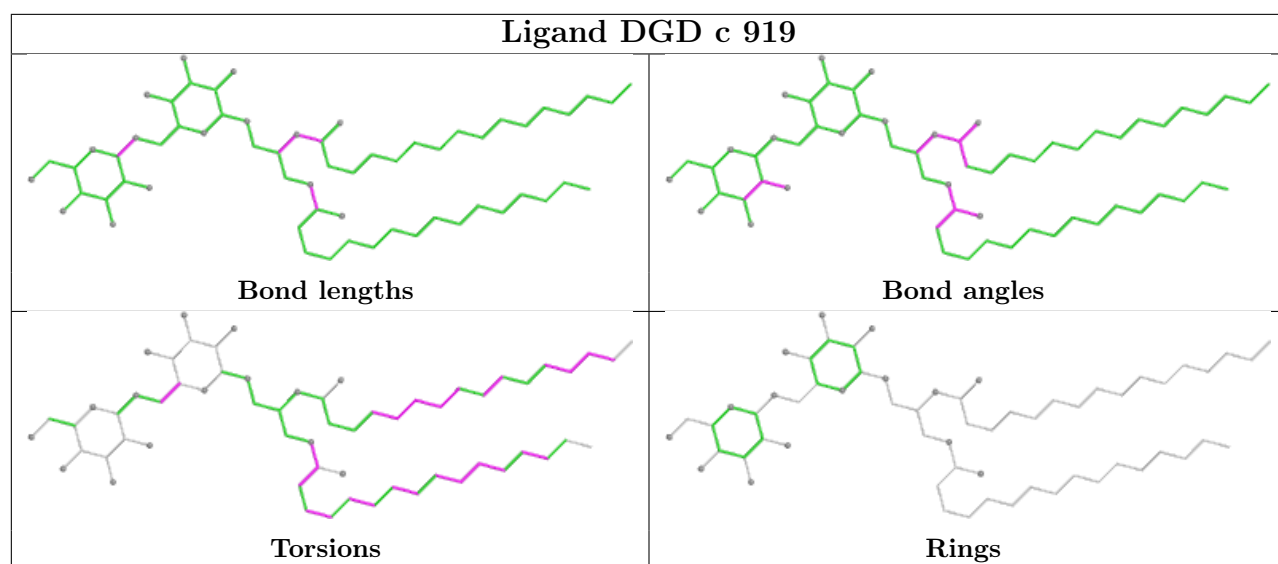




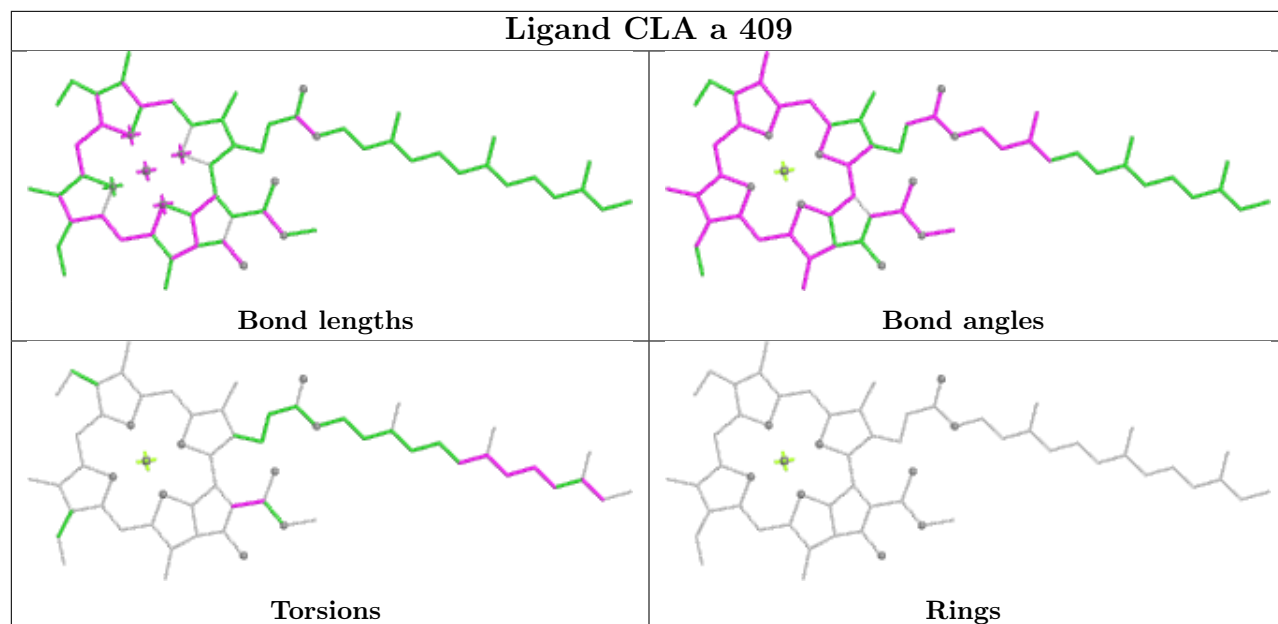
| Ligand CLA c 902                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR c 915                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

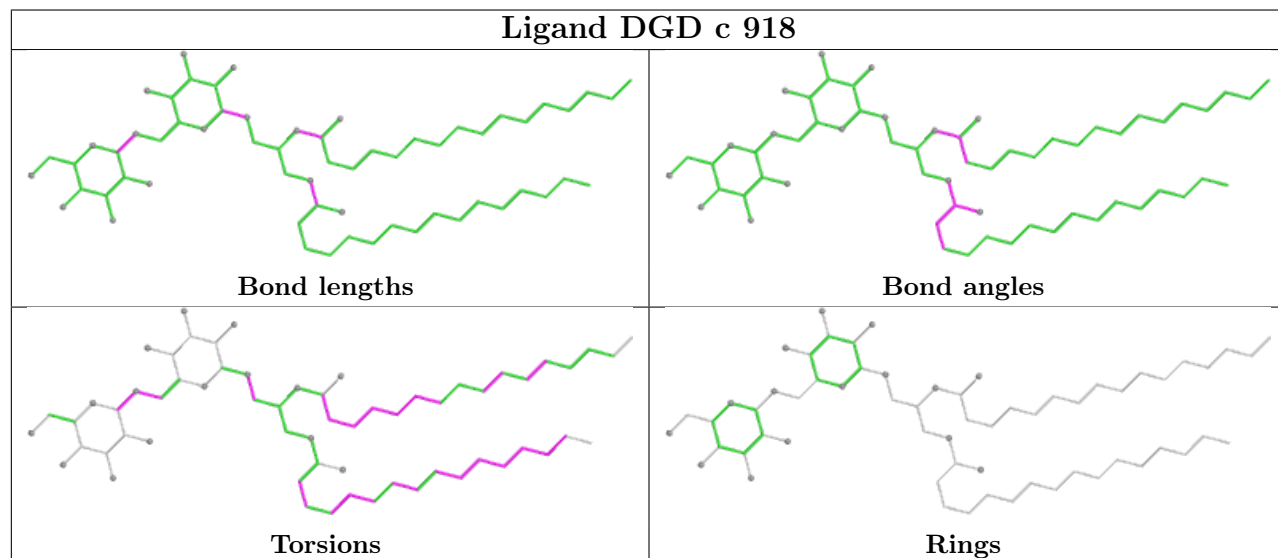




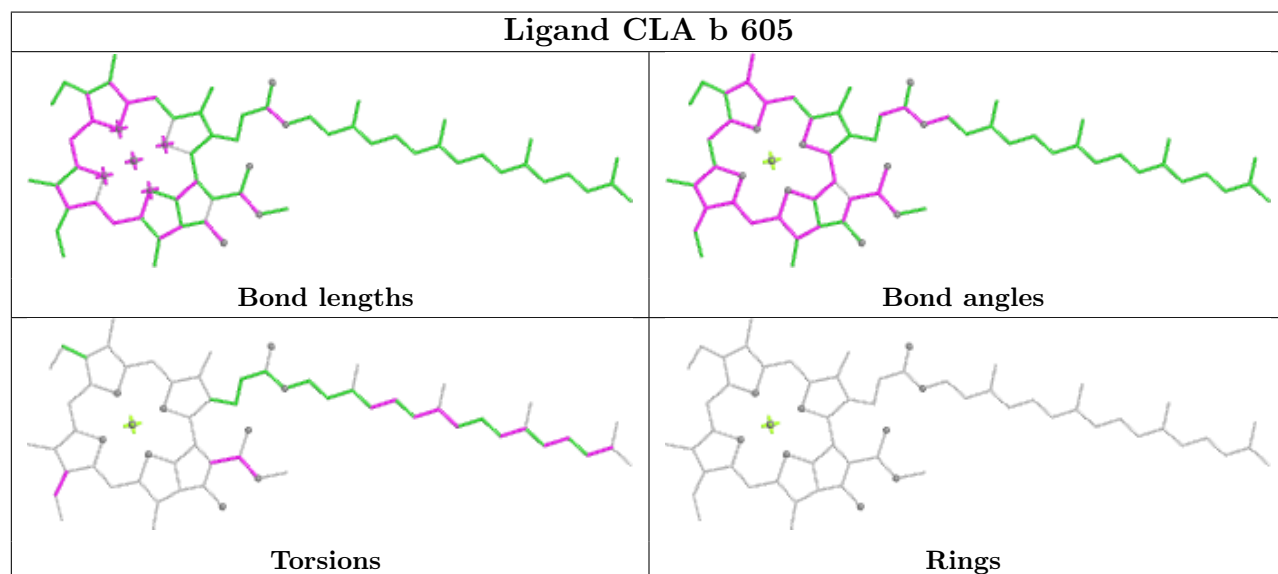
## Ligand CLA a 409

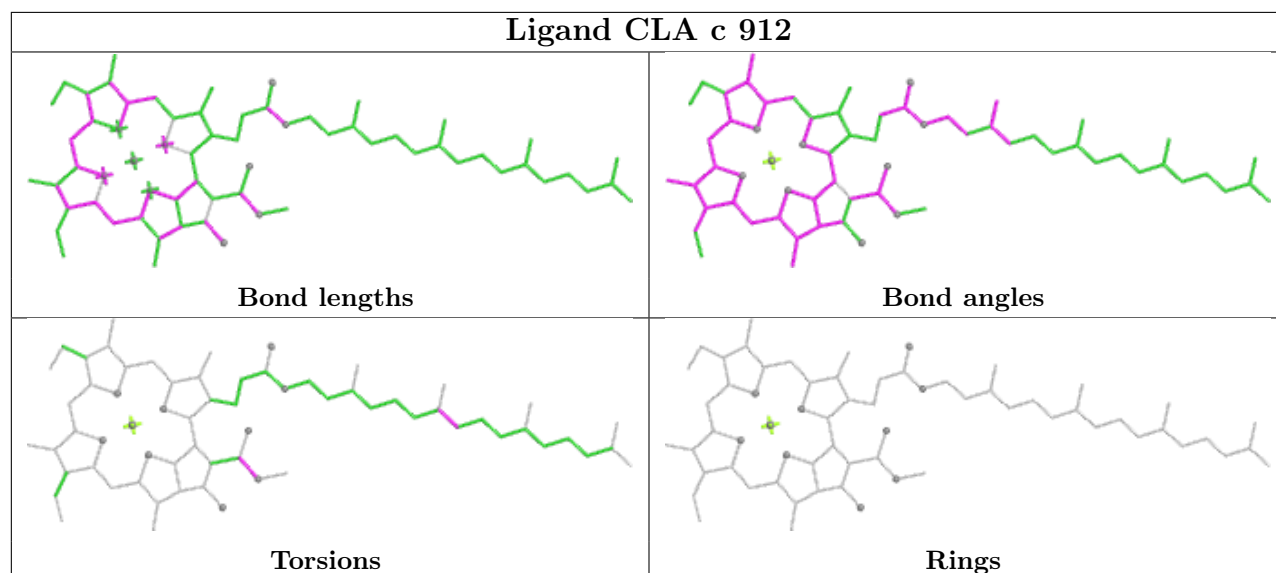
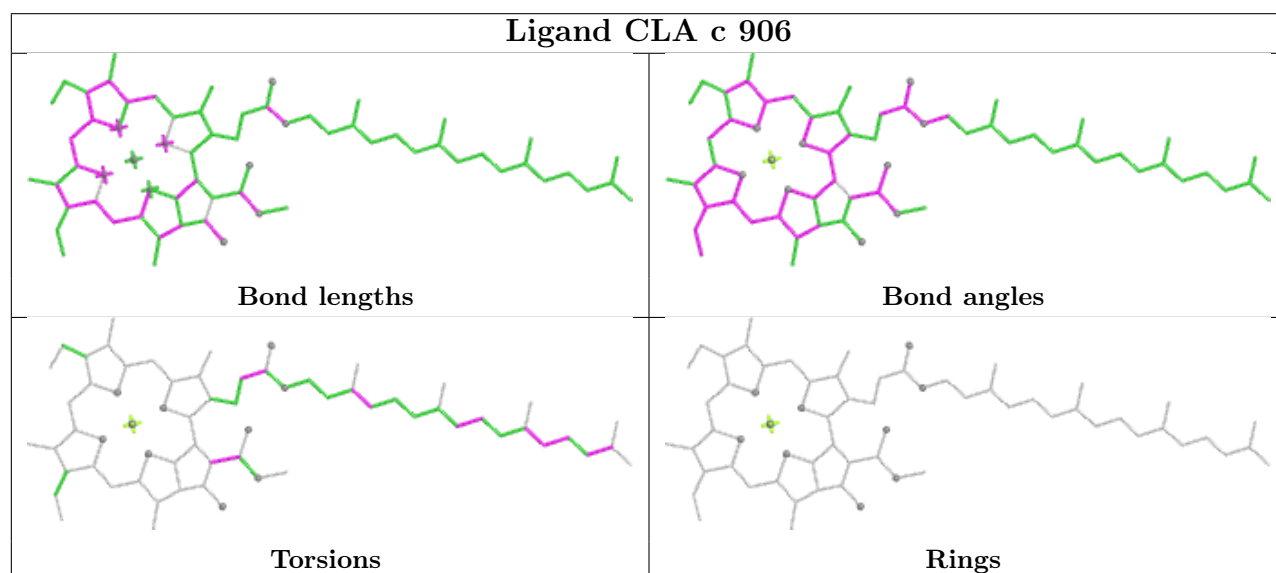
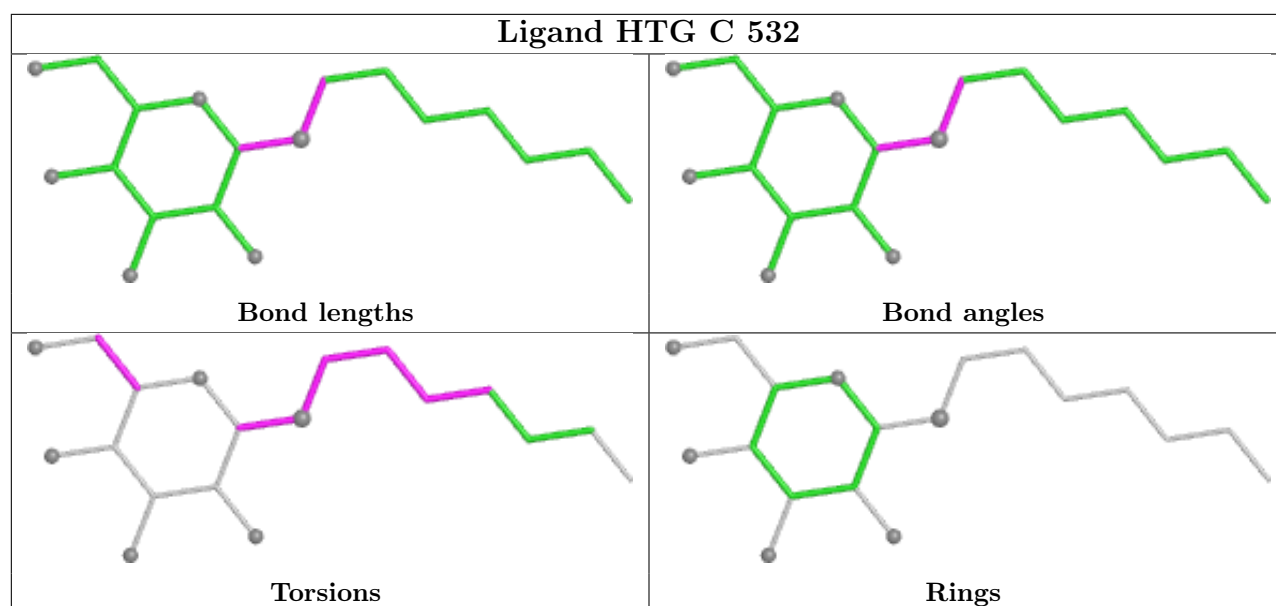


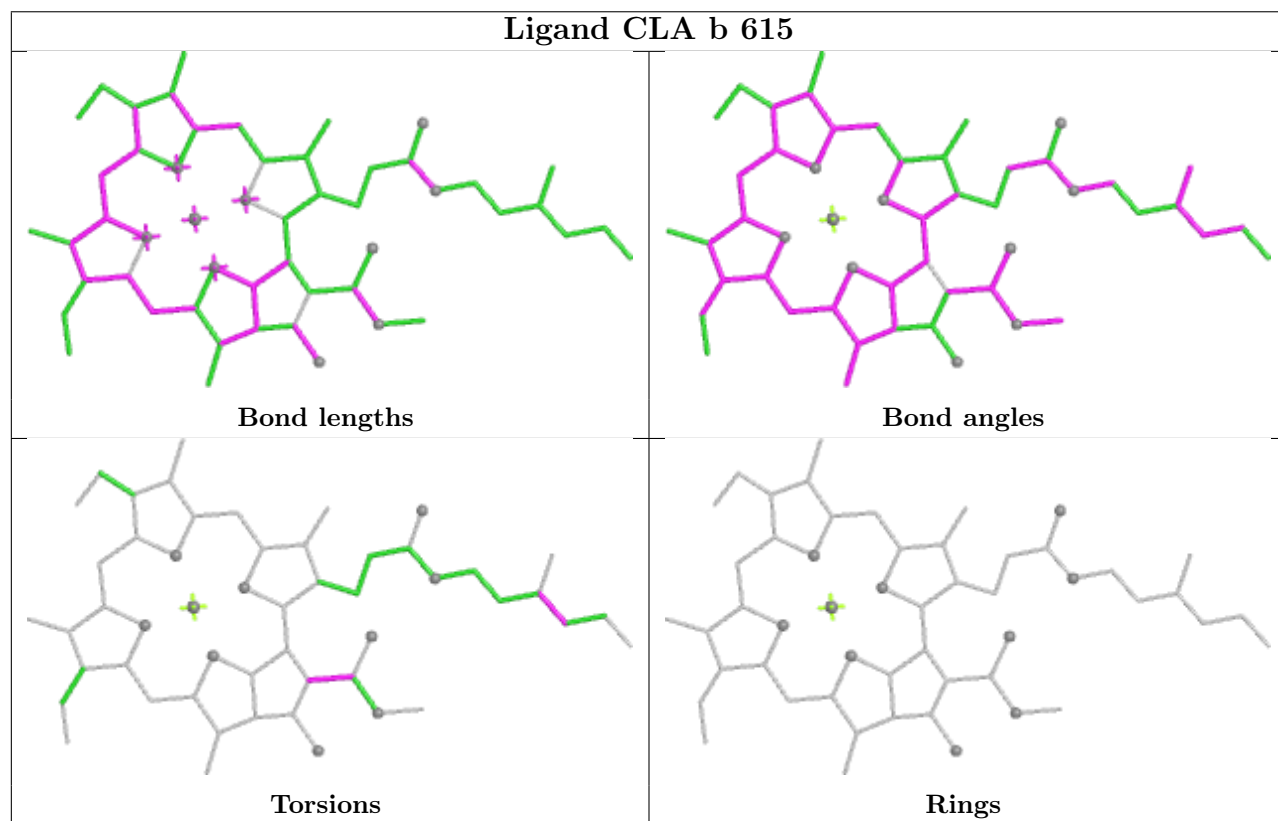
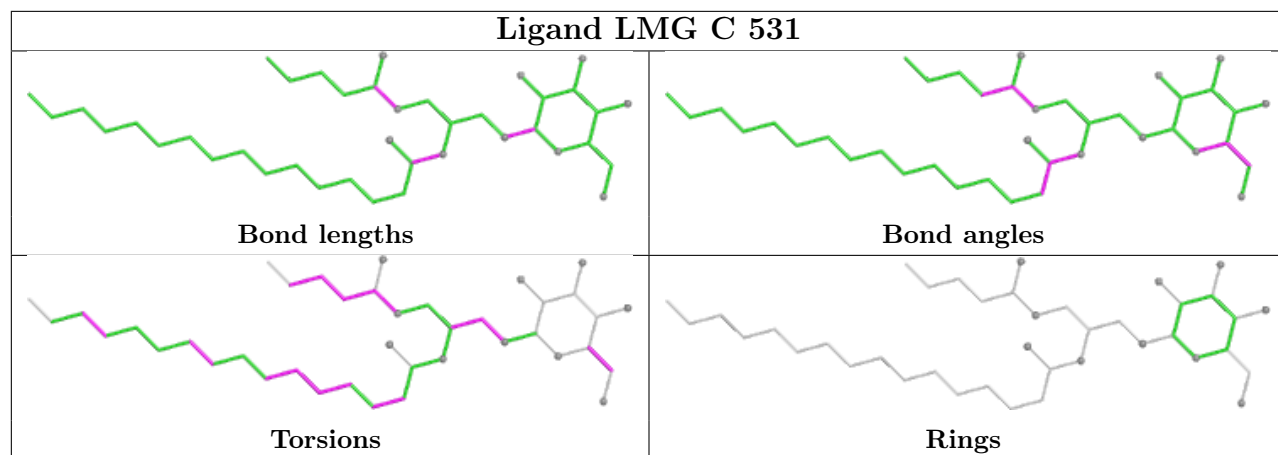
## Ligand DGD c 918



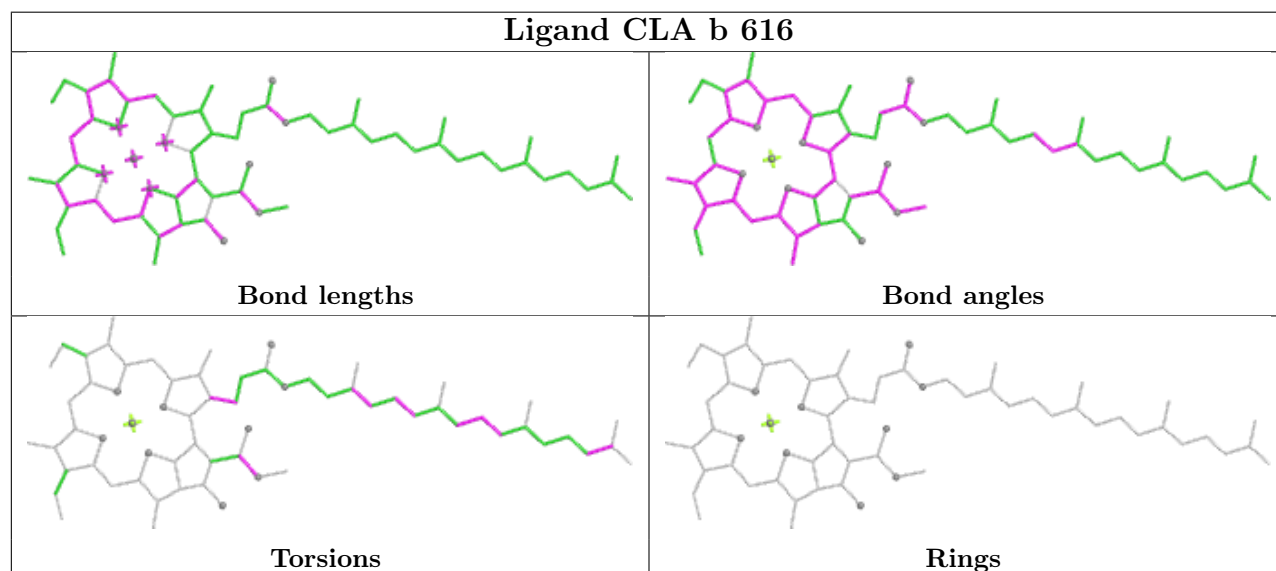
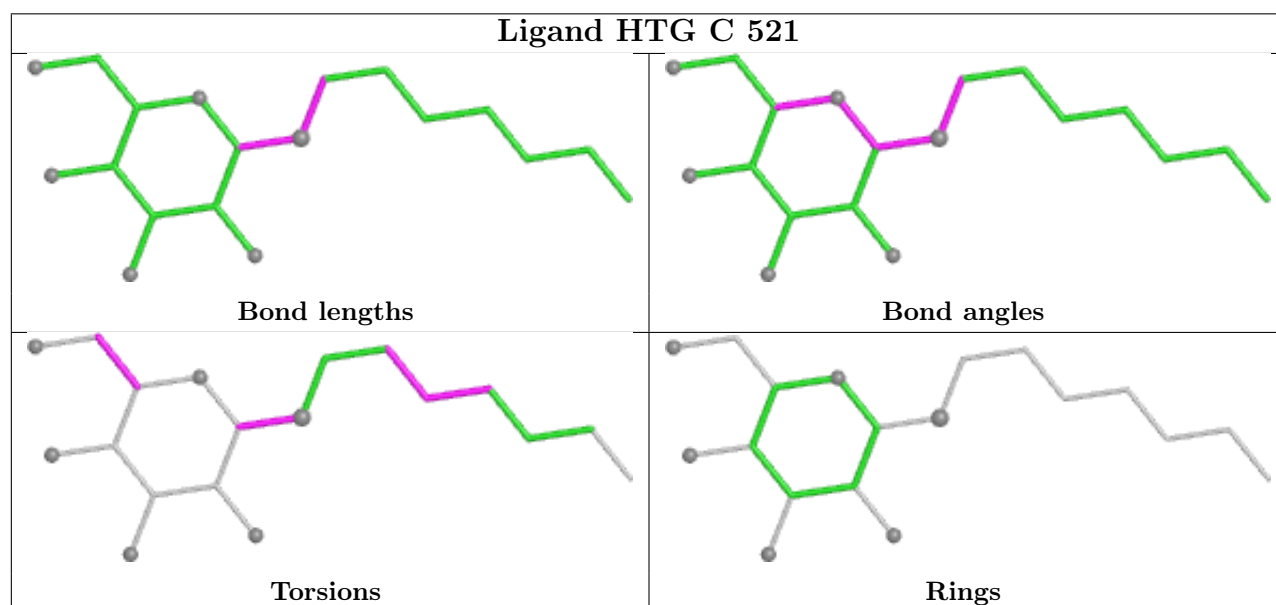
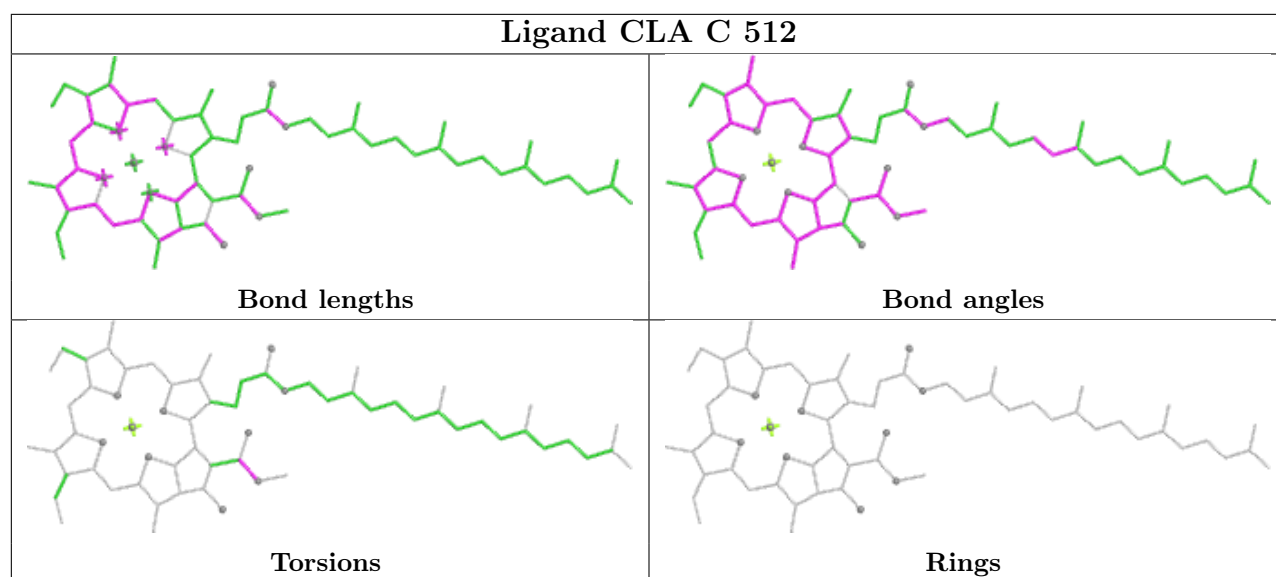
## Ligand CLA b 605



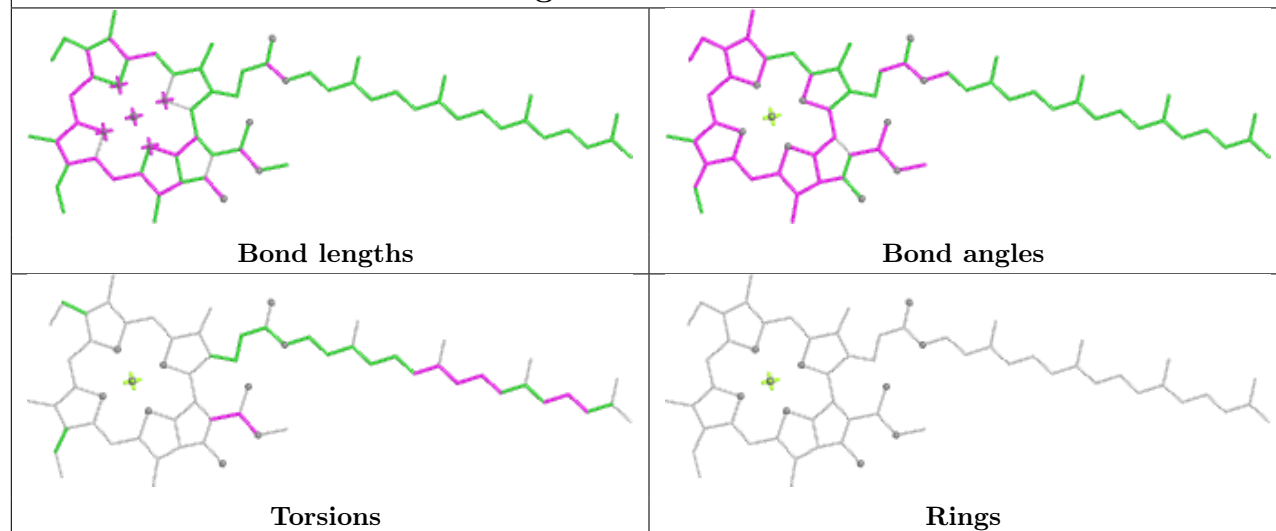




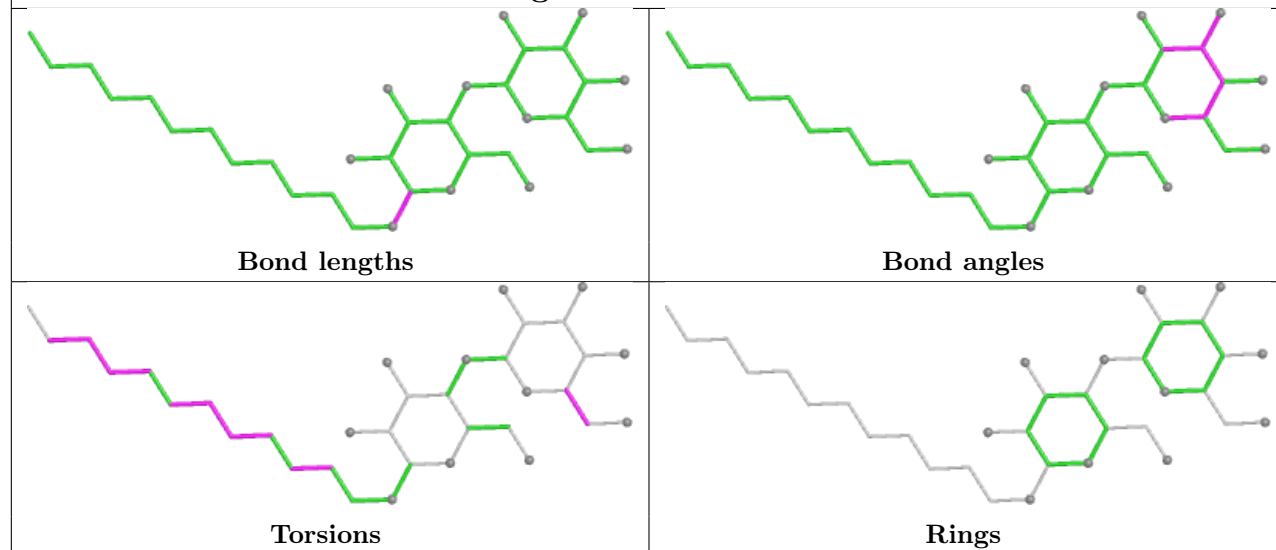




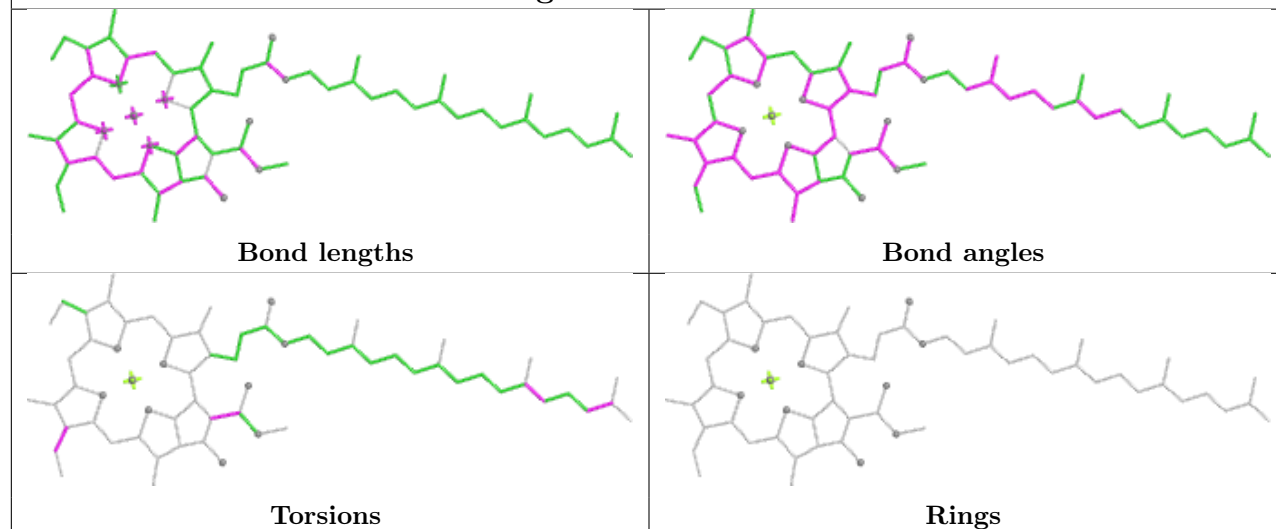
## Ligand CLA d 403

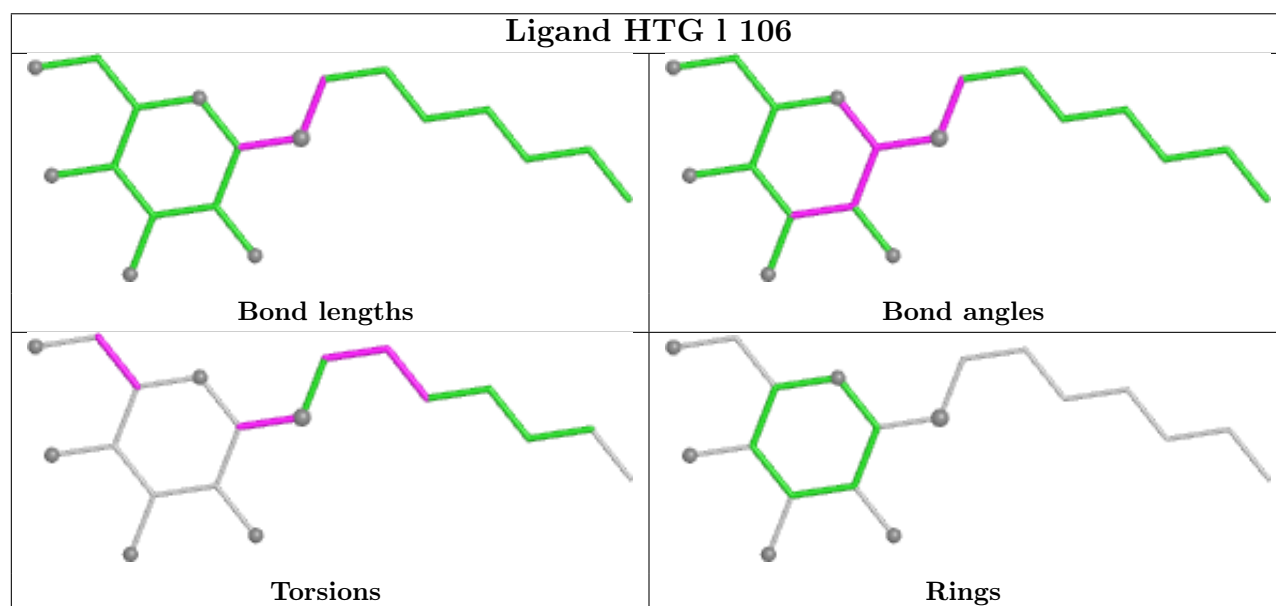
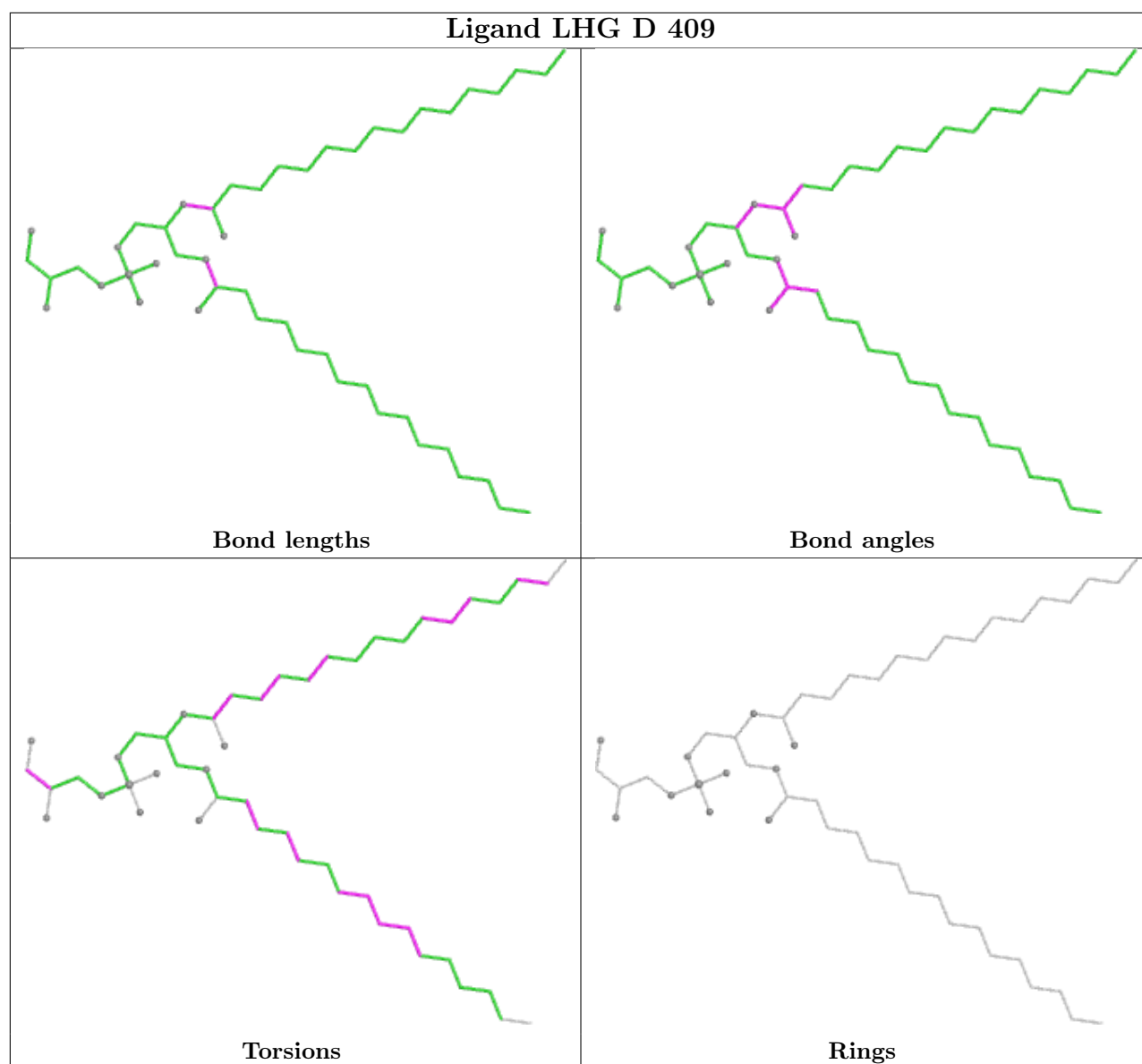


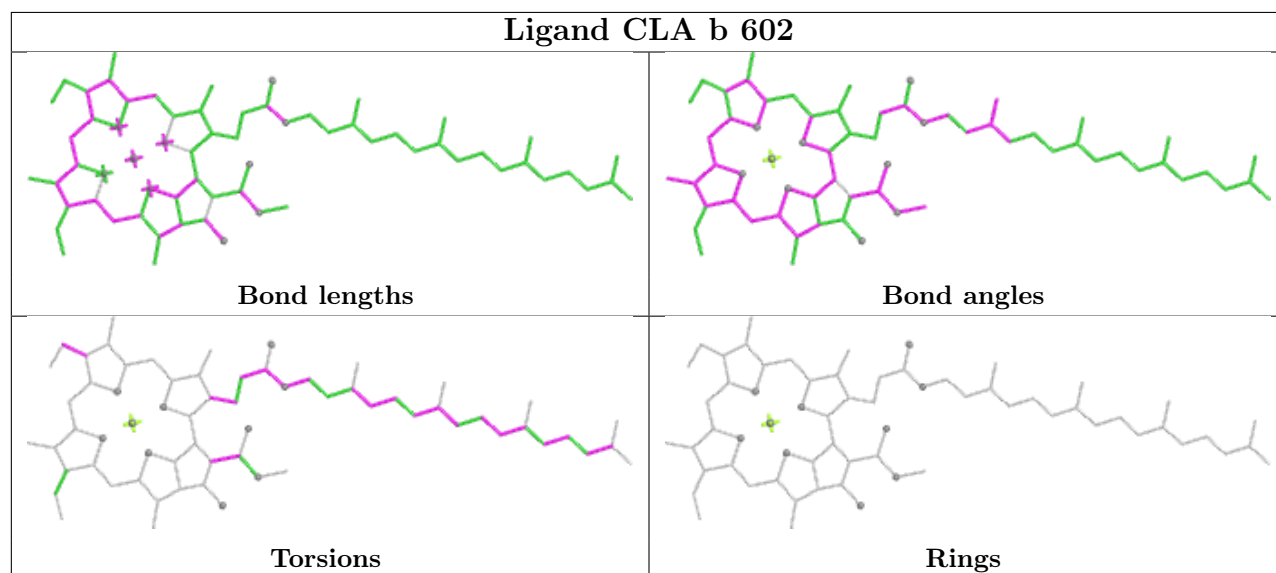
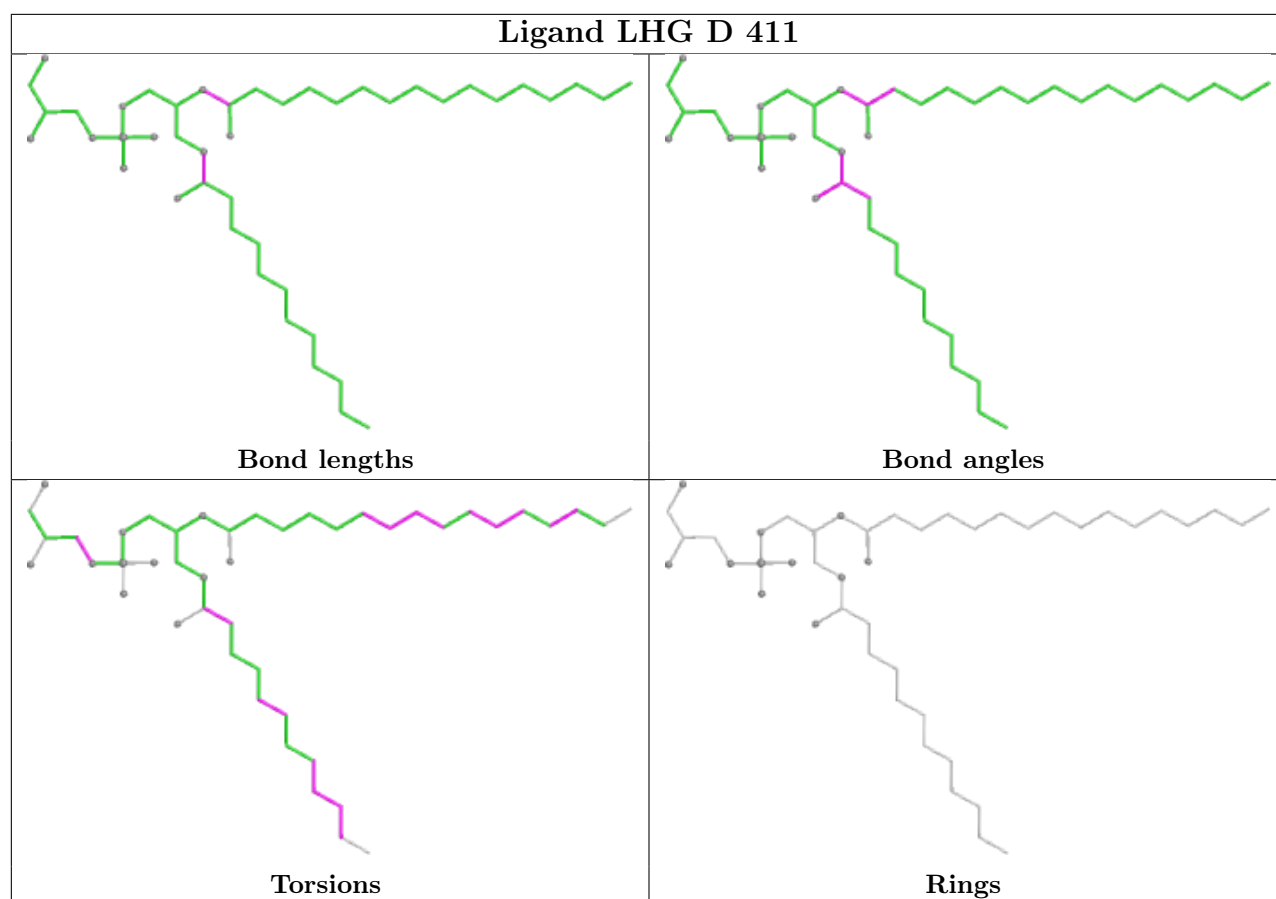
## Ligand LMT Z 101

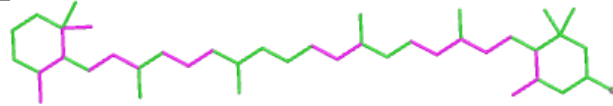
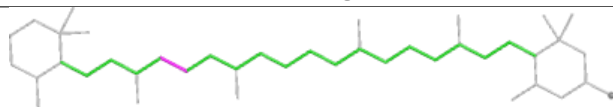
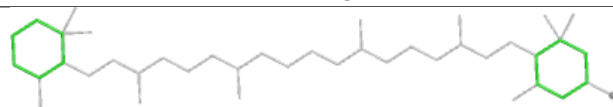


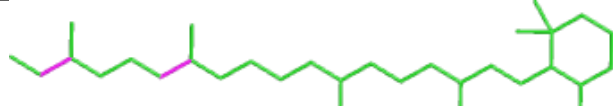
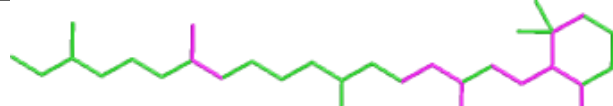
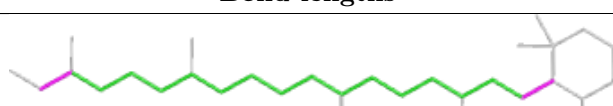
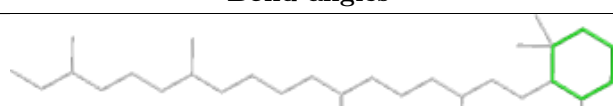
## Ligand CLA a 407



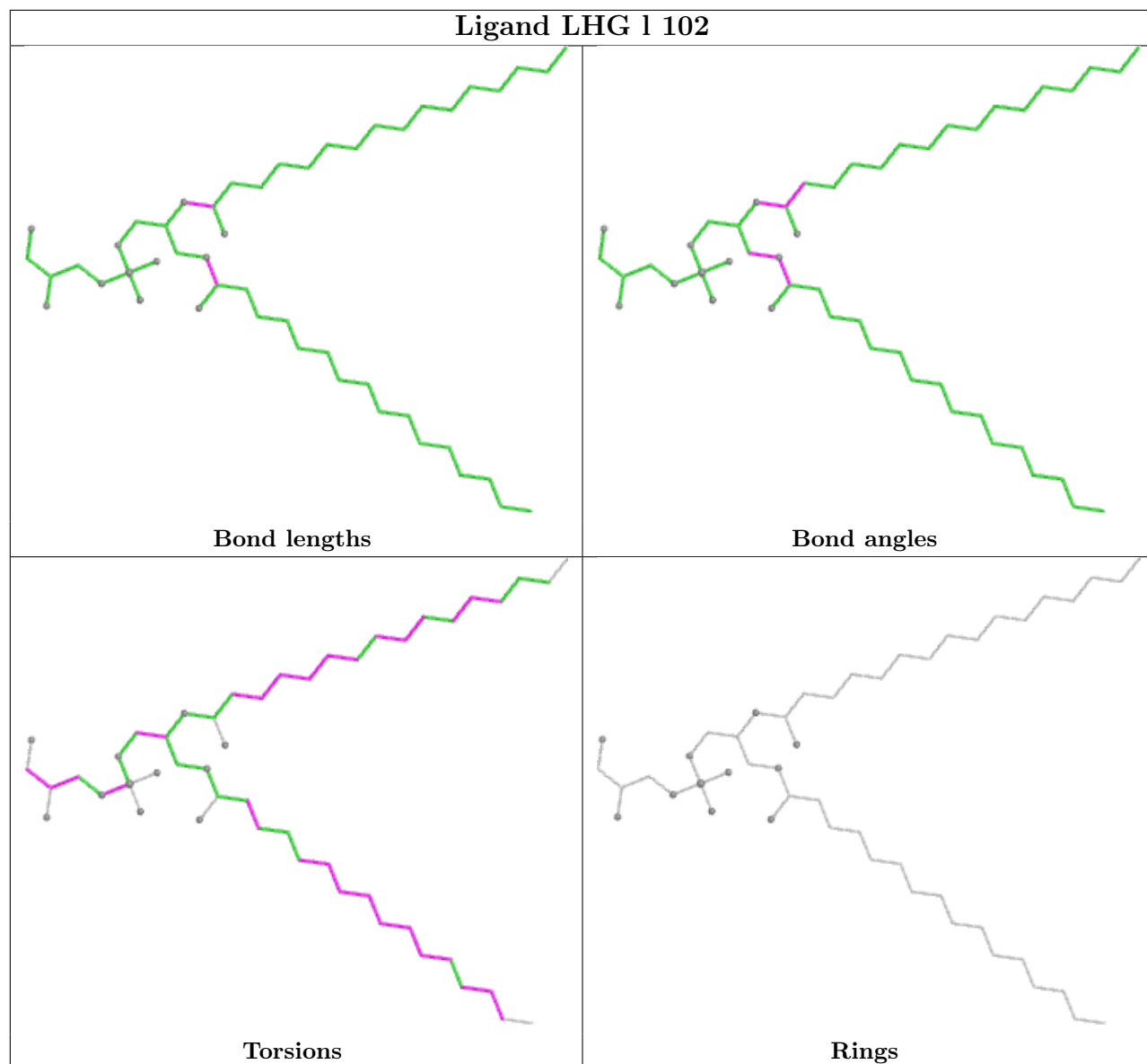




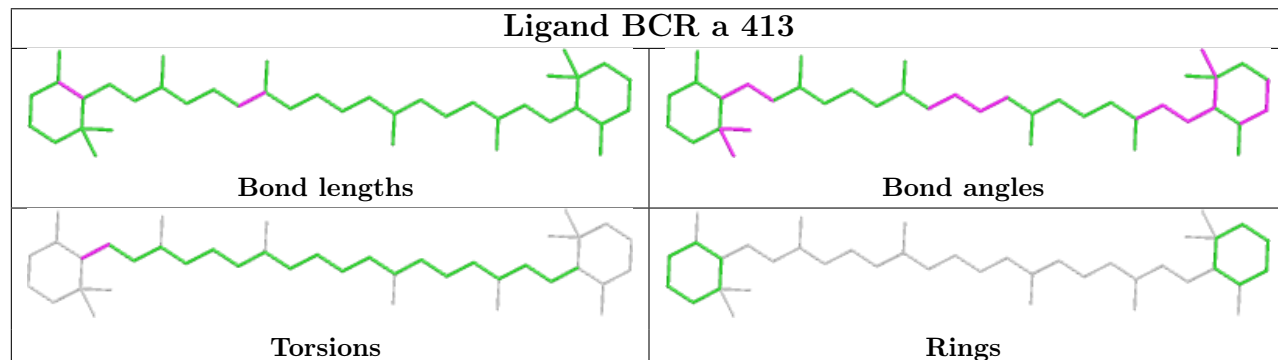
| Ligand RRX H 101                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

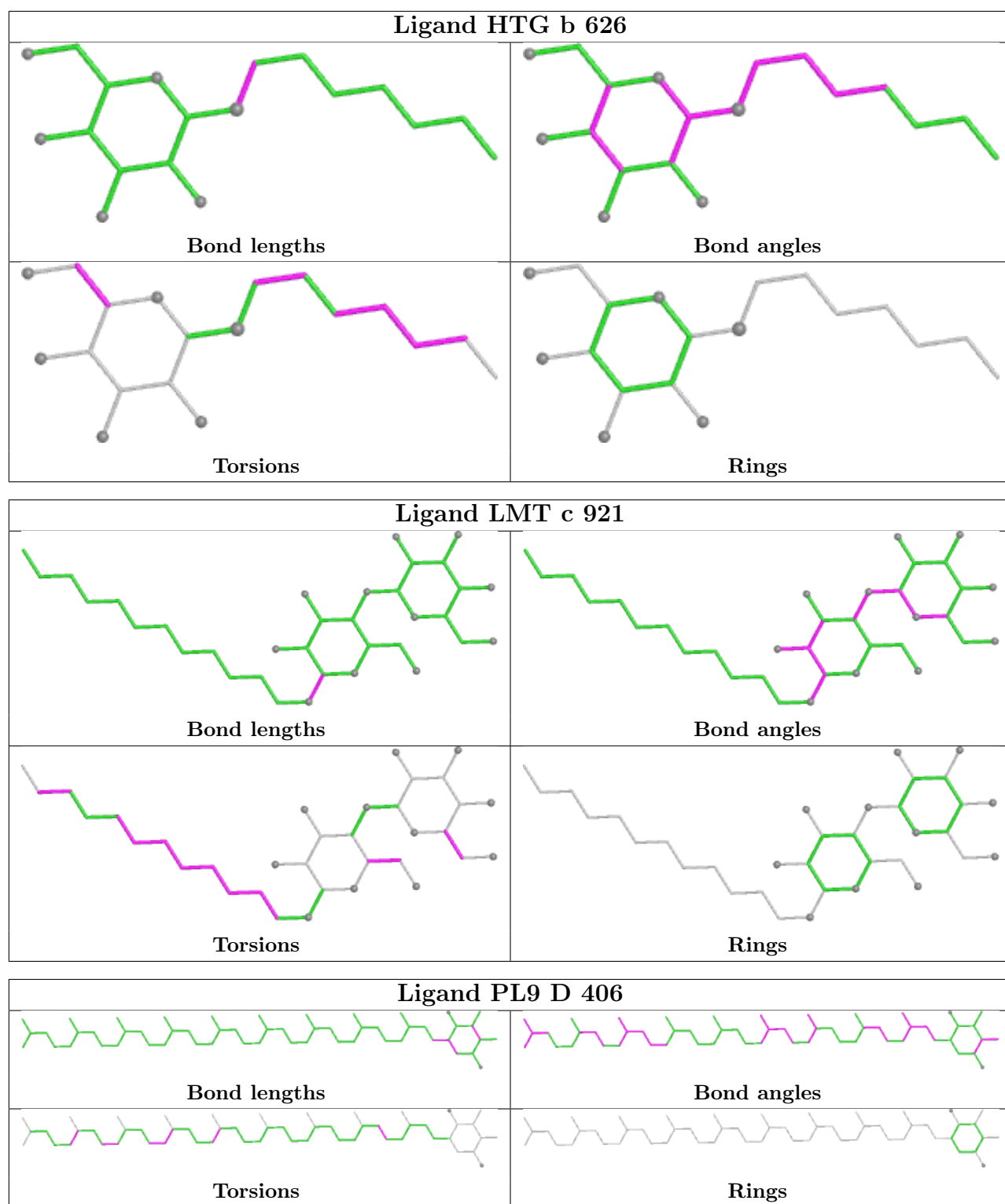
| Ligand BCR b 619                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

