



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 19, 2020 – 01:55 PM BST

PDB ID : 5B66  
Title : Crystal structure analysis of Photosystem II complex  
Authors : Tanaka, A.; Fukushima, Y.; Kamiya, N.  
Deposited on : 2016-05-25  
Resolution : 1.85 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

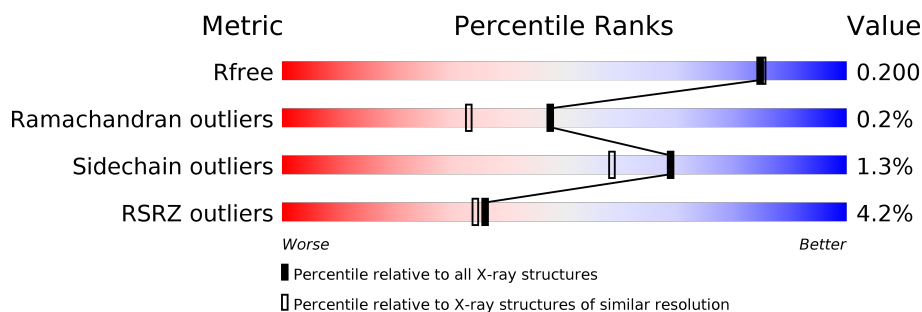
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 2469 (1.86-1.86)                                      |
| Ramachandran outliers | 138981                      | 2592 (1.86-1.86)                                      |
| Sidechain outliers    | 138945                      | 2592 (1.86-1.86)                                      |
| RSRZ outliers         | 127900                      | 2436 (1.86-1.86)                                      |

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 on 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     | 344    | <div> <div>%</div> <div>95%</div> <div>..</div> </div>  |
| 1   | a     | 344    | <div> <div>2%</div> <div>95%</div> <div>..</div> </div> |
| 2   | B     | 505    | <div> <div>4%</div> <div>97%</div> <div>.</div> </div>  |
| 2   | b     | 505    | <div> <div>4%</div> <div>95%</div> <div>..</div> </div> |
| 3   | C     | 455    | <div> <div>2%</div> <div>96%</div> <div>..</div> </div> |
| 3   | c     | 455    | <div> <div>%</div> <div>97%</div> <div>.</div> </div>   |
| 4   | D     | 342    | <div> <div>%</div> <div>98%</div> <div>.</div> </div>   |

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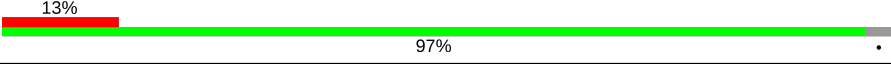
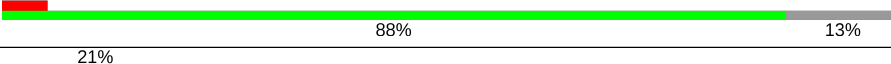
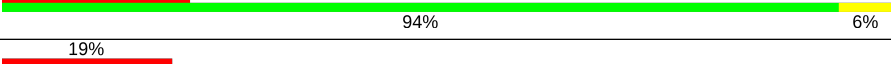
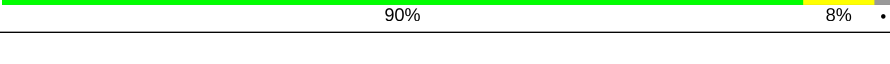


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | d     | 342    |                  |
| 5   | E     | 83     |                  |
| 5   | e     | 83     |                  |
| 6   | F     | 44     |                  |
| 6   | f     | 44     |                  |
| 7   | H     | 65     |                  |
| 7   | h     | 65     |                  |
| 8   | I     | 38     |                  |
| 8   | i     | 38     |                  |
| 9   | J     | 40     |                  |
| 9   | j     | 40     |                  |
| 10  | K     | 37     |                  |
| 10  | k     | 37     |                  |
| 11  | L     | 37     |                  |
| 11  | l     | 37     |                  |
| 12  | M     | 36     |                  |
| 12  | m     | 36     |                  |
| 13  | O     | 244    |                  |
| 13  | o     | 244    |                  |
| 14  | T     | 32     |                  |
| 14  | t     | 32     |                  |
| 15  | U     | 104    |                  |
| 15  | u     | 104    |                  |
| 16  | V     | 137    |                  |
| 16  | v     | 137    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 17  | Y     | 30     |  |
| 17  | y     | 30     |  |
| 18  | X     | 40     |  |
| 18  | x     | 40     |  |
| 19  | Z     | 62     |  |
| 19  | 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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 20  | CLA  | A     | 401 | X         | -        | -       | -                |
| 20  | CLA  | A     | 402 | X         | -        | -       | -                |
| 20  | CLA  | A     | 404 | X         | -        | -       | -                |
| 20  | CLA  | B     | 601 | X         | -        | -       | -                |
| 20  | CLA  | B     | 602 | X         | -        | -       | -                |
| 20  | CLA  | B     | 603 | X         | -        | -       | -                |
| 20  | CLA  | B     | 604 | X         | -        | -       | -                |
| 20  | CLA  | B     | 605 | X         | -        | -       | -                |
| 20  | CLA  | B     | 606 | X         | -        | -       | -                |
| 20  | CLA  | B     | 607 | X         | -        | -       | -                |
| 20  | CLA  | B     | 608 | X         | -        | -       | -                |
| 20  | CLA  | B     | 609 | X         | -        | -       | -                |
| 20  | CLA  | B     | 610 | X         | -        | -       | -                |
| 20  | CLA  | B     | 611 | X         | -        | -       | -                |
| 20  | CLA  | B     | 612 | X         | -        | -       | -                |
| 20  | CLA  | B     | 613 | X         | -        | -       | -                |
| 20  | CLA  | B     | 614 | X         | -        | -       | -                |
| 20  | CLA  | B     | 615 | X         | -        | -       | -                |
| 20  | CLA  | B     | 616 | X         | -        | -       | -                |
| 20  | CLA  | C     | 501 | X         | -        | -       | -                |
| 20  | CLA  | C     | 502 | X         | -        | -       | -                |
| 20  | CLA  | C     | 503 | X         | -        | -       | -                |
| 20  | CLA  | C     | 504 | X         | -        | -       | -                |
| 20  | CLA  | C     | 505 | X         | -        | -       | -                |
| 20  | CLA  | C     | 506 | X         | -        | -       | -                |
| 20  | CLA  | C     | 507 | X         | -        | -       | -                |
| 20  | CLA  | C     | 508 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 20  | CLA  | C     | 509 | X         | -        | -       | -                |
| 20  | CLA  | C     | 510 | X         | -        | -       | -                |
| 20  | CLA  | C     | 511 | X         | -        | -       | -                |
| 20  | CLA  | C     | 512 | X         | -        | -       | -                |
| 20  | CLA  | C     | 513 | X         | -        | -       | -                |
| 20  | CLA  | D     | 401 | X         | -        | -       | -                |
| 20  | CLA  | D     | 402 | X         | -        | -       | -                |
| 20  | CLA  | D     | 404 | X         | -        | -       | -                |
| 20  | CLA  | a     | 403 | X         | -        | -       | -                |
| 20  | CLA  | a     | 404 | X         | -        | -       | -                |
| 20  | CLA  | a     | 407 | X         | -        | -       | -                |
| 20  | CLA  | b     | 603 | X         | -        | -       | -                |
| 20  | CLA  | b     | 604 | X         | -        | -       | -                |
| 20  | CLA  | b     | 605 | X         | -        | -       | -                |
| 20  | CLA  | b     | 606 | X         | -        | -       | -                |
| 20  | CLA  | b     | 607 | X         | -        | -       | -                |
| 20  | CLA  | b     | 608 | X         | -        | -       | -                |
| 20  | CLA  | b     | 609 | X         | -        | -       | -                |
| 20  | CLA  | b     | 610 | X         | -        | -       | -                |
| 20  | CLA  | b     | 611 | X         | -        | -       | -                |
| 20  | CLA  | b     | 612 | X         | -        | -       | -                |
| 20  | CLA  | b     | 613 | X         | -        | -       | -                |
| 20  | CLA  | b     | 614 | X         | -        | -       | -                |
| 20  | CLA  | b     | 615 | X         | -        | -       | -                |
| 20  | CLA  | b     | 616 | X         | -        | -       | -                |
| 20  | CLA  | b     | 617 | X         | -        | -       | -                |
| 20  | CLA  | b     | 618 | X         | -        | -       | -                |
| 20  | CLA  | c     | 501 | X         | -        | -       | -                |
| 20  | CLA  | c     | 502 | X         | -        | -       | -                |
| 20  | CLA  | c     | 503 | X         | -        | -       | -                |
| 20  | CLA  | c     | 504 | X         | -        | -       | -                |
| 20  | CLA  | c     | 505 | X         | -        | -       | -                |
| 20  | CLA  | c     | 506 | X         | -        | -       | -                |
| 20  | CLA  | c     | 507 | X         | -        | -       | -                |
| 20  | CLA  | c     | 508 | X         | -        | -       | -                |
| 20  | CLA  | c     | 509 | X         | -        | -       | -                |
| 20  | CLA  | c     | 510 | X         | -        | -       | -                |
| 20  | CLA  | c     | 511 | X         | -        | -       | -                |
| 20  | CLA  | c     | 512 | X         | -        | -       | -                |
| 20  | CLA  | c     | 513 | X         | -        | -       | -                |
| 20  | CLA  | d     | 402 | X         | -        | -       | -                |
| 20  | CLA  | d     | 403 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 20  | CLA  | d     | 404 | X         | -        | -       | -                |

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54996 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.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 334      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2626  | 1721 | 430 | 460 | 15 |         |         |       |
| 1   | a     | 334      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2622  | 1719 | 431 | 457 | 15 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment              | Reference  |
|-------|---------|----------|--------|----------------------|------------|
| A     | 279     | PRO      | ARG    | see sequence details | UNP P51765 |
| a     | 279     | PRO      | ARG    | see sequence details | UNP P51765 |

- 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       | 11      | 0     |
|     |       |          | 4012  | 2632 | 668 | 699 | 13 |         |         |       |
| 2   | b     | 495      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 3884  | 2550 | 650 | 671 | 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       | 1       | 0     |
|     |       |          | 3483  | 2280 | 582 | 608 | 13 |         |         |       |
| 3   | c     | 455      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3523  | 2305 | 591 | 614 | 13 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment              | Reference  |
|-------|---------|----------|--------|----------------------|------------|
| C     | 19      | ASN      | -      | see sequence details | UNP D0VWR7 |
| C     | 20      | SER      | -      | see sequence details | UNP D0VWR7 |

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| Chain | Residue | Modelled | Actual | Comment              | Reference  |
|-------|---------|----------|--------|----------------------|------------|
| C     | 21      | ILE      | -      | see sequence details | UNP D0VWR7 |
| C     | 22      | PHE      | -      | see sequence details | UNP D0VWR7 |
| c     | 19      | ASN      | -      | see sequence details | UNP D0VWR7 |
| c     | 20      | SER      | -      | see sequence details | UNP D0VWR7 |
| c     | 21      | ILE      | -      | see sequence details | UNP D0VWR7 |
| c     | 22      | PHE      | -      | see sequence details | UNP D0VWR7 |

- 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       | 1       | 0     |
|     |       |          | 2728  | 1808 | 446 | 462 | 12 |         |         |       |
| 4   | d     | 342      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2722  | 1803 | 445 | 462 | 12 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5   | E     | 78       | Total | C   | N   | O   | 0       | 1       | 0     |
|     |       |          | 632   | 413 | 101 | 118 |         |         |       |
| 5   | e     | 78       | Total | C   | N   | O   | 0       | 2       | 0     |
|     |       |          | 636   | 419 | 99  | 118 |         |         |       |

- 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     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 257   | 175 | 43 | 38 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | H     | 64       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 508   | 339 | 81 | 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     |
|     |       |          | 284   | 194 | 45 | 44 | 1 |         |         |       |
| 8   | i     | 36       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 300   | 203 | 49 | 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     |
|     |       |          | 272   | 183 | 41 | 47 | 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 |         |         |       |
| 10  | k     | 37       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 285   | 199 | 42 | 44 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment              | Reference  |
|-------|---------|----------|--------|----------------------|------------|
| K     | 33      | LEU      | PHE    | see sequence details | UNP P19054 |
| K     | 39      | TRP      | VAL    | see sequence details | UNP P19054 |
| k     | 33      | LEU      | PHE    | see sequence details | UNP P19054 |
| k     | 39      | TRP      | VAL    | see sequence details | UNP P19054 |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 11  | L     | 37       | Total | C   | N  | O  | 0       | 1       | 0     |
|     |       |          | 302   | 203 | 48 | 51 |         |         |       |
| 11  | l     | 37       | Total | C   | N  | O  | 0       | 1       | 0     |
|     |       |          | 296   | 200 | 45 | 51 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | M     | 33       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 259   | 175 | 37 | 46 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | m     | 34       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 264   | 178 | 38 | 47 | 1 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment              | Reference  |
|-------|---------|----------|--------|----------------------|------------|
| M     | 8       | LEU      | PHE    | see sequence details | UNP P12312 |
| m     | 8       | LEU      | PHE    | see sequence details | UNP P12312 |

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | O     | 243      | Total | C    | N   | O   | S | 0       | 6       | 0     |
|     |       |          | 1870  | 1172 | 309 | 384 | 5 |         |         |       |
| 13  | o     | 243      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1838  | 1153 | 305 | 376 | 4 |         |         |       |

- Molecule 14 is a protein called Photosystem II reaction center protein T.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14  | T     | 29       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 257   | 181 | 35 | 39 | 2 |         |         |       |
| 14  | t     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 258   | 181 | 36 | 39 | 2 |         |         |       |

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 15  | U     | 97       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 766   | 486 | 128 | 152 |  |         |         |       |
| 15  | u     | 97       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 770   | 489 | 129 | 152 |  |         |         |       |

- Molecule 16 is a protein called Cytochrome c-550.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | V     | 137      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1080  | 685 | 181 | 210 | 4 |         |         |       |
| 16  | v     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1052  | 666 | 174 | 208 | 4 |         |         |       |

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.



| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 17  | Y     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 212   | 139 | 37 | 33 | 3 |         |         |       |
| 17  | y     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 213   | 140 | 37 | 33 | 3 |         |         |       |

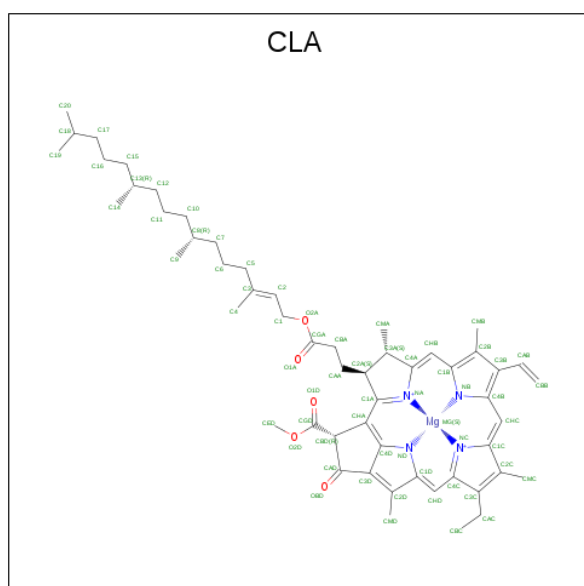
- Molecule 18 is a protein called Photosystem II reaction center protein X.

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 18  | X     | 38       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 274   | 183 | 44 | 47 |  |         |         |       |
| 18  | x     | 35       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 252   | 171 | 38 | 43 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 19  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 450   | 308 | 67 | 73 | 2 |         |         |       |
| 19  | z     | 61       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 433   | 297 | 66 | 69 | 1 |         |         |       |

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 20  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 20  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |         |
| 20  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 20  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | C     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | C     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | a     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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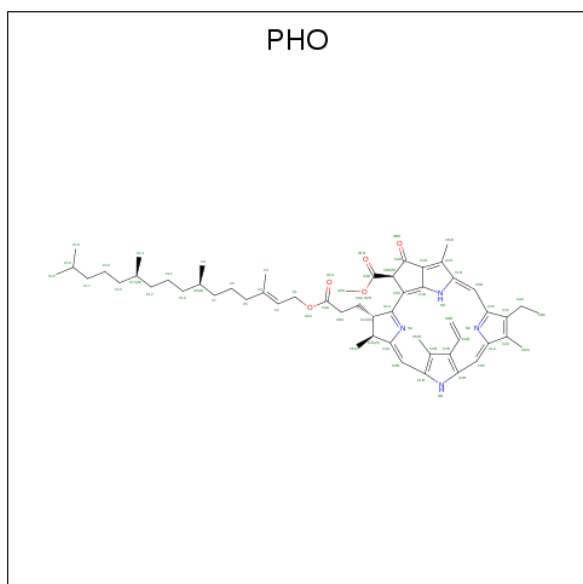
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | c     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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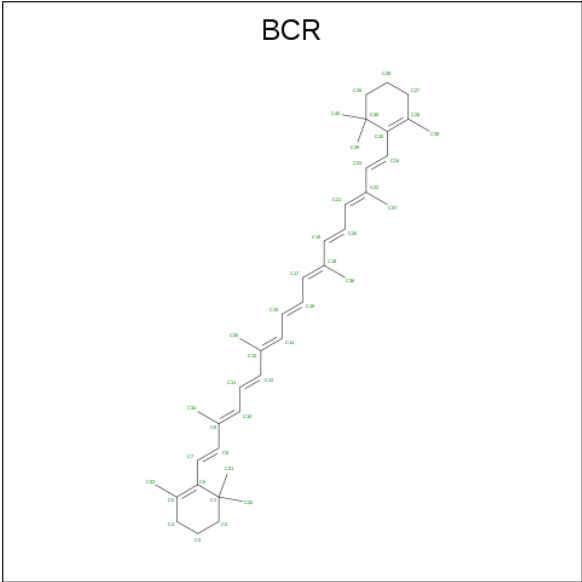
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 20  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |   |   |  | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|--|---------|---------|
| 21  | A     | 1        | Total | C  | N | O |  | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |  |         |         |
| 21  | D     | 1        | Total | C  | N | O |  | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |  |         |         |
| 21  | a     | 1        | Total | C  | N | O |  | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |  |         |         |
| 21  | a     | 1        | Total | C  | N | O |  | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |  |         |         |

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



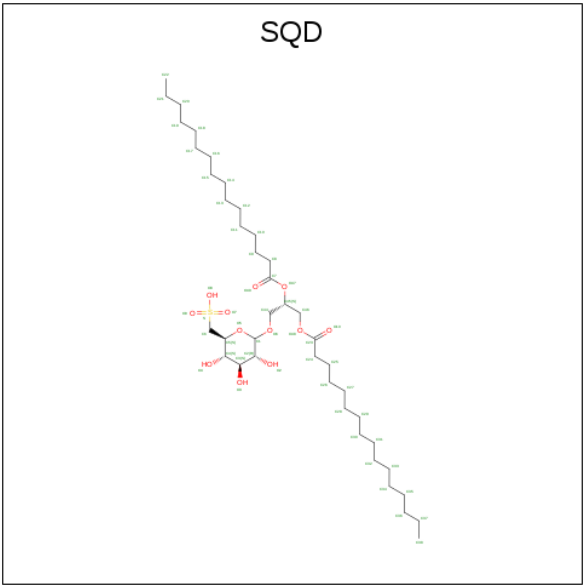
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 22  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | D     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | T     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | a     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | b     | 1        | Total C<br>40 40 | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 22  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | d     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | j     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | k     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | k     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | t     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



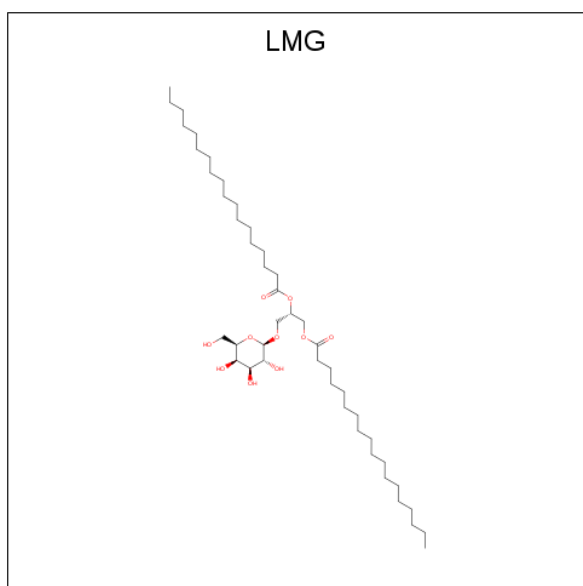
| Mol | Chain | Residues | Atoms                     | ZeroOcc | AltConf |
|-----|-------|----------|---------------------------|---------|---------|
| 23  | A     | 1        | Total C O S<br>54 41 12 1 | 0       | 0       |
| 23  | A     | 1        | Total C O S<br>54 41 12 1 | 0       | 0       |
| 23  | F     | 1        | Total C O S<br>35 23 11 1 | 0       | 0       |
| 23  | a     | 1        | Total C O S<br>54 41 12 1 | 0       | 0       |
| 23  | a     | 1        | Total C O S<br>54 41 12 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 23  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 23  | f     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 40    | 27 | 12 | 1 |         |         |
| 23  | l     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



| Mol | Chain | Residues | Atoms |    |    |  | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|--|---------|---------|
| 24  | A     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |
| 24  | B     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |
| 24  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |
| 24  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 45    | 35 | 10 |  |         |         |
| 24  | J     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 45    | 35 | 10 |  |         |         |
| 24  | a     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |
| 24  | b     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |  |         |         |
| 24  | c     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 24  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 24  | j     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 45    | 35 | 10 |         |         |

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 25  | A     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 25  | a     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

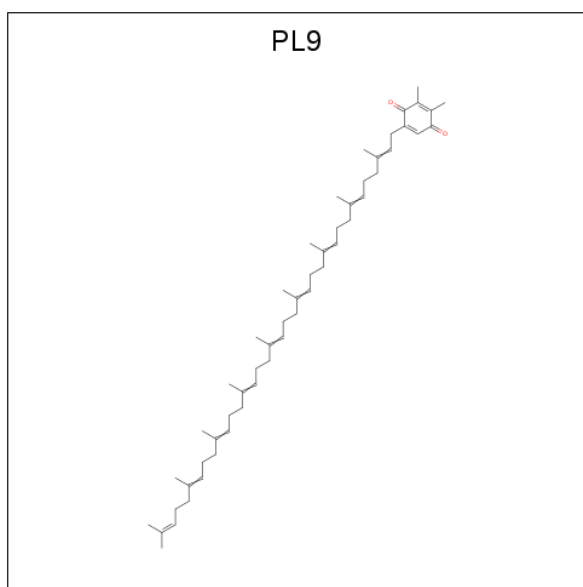
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 26  | h     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 16    | 16 |   |         |         |
| 26  | B     | 6        | Total | C  |   | 0       | 0       |
|     |       |          | 84    | 84 |   |         |         |
| 26  | c     | 3        | Total | C  | O | 0       | 0       |
|     |       |          | 48    | 43 | 5 |         |         |
| 26  | t     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 16    | 16 |   |         |         |
| 26  | X     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 16    | 16 |   |         |         |
| 26  | J     | 4        | Total | C  |   | 0       | 0       |
|     |       |          | 33    | 33 |   |         |         |
| 26  | E     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 15    | 15 |   |         |         |
| 26  | b     | 7        | Total | C  |   | 0       | 0       |
|     |       |          | 68    | 68 |   |         |         |
| 26  | A     | 2        | Total | C  | O | 0       | 0       |
|     |       |          | 40    | 35 | 5 |         |         |
| 26  | x     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 9     | 9  |   |         |         |
| 26  | M     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 12    | 12 |   |         |         |
| 26  | j     | 2        | Total | C  |   | 0       | 0       |
|     |       |          | 22    | 22 |   |         |         |
| 26  | D     | 2        | Total | C  | O | 0       | 0       |
|     |       |          | 53    | 48 | 5 |         |         |

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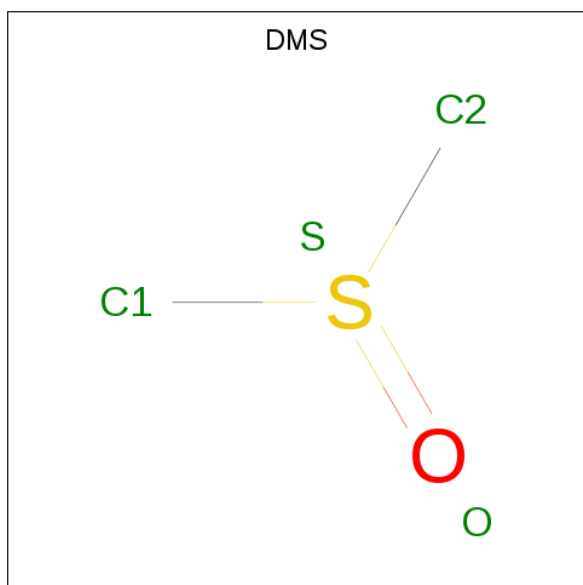
| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 26  | e     | 1        | Total C<br>7 7       | 0       | 0       |
| 26  | I     | 5        | Total C<br>61 61     | 0       | 0       |
| 26  | Z     | 1        | Total C<br>4 4       | 0       | 0       |
| 26  | a     | 3        | Total C O<br>45 40 5 | 0       | 0       |
| 26  | U     | 1        | Total C<br>14 14     | 0       | 0       |
| 26  | L     | 1        | Total C<br>14 14     | 0       | 0       |
| 26  | d     | 3        | Total C O<br>68 63 5 | 0       | 0       |
| 26  | H     | 2        | Total C<br>10 10     | 0       | 0       |
| 26  | i     | 3        | Total C<br>38 38     | 0       | 0       |
| 26  | C     | 1        | Total C O<br>34 29 5 | 0       | 0       |
| 26  | z     | 1        | Total C<br>6 6       | 0       | 0       |
| 26  | T     | 1        | Total C<br>13 13     | 0       | 0       |

- Molecule 27 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 (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 27  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 27  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 27  | a     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 27  | d     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |

- Molecule 28 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 28  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | C     | 1        | Total<br>8 | C<br>4 | O<br>2 | S<br>2 | 0       | 1       |
| 28  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 28  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | F     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | H     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | U     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | U     | 1        | Total<br>8 | C<br>4 | O<br>2 | S<br>2 | 0       | 1       |

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| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 28  | U     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | h     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | i     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | j     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 28  | u     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

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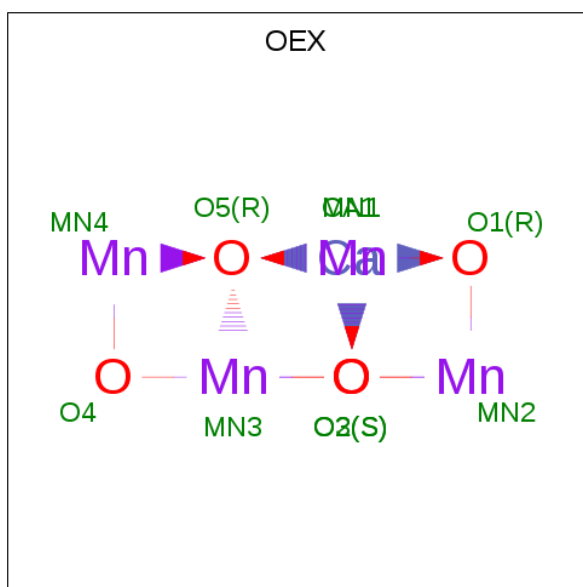
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 28  | u     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 28  | u     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 28  | v     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 28  | v     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 28  | v     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 28  | v     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 28  | v     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |
| 28  | v     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |

- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 29  | A     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 29  | a     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

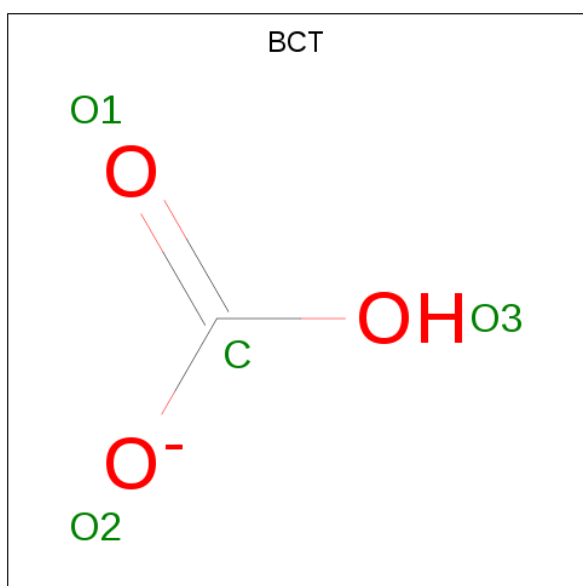
- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn<sub>4</sub>O<sub>5</sub>).





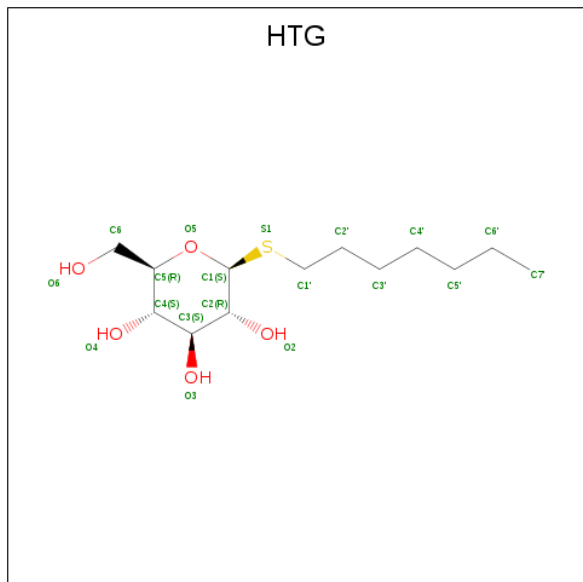
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 30  | A     | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |
| 30  | a     | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 31  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 31  | a     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 32  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | C     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | C     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | C     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | C     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | D     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | O     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 32  | V     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 13    | 7  | 5 | 1 |         |         |

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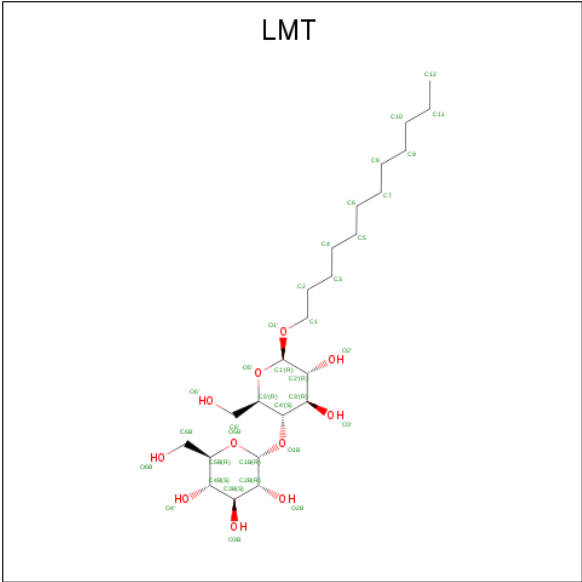
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| Mol | Chain | Residues | Atoms                    | ZeroOcc | AltConf |
|-----|-------|----------|--------------------------|---------|---------|
| 32  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 32  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 32  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 32  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 32  | c     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 32  | c     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 32  | d     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 32  | u     | 1        | Total C S<br>8 7 1       | 0       | 0       |
| 32  | v     | 1        | Total C O S<br>14 8 5 1  | 0       | 0       |

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



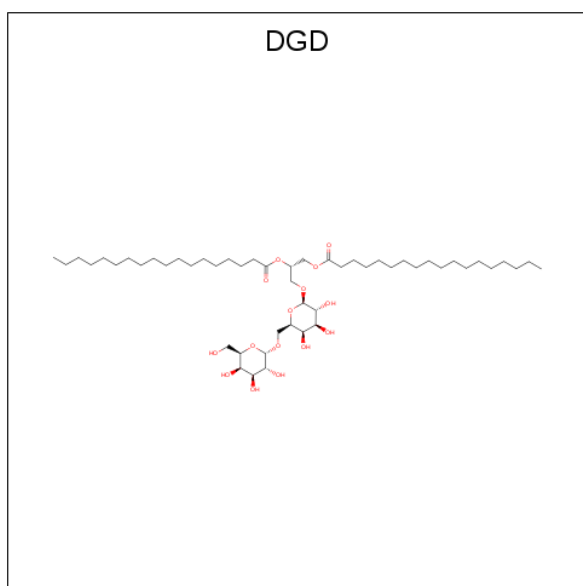
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 34  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 34  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 34  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 16    | 14 | 2  |         |         |
| 34  | E     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 34  | I     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 34  | J     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 34  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 34  | T     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 34  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 34  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 34  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 32    | 21 | 11 |         |         |
| 34  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 25    | 19 | 6  |         |         |
| 34  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 34  | f     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 34  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 34  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 34  | z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

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



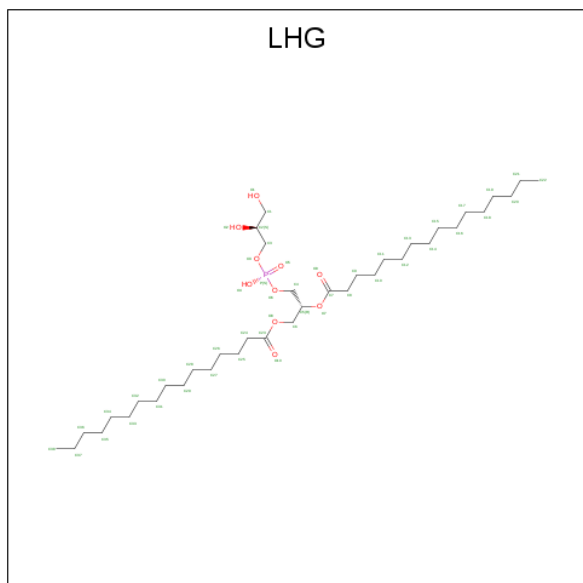
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 35  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 35  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 55    | 40 | 15 |         |         |
| 35  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 35  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 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       |
|     |       |          | 57    | 42 | 15 |         |         |
| 35  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |

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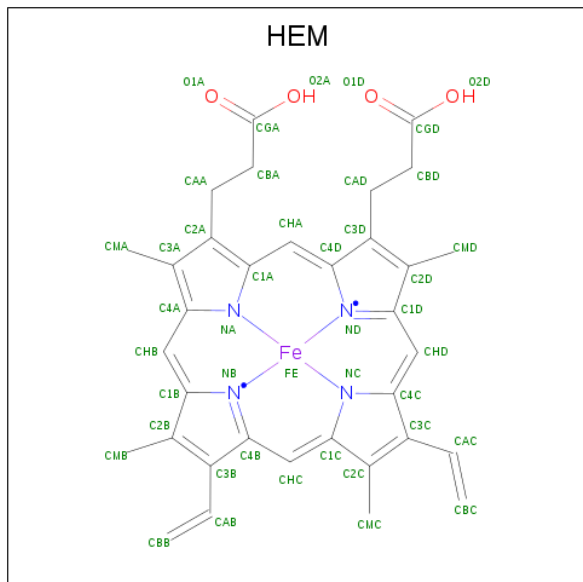
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 35  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 35  | h     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



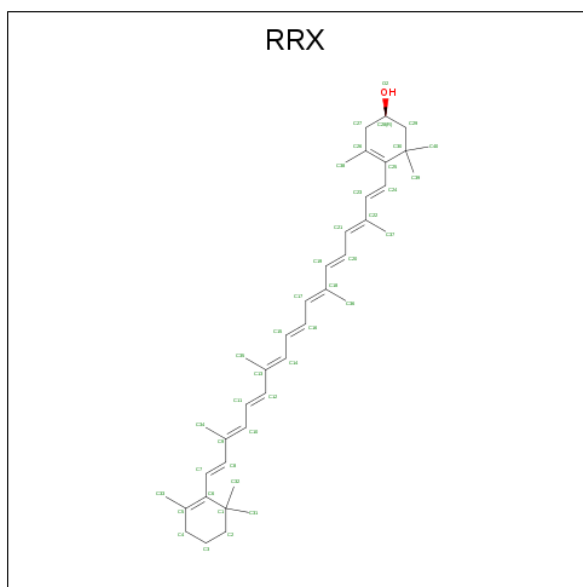
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 36  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 36  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 36  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 36  | E     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 48    | 37 | 10 | 1 |         |         |
| 36  | L     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 36  | d     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 36  | d     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 36  | d     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 36  | l     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 37  | E     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 37  | e     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula:  $C_{40}H_{56}O$ ).

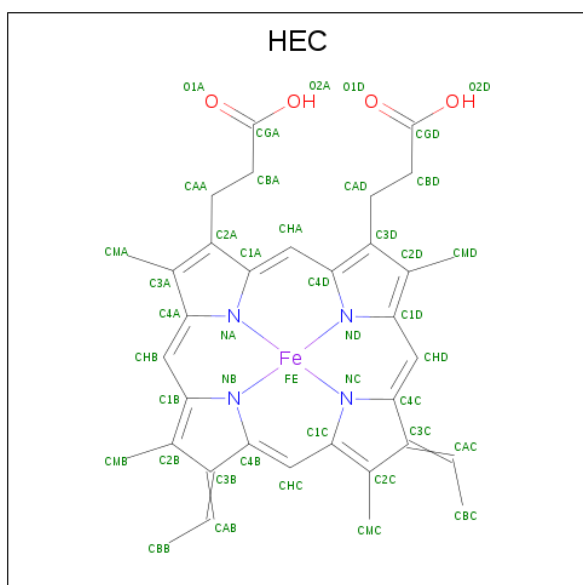


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 38  | H     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 41    | 40 | 1 |         |         |
| 38  | x     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 41    | 40 | 1 |         |         |

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 39  | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 39  | j     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 40 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 40  | V     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 40  | v     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 41 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 41  | A     | 177      | Total | O   | 0       | 5       |
|     |       |          | 182   | 182 |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 41  | B     | 447      | Total<br>473 | O<br>473 | 0       | 25      |
| 41  | C     | 317      | Total<br>324 | O<br>324 | 0       | 7       |
| 41  | D     | 175      | Total<br>180 | O<br>180 | 0       | 5       |
| 41  | E     | 62       | Total<br>66  | O<br>66  | 0       | 4       |
| 41  | F     | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 41  | H     | 62       | Total<br>65  | O<br>65  | 0       | 3       |
| 41  | I     | 16       | Total<br>16  | O<br>16  | 0       | 0       |
| 41  | J     | 23       | Total<br>23  | O<br>23  | 0       | 0       |
| 41  | K     | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 41  | L     | 19       | Total<br>21  | O<br>21  | 0       | 2       |
| 41  | M     | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 41  | O     | 263      | Total<br>273 | O<br>273 | 0       | 10      |
| 41  | T     | 19       | Total<br>20  | O<br>20  | 0       | 1       |
| 41  | U     | 133      | Total<br>136 | O<br>136 | 0       | 3       |
| 41  | V     | 177      | Total<br>183 | O<br>183 | 0       | 6       |
| 41  | Y     | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 41  | X     | 22       | Total<br>22  | O<br>22  | 0       | 0       |
| 41  | Z     | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 41  | a     | 182      | Total<br>185 | O<br>185 | 0       | 3       |
| 41  | b     | 451      | Total<br>465 | O<br>465 | 0       | 14      |
| 41  | c     | 362      | Total<br>374 | O<br>374 | 0       | 12      |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 41  | d     | 176      | Total<br>182 | O<br>182 | 0       | 6       |
| 41  | e     | 48       | Total<br>49  | O<br>49  | 0       | 1       |
| 41  | f     | 15       | Total<br>16  | O<br>16  | 0       | 1       |
| 41  | h     | 68       | Total<br>70  | O<br>70  | 0       | 2       |
| 41  | i     | 19       | Total<br>21  | O<br>21  | 0       | 2       |
| 41  | j     | 23       | Total<br>24  | O<br>24  | 0       | 1       |
| 41  | k     | 11       | Total<br>12  | O<br>12  | 0       | 1       |
| 41  | l     | 22       | Total<br>24  | O<br>24  | 0       | 2       |
| 41  | m     | 23       | Total<br>24  | O<br>24  | 0       | 1       |
| 41  | o     | 214      | Total<br>230 | O<br>230 | 0       | 15      |
| 41  | t     | 19       | Total<br>20  | O<br>20  | 0       | 1       |
| 41  | u     | 146      | Total<br>150 | O<br>150 | 0       | 4       |
| 41  | v     | 144      | Total<br>147 | O<br>147 | 0       | 3       |
| 41  | y     | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 41  | x     | 25       | Total<br>26  | O<br>26  | 0       | 1       |
| 41  | z     | 12       | Total<br>12  | O<br>12  | 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



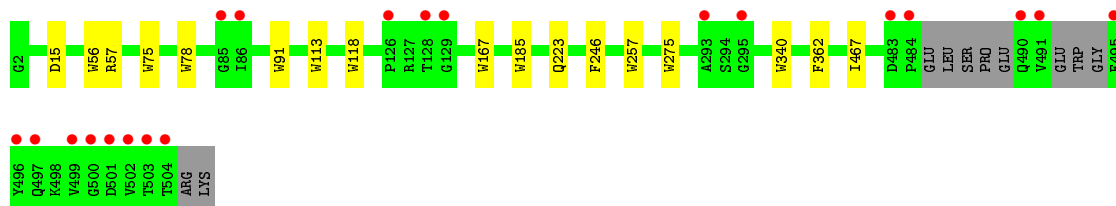
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

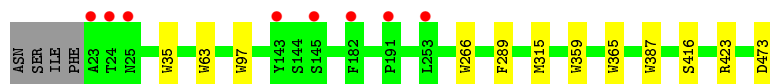


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein



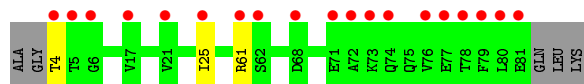
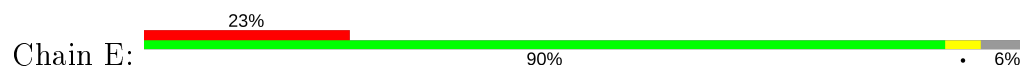
- Molecule 4: Photosystem II D2 protein



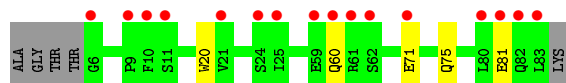
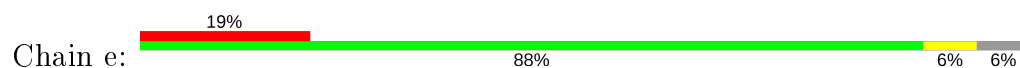
- Molecule 4: Photosystem II D2 protein



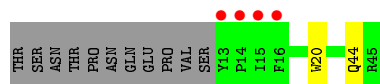
- Molecule 5: Cytochrome b559 subunit alpha



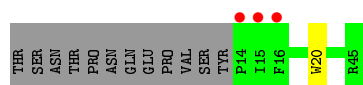
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



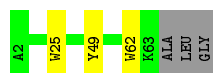
- Molecule 6: Cytochrome b559 subunit beta



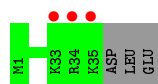
- Molecule 7: Photosystem II reaction center protein H



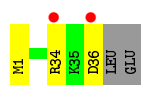
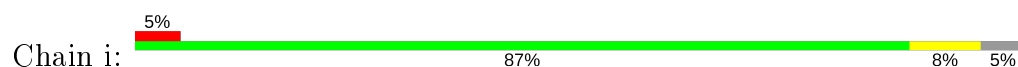
- Molecule 7: Photosystem II reaction center protein H



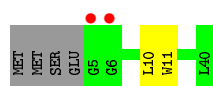
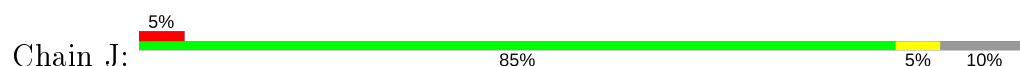
- Molecule 8: Photosystem II reaction center protein I



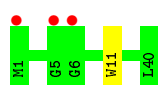
- Molecule 8: Photosystem II reaction center protein I



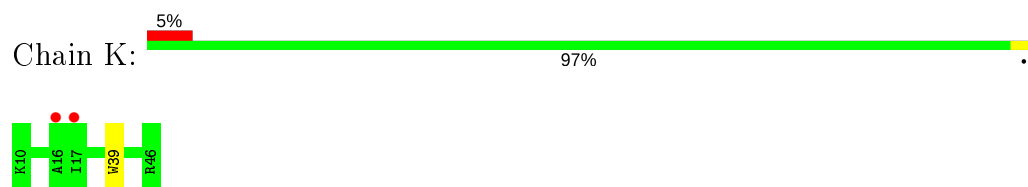
- Molecule 9: Photosystem II reaction center protein J



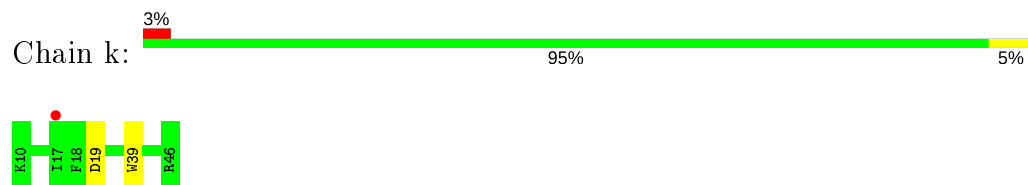
- Molecule 9: Photosystem II reaction center protein J



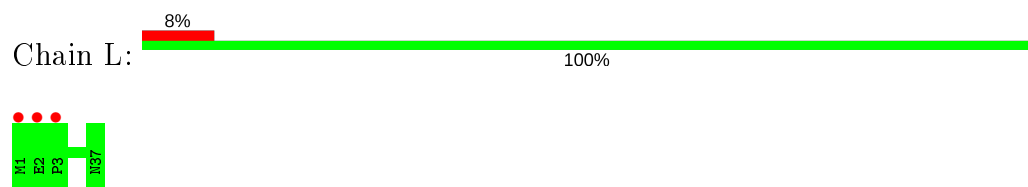
- Molecule 10: Photosystem II reaction center protein K



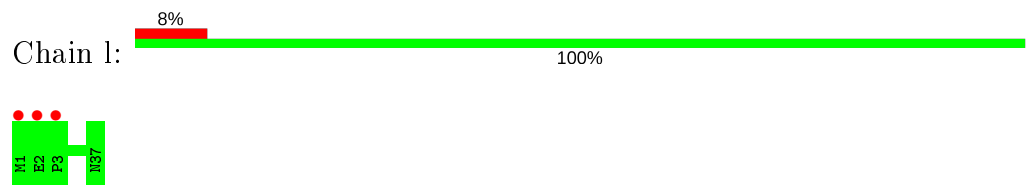
- Molecule 10: Photosystem II reaction center protein K



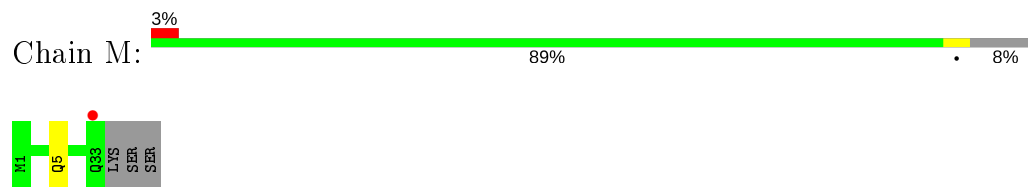
- Molecule 11: Photosystem II reaction center protein L



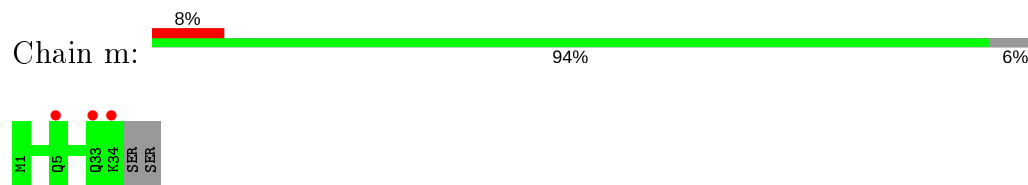
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

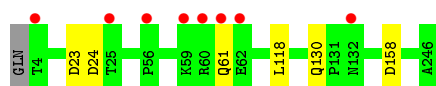


- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

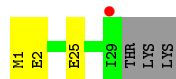
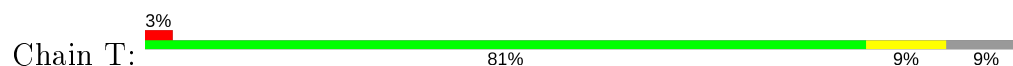




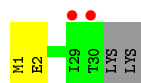
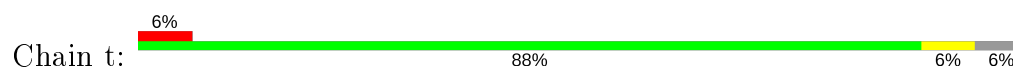
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



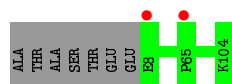
- Molecule 14: Photosystem II reaction center protein T



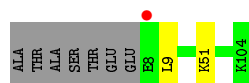
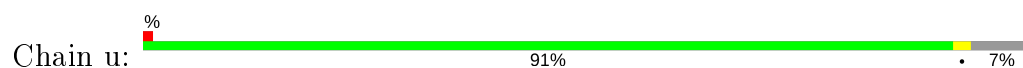
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



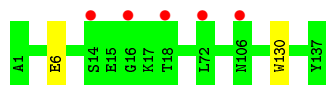
- Molecule 15: Photosystem II 12 kDa extrinsic protein



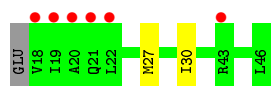
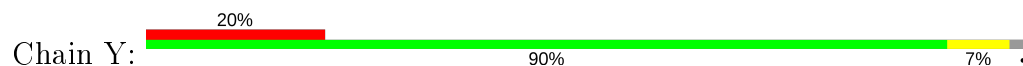
- Molecule 16: Cytochrome c-550



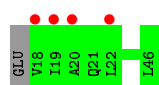
- Molecule 16: Cytochrome c-550



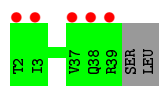
- Molecule 17: Photosystem II reaction center protein Ycf12



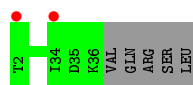
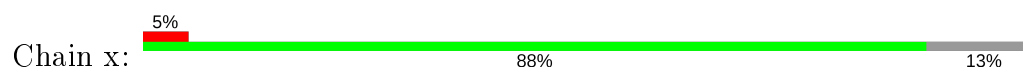
- Molecule 17: Photosystem II reaction center protein Ycf12



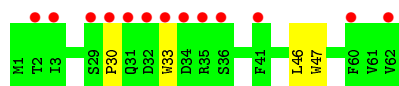
- Molecule 18: Photosystem II reaction center protein X



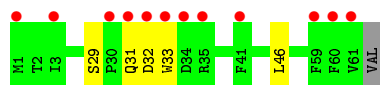
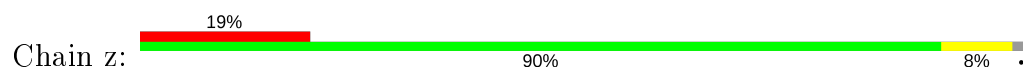
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: 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, $\alpha$ , $\beta$ , $\gamma$                | 121.47Å 228.18Å 286.42Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 19.99 – 1.85<br>19.99 – 1.85                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (19.99-1.85)<br>100.0 (19.99-1.85)                     | Depositor<br>EDS |
| $R_{merge}$   | 0.12  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.84 (at 1.85Å)   | Xtriage          |
| Refinement program  | REFMAC 5.6.0117   | Depositor        |
| R, $R_{free}$   | 0.162 , 0.201<br>0.162 , 0.200                              | Depositor<br>DCC |
| $R_{free}$ test set   | 33616 reflections (5.01%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 29.1  | Xtriage          |
| Anisotropy  | 0.087   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 70.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.97  | EDS              |
| Total number of atoms   | 54996   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 35.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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: PL9, DMS, BCT, BCR, DGD, FE2, RRX, LHG, CL, CA, CLA, HEC, HEM, FME, UNL, HTG, MG, OEX, PHO, LMT, LMG, SQD

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

| Mol | Chain | Bond lengths |                | Bond angles |               |
|-----|-------|--------------|----------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5       |
| 1   | A     | 0.95         | 5/2717 (0.2%)  | 0.77        | 1/3707 (0.0%) |
| 1   | a     | 0.93         | 4/2718 (0.1%)  | 0.79        | 2/3707 (0.1%) |
| 2   | B     | 0.90         | 9/4181 (0.2%)  | 0.77        | 1/5700 (0.0%) |
| 2   | b     | 0.91         | 11/4029 (0.3%) | 0.78        | 2/5490 (0.0%) |
| 3   | C     | 0.87         | 7/3599 (0.2%)  | 0.74        | 2/4901 (0.0%) |
| 3   | c     | 0.86         | 8/3640 (0.2%)  | 0.72        | 2/4956 (0.0%) |
| 4   | D     | 0.95         | 3/2826 (0.1%)  | 0.78        | 1/3850 (0.0%) |
| 4   | d     | 0.95         | 8/2817 (0.3%)  | 0.78        | 1/3839 (0.0%) |
| 5   | E     | 0.71         | 0/654          | 0.68        | 0/896         |
| 5   | e     | 0.69         | 1/661 (0.2%)   | 0.72        | 0/904         |
| 6   | F     | 0.79         | 1/278 (0.4%)   | 0.60        | 0/379         |
| 6   | f     | 0.81         | 1/265 (0.4%)   | 0.62        | 0/360         |
| 7   | H     | 0.84         | 2/524 (0.4%)   | 0.75        | 0/715         |
| 7   | h     | 0.86         | 2/517 (0.4%)   | 0.71        | 0/704         |
| 8   | I     | 0.63         | 0/281          | 0.69        | 0/380         |
| 8   | i     | 0.61         | 0/300          | 0.62        | 0/405         |
| 9   | J     | 0.82         | 1/257 (0.4%)   | 0.61        | 0/349         |
| 9   | j     | 0.81         | 1/278 (0.4%)   | 0.62        | 0/378         |
| 10  | K     | 0.70         | 1/303 (0.3%)   | 0.65        | 0/416         |
| 10  | k     | 0.72         | 1/295 (0.3%)   | 0.64        | 0/407         |
| 11  | L     | 0.88         | 0/312          | 0.76        | 0/425         |
| 11  | l     | 0.91         | 0/306          | 0.76        | 0/418         |
| 12  | M     | 0.70         | 0/265          | 0.74        | 0/362         |
| 12  | m     | 0.70         | 0/270          | 0.76        | 0/369         |
| 13  | O     | 0.72         | 0/1919         | 0.80        | 1/2607 (0.0%) |
| 13  | o     | 0.69         | 0/1875         | 0.77        | 2/2548 (0.1%) |
| 14  | T     | 0.78         | 0/259          | 0.77        | 0/352         |
| 14  | t     | 0.79         | 0/257          | 0.73        | 0/349         |
| 15  | U     | 0.77         | 0/777          | 0.78        | 0/1055        |
| 15  | u     | 0.76         | 0/781          | 0.77        | 0/1059        |
| 16  | V     | 0.80         | 0/1110         | 0.80        | 1/1506 (0.1%) |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 16  | v     | 0.71         | 1/1073 (0.1%)   | 0.75        | 0/1461          |
| 17  | Y     | 0.50         | 0/213           | 0.63        | 0/285           |
| 17  | y     | 0.45         | 0/214           | 0.60        | 0/286           |
| 18  | X     | 0.54         | 0/277           | 0.69        | 0/375           |
| 18  | x     | 0.57         | 0/255           | 0.66        | 0/345           |
| 19  | Z     | 0.70         | 2/461 (0.4%)    | 0.56        | 0/632           |
| 19  | z     | 0.61         | 1/444 (0.2%)    | 0.57        | 0/611           |
| All | All   | 0.85         | 70/42208 (0.2%) | 0.75        | 16/57488 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 13  | o     | 0                   | 1                   |

The worst 5 of 70 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | c     | 365 | TRP  | CD2-CE2 | 7.13 | 1.50        | 1.41     |
| 1   | A     | 343 | LEU  | C-N     | 6.74 | 1.49        | 1.34     |
| 1   | a     | 131 | TRP  | CD2-CE2 | 6.46 | 1.49        | 1.41     |
| 3   | C     | 266 | TRP  | CD2-CE2 | 6.43 | 1.49        | 1.41     |
| 2   | B     | 33  | TRP  | CD2-CE2 | 6.27 | 1.48        | 1.41     |

The worst 5 of 16 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | a     | 342 | ASP  | CB-CG-OD1 | 6.34  | 124.01      | 118.30   |
| 16  | V     | 128 | ASP  | CB-CG-OD1 | 6.14  | 123.82      | 118.30   |
| 3   | C     | 473 | ASP  | CB-CG-OD2 | 5.92  | 123.63      | 118.30   |
| 13  | o     | 152 | ARG  | NE-CZ-NH1 | -5.84 | 117.38      | 120.30   |
| 3   | c     | 423 | ARG  | NE-CZ-NH2 | -5.79 | 117.41      | 120.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 13  | o     | 60  | ARG  | Peptide |

## 5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 335/344 (97%)  | 329 (98%) | 5 (2%)  | 1 (0%)   | 41          | 26  |
| 1   | a     | 336/344 (98%)  | 330 (98%) | 5 (2%)  | 1 (0%)   | 41          | 26  |
| 2   | B     | 514/505 (102%) | 503 (98%) | 11 (2%) | 0        | 100         | 100 |
| 2   | b     | 493/505 (98%)  | 485 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 3   | C     | 450/455 (99%)  | 436 (97%) | 13 (3%) | 1 (0%)   | 47          | 33  |
| 3   | c     | 454/455 (100%) | 442 (97%) | 11 (2%) | 1 (0%)   | 47          | 33  |
| 4   | D     | 341/342 (100%) | 334 (98%) | 6 (2%)  | 1 (0%)   | 41          | 26  |
| 4   | d     | 340/342 (99%)  | 332 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 5   | E     | 77/83 (93%)    | 75 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 5   | e     | 78/83 (94%)    | 78 (100%) | 0       | 0        | 100         | 100 |
| 6   | F     | 31/44 (70%)    | 31 (100%) | 0       | 0        | 100         | 100 |
| 6   | f     | 30/44 (68%)    | 30 (100%) | 0       | 0        | 100         | 100 |
| 7   | H     | 63/65 (97%)    | 59 (94%)  | 4 (6%)  | 0        | 100         | 100 |
| 7   | h     | 61/65 (94%)    | 59 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 8   | I     | 33/38 (87%)    | 32 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 8   | i     | 35/38 (92%)    | 34 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 9   | J     | 34/40 (85%)    | 34 (100%) | 0       | 0        | 100         | 100 |
| 9   | j     | 38/40 (95%)    | 38 (100%) | 0       | 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     | 36/37 (97%)    | 36 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 11  | l     | 36/37 (97%)     | 36 (100%)  | 0        | 0        | 100         | 100 |
| 12  | M     | 32/36 (89%)     | 32 (100%)  | 0        | 0        | 100         | 100 |
| 12  | m     | 33/36 (92%)     | 32 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 13  | O     | 247/244 (101%)  | 235 (95%)  | 11 (4%)  | 1 (0%)   | 34          | 19  |
| 13  | o     | 243/244 (100%)  | 231 (95%)  | 9 (4%)   | 3 (1%)   | 13          | 3   |
| 14  | T     | 28/32 (88%)     | 28 (100%)  | 0        | 0        | 100         | 100 |
| 14  | t     | 28/32 (88%)     | 28 (100%)  | 0        | 0        | 100         | 100 |
| 15  | U     | 95/104 (91%)    | 93 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 15  | u     | 95/104 (91%)    | 92 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 16  | V     | 138/137 (101%)  | 133 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 16  | v     | 135/137 (98%)   | 131 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 17  | Y     | 27/30 (90%)     | 27 (100%)  | 0        | 0        | 100         | 100 |
| 17  | y     | 27/30 (90%)     | 27 (100%)  | 0        | 0        | 100         | 100 |
| 18  | X     | 36/40 (90%)     | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 18  | x     | 33/40 (82%)     | 32 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 19  | Z     | 60/62 (97%)     | 58 (97%)   | 1 (2%)   | 1 (2%)   | 9           | 2   |
| 19  | z     | 59/62 (95%)     | 54 (92%)   | 3 (5%)   | 2 (3%)   | 3           | 0   |
| All | All   | 5201/5350 (97%) | 5069 (98%) | 120 (2%) | 12 (0%)  | 47          | 33  |

5 of 12 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | o     | 60  | ARG  |
| 19  | z     | 32  | ASP  |
| 3   | C     | 416 | SER  |
| 4   | D     | 12  | ARG  |
| 13  | O     | 61  | 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     | 269/279 (96%)  | 268 (100%) | 1 (0%)   | 91          | 89  |
| 1   | a     | 270/279 (97%)  | 270 (100%) | 0        | 100         | 100 |
| 2   | B     | 405/403 (100%) | 401 (99%)  | 4 (1%)   | 76          | 69  |
| 2   | b     | 390/403 (97%)  | 386 (99%)  | 4 (1%)   | 76          | 69  |
| 3   | C     | 351/356 (99%)  | 349 (99%)  | 2 (1%)   | 86          | 83  |
| 3   | c     | 356/356 (100%) | 351 (99%)  | 5 (1%)   | 67          | 55  |
| 4   | D     | 277/277 (100%) | 274 (99%)  | 3 (1%)   | 73          | 65  |
| 4   | d     | 276/277 (100%) | 272 (99%)  | 4 (1%)   | 67          | 55  |
| 5   | E     | 68/72 (94%)    | 65 (96%)   | 3 (4%)   | 28          | 12  |
| 5   | e     | 68/72 (94%)    | 63 (93%)   | 5 (7%)   | 13          | 3   |
| 6   | F     | 27/38 (71%)    | 26 (96%)   | 1 (4%)   | 34          | 17  |
| 6   | f     | 26/38 (68%)    | 26 (100%)  | 0        | 100         | 100 |
| 7   | H     | 54/54 (100%)   | 52 (96%)   | 2 (4%)   | 34          | 17  |
| 7   | h     | 54/54 (100%)   | 53 (98%)   | 1 (2%)   | 57          | 43  |
| 8   | I     | 30/34 (88%)    | 30 (100%)  | 0        | 100         | 100 |
| 8   | i     | 32/34 (94%)    | 29 (91%)   | 3 (9%)   | 8           | 1   |
| 9   | J     | 23/28 (82%)    | 22 (96%)   | 1 (4%)   | 29          | 12  |
| 9   | j     | 24/28 (86%)    | 24 (100%)  | 0        | 100         | 100 |
| 10  | K     | 30/30 (100%)   | 30 (100%)  | 0        | 100         | 100 |
| 10  | k     | 28/30 (93%)    | 27 (96%)   | 1 (4%)   | 35          | 18  |
| 11  | L     | 34/35 (97%)    | 34 (100%)  | 0        | 100         | 100 |
| 11  | l     | 33/35 (94%)    | 33 (100%)  | 0        | 100         | 100 |
| 12  | M     | 30/33 (91%)    | 29 (97%)   | 1 (3%)   | 38          | 21  |
| 12  | m     | 30/33 (91%)    | 30 (100%)  | 0        | 100         | 100 |
| 13  | O     | 207/207 (100%) | 202 (98%)  | 5 (2%)   | 49          | 33  |
| 13  | o     | 199/207 (96%)  | 197 (99%)  | 2 (1%)   | 76          | 69  |
| 14  | T     | 26/28 (93%)    | 23 (88%)   | 3 (12%)  | 5           | 1   |
| 14  | t     | 26/28 (93%)    | 25 (96%)   | 1 (4%)   | 33          | 16  |
| 15  | U     | 82/89 (92%)    | 82 (100%)  | 0        | 100         | 100 |
| 15  | u     | 83/89 (93%)    | 81 (98%)   | 2 (2%)   | 49          | 33  |
| 16  | V     | 120/117 (103%) | 119 (99%)  | 1 (1%)   | 81          | 76  |
| 16  | v     | 114/117 (97%)  | 113 (99%)  | 1 (1%)   | 78          | 72  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 17  | Y     | 21/23 (91%)     | 19 (90%)   | 2 (10%)  | 8           | 1   |
| 17  | y     | 21/23 (91%)     | 21 (100%)  | 0        | 100         | 100 |
| 18  | X     | 29/33 (88%)     | 29 (100%)  | 0        | 100         | 100 |
| 18  | x     | 27/33 (82%)     | 27 (100%)  | 0        | 100         | 100 |
| 19  | Z     | 44/52 (85%)     | 43 (98%)   | 1 (2%)   | 50          | 34  |
| 19  | z     | 39/52 (75%)     | 37 (95%)   | 2 (5%)   | 24          | 9   |
| All | All   | 4223/4376 (96%) | 4162 (99%) | 61 (1%)  | 69          | 55  |