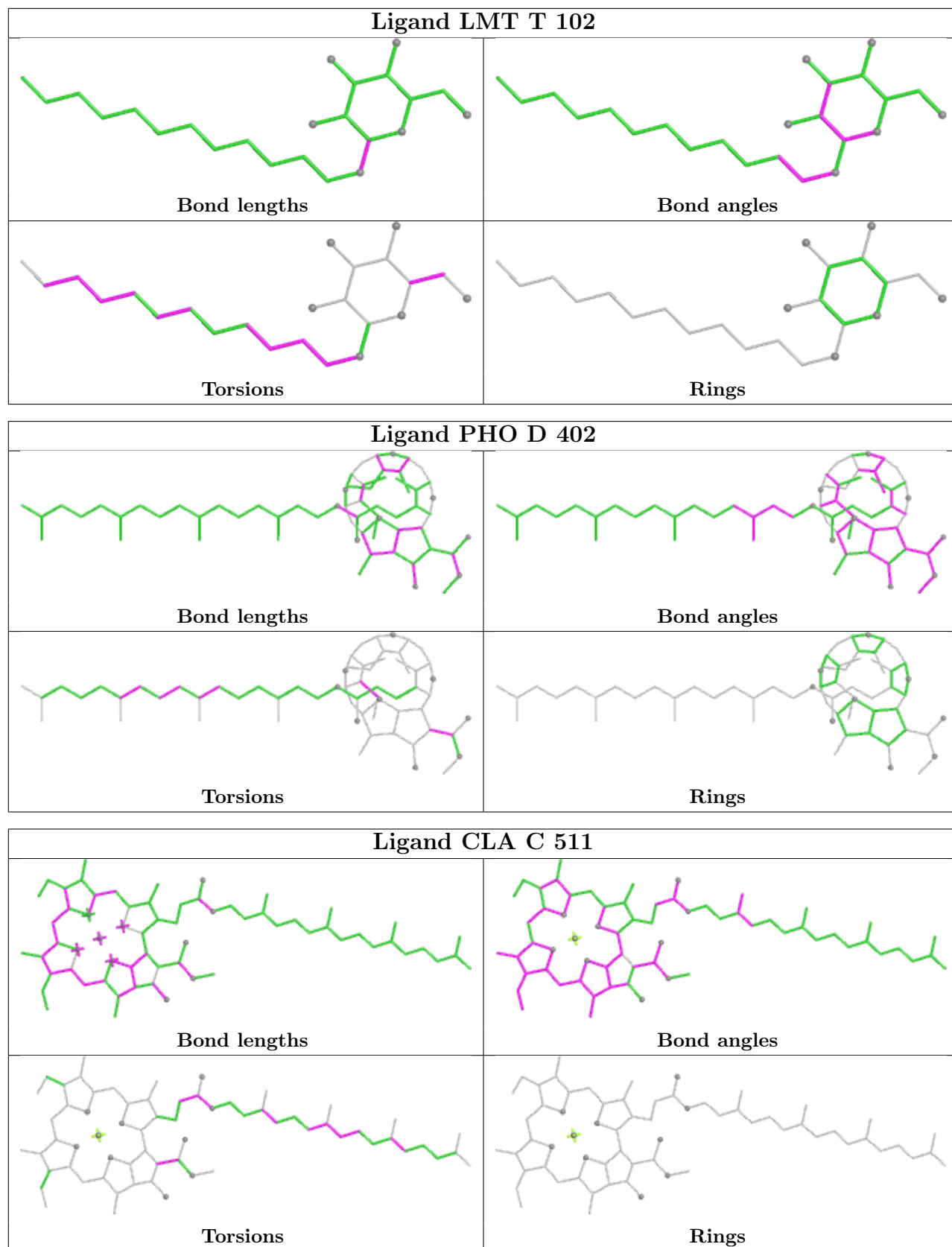
## Ligand LHG 1 102



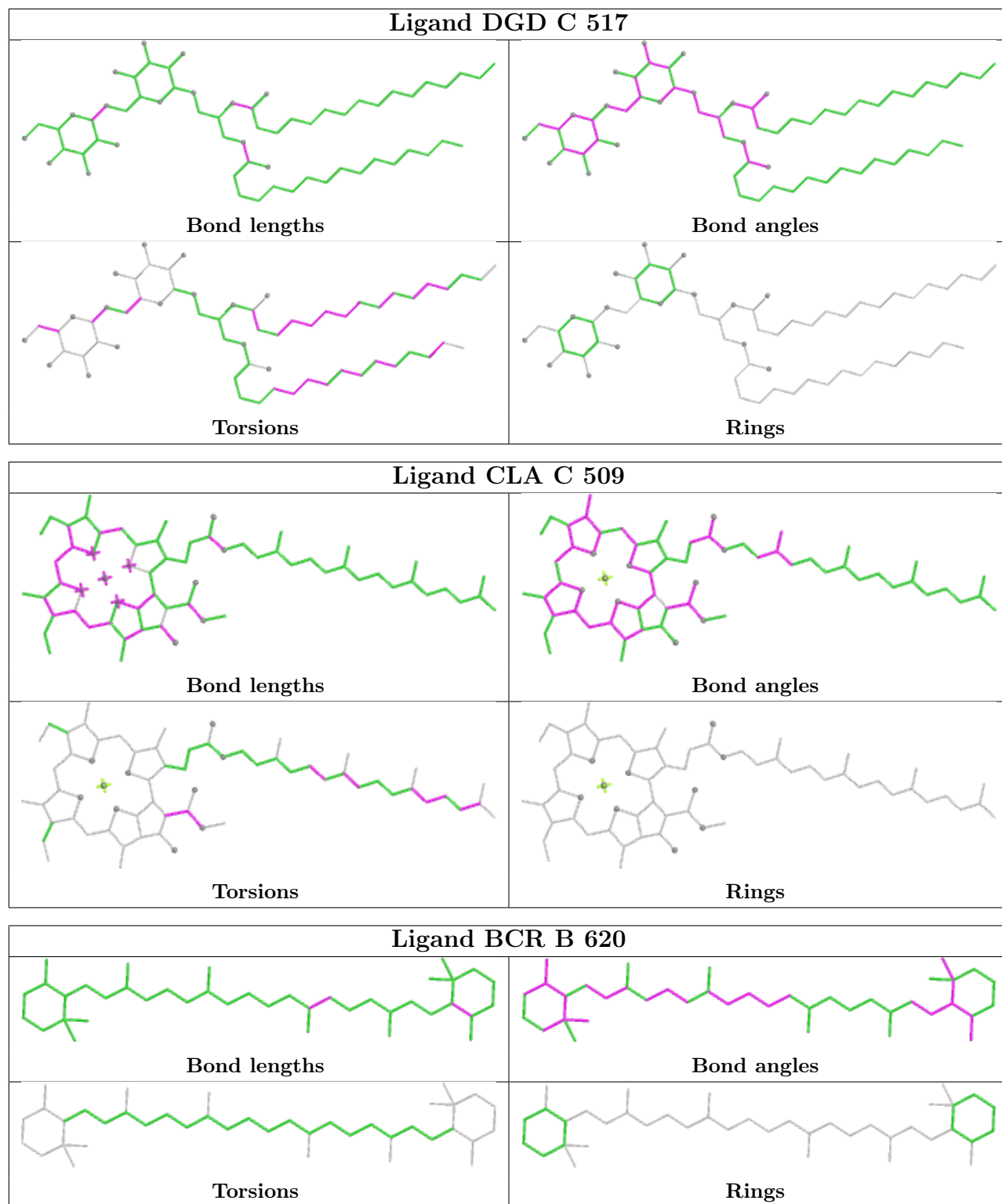
## Ligand BCR a 413

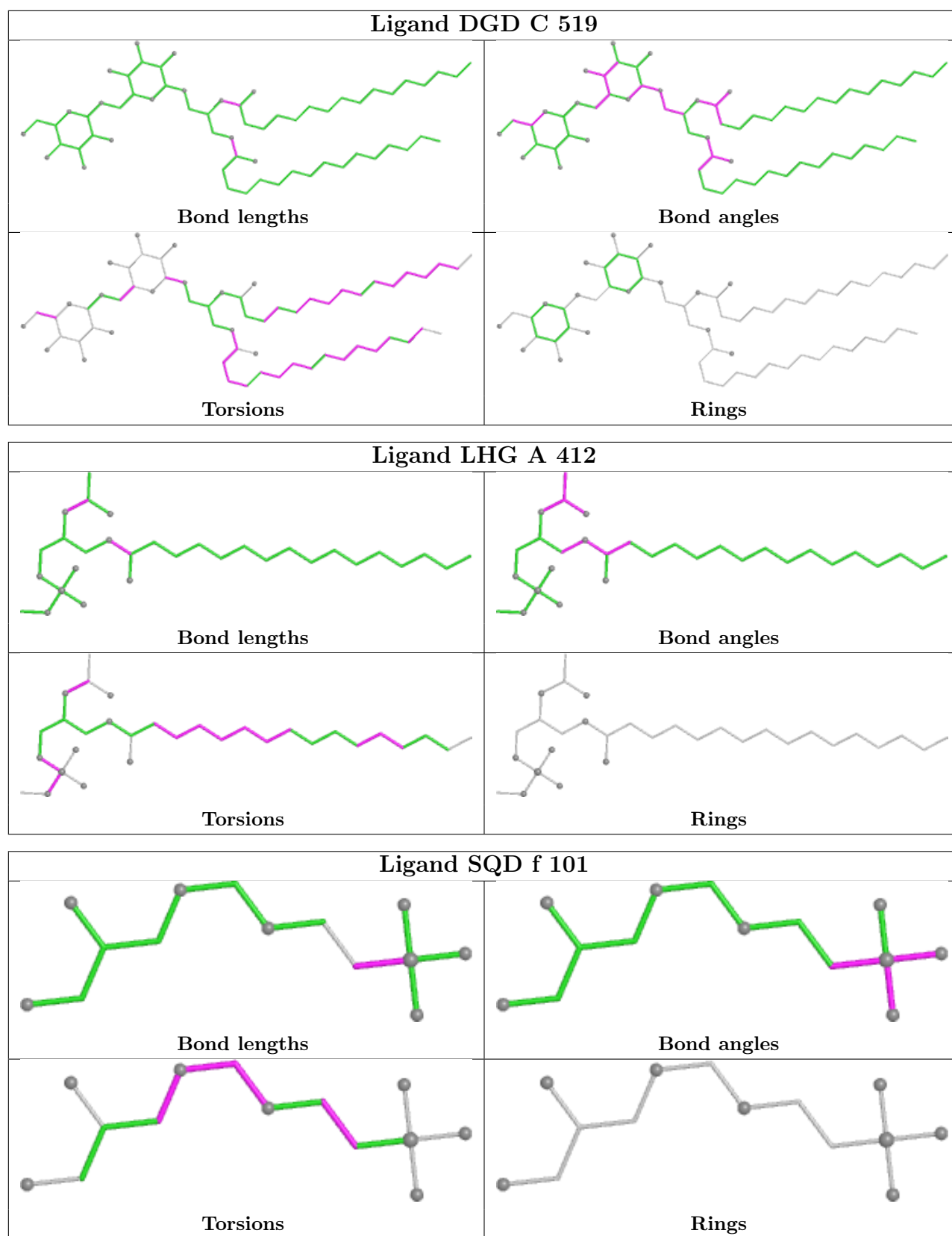


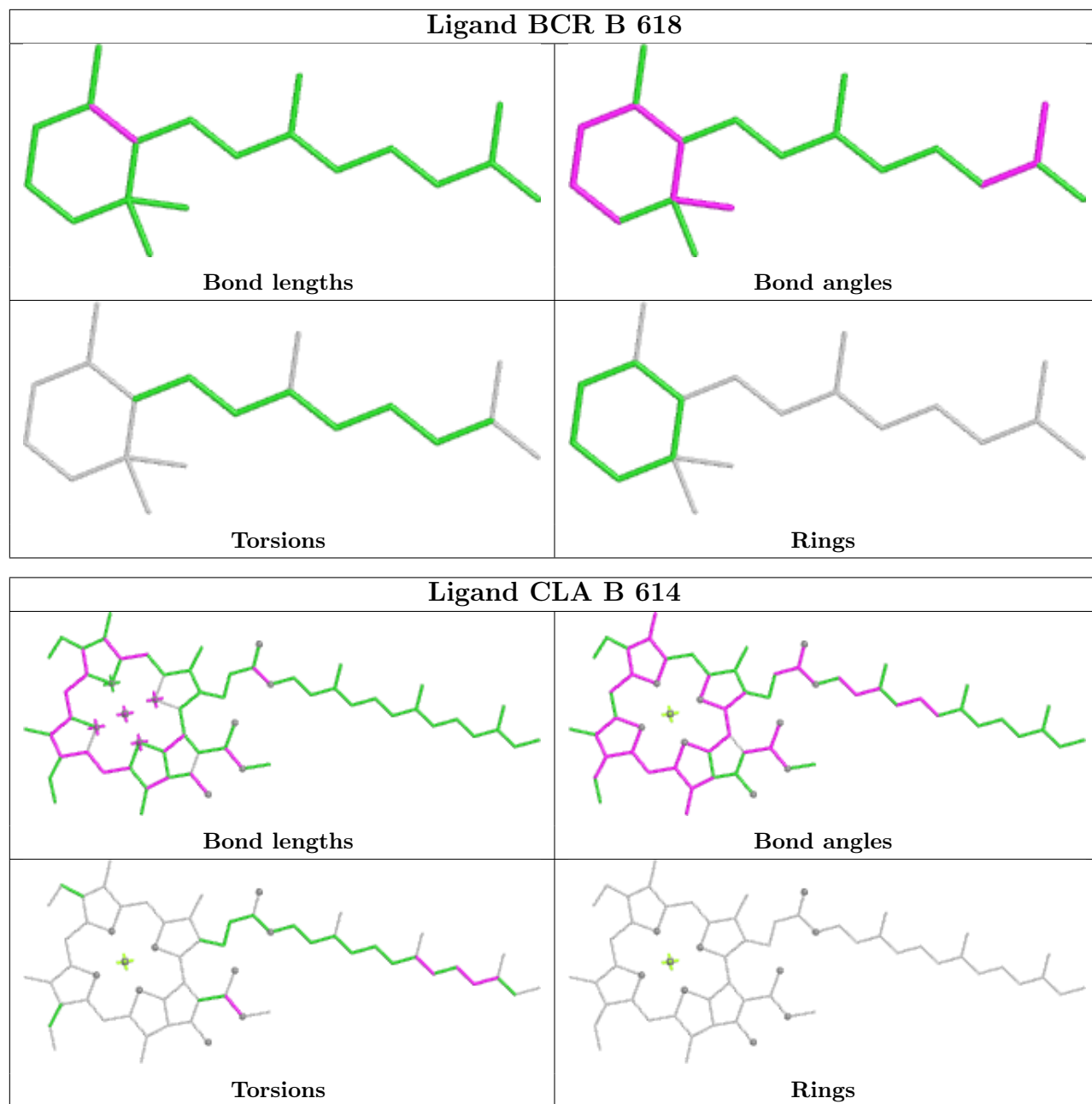


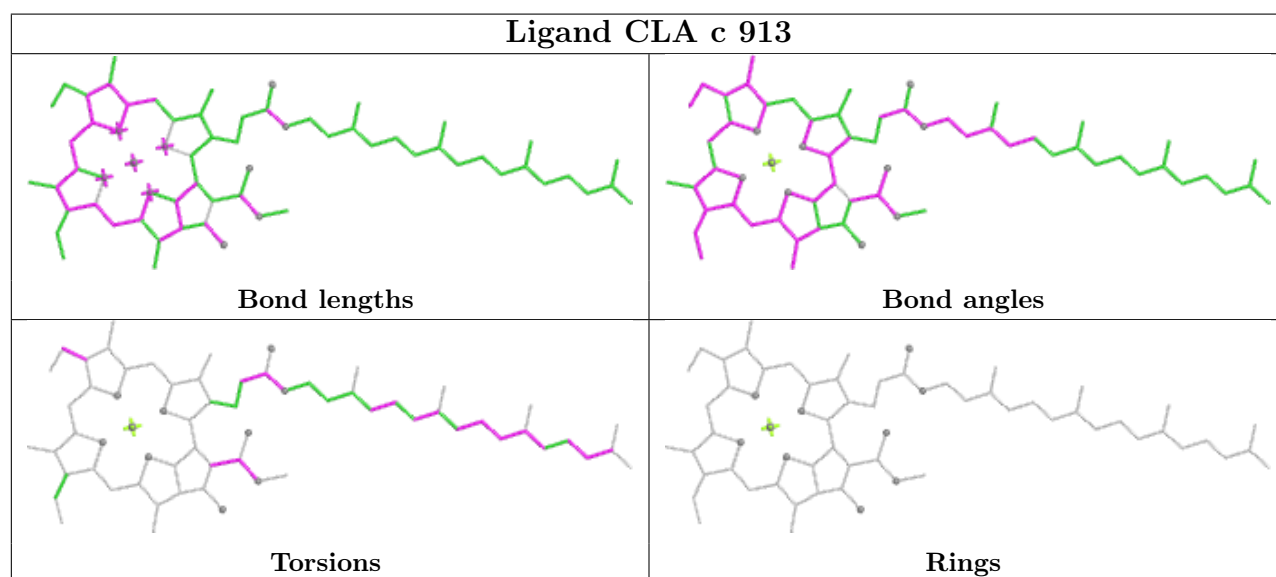
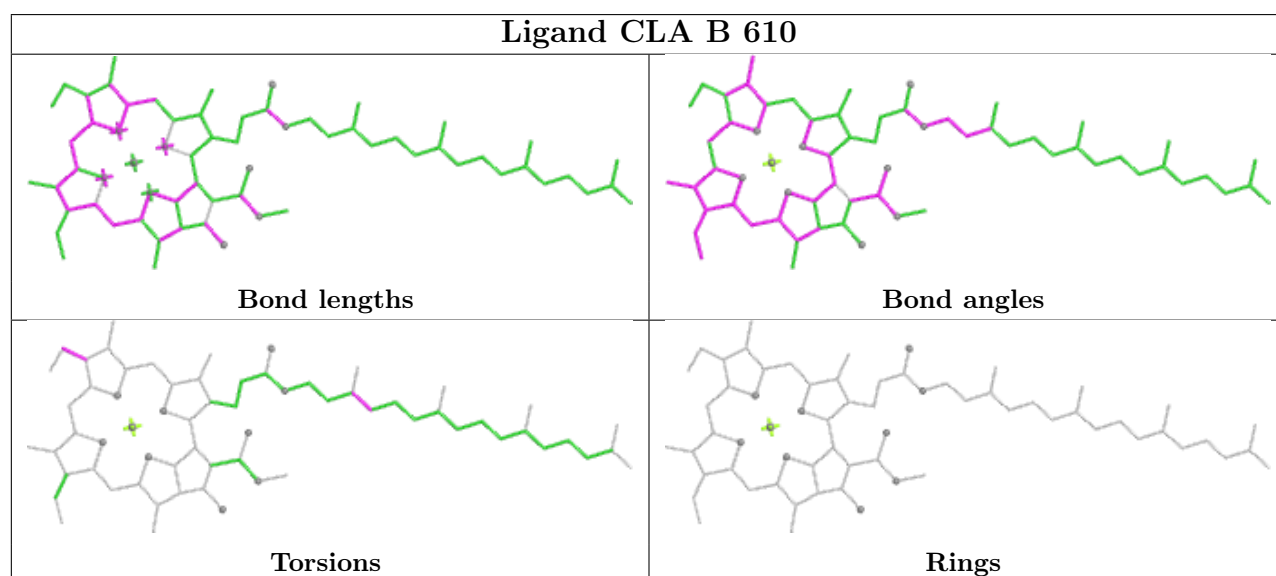
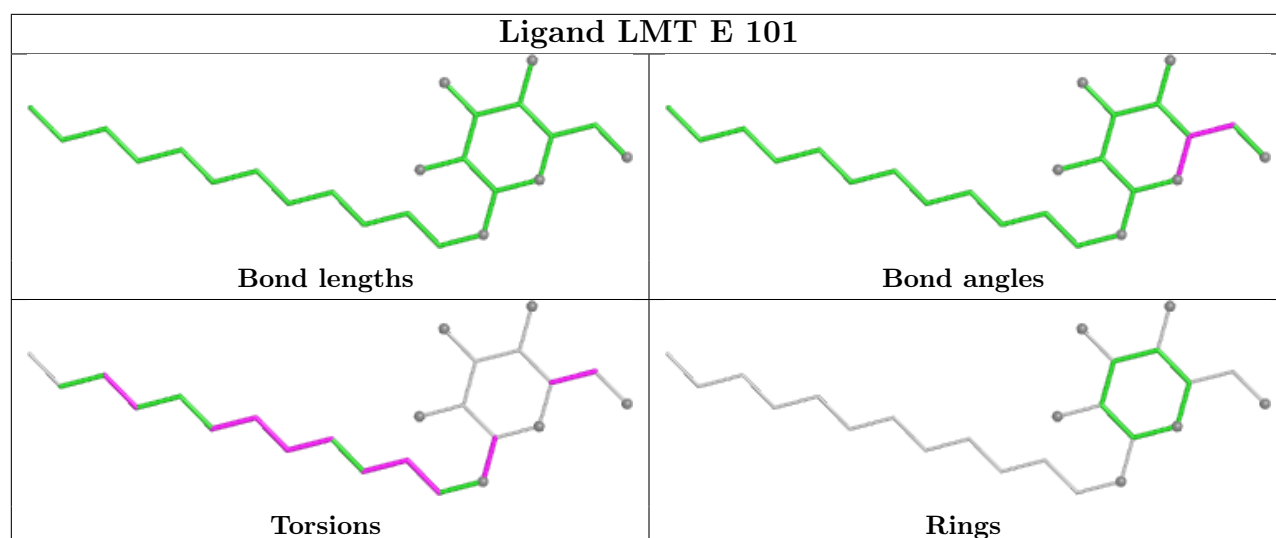




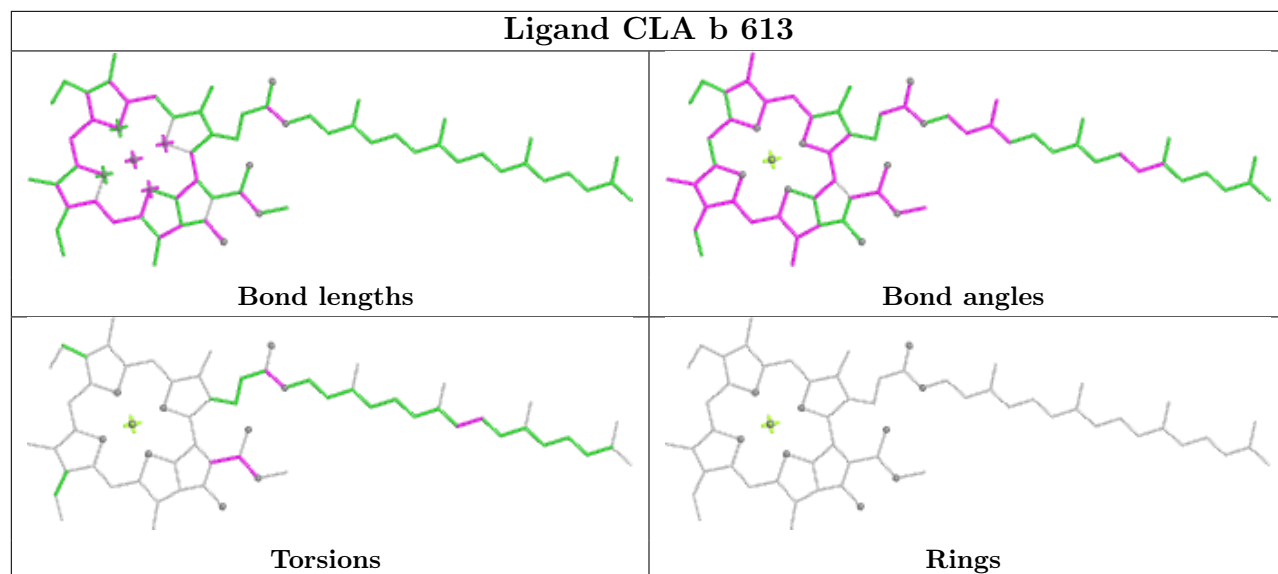




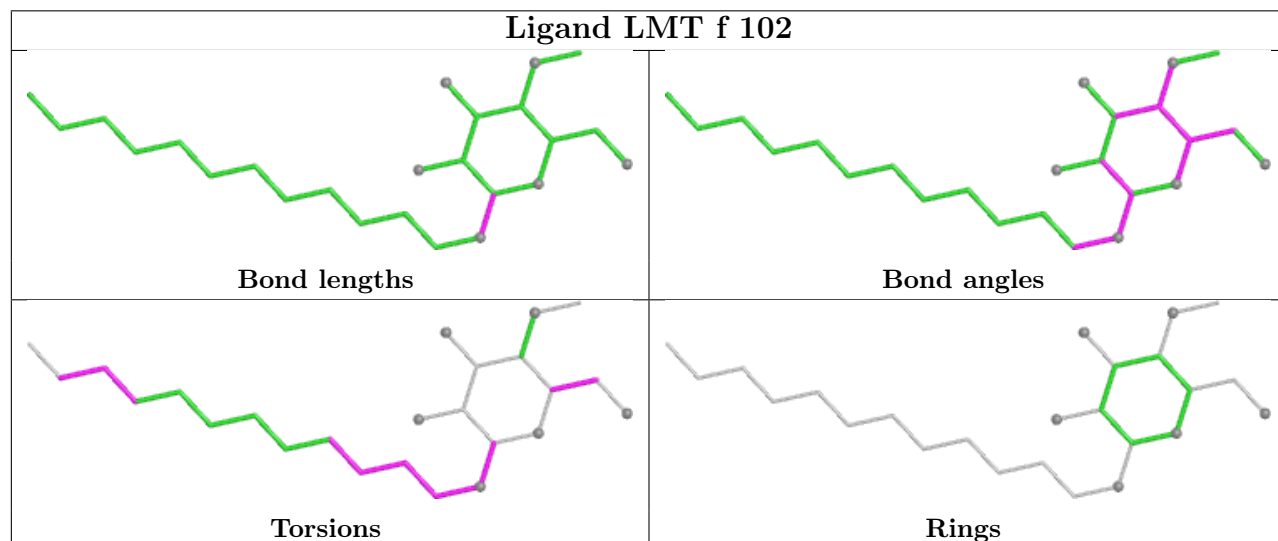




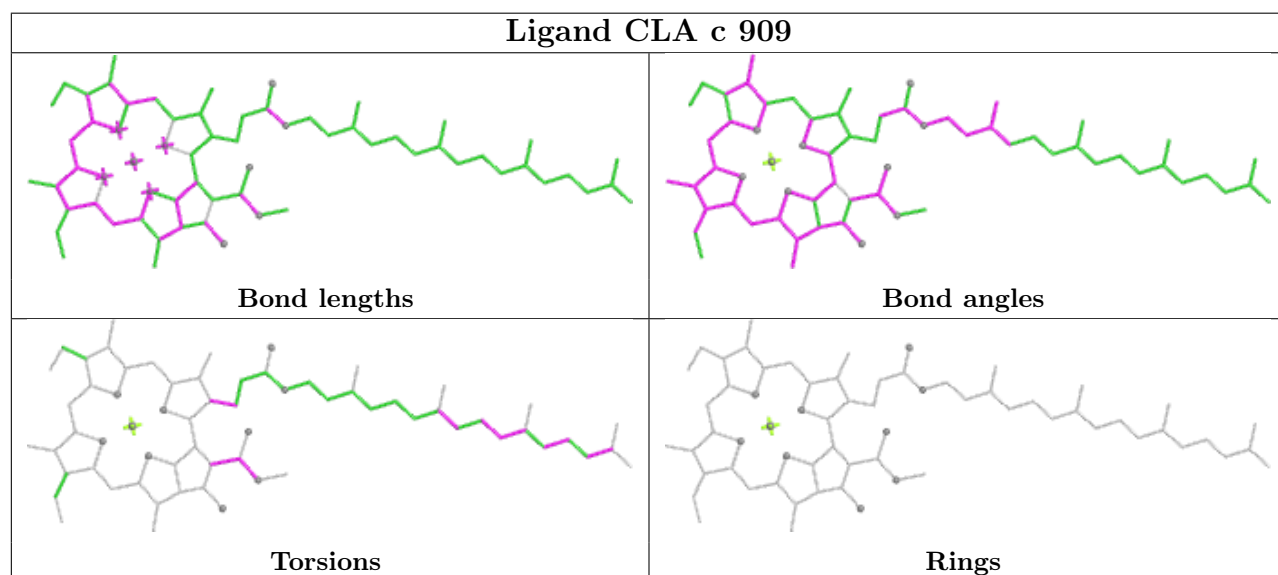
## Ligand CLA b 613

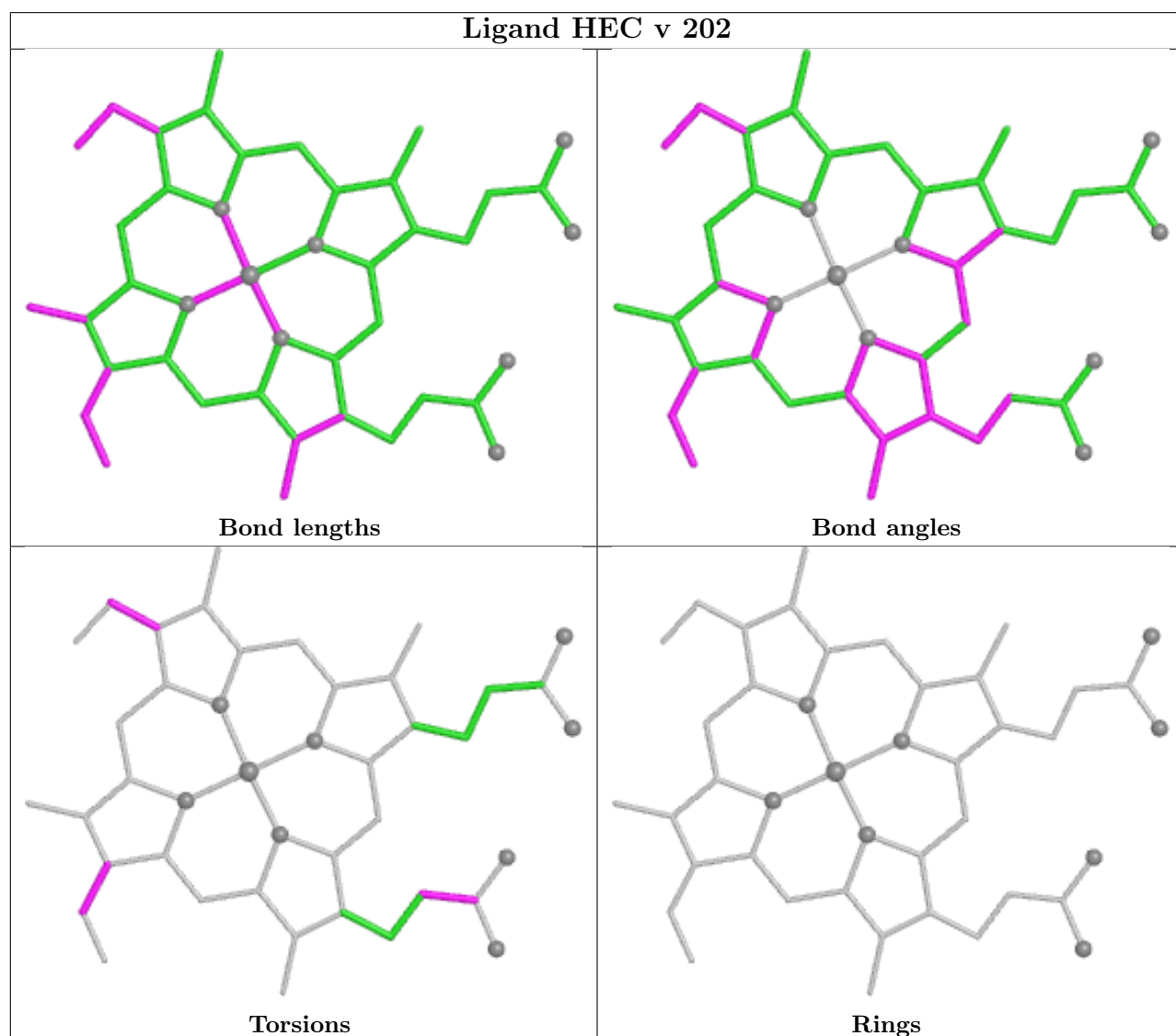
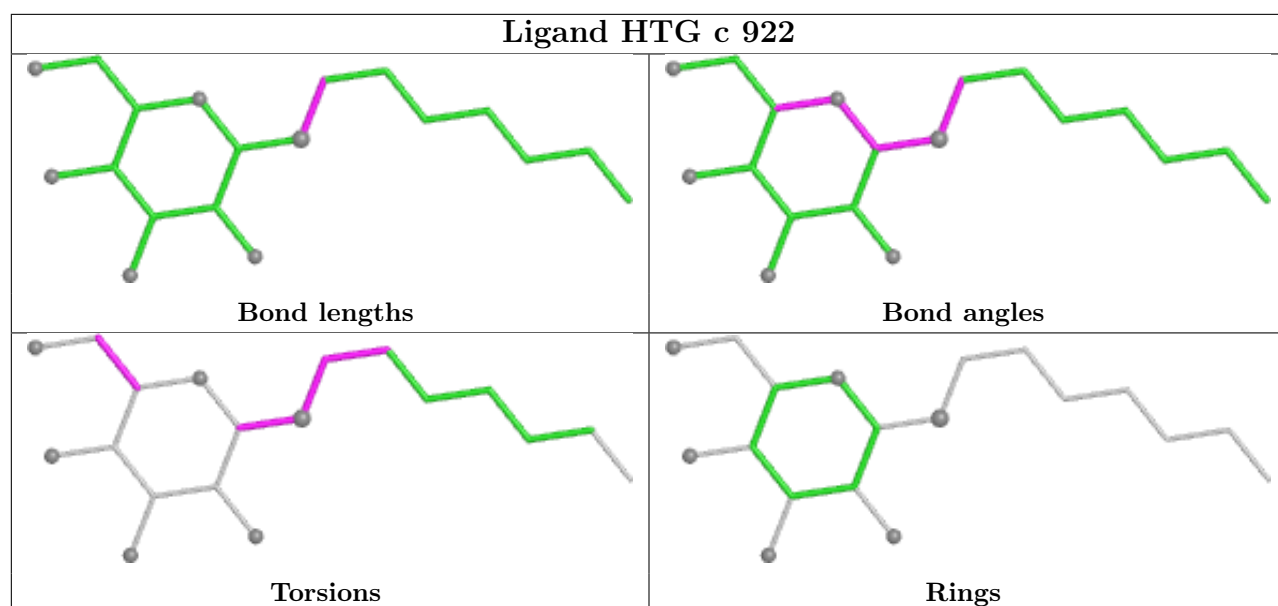


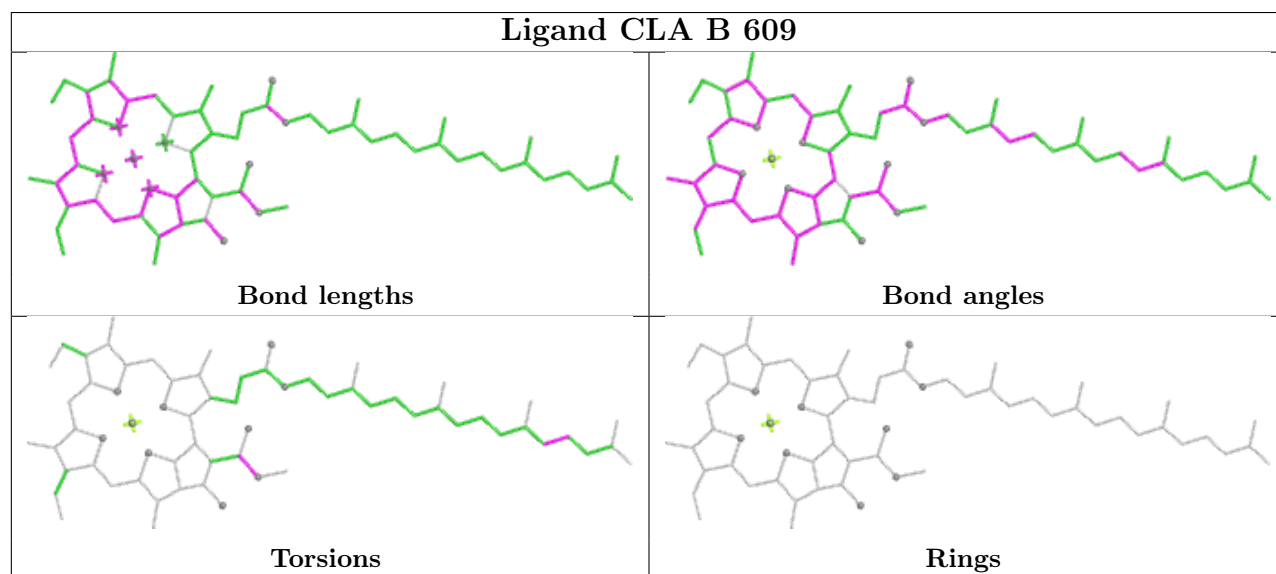
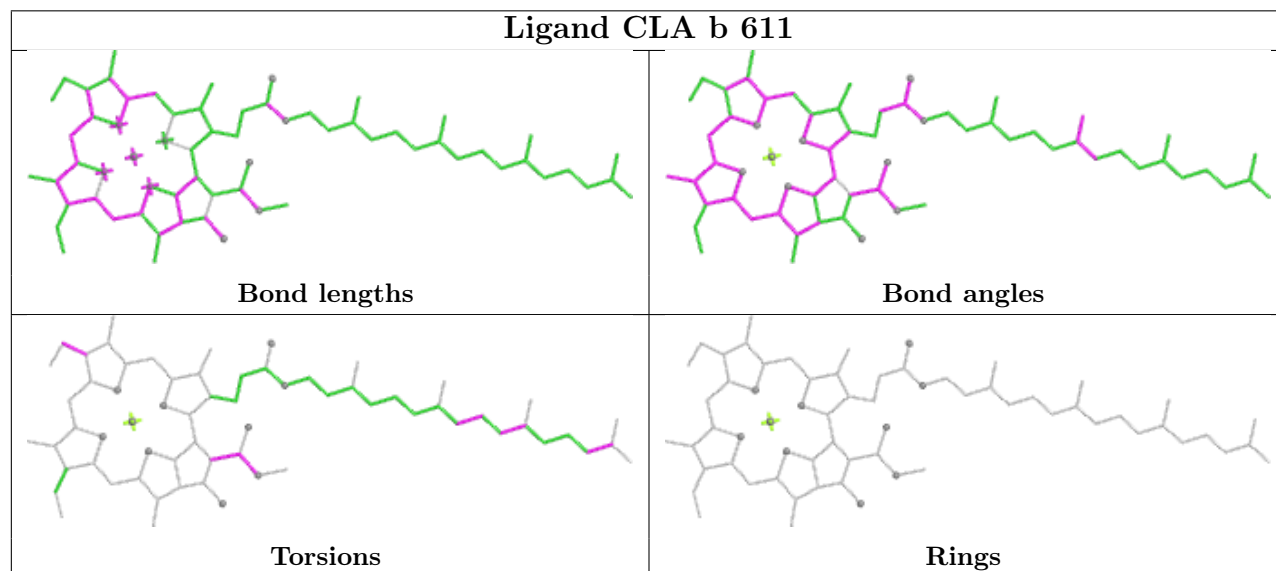
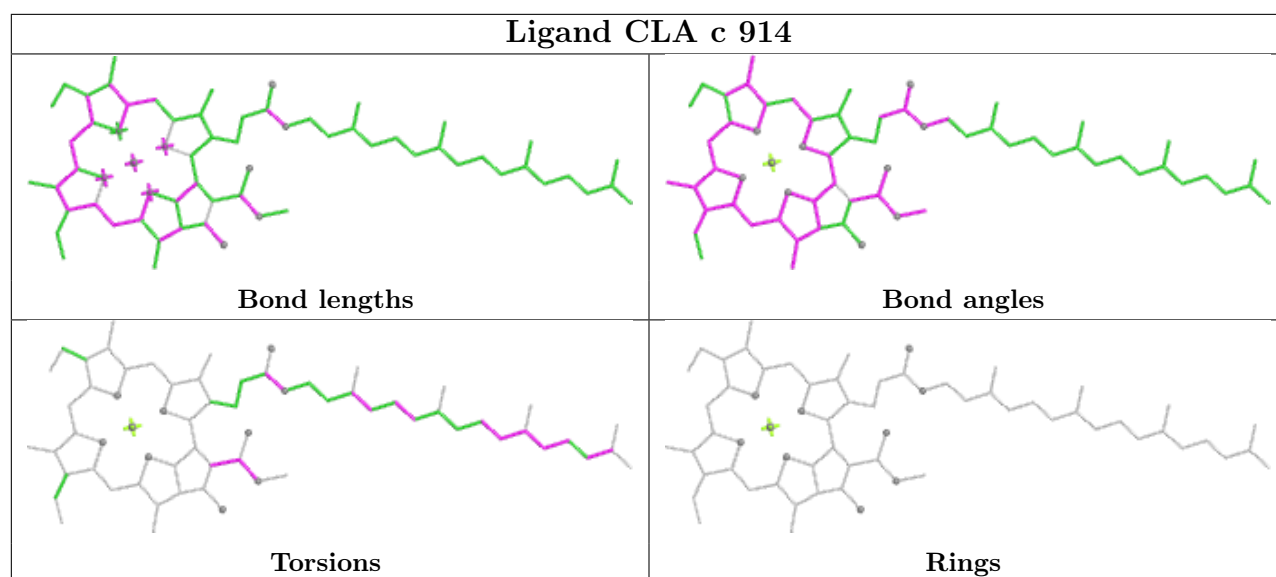
## Ligand LMT f 102

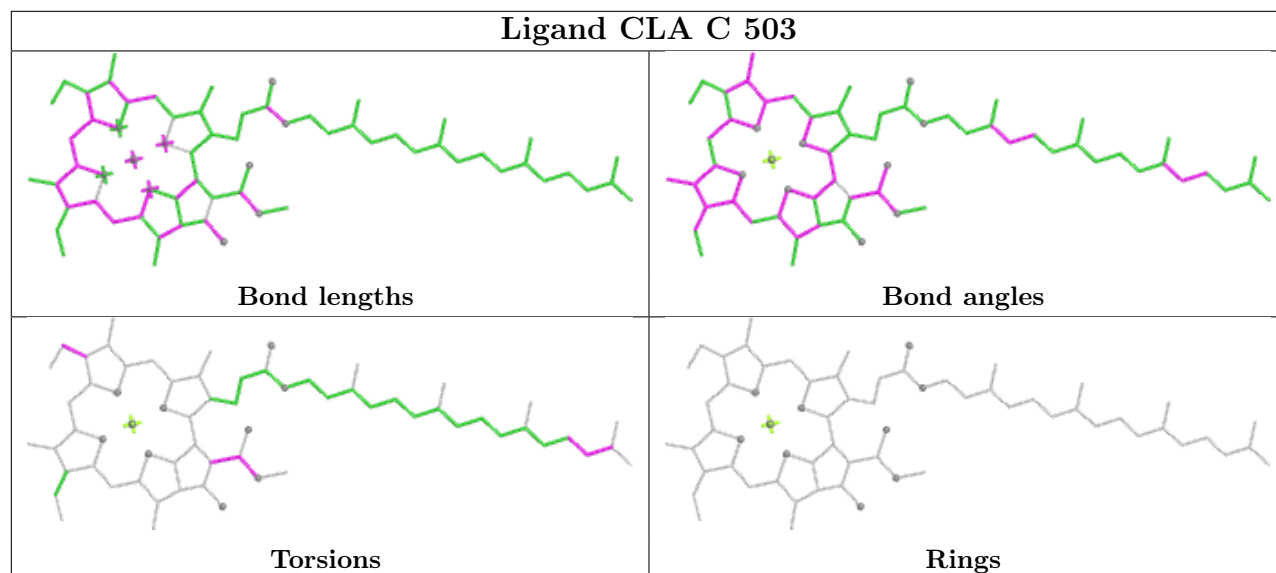
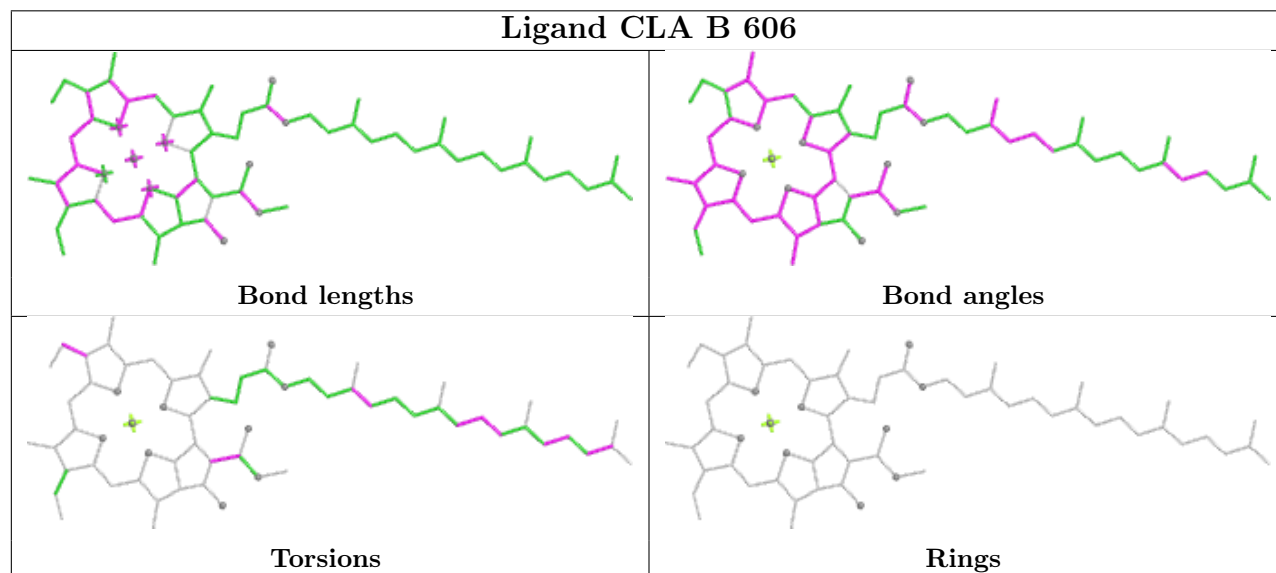
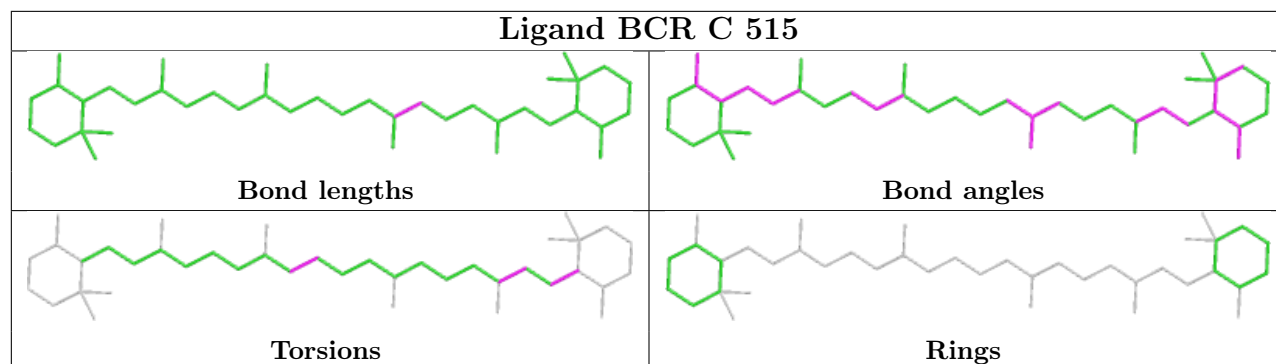


## Ligand CLA c 909

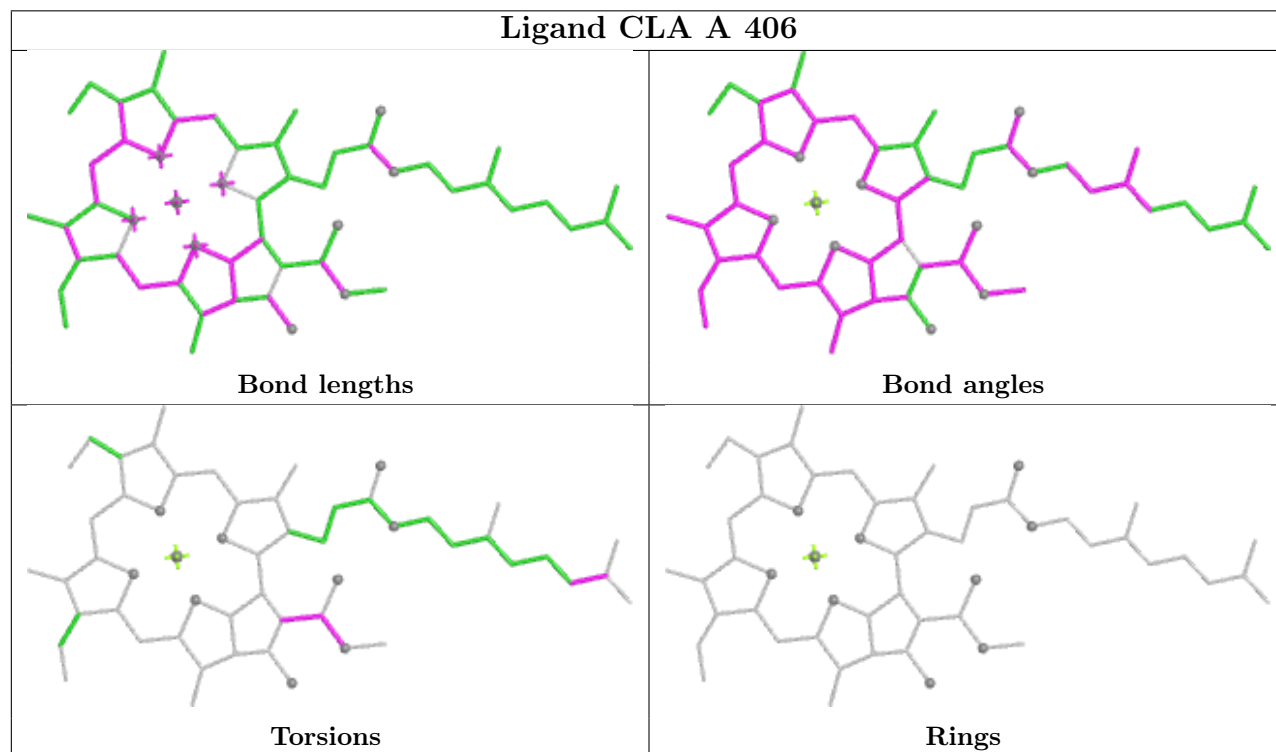
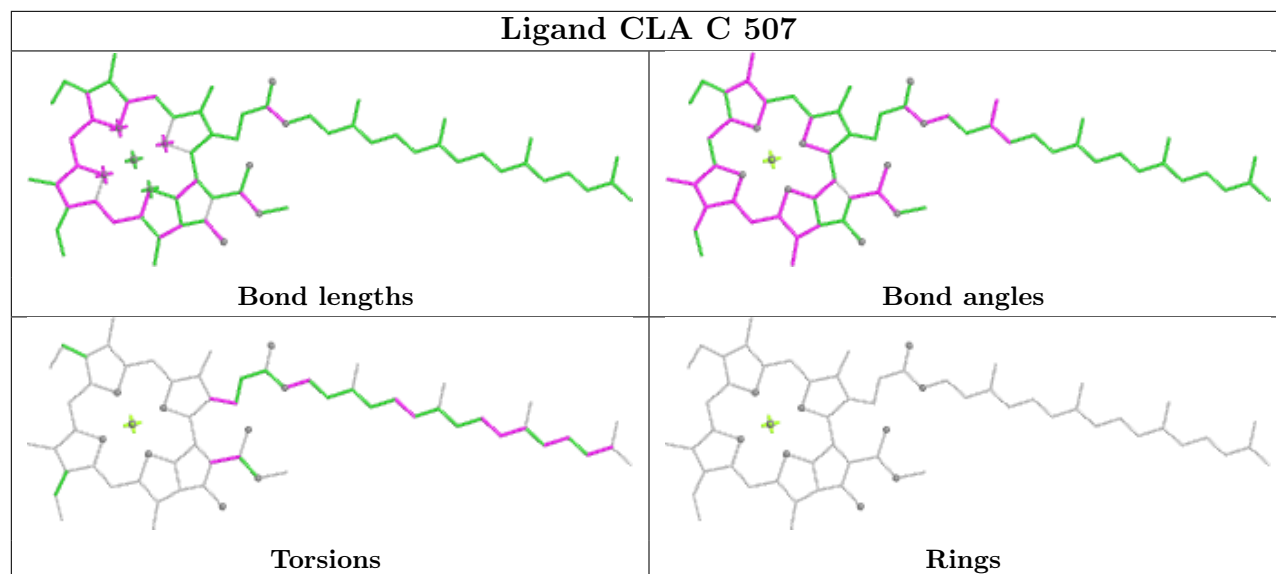