5 of 61 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | Y     | 27  | MET  |
| 3   | c     | 156 | LYS  |
| 15  | u     | 9   | LEU  |
| 17  | Y     | 30  | ILE  |
| 2   | b     | 223 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | O     | 82  | GLN  |
| 1   | a     | 315 | ASN  |
| 13  | o     | 231 | HIS  |
| 11  | L     | 6   | ASN  |
| 12  | M     | 5   | 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       | 0.69 | 0           | 7,9,11      | 1.11 | 0           |
| 14  | FME  | T     | 1   | 14   | 8,9,10       | 0.43 | 0           | 7,9,11      | 1.79 | 2 (28%)     |
| 8   | FME  | i     | 1   | 8    | 8,9,10       | 0.52 | 0           | 7,9,11      | 1.68 | 1 (14%)     |
| 14  | FME  | t     | 1   | 14   | 8,9,10       | 0.49 | 0           | 7,9,11      | 1.86 | 4 (57%)     |

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    | -       | 2/7/9/11 | -     |
| 14  | FME  | T     | 1   | 14   | -       | 3/7/9/11 | -     |
| 8   | FME  | i     | 1   | 8    | -       | 1/7/9/11 | -     |
| 14  | FME  | t     | 1   | 14   | -       | 3/7/9/11 | -     |

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | i     | 1   | FME  | C-CA-N   | 2.88  | 114.93      | 109.73   |
| 14  | T     | 1   | FME  | CE-SD-CG | 2.70  | 109.68      | 100.40   |
| 14  | T     | 1   | FME  | O-C-CA   | -2.46 | 118.34      | 124.78   |
| 14  | t     | 1   | FME  | CG-CB-CA | 2.44  | 119.72      | 112.95   |
| 14  | t     | 1   | FME  | CE-SD-CG | 2.32  | 108.38      | 100.40   |

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | I     | 1   | FME  | O1-CN-N-CA  |
| 14  | T     | 1   | FME  | N-CA-CB-CG  |
| 8   | i     | 1   | FME  | O1-CN-N-CA  |
| 14  | t     | 1   | FME  | N-CA-CB-CG  |
| 14  | T     | 1   | FME  | CB-CG-SD-CE |



There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 349 ligands modelled in this entry, 55 are unknown and 14 are monoatomic - leaving 280 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link   | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|--------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |        | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 24  | LMG  | B     | 620 | -      | 51,51,55     | 1.02 | 2 (3%)      | 59,59,63    | 1.31 | 5 (8%)      |
| 28  | DMS  | O     | 305 | -      | 3,3,3        | 2.63 | 1 (33%)     | 3,3,3       | 0.79 | 0           |
| 28  | DMS  | A     | 416 | -      | 3,3,3        | 2.68 | 1 (33%)     | 3,3,3       | 0.78 | 0           |
| 28  | DMS  | c     | 528 | -      | 3,3,3        | 2.57 | 1 (33%)     | 3,3,3       | 0.44 | 0           |
| 28  | DMS  | c     | 536 | -      | 3,3,3        | 2.84 | 1 (33%)     | 3,3,3       | 1.23 | 0           |
| 28  | DMS  | B     | 637 | -      | 3,3,3        | 2.56 | 1 (33%)     | 3,3,3       | 0.73 | 0           |
| 20  | CLA  | d     | 403 | 41     | 59,73,73     | 2.06 | 12 (20%)    | 67,113,113  | 2.07 | 16 (23%)    |
| 27  | PL9  | A     | 411 | -      | 55,55,55     | 0.83 | 3 (5%)      | 68,69,69    | 1.69 | 18 (26%)    |
| 28  | DMS  | c     | 527 | -      | 3,3,3        | 2.31 | 1 (33%)     | 3,3,3       | 0.49 | 0           |
| 35  | DGD  | C     | 518 | -      | 63,63,67     | 0.86 | 2 (3%)      | 77,77,81    | 1.04 | 3 (3%)      |
| 28  | DMS  | V     | 209 | -      | 3,3,3        | 2.61 | 1 (33%)     | 3,3,3       | 0.64 | 0           |
| 32  | HTG  | b     | 602 | -      | 19,19,19     | 1.00 | 2 (10%)     | 23,24,24    | 1.15 | 1 (4%)      |
| 20  | CLA  | B     | 604 | -      | 59,73,73     | 1.92 | 14 (23%)    | 67,113,113  | 2.20 | 17 (25%)    |
| 28  | DMS  | b     | 639 | -      | 3,3,3        | 2.81 | 1 (33%)     | 3,3,3       | 0.57 | 0           |
| 30  | OEX  | A     | 420 | 1,3,41 | 0,15,15      | 0.00 | -           | -           | -    | -           |
| 28  | DMS  | c     | 533 | -      | 3,3,3        | 2.74 | 1 (33%)     | 3,3,3       | 0.83 | 0           |
| 24  | LMG  | C     | 519 | -      | 51,51,55     | 1.03 | 2 (3%)      | 59,59,63    | 1.23 | 8 (13%)     |
| 20  | CLA  | C     | 503 | -      | 59,73,73     | 2.29 | 13 (22%)    | 67,113,113  | 1.85 | 18 (26%)    |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | DMS  | V     | 205    | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 21  | PHO  | A     | 403    | -    | 67,69,69     | 1.69 | 11 (16%) | 85,99,99    | 2.04 | 20 (23%) |
| 23  | SQD  | f     | 101    | -    | 39,40,54     | 1.37 | 3 (7%)   | 48,51,65    | 3.70 | 12 (25%) |
| 32  | HTG  | b     | 601    | -    | 19,19,19     | 1.04 | 2 (10%)  | 23,24,24    | 1.27 | 2 (8%)   |
| 20  | CLA  | c     | 504    | 41   | 59,73,73     | 2.14 | 13 (22%) | 67,113,113  | 2.30 | 15 (22%) |
| 35  | DGD  | D     | 406    | -    | 51,51,67     | 1.11 | 2 (3%)   | 59,59,81    | 1.21 | 5 (8%)   |
| 28  | DMS  | C     | 526    | -    | 3,3,3        | 2.56 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 28  | DMS  | c     | 530    | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 1.01 | 0        |
| 28  | DMS  | C     | 525[A] | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.85 | 0        |
| 22  | BCR  | b     | 620    | -    | 41,41,41     | 1.08 | 1 (2%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 34  | LMT  | B     | 626    | -    | 24,24,36     | 0.54 | 0        | 29,29,47    | 1.14 | 3 (10%)  |
| 40  | HEC  | v     | 201    | 16   | 26,50,50     | 2.25 | 8 (30%)  | 18,82,82    | 2.26 | 6 (33%)  |
| 20  | CLA  | C     | 507    | 41   | 59,73,73     | 2.42 | 16 (27%) | 67,113,113  | 2.26 | 17 (25%) |
| 20  | CLA  | c     | 502    | -    | 59,73,73     | 2.18 | 12 (20%) | 67,113,113  | 2.28 | 20 (29%) |
| 20  | CLA  | b     | 614    | -    | 59,73,73     | 1.88 | 12 (20%) | 67,113,113  | 2.14 | 18 (26%) |
| 28  | DMS  | C     | 528    | -    | 3,3,3        | 2.31 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 20  | CLA  | A     | 404    | -    | 59,73,73     | 2.00 | 14 (23%) | 67,113,113  | 1.92 | 16 (23%) |
| 24  | LMG  | A     | 407    | -    | 51,51,55     | 0.95 | 2 (3%)   | 59,59,63    | 1.06 | 3 (5%)   |
| 28  | DMS  | V     | 206    | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.67 | 0        |
| 28  | DMS  | c     | 532    | -    | 3,3,3        | 2.60 | 1 (33%)  | 3,3,3       | 0.47 | 0        |
| 20  | CLA  | D     | 402    | 41   | 59,73,73     | 1.86 | 15 (25%) | 67,113,113  | 2.14 | 16 (23%) |
| 20  | CLA  | C     | 504    | 41   | 59,73,73     | 2.14 | 11 (18%) | 67,113,113  | 2.07 | 19 (28%) |
| 20  | CLA  | a     | 404    | 41   | 54,68,73     | 1.86 | 12 (22%) | 61,107,113  | 2.13 | 18 (29%) |
| 28  | DMS  | C     | 529    | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 34  | LMT  | f     | 102    | -    | 24,24,36     | 0.79 | 1 (4%)   | 29,29,47    | 0.96 | 2 (6%)   |
| 28  | DMS  | b     | 635    | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.75 | 0        |
| 22  | BCR  | t     | 101    | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.74 | 19 (33%) |
| 20  | CLA  | D     | 404    | -    | 59,73,73     | 2.12 | 15 (25%) | 67,113,113  | 1.97 | 21 (31%) |
| 28  | DMS  | V     | 207    | -    | 3,3,3        | 2.58 | 1 (33%)  | 3,3,3       | 0.47 | 0        |
| 36  | LHG  | D     | 409    | -    | 48,48,48     | 0.95 | 2 (4%)   | 51,54,54    | 1.05 | 3 (5%)   |
| 20  | CLA  | B     | 603    | -    | 59,73,73     | 2.19 | 14 (23%) | 67,113,113  | 2.17 | 21 (31%) |
| 32  | HTG  | C     | 520    | -    | 19,19,19     | 0.89 | 1 (5%)   | 23,24,24    | 1.46 | 1 (4%)   |
| 34  | LMT  | b     | 628    | -    | 25,25,36     | 0.55 | 0        | 30,30,47    | 1.20 | 2 (6%)   |
| 27  | PL9  | D     | 412    | -    | 55,55,55     | 1.06 | 3 (5%)   | 68,69,69    | 1.51 | 12 (17%) |
| 28  | DMS  | D     | 413    | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.66 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | CLA  | c     | 513 | -    | 59,73,73     | 2.50 | 14 (23%) | 67,113,113  | 2.03 | 18 (26%) |
| 20  | CLA  | b     | 609 | 41   | 59,73,73     | 2.01 | 13 (22%) | 67,113,113  | 1.90 | 21 (31%) |
| 22  | BCR  | B     | 617 | -    | 41,41,41     | 0.98 | 0        | 56,56,56    | 1.62 | 11 (19%) |
| 28  | DMS  | b     | 634 | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.68 | 0        |
| 28  | DMS  | b     | 637 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 21  | PHO  | a     | 405 | -    | 67,69,69     | 1.81 | 12 (17%) | 85,99,99    | 1.84 | 17 (20%) |
| 20  | CLA  | C     | 511 | 3    | 59,73,73     | 2.35 | 15 (25%) | 67,113,113  | 2.29 | 19 (28%) |
| 20  | CLA  | b     | 606 | -    | 59,73,73     | 1.96 | 11 (18%) | 67,113,113  | 2.26 | 20 (29%) |
| 20  | CLA  | C     | 501 | -    | 59,73,73     | 1.98 | 14 (23%) | 67,113,113  | 1.98 | 13 (19%) |
| 28  | DMS  | d     | 415 | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 20  | CLA  | D     | 401 | -    | 59,73,73     | 1.79 | 11 (18%) | 67,113,113  | 2.22 | 20 (29%) |
| 28  | DMS  | A     | 414 | -    | 3,3,3        | 1.97 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 20  | CLA  | a     | 407 | -    | 41,55,73     | 2.30 | 9 (21%)  | 45,91,113   | 2.44 | 18 (40%) |
| 32  | HTG  | u     | 201 | -    | 7,7,19       | 0.43 | 0        | 6,6,24      | 0.70 | 0        |
| 35  | DGD  | C     | 516 | -    | 63,63,67     | 0.89 | 2 (3%)   | 77,77,81    | 1.20 | 7 (9%)   |
| 28  | DMS  | A     | 415 | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 1.01 | 0        |
| 23  | SQD  | F     | 101 | -    | 34,35,54     | 1.01 | 2 (5%)   | 42,45,65    | 1.59 | 7 (16%)  |
| 28  | DMS  | b     | 640 | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 1.38 | 1 (33%)  |
| 37  | HEM  | e     | 102 | 5,6  | 27,50,50     | 2.06 | 8 (29%)  | 17,82,82    | 2.69 | 8 (47%)  |
| 28  | DMS  | v     | 207 | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 32  | HTG  | b     | 624 | -    | 19,19,19     | 1.15 | 2 (10%)  | 23,24,24    | 1.60 | 2 (8%)   |
| 35  | DGD  | C     | 517 | -    | 56,56,67     | 0.98 | 2 (3%)   | 70,70,81    | 0.93 | 4 (5%)   |
| 28  | DMS  | B     | 644 | -    | 3,3,3        | 2.87 | 1 (33%)  | 3,3,3       | 1.26 | 0        |
| 20  | CLA  | B     | 610 | -    | 59,73,73     | 2.14 | 13 (22%) | 67,113,113  | 2.09 | 19 (28%) |
| 28  | DMS  | v     | 204 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 28  | DMS  | C     | 533 | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 28  | DMS  | d     | 414 | -    | 3,3,3        | 2.50 | 1 (33%)  | 3,3,3       | 0.24 | 0        |
| 20  | CLA  | b     | 610 | -    | 59,73,73     | 1.99 | 12 (20%) | 67,113,113  | 2.09 | 19 (28%) |
| 28  | DMS  | c     | 535 | -    | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.79 | 0        |
| 28  | DMS  | j     | 105 | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.85 | 0        |
| 35  | DGD  | H     | 102 | -    | 63,63,67     | 1.04 | 3 (4%)   | 77,77,81    | 1.27 | 8 (10%)  |
| 32  | HTG  | d     | 401 | -    | 19,19,19     | 1.08 | 1 (5%)   | 23,24,24    | 2.36 | 4 (17%)  |
| 36  | LHG  | L     | 101 | -    | 48,48,48     | 0.90 | 3 (6%)   | 51,54,54    | 0.90 | 1 (1%)   |
| 20  | CLA  | B     | 602 | 41   | 59,73,73     | 2.54 | 17 (28%) | 67,113,113  | 2.37 | 20 (29%) |
| 22  | BCR  | C     | 515 | -    | 41,41,41     | 0.97 | 0        | 56,56,56    | 1.19 | 6 (10%)  |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | DMS  | O     | 309    | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 1.16 | 0        |
| 20  | CLA  | C     | 505    | -    | 59,73,73     | 2.09 | 16 (27%) | 67,113,113  | 1.93 | 15 (22%) |
| 28  | DMS  | V     | 204    | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 22  | BCR  | A     | 405    | -    | 41,41,41     | 0.95 | 3 (7%)   | 56,56,56    | 1.27 | 7 (12%)  |
| 22  | BCR  | C     | 514    | -    | 41,41,41     | 0.85 | 0        | 56,56,56    | 1.31 | 7 (12%)  |
| 28  | DMS  | o     | 304    | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.65 | 0        |
| 20  | CLA  | B     | 605    | -    | 59,73,73     | 2.02 | 12 (20%) | 67,113,113  | 1.89 | 16 (23%) |
| 28  | DMS  | u     | 203    | -    | 3,3,3        | 2.57 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 20  | CLA  | b     | 618    | -    | 59,73,73     | 2.14 | 14 (23%) | 67,113,113  | 2.21 | 21 (31%) |
| 31  | BCT  | a     | 413    | 29   | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 22  | BCR  | j     | 102    | -    | 41,41,41     | 0.85 | 0        | 56,56,56    | 1.38 | 9 (16%)  |
| 28  | DMS  | b     | 638    | -    | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.94 | 0        |
| 28  | DMS  | B     | 643    | -    | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.74 | 0        |
| 28  | DMS  | B     | 635    | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.46 | 0        |
| 28  | DMS  | F     | 102    | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.61 | 0        |
| 32  | HTG  | B     | 621    | -    | 19,19,19     | 1.45 | 3 (15%)  | 23,24,24    | 1.79 | 6 (26%)  |
| 28  | DMS  | B     | 640    | -    | 3,3,3        | 2.55 | 1 (33%)  | 3,3,3       | 0.97 | 0        |
| 28  | DMS  | c     | 534    | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.76 | 0        |
| 28  | DMS  | H     | 103    | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.63 | 0        |
| 20  | CLA  | b     | 603    | 41   | 59,73,73     | 2.45 | 16 (27%) | 67,113,113  | 2.11 | 19 (28%) |
| 32  | HTG  | c     | 521    | -    | 19,19,19     | 0.96 | 1 (5%)   | 23,24,24    | 2.03 | 3 (13%)  |
| 35  | DGD  | c     | 515    | -    | 63,63,67     | 0.85 | 3 (4%)   | 77,77,81    | 1.19 | 8 (10%)  |
| 34  | LMT  | M     | 101    | -    | 36,36,36     | 0.64 | 0        | 47,47,47    | 0.93 | 2 (4%)   |
| 28  | DMS  | v     | 205    | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 20  | CLA  | b     | 613    | -    | 59,73,73     | 2.03 | 9 (15%)  | 67,113,113  | 1.97 | 19 (28%) |
| 28  | DMS  | U     | 903[B] | -    | 3,3,3        | 2.44 | 1 (33%)  | 3,3,3       | 0.17 | 0        |
| 28  | DMS  | B     | 642    | -    | 3,3,3        | 2.79 | 1 (33%)  | 3,3,3       | 0.75 | 0        |
| 20  | CLA  | d     | 402    | -    | 59,73,73     | 1.90 | 12 (20%) | 67,113,113  | 1.89 | 19 (28%) |
| 28  | DMS  | o     | 305    | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.77 | 0        |
| 28  | DMS  | o     | 306    | -    | 3,3,3        | 2.79 | 1 (33%)  | 3,3,3       | 1.03 | 0        |
| 28  | DMS  | c     | 529    | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 36  | LHG  | D     | 407    | -    | 48,48,48     | 0.86 | 1 (2%)   | 51,54,54    | 1.26 | 5 (9%)   |
| 34  | LMT  | Z     | 101    | -    | 36,36,36     | 0.68 | 1 (2%)   | 47,47,47    | 0.98 | 3 (6%)   |
| 20  | CLA  | A     | 401    | -    | 59,73,73     | 1.85 | 13 (22%) | 67,113,113  | 2.01 | 18 (26%) |
| 28  | DMS  | U     | 903[A] | -    | 3,3,3        | 2.56 | 1 (33%)  | 3,3,3       | 0.75 | 0        |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | BCR  | k     | 102    | -    | 41,41,41     | 0.79 | 0        | 56,56,56    | 1.29 | 9 (16%)  |
| 32  | HTG  | C     | 521    | -    | 19,19,19     | 0.98 | 2 (10%)  | 23,24,24    | 1.97 | 4 (17%)  |
| 20  | CLA  | c     | 507    | 41   | 59,73,73     | 2.31 | 13 (22%) | 67,113,113  | 2.11 | 16 (23%) |
| 20  | CLA  | B     | 606    | -    | 59,73,73     | 1.85 | 10 (16%) | 67,113,113  | 2.11 | 19 (28%) |
| 34  | LMT  | m     | 101    | -    | 36,36,36     | 0.61 | 1 (2%)   | 47,47,47    | 0.96 | 1 (2%)   |
| 20  | CLA  | b     | 608    | -    | 59,73,73     | 2.43 | 16 (27%) | 67,113,113  | 1.99 | 16 (23%) |
| 20  | CLA  | a     | 403    | -    | 59,73,73     | 1.86 | 13 (22%) | 67,113,113  | 2.05 | 18 (26%) |
| 27  | PL9  | d     | 412    | -    | 55,55,55     | 1.09 | 3 (5%)   | 68,69,69    | 1.59 | 16 (23%) |
| 28  | DMS  | v     | 203    | -    | 3,3,3        | 2.59 | 1 (33%)  | 3,3,3       | 0.85 | 0        |
| 28  | DMS  | O     | 311    | -    | 3,3,3        | 2.87 | 1 (33%)  | 3,3,3       | 0.92 | 0        |
| 23  | SQD  | a     | 409    | -    | 53,54,54     | 1.01 | 4 (7%)   | 62,65,65    | 2.11 | 11 (17%) |
| 28  | DMS  | O     | 306    | -    | 3,3,3        | 2.53 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 32  | HTG  | B     | 631    | -    | 19,19,19     | 0.94 | 2 (10%)  | 23,24,24    | 2.09 | 6 (26%)  |
| 21  | PHO  | D     | 403    | -    | 67,69,69     | 1.92 | 14 (20%) | 85,99,99    | 1.90 | 19 (22%) |
| 22  | BCR  | B     | 619    | -    | 41,41,41     | 1.06 | 1 (2%)   | 56,56,56    | 1.58 | 9 (16%)  |
| 20  | CLA  | c     | 508    | -    | 54,68,73     | 2.45 | 16 (29%) | 61,107,113  | 2.05 | 19 (31%) |
| 22  | BCR  | K     | 102    | -    | 41,41,41     | 0.92 | 1 (2%)   | 56,56,56    | 1.48 | 6 (10%)  |
| 20  | CLA  | C     | 506    | -    | 59,73,73     | 2.38 | 14 (23%) | 67,113,113  | 2.17 | 19 (28%) |
| 20  | CLA  | c     | 510    | -    | 59,73,73     | 1.77 | 13 (22%) | 67,113,113  | 1.98 | 20 (29%) |
| 20  | CLA  | C     | 509    | -    | 59,73,73     | 2.24 | 11 (18%) | 67,113,113  | 2.11 | 18 (26%) |
| 28  | DMS  | O     | 308    | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.79 | 0        |
| 20  | CLA  | B     | 601    | -    | 59,73,73     | 2.02 | 13 (22%) | 67,113,113  | 1.90 | 19 (28%) |
| 28  | DMS  | A     | 418    | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.73 | 0        |
| 20  | CLA  | b     | 617    | -    | 59,73,73     | 2.23 | 14 (23%) | 67,113,113  | 2.18 | 22 (32%) |
| 28  | DMS  | d     | 413    | -    | 3,3,3        | 2.57 | 1 (33%)  | 3,3,3       | 0.91 | 0        |
| 24  | LMG  | J     | 101    | 39   | 45,45,55     | 1.01 | 2 (4%)   | 53,53,63    | 0.98 | 3 (5%)   |
| 28  | DMS  | C     | 525[B] | -    | 3,3,3        | 2.59 | 1 (33%)  | 3,3,3       | 0.79 | 0        |
| 28  | DMS  | b     | 632    | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 35  | DGD  | d     | 416    | -    | 51,51,67     | 1.11 | 3 (5%)   | 59,59,81    | 1.20 | 6 (10%)  |
| 34  | LMT  | J     | 103    | -    | 24,24,36     | 0.65 | 1 (4%)   | 29,29,47    | 1.12 | 1 (3%)   |
| 28  | DMS  | C     | 530    | -    | 3,3,3        | 2.61 | 1 (33%)  | 3,3,3       | 1.00 | 0        |
| 34  | LMT  | c     | 523    | -    | 36,36,36     | 0.81 | 1 (2%)   | 47,47,47    | 1.60 | 6 (12%)  |
| 28  | DMS  | B     | 636    | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 22  | BCR  | D     | 405    | -    | 41,41,41     | 1.03 | 3 (7%)   | 56,56,56    | 1.73 | 13 (23%) |
| 28  | DMS  | B     | 639    | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.63 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 37  | HEM  | E     | 104 | 5,6  | 27,50,50     | 2.12 | 8 (29%)  | 17,82,82    | 2.43 | 6 (35%)  |
| 20  | CLA  | c     | 512 | -    | 59,73,73     | 2.32 | 15 (25%) | 67,113,113  | 2.09 | 16 (23%) |
| 23  | SQD  | l     | 101 | -    | 53,54,54     | 1.08 | 4 (7%)   | 62,65,65    | 1.68 | 8 (12%)  |
| 32  | HTG  | c     | 520 | -    | 19,19,19     | 0.89 | 2 (10%)  | 23,24,24    | 1.32 | 2 (8%)   |
| 34  | LMT  | a     | 418 | -    | 36,36,36     | 0.68 | 2 (5%)   | 47,47,47    | 1.54 | 6 (12%)  |
| 32  | HTG  | v     | 210 | -    | 14,14,19     | 0.62 | 0        | 18,19,24    | 2.19 | 4 (22%)  |
| 22  | BCR  | K     | 101 | -    | 41,41,41     | 0.83 | 1 (2%)   | 56,56,56    | 1.48 | 13 (23%) |
| 22  | BCR  | b     | 621 | -    | 41,41,41     | 0.80 | 1 (2%)   | 56,56,56    | 1.47 | 8 (14%)  |
| 20  | CLA  | B     | 616 | -    | 59,73,73     | 2.15 | 14 (23%) | 67,113,113  | 1.97 | 19 (28%) |
| 28  | DMS  | c     | 531 | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 32  | HTG  | B     | 622 | -    | 19,19,19     | 1.34 | 3 (15%)  | 23,24,24    | 1.93 | 6 (26%)  |
| 32  | HTG  | C     | 522 | -    | 19,19,19     | 1.06 | 2 (10%)  | 23,24,24    | 1.56 | 1 (4%)   |
| 28  | DMS  | D     | 415 | -    | 3,3,3        | 2.92 | 1 (33%)  | 3,3,3       | 0.73 | 0        |
| 20  | CLA  | c     | 505 | -    | 59,73,73     | 2.07 | 14 (23%) | 67,113,113  | 1.95 | 16 (23%) |
| 34  | LMT  | B     | 627 | -    | 15,15,36     | 0.48 | 0        | 14,14,47    | 0.67 | 0        |
| 24  | LMG  | j     | 101 | 39   | 45,45,55     | 1.00 | 3 (6%)   | 53,53,63    | 1.02 | 6 (11%)  |
| 36  | LHG  | l     | 102 | -    | 48,48,48     | 0.78 | 2 (4%)   | 51,54,54    | 1.00 | 2 (3%)   |
| 28  | DMS  | O     | 304 | -    | 3,3,3        | 2.61 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 23  | SQD  | b     | 622 | -    | 53,54,54     | 1.10 | 3 (5%)   | 62,65,65    | 1.55 | 11 (17%) |
| 24  | LMG  | C     | 524 | -    | 45,45,55     | 1.10 | 3 (6%)   | 53,53,63    | 1.36 | 5 (9%)   |
| 35  | DGD  | c     | 516 | -    | 58,58,67     | 0.86 | 2 (3%)   | 72,72,81    | 1.13 | 6 (8%)   |
| 28  | DMS  | b     | 636 | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.75 | 0        |
| 36  | LHG  | d     | 408 | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 0.99 | 5 (9%)   |
| 23  | SQD  | A     | 406 | -    | 53,54,54     | 1.00 | 3 (5%)   | 62,65,65    | 1.75 | 14 (22%) |
| 22  | BCR  | a     | 408 | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.44 | 7 (12%)  |
| 28  | DMS  | B     | 638 | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.82 | 0        |
| 32  | HTG  | C     | 534 | -    | 19,19,19     | 1.08 | 1 (5%)   | 23,24,24    | 1.47 | 5 (21%)  |
| 35  | DGD  | c     | 517 | -    | 63,63,67     | 1.04 | 4 (6%)   | 77,77,81    | 1.19 | 8 (10%)  |
| 27  | PL9  | a     | 415 | -    | 55,55,55     | 0.83 | 3 (5%)   | 68,69,69    | 1.67 | 16 (23%) |
| 32  | HTG  | b     | 625 | -    | 19,19,19     | 1.21 | 2 (10%)  | 23,24,24    | 1.34 | 4 (17%)  |
| 22  | BCR  | b     | 619 | -    | 41,41,41     | 0.95 | 0        | 56,56,56    | 1.77 | 11 (19%) |
| 34  | LMT  | z     | 102 | -    | 36,36,36     | 0.76 | 1 (2%)   | 47,47,47    | 1.49 | 8 (17%)  |
| 32  | HTG  | O     | 302 | -    | 19,19,19     | 1.29 | 2 (10%)  | 23,24,24    | 1.18 | 2 (8%)   |
| 28  | DMS  | b     | 633 | -    | 3,3,3        | 2.55 | 1 (33%)  | 3,3,3       | 1.05 | 0        |
| 28  | DMS  | u     | 202 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 1.29 | 0        |

| Mol | Type | Chain | Res | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | LMT  | b     | 627 | -      | 33,33,36     | 0.88 | 1 (3%)   | 44,44,47    | 1.80 | 10 (22%) |
| 30  | OEX  | a     | 419 | 1,3,41 | 0,15,15      | 0.00 | -        | -           |      |          |
| 28  | DMS  | U     | 902 | -      | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 1.63 | 1 (33%)  |
| 28  | DMS  | U     | 904 | -      | 3,3,3        | 2.85 | 1 (33%)  | 3,3,3       | 0.70 | 0        |
| 22  | BCR  | T     | 101 | -      | 41,41,41     | 0.81 | 0        | 56,56,56    | 1.50 | 11 (19%) |
| 28  | DMS  | V     | 208 | -      | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.74 | 0        |
| 24  | LMG  | c     | 519 | -      | 51,51,55     | 1.01 | 3 (5%)   | 59,59,63    | 1.17 | 7 (11%)  |
| 20  | CLA  | C     | 512 | -      | 49,63,73     | 2.69 | 15 (30%) | 55,101,113  | 2.35 | 17 (30%) |
| 34  | LMT  | T     | 102 | -      | 24,24,36     | 0.45 | 0        | 29,29,47    | 1.15 | 2 (6%)   |
| 21  | PHO  | a     | 406 | -      | 67,69,69     | 1.89 | 14 (20%) | 85,99,99    | 1.92 | 22 (25%) |
| 20  | CLA  | C     | 508 | -      | 54,68,73     | 2.47 | 15 (27%) | 61,107,113  | 2.01 | 18 (29%) |
| 32  | HTG  | B     | 623 | -      | 19,19,19     | 0.96 | 1 (5%)   | 23,24,24    | 1.56 | 2 (8%)   |
| 20  | CLA  | B     | 609 | -      | 59,73,73     | 1.90 | 13 (22%) | 67,113,113  | 2.07 | 20 (29%) |
| 31  | BCT  | A     | 421 | 29     | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 28  | DMS  | B     | 634 | -      | 3,3,3        | 1.94 | 1 (33%)  | 3,3,3       | 0.29 | 0        |
| 28  | DMS  | O     | 307 | -      | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.42 | 0        |
| 28  | DMS  | o     | 303 | -      | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.50 | 0        |
| 36  | LHG  | d     | 407 | -      | 48,48,48     | 0.73 | 2 (4%)   | 51,54,54    | 0.99 | 4 (7%)   |
| 20  | CLA  | b     | 607 | -      | 59,73,73     | 1.79 | 9 (15%)  | 67,113,113  | 2.13 | 17 (25%) |
| 20  | CLA  | b     | 615 | -      | 59,73,73     | 1.87 | 13 (22%) | 67,113,113  | 2.13 | 18 (26%) |
| 32  | HTG  | B     | 632 | -      | 19,19,19     | 1.02 | 1 (5%)   | 23,24,24    | 1.26 | 2 (8%)   |
| 20  | CLA  | c     | 501 | -      | 59,73,73     | 2.15 | 13 (22%) | 67,113,113  | 2.44 | 17 (25%) |
| 28  | DMS  | v     | 209 | -      | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 28  | DMS  | h     | 102 | -      | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 20  | CLA  | C     | 502 | -      | 59,73,73     | 2.26 | 14 (23%) | 67,113,113  | 2.02 | 16 (23%) |
| 20  | CLA  | B     | 611 | 41     | 59,73,73     | 2.27 | 15 (25%) | 67,113,113  | 2.18 | 16 (23%) |
| 38  | RRX  | H     | 101 | -      | 42,42,42     | 0.77 | 1 (2%)   | 57,58,58    | 1.49 | 8 (14%)  |
| 36  | LHG  | E     | 103 | -      | 46,46,48     | 1.03 | 2 (4%)   | 49,50,54    | 1.14 | 5 (10%)  |
| 28  | DMS  | v     | 206 | -      | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.66 | 0        |
| 28  | DMS  | C     | 532 | -      | 3,3,3        | 3.28 | 1 (33%)  | 3,3,3       | 1.29 | 1 (33%)  |
| 22  | BCR  | B     | 618 | -      | 41,41,41     | 1.05 | 0        | 56,56,56    | 1.26 | 7 (12%)  |
| 20  | CLA  | A     | 402 | 41     | 53,67,73     | 1.76 | 10 (18%) | 59,105,113  | 2.38 | 16 (27%) |
| 28  | DMS  | o     | 302 | -      | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.90 | 0        |
| 20  | CLA  | c     | 511 | 3      | 59,73,73     | 2.56 | 17 (28%) | 67,113,113  | 2.18 | 16 (23%) |
| 24  | LMG  | b     | 623 | -      | 49,49,55     | 0.96 | 2 (4%)   | 57,57,63    | 1.31 | 6 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | LMT  | B     | 625 | -    | 24,24,36     | 0.53 | 0        | 29,29,47    | 1.26 | 4 (13%)  |
| 38  | RRX  | x     | 101 | -    | 42,42,42     | 0.82 | 0        | 57,58,58    | 1.22 | 6 (10%)  |
| 20  | CLA  | B     | 607 | -    | 59,73,73     | 2.39 | 15 (25%) | 67,113,113  | 2.09 | 19 (28%) |
| 23  | SQD  | A     | 412 | -    | 53,54,54     | 1.02 | 3 (5%)   | 62,65,65    | 1.71 | 10 (16%) |
| 28  | DMS  | o     | 307 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.85 | 0        |
| 34  | LMT  | I     | 101 | -    | 36,36,36     | 0.65 | 1 (2%)   | 47,47,47    | 1.28 | 6 (12%)  |
| 28  | DMS  | i     | 104 | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.33 | 0        |
| 20  | CLA  | c     | 506 | -    | 59,73,73     | 1.99 | 14 (23%) | 67,113,113  | 1.91 | 19 (28%) |
| 28  | DMS  | A     | 417 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.45 | 0        |
| 34  | LMT  | m     | 102 | -    | 36,36,36     | 0.58 | 0        | 47,47,47    | 1.14 | 4 (8%)   |
| 20  | CLA  | c     | 509 | -    | 59,73,73     | 2.32 | 15 (25%) | 67,113,113  | 2.25 | 20 (29%) |
| 20  | CLA  | c     | 503 | -    | 59,73,73     | 2.42 | 16 (27%) | 67,113,113  | 2.17 | 15 (22%) |
| 20  | CLA  | b     | 605 | -    | 59,73,73     | 2.04 | 11 (18%) | 67,113,113  | 2.18 | 22 (32%) |
| 28  | DMS  | B     | 641 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 28  | DMS  | u     | 204 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.49 | 0        |
| 36  | LHG  | D     | 408 | -    | 48,48,48     | 0.82 | 2 (4%)   | 51,54,54    | 1.03 | 1 (1%)   |
| 20  | CLA  | C     | 513 | -    | 59,73,73     | 2.48 | 15 (25%) | 67,113,113  | 2.01 | 14 (20%) |
| 32  | HTG  | V     | 202 | -    | 12,13,19     | 0.76 | 1 (8%)   | 16,18,24    | 2.50 | 6 (37%)  |
| 28  | DMS  | C     | 531 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.97 | 0        |
| 28  | DMS  | D     | 416 | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 20  | CLA  | b     | 611 | -    | 59,73,73     | 2.64 | 15 (25%) | 67,113,113  | 1.70 | 15 (22%) |
| 32  | HTG  | D     | 417 | -    | 19,19,19     | 1.05 | 1 (5%)   | 23,24,24    | 1.49 | 3 (13%)  |
| 28  | DMS  | O     | 303 | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 23  | SQD  | a     | 401 | -    | 53,54,54     | 1.12 | 3 (5%)   | 62,65,65    | 1.40 | 7 (11%)  |
| 22  | BCR  | d     | 405 | -    | 41,41,41     | 0.94 | 0        | 56,56,56    | 1.84 | 11 (19%) |
| 40  | HEC  | V     | 201 | 16   | 26,50,50     | 1.99 | 8 (30%)  | 18,82,82    | 1.88 | 4 (22%)  |
| 28  | DMS  | D     | 414 | -    | 3,3,3        | 2.53 | 1 (33%)  | 3,3,3       | 0.25 | 0        |
| 28  | DMS  | B     | 645 | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.93 | 0        |
| 22  | BCR  | k     | 101 | -    | 41,41,41     | 0.94 | 0        | 56,56,56    | 1.12 | 6 (10%)  |
| 28  | DMS  | v     | 202 | -    | 3,3,3        | 2.50 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 28  | DMS  | b     | 641 | -    | 3,3,3        | 2.79 | 1 (33%)  | 3,3,3       | 1.11 | 0        |
| 28  | DMS  | b     | 631 | -    | 3,3,3        | 2.88 | 1 (33%)  | 3,3,3       | 1.24 | 0        |
| 20  | CLA  | b     | 612 | 41   | 59,73,73     | 1.97 | 13 (22%) | 67,113,113  | 1.86 | 17 (25%) |
| 28  | DMS  | v     | 208 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.66 | 0        |
| 24  | LMG  | c     | 518 | -    | 51,51,55     | 1.11 | 3 (5%)   | 59,59,63    | 1.31 | 7 (11%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | BCR  | c     | 514 | -    | 41,41,41     | 0.85 | 1 (2%)   | 56,56,56    | 1.49 | 7 (12%)  |
| 28  | DMS  | O     | 310 | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.70 | 0        |
| 20  | CLA  | B     | 608 | 41   | 59,73,73     | 1.95 | 12 (20%) | 67,113,113  | 1.92 | 14 (20%) |
| 20  | CLA  | B     | 614 | -    | 59,73,73     | 1.96 | 16 (27%) | 67,113,113  | 1.90 | 17 (25%) |
| 28  | DMS  | C     | 527 | -    | 3,3,3        | 2.56 | 1 (33%)  | 3,3,3       | 0.49 | 0        |
| 24  | LMG  | a     | 410 | -    | 51,51,55     | 0.89 | 2 (3%)   | 59,59,63    | 1.08 | 2 (3%)   |
| 36  | LHG  | d     | 406 | -    | 48,48,48     | 0.94 | 2 (4%)   | 51,54,54    | 1.16 | 5 (9%)   |
| 20  | CLA  | b     | 604 | -    | 59,73,73     | 1.92 | 14 (23%) | 67,113,113  | 2.16 | 25 (37%) |
| 20  | CLA  | b     | 616 | -    | 59,73,73     | 2.03 | 13 (22%) | 67,113,113  | 2.22 | 23 (34%) |
| 20  | CLA  | C     | 510 | -    | 59,73,73     | 2.13 | 13 (22%) | 67,113,113  | 2.07 | 17 (25%) |
| 20  | CLA  | d     | 404 | -    | 59,73,73     | 1.98 | 14 (23%) | 67,113,113  | 1.93 | 17 (25%) |
| 28  | DMS  | o     | 308 | -    | 3,3,3        | 2.85 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 34  | LMT  | E     | 101 | -    | 24,24,36     | 0.62 | 1 (4%)   | 29,29,47    | 1.01 | 3 (10%)  |
| 20  | CLA  | B     | 613 | -    | 59,73,73     | 2.07 | 12 (20%) | 67,113,113  | 2.08 | 18 (26%) |
| 20  | CLA  | B     | 612 | -    | 59,73,73     | 1.86 | 13 (22%) | 67,113,113  | 2.10 | 19 (28%) |
| 35  | DGD  | h     | 101 | -    | 63,63,67     | 0.98 | 3 (4%)   | 77,77,81    | 1.04 | 4 (5%)   |
| 20  | CLA  | B     | 615 | -    | 59,73,73     | 1.97 | 13 (22%) | 67,113,113  | 2.13 | 19 (28%) |

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  | LMG  | B     | 620 | -    | -         | 19/46/66/70  | 0/1/1/1 |
| 22  | BCR  | k     | 101 | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 20  | CLA  | d     | 403 | 41   | 1/1/20/25 | 5/37/135/135 | -       |
| 27  | PL9  | A     | 411 | -    | -         | 10/53/73/73  | 0/1/1/1 |
| 20  | CLA  | a     | 404 | 41   | 2/2/19/25 | 6/31/129/135 | -       |
| 35  | DGD  | C     | 518 | -    | -         | 12/51/91/95  | 0/2/2/2 |
| 32  | HTG  | b     | 602 | -    | -         | 3/10/30/30   | 0/1/1/1 |
| 20  | CLA  | B     | 604 | -    | 3/3/20/25 | 3/37/135/135 | -       |
| 24  | LMG  | C     | 519 | -    | -         | 19/46/66/70  | 0/1/1/1 |
| 20  | CLA  | C     | 503 | -    | 2/2/20/25 | 4/37/135/135 | -       |
| 21  | PHO  | A     | 403 | -    | -         | 2/53/103/103 | 0/5/6/6 |
| 23  | SQD  | f     | 101 | -    | -         | 16/34/54/69  | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32  | HTG  | b     | 601 | -    | -         | 2/10/30/30    | 0/1/1/1 |
| 20  | CLA  | c     | 504 | 41   | 3/3/20/25 | 5/37/135/135  | -       |
| 35  | DGD  | D     | 406 | -    | -         | 26/46/66/95   | 0/1/1/2 |
| 34  | LMT  | Z     | 101 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 22  | BCR  | b     | 620 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 34  | LMT  | B     | 626 | -    | -         | 7/15/35/61    | 0/1/1/2 |
| 40  | HEC  | v     | 201 | 16   | -         | 0/6/54/54     | -       |
| 20  | CLA  | c     | 502 | -    | 2/2/20/25 | 6/37/135/135  | -       |
| 20  | CLA  | b     | 606 | -    | 3/3/20/25 | 3/37/135/135  | -       |
| 35  | DGD  | H     | 102 | -    | -         | 15/51/91/95   | 0/2/2/2 |
| 24  | LMG  | A     | 407 | -    | -         | 28/46/66/70   | 0/1/1/1 |
| 20  | CLA  | D     | 402 | 41   | 1/1/20/25 | 5/37/135/135  | -       |
| 34  | LMT  | f     | 102 | -    | -         | 8/15/35/61    | 0/1/1/2 |
| 22  | BCR  | t     | 101 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 20  | CLA  | D     | 404 | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 36  | LHG  | D     | 409 | -    | -         | 14/53/53/53   | -       |
| 34  | LMT  | m     | 102 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 32  | HTG  | C     | 520 | -    | -         | 4/10/30/30    | 0/1/1/1 |
| 34  | LMT  | b     | 628 | -    | -         | 9/17/37/61    | 0/1/1/2 |
| 27  | PL9  | D     | 412 | -    | -         | 3/53/73/73    | 0/1/1/1 |
| 20  | CLA  | c     | 513 | -    | 1/1/20/25 | 14/37/135/135 | -       |
| 20  | CLA  | b     | 609 | 41   | 3/3/20/25 | 2/37/135/135  | -       |
| 22  | BCR  | B     | 617 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 27  | PL9  | a     | 415 | -    | -         | 11/53/73/73   | 0/1/1/1 |
| 21  | PHO  | a     | 405 | -    | -         | 4/53/103/103  | 0/5/6/6 |
| 20  | CLA  | C     | 501 | -    | 3/3/20/25 | 3/37/135/135  | -       |
| 36  | LHG  | l     | 102 | -    | -         | 19/53/53/53   | -       |
| 20  | CLA  | D     | 401 | -    | 1/1/20/25 | 7/37/135/135  | -       |
| 20  | CLA  | a     | 407 | -    | 1/1/16/25 | 0/16/114/135  | -       |
| 32  | HTG  | u     | 201 | -    | -         | 1/5/5/30      | -       |
| 35  | DGD  | C     | 516 | -    | -         | 18/51/91/95   | 0/2/2/2 |
| 23  | SQD  | F     | 101 | -    | -         | 17/28/48/69   | 0/1/1/1 |
| 20  | CLA  | B     | 606 | -    | 3/3/20/25 | 4/37/135/135  | -       |
| 35  | DGD  | C     | 517 | -    | -         | 14/44/84/95   | 0/2/2/2 |
| 23  | SQD  | b     | 622 | -    | -         | 23/49/69/69   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 35  | DGD  | h     | 101 | -    | -         | 15/51/91/95   | 0/2/2/2 |
| 20  | CLA  | b     | 610 | -    | 1/1/20/25 | 1/37/135/135  | -       |
| 32  | HTG  | d     | 401 | -    | -         | 9/10/30/30    | 0/1/1/1 |
| 36  | LHG  | L     | 101 | -    | -         | 17/53/53/53   | -       |
| 20  | CLA  | B     | 602 | 41   | 2/2/20/25 | 21/37/135/135 | -       |
| 22  | BCR  | C     | 515 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 20  | CLA  | C     | 505 | -    | 2/2/20/25 | 1/37/135/135  | -       |
| 20  | CLA  | B     | 615 | -    | 3/3/20/25 | 10/37/135/135 | -       |
| 22  | BCR  | A     | 405 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 22  | BCR  | C     | 514 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 20  | CLA  | B     | 605 | -    | 3/3/20/25 | 8/37/135/135  | -       |
| 22  | BCR  | j     | 102 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 20  | CLA  | b     | 614 | -    | 3/3/20/25 | 4/37/135/135  | -       |
| 22  | BCR  | K     | 101 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 32  | HTG  | B     | 622 | -    | -         | 5/10/30/30    | 0/1/1/1 |
| 32  | HTG  | B     | 621 | -    | -         | 5/10/30/30    | 0/1/1/1 |
| 20  | CLA  | b     | 603 | 41   | 3/3/20/25 | 18/37/135/135 | -       |
| 23  | SQD  | l     | 101 | -    | -         | 28/49/69/69   | 0/1/1/1 |
| 35  | DGD  | c     | 515 | -    | -         | 18/51/91/95   | 0/2/2/2 |
| 34  | LMT  | M     | 101 | -    | -         | 1/21/61/61    | 0/2/2/2 |
| 20  | CLA  | b     | 613 | -    | 1/1/20/25 | 7/37/135/135  | -       |
| 20  | CLA  | b     | 608 | -    | 3/3/20/25 | 9/37/135/135  | -       |
| 20  | CLA  | d     | 402 | -    | 2/2/20/25 | 3/37/135/135  | -       |
| 36  | LHG  | D     | 407 | -    | -         | 9/53/53/53    | -       |
| 20  | CLA  | A     | 404 | -    | 1/1/20/25 | 10/37/135/135 | -       |
| 20  | CLA  | A     | 401 | -    | 3/3/20/25 | 4/37/135/135  | -       |
| 32  | HTG  | c     | 521 | -    | -         | 5/10/30/30    | 0/1/1/1 |
| 22  | BCR  | k     | 102 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 32  | HTG  | C     | 521 | -    | -         | 6/10/30/30    | 0/1/1/1 |
| 20  | CLA  | c     | 507 | 41   | 3/3/20/25 | 6/37/135/135  | -       |
| 32  | HTG  | B     | 623 | -    | -         | 6/10/30/30    | 0/1/1/1 |
| 34  | LMT  | m     | 101 | -    | -         | 15/21/61/61   | 0/2/2/2 |
| 20  | CLA  | a     | 403 | -    | 3/3/20/25 | 4/37/135/135  | -       |
| 20  | CLA  | B     | 608 | 41   | 3/3/20/25 | 1/37/135/135  | -       |
| 23  | SQD  | a     | 409 | -    | -         | 20/49/69/69   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32  | HTG  | B     | 631 | -    | -         | 5/10/30/30    | 0/1/1/1 |
| 21  | PHO  | D     | 403 | -    | -         | 5/53/103/103  | 0/5/6/6 |
| 22  | BCR  | B     | 619 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 20  | CLA  | c     | 508 | -    | 2/2/19/25 | 2/31/129/135  | -       |
| 22  | BCR  | K     | 102 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 20  | CLA  | C     | 506 | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 20  | CLA  | c     | 510 | -    | 3/3/20/25 | 3/37/135/135  | -       |
| 20  | CLA  | C     | 509 | -    | 3/3/20/25 | 8/37/135/135  | -       |
| 20  | CLA  | B     | 601 | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 20  | CLA  | b     | 617 | -    | 3/3/20/25 | 8/37/135/135  | -       |
| 37  | HEM  | e     | 102 | 5,6  | -         | 0/6/54/54     | -       |
| 24  | LMG  | J     | 101 | 39   | -         | 9/40/60/70    | 0/1/1/1 |
| 35  | DGD  | d     | 416 | -    | -         | 30/46/66/95   | 0/1/1/2 |
| 34  | LMT  | J     | 103 | -    | -         | 7/15/35/61    | 0/1/1/2 |
| 34  | LMT  | c     | 523 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 22  | BCR  | D     | 405 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 37  | HEM  | E     | 104 | 5,6  | -         | 0/6/54/54     | -       |
| 20  | CLA  | c     | 512 | -    | 3/3/20/25 | 7/37/135/135  | -       |
| 32  | HTG  | c     | 520 | -    | -         | 5/10/30/30    | 0/1/1/1 |
| 34  | LMT  | a     | 418 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 32  | HTG  | v     | 210 | -    | -         | 3/5/25/30     | 0/1/1/1 |
| 22  | BCR  | b     | 621 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 20  | CLA  | B     | 616 | -    | 3/3/20/25 | 5/37/135/135  | -       |
| 20  | CLA  | A     | 402 | 41   | 2/2/18/25 | 3/30/128/135  | -       |
| 32  | HTG  | C     | 522 | -    | -         | 4/10/30/30    | 0/1/1/1 |
| 20  | CLA  | c     | 505 | -    | 2/2/20/25 | 1/37/135/135  | -       |
| 34  | LMT  | B     | 627 | -    | -         | 7/13/13/61    | -       |
| 20  | CLA  | C     | 511 | 3    | 2/2/20/25 | 0/37/135/135  | -       |
| 24  | LMG  | C     | 524 | -    | -         | 22/40/60/70   | 0/1/1/1 |
| 35  | DGD  | c     | 516 | -    | -         | 13/46/86/95   | 0/2/2/2 |
| 36  | LHG  | d     | 408 | -    | -         | 14/53/53/53   | -       |
| 23  | SQD  | A     | 406 | -    | -         | 21/49/69/69   | 0/1/1/1 |
| 22  | BCR  | a     | 408 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 32  | HTG  | C     | 534 | -    | -         | 6/10/30/30    | 0/1/1/1 |
| 35  | DGD  | c     | 517 | -    | -         | 14/51/91/95   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 20  | CLA  | B     | 611 | 41   | 3/3/20/25 | 4/37/135/135  | -       |
| 32  | HTG  | b     | 625 | -    | -         | 4/10/30/30    | 0/1/1/1 |
| 22  | BCR  | b     | 619 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 34  | LMT  | z     | 102 | -    | -         | 13/21/61/61   | 0/2/2/2 |
| 20  | CLA  | B     | 603 | -    | 3/3/20/25 | 3/37/135/135  | -       |
| 34  | LMT  | b     | 627 | -    | -         | 10/18/58/61   | 0/2/2/2 |
| 21  | PHO  | a     | 406 | -    | -         | 4/53/103/103  | 0/5/6/6 |
| 22  | BCR  | T     | 101 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 27  | PL9  | d     | 412 | -    | -         | 3/53/73/73    | 0/1/1/1 |
| 24  | LMG  | c     | 519 | -    | -         | 26/46/66/70   | 0/1/1/1 |
| 34  | LMT  | T     | 102 | -    | -         | 11/15/35/61   | 0/1/1/2 |
| 20  | CLA  | C     | 504 | 41   | 2/2/20/25 | 11/37/135/135 | -       |
| 20  | CLA  | B     | 609 | -    | 1/1/20/25 | 1/37/135/135  | -       |
| 36  | LHG  | d     | 407 | -    | -         | 11/53/53/53   | -       |
| 20  | CLA  | b     | 607 | -    | 3/3/20/25 | 4/37/135/135  | -       |
| 20  | CLA  | b     | 615 | -    | 3/3/20/25 | 6/37/135/135  | -       |
| 32  | HTG  | B     | 632 | -    | -         | 2/10/30/30    | 0/1/1/1 |
| 20  | CLA  | c     | 501 | -    | 3/3/20/25 | 3/37/135/135  | -       |
| 32  | HTG  | b     | 624 | -    | -         | 0/10/30/30    | 0/1/1/1 |
| 22  | BCR  | c     | 514 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 20  | CLA  | C     | 502 | -    | 1/1/20/25 | 5/37/135/135  | -       |
| 24  | LMG  | b     | 623 | -    | -         | 14/44/64/70   | 0/1/1/1 |
| 38  | RRX  | H     | 101 | -    | -         | 1/29/65/65    | 0/2/2/2 |
| 36  | LHG  | E     | 103 | -    | -         | 27/45/45/53   | -       |
| 22  | BCR  | B     | 618 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 20  | CLA  | b     | 616 | -    | 3/3/20/25 | 18/37/135/135 | -       |
| 20  | CLA  | c     | 511 | 3    | 3/3/20/25 | 0/37/135/135  | -       |
| 34  | LMT  | B     | 625 | -    | -         | 4/15/35/61    | 0/1/1/2 |
| 38  | RRX  | x     | 101 | -    | -         | 3/29/65/65    | 0/2/2/2 |
| 20  | CLA  | B     | 607 | -    | 3/3/20/25 | 11/37/135/135 | -       |
| 23  | SQD  | A     | 412 | -    | -         | 24/49/69/69   | 0/1/1/1 |
| 20  | CLA  | c     | 506 | -    | 2/2/20/25 | 10/37/135/135 | -       |
| 20  | CLA  | B     | 610 | -    | 2/2/20/25 | 1/37/135/135  | -       |
| 20  | CLA  | C     | 507 | 41   | 3/3/20/25 | 11/37/135/135 | -       |
| 20  | CLA  | c     | 509 | -    | 3/3/20/25 | 10/37/135/135 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 20  | CLA  | c     | 503 | -    | 1/1/20/25 | 3/37/135/135  | -       |
| 20  | CLA  | b     | 605 | -    | 3/3/20/25 | 1/37/135/135  | -       |
| 36  | LHG  | D     | 408 | -    | -         | 10/53/53/53   | -       |
| 20  | CLA  | C     | 513 | -    | 1/1/20/25 | 10/37/135/135 | -       |
| 32  | HTG  | V     | 202 | -    | -         | 1/4/24/30     | 0/1/1/1 |
| 20  | CLA  | b     | 611 | -    | 2/2/20/25 | 0/37/135/135  | -       |
| 32  | HTG  | D     | 417 | -    | -         | 5/10/30/30    | 0/1/1/1 |
| 20  | CLA  | b     | 618 | -    | 3/3/20/25 | 17/37/135/135 | -       |
| 23  | SQD  | a     | 401 | -    | -         | 20/49/69/69   | 0/1/1/1 |
| 22  | BCR  | d     | 405 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 40  | HEC  | V     | 201 | 16   | -         | 0/6/54/54     | -       |
| 20  | CLA  | B     | 614 | -    | 3/3/20/25 | 6/37/135/135  | -       |
| 20  | CLA  | b     | 612 | 41   | 3/3/20/25 | 5/37/135/135  | -       |
| 24  | LMG  | c     | 518 | -    | -         | 8/46/66/70    | 0/1/1/1 |
| 24  | LMG  | j     | 101 | 39   | -         | 15/40/60/70   | 0/1/1/1 |
| 32  | HTG  | O     | 302 | -    | -         | 5/10/30/30    | 0/1/1/1 |
| 20  | CLA  | C     | 512 | -    | 3/3/18/25 | 6/25/123/135  | -       |
| 20  | CLA  | C     | 508 | -    | 3/3/19/25 | 6/31/129/135  | -       |
| 24  | LMG  | a     | 410 | -    | -         | 18/46/66/70   | 0/1/1/1 |
| 36  | LHG  | d     | 406 | -    | -         | 11/53/53/53   | -       |
| 20  | CLA  | b     | 604 | -    | 3/3/20/25 | 7/37/135/135  | -       |
| 34  | LMT  | I     | 101 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 20  | CLA  | C     | 510 | -    | 3/3/20/25 | 2/37/135/135  | -       |
| 20  | CLA  | d     | 404 | -    | 1/1/20/25 | 8/37/135/135  | -       |
| 34  | LMT  | E     | 101 | -    | -         | 8/15/35/61    | 0/1/1/2 |
| 20  | CLA  | B     | 613 | -    | 3/3/20/25 | 0/37/135/135  | -       |
| 20  | CLA  | B     | 612 | -    | 3/3/20/25 | 3/37/135/135  | -       |

The worst 5 of 1283 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 20  | b     | 611 | CLA  | MG-NA | 12.91 | 2.36        | 2.06     |
| 20  | c     | 513 | CLA  | MG-NA | 12.66 | 2.36        | 2.06     |
| 20  | B     | 602 | CLA  | MG-NA | 11.66 | 2.34        | 2.06     |
| 20  | c     | 507 | CLA  | MG-NA | 10.98 | 2.32        | 2.06     |
| 20  | c     | 511 | CLA  | MG-NC | 10.70 | 2.31        | 2.06     |

The worst 5 of 1978 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 23  | f     | 101 | SQD  | O9-S-C6    | -14.05 | 90.24       | 106.94   |
| 20  | c     | 504 | CLA  | C4A-NA-C1A | 12.19  | 112.19      | 106.71   |
| 20  | C     | 511 | CLA  | C4A-NA-C1A | 11.76  | 111.99      | 106.71   |
| 20  | c     | 501 | CLA  | C4A-NA-C1A | 11.42  | 111.84      | 106.71   |
| 20  | c     | 509 | CLA  | C4A-NA-C1A | 10.78  | 111.55      | 106.71   |

5 of 170 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 20  | c     | 502 | CLA  | NC   |
| 20  | c     | 502 | CLA  | NA   |
| 20  | b     | 614 | CLA  | NA   |
| 20  | b     | 614 | CLA  | NC   |
| 20  | b     | 614 | CLA  | ND   |

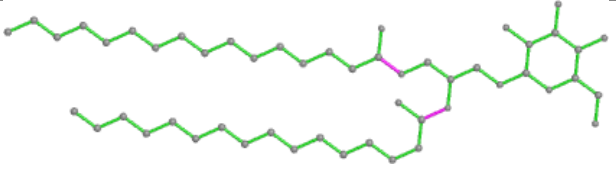
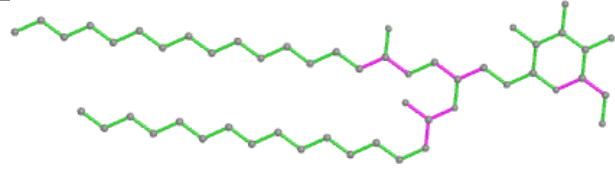
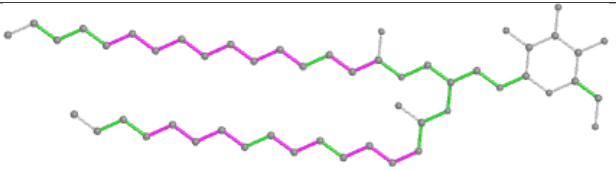
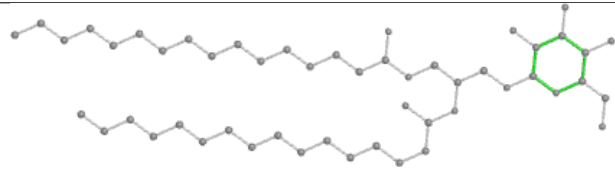
5 of 1383 torsion outliers are listed below:

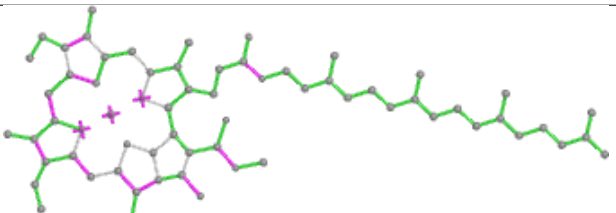
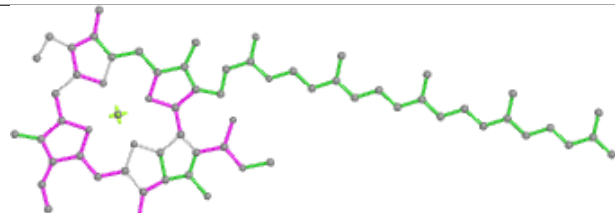
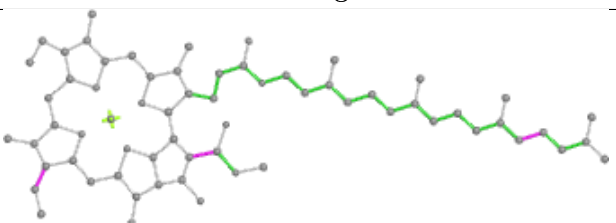
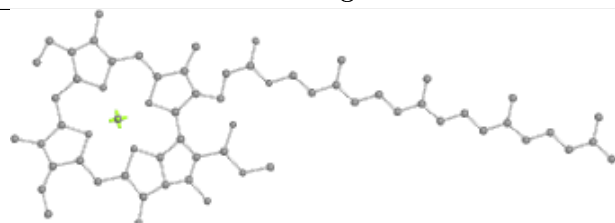
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | k     | 101 | BCR  | C7-C8-C9-C10    |
| 22  | k     | 101 | BCR  | C7-C8-C9-C34    |
| 20  | c     | 502 | CLA  | CHA-CBD-CGD-O2D |
| 32  | C     | 520 | HTG  | C2'-C1'-S1-C1   |
| 23  | F     | 101 | SQD  | C44-C45-C46-O48 |


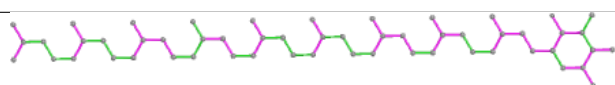
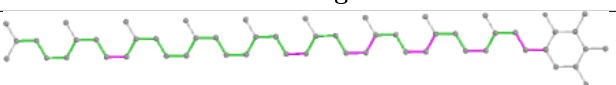
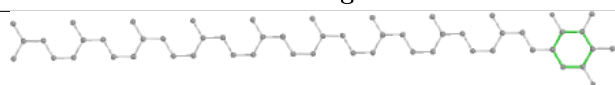
There are no ring outliers.

No monomer is involved in short contacts.