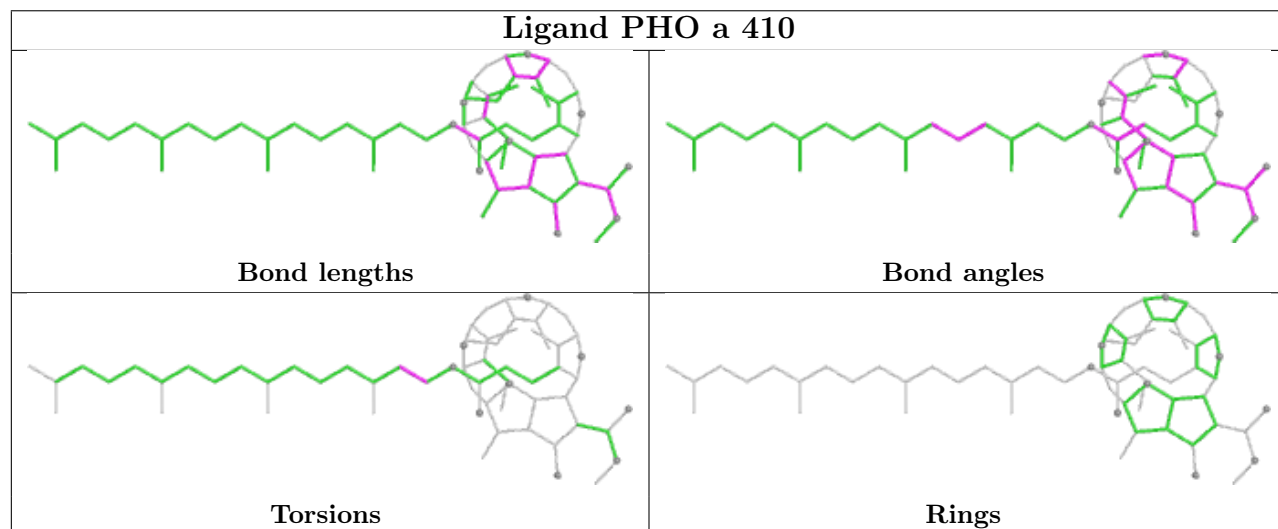
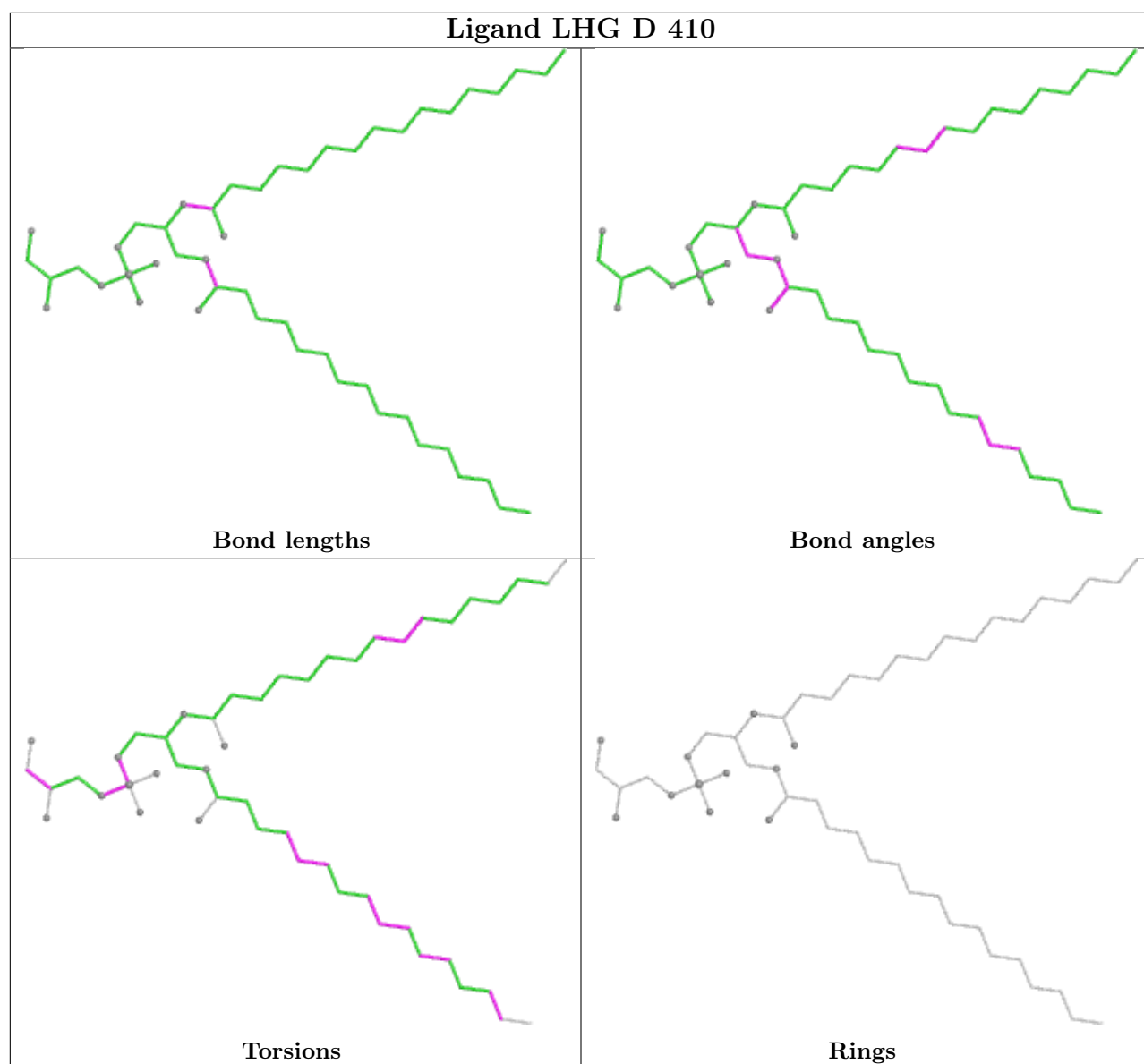


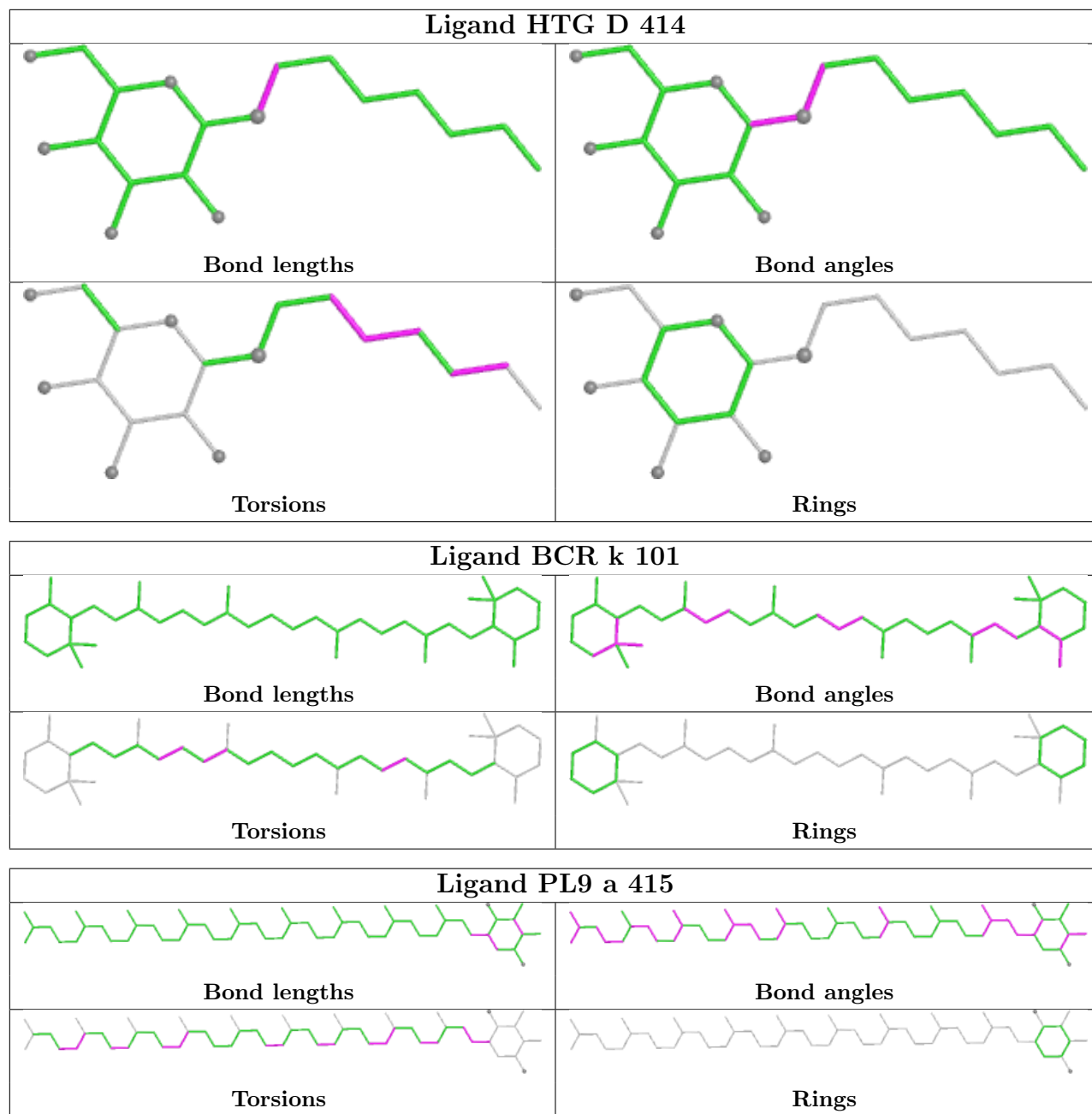




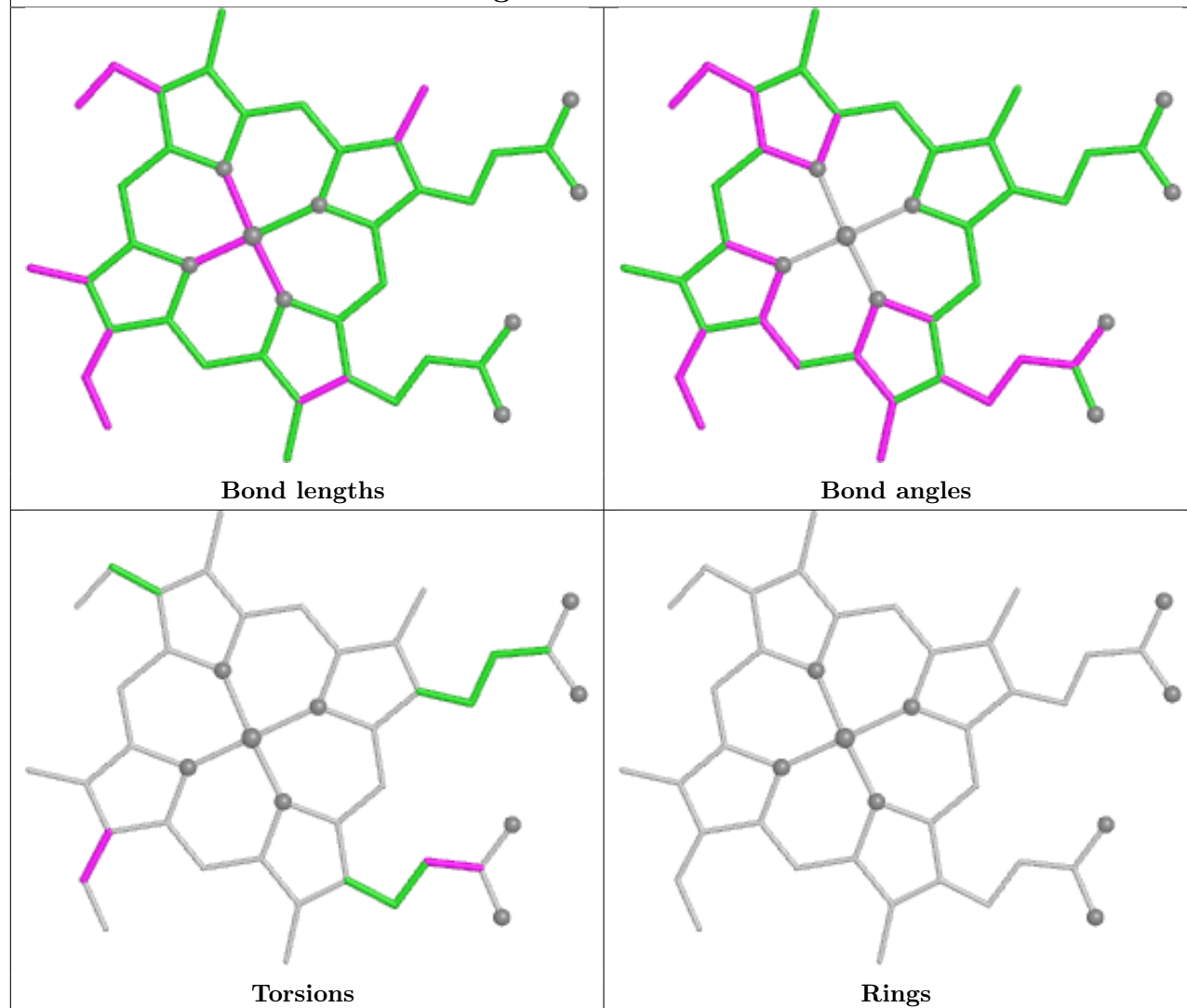




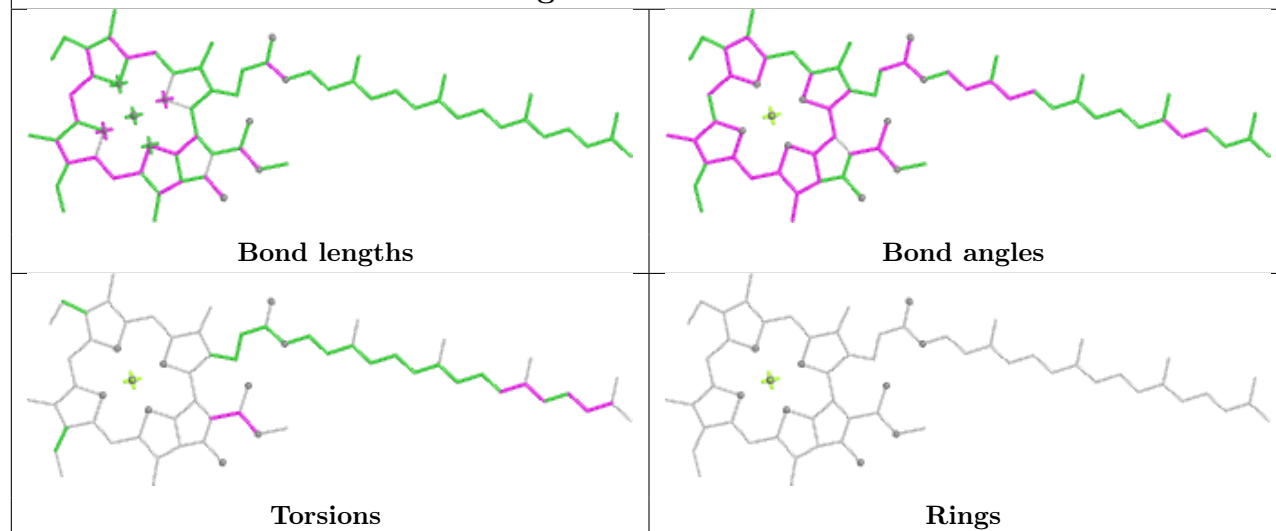


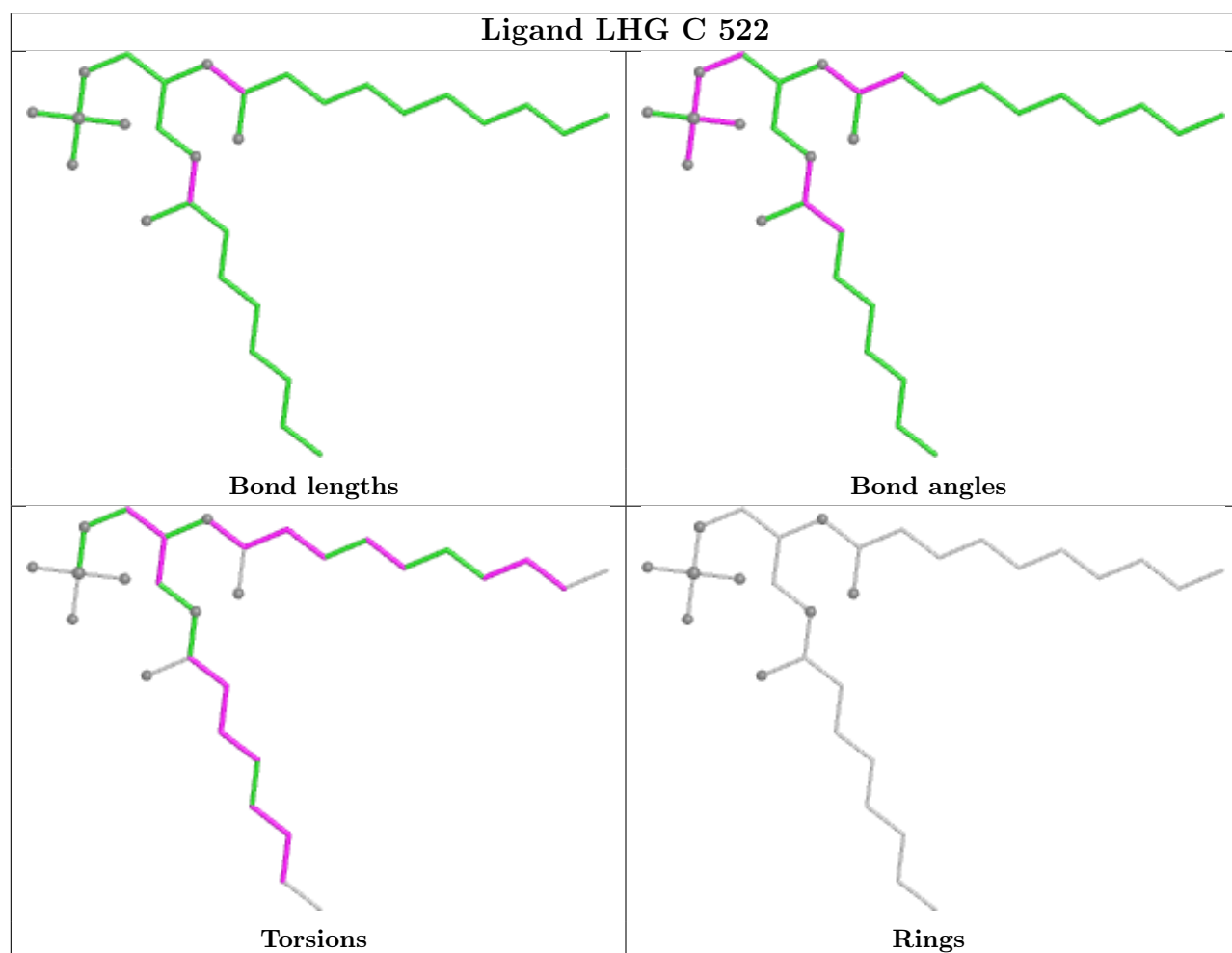
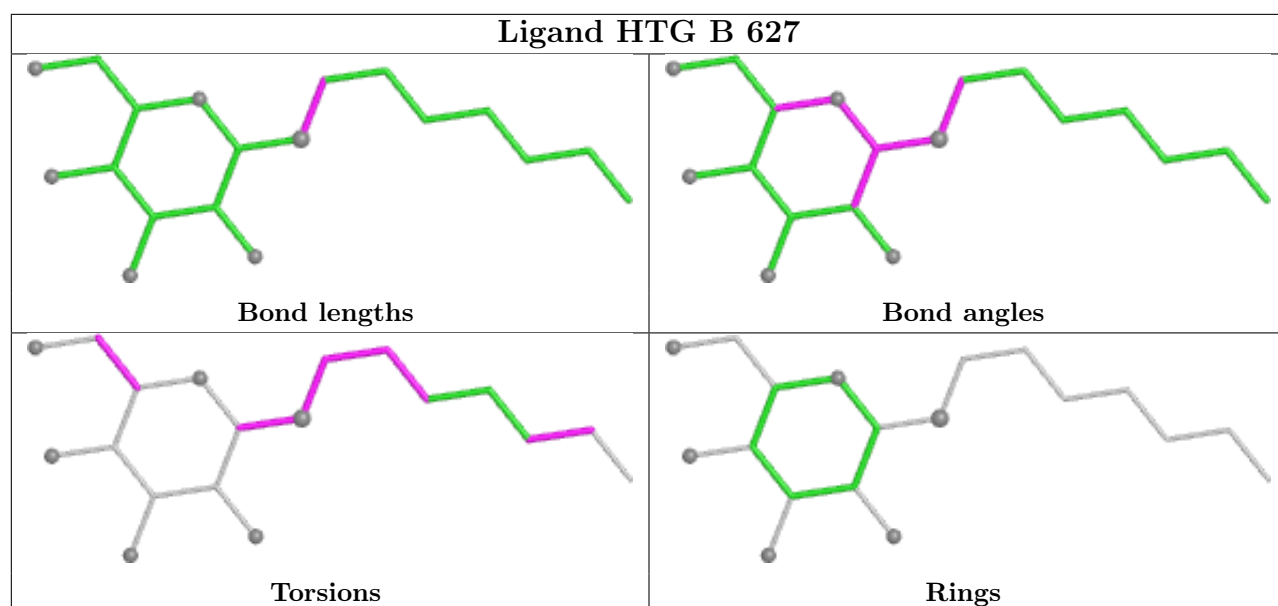


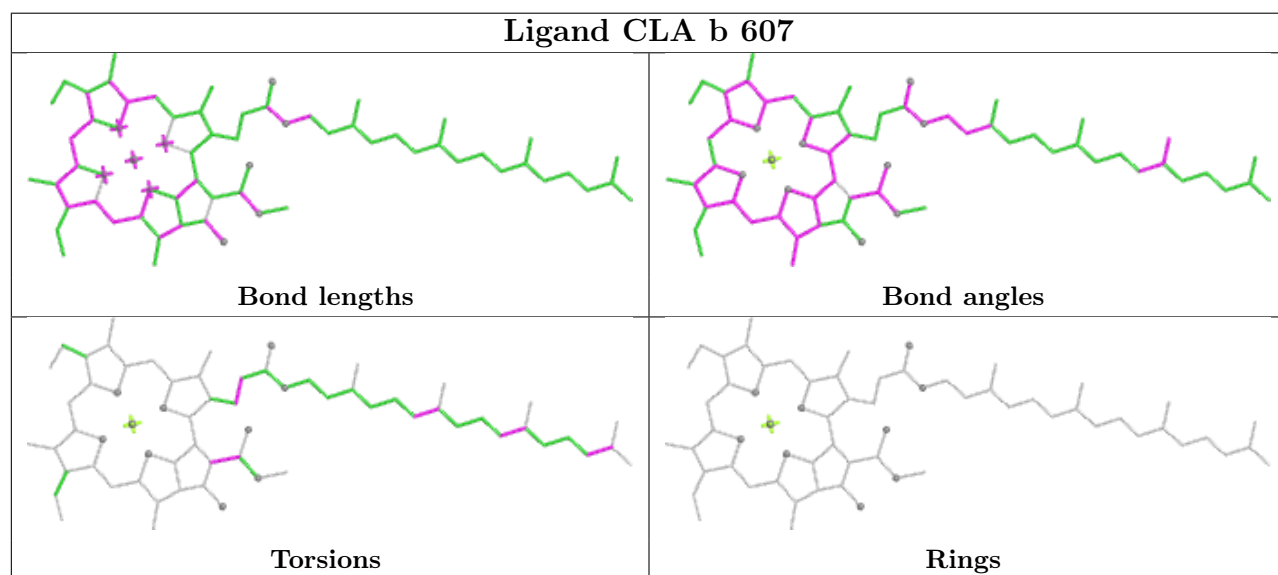
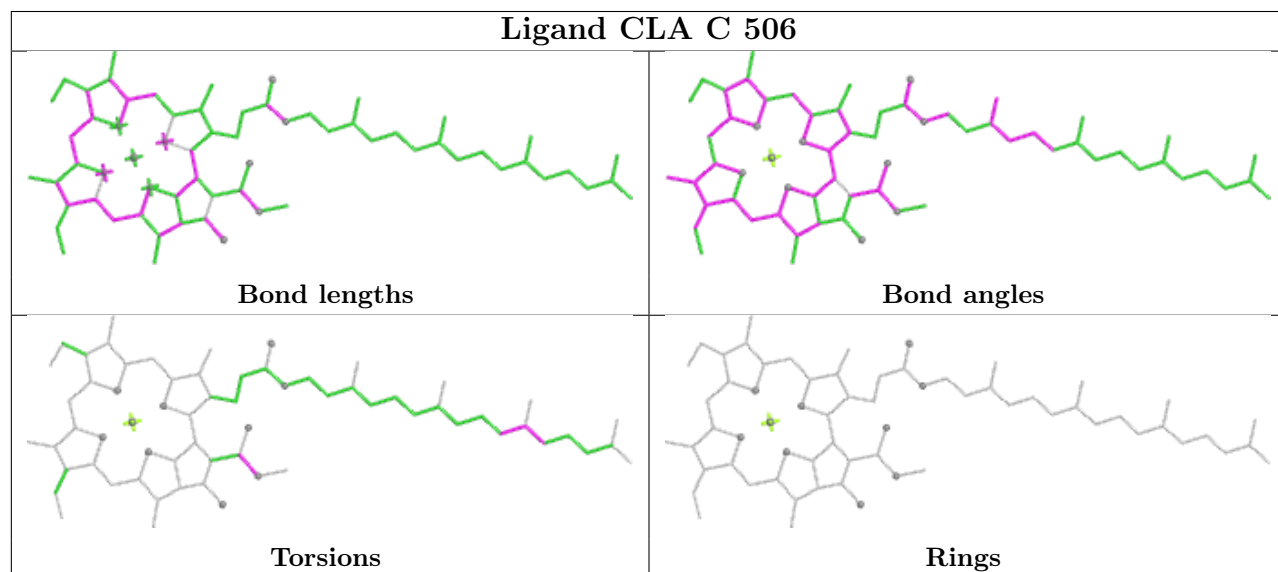
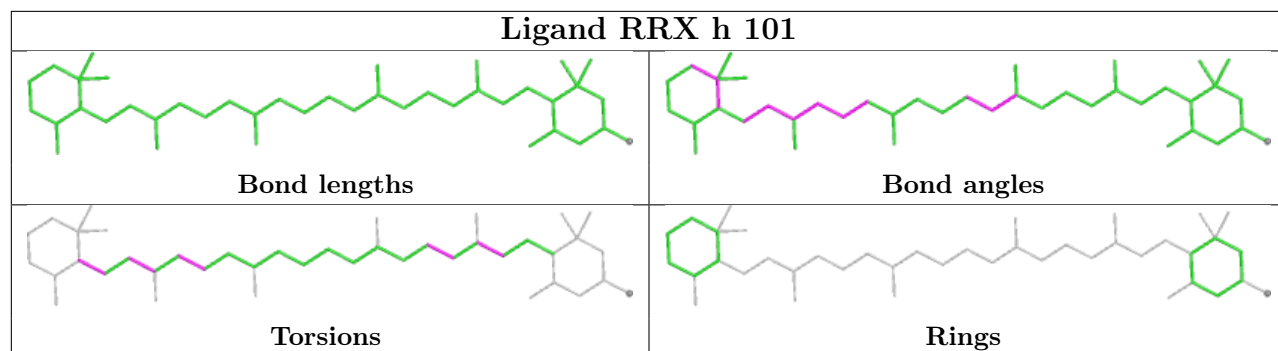
## Ligand HEC V 202

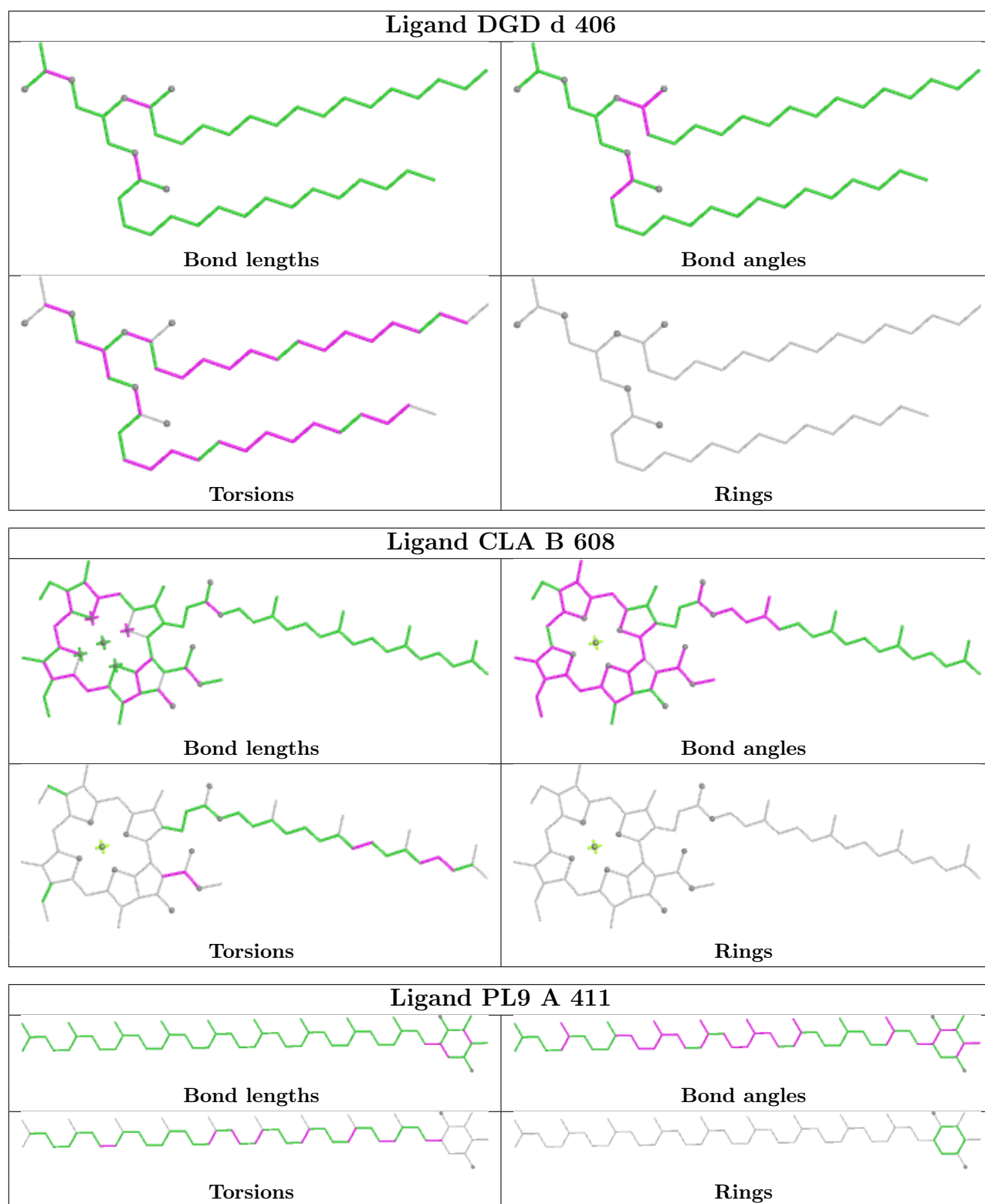


## Ligand CLA c 903









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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   | A     | 334/334 (100%) | -0.48  | 7 (2%) 63 60  | 17, 28, 66, 87        | 1 (0%) |
| 1   | a     | 334/334 (100%) | -0.18  | 33 (9%) 13 10 | 17, 30, 96, 135       | 1 (0%) |
| 2   | B     | 505/505 (100%) | -0.32  | 16 (3%) 50 47 | 21, 33, 67, 109       | 3 (0%) |
| 2   | b     | 483/505 (95%)  | -0.32  | 5 (1%) 79 77  | 19, 35, 57, 124       | 1 (0%) |
| 3   | C     | 451/455 (99%)  | -0.29  | 3 (0%) 84 82  | 24, 37, 55, 106       | 0      |
| 3   | c     | 455/455 (100%) | -0.14  | 2 (0%) 88 87  | 27, 41, 57, 89        | 1 (0%) |
| 4   | D     | 342/342 (100%) | -0.55  | 0 100 100     | 14, 29, 51, 86        | 3 (0%) |
| 4   | d     | 341/342 (99%)  | -0.41  | 4 (1%) 76 74  | 16, 32, 59, 85        | 2 (0%) |
| 5   | E     | 79/80 (98%)    | 0.19   | 3 (3%) 44 41  | 30, 53, 77, 89        | 0      |
| 5   | e     | 79/80 (98%)    | 0.43   | 3 (3%) 44 41  | 35, 54, 91, 96        | 0      |
| 6   | F     | 33/33 (100%)   | 0.03   | 1 (3%) 52 49  | 32, 38, 68, 87        | 0      |
| 6   | f     | 31/33 (93%)    | 0.18   | 1 (3%) 50 47  | 34, 42, 62, 95        | 0      |
| 7   | H     | 63/63 (100%)   | 0.11   | 1 (1%) 70 67  | 22, 41, 51, 104       | 3 (4%) |
| 7   | h     | 62/63 (98%)    | 0.31   | 1 (1%) 70 67  | 26, 48, 62, 74        | 1 (1%) |
| 8   | I     | 34/36 (94%)    | -0.08  | 0 100 100     | 33, 42, 60, 78        | 0      |
| 8   | i     | 35/36 (97%)    | -0.19  | 0 100 100     | 34, 43, 71, 95        | 0      |
| 9   | J     | 36/40 (90%)    | 0.02   | 2 (5%) 30 27  | 29, 46, 73, 82        | 0      |
| 9   | j     | 40/40 (100%)   | 0.25   | 2 (5%) 34 31  | 34, 47, 81, 92        | 0      |
| 10  | K     | 37/37 (100%)   | -0.11  | 0 100 100     | 36, 44, 55, 70        | 0      |
| 10  | k     | 37/37 (100%)   | 0.18   | 1 (2%) 56 53  | 39, 47, 68, 81        | 0      |
| 11  | L     | 35/35 (100%)   | -0.25  | 1 (2%) 53 50  | 23, 32, 66, 78        | 0      |
| 11  | l     | 35/35 (100%)   | -0.04  | 1 (2%) 53 50  | 25, 35, 75, 92        | 0      |
| 12  | O     | 243/243 (100%) | -0.20  | 1 (0%) 88 87  | 20, 39, 69, 104       | 1 (0%) |
| 12  | o     | 243/243 (100%) | -0.19  | 4 (1%) 70 67  | 24, 42, 71, 102       | 0      |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|----------------|-----------------------|---------|
| 13  | T     | 29/30 (96%)     | -0.24  | 2 (6%) 23 20   | 26, 32, 59, 89        | 0       |
| 13  | t     | 29/30 (96%)     | -0.16  | 2 (6%) 23 20   | 27, 34, 66, 98        | 0       |
| 14  | U     | 97/97 (100%)    | -0.32  | 0 100 100      | 26, 36, 58, 89        | 1 (1%)  |
| 14  | u     | 97/97 (100%)    | -0.31  | 1 (1%) 79 77   | 28, 37, 51, 76        | 0       |
| 15  | V     | 137/137 (100%)  | -0.53  | 0 100 100      | 22, 34, 50, 70        | 1 (0%)  |
| 15  | v     | 137/137 (100%)  | -0.11  | 0 100 100      | 24, 44, 61, 84        | 1 (0%)  |
| 16  | Y     | 29/29 (100%)    | 0.28   | 1 (3%) 48 45   | 40, 54, 69, 81        | 0       |
| 16  | y     | 29/29 (100%)    | 0.53   | 1 (3%) 48 45   | 51, 62, 70, 74        | 0       |
| 17  | X     | 37/37 (100%)    | 0.31   | 1 (2%) 56 53   | 27, 50, 72, 83        | 1 (2%)  |
| 17  | x     | 36/37 (97%)     | 0.63   | 1 (2%) 55 52   | 41, 54, 88, 89        | 0       |
| 18  | Z     | 62/62 (100%)    | 0.70   | 6 (9%) 13 10   | 42, 54, 88, 106       | 0       |
| 18  | z     | 61/62 (98%)     | 1.04   | 10 (16%) 4 3   | 49, 64, 98, 102       | 0       |
| All | All   | 5147/5190 (99%) | -0.21  | 117 (2%) 61 58 | 14, 37, 70, 135       | 21 (0%) |

The worst 5 of 117 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 486 | LEU  | 5.6  |
| 1   | a     | 230 | THR  | 5.5  |
| 17  | x     | 37  | VAL  | 5.2  |
| 7   | H     | 64  | ALA  | 4.8  |
| 1   | A     | 246 | TYR  | 4.6  |

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

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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 13  | FME  | T     | 1   | 10/11 | 0.88 | 0.14 | 38,42,72,75                | 0     |
| 13  | FME  | t     | 1   | 10/11 | 0.92 | 0.10 | 33,38,80,91                | 0     |
| 8   | FME  | I     | 1   | 10/11 | 0.96 | 0.09 | 33,37,40,41                | 0     |
| 8   | FME  | i     | 1   | 10/11 | 0.97 | 0.09 | 36,41,45,48                | 0     |

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 31  | DMS  | c     | 942 | 4/4   | 0.60 | 0.24 | 101,103,111,117            | 0     |
| 31  | DMS  | c     | 936 | 4/4   | 0.64 | 0.22 | 106,116,116,124            | 0     |
| 31  | DMS  | C     | 537 | 4/4   | 0.67 | 0.29 | 88,103,104,113             | 0     |
| 30  | UNL  | c     | 932 | 10/-  | 0.70 | 0.23 | 56,74,80,83                | 0     |
| 31  | DMS  | O     | 307 | 4/4   | 0.70 | 0.24 | 84,97,98,104               | 0     |
| 30  | UNL  | i     | 104 | 16/-  | 0.70 | 0.23 | 67,76,87,89                | 0     |
| 31  | DMS  | c     | 937 | 4/4   | 0.70 | 0.25 | 80,90,91,100               | 0     |
| 31  | DMS  | B     | 639 | 4/4   | 0.70 | 0.20 | 72,87,90,102               | 0     |
| 34  | HTG  | b     | 624 | 19/19 | 0.70 | 0.18 | 69,97,109,110              | 0     |
| 31  | DMS  | O     | 305 | 4/4   | 0.71 | 0.20 | 68,70,79,99                | 0     |
| 29  | LMT  | f     | 102 | 25/35 | 0.71 | 0.21 | 61,93,105,108              | 0     |
| 34  | HTG  | c     | 922 | 19/19 | 0.71 | 0.16 | 70,93,109,112              | 0     |
| 30  | UNL  | t     | 102 | 16/-  | 0.72 | 0.16 | 59,71,78,80                | 0     |
| 30  | UNL  | i     | 105 | 10/-  | 0.72 | 0.22 | 67,78,86,87                | 0     |
| 31  | DMS  | u     | 205 | 4/4   | 0.73 | 0.26 | 64,67,73,83                | 0     |
| 31  | DMS  | b     | 637 | 4/4   | 0.73 | 0.20 | 90,97,101,112              | 0     |
| 30  | UNL  | a     | 417 | 10/-  | 0.73 | 0.24 | 75,80,84,87                | 0     |
| 30  | UNL  | Z     | 102 | 9/-   | 0.74 | 0.17 | 57,71,79,81                | 0     |
| 34  | HTG  | b     | 627 | 19/19 | 0.74 | 0.16 | 50,92,108,109              | 0     |
| 34  | HTG  | D     | 415 | 19/19 | 0.74 | 0.19 | 39,69,80,87                | 0     |
| 35  | DGD  | d     | 406 | 43/66 | 0.74 | 0.22 | 58,85,139,146              | 0     |
| 34  | HTG  | D     | 414 | 19/19 | 0.75 | 0.18 | 63,103,114,115             | 0     |
| 34  | HTG  | b     | 632 | 19/19 | 0.75 | 0.20 | 56,74,91,92                | 0     |
| 31  | DMS  | b     | 636 | 4/4   | 0.75 | 0.23 | 88,95,109,113              | 0     |
| 31  | DMS  | c     | 938 | 4/4   | 0.75 | 0.20 | 86,91,98,103               | 0     |
| 34  | HTG  | B     | 627 | 19/19 | 0.76 | 0.16 | 51,104,113,116             | 0     |
| 31  | DMS  | v     | 207 | 4/4   | 0.76 | 0.31 | 84,93,97,117               | 0     |
| 29  | LMT  | I     | 102 | 35/35 | 0.77 | 0.15 | 76,88,100,102              | 0     |
| 31  | DMS  | d     | 414 | 4/4   | 0.77 | 0.28 | 102,112,113,120            | 0     |
| 30  | UNL  | I     | 105 | 16/-  | 0.77 | 0.20 | 70,82,88,90                | 0     |
| 30  | UNL  | a     | 420 | 6/-   | 0.77 | 0.20 | 56,59,60,60                | 0     |
| 30  | UNL  | b     | 628 | 11/-  | 0.77 | 0.16 | 58,63,78,79                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 31  | DMS  | V     | 211 | 4/4   | 0.77 | 0.23 | 77,84,85,85                 | 0     |
| 31  | DMS  | u     | 204 | 4/4   | 0.78 | 0.20 | 50,68,69,75                 | 0     |
| 27  | LHG  | A     | 412 | 31/49 | 0.78 | 0.19 | 66,83,107,117               | 0     |
| 31  | DMS  | v     | 204 | 4/4   | 0.78 | 0.19 | 87,88,90,91                 | 0     |
| 31  | DMS  | a     | 401 | 4/4   | 0.78 | 0.28 | 75,84,85,104                | 0     |
| 30  | UNL  | u     | 201 | 11/-  | 0.78 | 0.20 | 47,53,69,69                 | 0     |
| 34  | HTG  | v     | 203 | 16/19 | 0.78 | 0.15 | 52,69,81,97                 | 0     |
| 35  | DGD  | D     | 407 | 50/66 | 0.78 | 0.20 | 60,87,120,123               | 0     |
| 31  | DMS  | l     | 105 | 4/4   | 0.78 | 0.26 | 100,103,110,115             | 0     |
| 31  | DMS  | c     | 943 | 4/4   | 0.79 | 0.21 | 77,82,87,92                 | 0     |
| 22  | CLA  | b     | 602 | 65/65 | 0.79 | 0.16 | 49,67,89,98                 | 0     |
| 31  | DMS  | l     | 103 | 4/4   | 0.79 | 0.24 | 91,95,97,99                 | 0     |
| 31  | DMS  | c     | 935 | 4/4   | 0.79 | 0.16 | 71,78,81,84                 | 0     |
| 31  | DMS  | u     | 203 | 4/4   | 0.79 | 0.21 | 56,68,72,84                 | 0     |
| 29  | LMT  | A     | 414 | 35/35 | 0.79 | 0.17 | 59,86,109,114               | 0     |
| 31  | DMS  | C     | 540 | 4/4   | 0.79 | 0.22 | 82,83,91,97                 | 0     |
| 31  | DMS  | H     | 103 | 4/4   | 0.79 | 0.21 | 63,67,69,74                 | 0     |
| 31  | DMS  | v     | 205 | 4/4   | 0.79 | 0.19 | 70,72,78,80                 | 0     |
| 31  | DMS  | L     | 102 | 4/4   | 0.79 | 0.23 | 79,80,91,100                | 0     |
| 29  | LMT  | T     | 102 | 24/35 | 0.80 | 0.17 | 42,80,98,101                | 0     |
| 31  | DMS  | f     | 103 | 4/4   | 0.80 | 0.24 | 87,89,90,100                | 0     |
| 31  | DMS  | O     | 313 | 4/4   | 0.80 | 0.26 | 89,100,100,107              | 0     |
| 27  | LHG  | a     | 416 | 49/49 | 0.80 | 0.17 | 60,84,100,108               | 0     |
| 34  | HTG  | V     | 203 | 14/19 | 0.81 | 0.15 | 48,52,79,84                 | 0     |
| 31  | DMS  | c     | 944 | 4/4   | 0.81 | 0.20 | 79,82,89,92                 | 0     |
| 29  | LMT  | Z     | 101 | 35/35 | 0.81 | 0.16 | 40,105,123,128              | 0     |
| 31  | DMS  | C     | 539 | 4/4   | 0.81 | 0.23 | 88,90,93,95                 | 0     |
| 25  | LMG  | D     | 412 | 46/55 | 0.81 | 0.19 | 41,68,138,142               | 0     |
| 31  | DMS  | B     | 634 | 4/4   | 0.81 | 0.23 | 57,68,73,95                 | 0     |
| 30  | UNL  | j     | 103 | 16/-  | 0.81 | 0.16 | 59,67,71,74                 | 0     |
| 31  | DMS  | C     | 534 | 4/4   | 0.81 | 0.17 | 105,111,112,121             | 0     |
| 31  | DMS  | B     | 631 | 4/4   | 0.82 | 0.19 | 78,80,84,87                 | 0     |
| 28  | SQD  | D     | 408 | 20/54 | 0.82 | 0.15 | 65,97,105,108               | 0     |
| 31  | DMS  | B     | 637 | 4/4   | 0.82 | 0.20 | 69,76,80,88                 | 0     |
| 34  | HTG  | l     | 106 | 19/19 | 0.82 | 0.17 | 63,97,108,109               | 0     |
| 31  | DMS  | U     | 203 | 4/4   | 0.82 | 0.23 | 62,73,74,76                 | 0     |
| 30  | UNL  | T     | 101 | 13/-  | 0.82 | 0.16 | 63,71,77,79                 | 0     |
| 24  | BCR  | B     | 618 | 19/40 | 0.82 | 0.15 | 50,59,74,77                 | 0     |
| 30  | UNL  | I     | 104 | 16/-  | 0.83 | 0.18 | 60,71,84,86                 | 0     |
| 34  | HTG  | C     | 532 | 19/19 | 0.83 | 0.14 | 69,98,111,112               | 0     |
| 26  | PL9  | A     | 411 | 55/55 | 0.83 | 0.20 | 61,73,87,92                 | 0     |
| 28  | SQD  | l     | 101 | 54/54 | 0.83 | 0.16 | 53,82,119,123               | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 30  | UNL  | U     | 201 | 14/-  | 0.83 | 0.17 | 44,57,65,66                 | 0     |
| 27  | LHG  | d     | 401 | 33/49 | 0.83 | 0.14 | 62,94,138,142               | 0     |
| 31  | DMS  | t     | 105 | 4/4   | 0.83 | 0.23 | 89,93,101,108               | 0     |
| 29  | LMT  | a     | 419 | 35/35 | 0.83 | 0.18 | 46,69,93,100                | 0     |
| 29  | LMT  | E     | 101 | 24/35 | 0.83 | 0.17 | 61,82,97,113                | 0     |
| 29  | LMT  | t     | 101 | 24/35 | 0.83 | 0.13 | 50,71,109,119               | 0     |
| 31  | DMS  | c     | 940 | 4/4   | 0.83 | 0.19 | 74,74,75,80                 | 0     |
| 30  | UNL  | I     | 103 | 13/-  | 0.83 | 0.17 | 53,57,77,82                 | 0     |
| 31  | DMS  | C     | 533 | 4/4   | 0.83 | 0.19 | 79,84,85,89                 | 0     |
| 29  | LMT  | c     | 931 | 24/35 | 0.84 | 0.18 | 50,84,95,98                 | 0     |
| 28  | SQD  | b     | 621 | 38/54 | 0.84 | 0.16 | 58,90,110,112               | 0     |
| 31  | DMS  | C     | 536 | 4/4   | 0.84 | 0.20 | 77,80,94,95                 | 0     |
| 25  | LMG  | b     | 622 | 43/55 | 0.84 | 0.17 | 48,78,88,98                 | 0     |
| 31  | DMS  | d     | 415 | 4/4   | 0.84 | 0.17 | 60,63,67,79                 | 0     |
| 31  | DMS  | C     | 538 | 4/4   | 0.84 | 0.14 | 79,86,86,87                 | 0     |
| 30  | UNL  | b     | 625 | 16/-  | 0.84 | 0.15 | 43,52,64,67                 | 0     |
| 34  | HTG  | C     | 523 | 9/19  | 0.84 | 0.17 | 63,69,81,86                 | 0     |
| 31  | DMS  | V     | 207 | 4/4   | 0.84 | 0.18 | 64,71,71,76                 | 0     |
| 29  | LMT  | c     | 921 | 35/35 | 0.84 | 0.15 | 74,90,99,103                | 0     |
| 31  | DMS  | o     | 308 | 4/4   | 0.85 | 0.16 | 76,77,82,91                 | 0     |
| 31  | DMS  | V     | 210 | 4/4   | 0.85 | 0.19 | 70,73,78,88                 | 0     |
| 26  | PL9  | a     | 415 | 55/55 | 0.85 | 0.22 | 64,84,106,111               | 0     |
| 25  | LMG  | c     | 930 | 49/55 | 0.85 | 0.13 | 44,78,96,106                | 0     |
| 31  | DMS  | b     | 634 | 4/4   | 0.85 | 0.15 | 68,76,79,86                 | 0     |
| 28  | SQD  | f     | 101 | 14/54 | 0.85 | 0.12 | 77,89,96,96                 | 0     |
| 27  | LHG  | C     | 522 | 30/49 | 0.85 | 0.14 | 55,79,127,134               | 0     |
| 31  | DMS  | c     | 929 | 4/4   | 0.85 | 0.25 | 69,73,76,78                 | 0     |
| 31  | DMS  | O     | 314 | 4/4   | 0.85 | 0.19 | 78,80,86,91                 | 0     |
| 25  | LMG  | d     | 409 | 47/55 | 0.85 | 0.15 | 49,76,113,114               | 0     |
| 25  | LMG  | C     | 531 | 40/55 | 0.85 | 0.14 | 37,81,103,107               | 0     |
| 31  | DMS  | V     | 209 | 4/4   | 0.86 | 0.21 | 76,87,89,93                 | 0     |
| 30  | UNL  | x     | 101 | 15/-  | 0.86 | 0.11 | 43,50,56,58                 | 0     |
| 31  | DMS  | o     | 305 | 4/4   | 0.86 | 0.17 | 78,82,86,87                 | 0     |
| 30  | UNL  | B     | 624 | 7/-   | 0.86 | 0.18 | 30,45,51,56                 | 0     |
| 31  | DMS  | t     | 103 | 4/4   | 0.86 | 0.17 | 89,102,103,103              | 0     |
| 28  | SQD  | a     | 418 | 51/54 | 0.86 | 0.14 | 47,70,91,97                 | 0     |
| 31  | DMS  | c     | 941 | 4/4   | 0.86 | 0.15 | 73,79,87,88                 | 0     |
| 31  | DMS  | O     | 308 | 4/4   | 0.86 | 0.17 | 64,72,73,80                 | 0     |
| 31  | DMS  | B     | 636 | 4/4   | 0.86 | 0.14 | 60,62,67,69                 | 0     |
| 25  | LMG  | B     | 621 | 40/55 | 0.86 | 0.16 | 47,82,108,112               | 0     |
| 31  | DMS  | c     | 927 | 4/4   | 0.86 | 0.21 | 87,89,91,97                 | 0     |
| 30  | UNL  | A     | 415 | 5/-   | 0.86 | 0.18 | 68,72,73,75                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 30  | UNL  | i     | 103 | 16/-  | 0.86 | 0.14 | 53,64,79,82                 | 0     |
| 31  | DMS  | a     | 421 | 4/4   | 0.87 | 0.19 | 85,87,87,94                 | 0     |
| 31  | DMS  | o     | 302 | 4/4   | 0.87 | 0.17 | 59,64,71,75                 | 0     |
| 31  | DMS  | o     | 303 | 4/4   | 0.87 | 0.21 | 60,77,80,83                 | 0     |
| 31  | DMS  | D     | 417 | 4/4   | 0.87 | 0.16 | 72,72,77,86                 | 0     |
| 31  | DMS  | b     | 635 | 4/4   | 0.87 | 0.16 | 62,69,76,86                 | 0     |
| 31  | DMS  | U     | 202 | 4/4   | 0.87 | 0.21 | 42,49,58,67                 | 0     |
| 24  | BCR  | b     | 618 | 20/40 | 0.87 | 0.18 | 57,65,70,71                 | 0     |
| 27  | LHG  | l     | 102 | 49/49 | 0.87 | 0.14 | 38,61,91,95                 | 0     |
| 30  | UNL  | J     | 103 | 16/-  | 0.87 | 0.13 | 44,57,77,77                 | 0     |
| 31  | DMS  | B     | 642 | 4/4   | 0.87 | 0.16 | 65,66,75,82                 | 0     |
| 31  | DMS  | C     | 529 | 4/4   | 0.87 | 0.16 | 72,78,78,86                 | 0     |
| 29  | LMT  | B     | 622 | 24/35 | 0.87 | 0.12 | 57,67,73,78                 | 0     |
| 31  | DMS  | l     | 104 | 4/4   | 0.87 | 0.20 | 79,80,86,87                 | 0     |
| 31  | DMS  | v     | 210 | 4/4   | 0.87 | 0.25 | 63,71,80,91                 | 0     |
| 31  | DMS  | t     | 104 | 4/4   | 0.88 | 0.15 | 101,101,104,111             | 0     |
| 30  | UNL  | i     | 102 | 16/-  | 0.88 | 0.15 | 41,51,80,81                 | 0     |
| 24  | BCR  | b     | 619 | 31/40 | 0.88 | 0.11 | 47,54,63,67                 | 0     |
| 31  | DMS  | A     | 416 | 4/4   | 0.88 | 0.19 | 60,67,69,72                 | 0     |
| 31  | DMS  | C     | 535 | 4/4   | 0.88 | 0.16 | 70,79,83,86                 | 0     |
| 31  | DMS  | A     | 417 | 4/4   | 0.88 | 0.15 | 76,82,83,85                 | 0     |
| 31  | DMS  | V     | 204 | 4/4   | 0.88 | 0.16 | 66,73,76,76                 | 0     |
| 31  | DMS  | O     | 303 | 4/4   | 0.88 | 0.15 | 68,71,78,79                 | 0     |
| 31  | DMS  | b     | 638 | 4/4   | 0.88 | 0.20 | 49,52,54,70                 | 0     |
| 28  | SQD  | A     | 413 | 49/54 | 0.88 | 0.15 | 46,65,91,95                 | 0     |
| 34  | HTG  | C     | 521 | 19/19 | 0.88 | 0.12 | 55,80,93,96                 | 0     |
| 31  | DMS  | C     | 528 | 4/4   | 0.88 | 0.21 | 88,89,90,90                 | 0     |
| 31  | DMS  | V     | 212 | 4/4   | 0.89 | 0.17 | 51,54,55,72                 | 0     |
| 27  | LHG  | D     | 409 | 49/49 | 0.89 | 0.15 | 38,56,85,97                 | 0     |
| 31  | DMS  | v     | 206 | 4/4   | 0.89 | 0.17 | 69,72,72,77                 | 0     |
| 31  | DMS  | C     | 530 | 4/4   | 0.89 | 0.17 | 71,79,82,83                 | 0     |
| 31  | DMS  | b     | 631 | 4/4   | 0.89 | 0.16 | 68,72,79,80                 | 0     |
| 31  | DMS  | V     | 205 | 4/4   | 0.89 | 0.13 | 64,66,67,71                 | 0     |
| 31  | DMS  | O     | 311 | 4/4   | 0.89 | 0.15 | 48,56,59,61                 | 0     |
| 31  | DMS  | B     | 632 | 4/4   | 0.89 | 0.14 | 49,57,67,69                 | 0     |
| 30  | UNL  | D     | 413 | 16/-  | 0.89 | 0.12 | 38,46,52,58                 | 0     |
| 30  | UNL  | O     | 301 | 16/-  | 0.89 | 0.16 | 39,47,73,74                 | 0     |
| 37  | RRX  | h     | 101 | 41/41 | 0.89 | 0.12 | 40,49,75,82                 | 0     |
| 31  | DMS  | c     | 928 | 4/4   | 0.90 | 0.15 | 73,74,74,80                 | 0     |
| 30  | UNL  | B     | 625 | 16/-  | 0.90 | 0.12 | 40,47,59,59                 | 0     |
| 22  | CLA  | B     | 602 | 65/65 | 0.90 | 0.11 | 39,56,101,107               | 0     |
| 24  | BCR  | B     | 619 | 30/40 | 0.90 | 0.10 | 44,51,61,63                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 31  | DMS  | i     | 106 | 4/4   | 0.90 | 0.19 | 72,76,79,89                 | 0     |
| 28  | SQD  | a     | 414 | 54/54 | 0.90 | 0.13 | 36,69,81,87                 | 0     |
| 31  | DMS  | V     | 208 | 4/4   | 0.90 | 0.15 | 73,74,77,78                 | 0     |
| 31  | DMS  | c     | 939 | 4/4   | 0.90 | 0.15 | 88,92,95,102                | 0     |
| 30  | UNL  | X     | 101 | 16/-  | 0.90 | 0.12 | 35,53,62,64                 | 0     |
| 31  | DMS  | I     | 101 | 4/4   | 0.90 | 0.19 | 64,69,74,76                 | 0     |
| 31  | DMS  | o     | 304 | 4/4   | 0.90 | 0.18 | 70,70,70,74                 | 0     |
| 34  | HTG  | B     | 626 | 19/19 | 0.90 | 0.12 | 42,69,81,87                 | 0     |
| 31  | DMS  | I     | 106 | 4/4   | 0.90 | 0.18 | 64,74,78,80                 | 0     |
| 22  | CLA  | c     | 914 | 65/65 | 0.90 | 0.12 | 47,60,95,108                | 0     |
| 25  | LMG  | i     | 101 | 51/55 | 0.91 | 0.12 | 45,57,80,81                 | 0     |
| 25  | LMG  | c     | 920 | 51/55 | 0.91 | 0.13 | 37,61,87,91                 | 0     |
| 31  | DMS  | d     | 412 | 4/4   | 0.91 | 0.13 | 58,59,66,66                 | 0     |
| 31  | DMS  | F     | 101 | 4/4   | 0.91 | 0.16 | 69,70,74,77                 | 0     |
| 31  | DMS  | B     | 638 | 4/4   | 0.91 | 0.16 | 81,82,86,93                 | 0     |
| 31  | DMS  | u     | 202 | 4/4   | 0.91 | 0.15 | 47,53,55,68                 | 0     |
| 31  | DMS  | A     | 420 | 4/4   | 0.91 | 0.16 | 37,39,39,57                 | 0     |
| 31  | DMS  | B     | 641 | 4/4   | 0.91 | 0.14 | 46,49,61,66                 | 0     |
| 31  | DMS  | a     | 425 | 4/4   | 0.91 | 0.17 | 39,47,51,62                 | 0     |
| 25  | LMG  | C     | 520 | 51/55 | 0.91 | 0.12 | 34,60,90,92                 | 0     |
| 27  | LHG  | a     | 423 | 45/49 | 0.91 | 0.11 | 39,58,72,74                 | 0     |
| 31  | DMS  | O     | 304 | 4/4   | 0.91 | 0.15 | 74,80,84,88                 | 0     |
| 24  | BCR  | c     | 915 | 40/40 | 0.91 | 0.11 | 43,59,68,69                 | 0     |
| 31  | DMS  | v     | 208 | 4/4   | 0.91 | 0.17 | 88,90,91,94                 | 0     |
| 31  | DMS  | v     | 209 | 4/4   | 0.91 | 0.14 | 72,74,76,81                 | 0     |
| 31  | DMS  | O     | 306 | 4/4   | 0.91 | 0.15 | 69,69,70,81                 | 0     |
| 31  | DMS  | v     | 211 | 4/4   | 0.91 | 0.14 | 65,77,82,90                 | 0     |
| 30  | UNL  | d     | 410 | 16/-  | 0.92 | 0.10 | 40,49,57,60                 | 0     |
| 25  | LMG  | A     | 410 | 51/55 | 0.92 | 0.11 | 47,62,83,91                 | 0     |
| 27  | LHG  | L     | 101 | 40/49 | 0.92 | 0.11 | 37,53,63,66                 | 0     |
| 27  | LHG  | d     | 408 | 46/49 | 0.92 | 0.13 | 29,41,93,97                 | 0     |
| 31  | DMS  | O     | 309 | 4/4   | 0.92 | 0.16 | 61,70,70,74                 | 0     |
| 34  | HTG  | b     | 626 | 19/19 | 0.92 | 0.11 | 47,69,86,90                 | 0     |
| 22  | CLA  | c     | 913 | 65/65 | 0.92 | 0.11 | 42,54,96,98                 | 0     |
| 24  | BCR  | d     | 404 | 40/40 | 0.93 | 0.09 | 27,38,63,66                 | 0     |
| 31  | DMS  | d     | 413 | 4/4   | 0.93 | 0.24 | 67,69,73,80                 | 0     |
| 31  | DMS  | o     | 306 | 4/4   | 0.93 | 0.15 | 66,71,74,83                 | 0     |
| 24  | BCR  | k     | 101 | 40/40 | 0.93 | 0.09 | 36,45,51,52                 | 0     |
| 24  | BCR  | y     | 101 | 40/40 | 0.93 | 0.09 | 32,41,51,53                 | 0     |
| 24  | BCR  | Y     | 101 | 39/40 | 0.93 | 0.08 | 34,40,48,50                 | 0     |
| 31  | DMS  | C     | 527 | 4/4   | 0.93 | 0.16 | 74,80,80,81                 | 0     |
| 32  | BCT  | a     | 422 | 4/4   | 0.93 | 0.10 | 51,52,56,57                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 22  | CLA  | C     | 507    | 65/65 | 0.93 | 0.11 | 37,45,85,88                 | 0     |
| 31  | DMS  | c     | 926    | 4/4   | 0.93 | 0.14 | 63,64,67,68                 | 0     |
| 31  | DMS  | B     | 635    | 4/4   | 0.93 | 0.15 | 61,63,66,73                 | 0     |
| 35  | DGD  | c     | 918    | 62/66 | 0.93 | 0.10 | 34,42,98,113                | 0     |
| 22  | CLA  | b     | 617    | 60/65 | 0.93 | 0.10 | 32,41,75,80                 | 0     |
| 37  | RRX  | H     | 101    | 41/41 | 0.93 | 0.10 | 32,42,58,62                 | 0     |
| 22  | CLA  | C     | 514    | 65/65 | 0.93 | 0.10 | 44,55,83,86                 | 0     |
| 22  | CLA  | B     | 615    | 53/65 | 0.94 | 0.09 | 31,36,71,84                 | 0     |
| 22  | CLA  | b     | 607    | 65/65 | 0.94 | 0.08 | 29,37,58,65                 | 0     |
| 31  | DMS  | a     | 424    | 4/4   | 0.94 | 0.12 | 38,47,50,65                 | 0     |
| 24  | BCR  | C     | 515    | 40/40 | 0.94 | 0.09 | 37,50,58,59                 | 0     |
| 31  | DMS  | B     | 633    | 4/4   | 0.94 | 0.17 | 65,71,71,73                 | 0     |
| 22  | CLA  | b     | 615    | 52/65 | 0.94 | 0.09 | 36,42,71,76                 | 0     |
| 22  | CLA  | B     | 617    | 55/65 | 0.94 | 0.09 | 28,35,72,76                 | 0     |
| 34  | HTG  | b     | 623    | 19/19 | 0.94 | 0.09 | 42,46,54,63                 | 0     |
| 22  | CLA  | c     | 904    | 65/65 | 0.94 | 0.08 | 32,44,50,54                 | 0     |
| 22  | CLA  | c     | 907    | 65/65 | 0.94 | 0.11 | 39,47,102,108               | 0     |
| 24  | BCR  | c     | 916    | 40/40 | 0.94 | 0.08 | 33,42,48,49                 | 0     |
| 22  | CLA  | c     | 908    | 65/65 | 0.94 | 0.09 | 34,39,53,61                 | 0     |
| 31  | DMS  | B     | 640    | 4/4   | 0.94 | 0.17 | 47,53,57,63                 | 0     |
| 28  | SQD  | C     | 501    | 54/54 | 0.94 | 0.11 | 32,64,83,89                 | 0     |
| 25  | LMG  | j     | 101    | 47/55 | 0.94 | 0.10 | 33,43,69,74                 | 0     |
| 35  | DGD  | C     | 518    | 62/66 | 0.94 | 0.10 | 29,40,89,109                | 0     |
| 31  | DMS  | c     | 934    | 4/4   | 0.94 | 0.11 | 64,73,74,77                 | 0     |
| 22  | CLA  | B     | 607    | 65/65 | 0.94 | 0.08 | 28,34,56,65                 | 0     |
| 22  | CLA  | B     | 608    | 65/65 | 0.94 | 0.09 | 24,29,64,79                 | 0     |
| 35  | DGD  | h     | 102    | 62/66 | 0.94 | 0.09 | 28,42,53,58                 | 0     |
| 22  | CLA  | d     | 403    | 65/65 | 0.94 | 0.10 | 35,40,85,90                 | 0     |
| 31  | DMS  | A     | 419    | 4/4   | 0.94 | 0.17 | 58,60,70,72                 | 0     |
| 31  | DMS  | c     | 933    | 4/4   | 0.95 | 0.12 | 57,64,66,70                 | 0     |
| 22  | CLA  | b     | 614    | 59/65 | 0.95 | 0.08 | 26,32,76,82                 | 0     |
| 31  | DMS  | O     | 310    | 4/4   | 0.95 | 0.14 | 66,68,68,73                 | 0     |
| 24  | BCR  | B     | 620    | 40/40 | 0.95 | 0.07 | 30,37,49,50                 | 0     |
| 22  | CLA  | C     | 509    | 65/65 | 0.95 | 0.09 | 29,35,81,102                | 0     |
| 24  | BCR  | C     | 516    | 40/40 | 0.95 | 0.08 | 32,39,47,54                 | 0     |
| 24  | BCR  | D     | 405    | 40/40 | 0.95 | 0.08 | 26,35,62,66                 | 0     |
| 24  | BCR  | K     | 101    | 40/40 | 0.95 | 0.08 | 31,39,43,43                 | 0     |
| 31  | DMS  | V     | 201    | 4/4   | 0.95 | 0.10 | 46,48,54,58                 | 0     |
| 32  | BCT  | A     | 421[A] | 4/4   | 0.95 | 0.10 | 34,36,39,39                 | 4     |
| 32  | BCT  | A     | 421[B] | 4/4   | 0.95 | 0.10 | 27,29,30,34                 | 4     |
| 26  | PL9  | D     | 406    | 55/55 | 0.95 | 0.07 | 21,30,37,51                 | 0     |
| 33  | CA   | B     | 601    | 1/1   | 0.95 | 0.05 | 64,64,64,64                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 33  | CA   | O     | 302 | 1/1   | 0.95 | 0.06 | 59,59,59,59                 | 0     |
| 34  | HTG  | B     | 623 | 19/19 | 0.95 | 0.09 | 41,47,64,66                 | 0     |
| 22  | CLA  | C     | 512 | 65/65 | 0.95 | 0.08 | 31,39,48,51                 | 0     |
| 26  | PL9  | d     | 405 | 55/55 | 0.95 | 0.07 | 23,32,39,43                 | 0     |
| 24  | BCR  | a     | 413 | 40/40 | 0.95 | 0.07 | 26,31,38,39                 | 0     |
| 22  | CLA  | c     | 902 | 65/65 | 0.95 | 0.08 | 34,39,50,51                 | 0     |
| 22  | CLA  | C     | 513 | 56/65 | 0.95 | 0.08 | 37,48,62,65                 | 0     |
| 27  | LHG  | D     | 411 | 45/49 | 0.95 | 0.10 | 31,39,90,94                 | 0     |
| 24  | BCR  | b     | 620 | 40/40 | 0.95 | 0.07 | 33,39,48,49                 | 0     |
| 22  | CLA  | c     | 906 | 65/65 | 0.95 | 0.08 | 30,40,50,54                 | 0     |
| 31  | DMS  | D     | 416 | 4/4   | 0.95 | 0.12 | 55,59,60,69                 | 0     |
| 22  | CLA  | B     | 611 | 65/65 | 0.95 | 0.08 | 26,33,41,46                 | 0     |
| 22  | CLA  | D     | 404 | 65/65 | 0.95 | 0.09 | 30,37,94,104                | 0     |
| 31  | DMS  | b     | 630 | 4/4   | 0.95 | 0.15 | 56,63,63,64                 | 0     |
| 31  | DMS  | B     | 629 | 4/4   | 0.95 | 0.14 | 48,52,58,65                 | 0     |
| 31  | DMS  | b     | 633 | 4/4   | 0.95 | 0.14 | 68,68,70,78                 | 0     |
| 22  | CLA  | c     | 909 | 65/65 | 0.95 | 0.08 | 31,37,80,97                 | 0     |
| 22  | CLA  | c     | 910 | 65/65 | 0.95 | 0.09 | 28,38,58,64                 | 0     |
| 22  | CLA  | c     | 912 | 65/65 | 0.95 | 0.08 | 35,45,50,53                 | 0     |
| 35  | DGD  | C     | 519 | 62/66 | 0.95 | 0.09 | 23,36,76,85                 | 0     |
| 22  | CLA  | a     | 412 | 65/65 | 0.95 | 0.11 | 27,32,102,116               | 0     |
| 35  | DGD  | H     | 102 | 62/66 | 0.95 | 0.08 | 28,37,46,50                 | 0     |
| 22  | CLA  | B     | 604 | 65/65 | 0.95 | 0.08 | 26,30,40,47                 | 0     |
| 35  | DGD  | c     | 919 | 62/66 | 0.95 | 0.09 | 29,40,73,79                 | 0     |
| 22  | CLA  | C     | 508 | 65/65 | 0.95 | 0.08 | 32,42,55,59                 | 0     |
| 23  | PHO  | a     | 411 | 64/64 | 0.95 | 0.06 | 26,33,40,48                 | 0     |
| 25  | LMG  | J     | 101 | 45/55 | 0.95 | 0.09 | 28,36,71,79                 | 0     |
| 22  | CLA  | b     | 610 | 65/65 | 0.95 | 0.08 | 32,41,45,54                 | 0     |
| 22  | CLA  | A     | 408 | 65/65 | 0.96 | 0.09 | 19,29,99,110                | 0     |
| 27  | LHG  | d     | 407 | 49/49 | 0.96 | 0.07 | 28,36,56,63                 | 0     |
| 31  | DMS  | d     | 411 | 4/4   | 0.96 | 0.12 | 60,62,64,64                 | 0     |
| 22  | CLA  | b     | 608 | 65/65 | 0.96 | 0.08 | 27,31,73,74                 | 0     |
| 31  | DMS  | B     | 630 | 4/4   | 0.96 | 0.13 | 63,67,68,75                 | 0     |
| 22  | CLA  | b     | 609 | 65/65 | 0.96 | 0.06 | 27,34,42,45                 | 0     |
| 23  | PHO  | A     | 407 | 64/64 | 0.96 | 0.06 | 20,25,30,32                 | 0     |
| 23  | PHO  | D     | 402 | 64/64 | 0.96 | 0.06 | 25,29,35,39                 | 0     |
| 23  | PHO  | a     | 410 | 64/64 | 0.96 | 0.06 | 21,28,32,36                 | 0     |
| 22  | CLA  | B     | 614 | 61/65 | 0.96 | 0.07 | 25,31,70,83                 | 0     |
| 24  | BCR  | A     | 409 | 40/40 | 0.96 | 0.06 | 25,30,37,38                 | 0     |
| 22  | CLA  | b     | 611 | 65/65 | 0.96 | 0.07 | 28,35,40,43                 | 0     |
| 22  | CLA  | b     | 612 | 65/65 | 0.96 | 0.08 | 27,31,72,83                 | 0     |
| 22  | CLA  | B     | 606 | 65/65 | 0.96 | 0.07 | 24,30,42,46                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 22  | CLA  | C     | 510 | 65/65 | 0.96 | 0.09 | 31,36,59,64                 | 0     |
| 22  | CLA  | b     | 616 | 65/65 | 0.96 | 0.07 | 30,37,53,57                 | 0     |
| 31  | DMS  | c     | 924 | 4/4   | 0.96 | 0.14 | 37,42,47,49                 | 0     |
| 31  | DMS  | c     | 925 | 4/4   | 0.96 | 0.11 | 51,58,60,61                 | 0     |
| 22  | CLA  | C     | 511 | 65/65 | 0.96 | 0.06 | 31,36,41,46                 | 0     |
| 22  | CLA  | B     | 610 | 65/65 | 0.96 | 0.06 | 30,37,42,46                 | 0     |
| 31  | DMS  | O     | 312 | 4/4   | 0.96 | 0.14 | 37,51,56,59                 | 0     |
| 22  | CLA  | C     | 502 | 65/65 | 0.96 | 0.07 | 33,39,52,62                 | 0     |
| 22  | CLA  | c     | 905 | 65/65 | 0.96 | 0.08 | 30,35,62,66                 | 0     |
| 35  | DGD  | C     | 517 | 62/66 | 0.96 | 0.09 | 24,35,80,88                 | 0     |
| 22  | CLA  | C     | 503 | 65/65 | 0.96 | 0.07 | 28,32,47,56                 | 0     |
| 22  | CLA  | C     | 504 | 65/65 | 0.96 | 0.06 | 29,37,42,51                 | 0     |
| 31  | DMS  | v     | 201 | 4/4   | 0.96 | 0.16 | 42,48,50,51                 | 0     |
| 22  | CLA  | C     | 505 | 65/65 | 0.96 | 0.07 | 28,34,58,60                 | 0     |
| 35  | DGD  | c     | 917 | 62/66 | 0.96 | 0.08 | 26,42,81,94                 | 0     |
| 27  | LHG  | D     | 410 | 49/49 | 0.96 | 0.07 | 29,36,51,61                 | 0     |
| 22  | CLA  | C     | 506 | 65/65 | 0.96 | 0.07 | 30,37,50,54                 | 0     |
| 31  | DMS  | V     | 206 | 4/4   | 0.96 | 0.09 | 45,48,51,62                 | 0     |
| 22  | CLA  | b     | 603 | 65/65 | 0.96 | 0.07 | 29,36,46,49                 | 0     |
| 36  | HEM  | E     | 102 | 43/43 | 0.96 | 0.09 | 48,56,62,65                 | 0     |
| 22  | CLA  | c     | 911 | 65/65 | 0.96 | 0.06 | 29,38,46,52                 | 0     |
| 22  | CLA  | b     | 604 | 65/65 | 0.96 | 0.07 | 26,32,45,50                 | 0     |
| 38  | MG   | J     | 102 | 1/1   | 0.96 | 0.06 | 30,30,30,30                 | 0     |
| 22  | CLA  | B     | 609 | 65/65 | 0.97 | 0.06 | 25,30,38,39                 | 0     |
| 31  | DMS  | C     | 526 | 4/4   | 0.97 | 0.09 | 48,48,50,51                 | 0     |
| 22  | CLA  | B     | 616 | 65/65 | 0.97 | 0.06 | 30,36,50,57                 | 0     |
| 22  | CLA  | A     | 406 | 55/65 | 0.97 | 0.06 | 21,27,49,60                 | 0     |
| 31  | DMS  | b     | 629 | 4/4   | 0.97 | 0.09 | 29,31,36,45                 | 0     |
| 22  | CLA  | a     | 408 | 65/65 | 0.97 | 0.05 | 20,26,35,41                 | 0     |
| 22  | CLA  | a     | 409 | 61/65 | 0.97 | 0.07 | 25,29,80,87                 | 0     |
| 22  | CLA  | B     | 603 | 65/65 | 0.97 | 0.06 | 27,36,43,47                 | 0     |
| 22  | CLA  | b     | 613 | 65/65 | 0.97 | 0.06 | 26,32,37,40                 | 0     |
| 22  | CLA  | B     | 612 | 65/65 | 0.97 | 0.06 | 23,29,55,60                 | 0     |
| 22  | CLA  | B     | 613 | 65/65 | 0.97 | 0.06 | 24,30,37,40                 | 0     |
| 22  | CLA  | A     | 405 | 65/65 | 0.97 | 0.06 | 18,23,36,54                 | 0     |
| 22  | CLA  | b     | 605 | 65/65 | 0.97 | 0.07 | 23,29,63,65                 | 0     |
| 22  | CLA  | d     | 402 | 65/65 | 0.97 | 0.05 | 21,27,42,50                 | 0     |
| 36  | HEM  | e     | 101 | 43/43 | 0.97 | 0.09 | 43,55,85,93                 | 0     |
| 31  | DMS  | o     | 307 | 4/4   | 0.97 | 0.19 | 48,56,62,64                 | 0     |
| 22  | CLA  | b     | 606 | 65/65 | 0.97 | 0.06 | 24,28,40,40                 | 0     |
| 22  | CLA  | c     | 903 | 65/65 | 0.97 | 0.07 | 27,34,54,65                 | 0     |
| 38  | MG   | k     | 102 | 1/1   | 0.97 | 0.07 | 48,48,48,48                 | 0     |