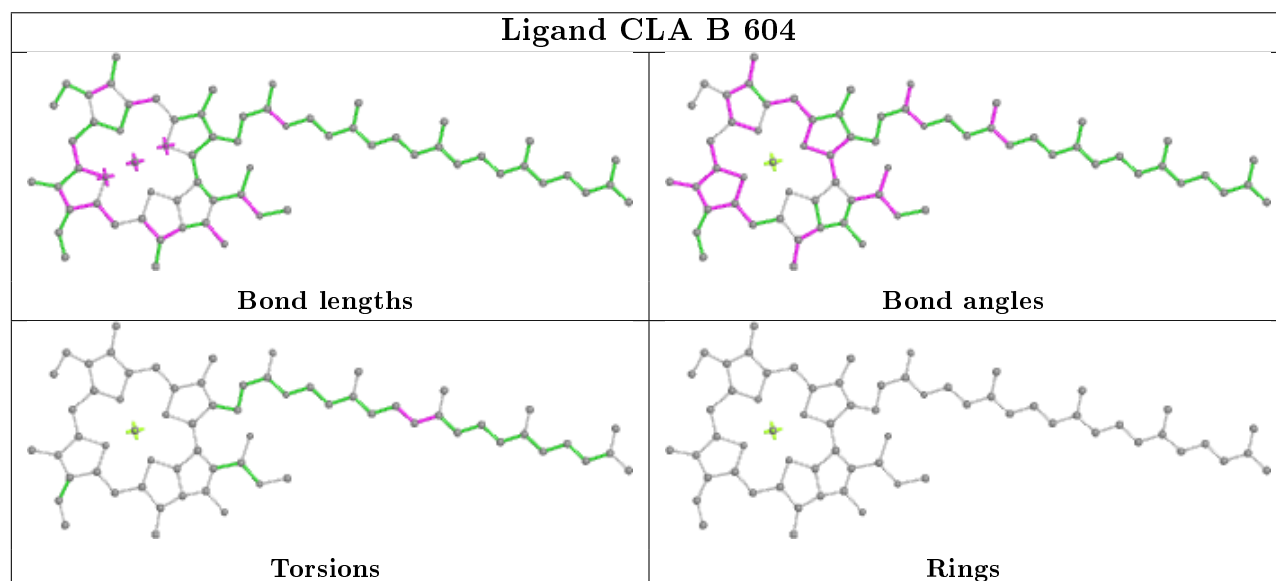
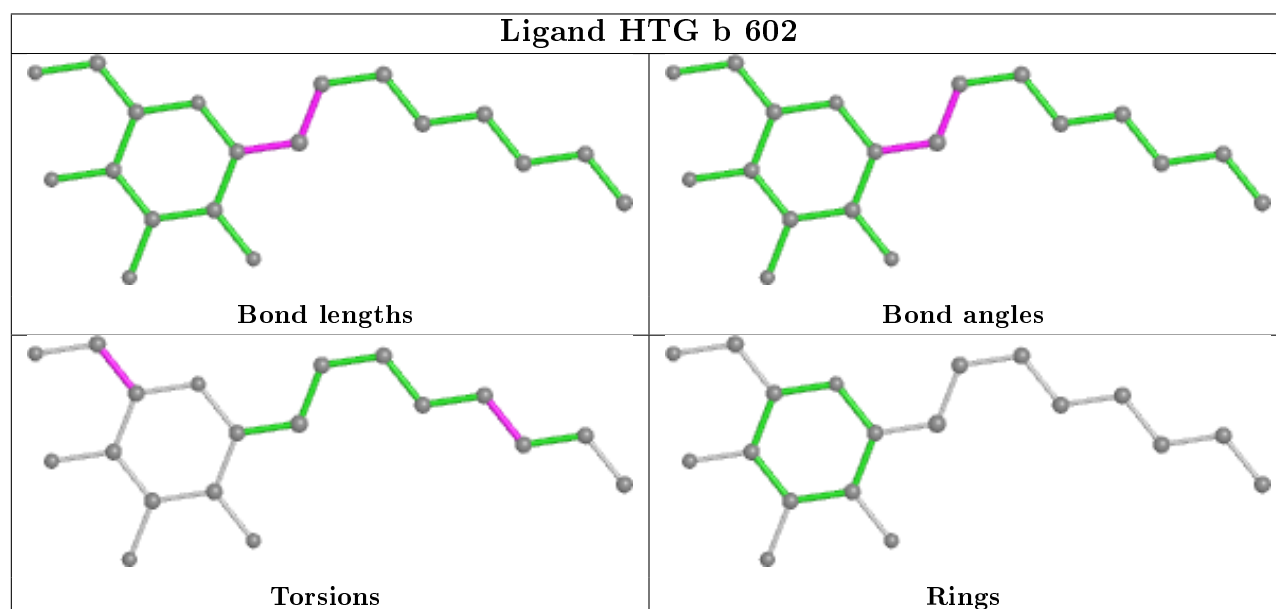
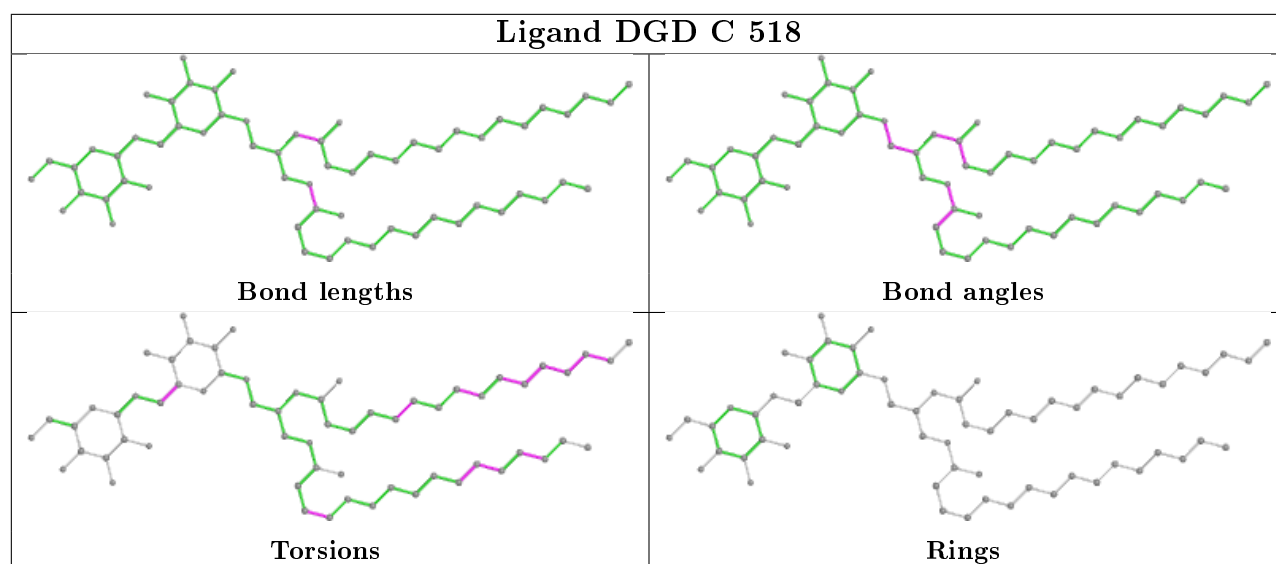
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

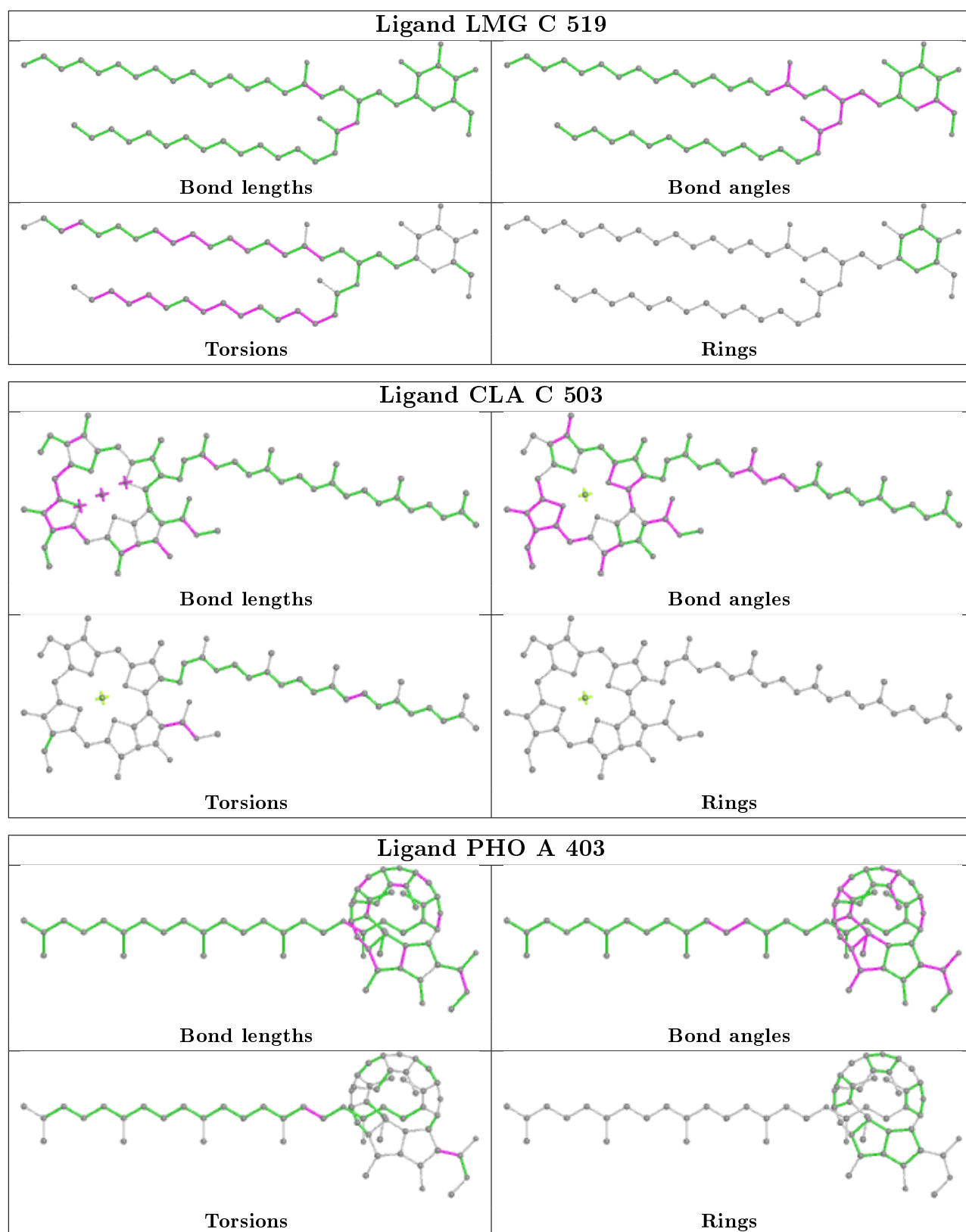
| Ligand LMG B 620  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

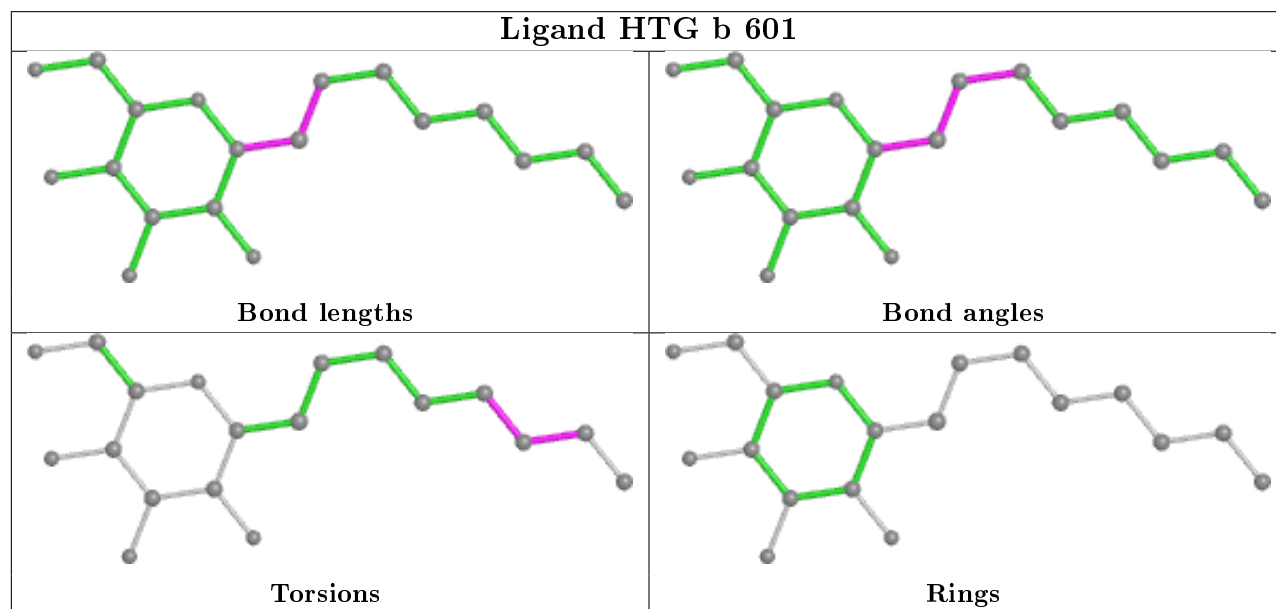
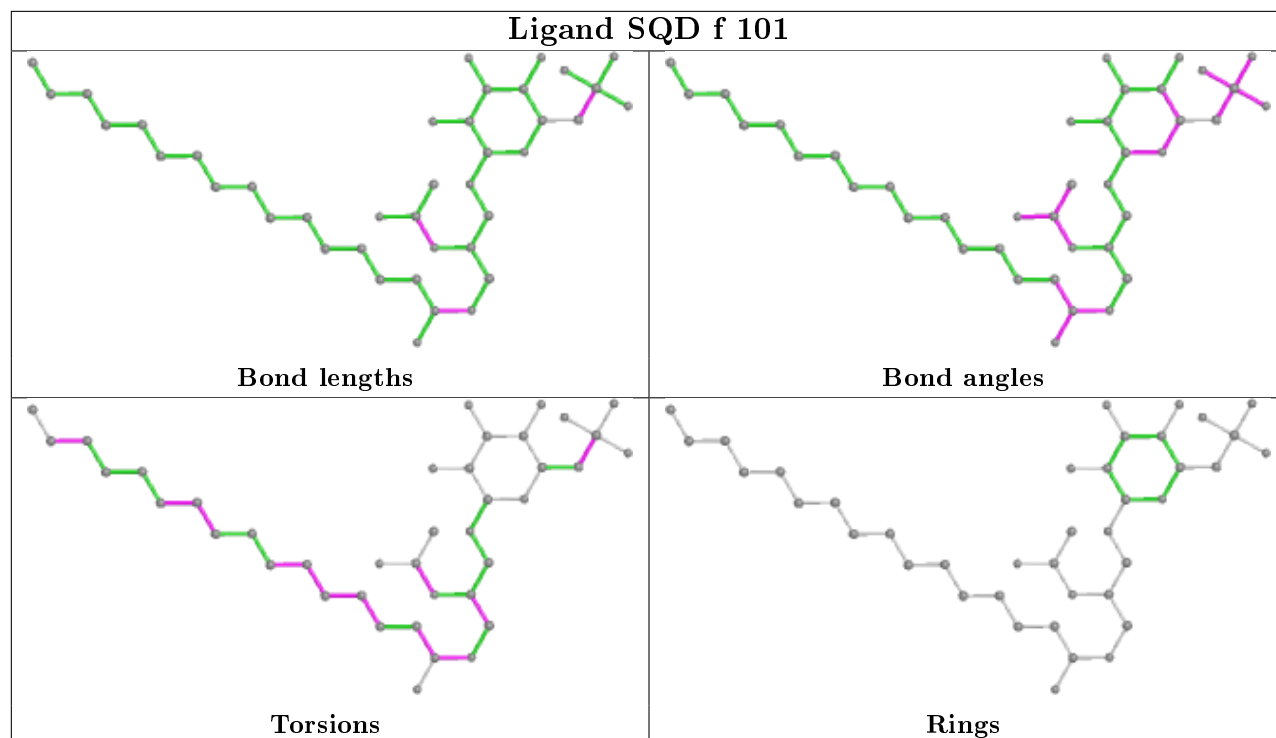
| Ligand CLA d 403   |   |
|--|---|
|   |   |
| Bond lengths   | Bond angles   |
|  |  |
| Torsions   | Rings   |

| Ligand PL9 A 411  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

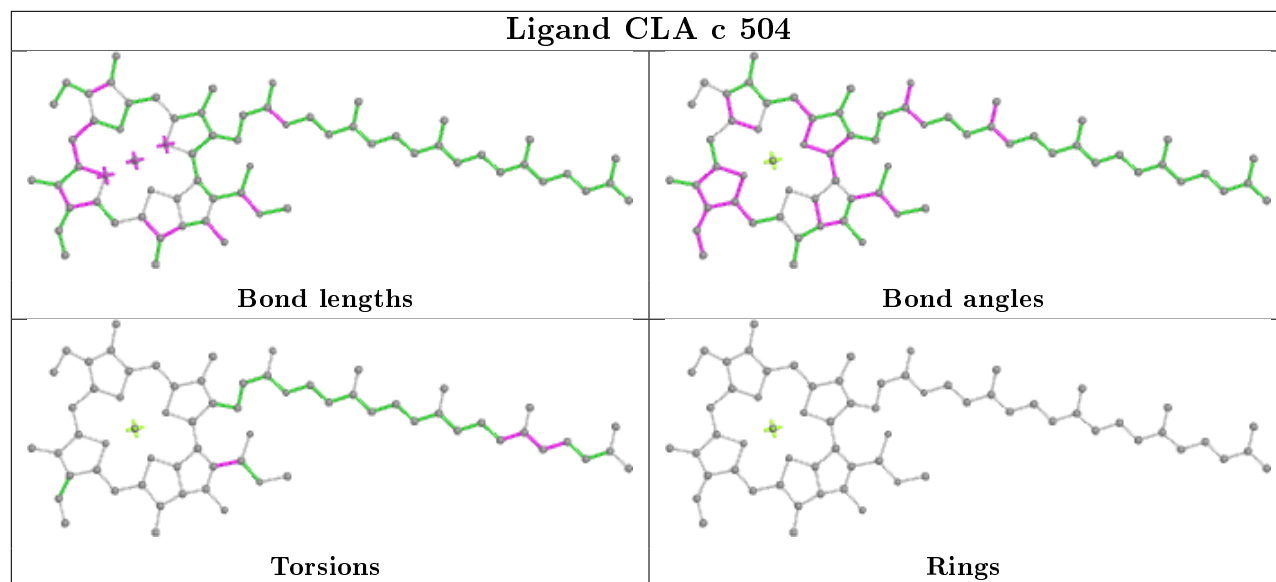




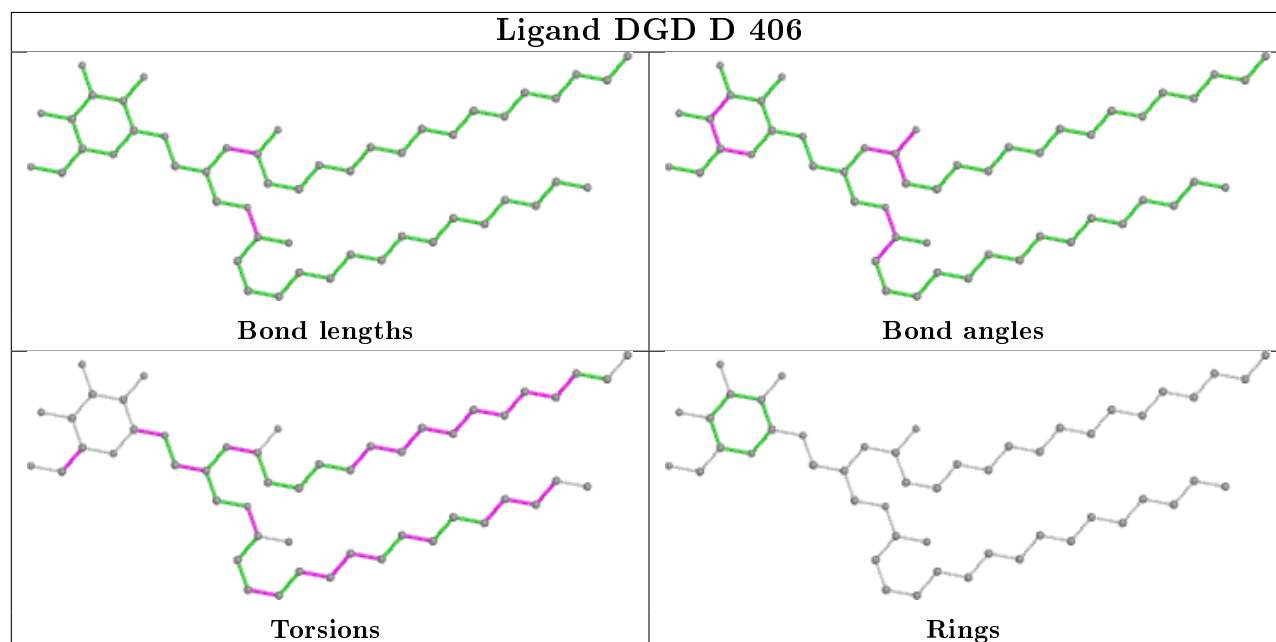




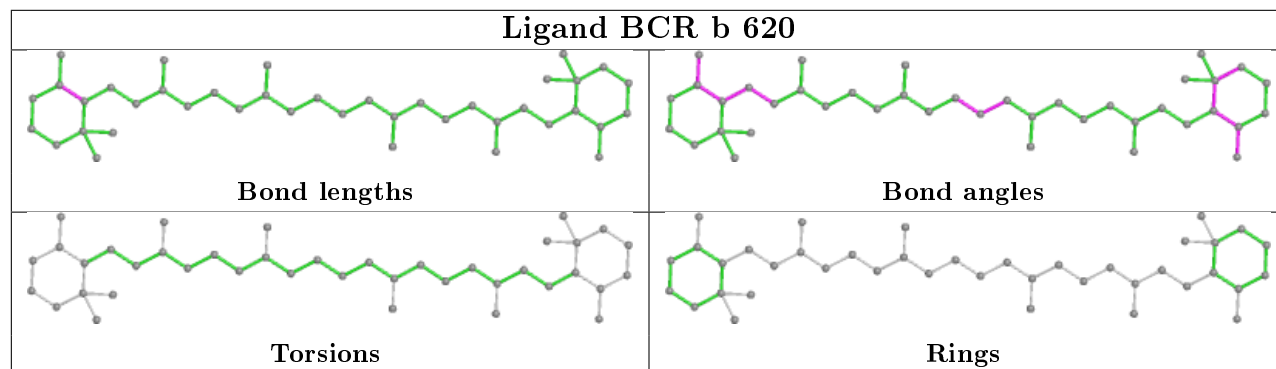
## Ligand CLA c 504

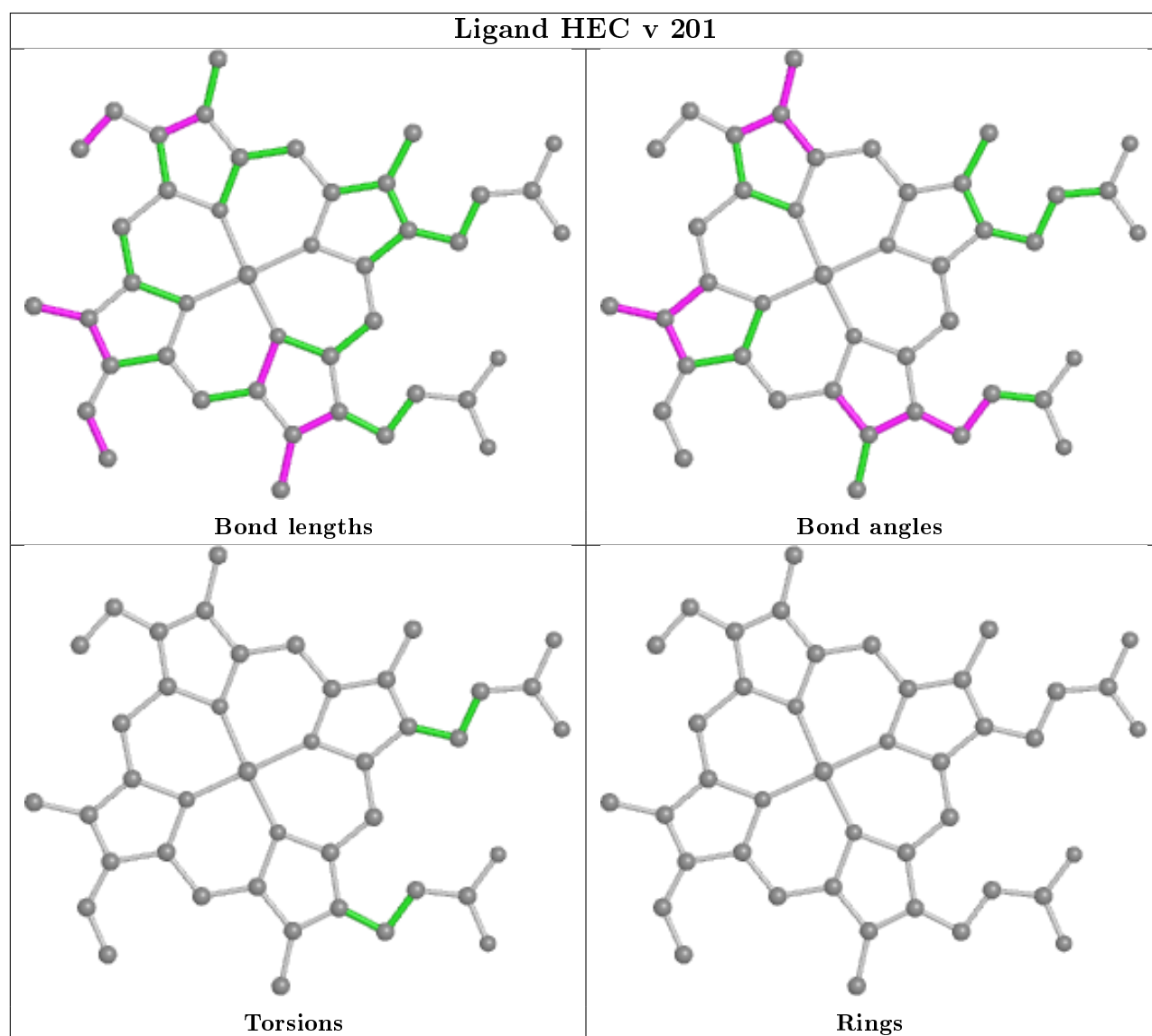
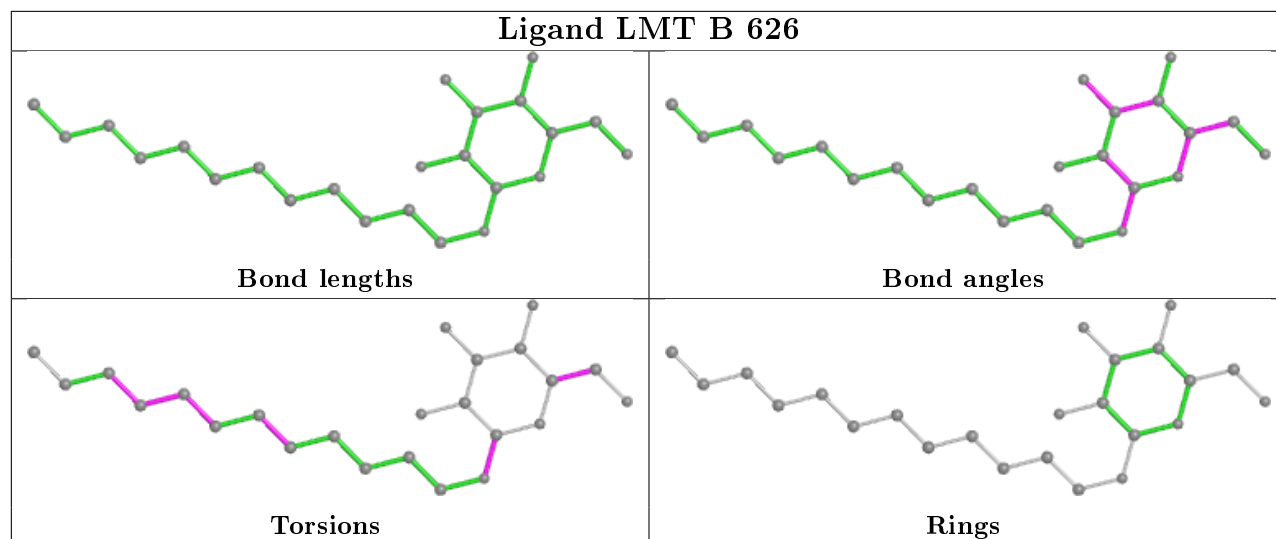


## Ligand DGD D 406

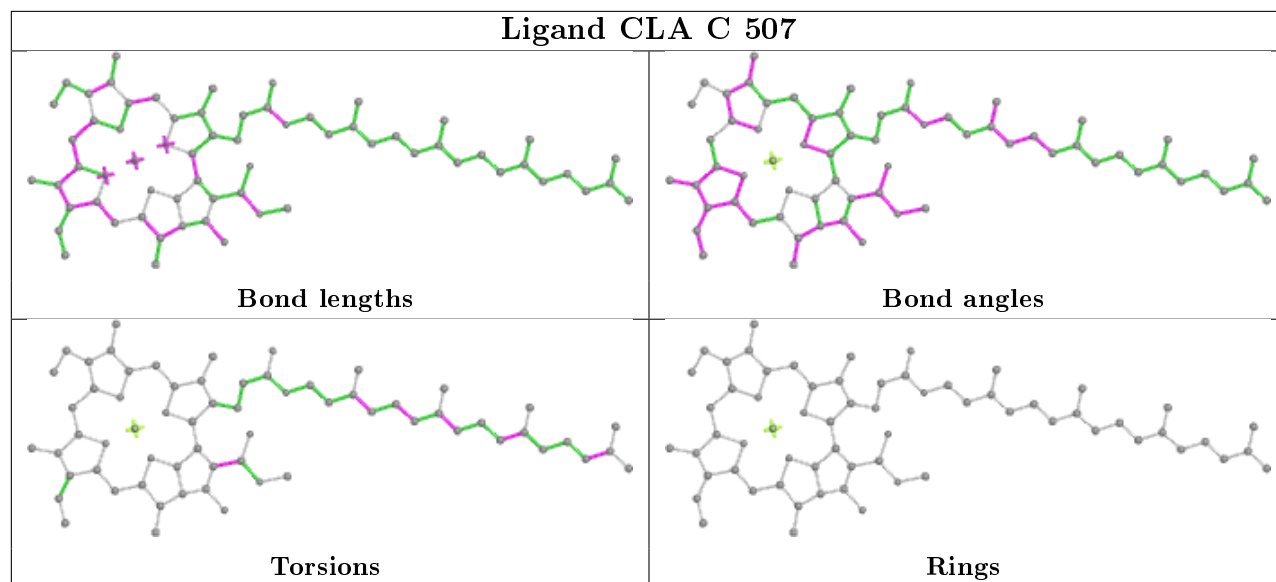


## Ligand BCR b 620

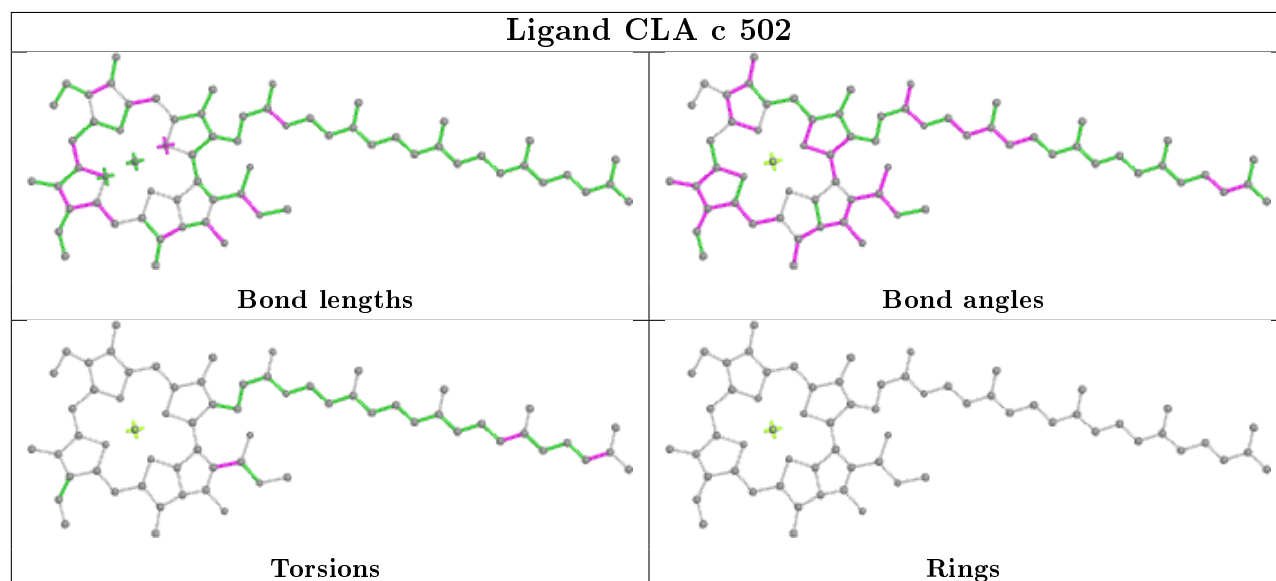




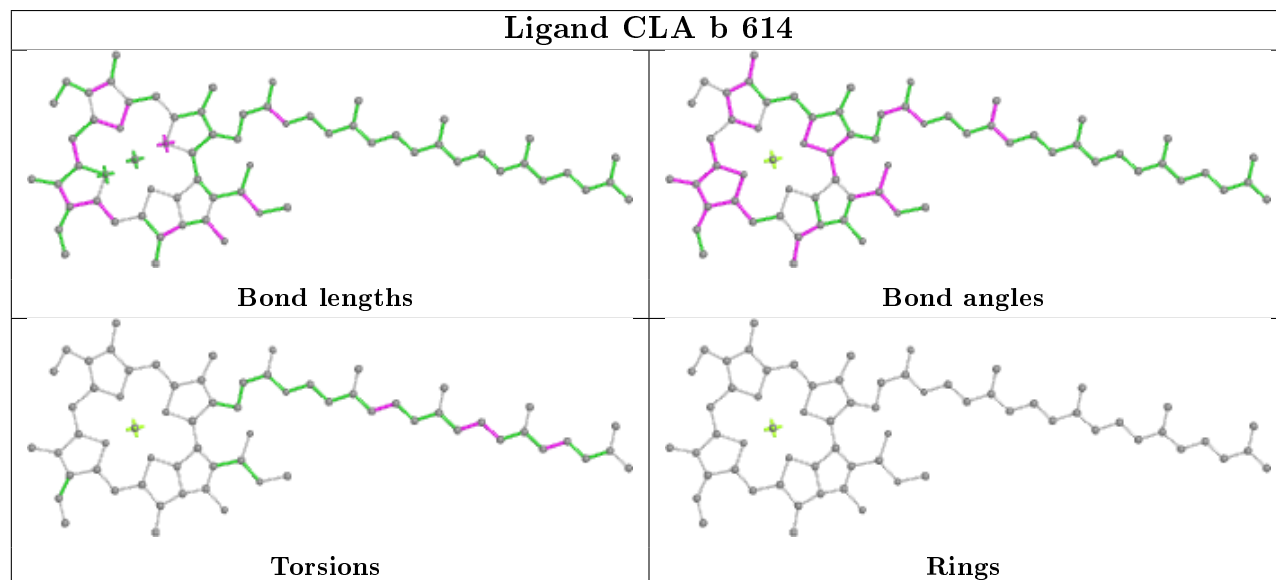
## Ligand CLA C 507

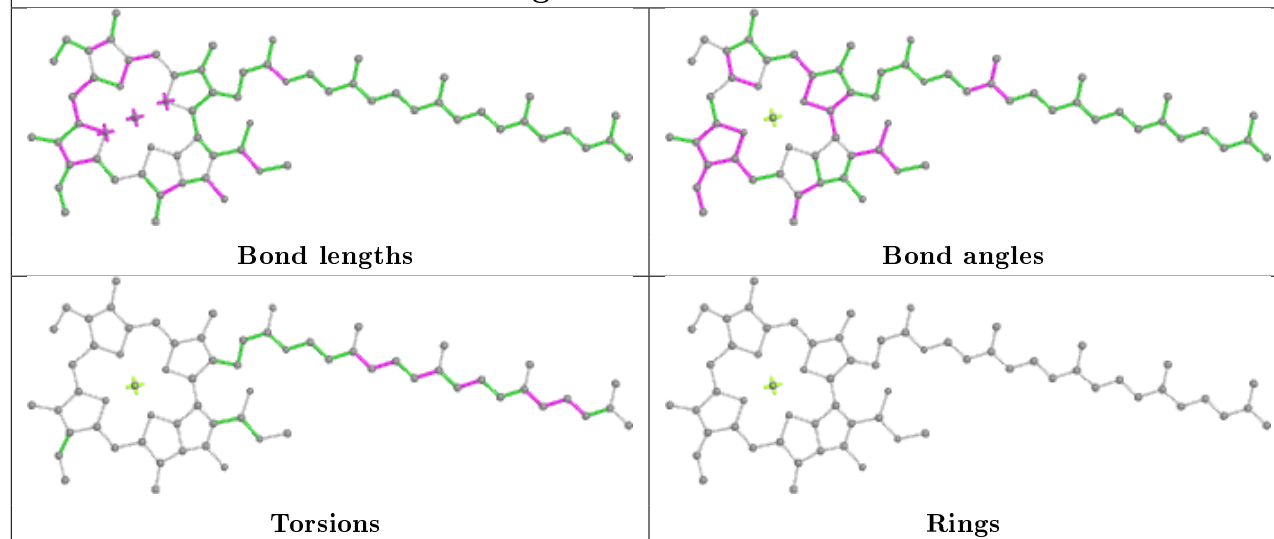
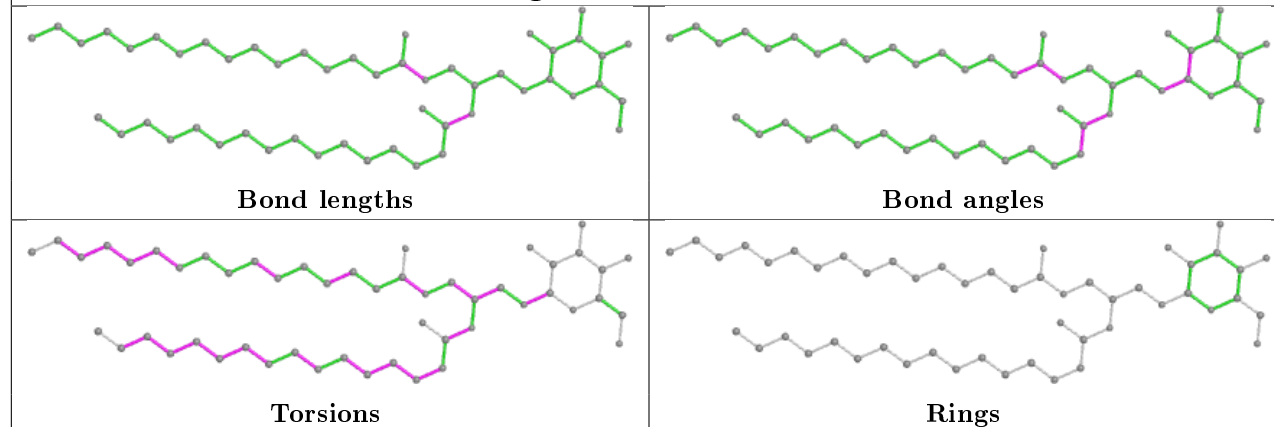
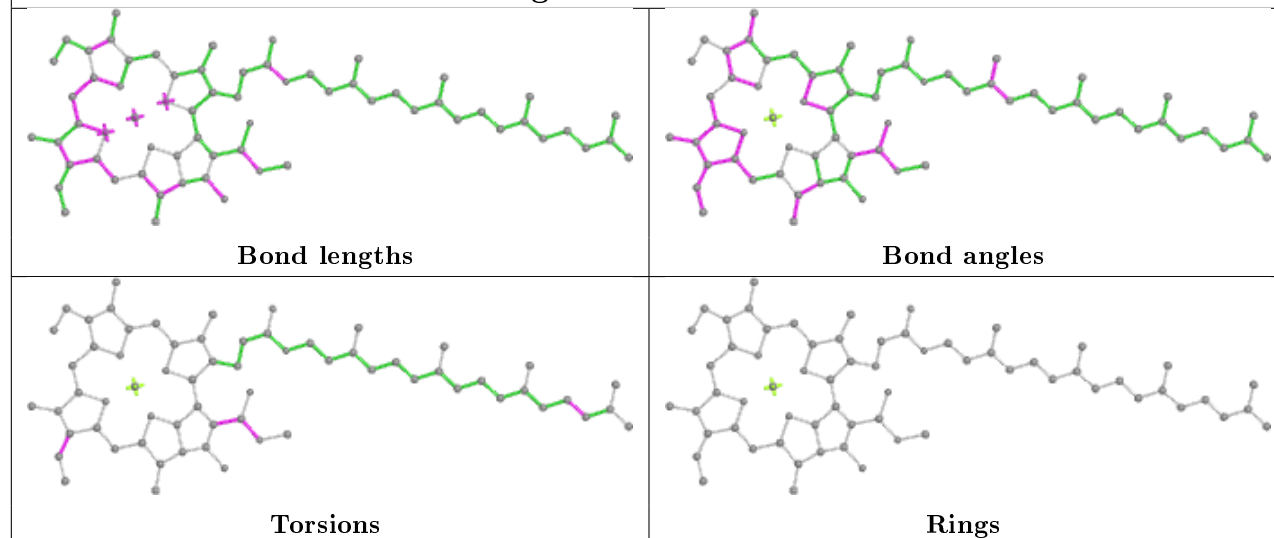


## Ligand CLA c 502

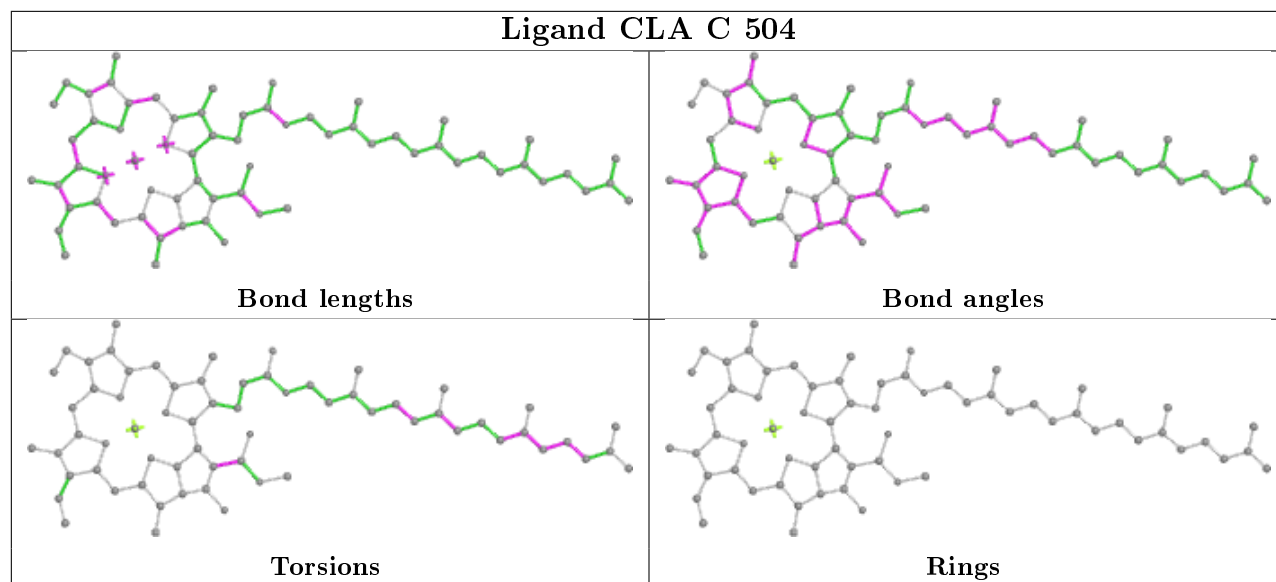


## Ligand CLA b 614

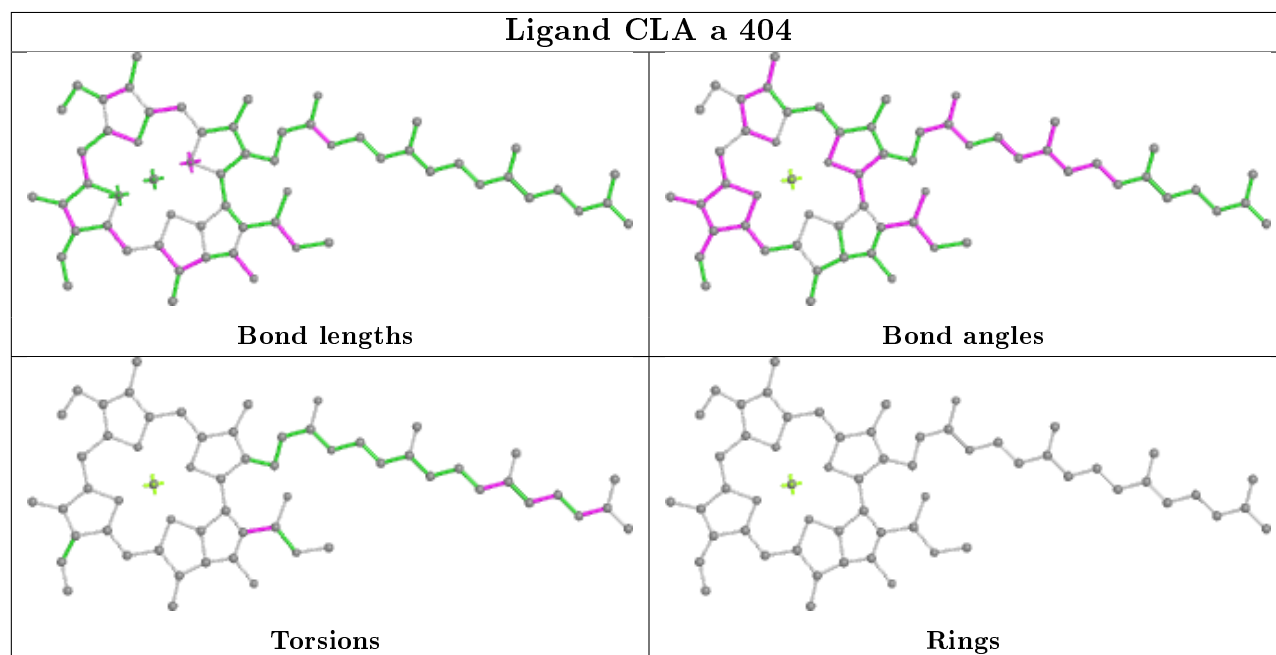


**Ligand CLA A 404****Ligand LMG A 407****Ligand CLA D 402**

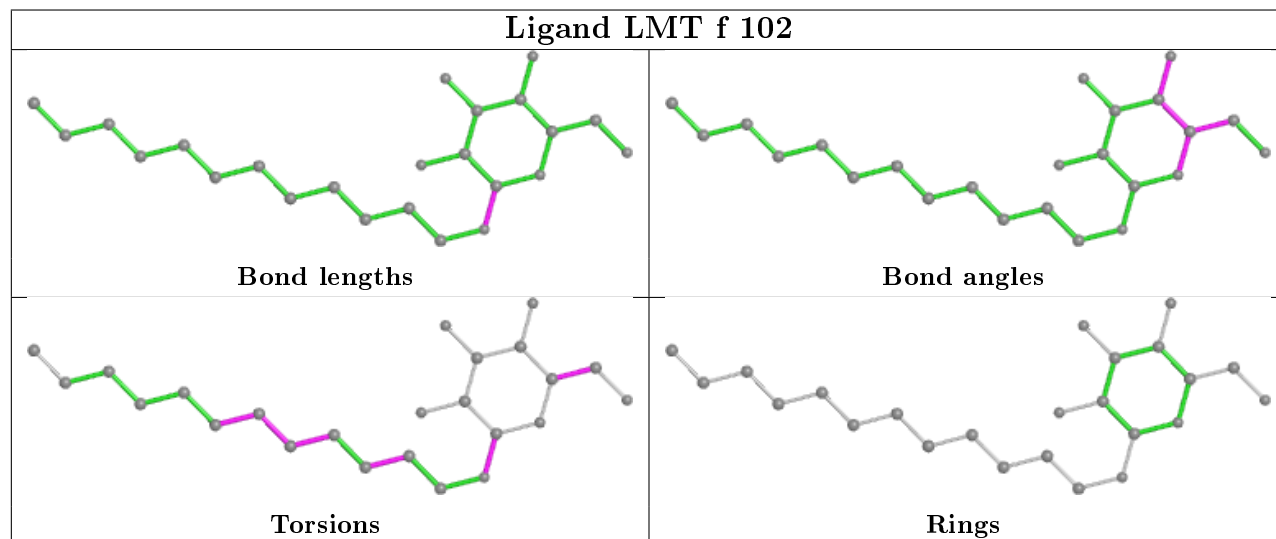
## Ligand CLA C 504



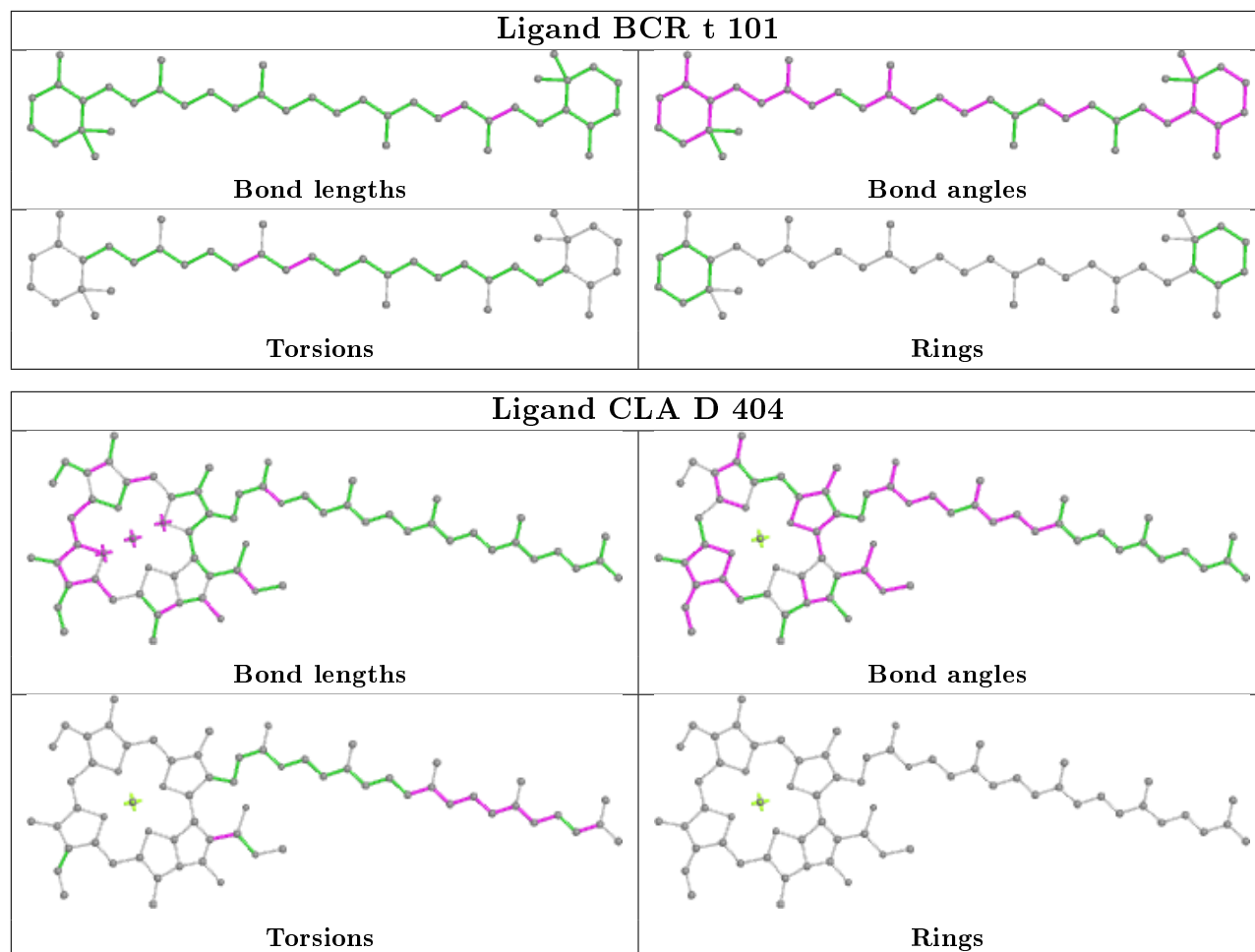
## Ligand CLA a 404

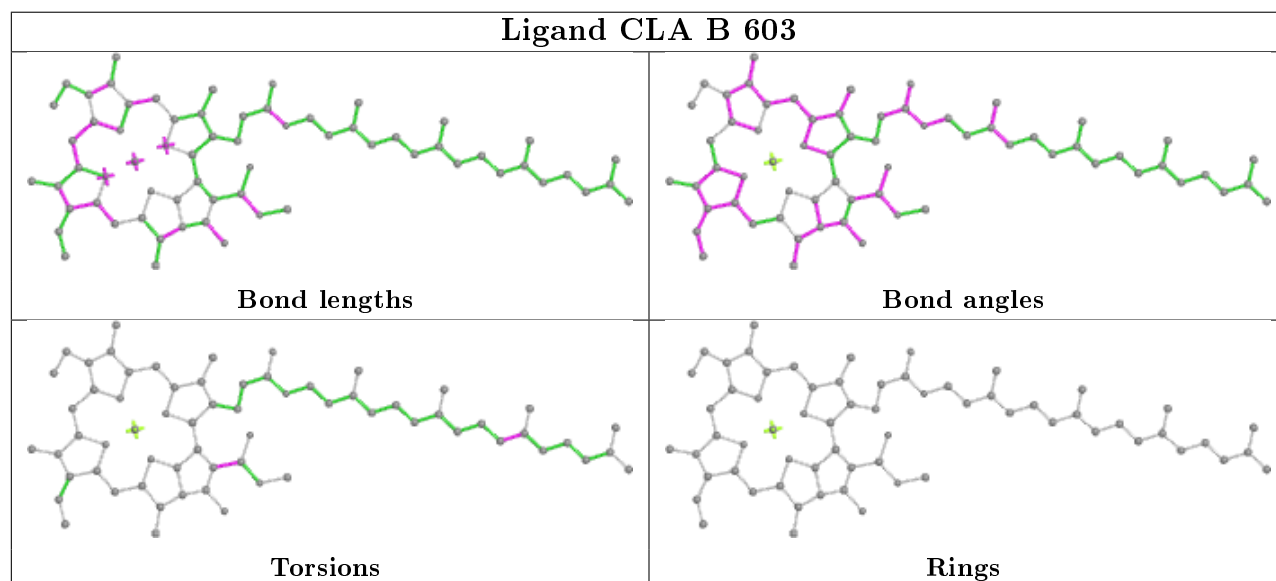
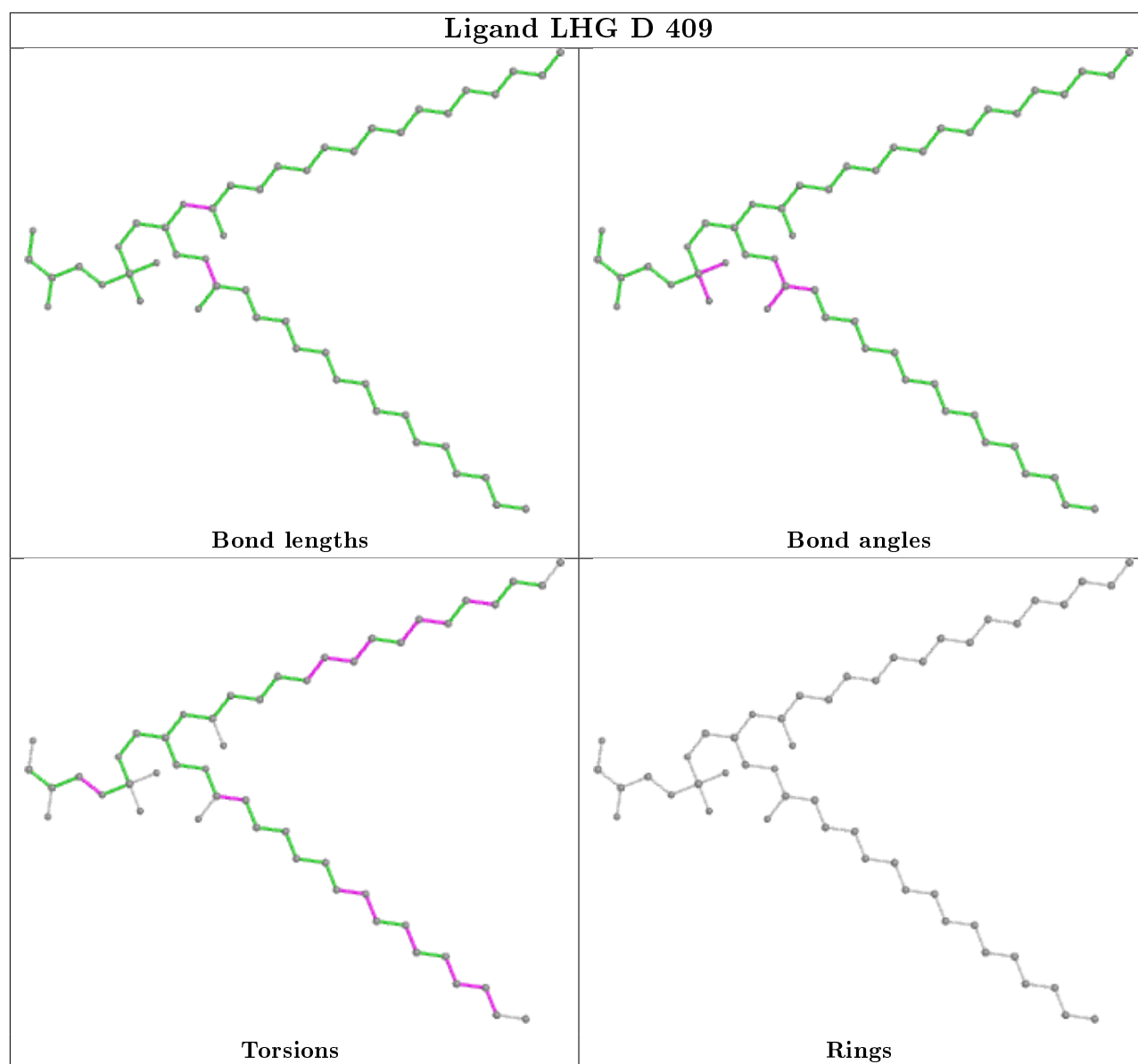


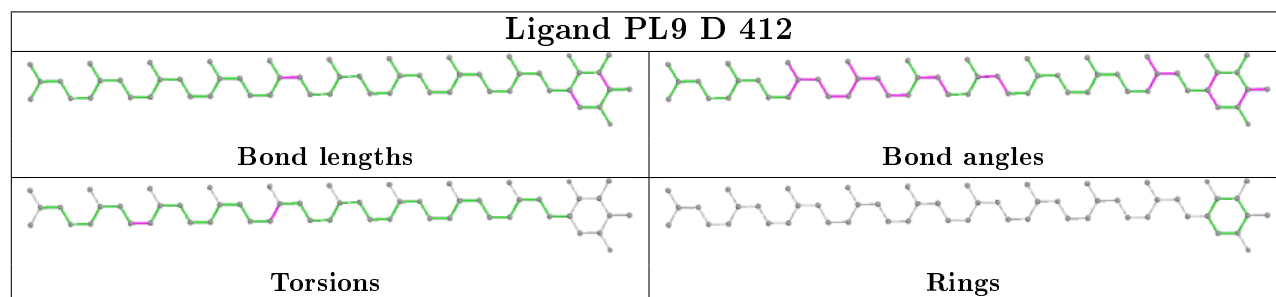
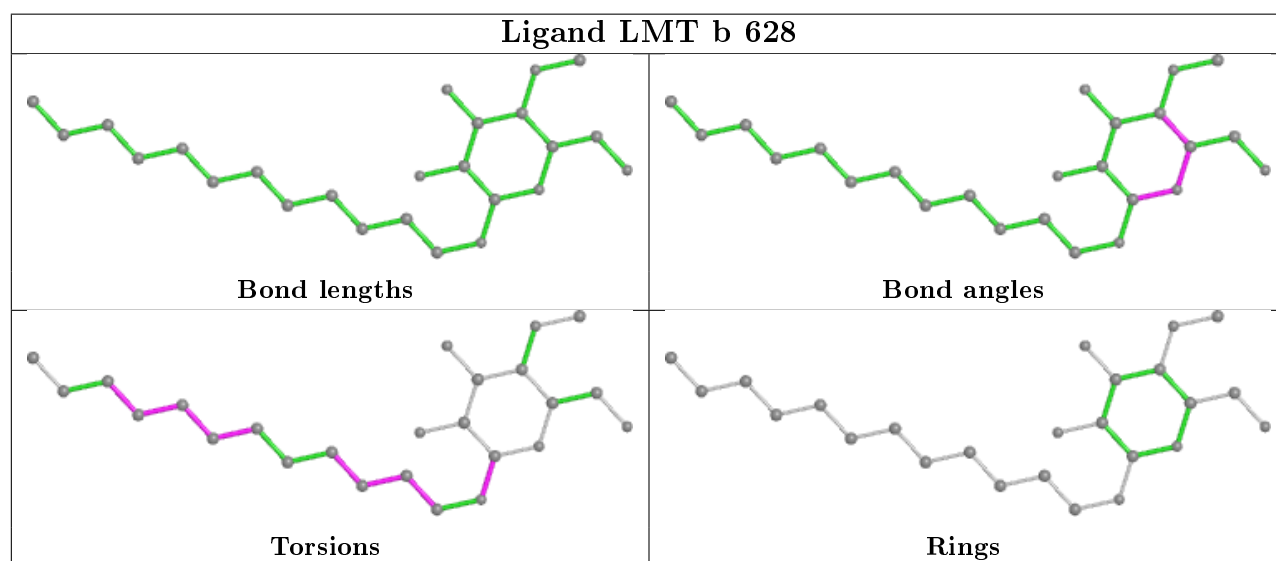
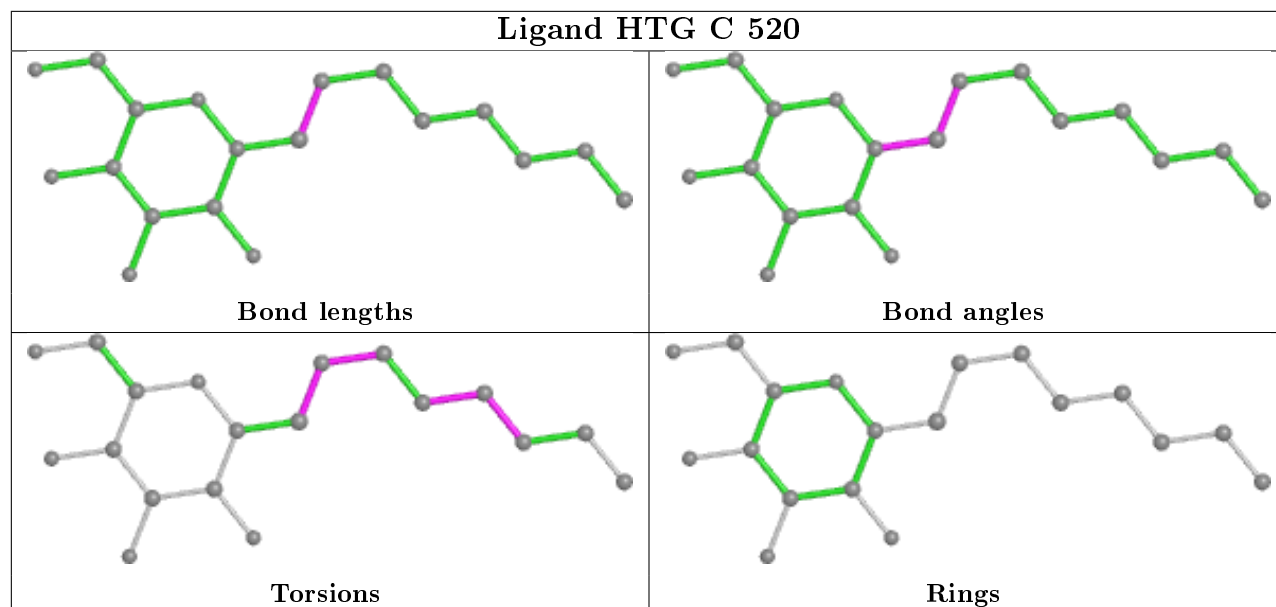
## Ligand LMT f 102

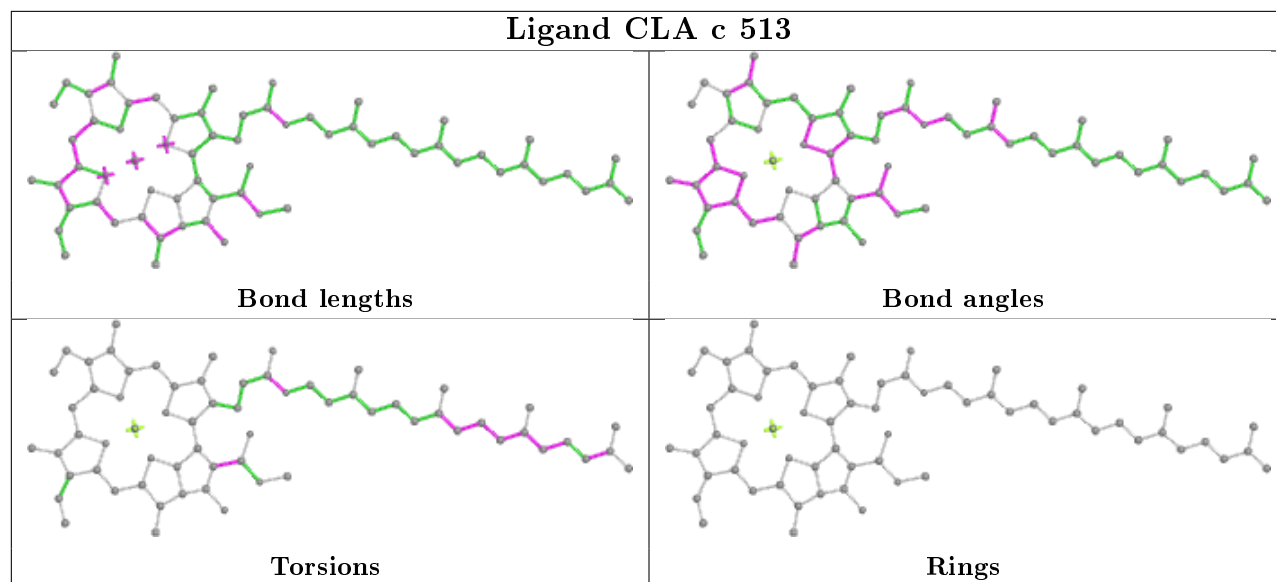
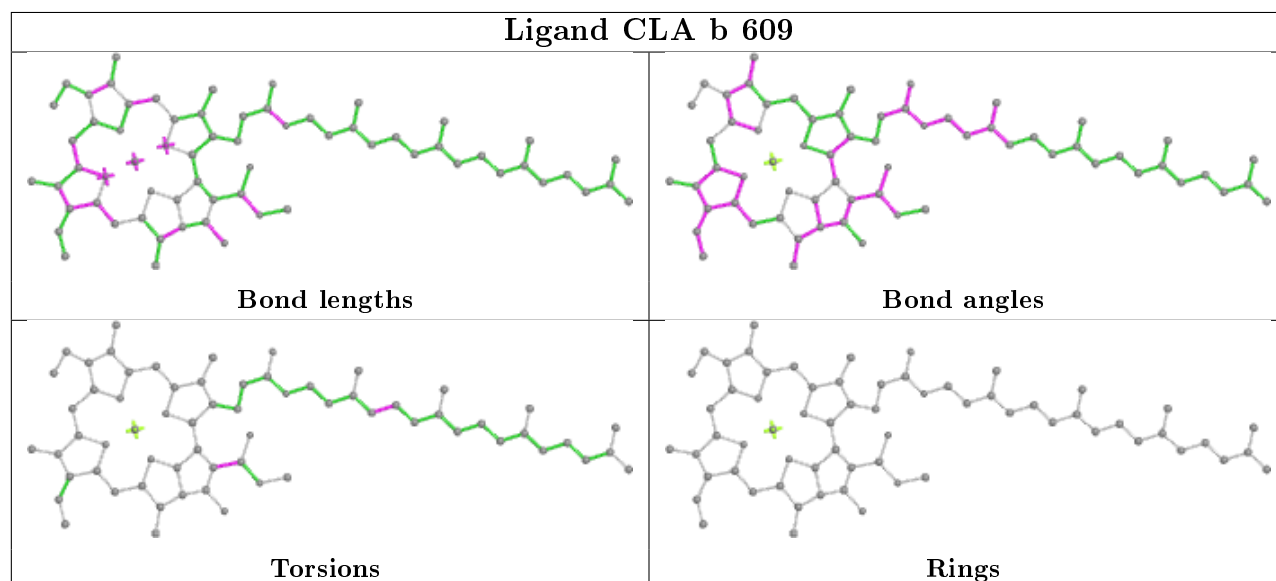
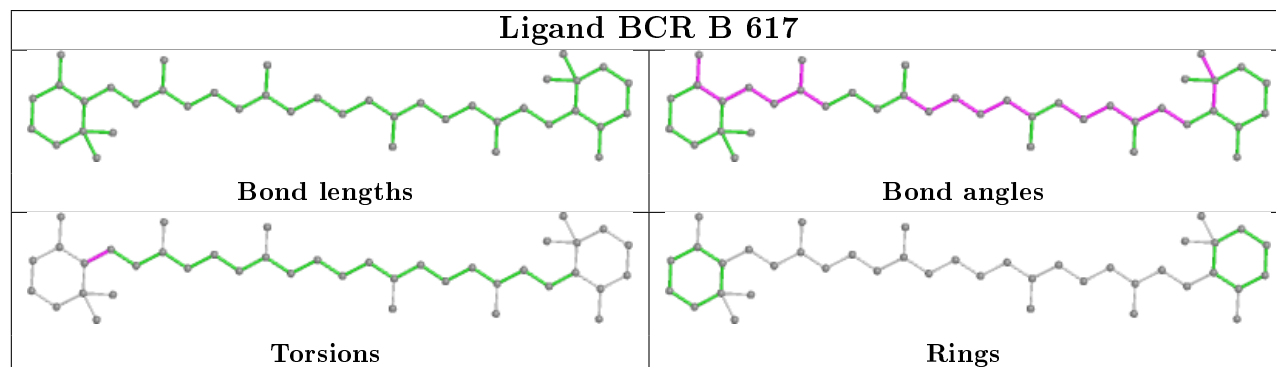