*Continued on next page...*

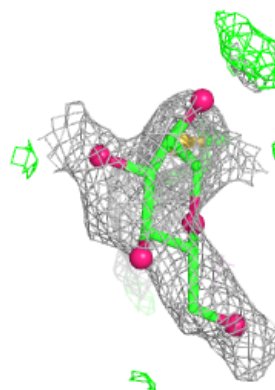
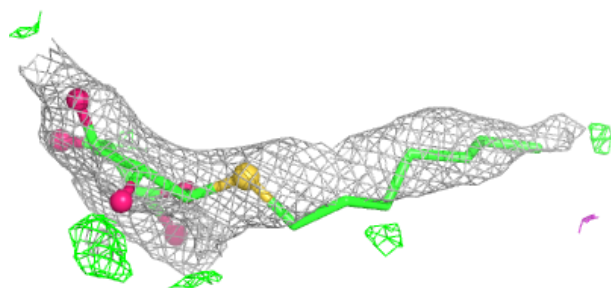
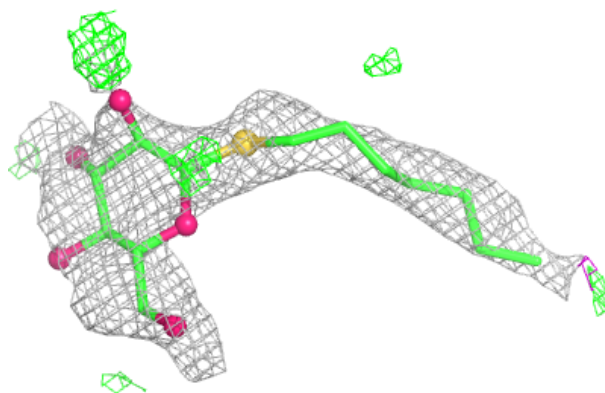
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 31  | DMS  | c     | 923 | 4/4   | 0.98 | 0.09 | 37,40,42,43                 | 0     |
| 22  | CLA  | B     | 605 | 65/65 | 0.98 | 0.06 | 24,28,60,66                 | 0     |
| 31  | DMS  | B     | 628 | 4/4   | 0.98 | 0.07 | 27,29,32,38                 | 0     |
| 31  | DMS  | D     | 418 | 4/4   | 0.98 | 0.06 | 35,39,42,43                 | 0     |
| 31  | DMS  | C     | 525 | 4/4   | 0.98 | 0.08 | 34,35,38,40                 | 0     |
| 22  | CLA  | a     | 407 | 65/65 | 0.98 | 0.05 | 23,26,45,61                 | 0     |
| 21  | CL   | A     | 404 | 1/1   | 0.98 | 0.04 | 28,28,28,28                 | 0     |
| 22  | CLA  | D     | 401 | 65/65 | 0.98 | 0.05 | 19,23,31,36                 | 0     |
| 31  | DMS  | A     | 418 | 4/4   | 0.98 | 0.05 | 29,30,31,31                 | 0     |
| 38  | MG   | K     | 102 | 1/1   | 0.98 | 0.05 | 51,51,51,51                 | 0     |
| 22  | CLA  | D     | 403 | 65/65 | 0.98 | 0.05 | 18,24,45,52                 | 0     |
| 39  | HEC  | V     | 202 | 43/43 | 0.98 | 0.06 | 23,29,36,40                 | 0     |
| 39  | HEC  | v     | 202 | 43/43 | 0.98 | 0.06 | 33,37,42,46                 | 0     |
| 21  | CL   | a     | 406 | 1/1   | 0.99 | 0.03 | 32,32,32,32                 | 0     |
| 33  | CA   | b     | 601 | 1/1   | 0.99 | 0.03 | 59,59,59,59                 | 0     |
| 33  | CA   | c     | 901 | 1/1   | 0.99 | 0.05 | 48,48,48,48                 | 0     |
| 33  | CA   | o     | 301 | 1/1   | 0.99 | 0.04 | 55,55,55,55                 | 0     |
| 31  | DMS  | a     | 402 | 4/4   | 0.99 | 0.07 | 30,32,34,34                 | 0     |
| 38  | MG   | j     | 102 | 1/1   | 0.99 | 0.08 | 40,40,40,40                 | 0     |
| 31  | DMS  | C     | 524 | 4/4   | 0.99 | 0.06 | 38,42,43,43                 | 0     |
| 21  | CL   | A     | 403 | 1/1   | 0.99 | 0.04 | 29,29,29,29                 | 0     |
| 21  | CL   | a     | 405 | 1/1   | 0.99 | 0.04 | 31,31,31,31                 | 0     |
| 19  | OEX  | A     | 401 | 10/10 | 1.00 | 0.05 | 25,27,31,32                 | 0     |
| 19  | OEX  | a     | 403 | 10/10 | 1.00 | 0.03 | 29,31,32,33                 | 0     |
| 20  | FE2  | A     | 402 | 1/1   | 1.00 | 0.01 | 39,39,39,39                 | 0     |
| 20  | FE2  | a     | 404 | 1/1   | 1.00 | 0.01 | 42,42,42,42                 | 0     |

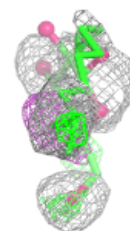
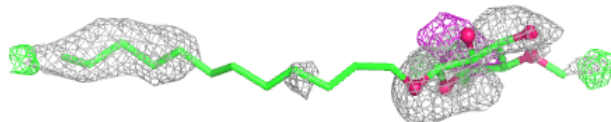
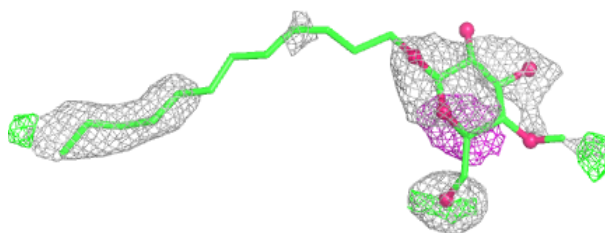
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HTG b 624:**

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

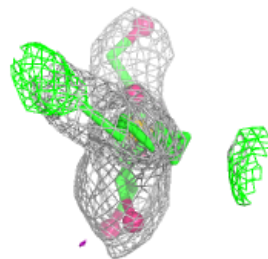
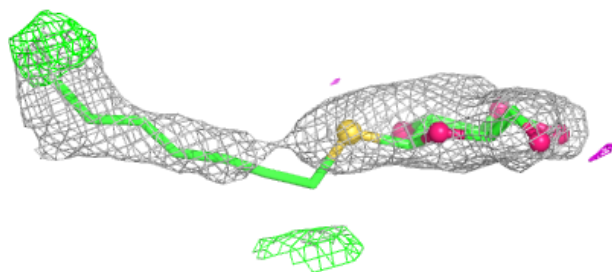
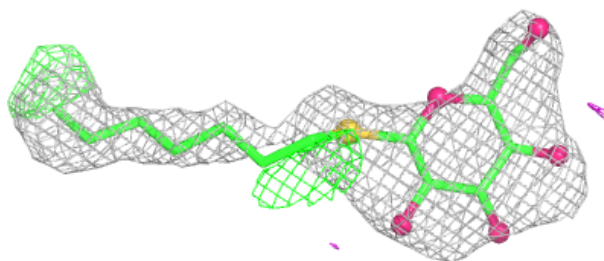
**Electron density around LMT f 102:**

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

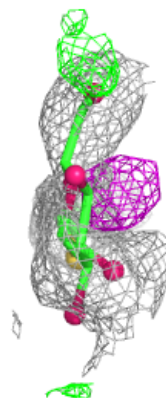
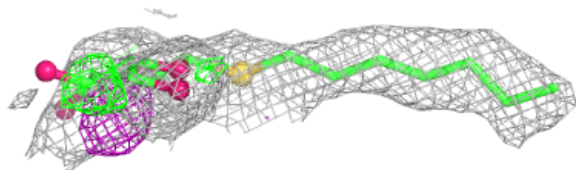
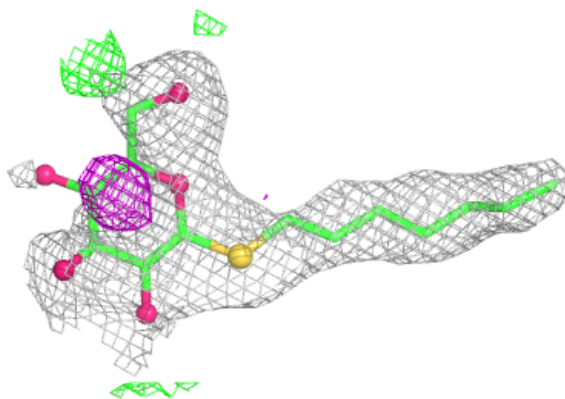


**Electron density around HTG c 922:**

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

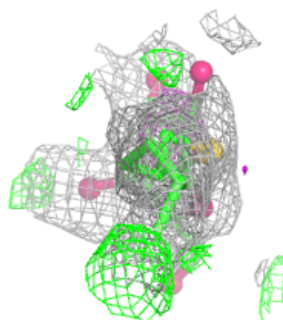
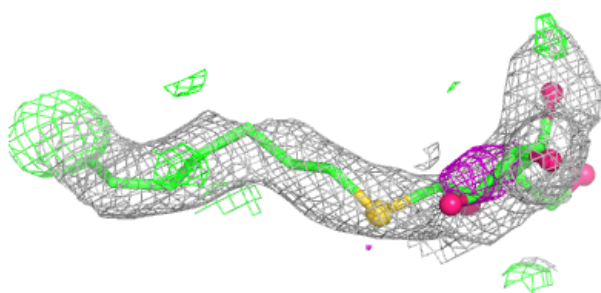
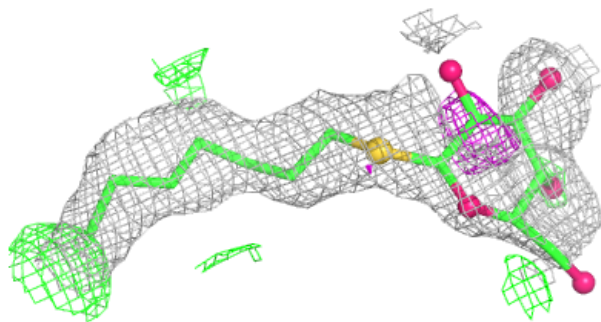
**Electron density around HTG b 627:**

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

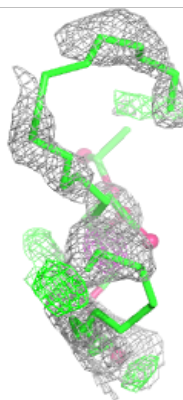
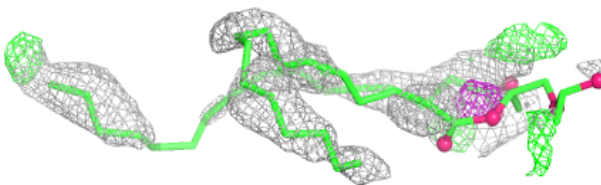
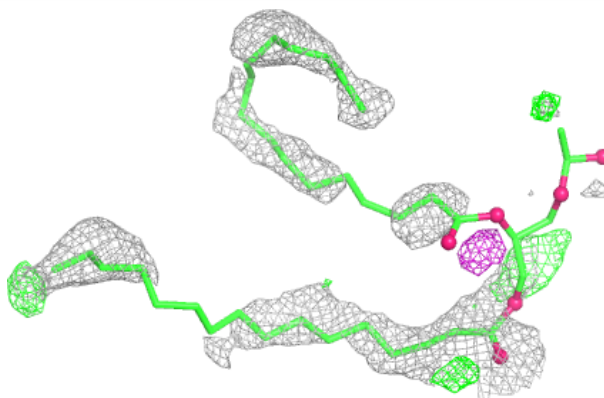


**Electron density around HTG D 415:**

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

**Electron density around DGD d 406:**

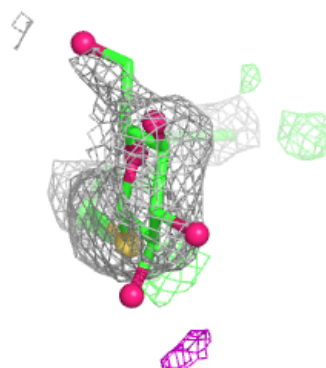
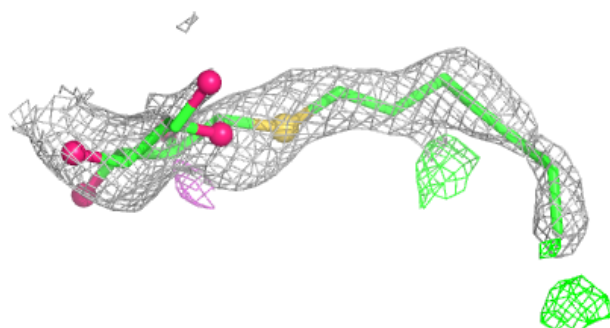
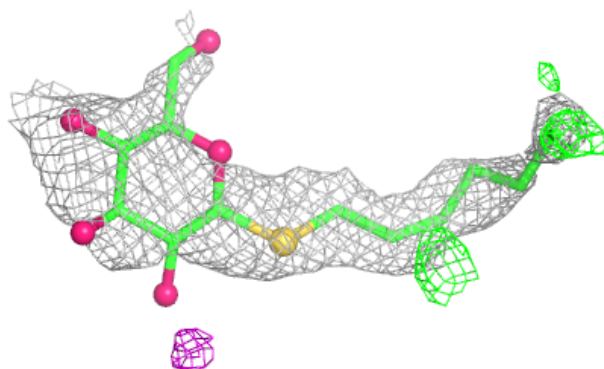
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



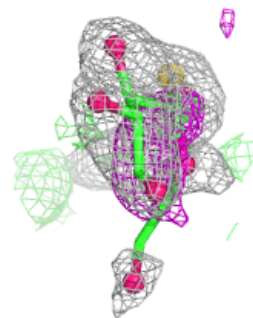
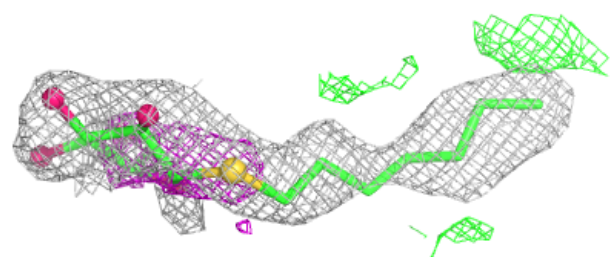
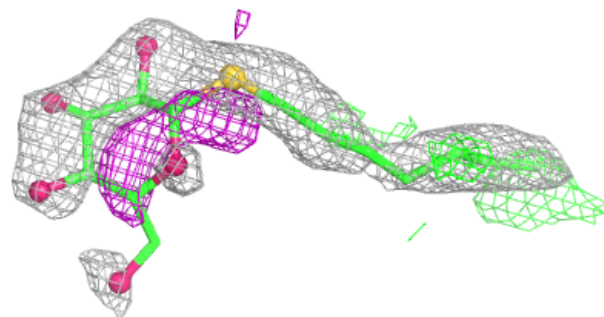


**Electron density around HTG D 414:**

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

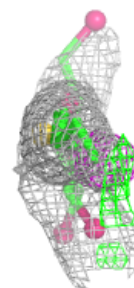
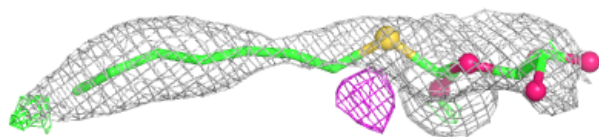
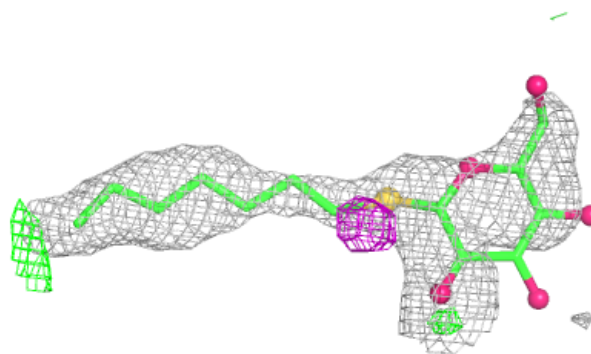
**Electron density around HTG b 632:**

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

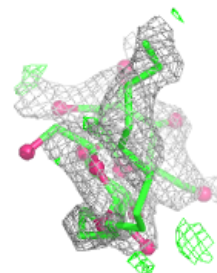
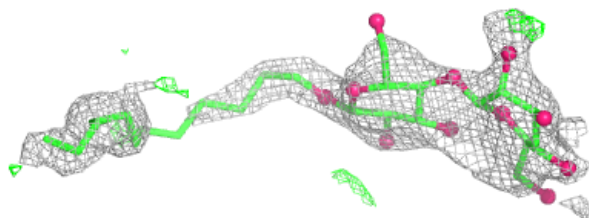
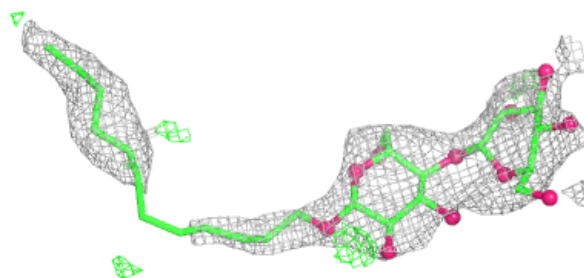


**Electron density around HTG B 627:**

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

**Electron density around LMT I 102:**

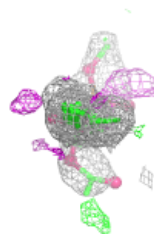
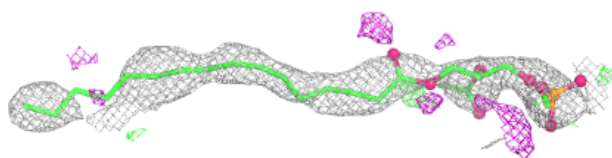
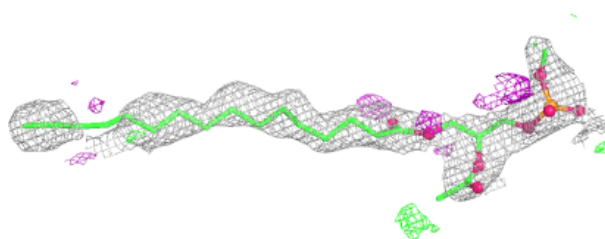
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





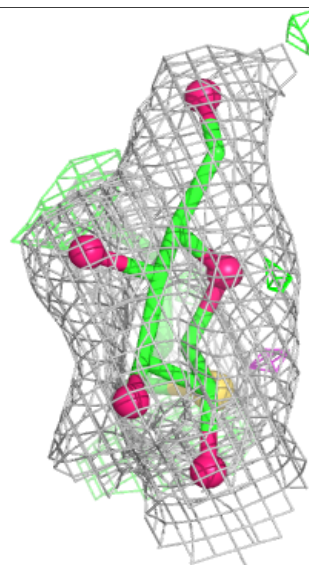
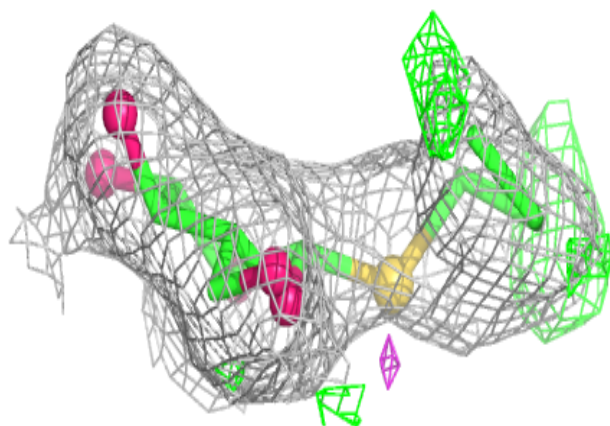
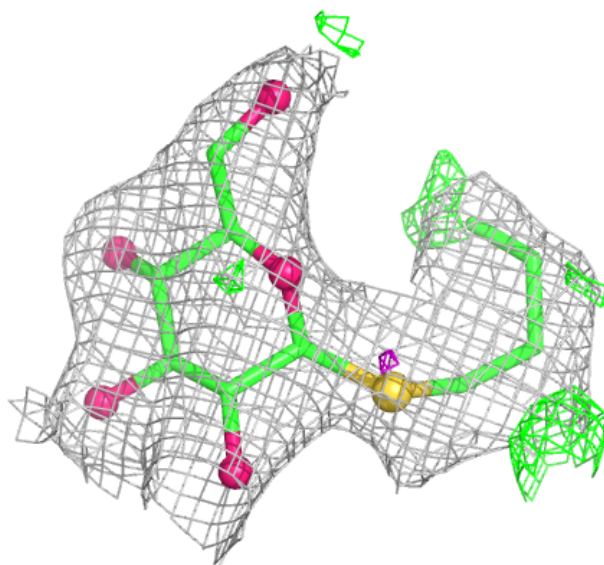
**Electron density around LHG A 412:**

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



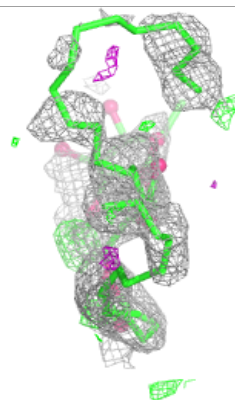
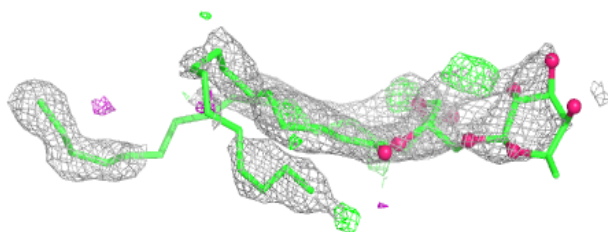
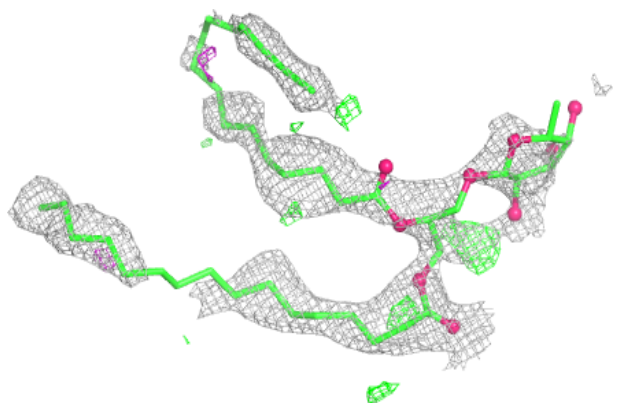
**Electron density around HTG v 203:**

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

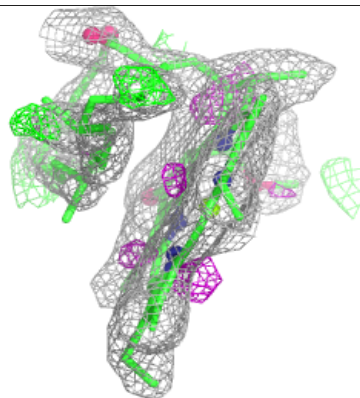
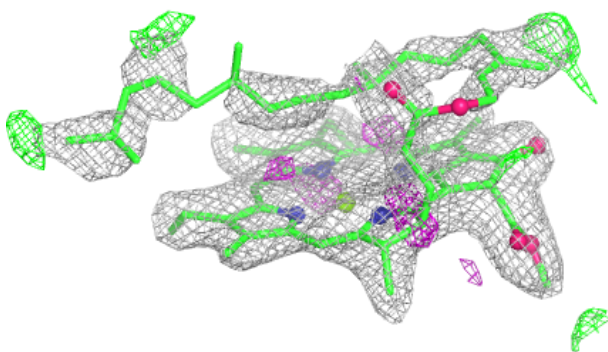
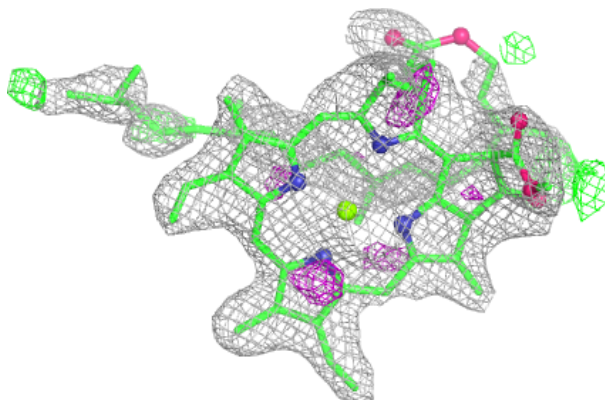


**Electron density around DGD D 407:**

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

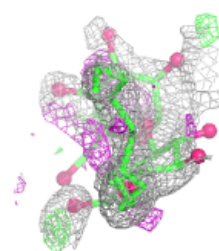
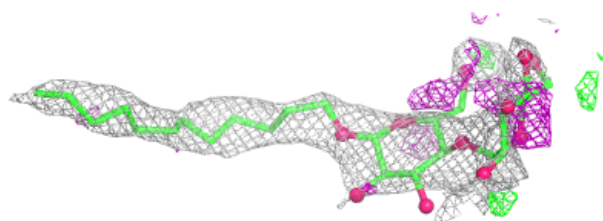
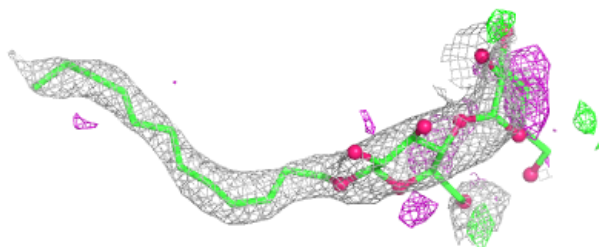
**Electron density around CLA b 602:**

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

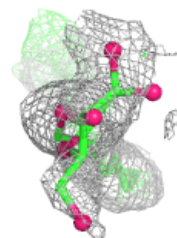
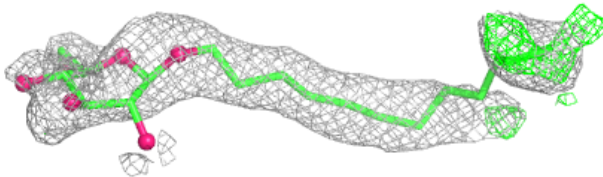
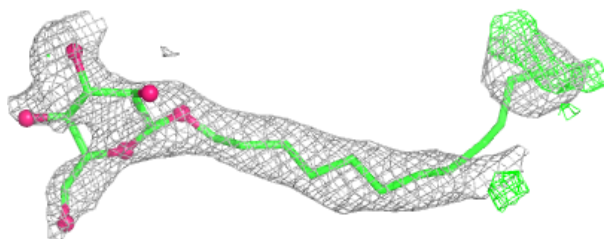


**Electron density around LMT A 414:**

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

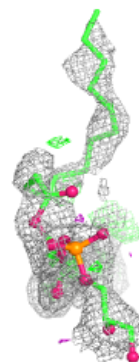
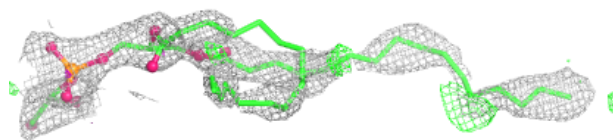
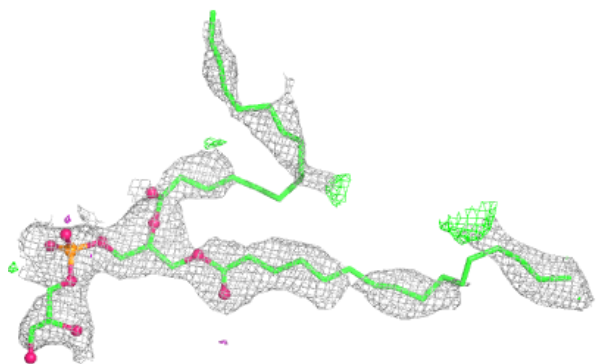
**Electron density around LMT T 102:**

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



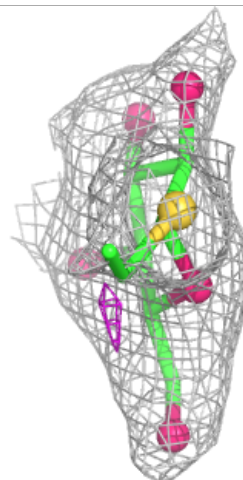
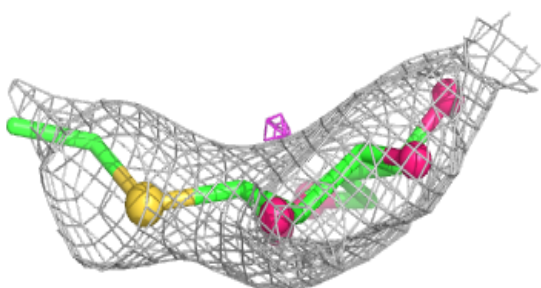
**Electron density around LHG a 416:**

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



**Electron density around HTG V 203:**

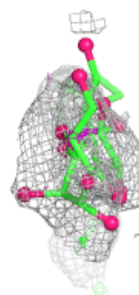
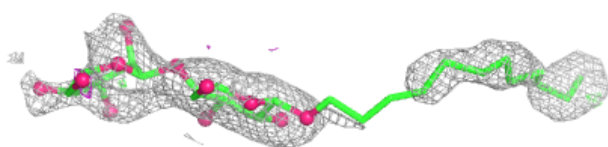
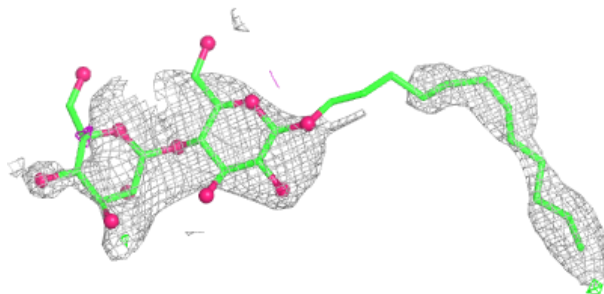
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



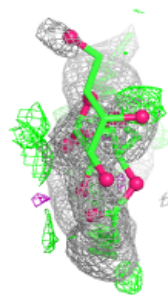
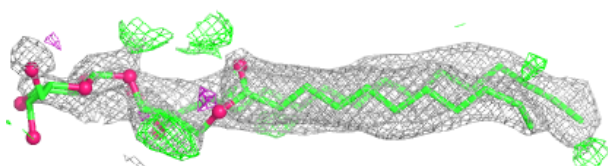
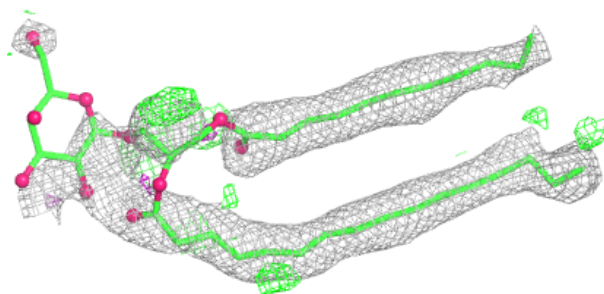


**Electron density around LMT Z 101:**

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

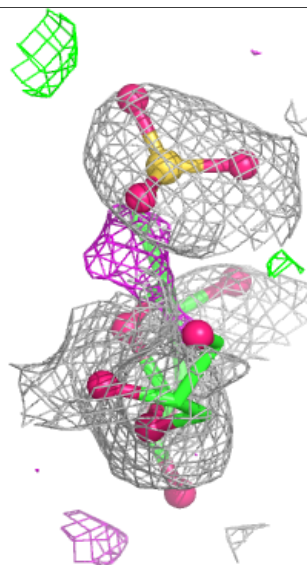
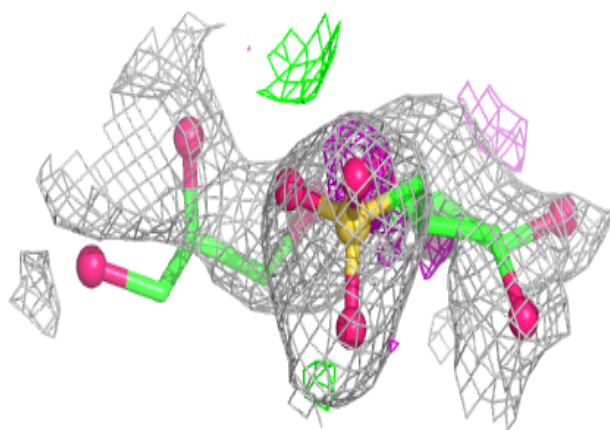
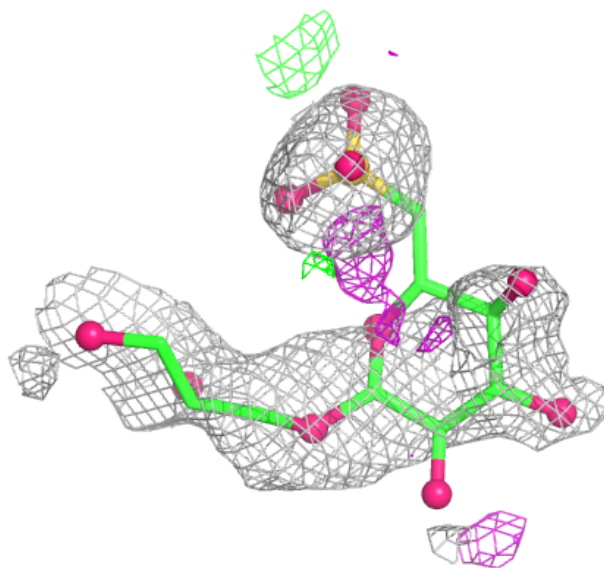
**Electron density around LMG D 412:**

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



**Electron density around SQD D 408:**

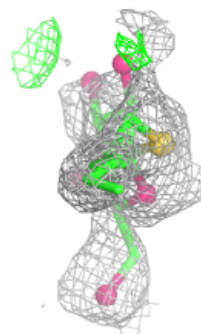
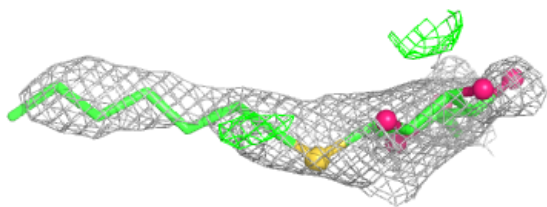
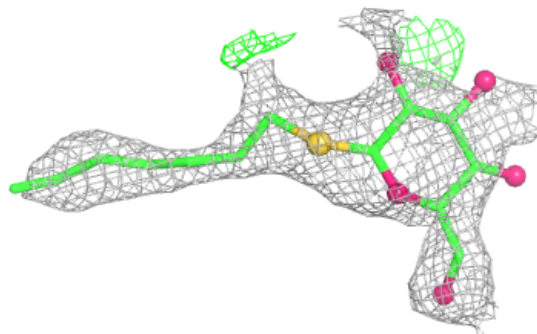
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



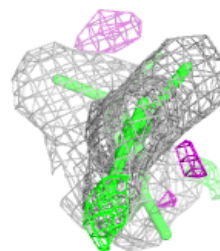
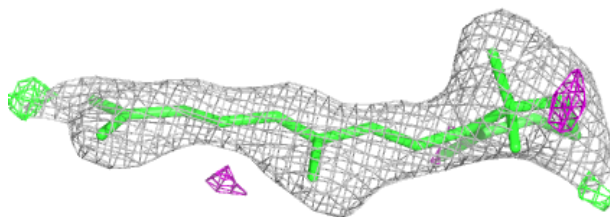
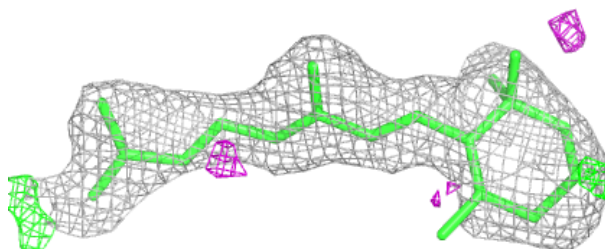


**Electron density around HTG 1 106:**

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

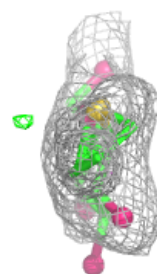
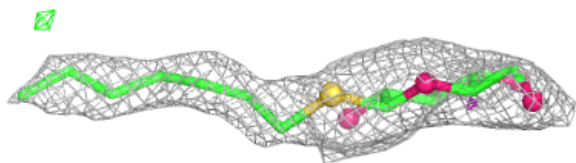
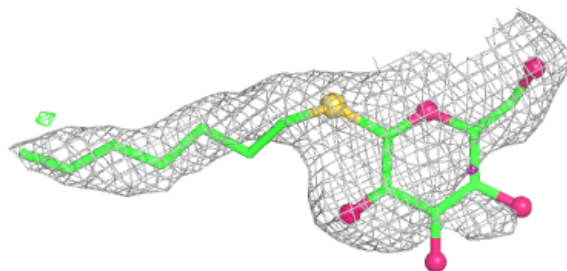
**Electron density around BCR B 618:**

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

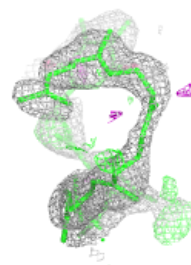
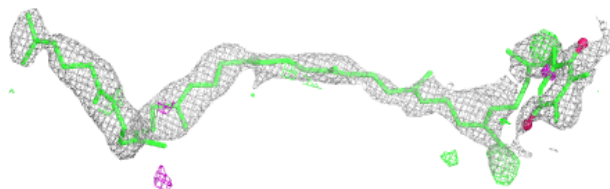
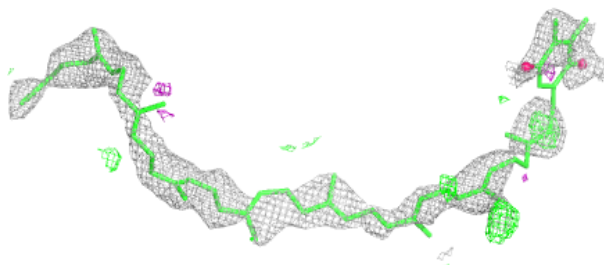