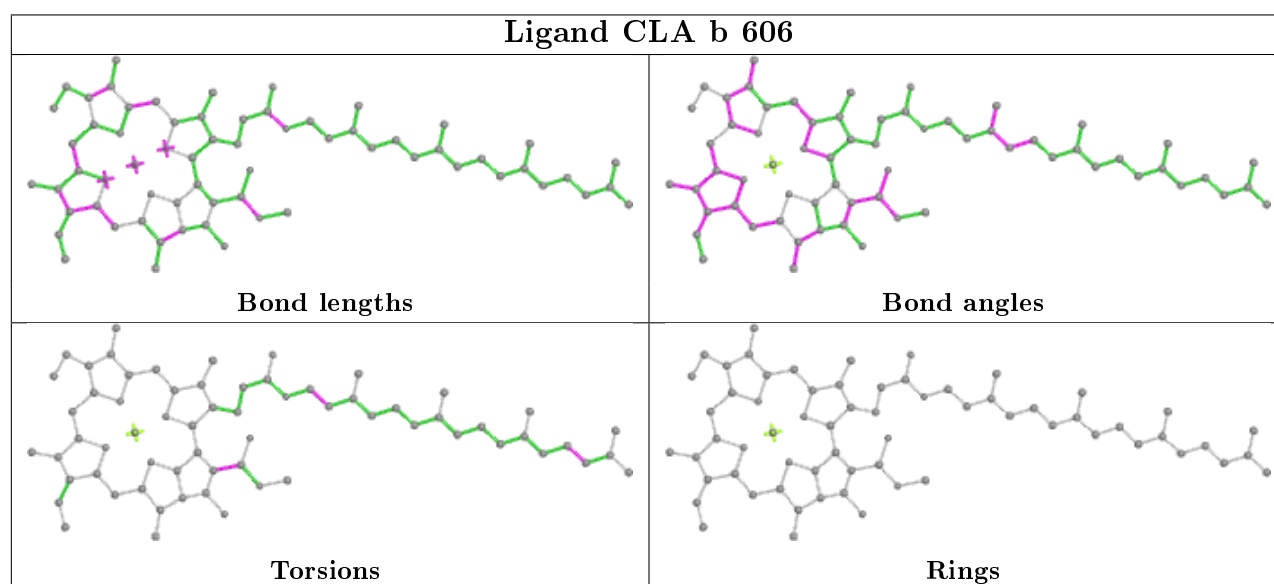
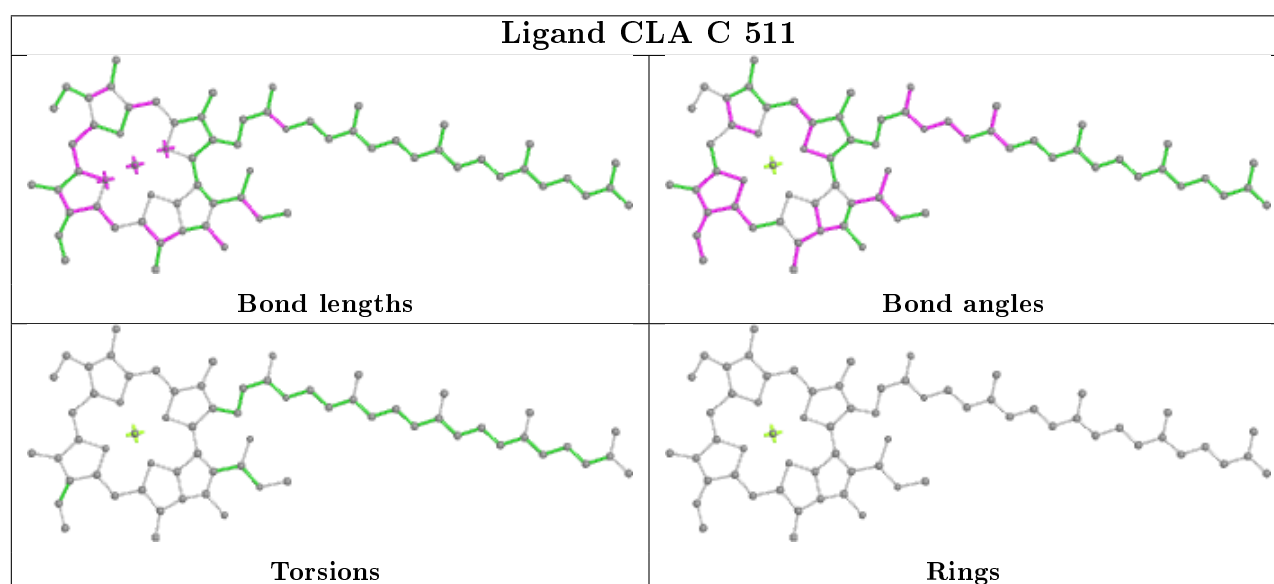
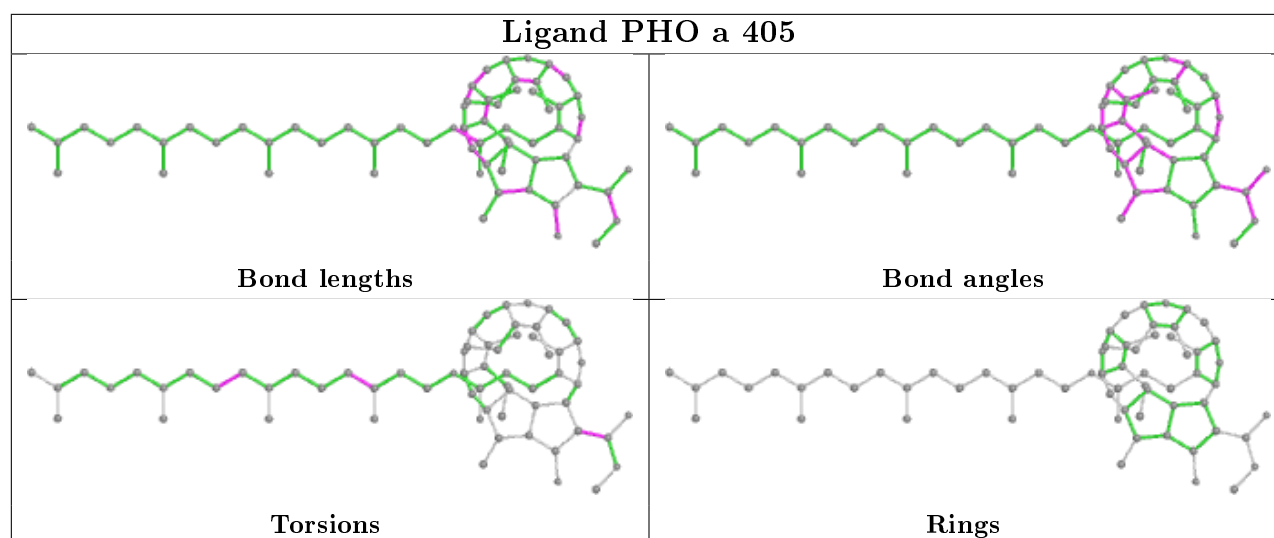


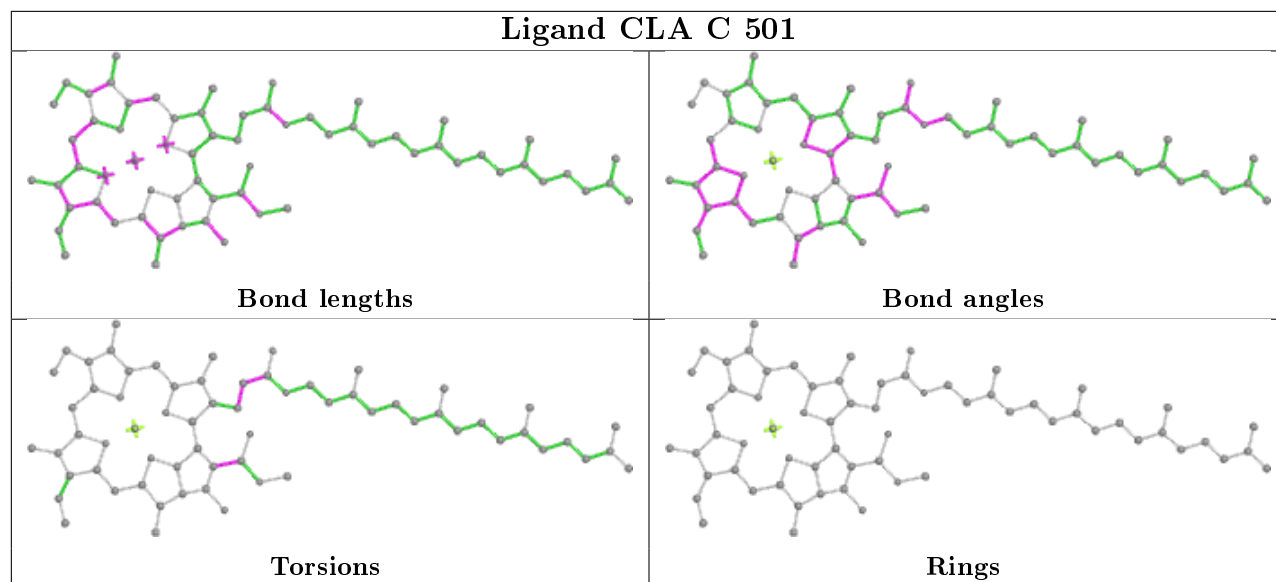
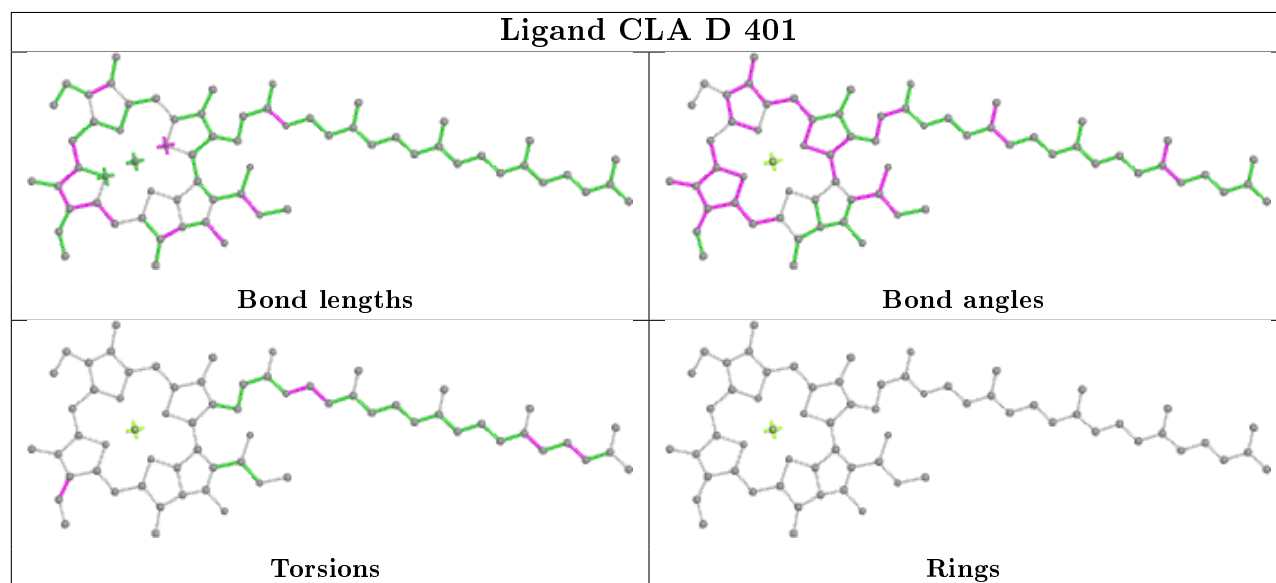




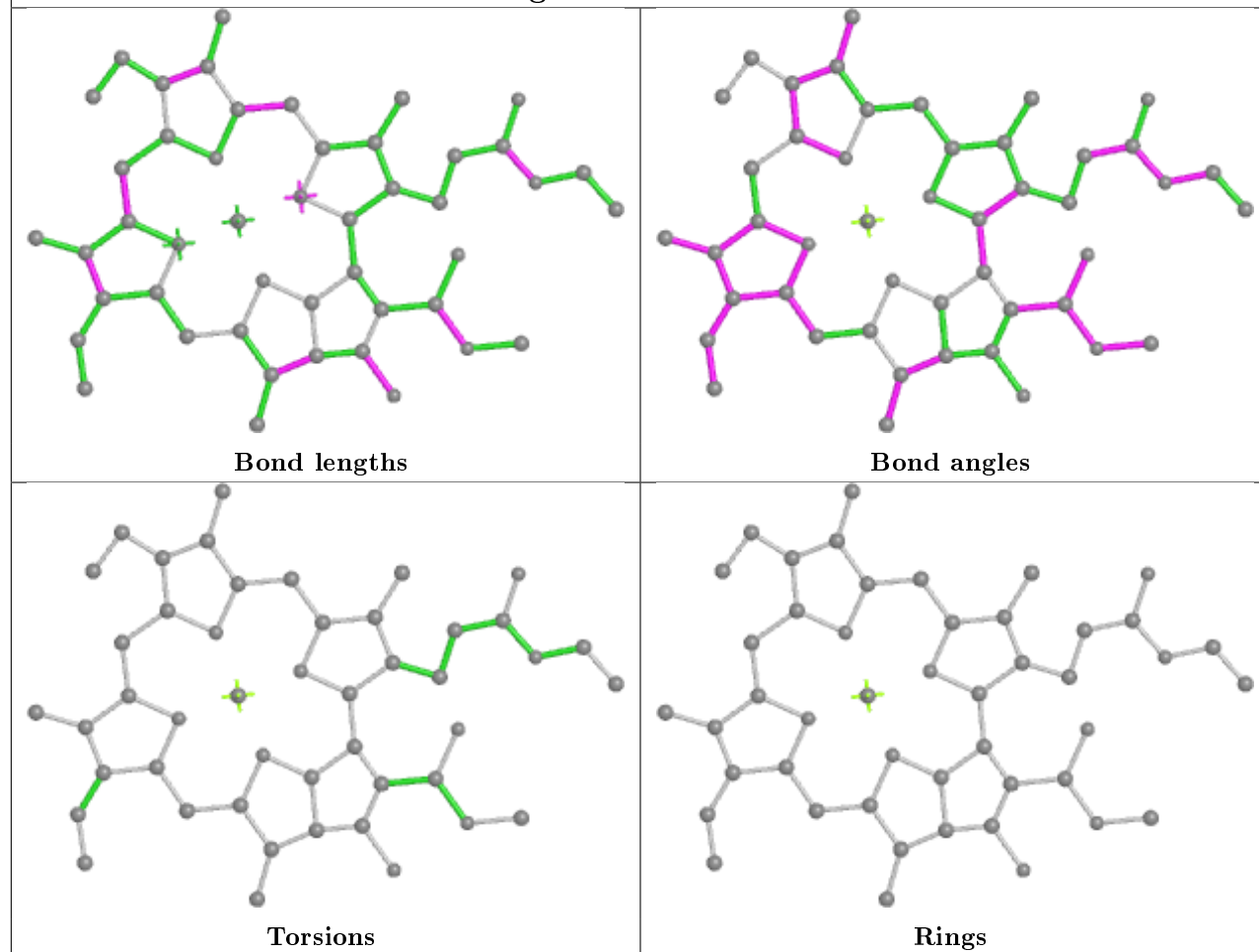


**Ligand CLA c 513****Ligand CLA b 609****Ligand BCR B 617**

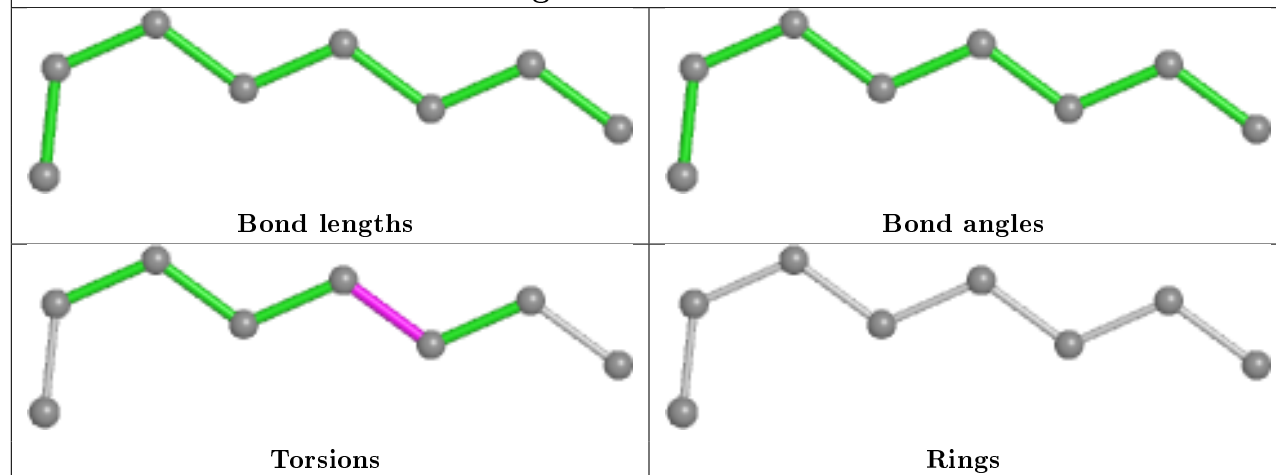


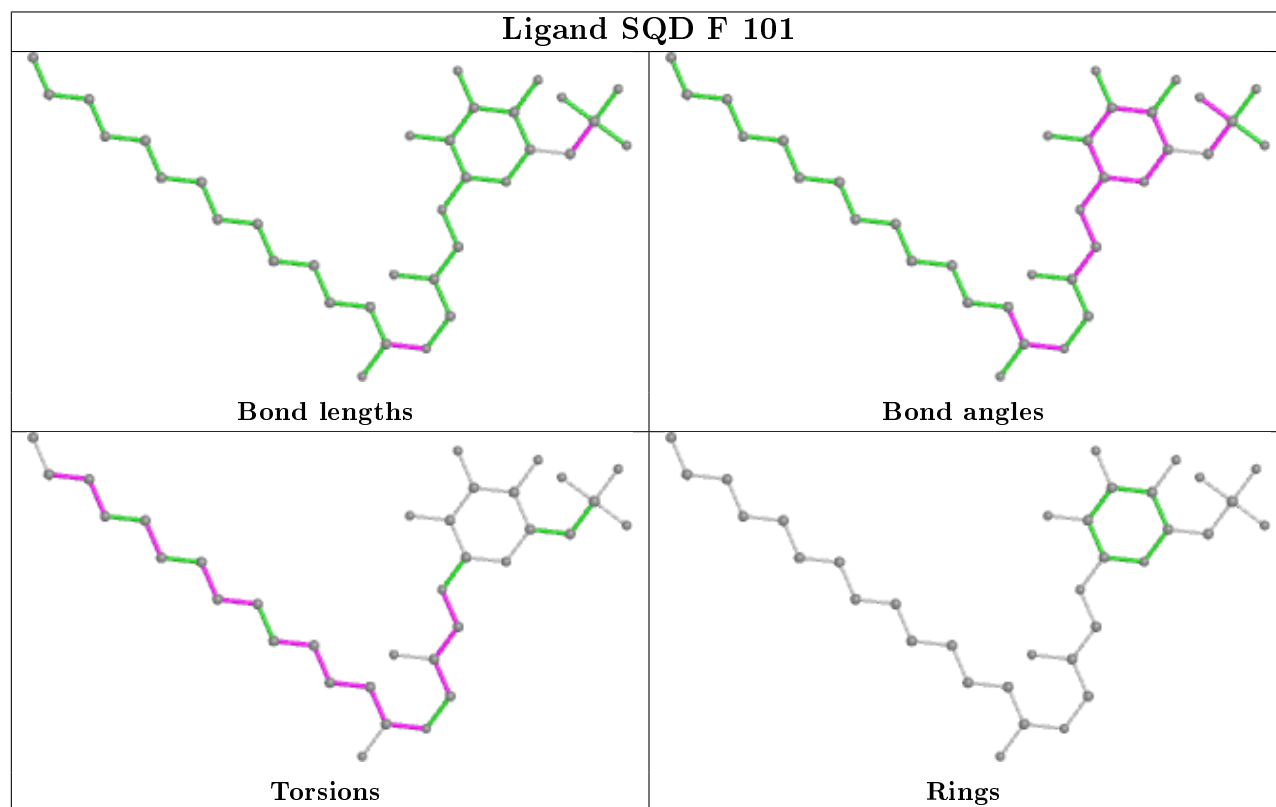
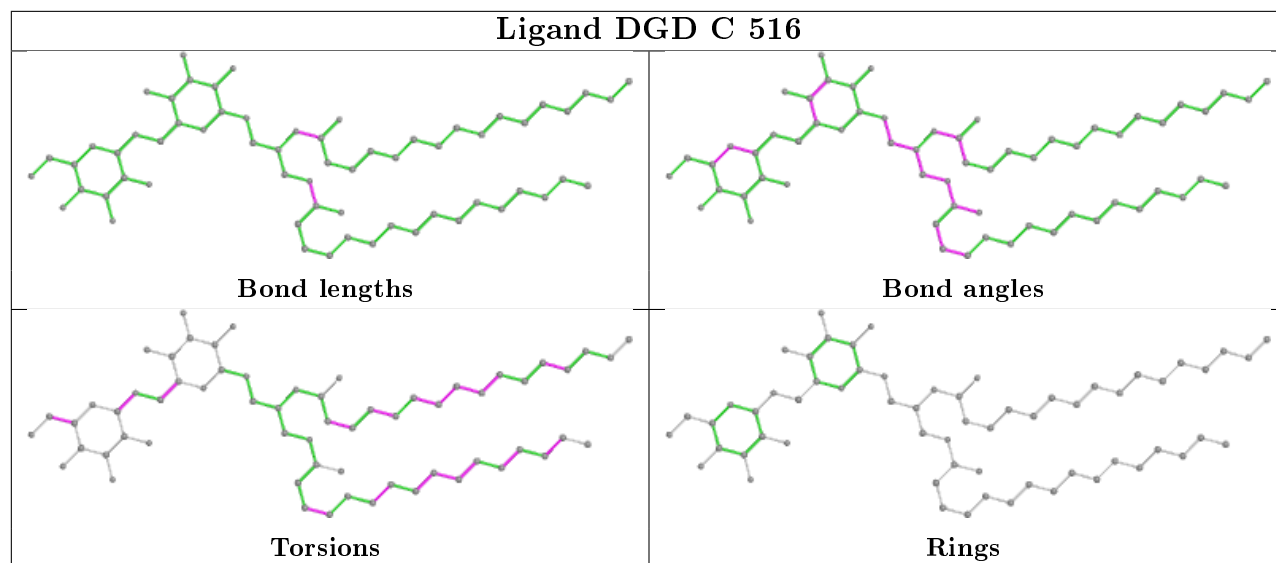
**Ligand CLA C 501****Ligand CLA D 401**

## Ligand CLA a 407

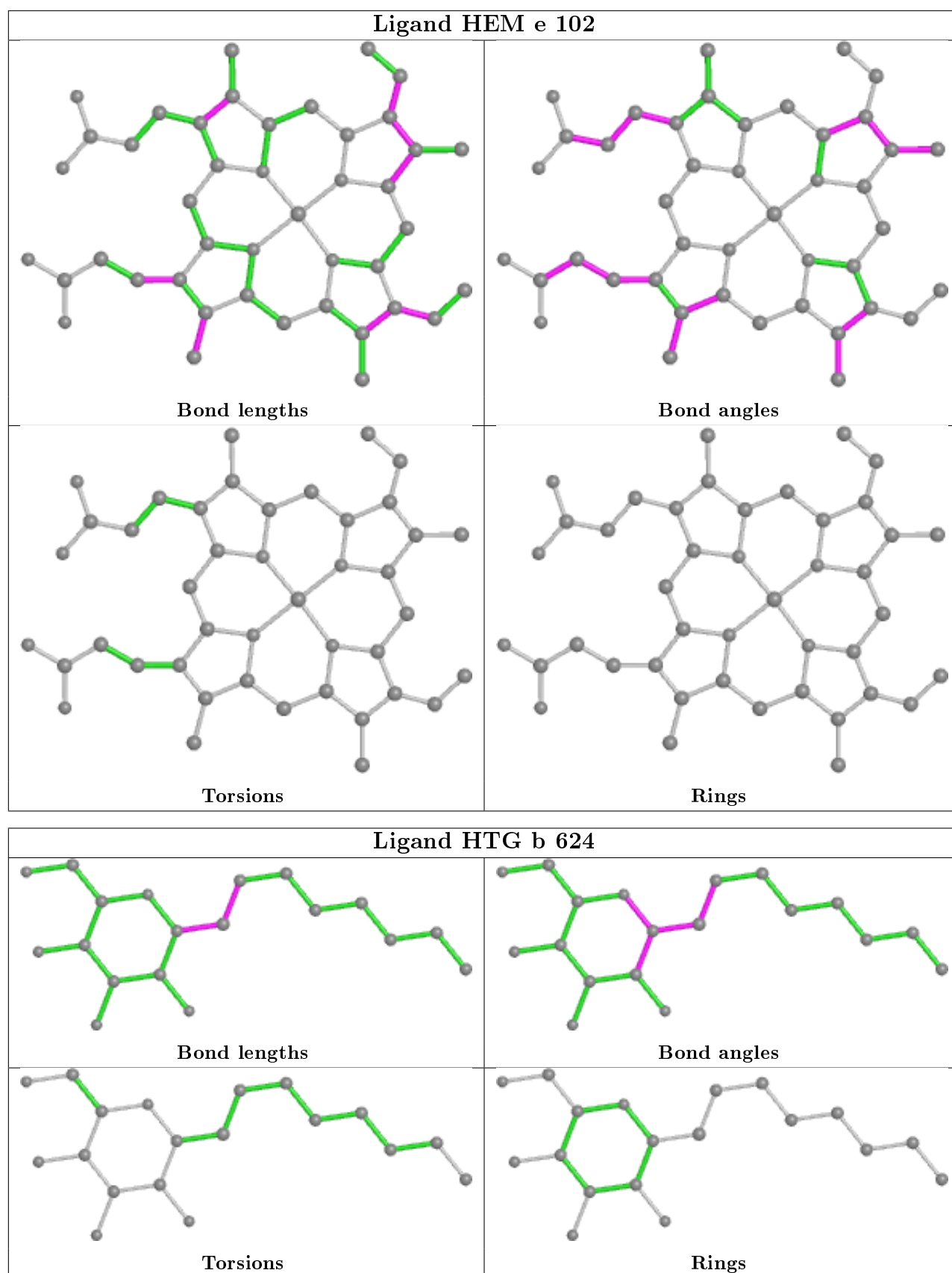


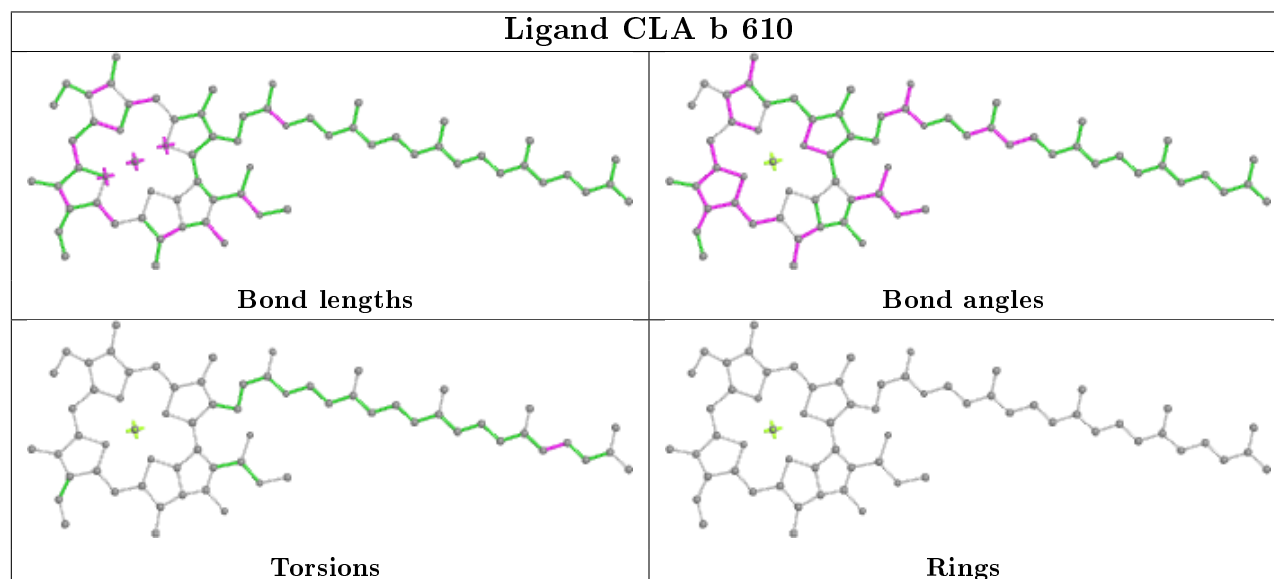
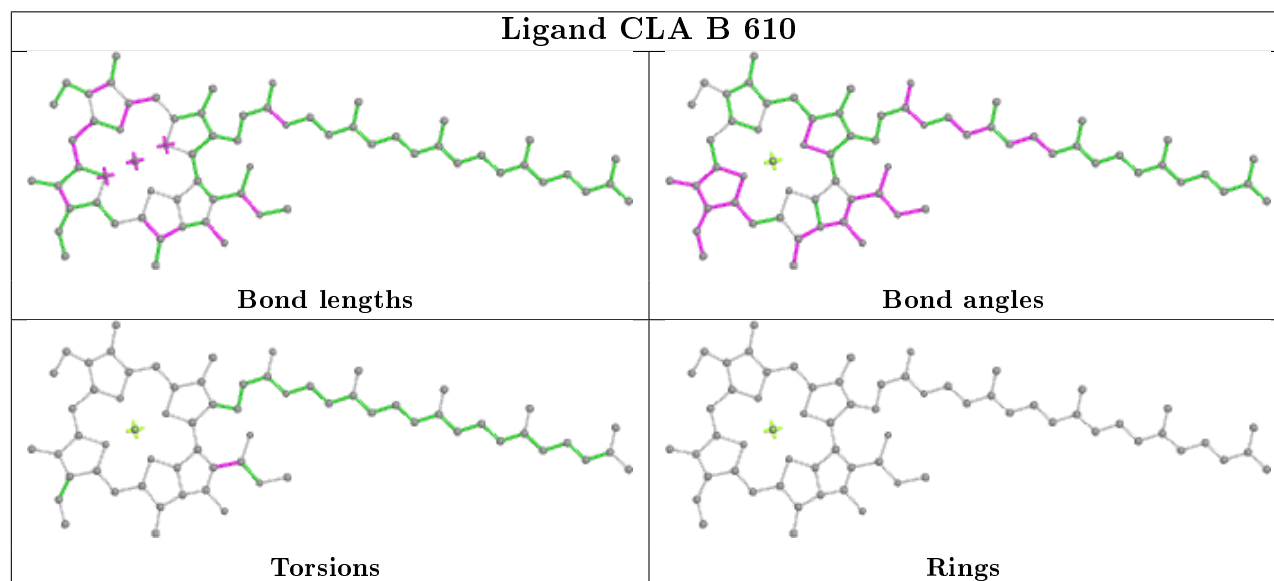
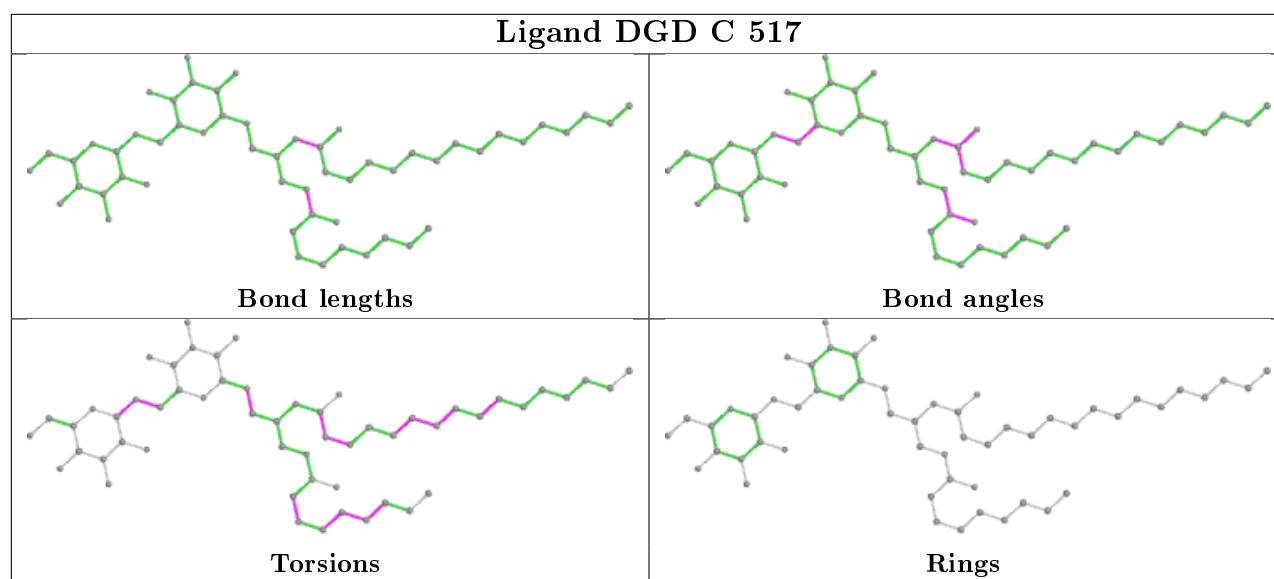
## Ligand HTG u 201