**Electron density around HTG C 532:**

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

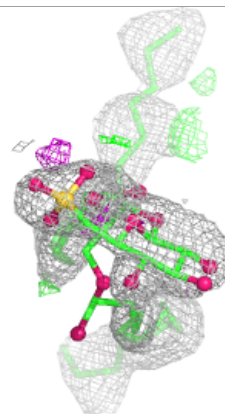
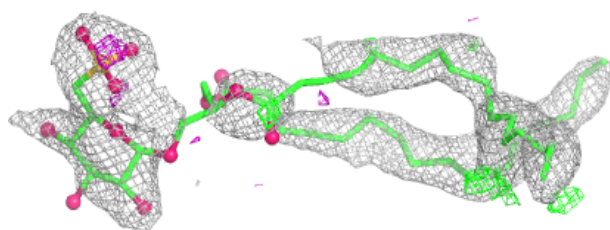
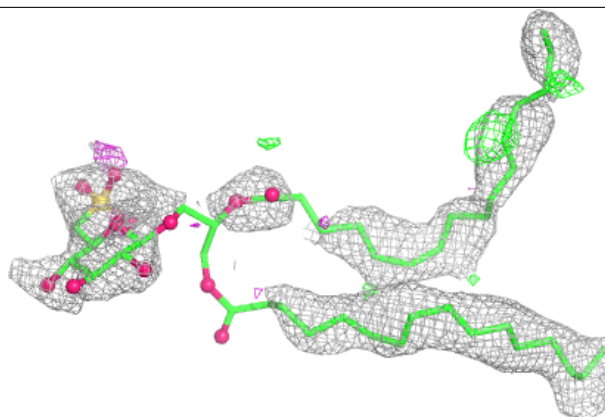
**Electron density around PL9 A 411:**

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

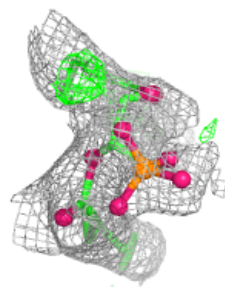
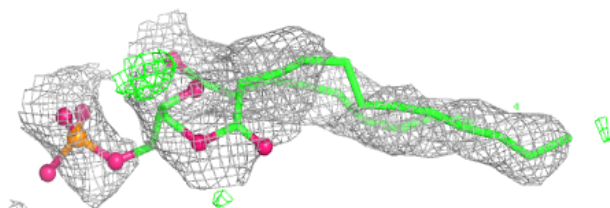
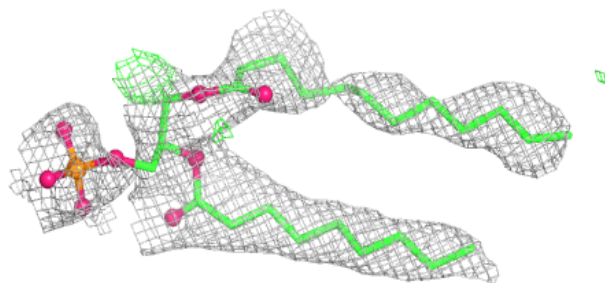


**Electron density around SQD 1 101:**

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

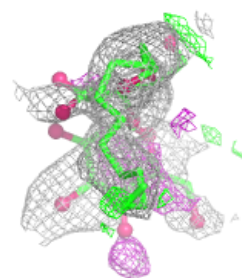
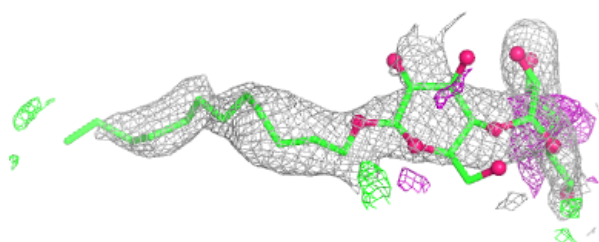
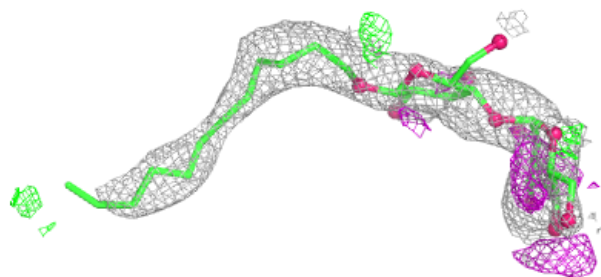
**Electron density around LHG d 401:**

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

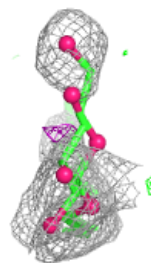
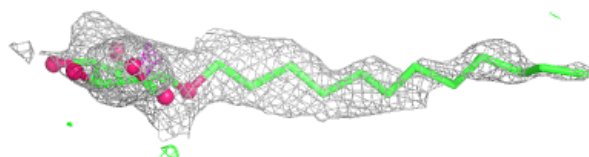
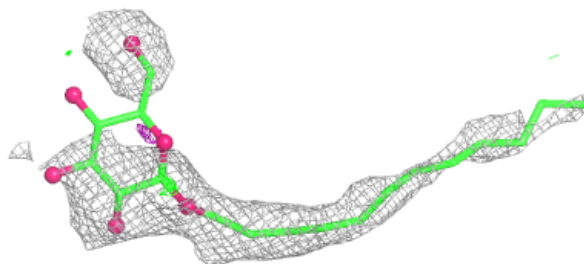


**Electron density around LMT a 419:**

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

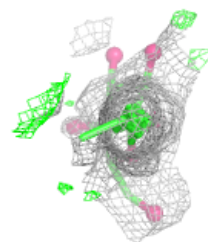
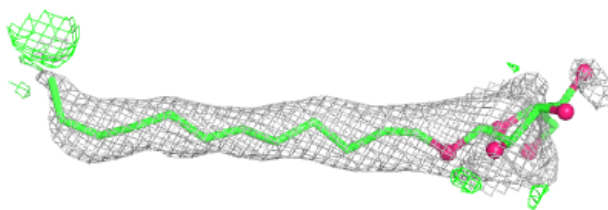
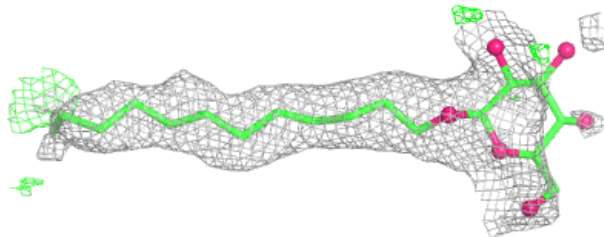
**Electron density around LMT E 101:**

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

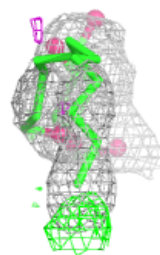
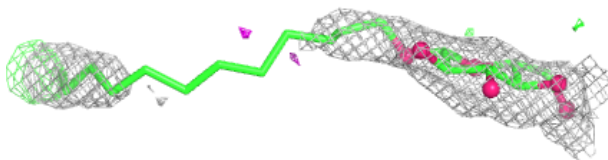
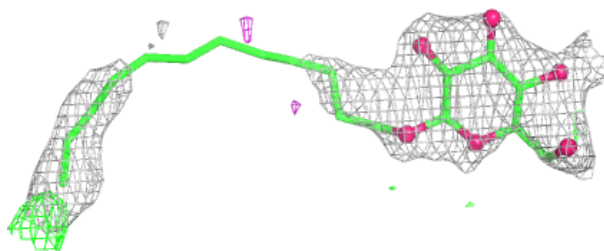


**Electron density around LMT t 101:**

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

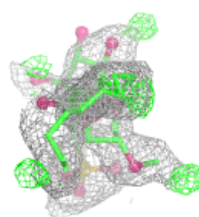
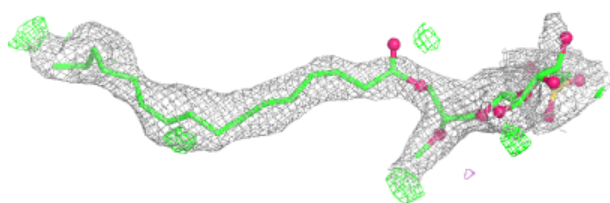
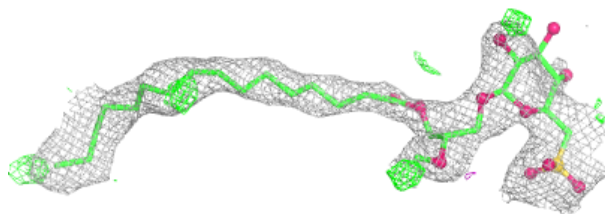
**Electron density around LMT c 931:**

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

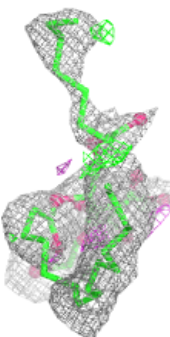
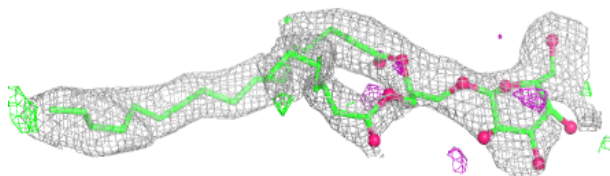
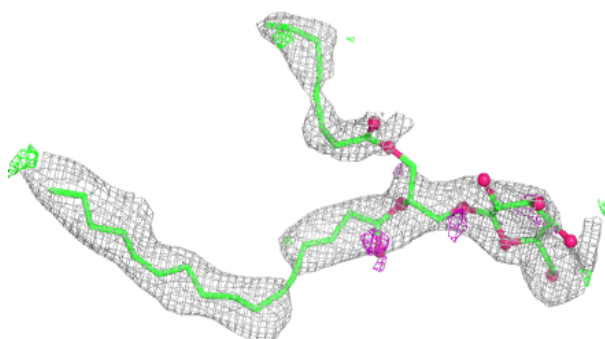


**Electron density around SQD b 621:**

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

**Electron density around LMG b 622:**

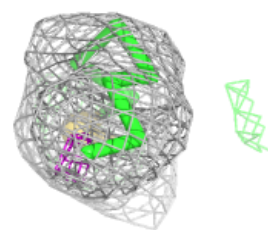
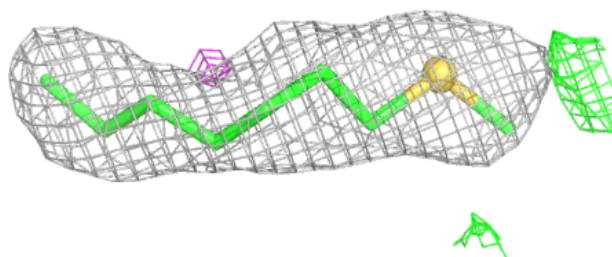
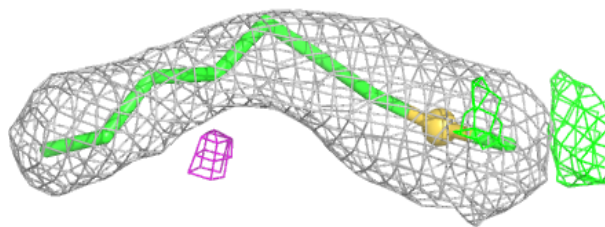
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



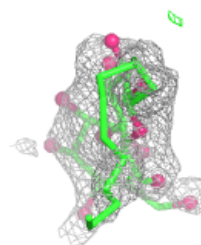
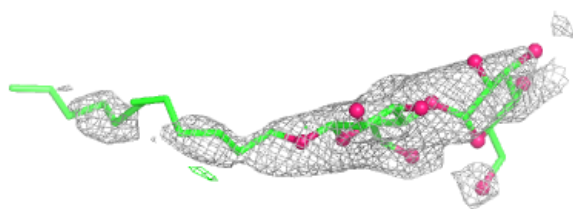
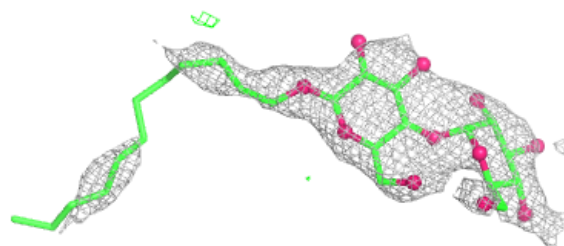


**Electron density around HTG C 523:**

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

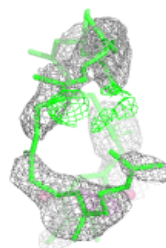
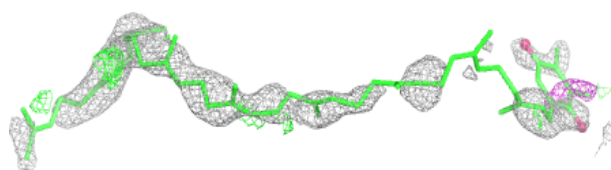
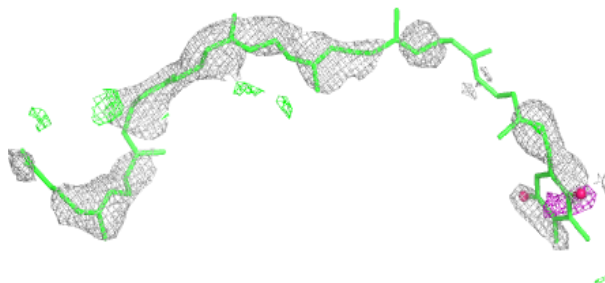
**Electron density around LMT c 921:**

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

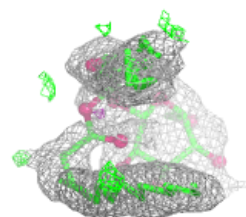
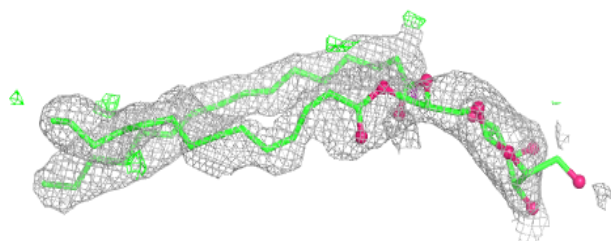
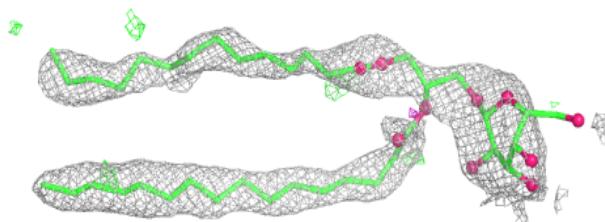


**Electron density around PL9 a 415:**

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

**Electron density around LMG c 930:**

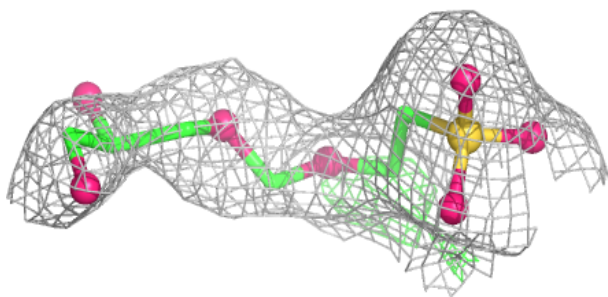
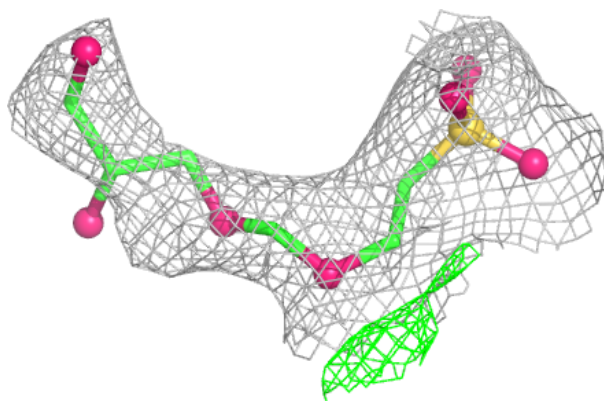
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



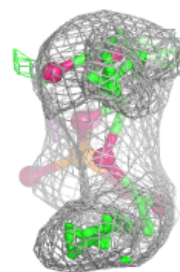
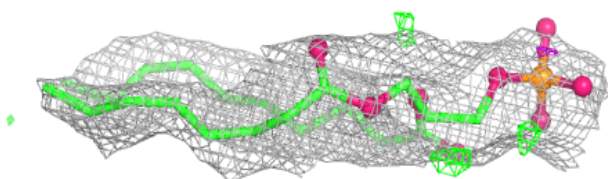
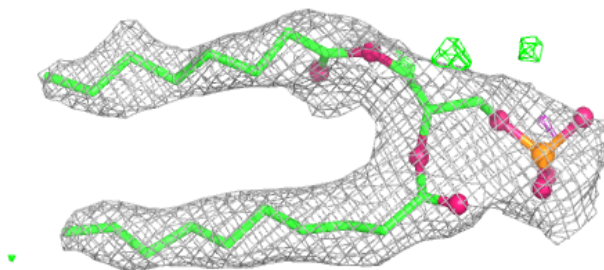


**Electron density around SQD f 101:**

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

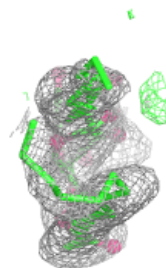
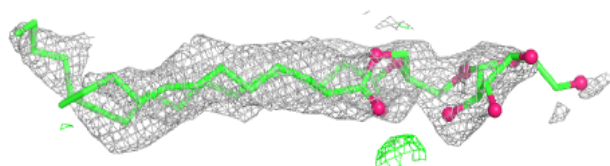
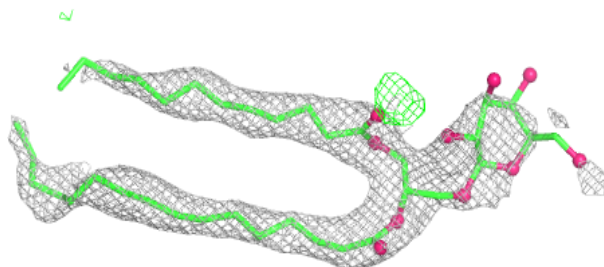
**Electron density around LHG C 522:**

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

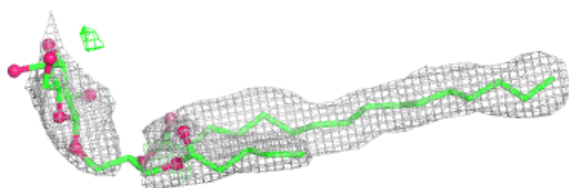


**Electron density around LMG d 409:**

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

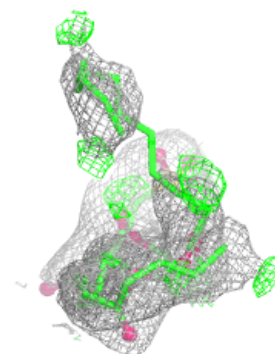
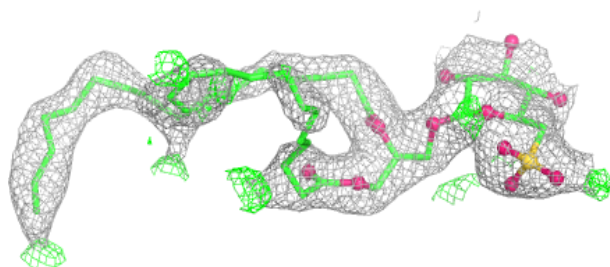
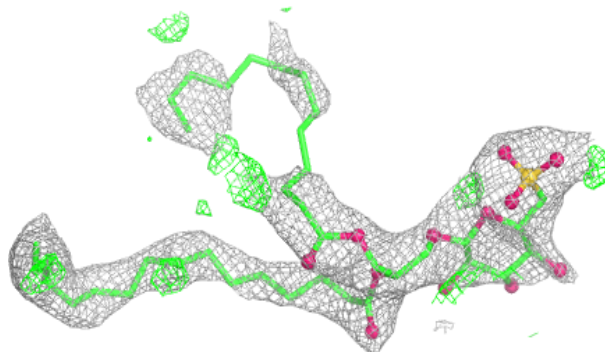
**Electron density around LMG C 531:**

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

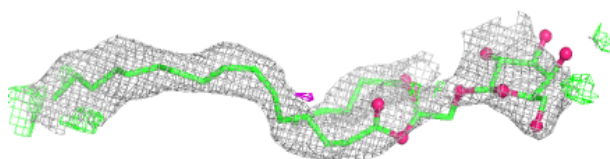
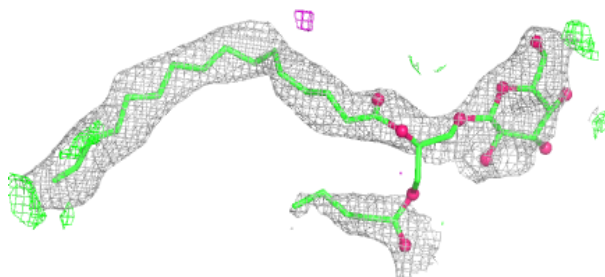


**Electron density around SQD a 418:**

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

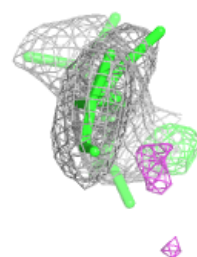
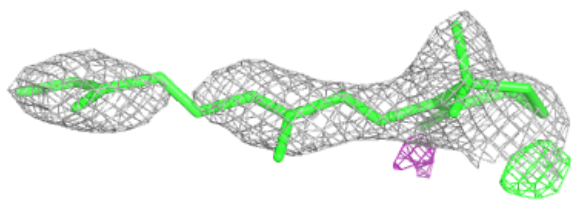
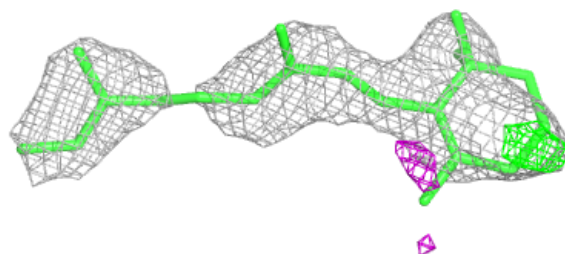
**Electron density around LMG B 621:**

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



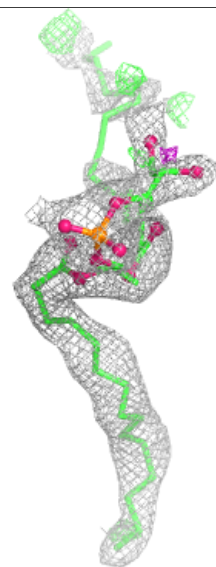
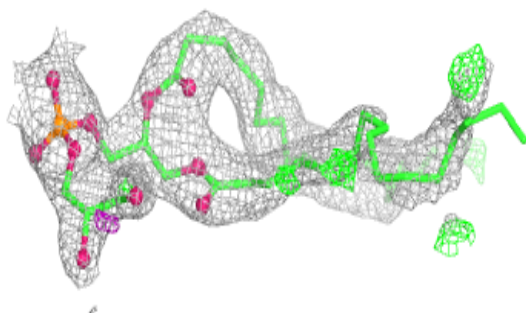
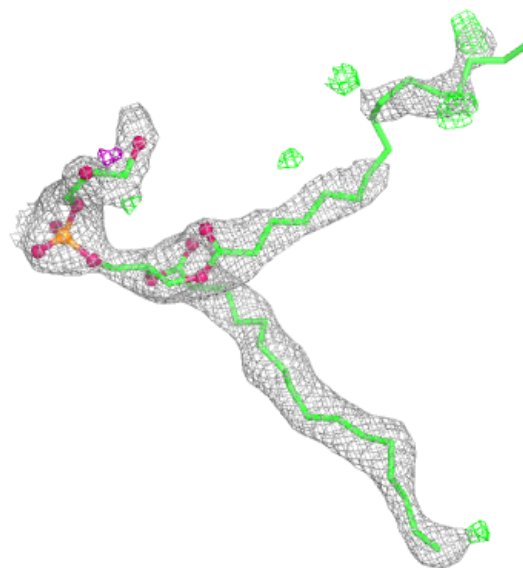
**Electron density around BCR b 618:**

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



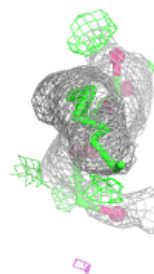
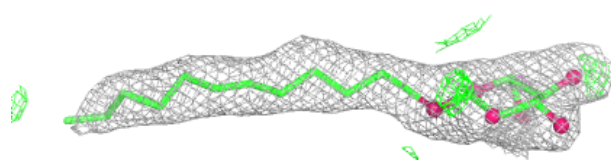
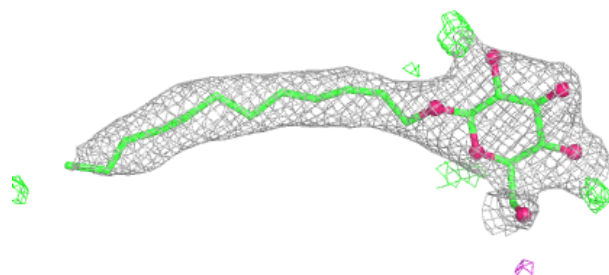
**Electron density around LHG 1 102:**

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

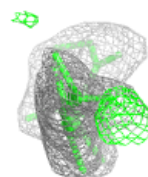
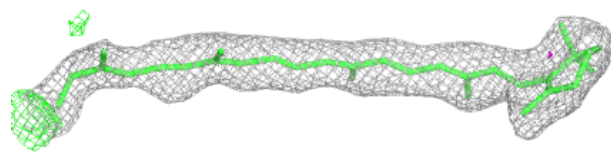
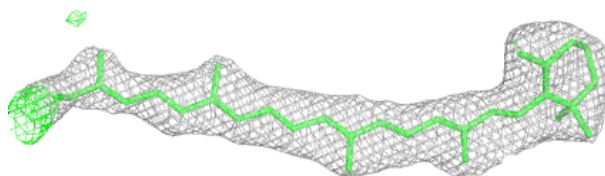


**Electron density around LMT B 622:**

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

**Electron density around BCR b 619:**

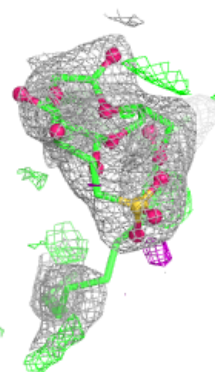
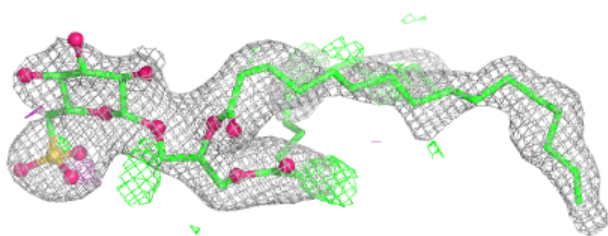
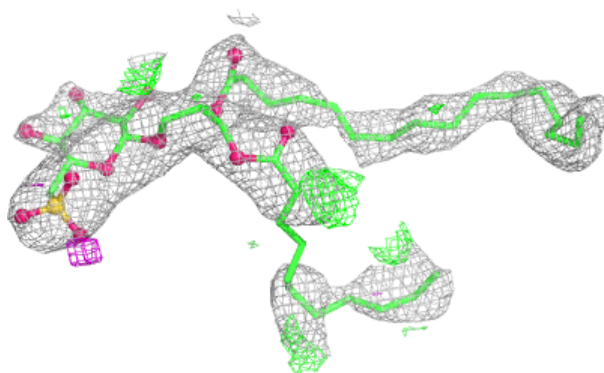
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



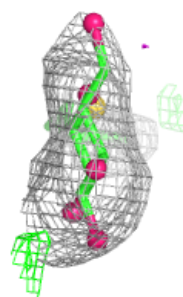
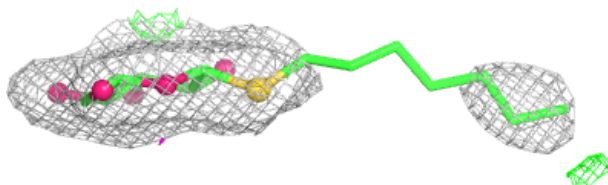
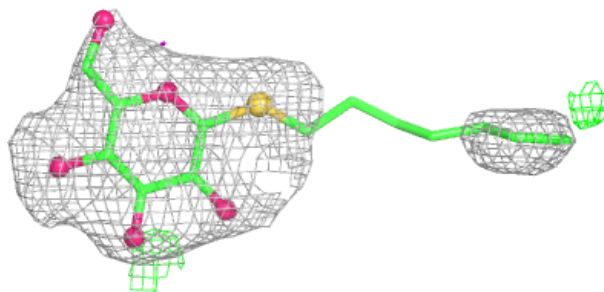


**Electron density around SQD A 413:**

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

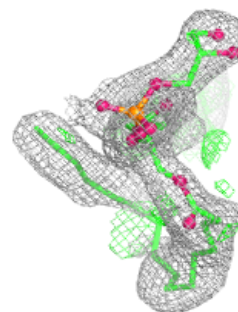
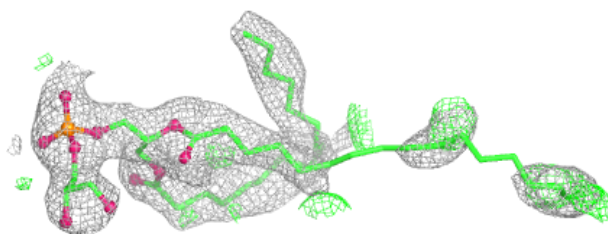
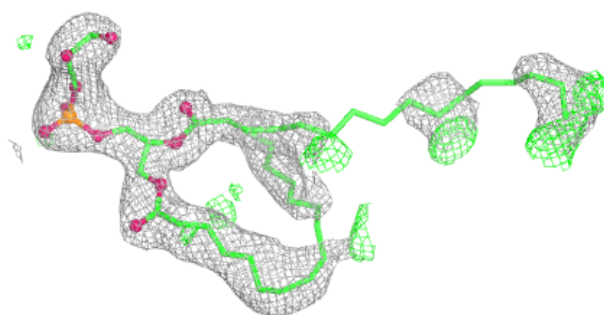
**Electron density around HTG C 521:**

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

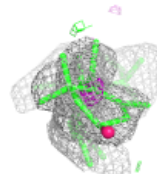
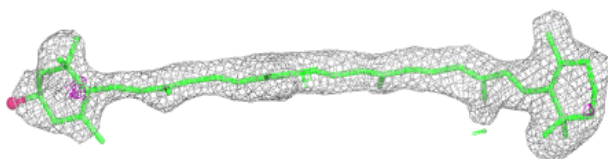
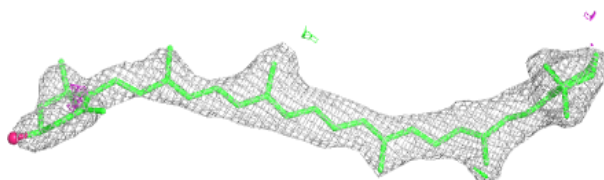


**Electron density around LHG D 409:**

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

**Electron density around RRX h 101:**

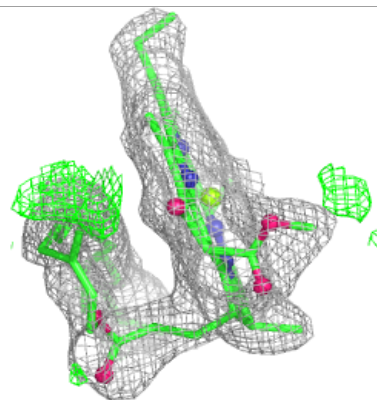
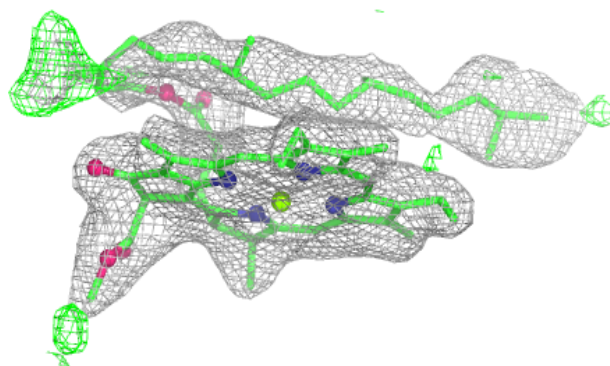
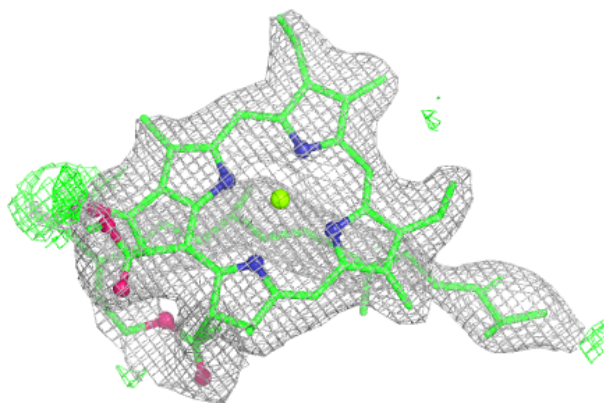
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



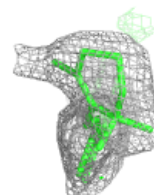
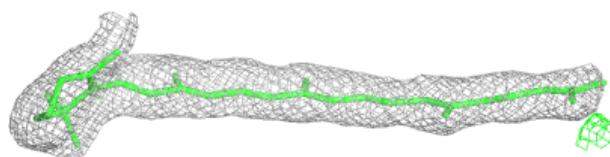
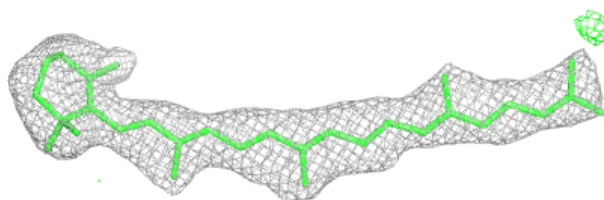


**Electron density around CLA B 602:**

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

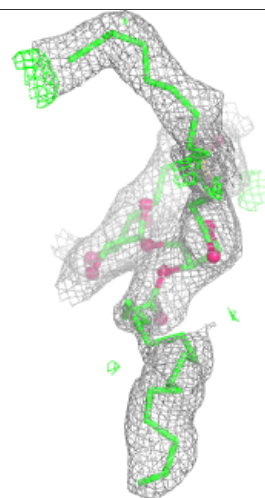
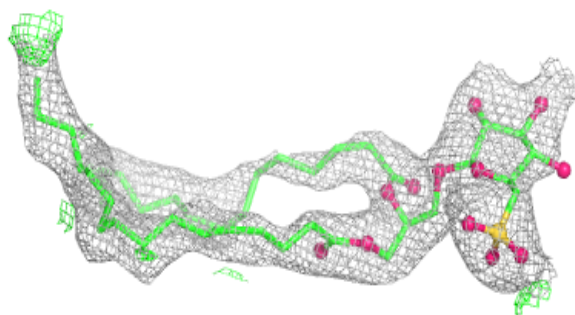
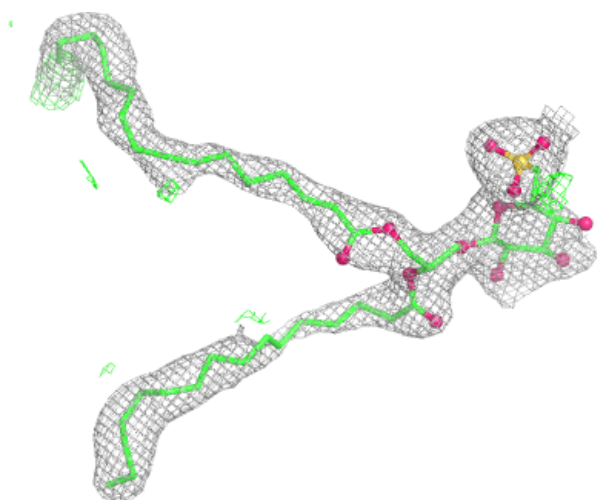
**Electron density around BCR B 619:**

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



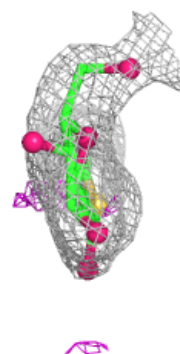
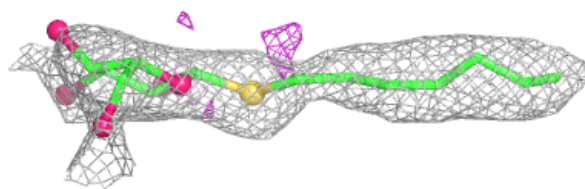
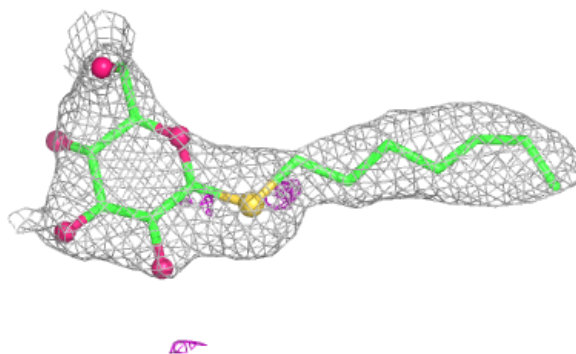
**Electron density around SQD a 414:**

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

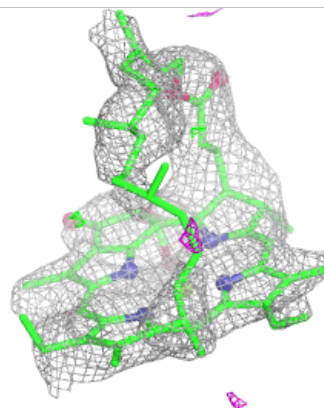
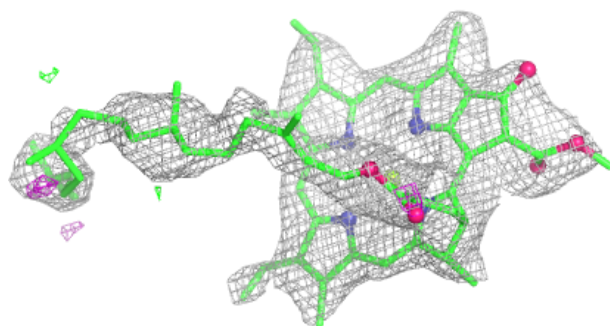
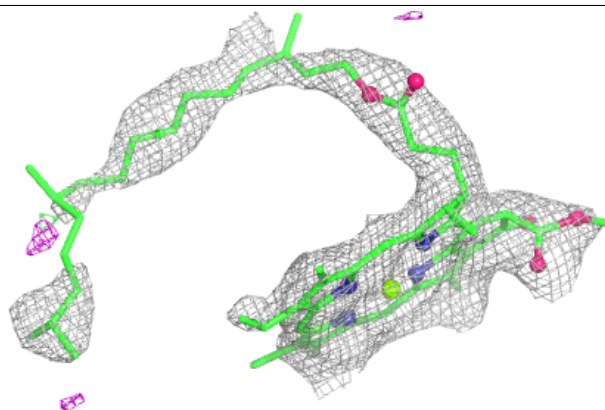


**Electron density around HTG B 626:**

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

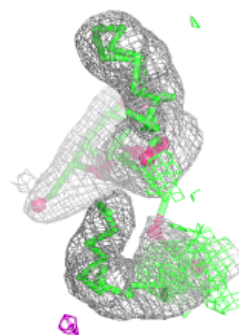
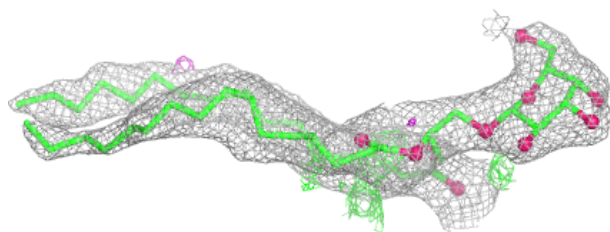
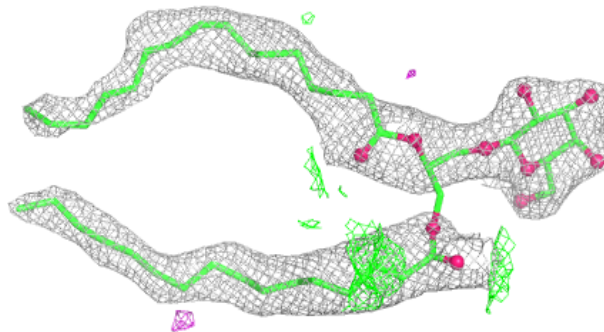
**Electron density around CLA c 914:**

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



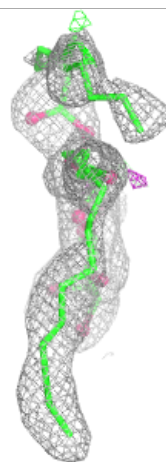
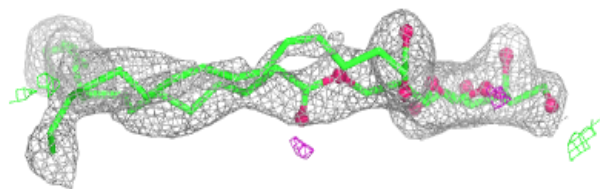
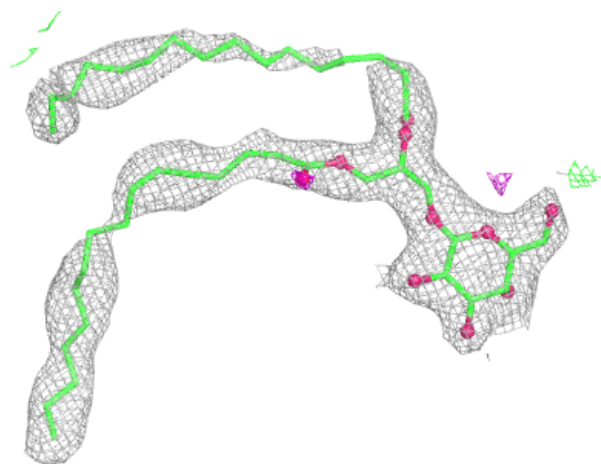
**Electron density around LMG i 101:**

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



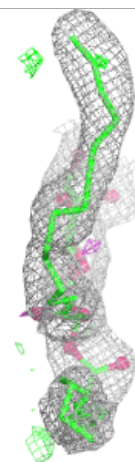
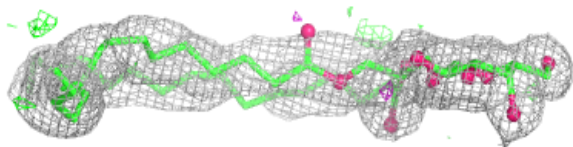
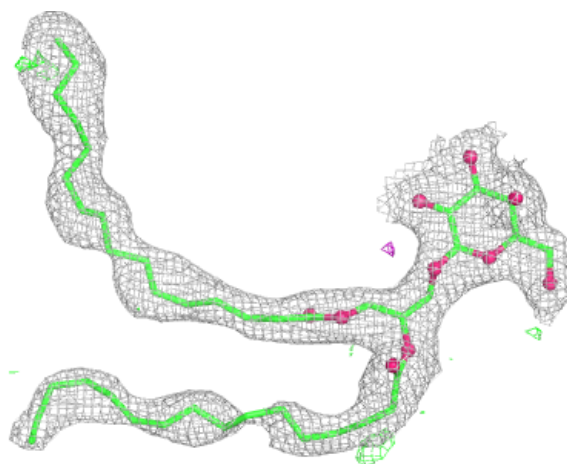
**Electron density around LMG c 920:**

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



**Electron density around LMG C 520:**

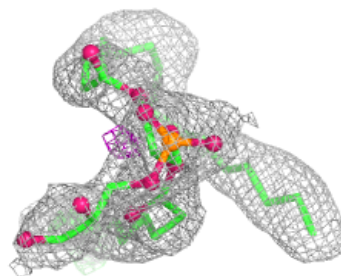
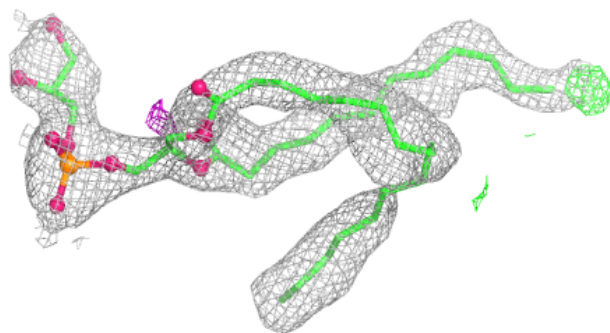
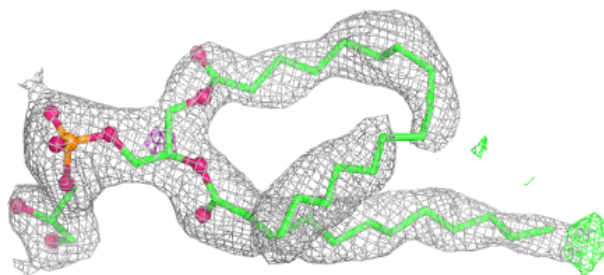
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



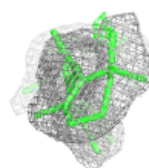
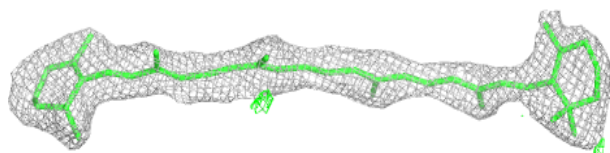
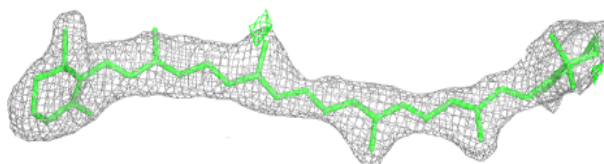


**Electron density around LHG a 423:**

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

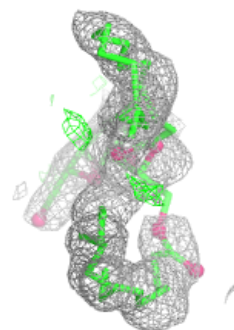
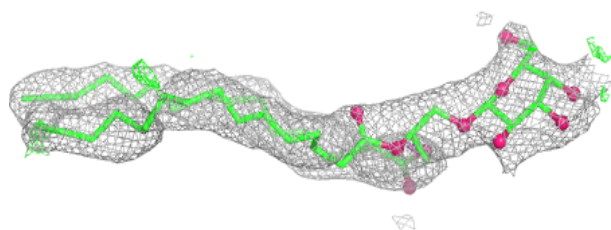
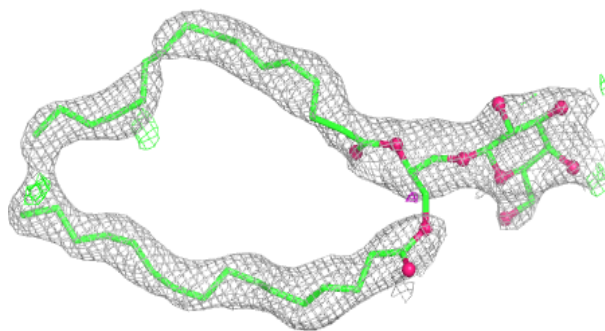
**Electron density around BCR c 915:**

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

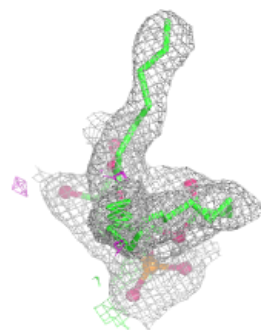
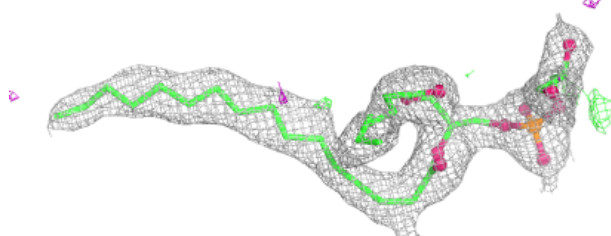
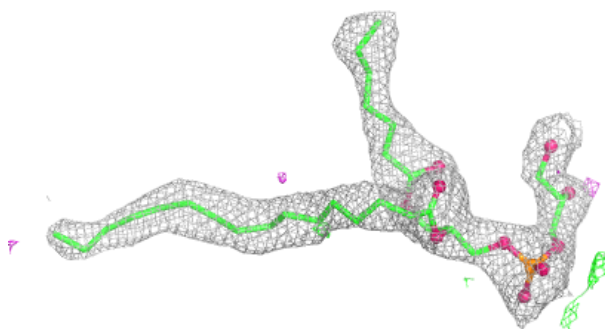


**Electron density around LMG A 410:**

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

**Electron density around LHG L 101:**

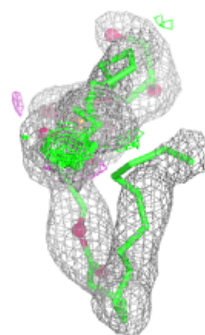
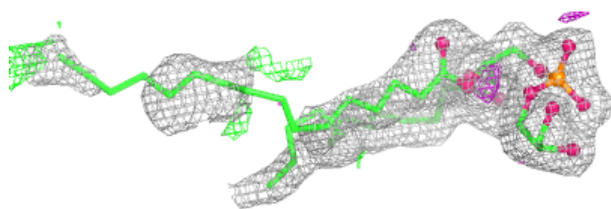
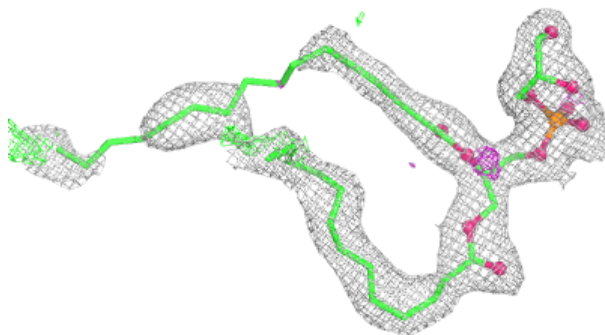
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



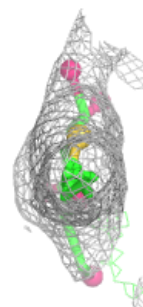
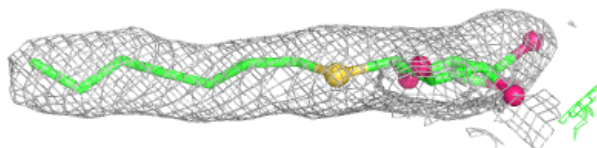
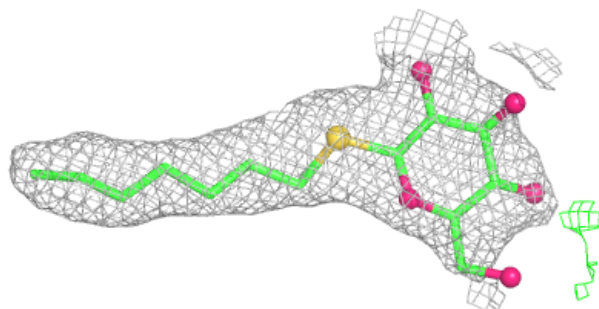


**Electron density around LHG d 408:**

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

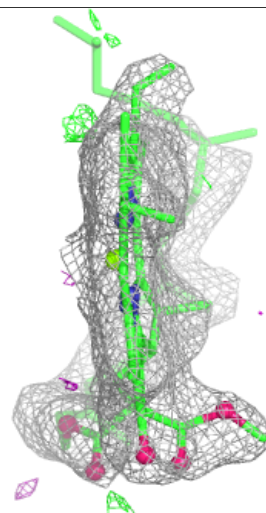
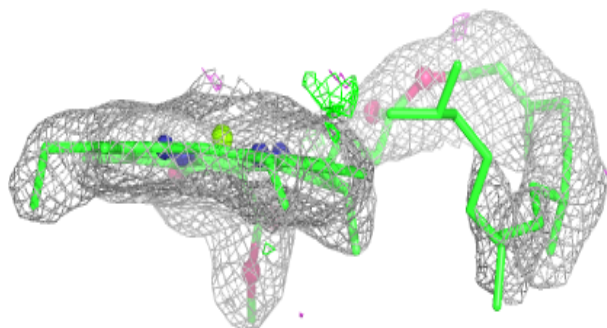
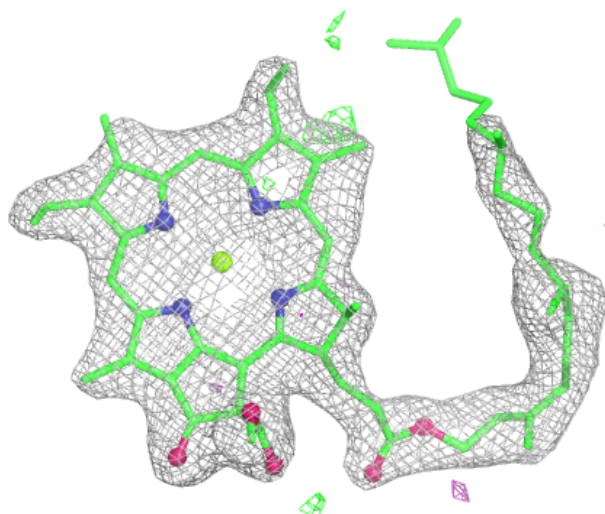
**Electron density around HTG b 626:**

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



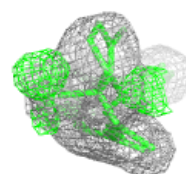
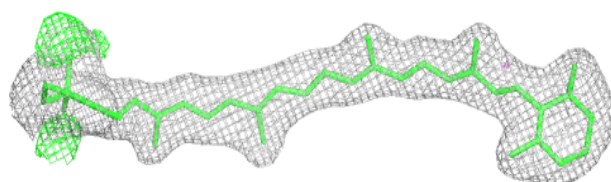
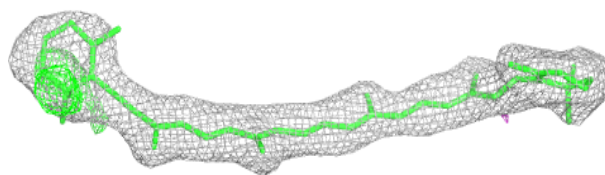
**Electron density around CLA c 913:**

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

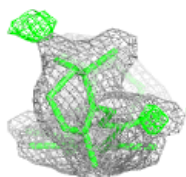
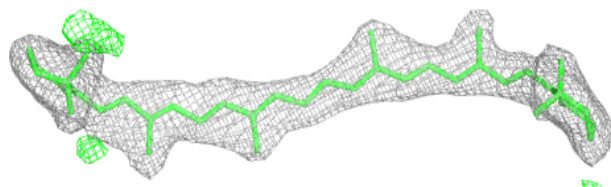
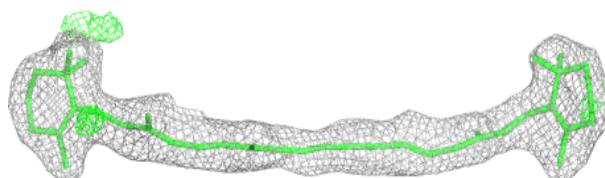


**Electron density around BCR d 404:**

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

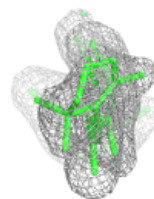
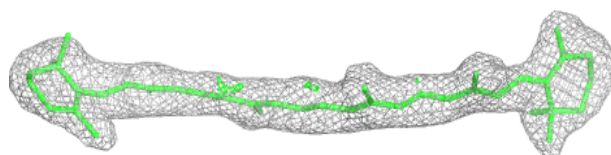
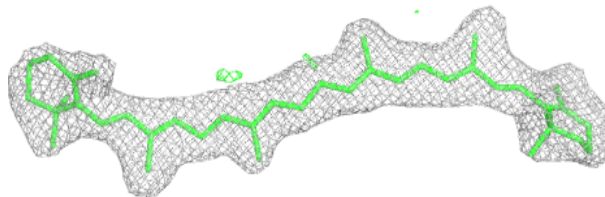
**Electron density around BCR k 101:**

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

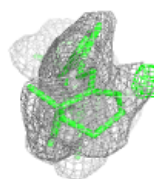
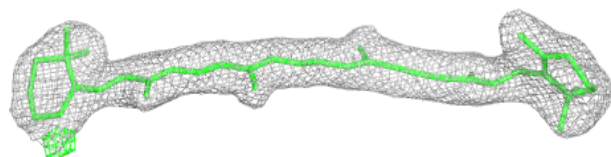
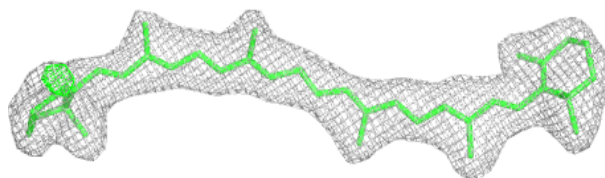


**Electron density around BCR y 101:**

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

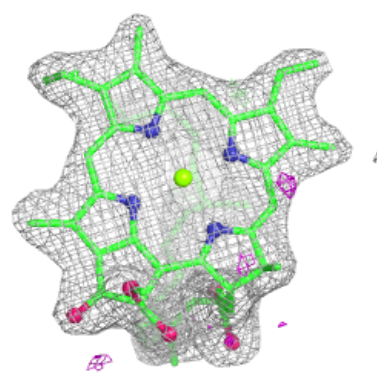
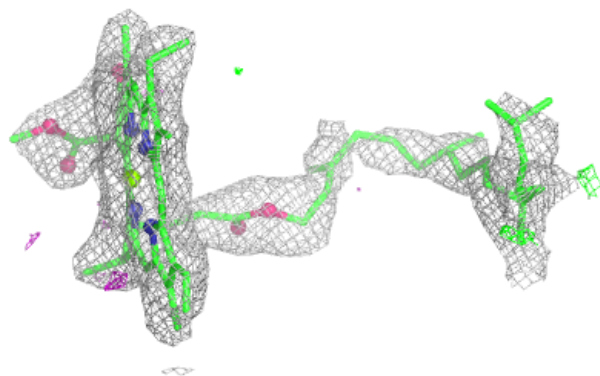
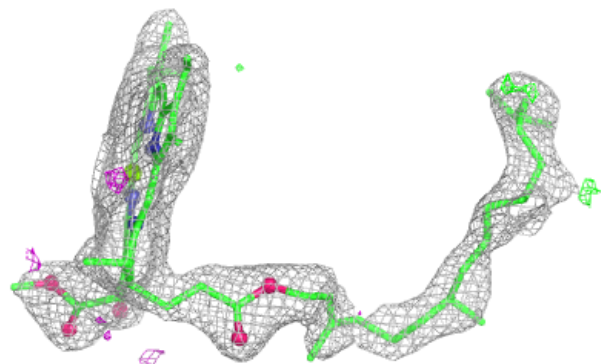
**Electron density around BCR Y 101:**

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

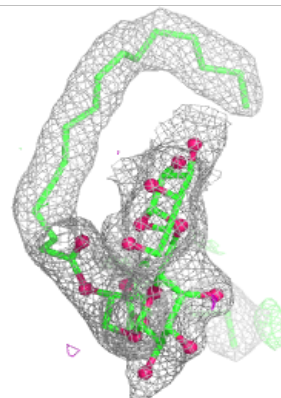
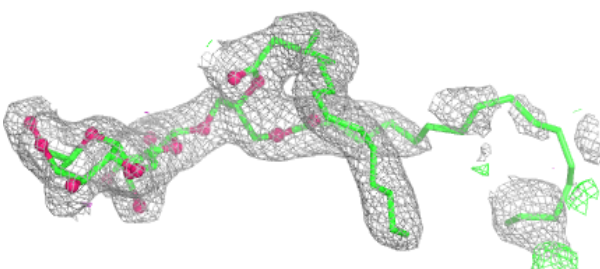
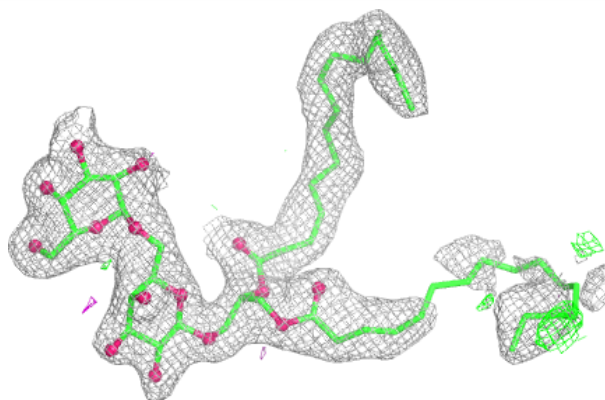


**Electron density around CLA C 507:**

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

**Electron density around DGD c 918:**

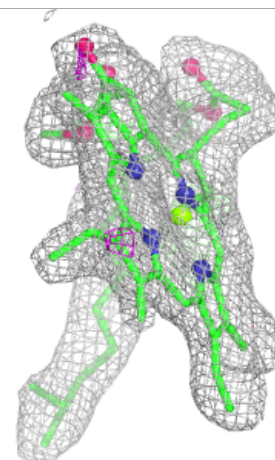
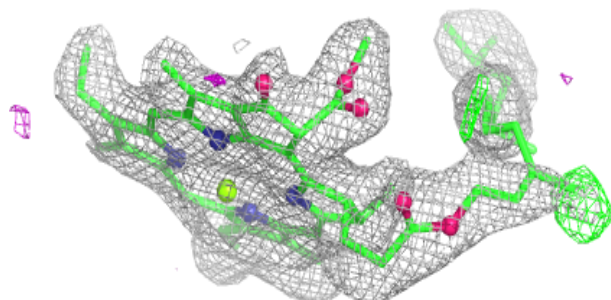
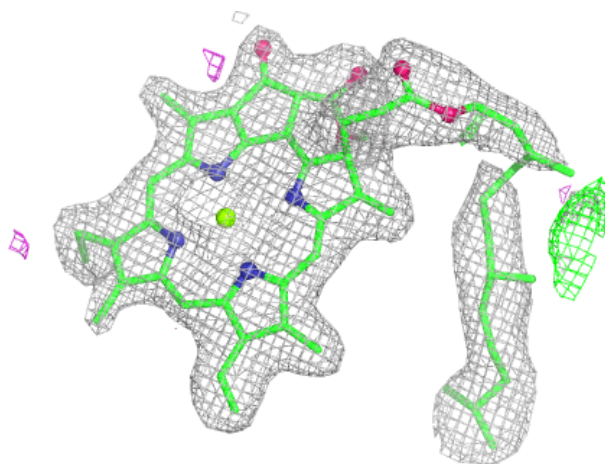
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





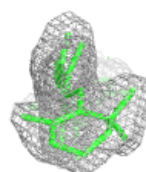
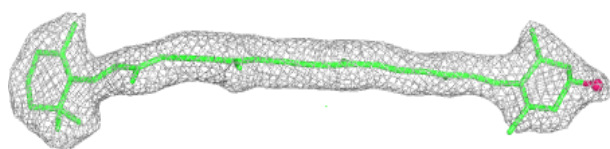
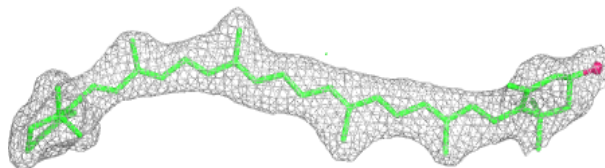
**Electron density around CLA b 617:**

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

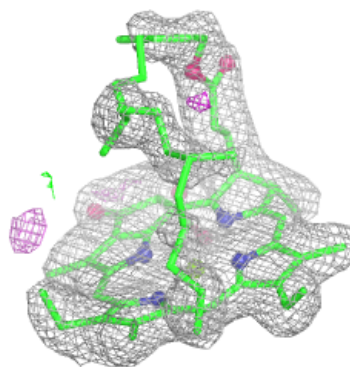
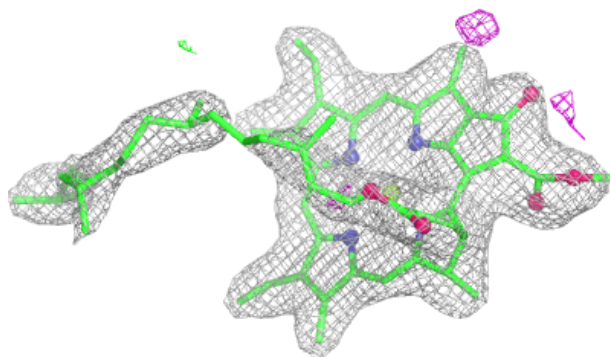
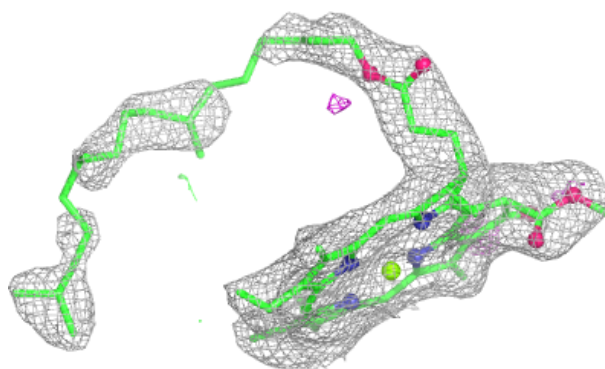


**Electron density around RRX H 101:**

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

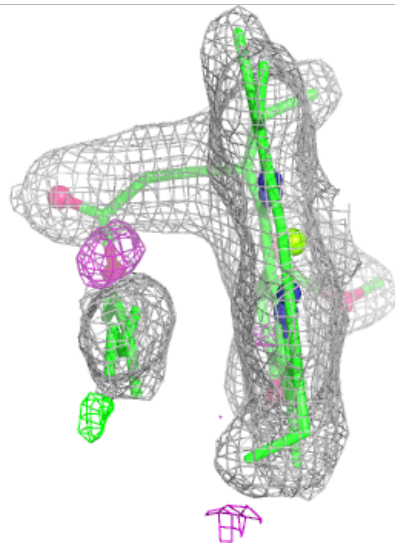
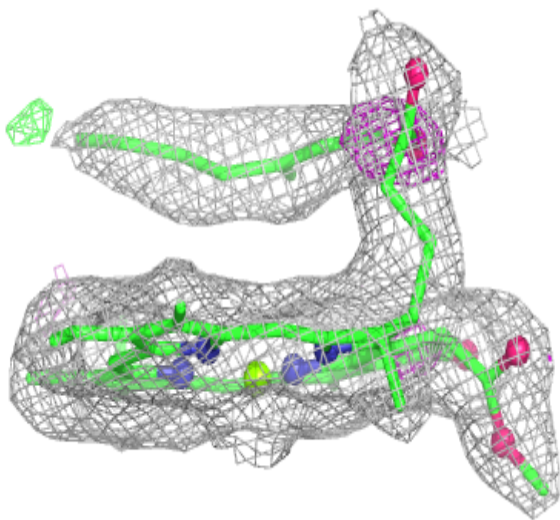
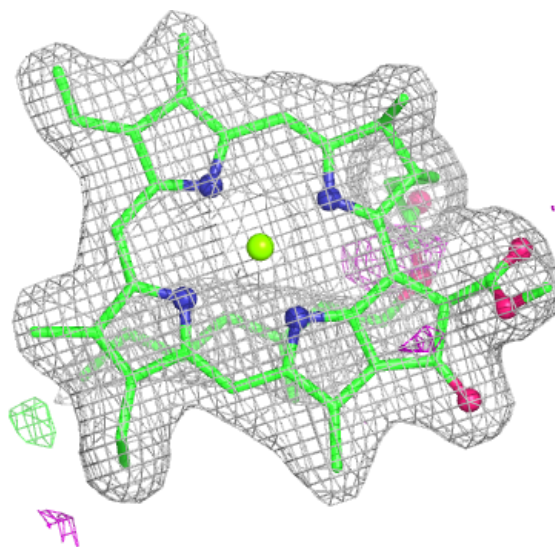
**Electron density around CLA C 514:**

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



**Electron density around CLA B 615:**

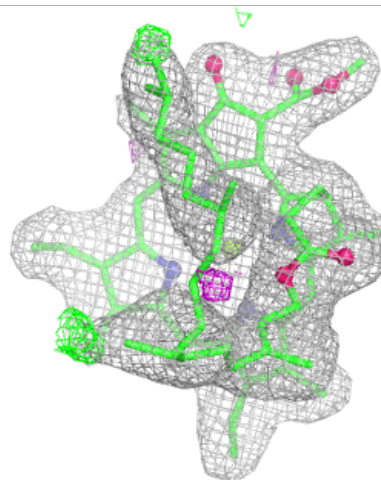
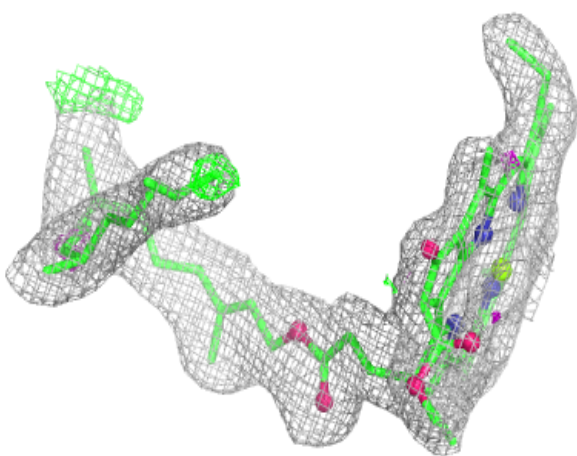
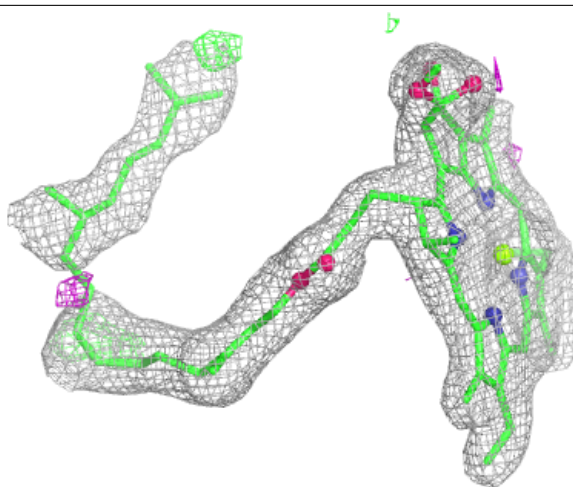
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





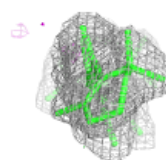
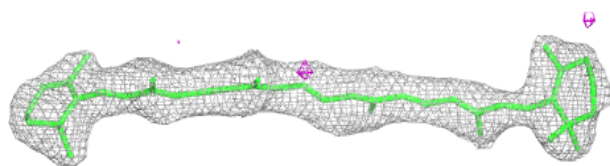
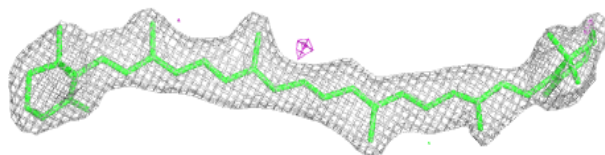
**Electron density around CLA b 607:**

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

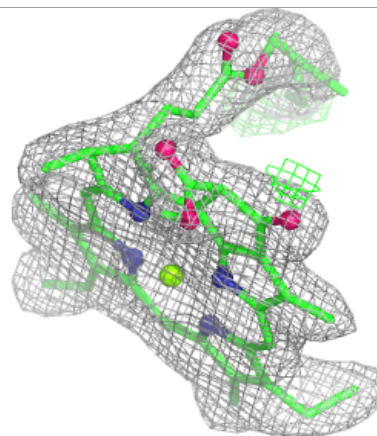
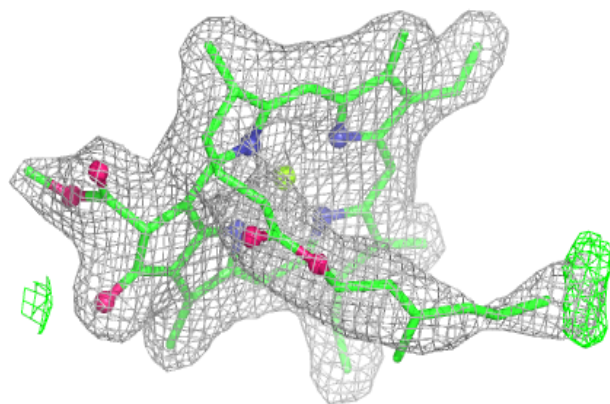
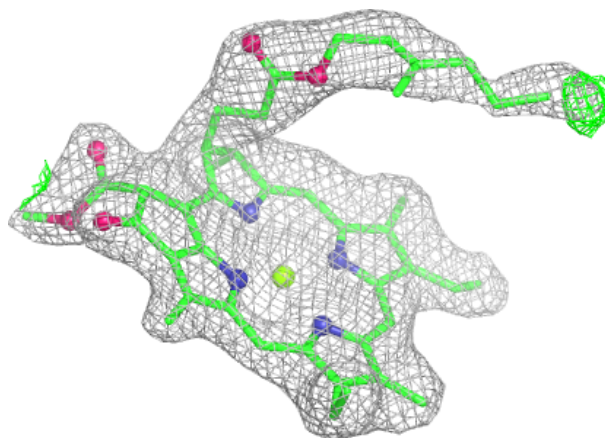


**Electron density around BCR C 515:**

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

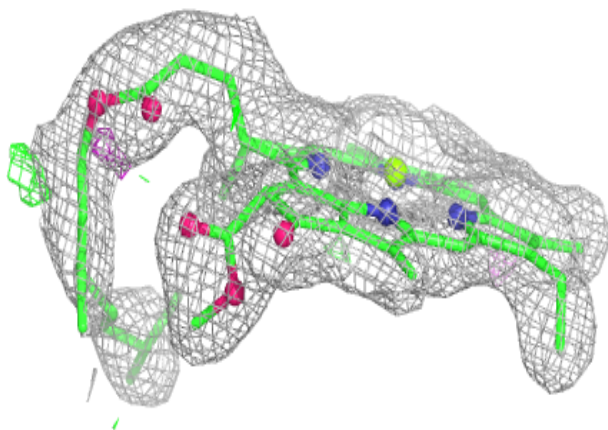
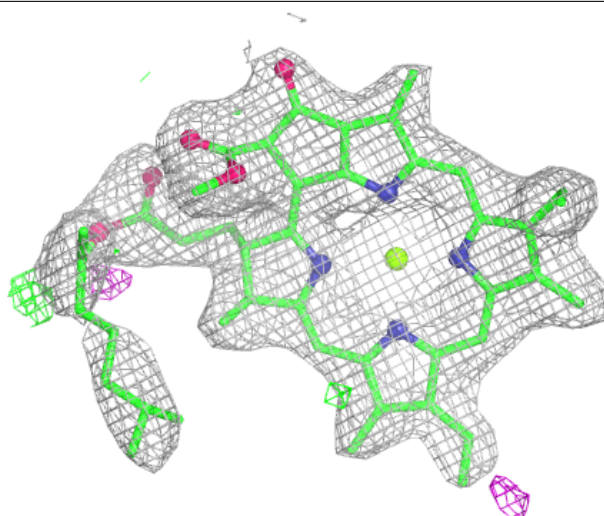
**Electron density around CLA b 615:**

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



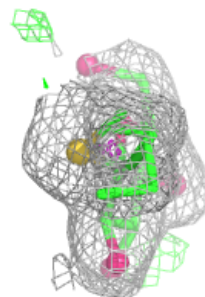
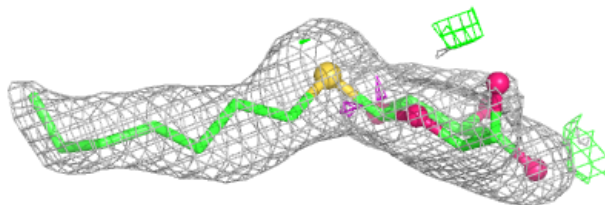
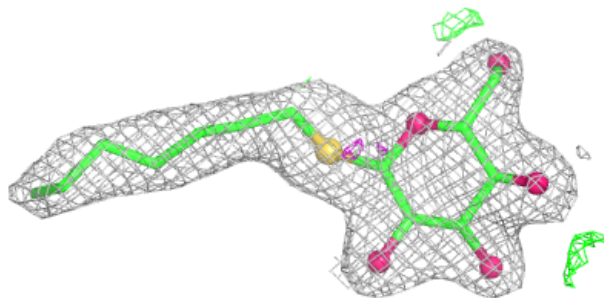
**Electron density around CLA B 617:**

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



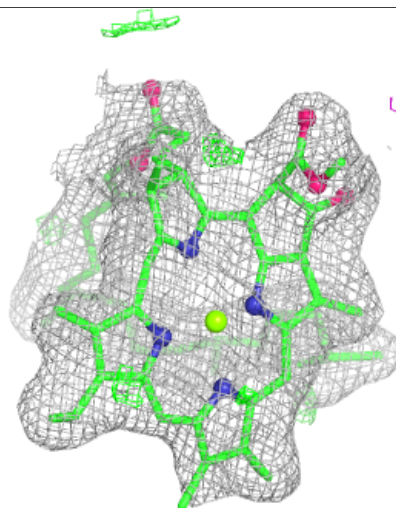
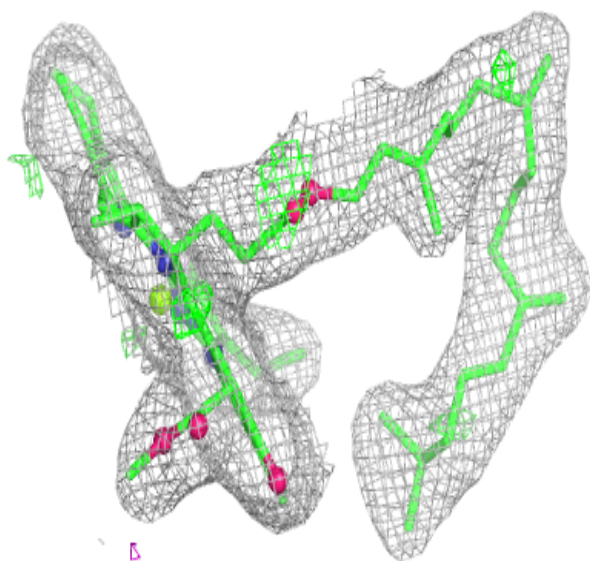
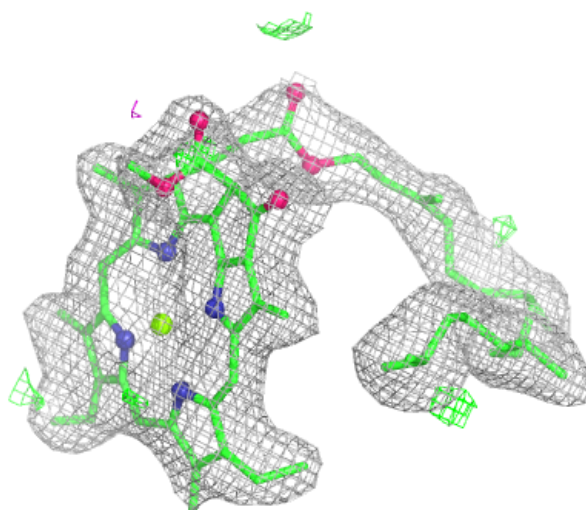
**Electron density around HTG b 623:**

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



**Electron density around CLA c 904:**

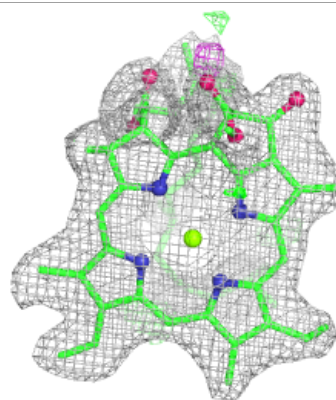
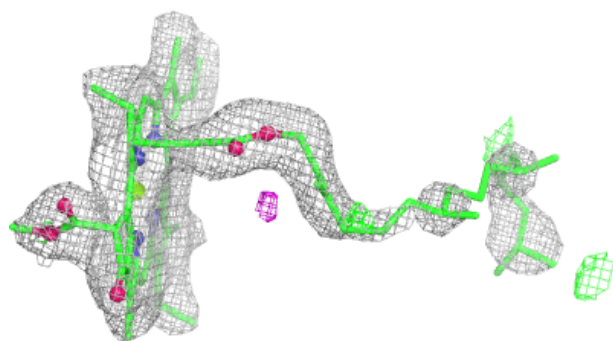
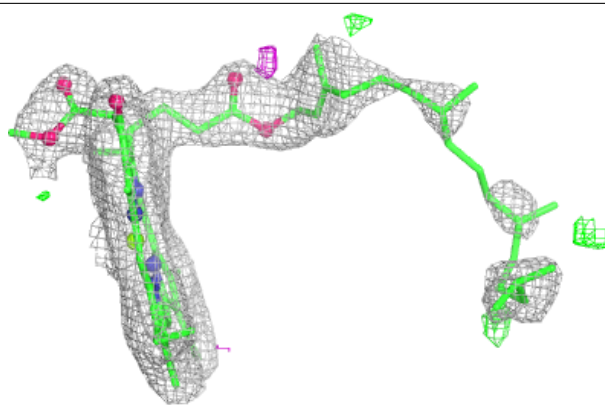
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



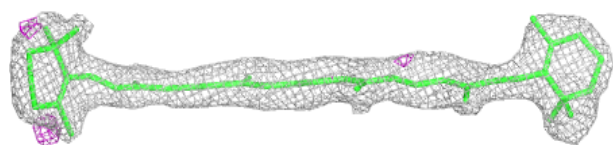
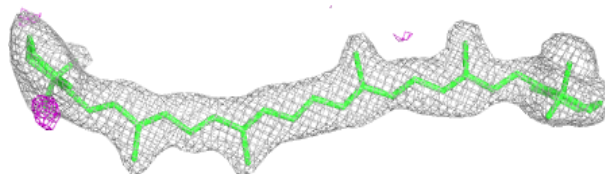


**Electron density around CLA c 907:**

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

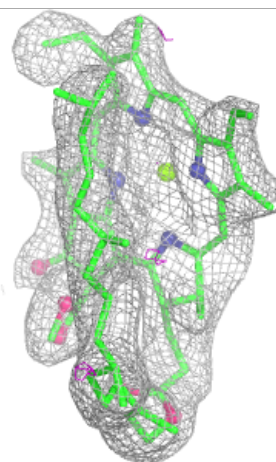
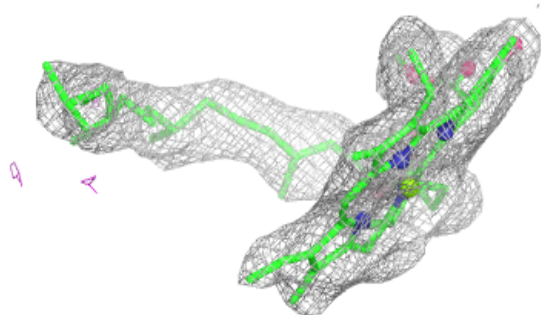
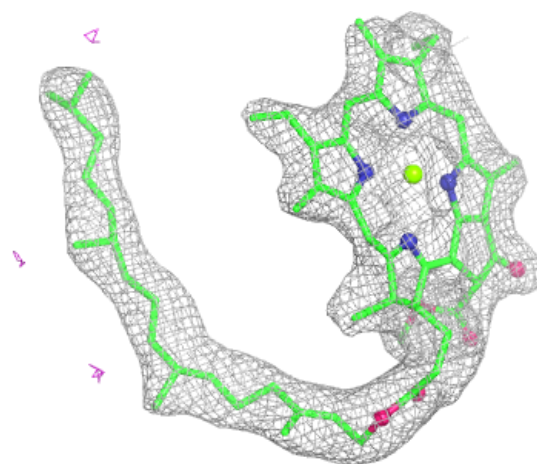
**Electron density around BCR c 916:**

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



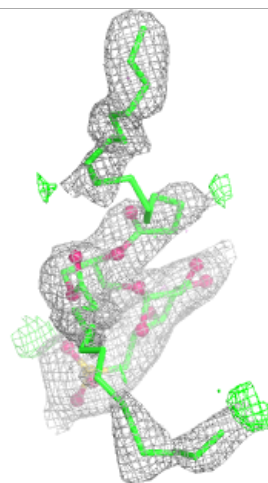
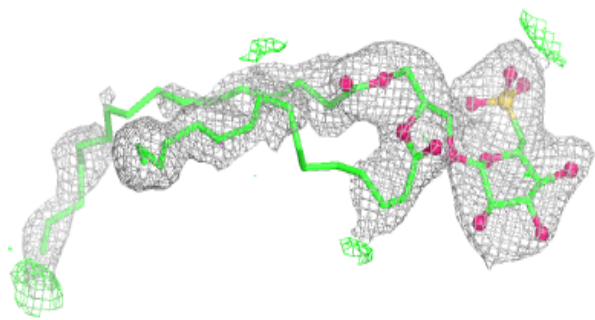
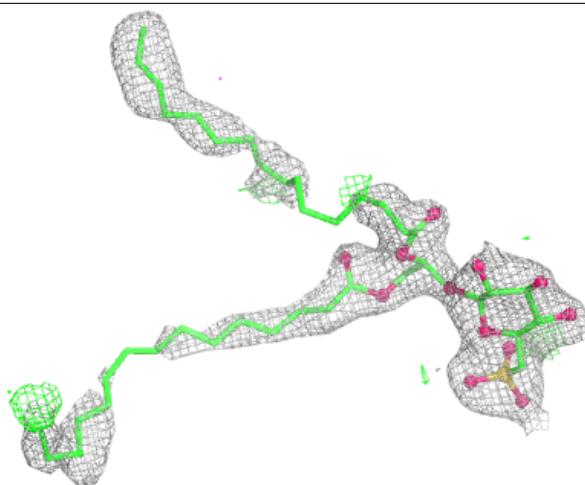
**Electron density around CLA c 908:**

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



**Electron density around SQD C 501:**

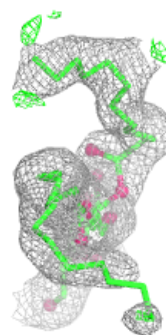
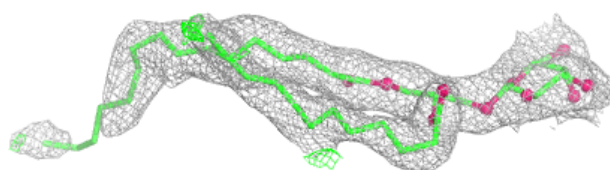
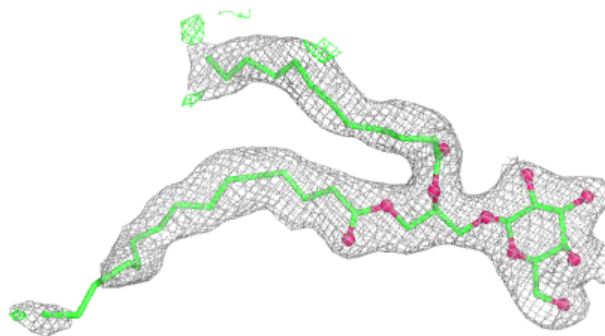
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



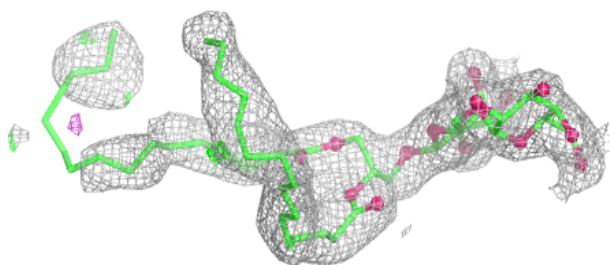
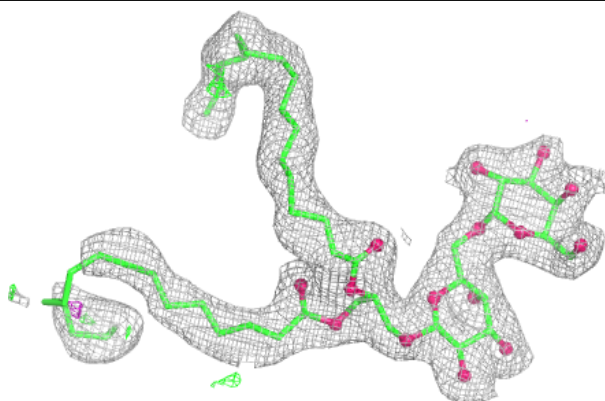


**Electron density around LMG j 101:**

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

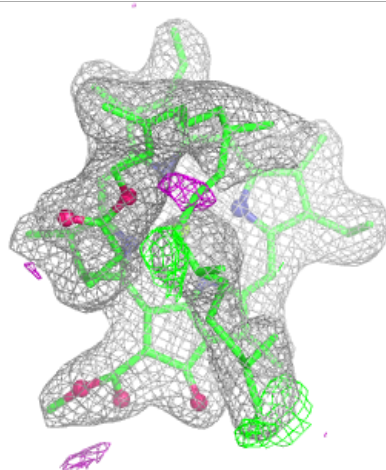
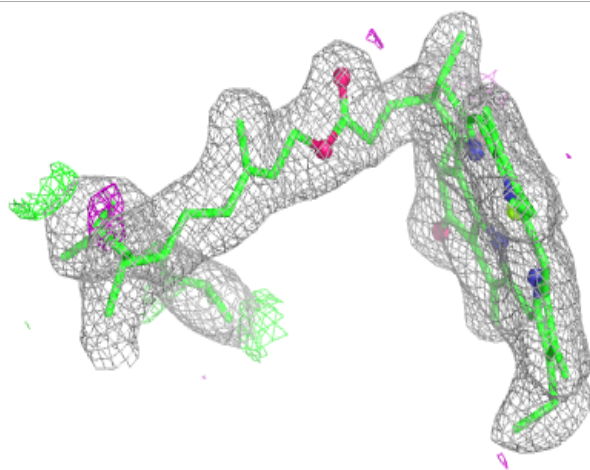
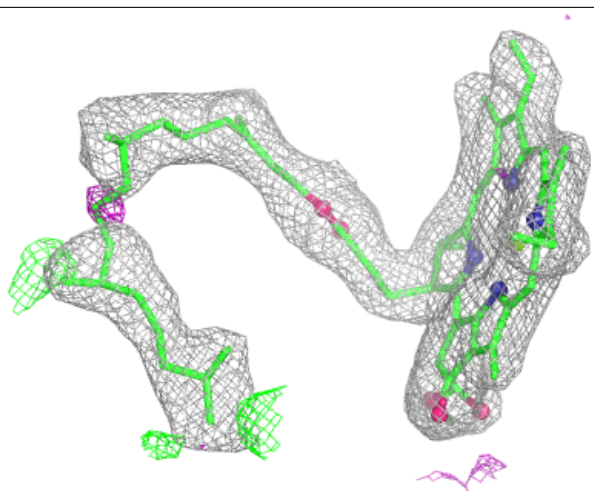
**Electron density around DGD C 518:**

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



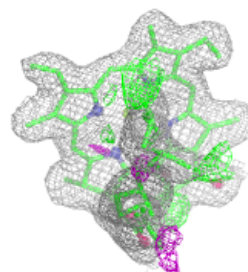
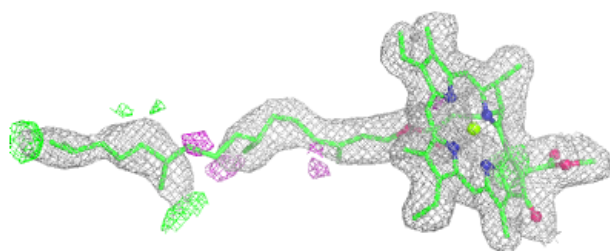
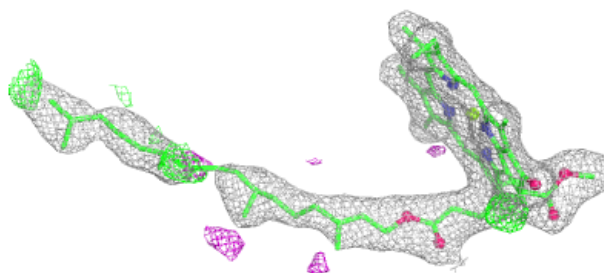
**Electron density around CLA B 607:**

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

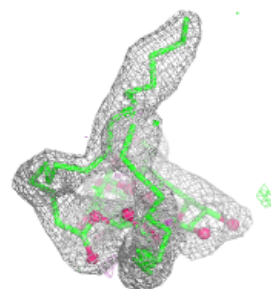
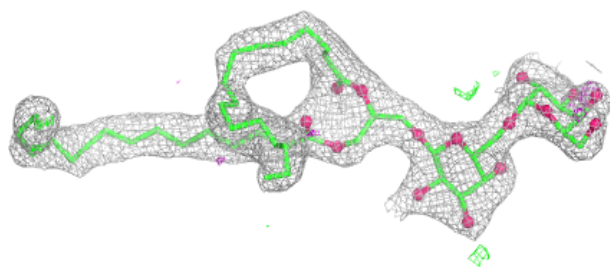
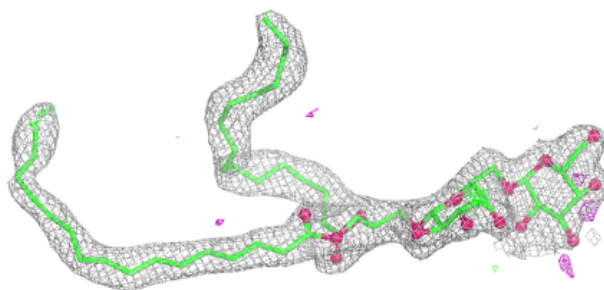


**Electron density around CLA B 608:**

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

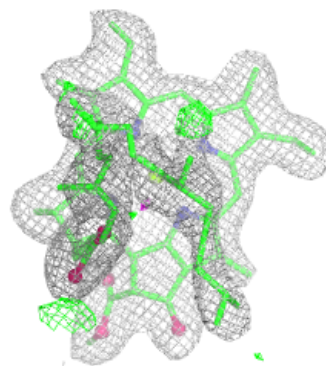
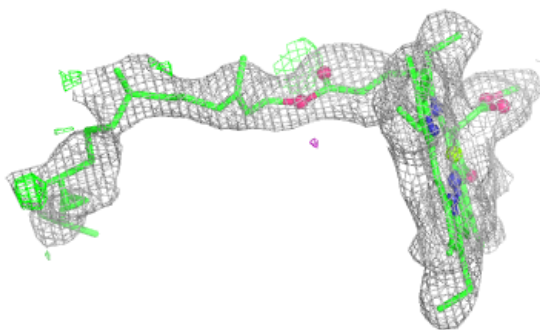
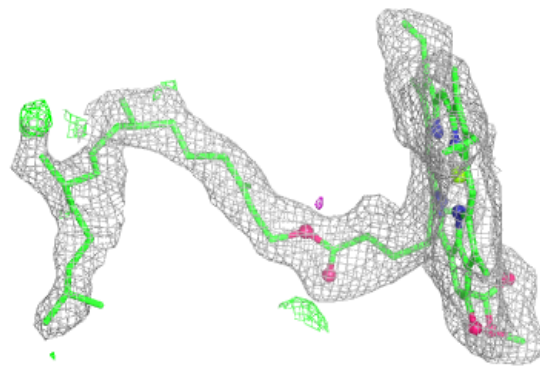
**Electron density around DGD h 102:**

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



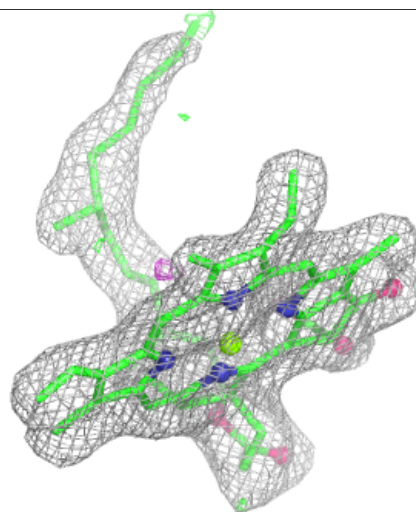
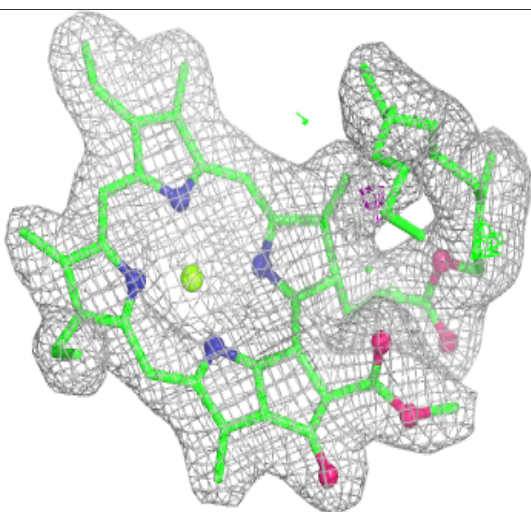
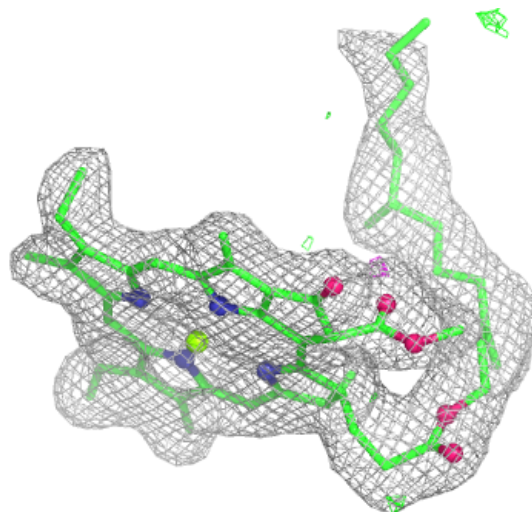
**Electron density around CLA d 403:**

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



**Electron density around CLA b 614:**

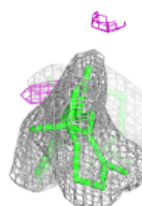
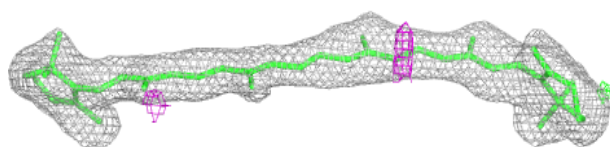
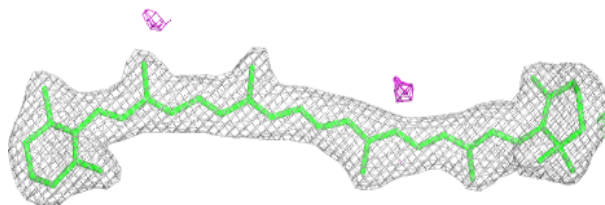
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



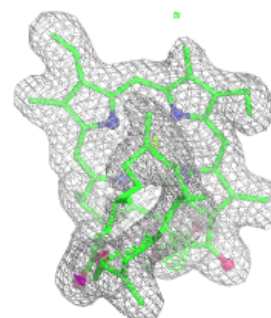
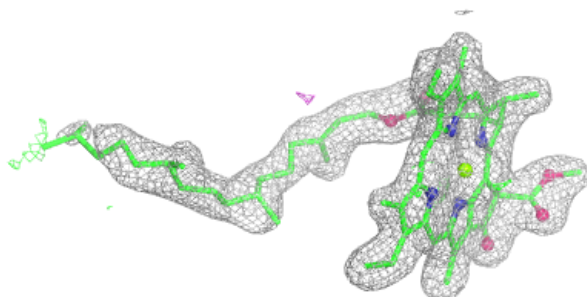
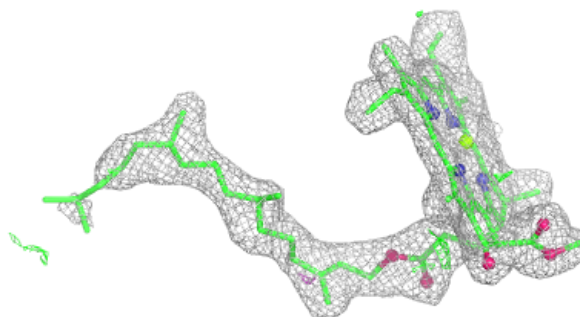


**Electron density around BCR B 620:**

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

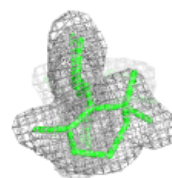
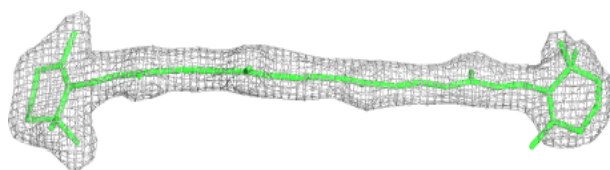
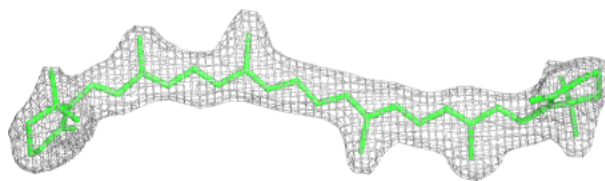
**Electron density around CLA C 509:**

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

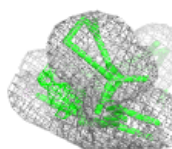
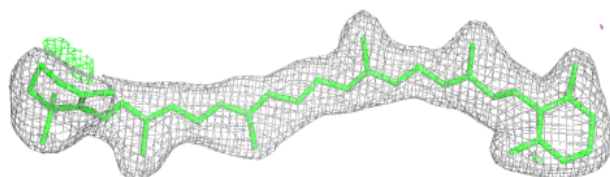
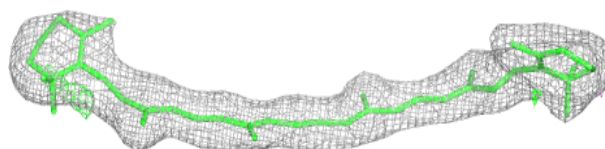


**Electron density around BCR C 516:**

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

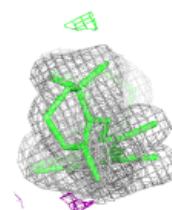
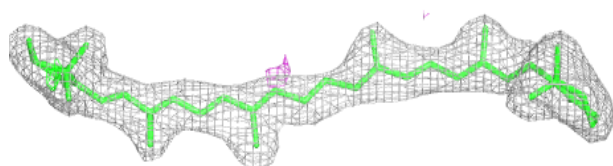
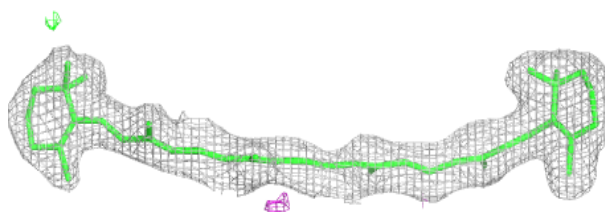
**Electron density around BCR D 405:**

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

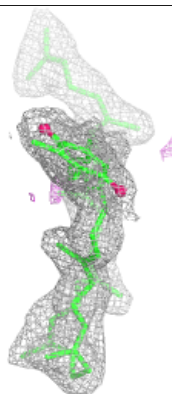
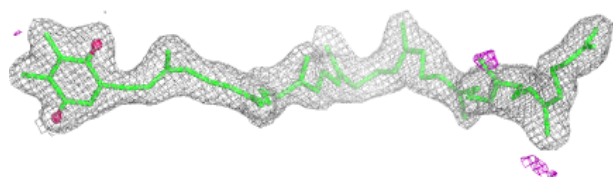
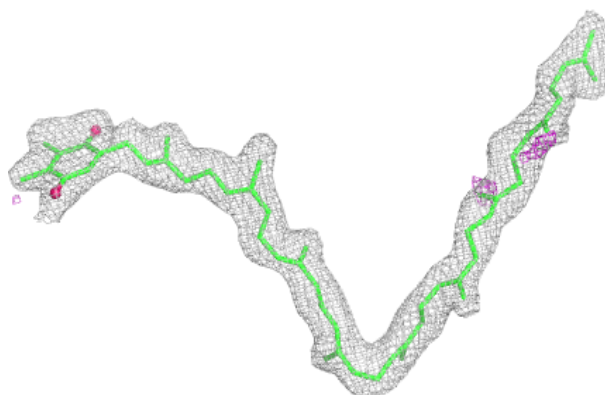


**Electron density around BCR K 101:**

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

**Electron density around PL9 D 406:**

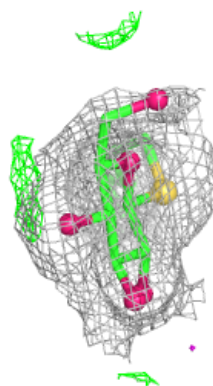
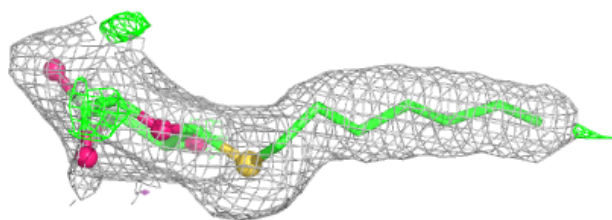
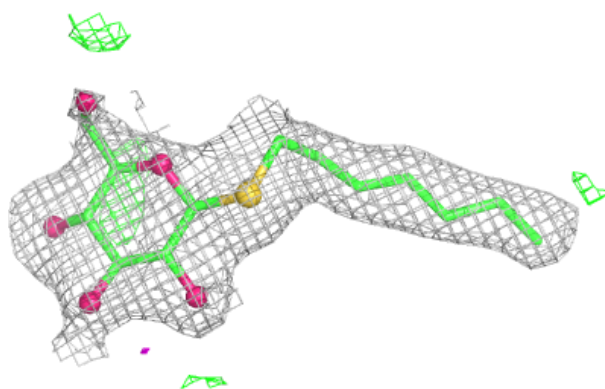
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



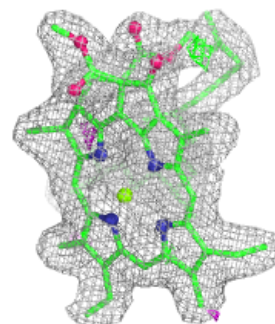
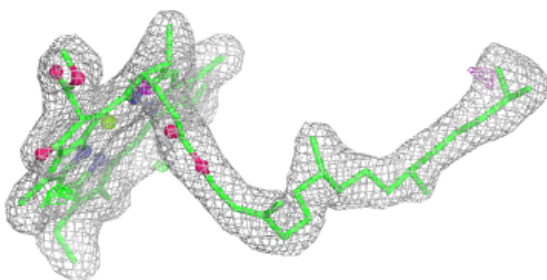
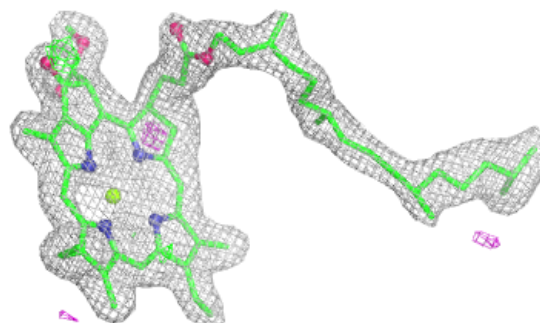


**Electron density around HTG B 623:**

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

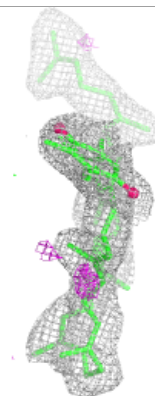
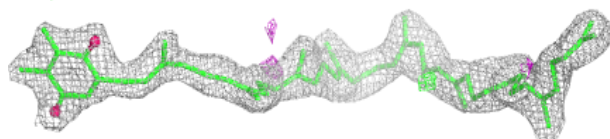
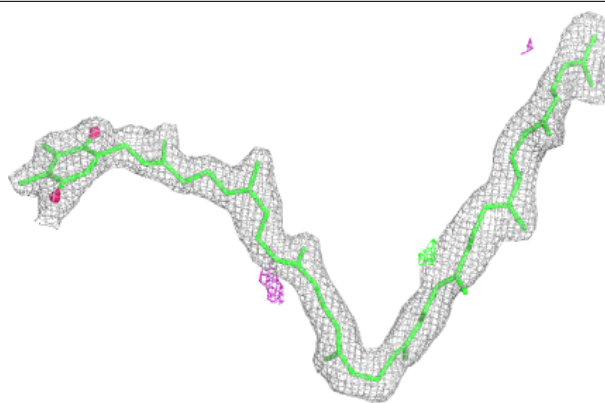
**Electron density around CLA C 512:**

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

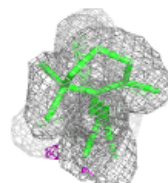
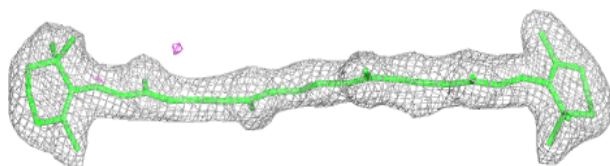
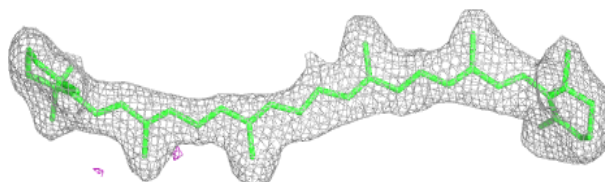


**Electron density around PL9 d 405:**

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

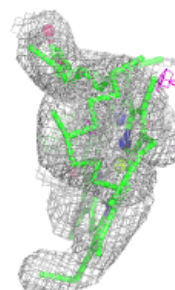
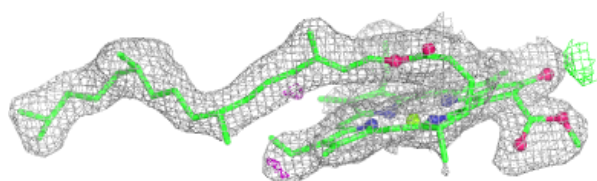
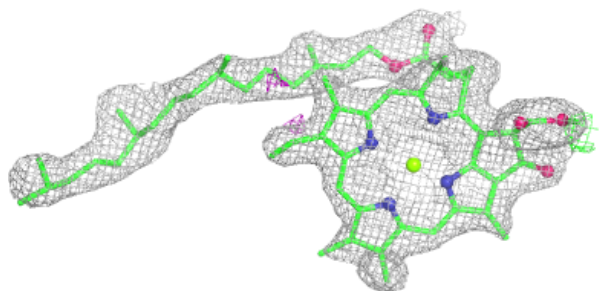
**Electron density around BCR a 413:**

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



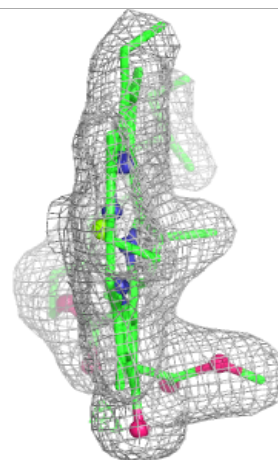
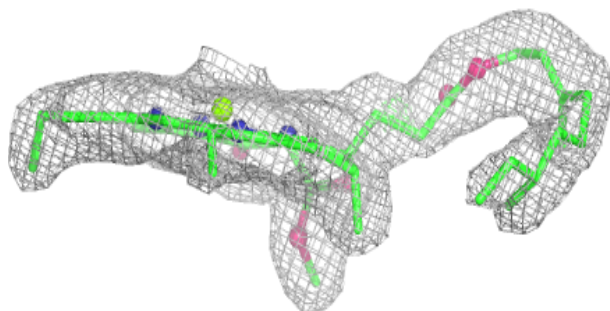
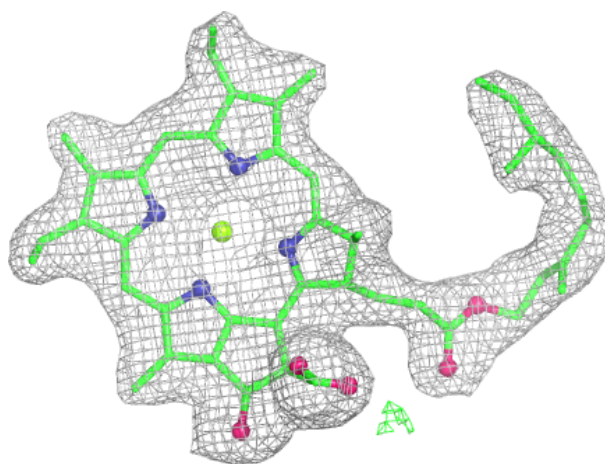
**Electron density around CLA c 902:**

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



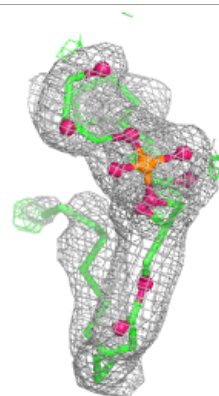
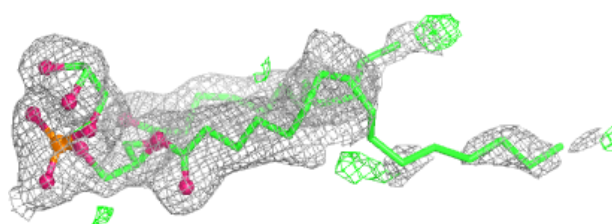
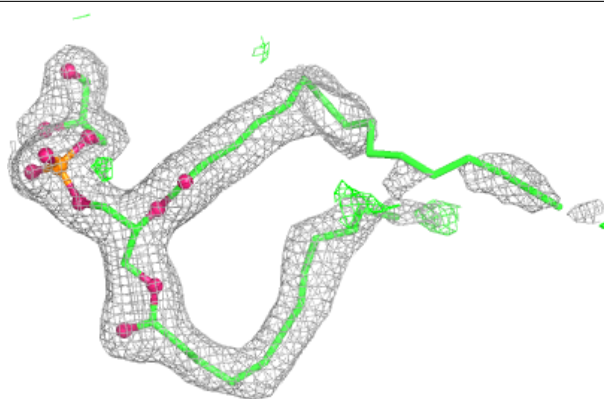
**Electron density around CLA C 513:**

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

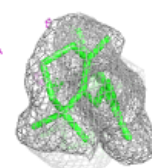
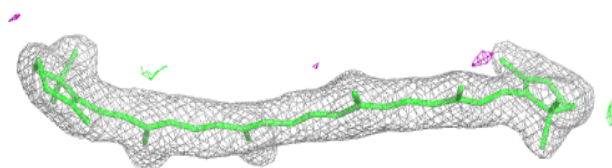
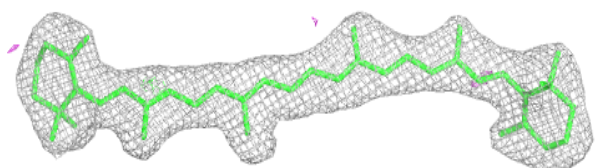


**Electron density around LHG D 411:**

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

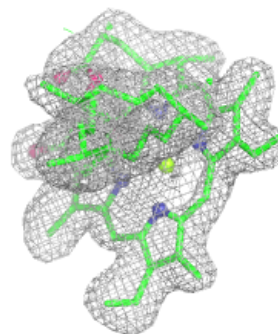
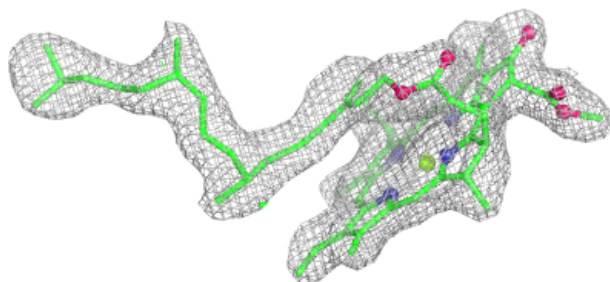
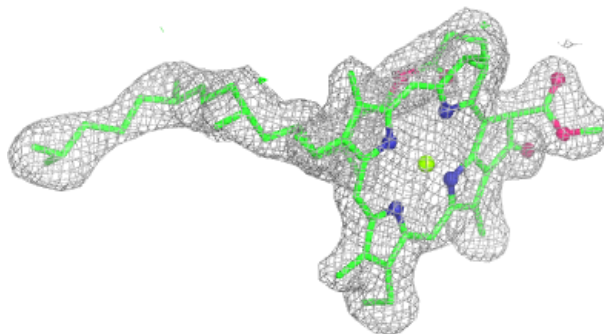
**Electron density around BCR b 620:**

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



**Electron density around CLA c 906:**

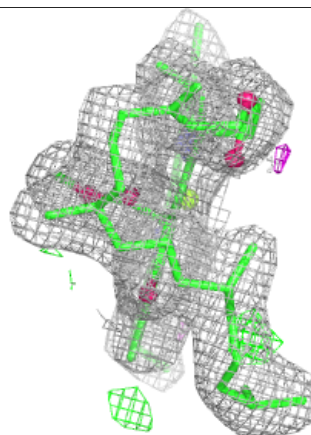
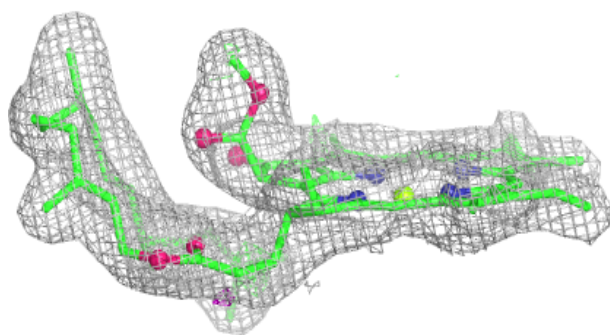
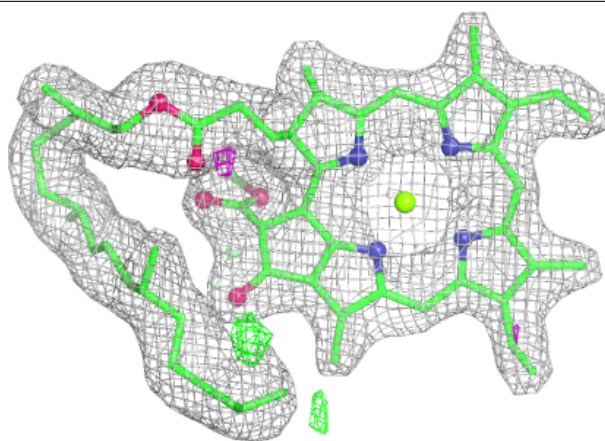
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





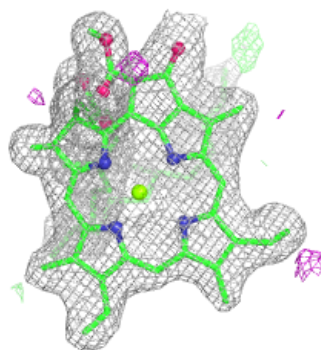
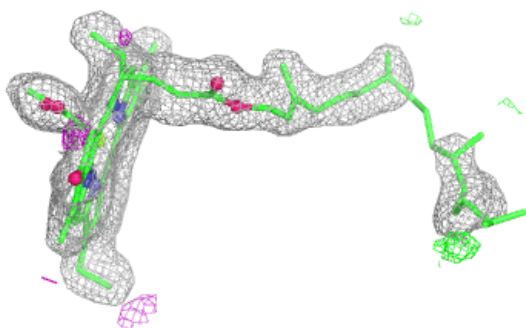
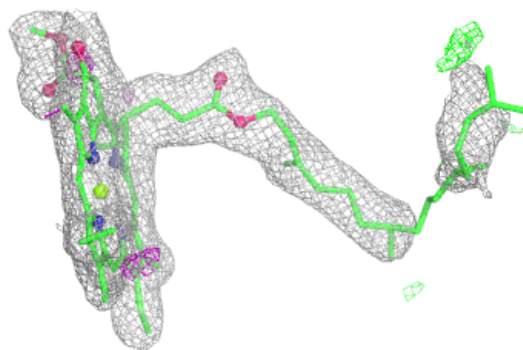
**Electron density around CLA B 611:**

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

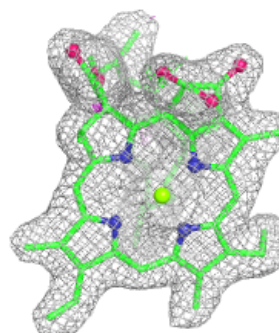
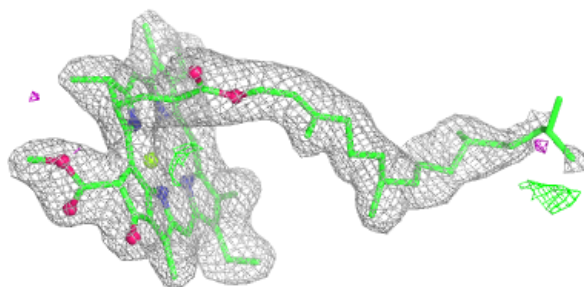
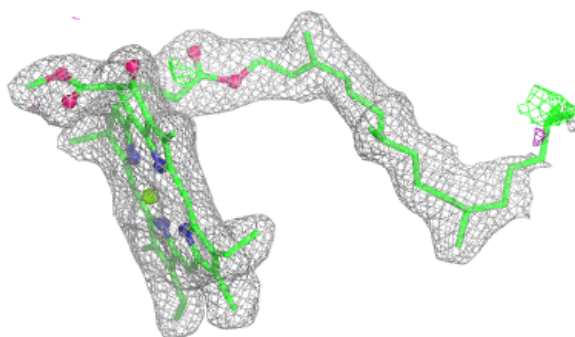


**Electron density around CLA D 404:**

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

**Electron density around CLA c 909:**

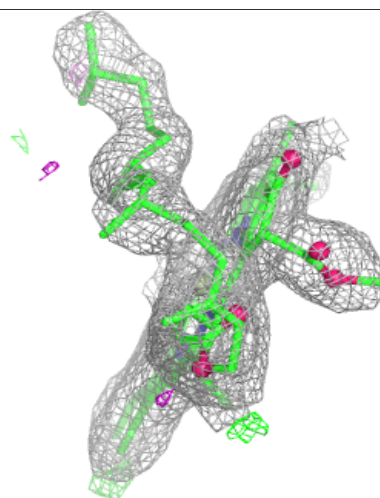
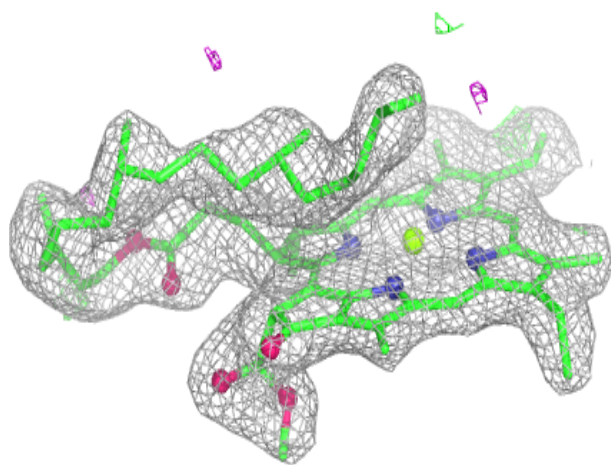
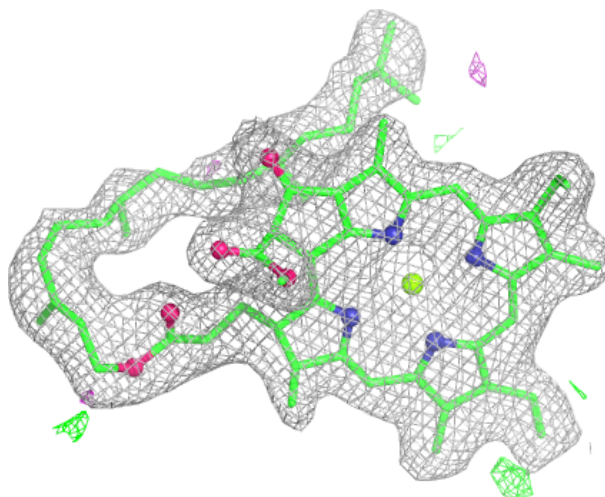
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





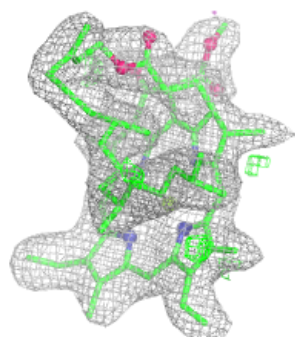
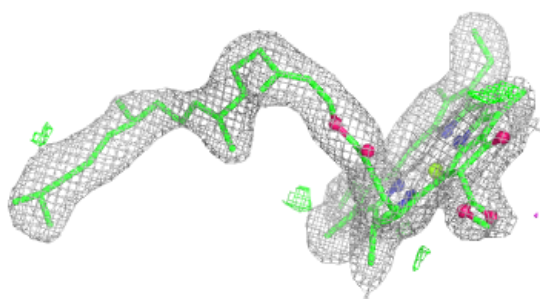
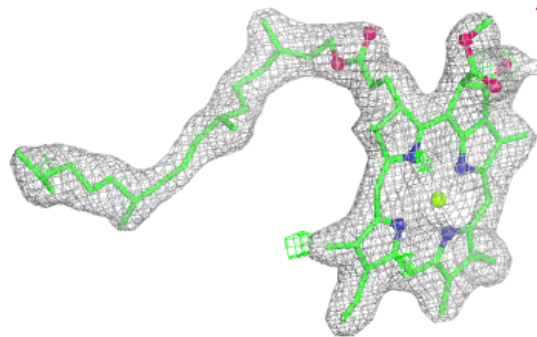
**Electron density around CLA c 910:**

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

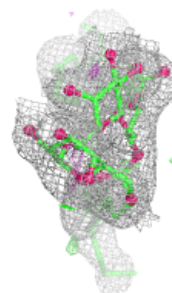
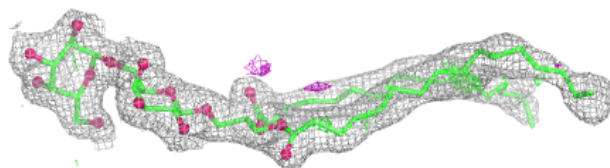
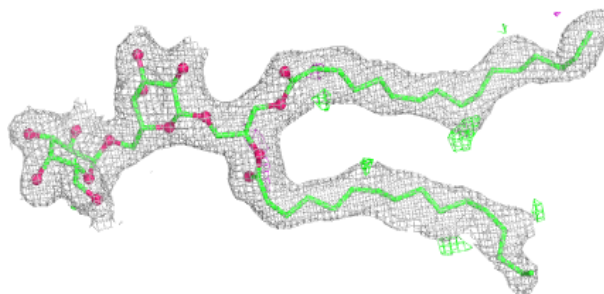


**Electron density around CLA c 912:**

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

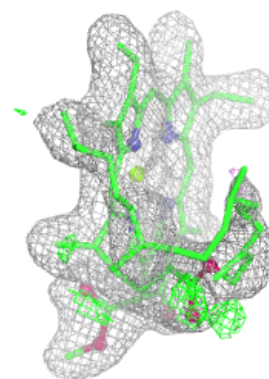
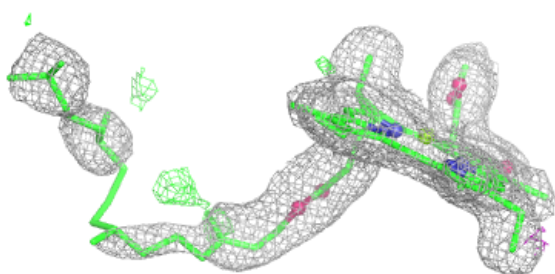
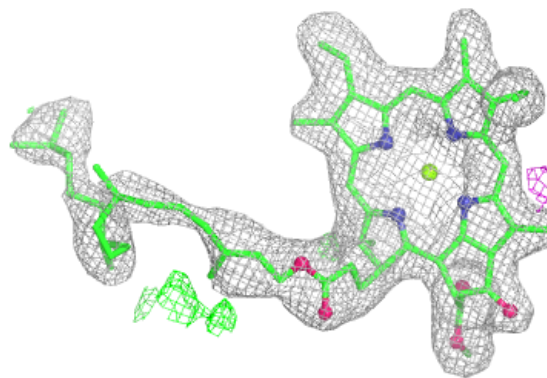
**Electron density around DGD C 519:**

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

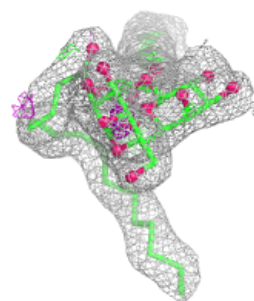
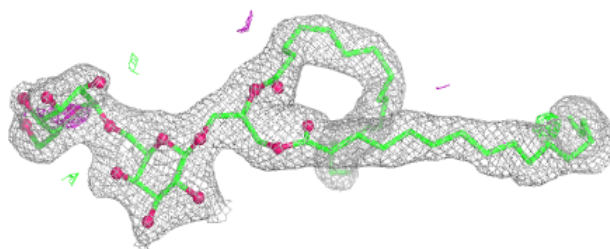
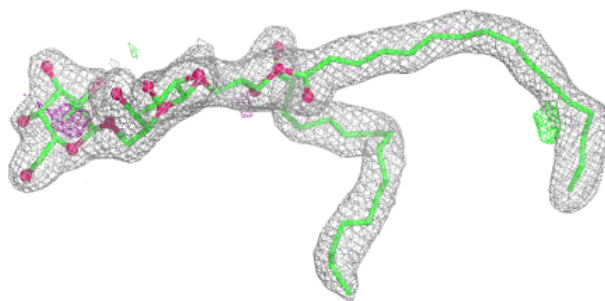


**Electron density around CLA a 412:**

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

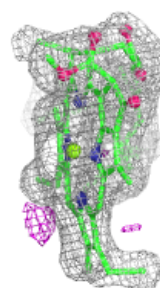
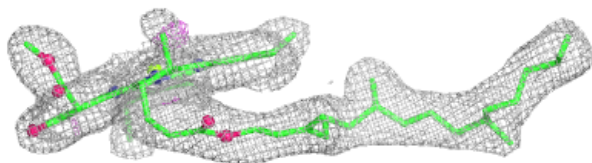
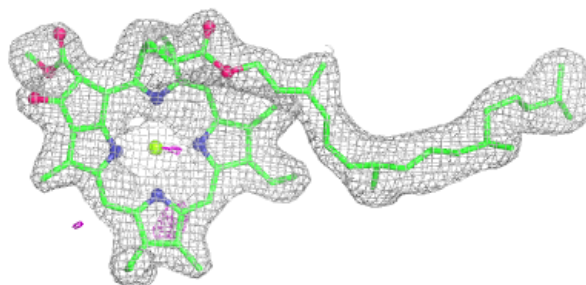
**Electron density around DGD H 102:**

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

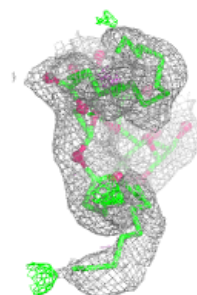
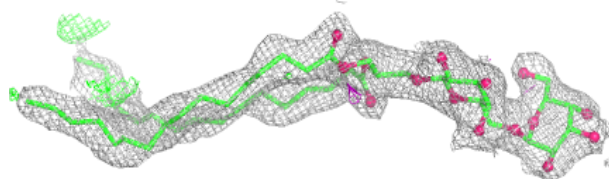
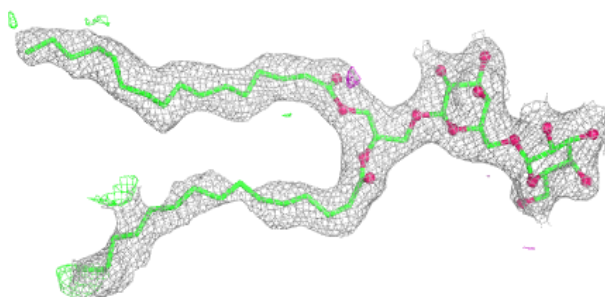


**Electron density around CLA B 604:**

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

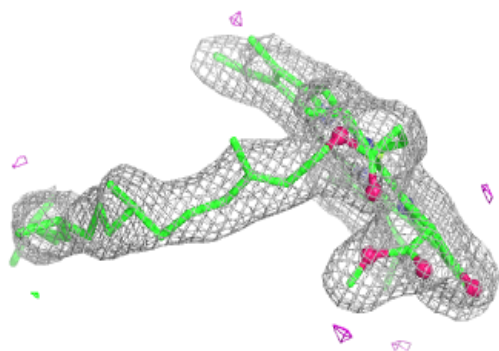
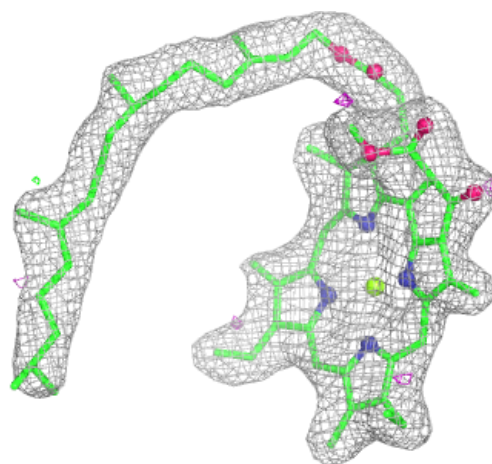
**Electron density around DGD c 919:**

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



**Electron density around CLA C 508:**

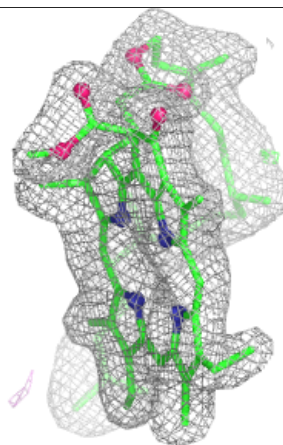
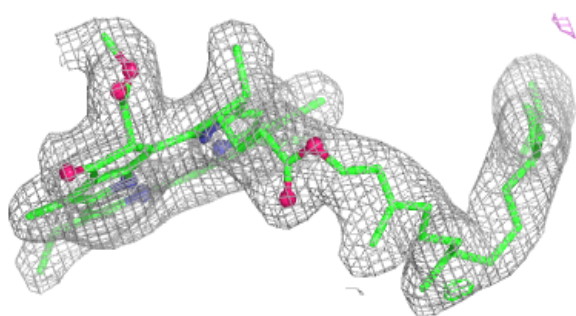
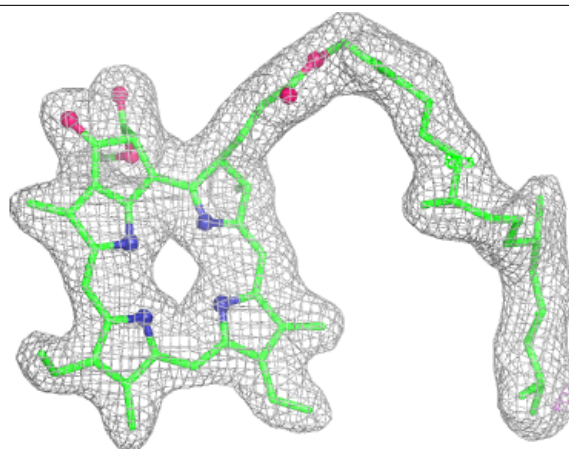
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



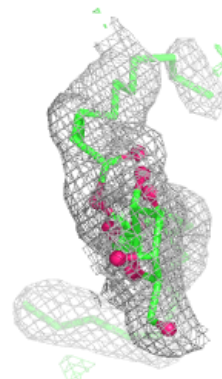
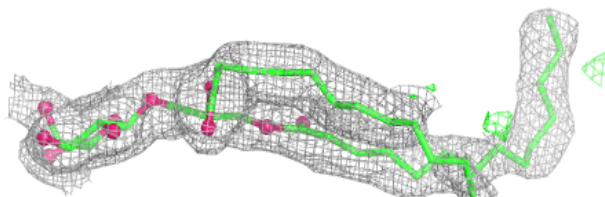
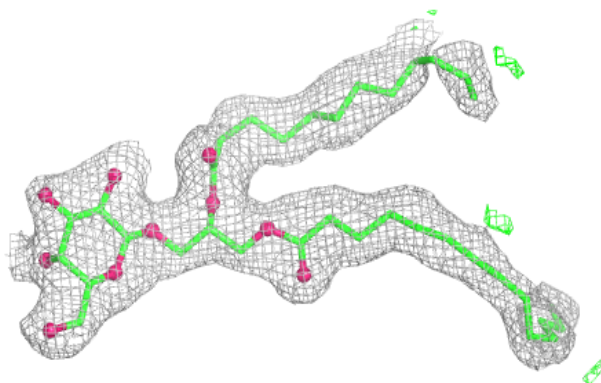


**Electron density around PHO a 411:**

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

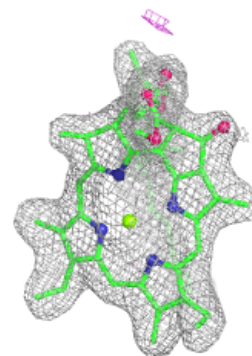
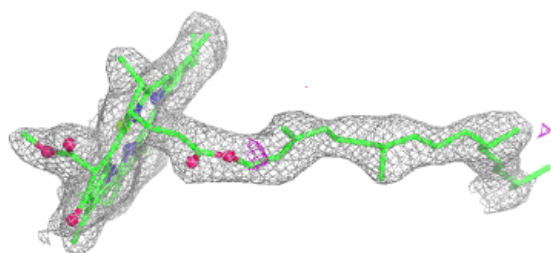
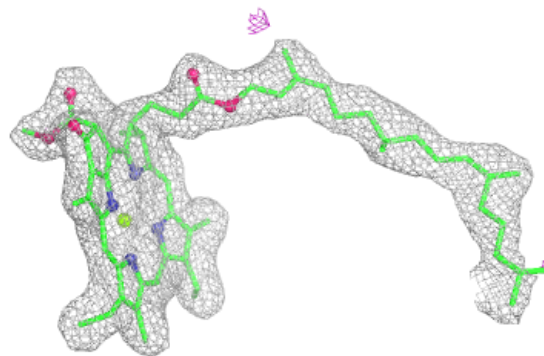
**Electron density around LMG J 101:**

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

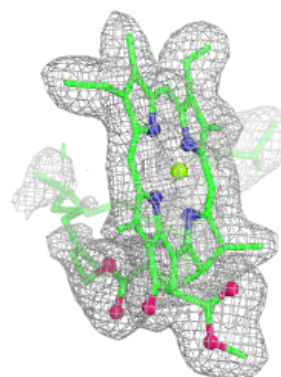
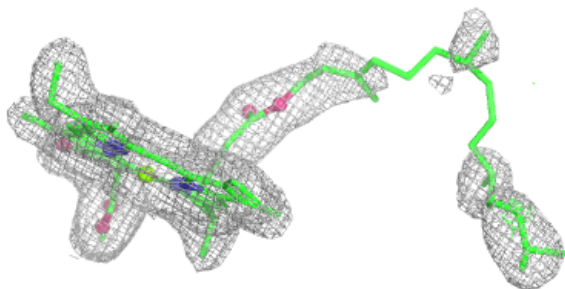
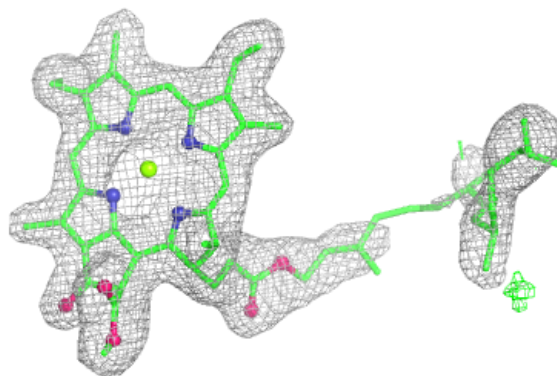


**Electron density around CLA b 610:**

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

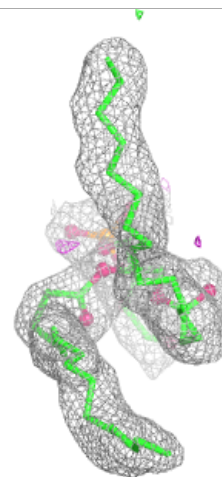
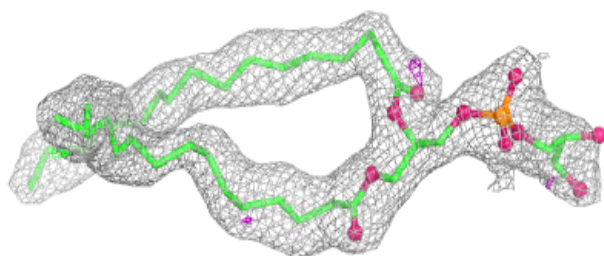
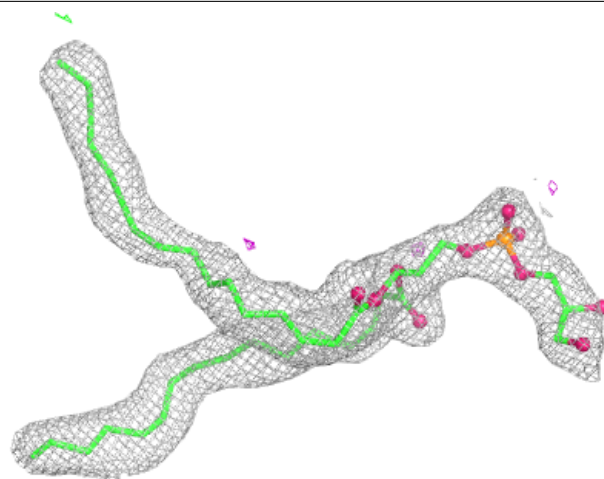
**Electron density around CLA A 408:**

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



**Electron density around LHG d 407:**

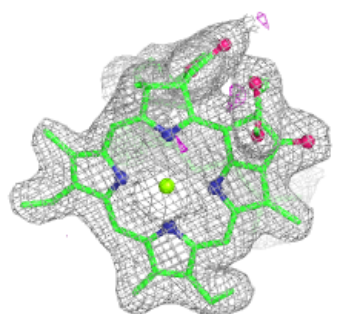
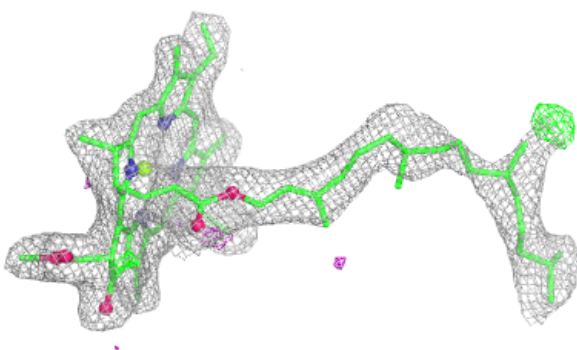
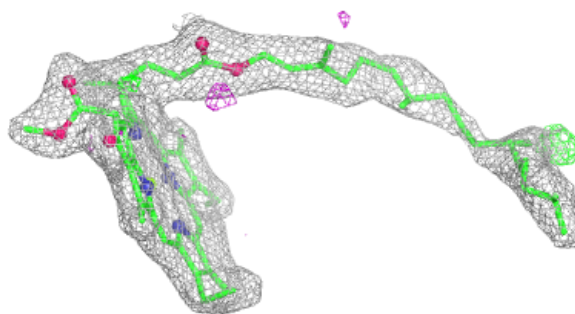
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



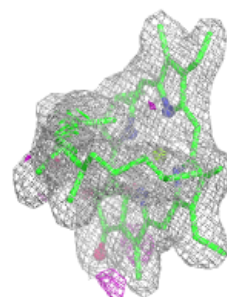
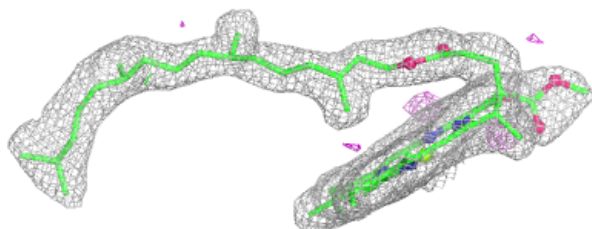
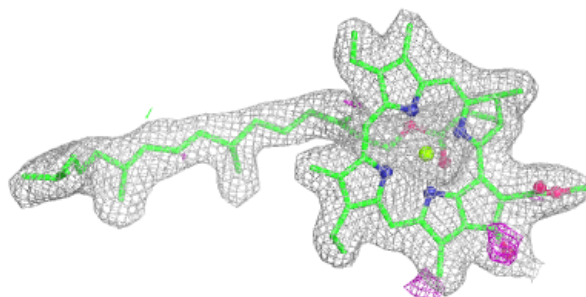


**Electron density around CLA b 608:**

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

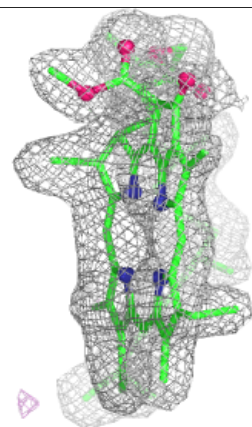
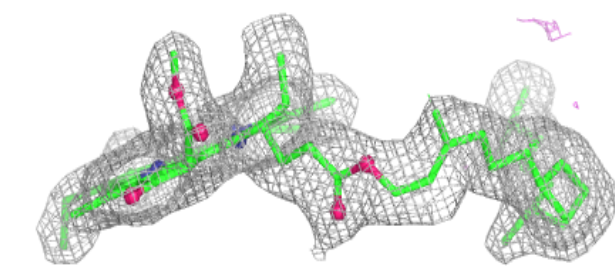
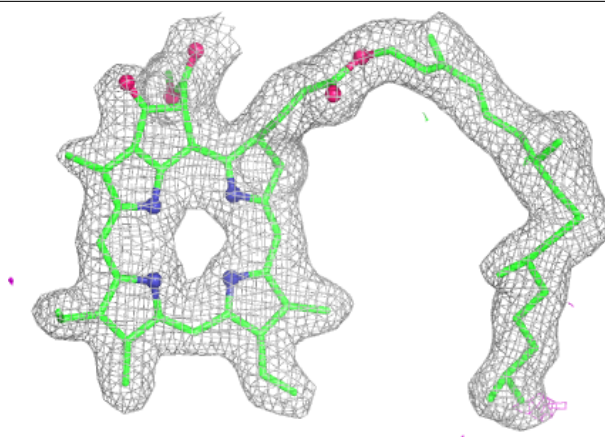
**Electron density around CLA b 609:**

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



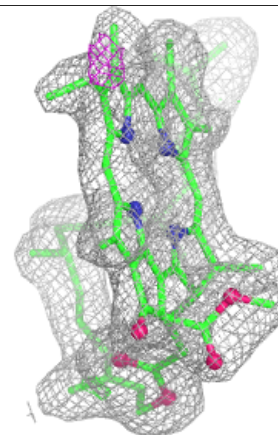
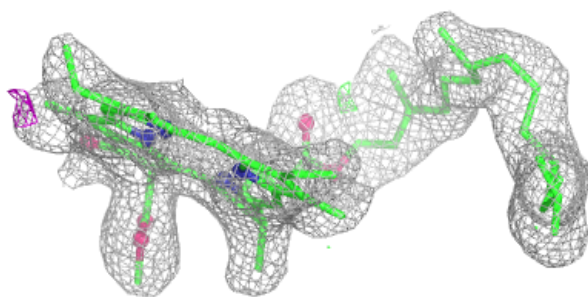
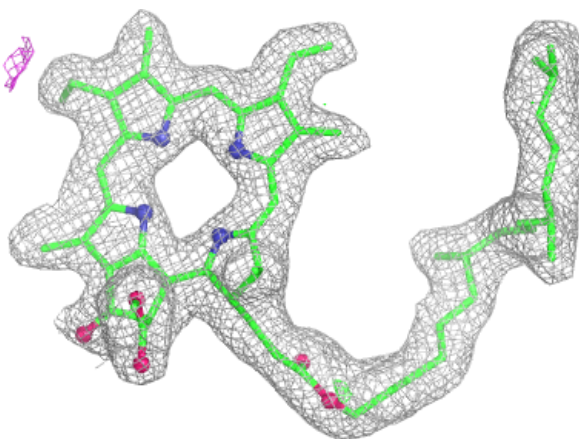
**Electron density around PHO A 407:**

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



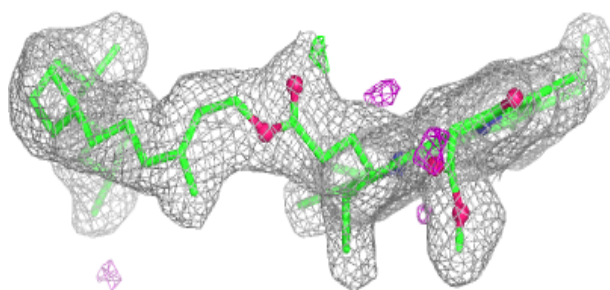
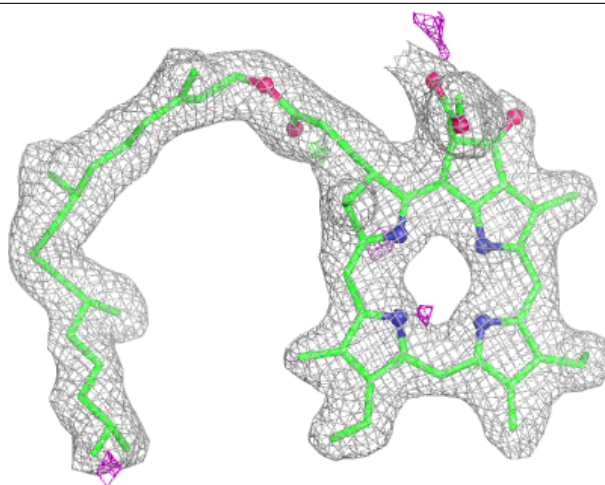
**Electron density around PHO D 402:**

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



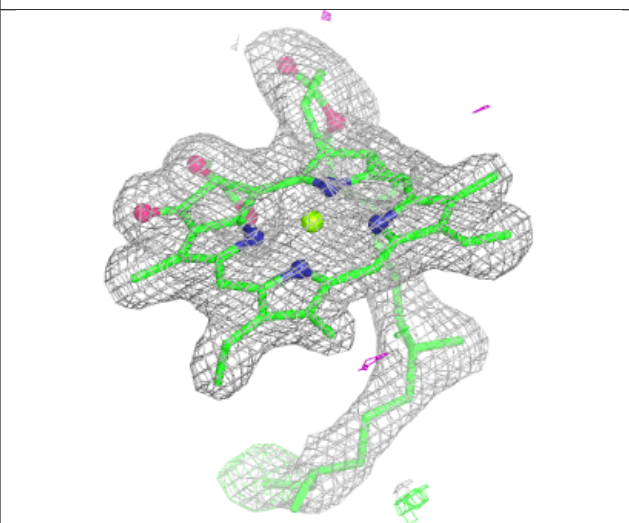
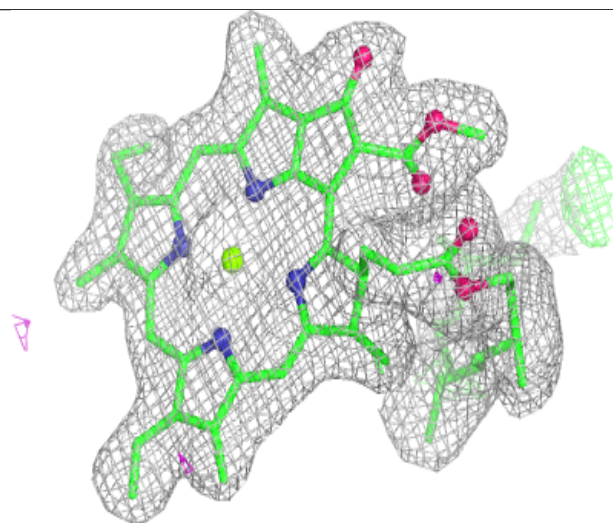
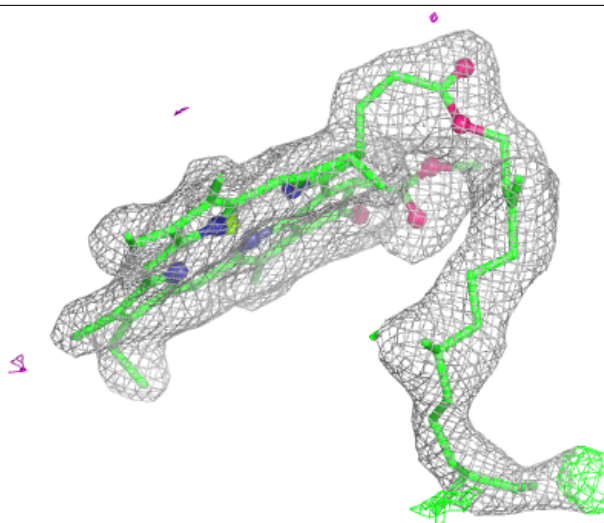
**Electron density around PHO a 410:**

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



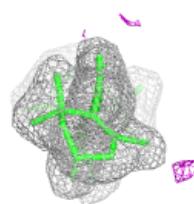
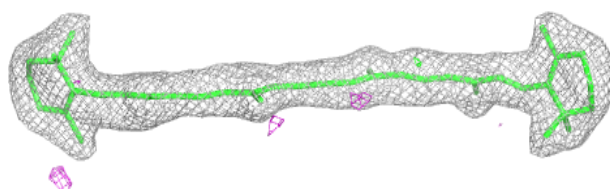
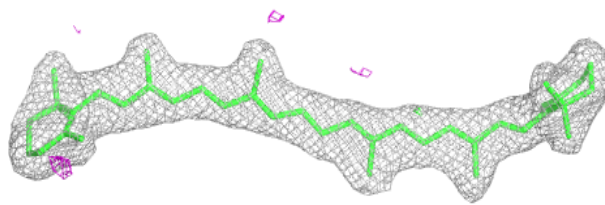
**Electron density around CLA B 614:**

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



**Electron density around BCR A 409:**

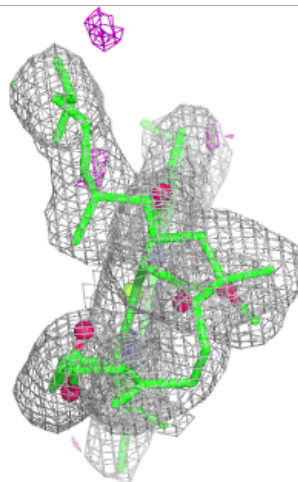
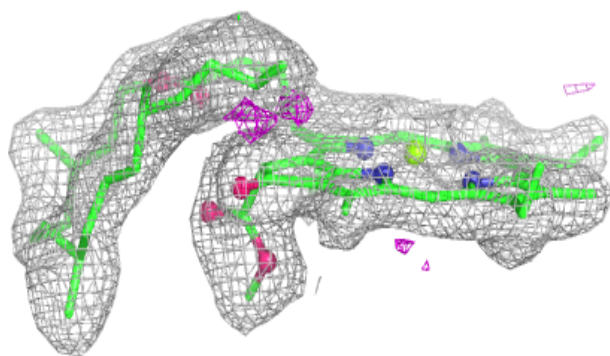
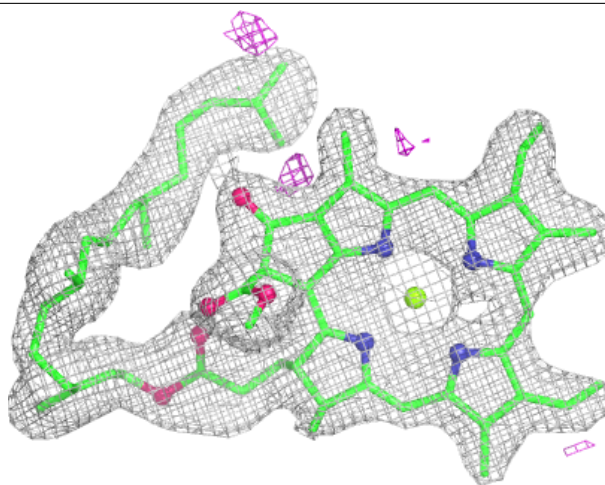
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





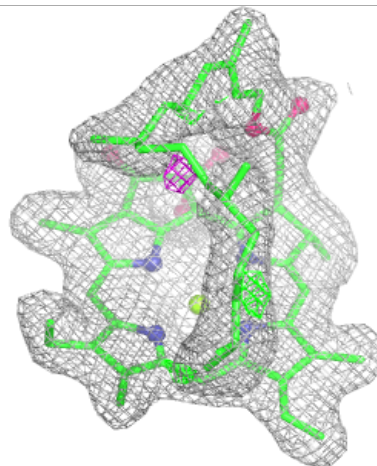
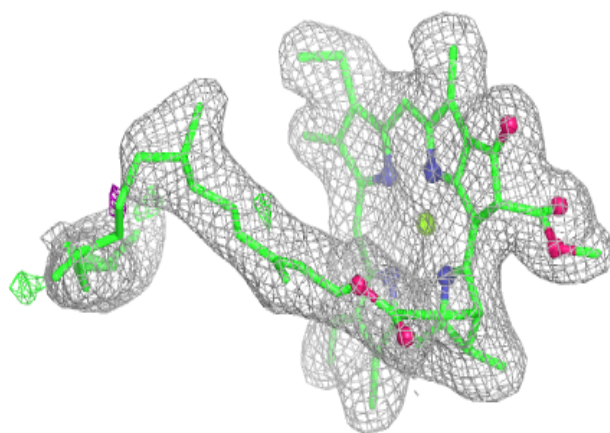
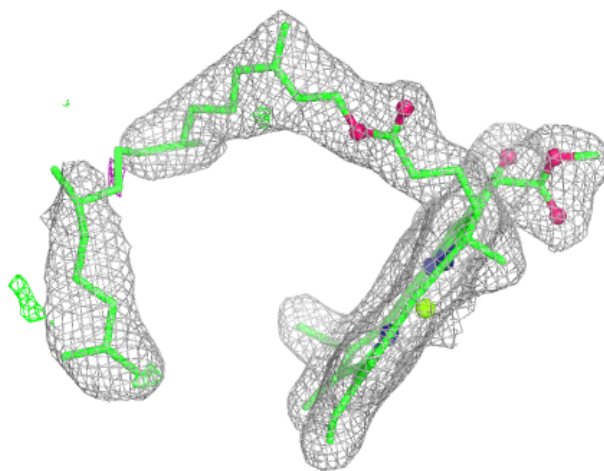
**Electron density around CLA b 611:**

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



**Electron density around CLA b 612:**

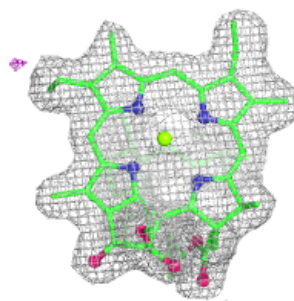
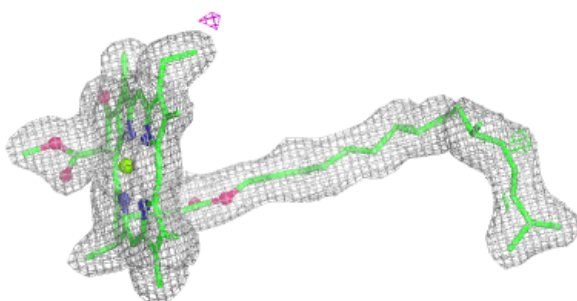
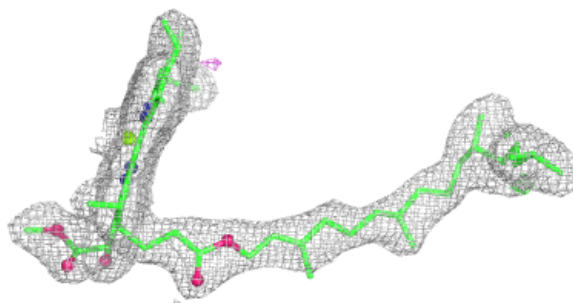
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





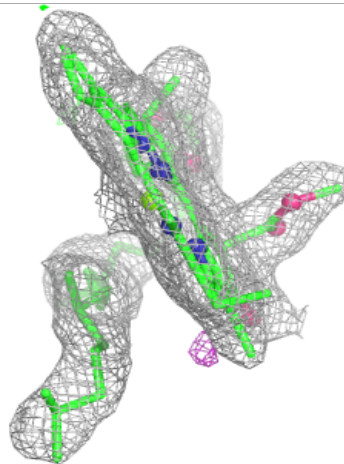
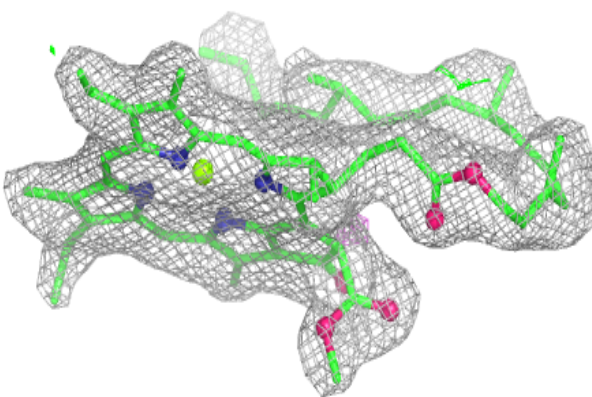
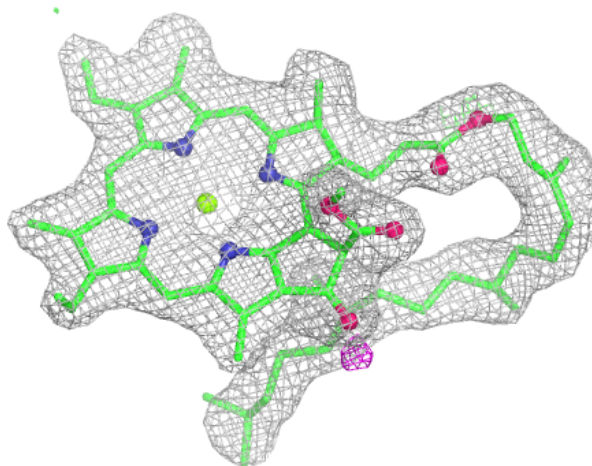
**Electron density around CLA B 606:**

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



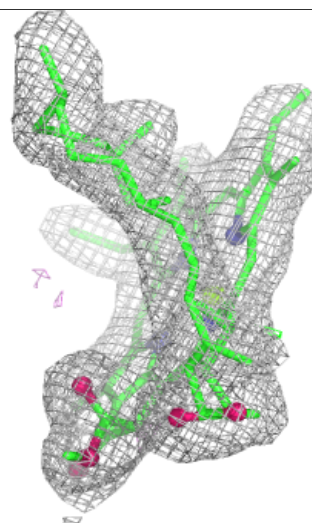
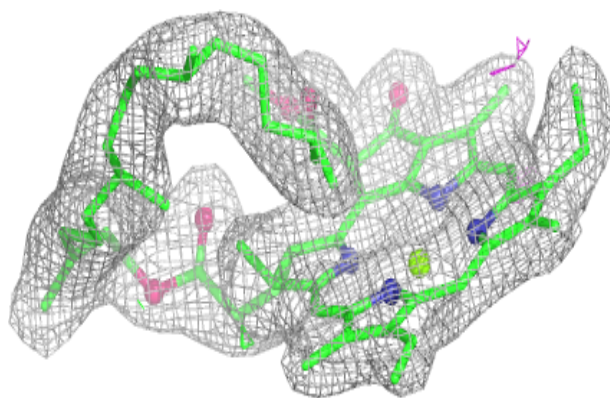
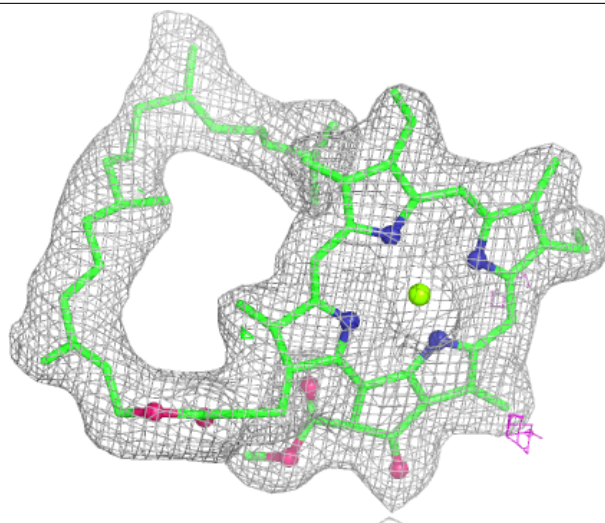
**Electron density around CLA C 510:**

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



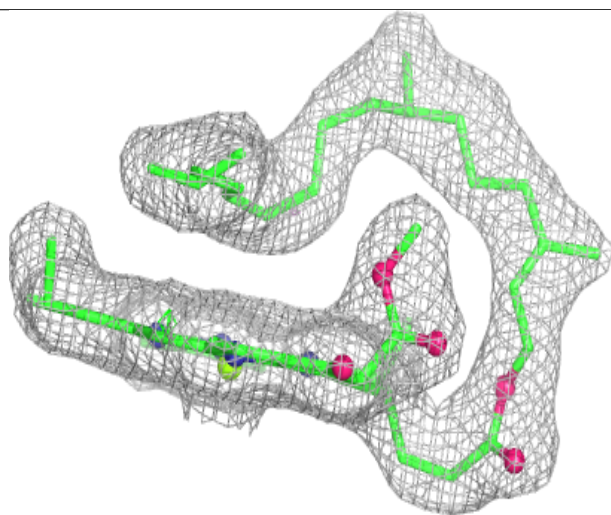
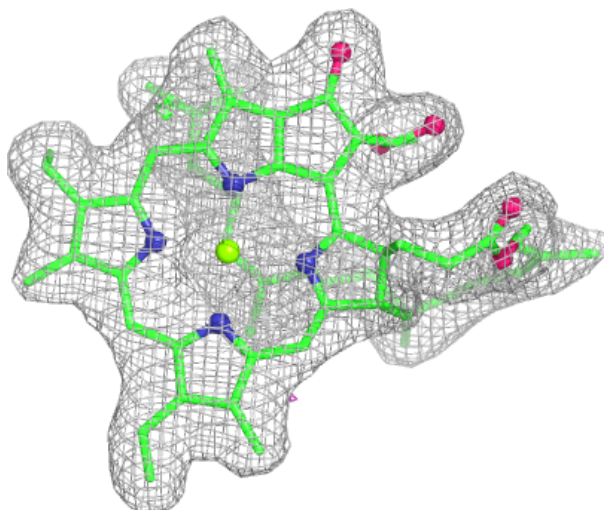
**Electron density around CLA b 616:**

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



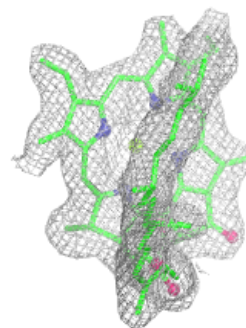
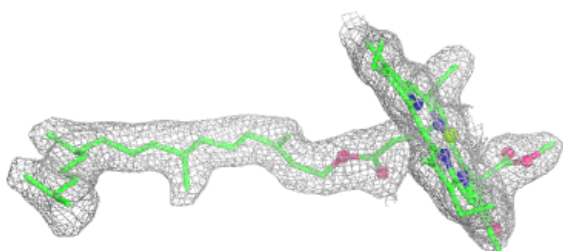
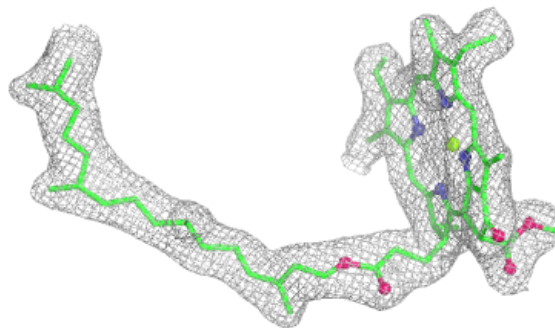
**Electron density around CLA C 511:**

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

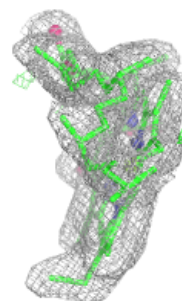
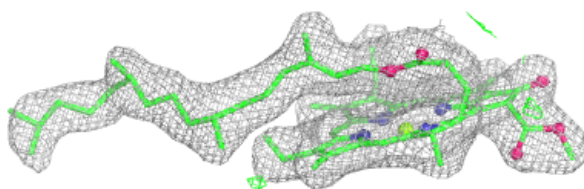
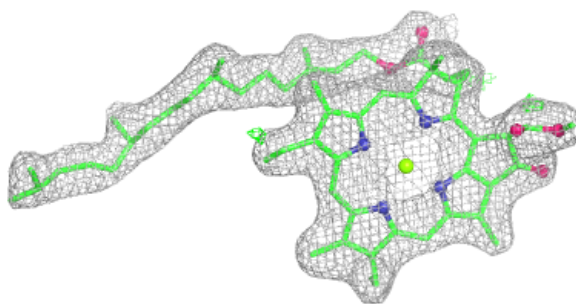


**Electron density around CLA B 610:**

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

**Electron density around CLA C 502:**

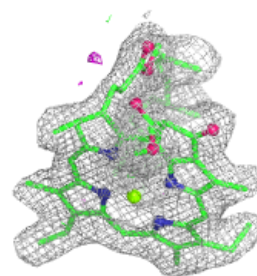
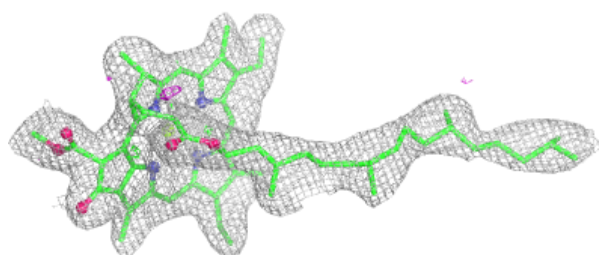
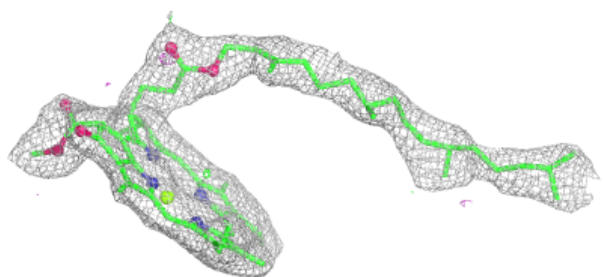
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



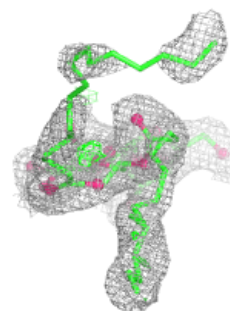
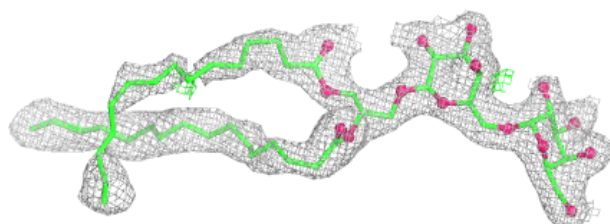
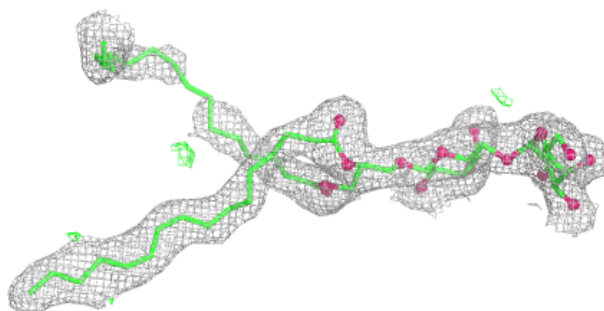


**Electron density around CLA c 905:**

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

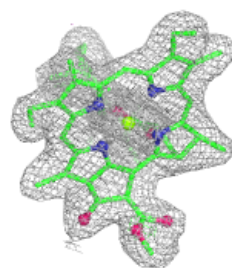
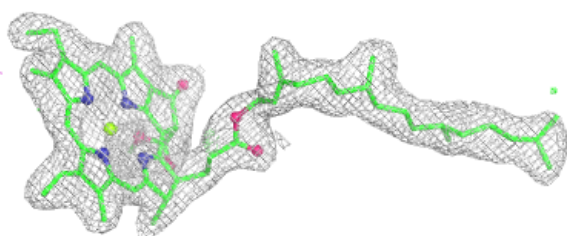
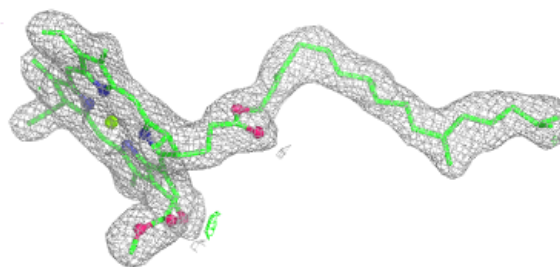
**Electron density around DGD C 517:**

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



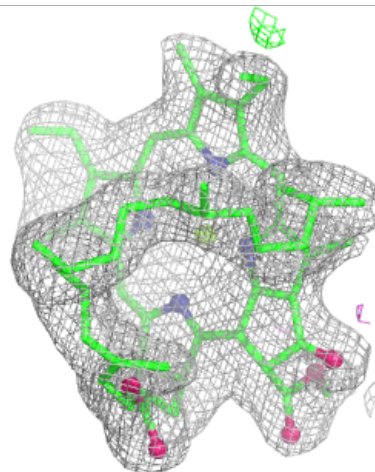
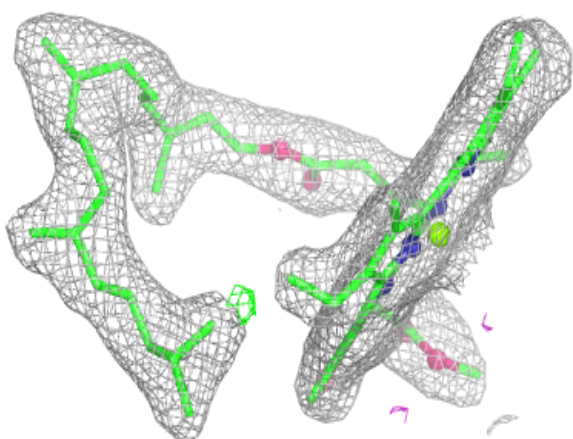
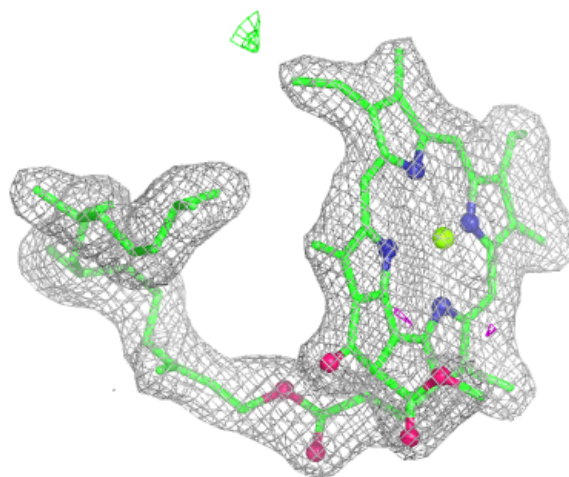
**Electron density around CLA C 503:**

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



**Electron density around CLA C 504:**

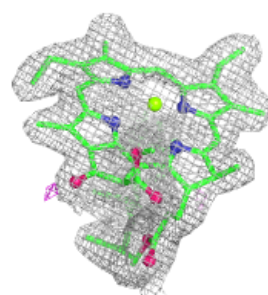
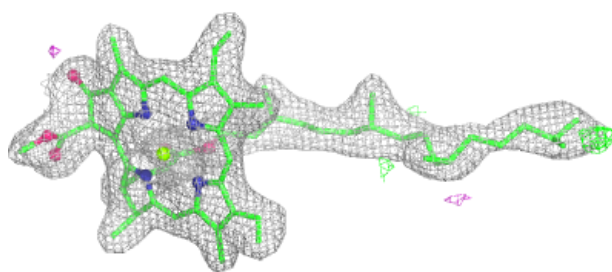
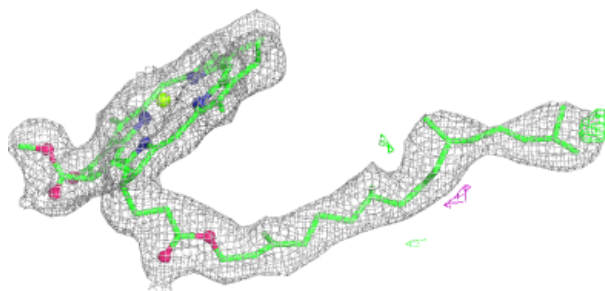
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



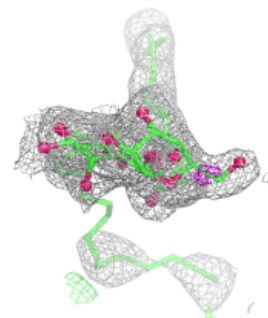
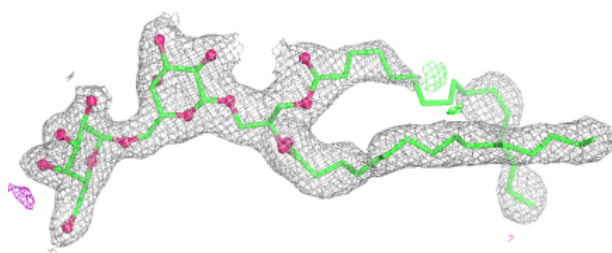
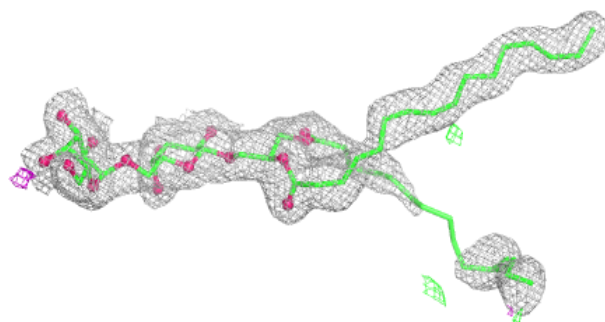


**Electron density around CLA C 505:**

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

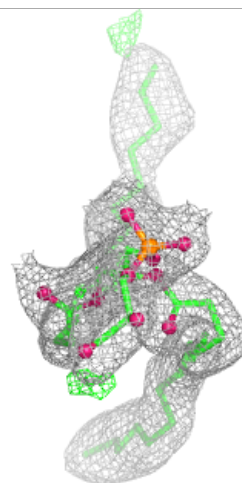
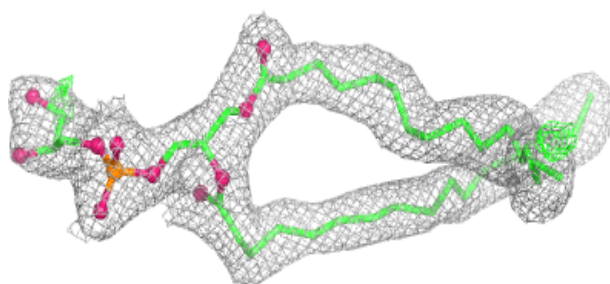
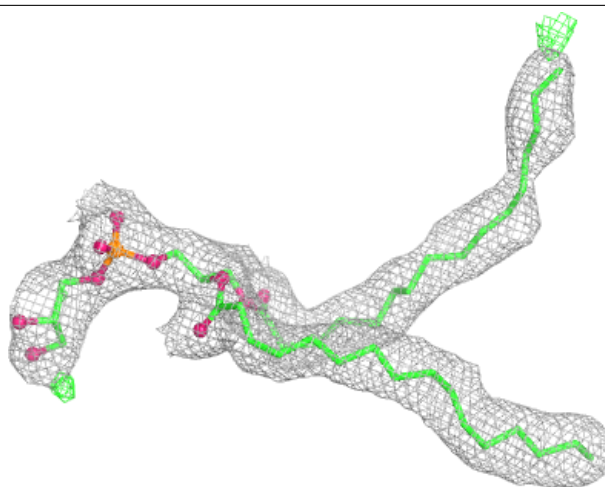
**Electron density around DGD c 917:**

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



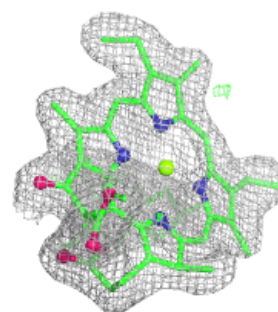
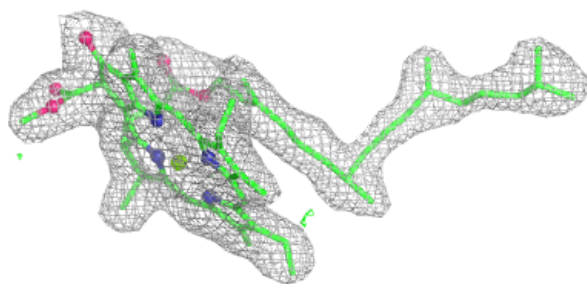
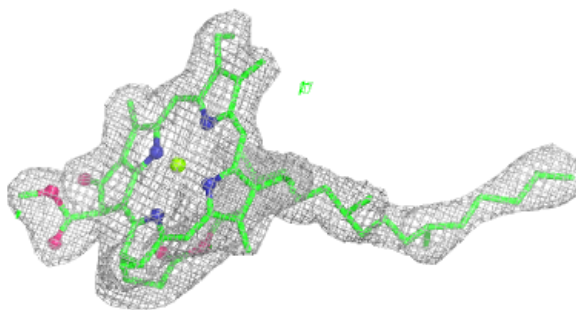
**Electron density around LHG D 410:**

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

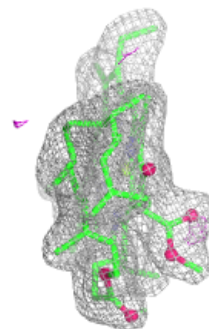
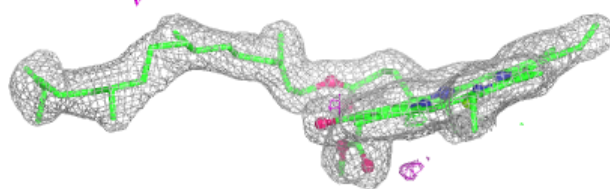
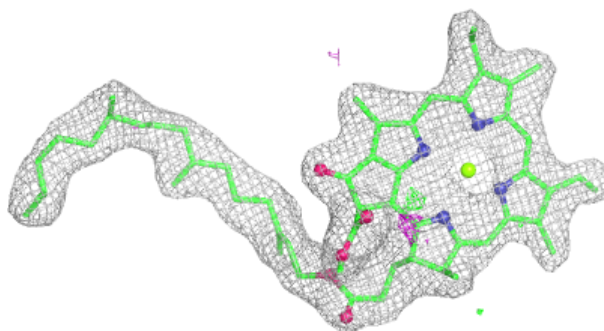


**Electron density around CLA C 506:**

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

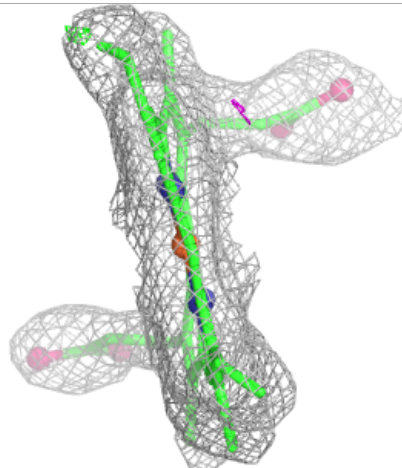
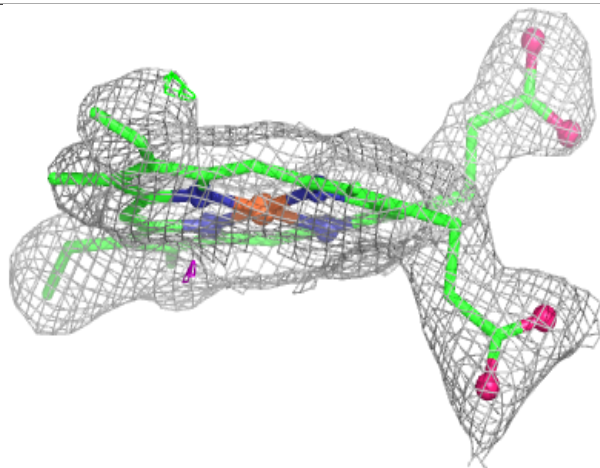
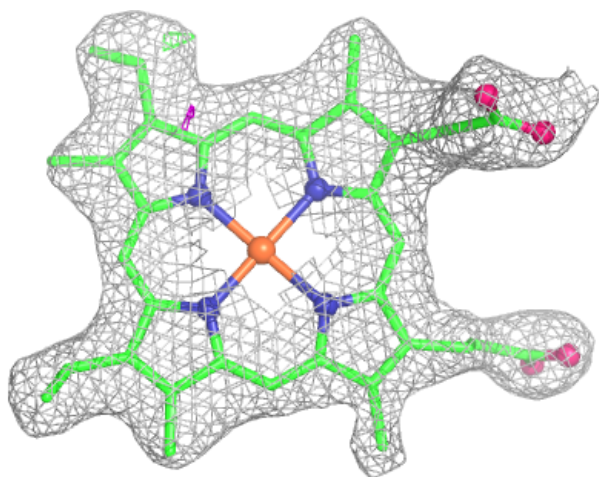
**Electron density around CLA b 603:**

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



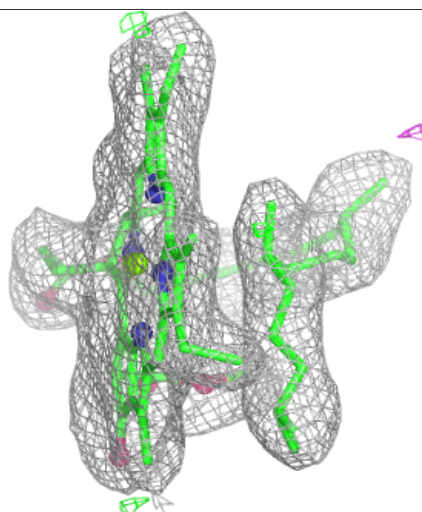
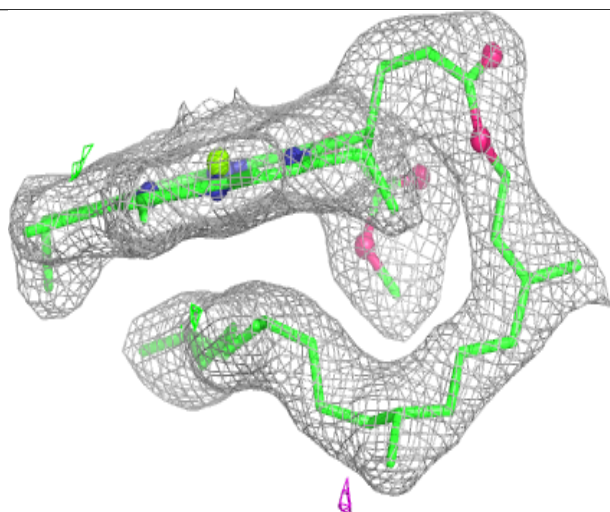
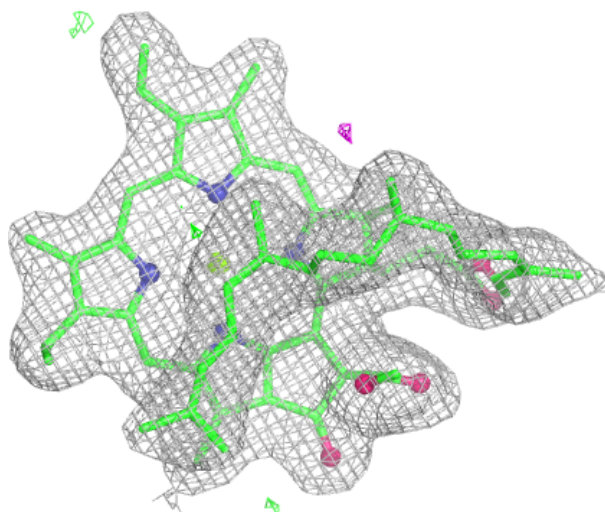
**Electron density around HEM E 102:**

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



**Electron density around CLA c 911:**

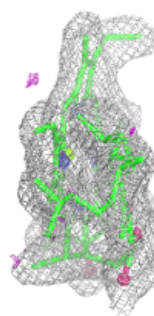
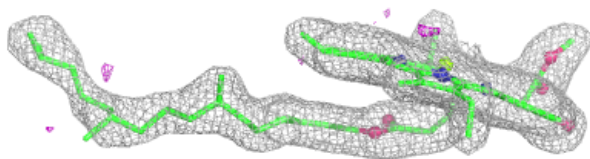
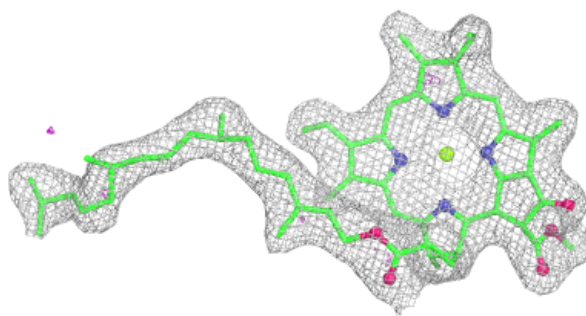
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



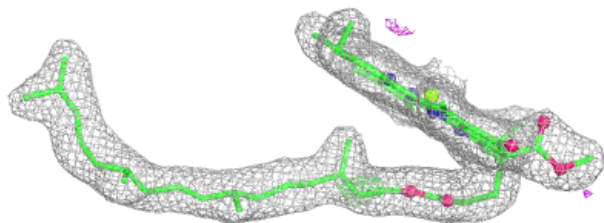
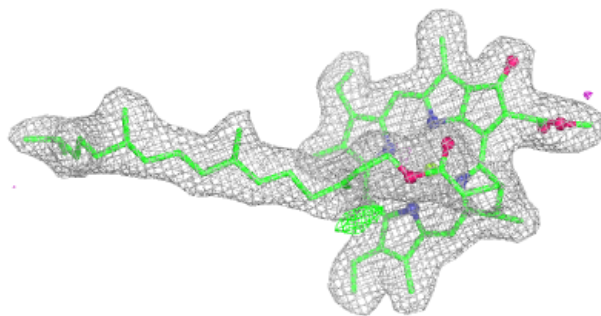


**Electron density around CLA b 604:**

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

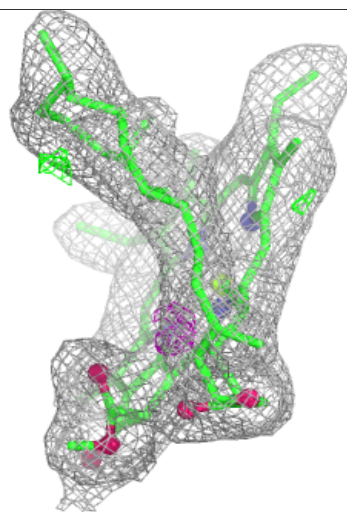
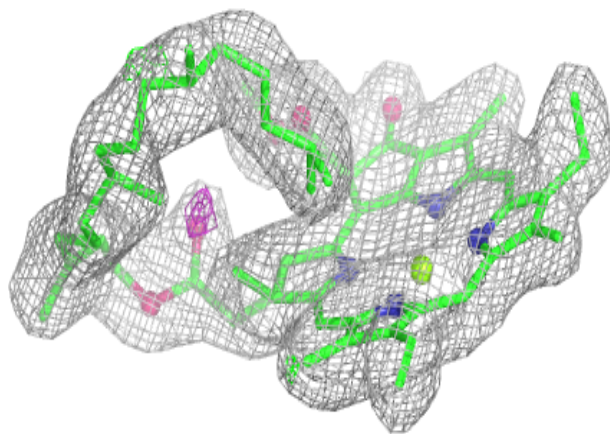
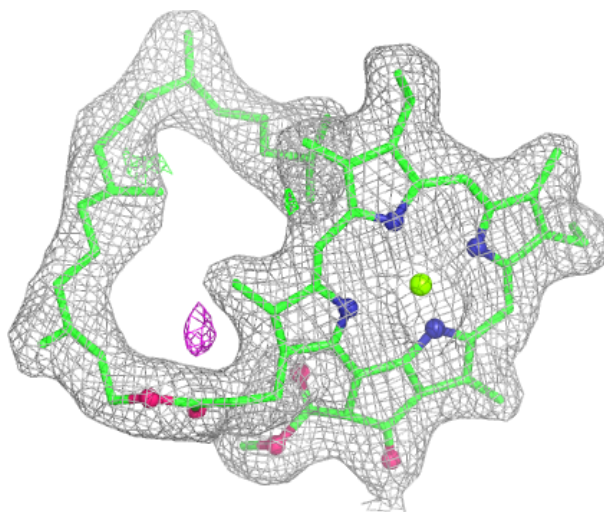
**Electron density around CLA B 609:**

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



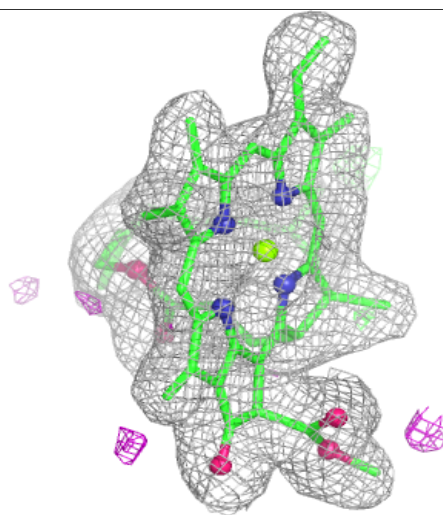
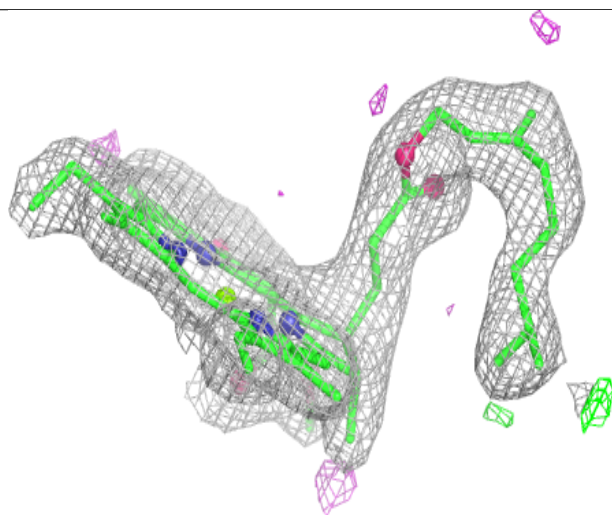
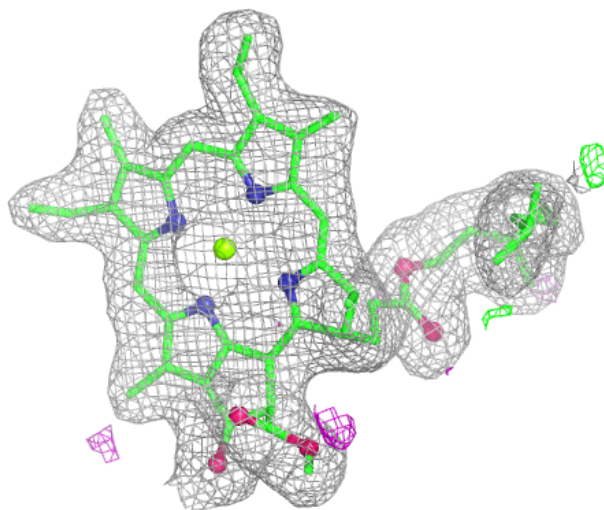
**Electron density around CLA B 616:**

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



**Electron density around CLA A 406:**

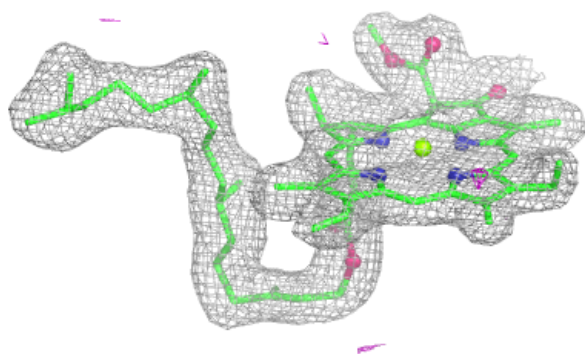
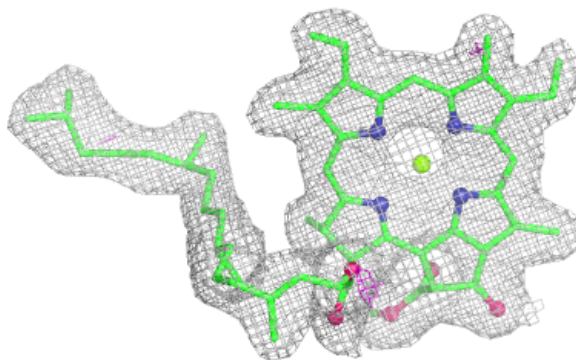
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



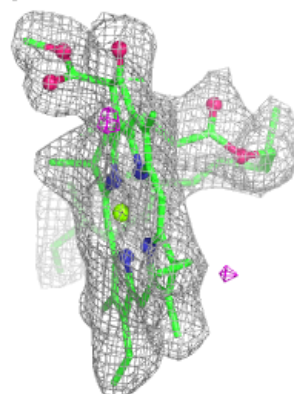
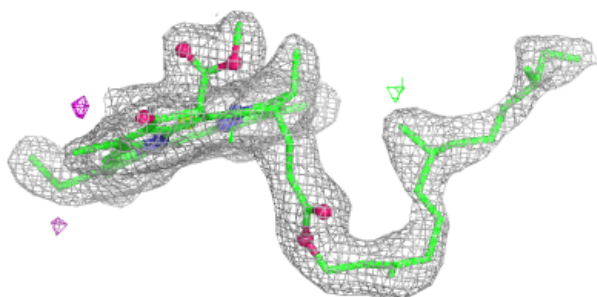
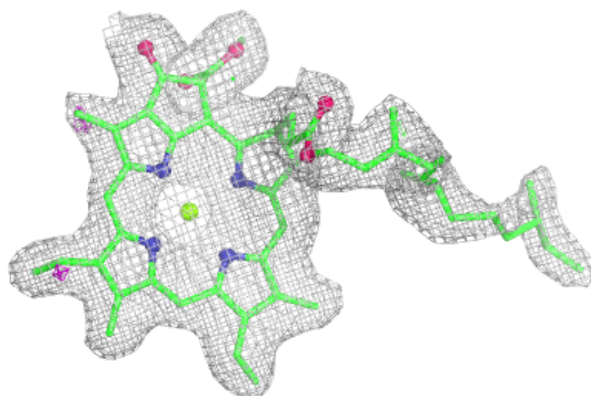


**Electron density around CLA a 408:**

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

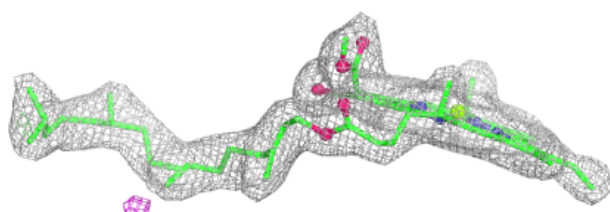
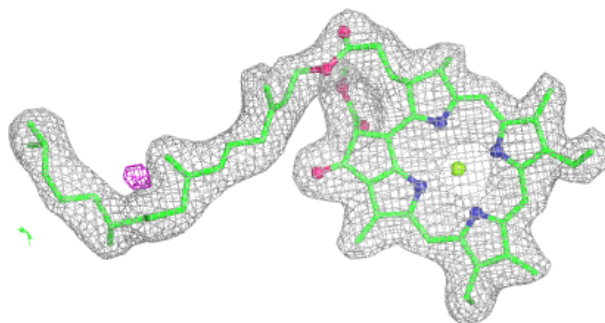
**Electron density around CLA a 409:**

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

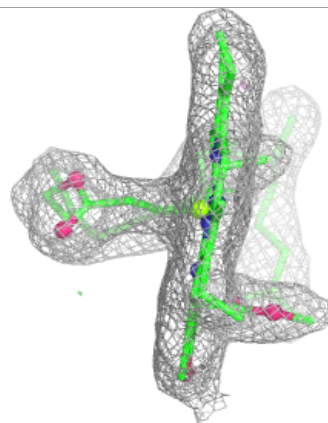
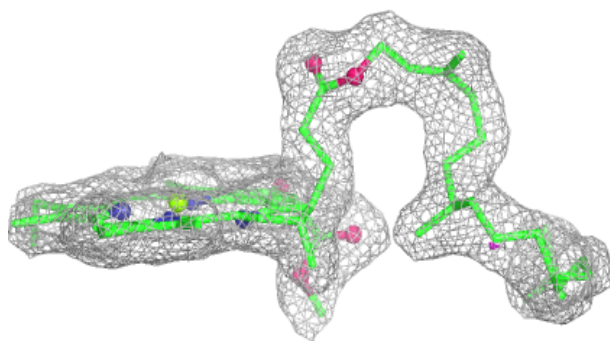
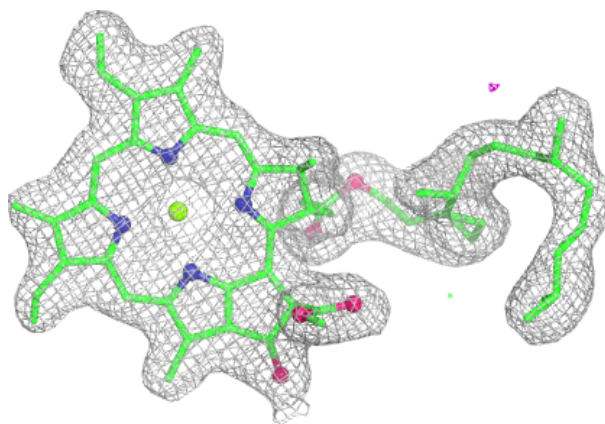


**Electron density around CLA B 603:**

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

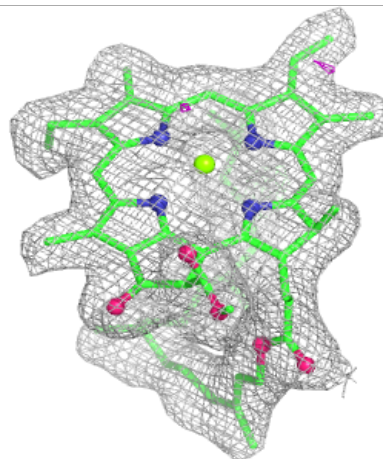
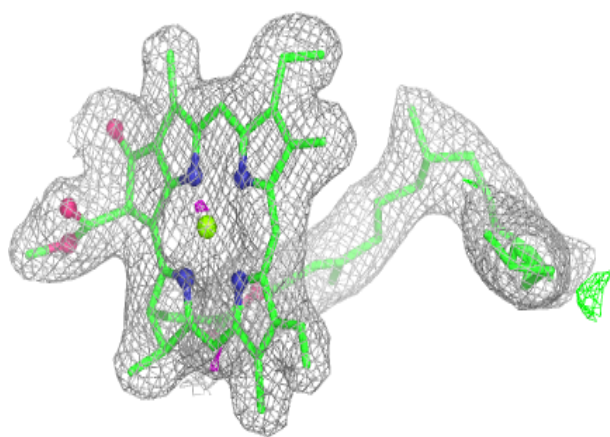
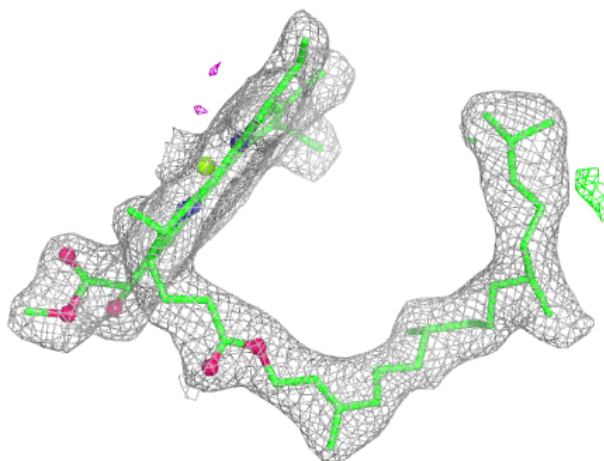
**Electron density around CLA b 613:**

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



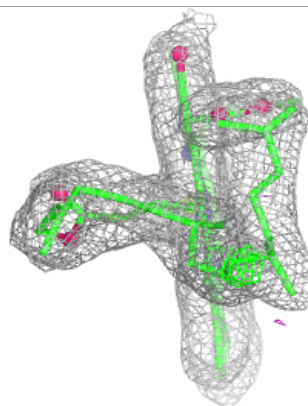
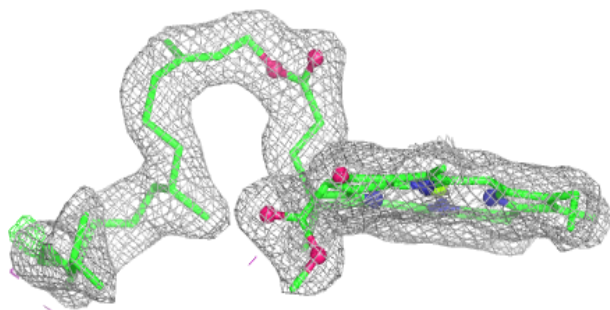
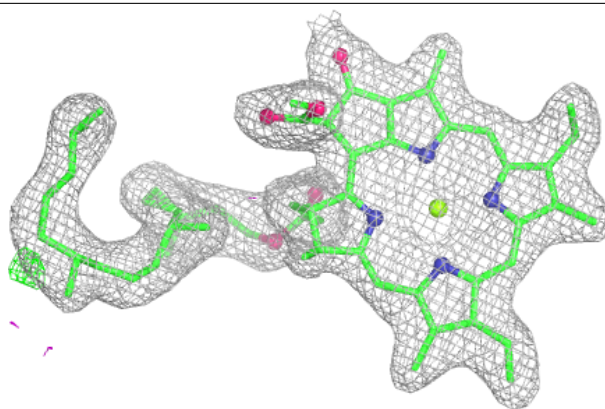
**Electron density around CLA B 612:**

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

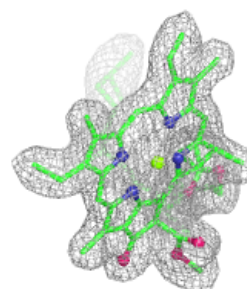
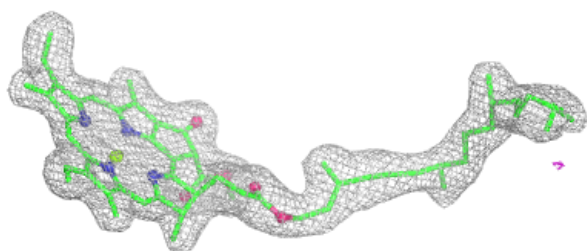
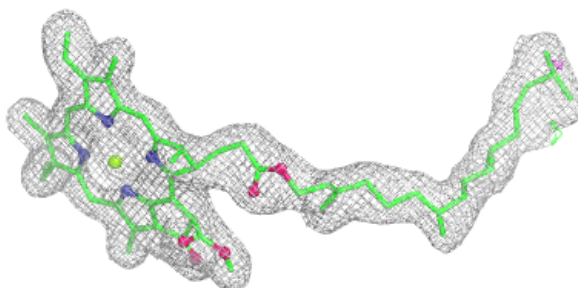


**Electron density around CLA B 613:**

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

**Electron density around CLA A 405:**

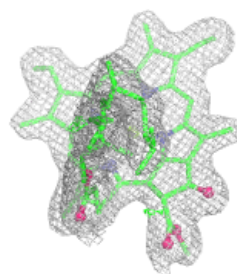
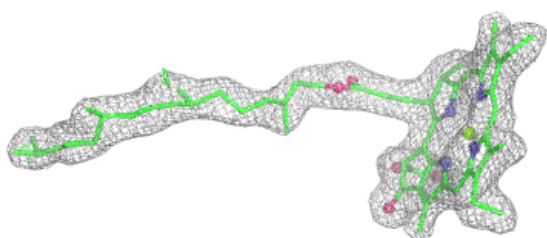
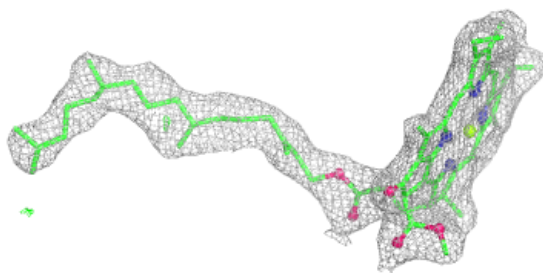
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



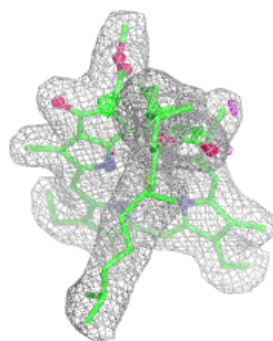
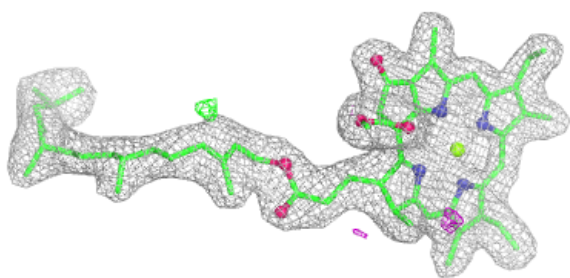
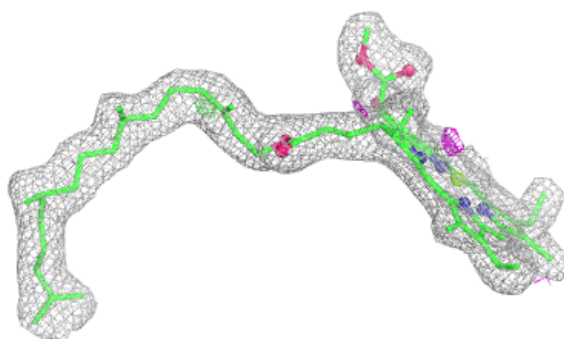


**Electron density around CLA b 605:**

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

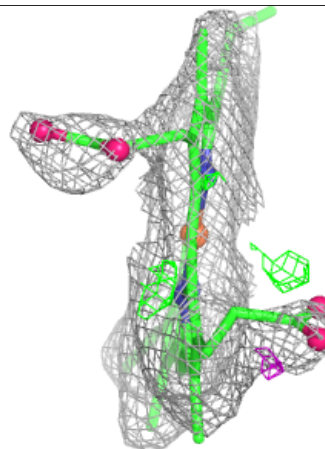
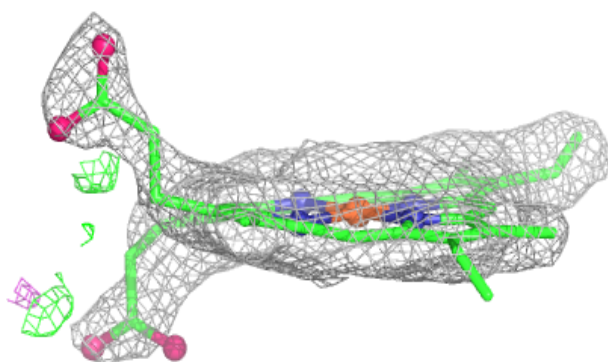
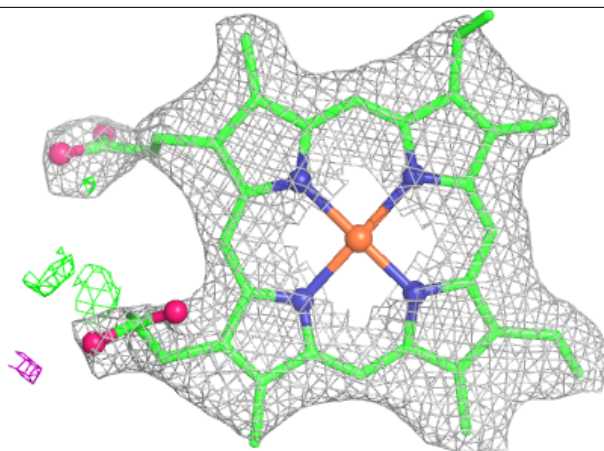
**Electron density around CLA d 402:**

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



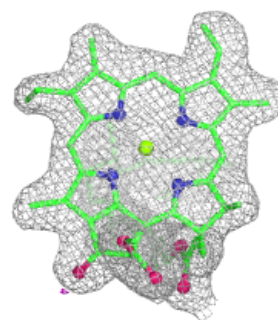
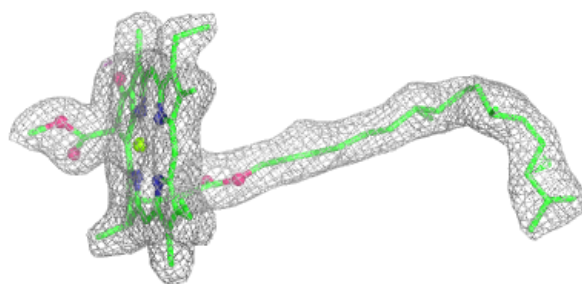
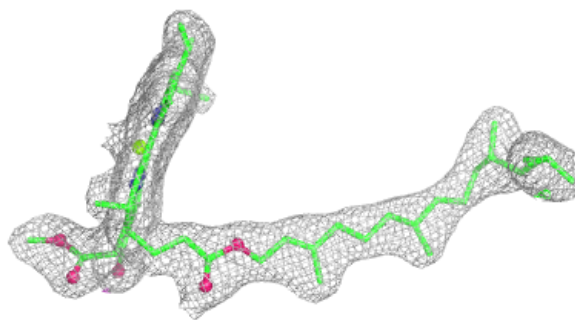
**Electron density around HEM e 101:**

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

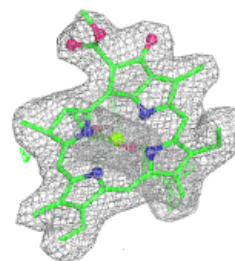
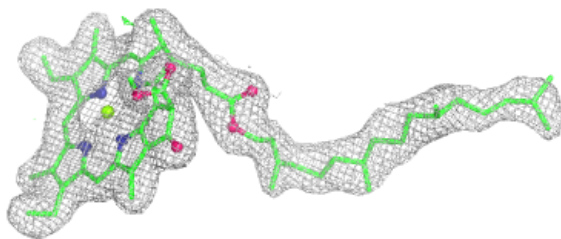
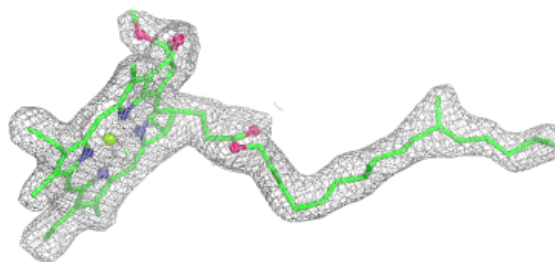


**Electron density around CLA b 606:**

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

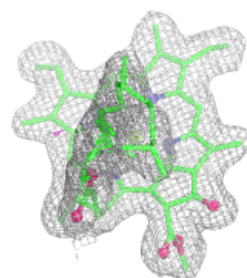
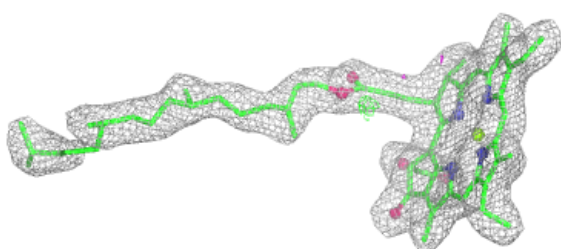
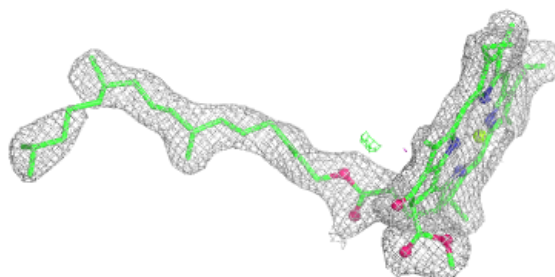
**Electron density around CLA c 903:**

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

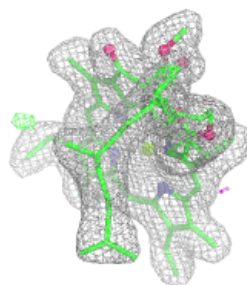
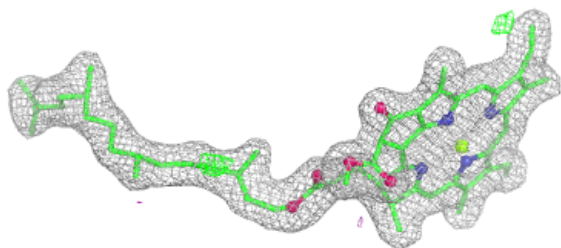
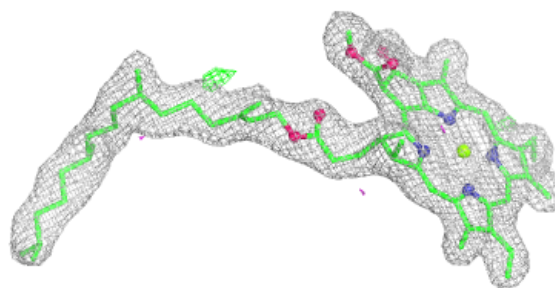


**Electron density around CLA B 605:**

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

**Electron density around CLA a 407:**

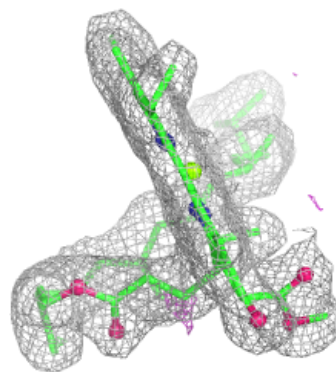
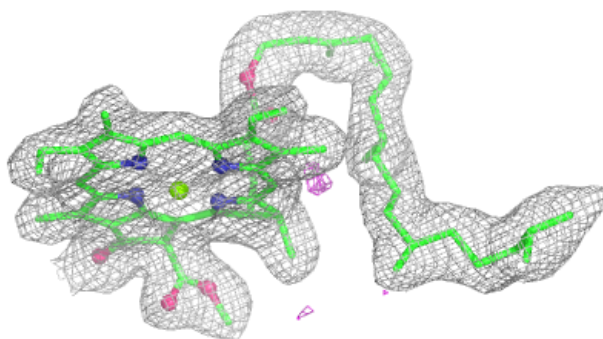
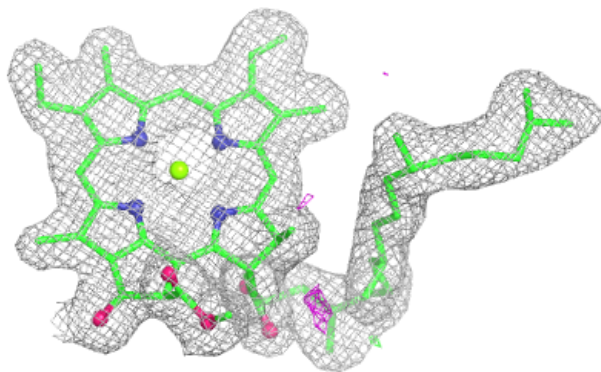
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



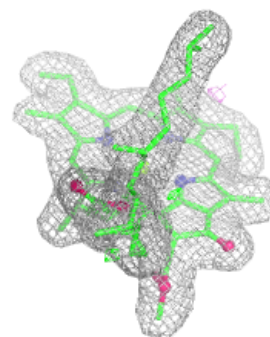
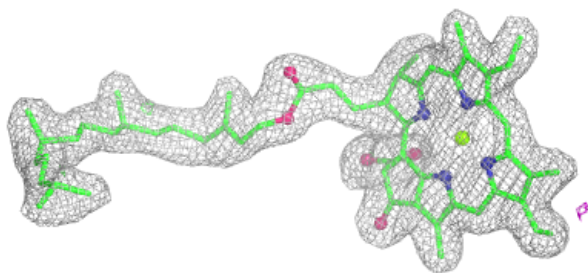
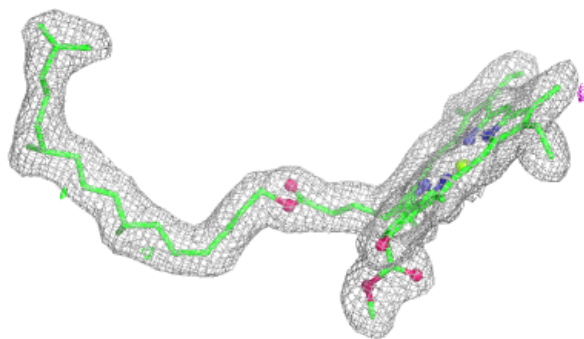


**Electron density around CLA D 401:**

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

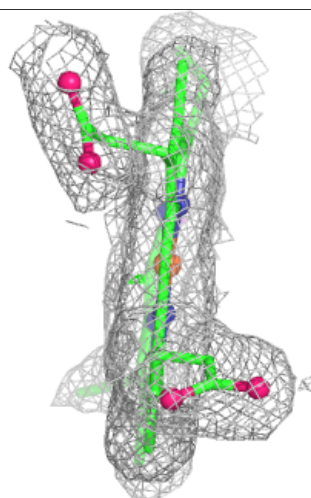
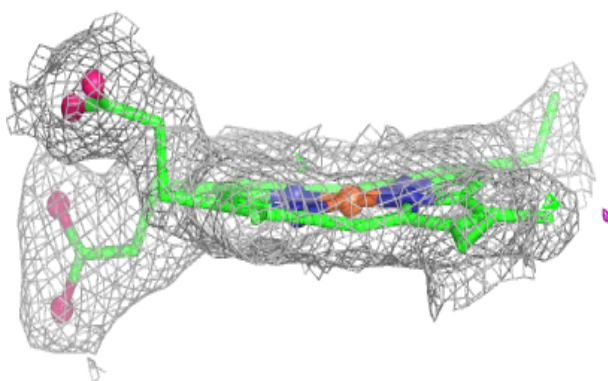
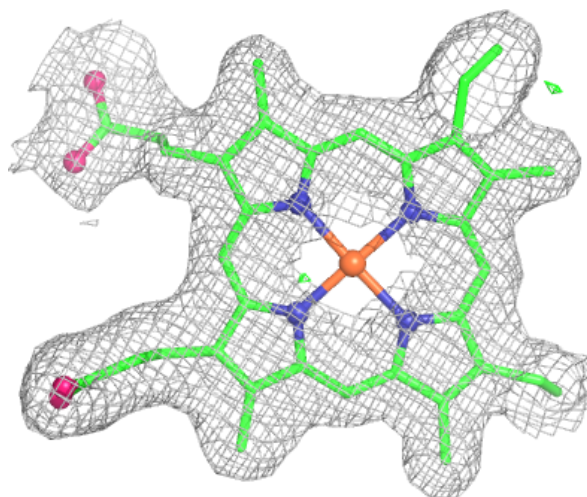
**Electron density around CLA D 403:**

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



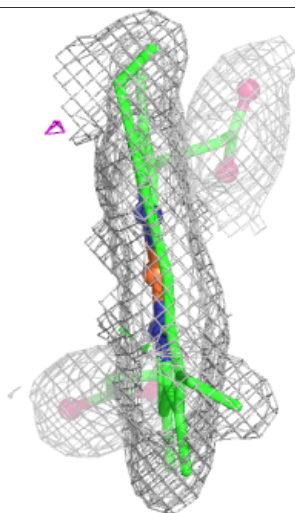
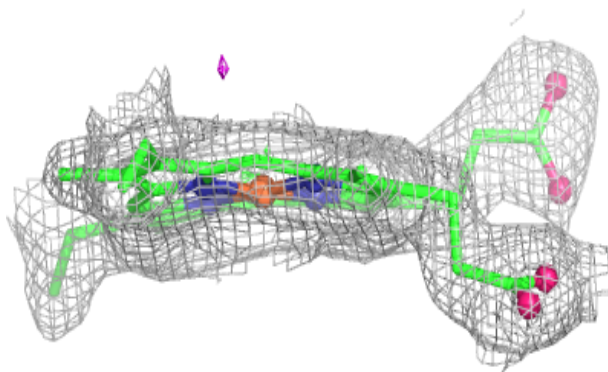
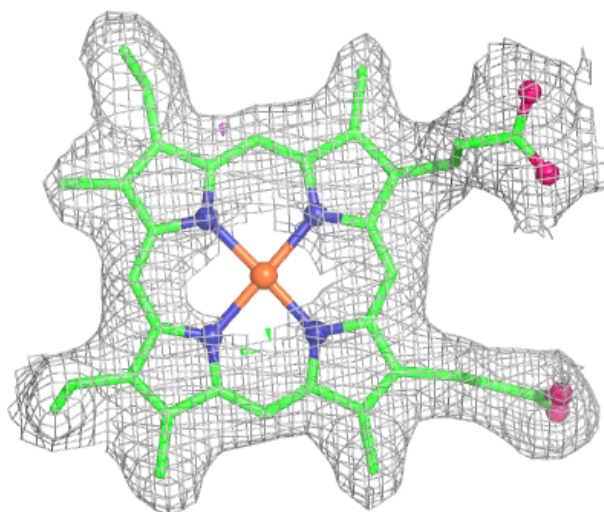
**Electron density around HEC V 202:**

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



**Electron density around HEC v 202:**

$2mF_o-DF_c$  (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.