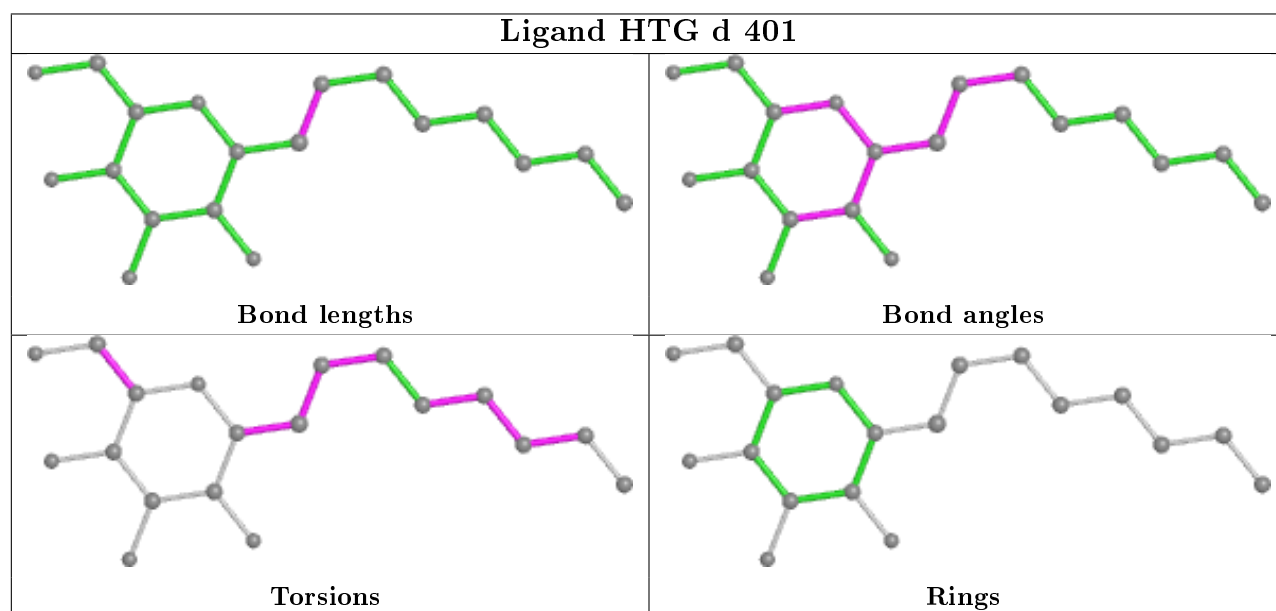
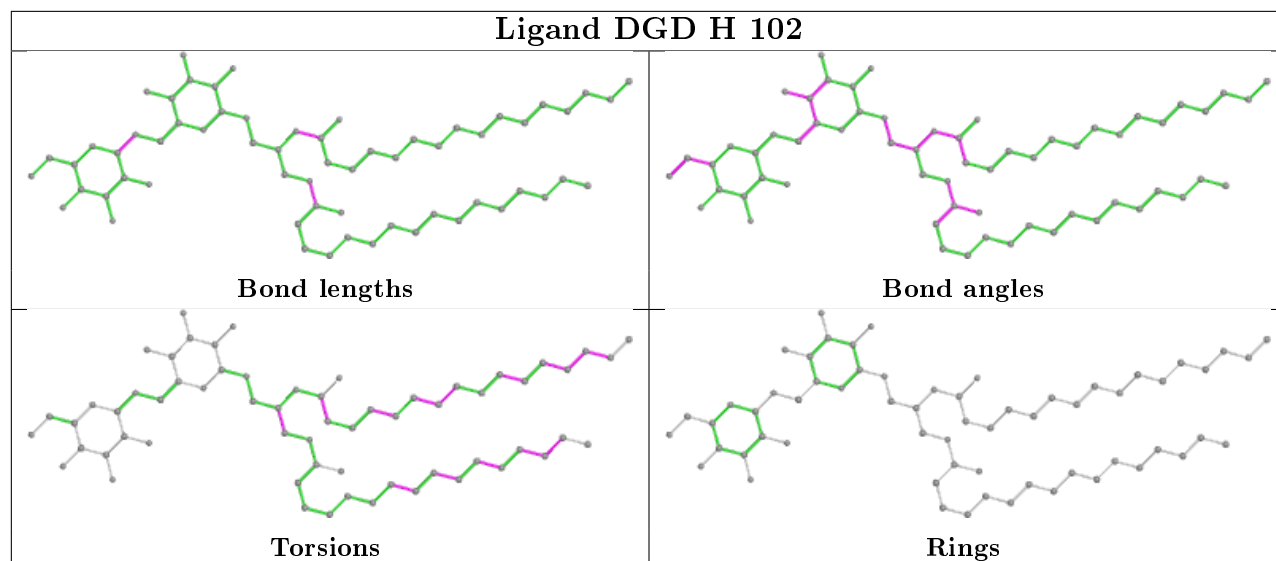


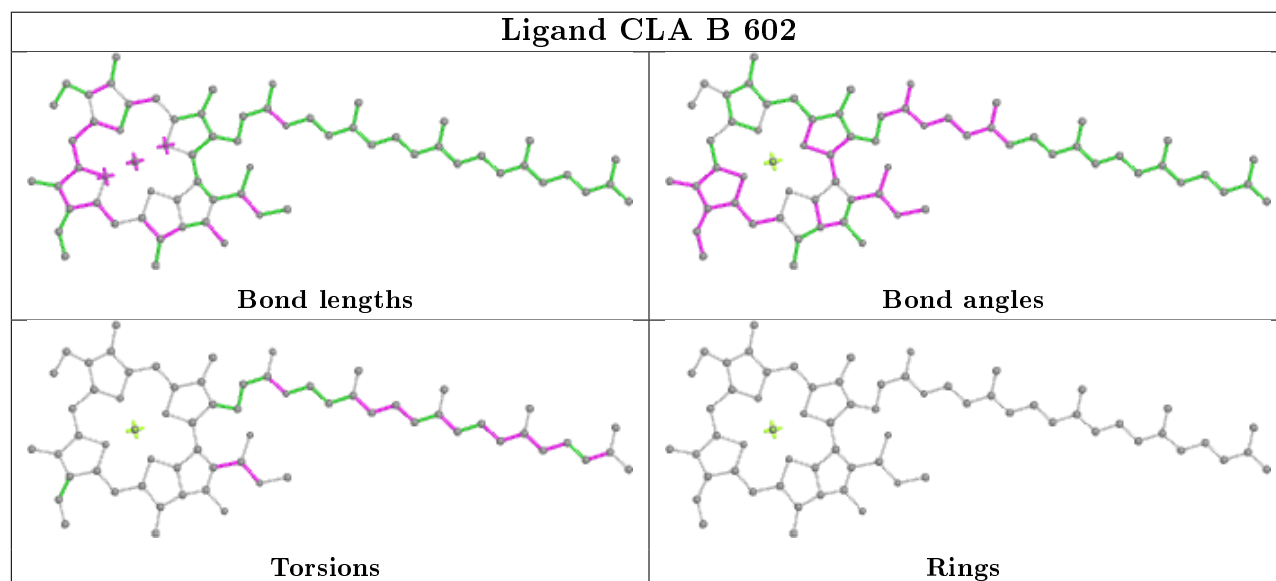
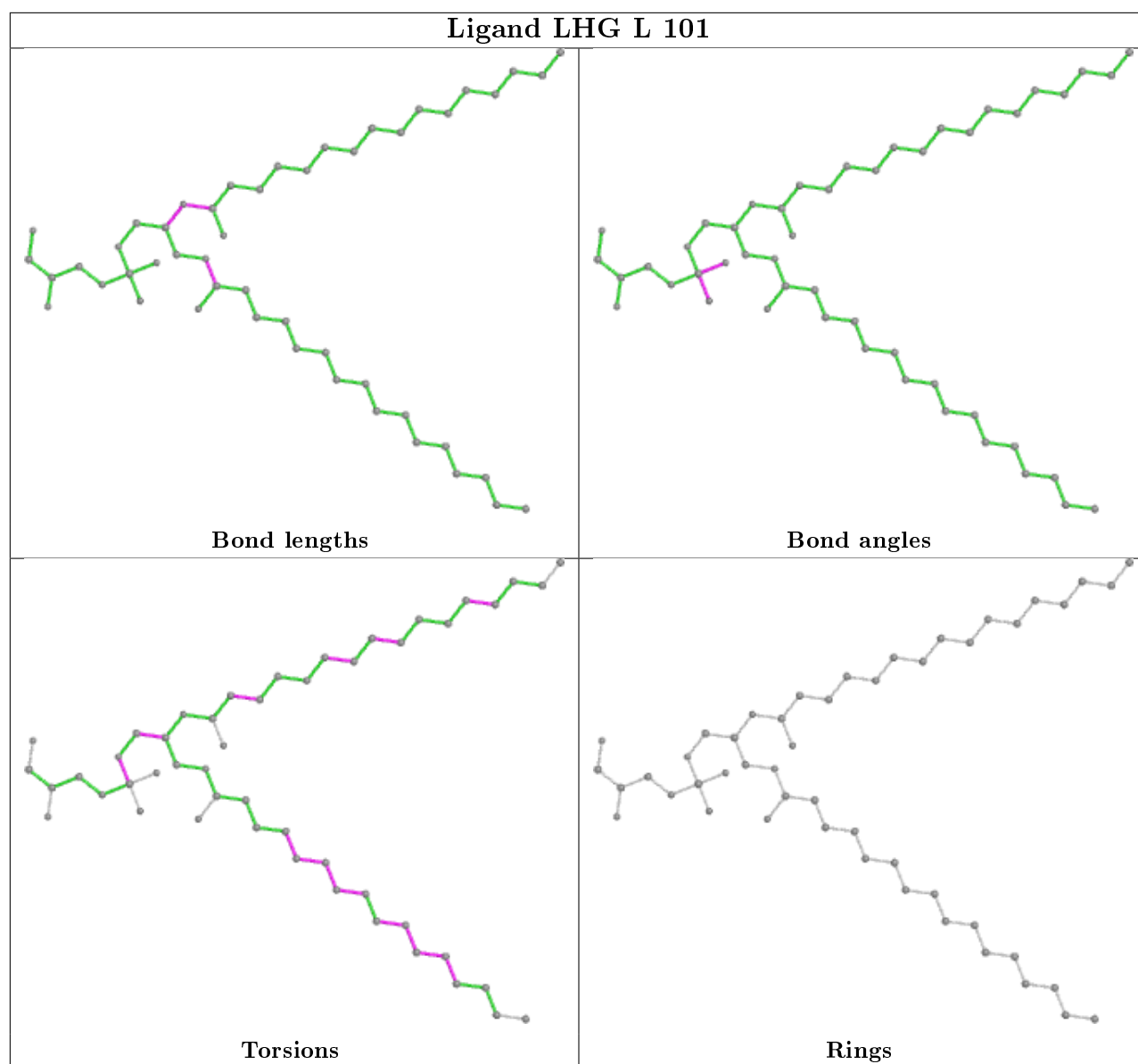


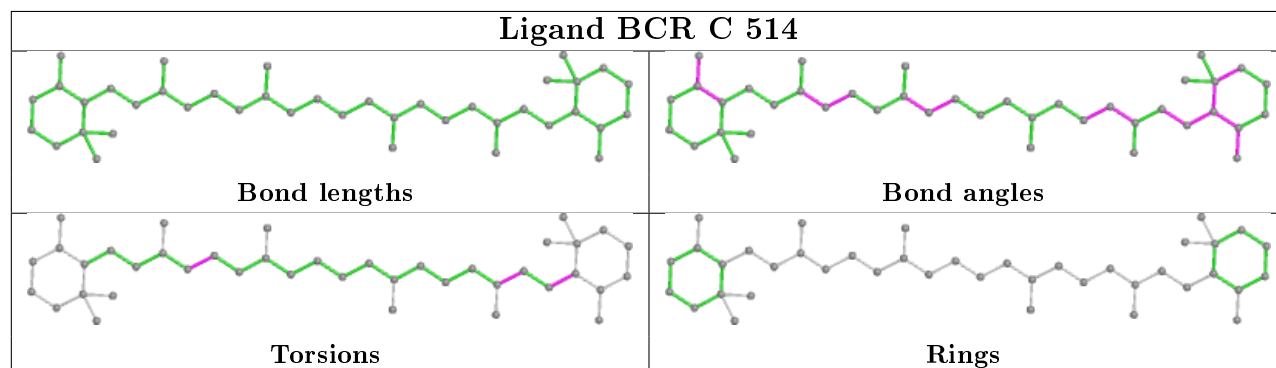
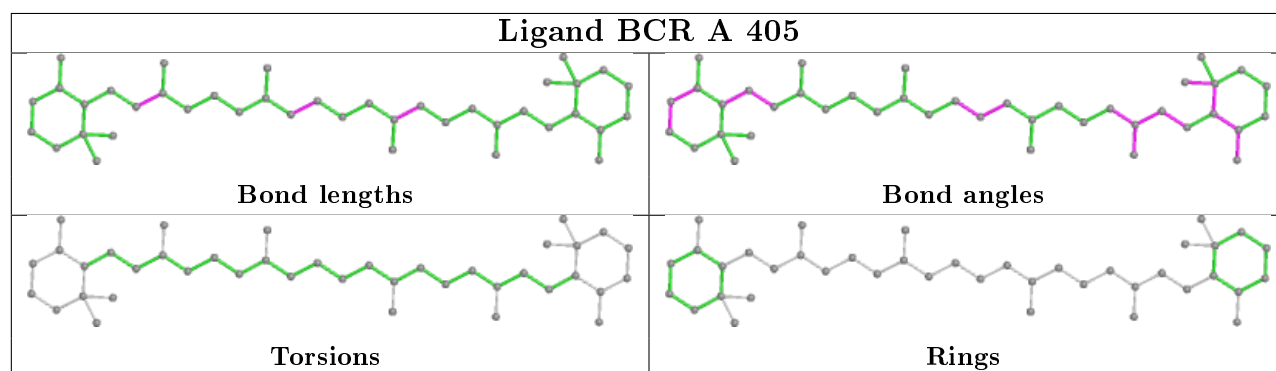
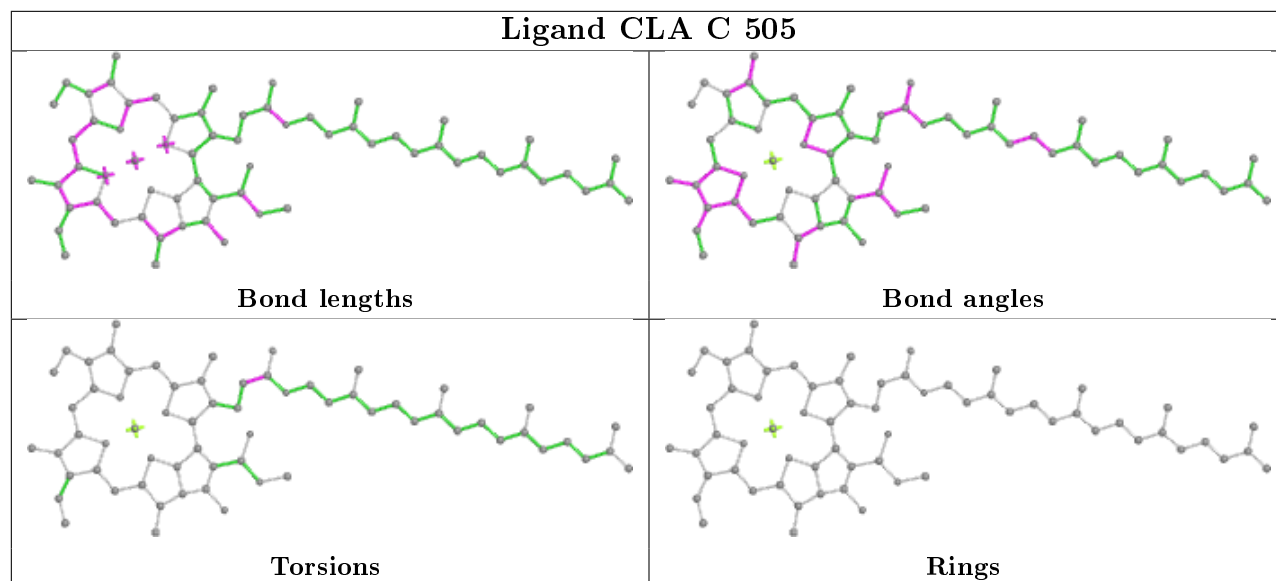
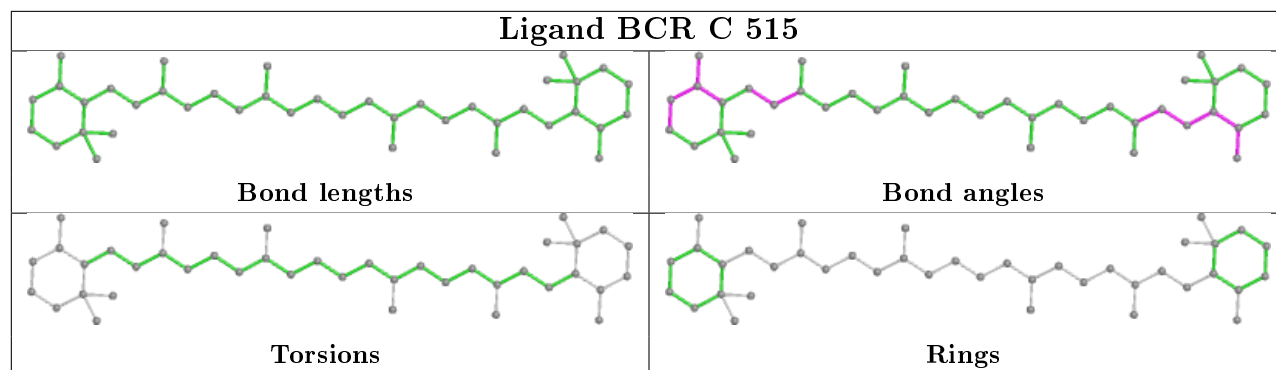


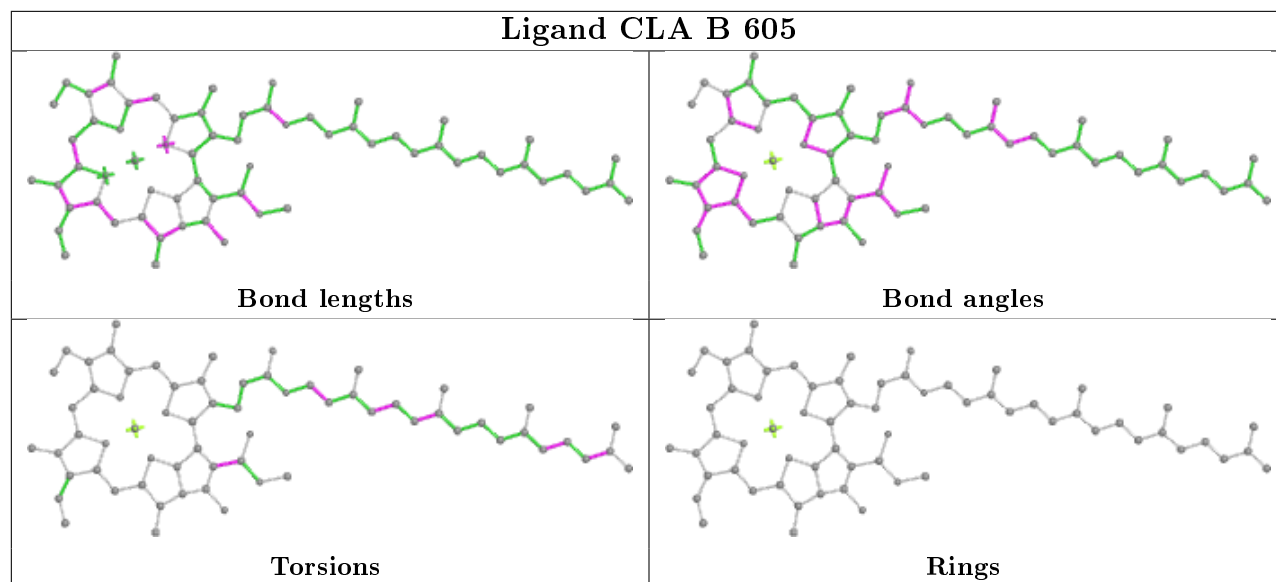
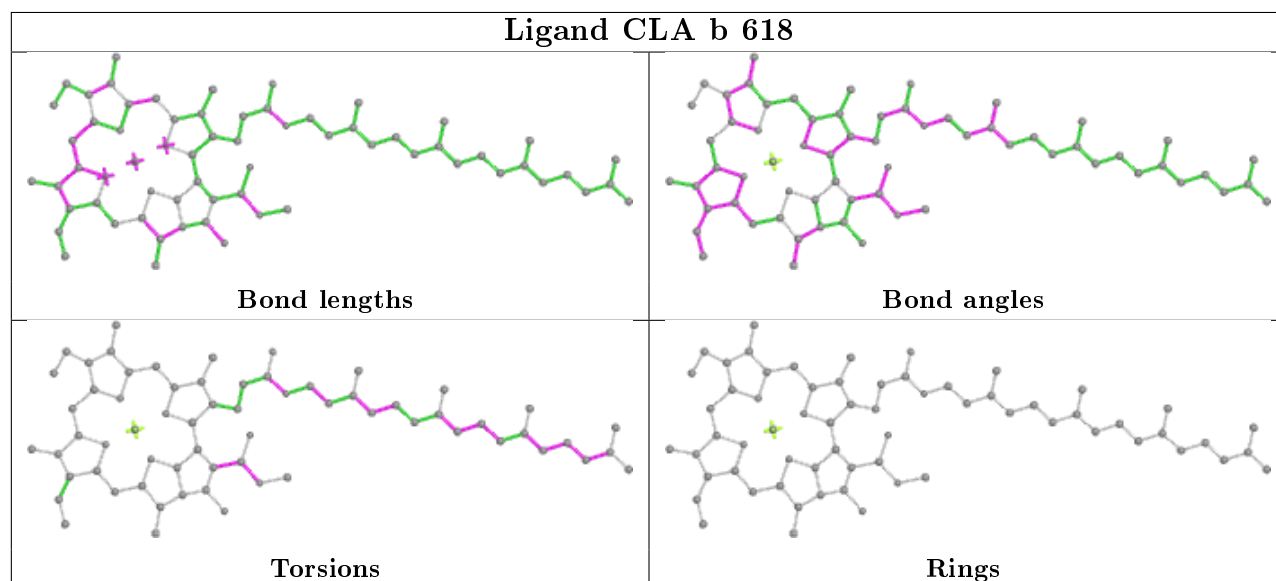
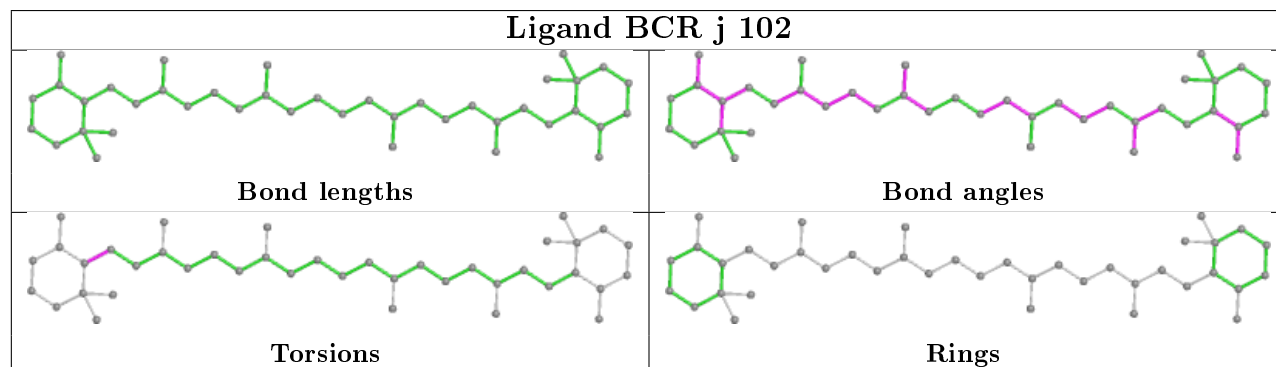


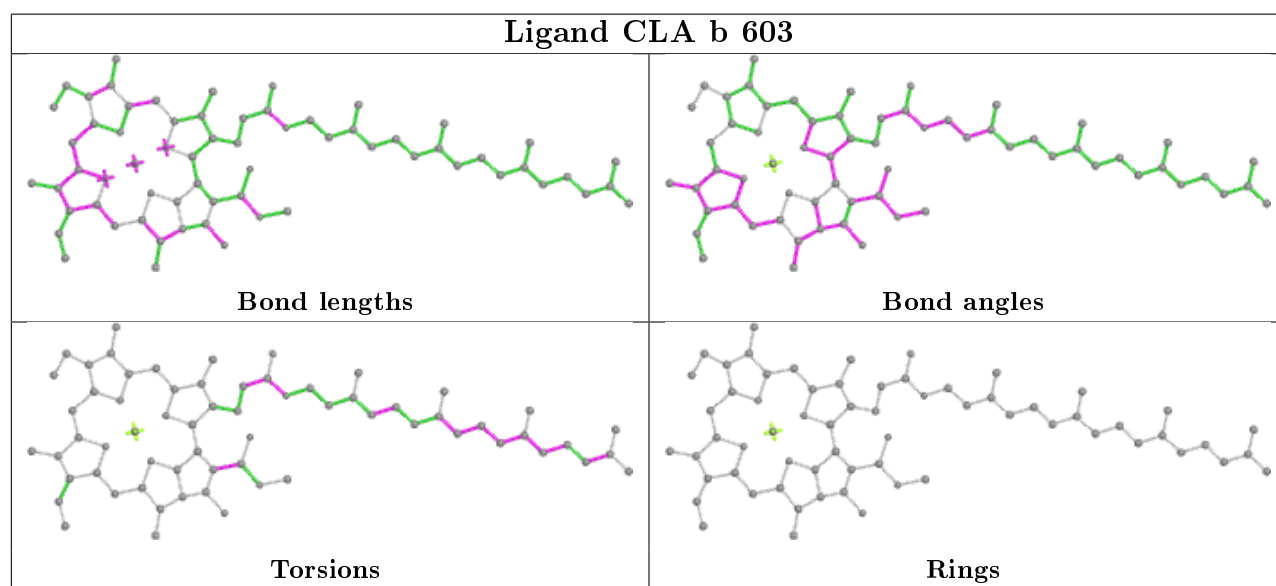
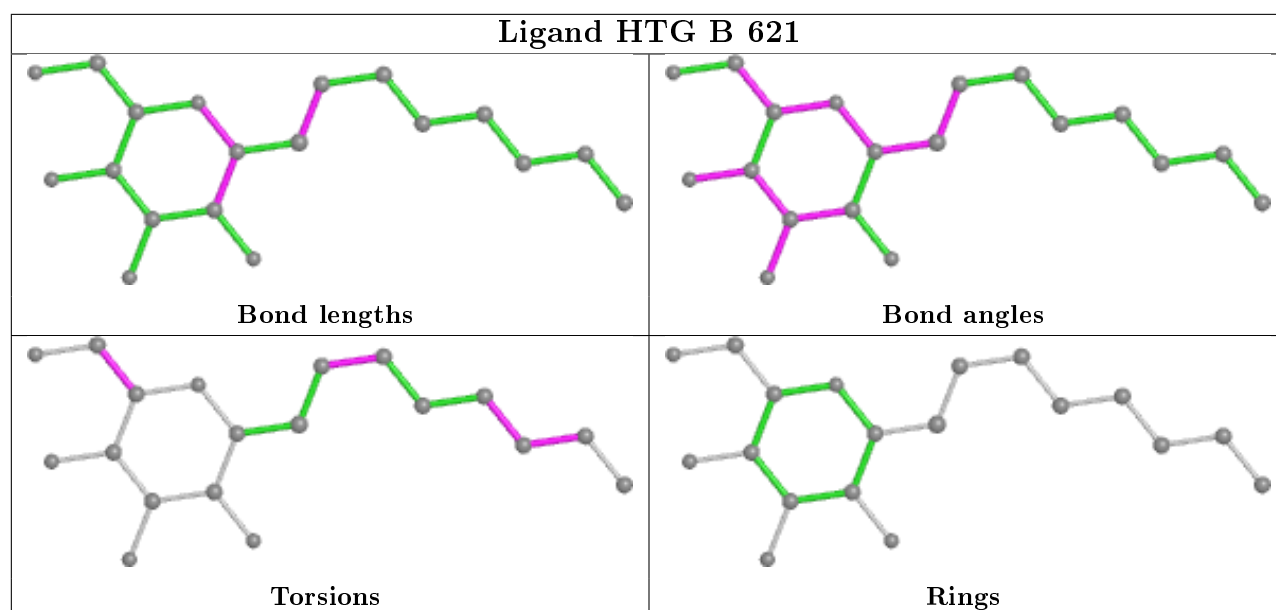


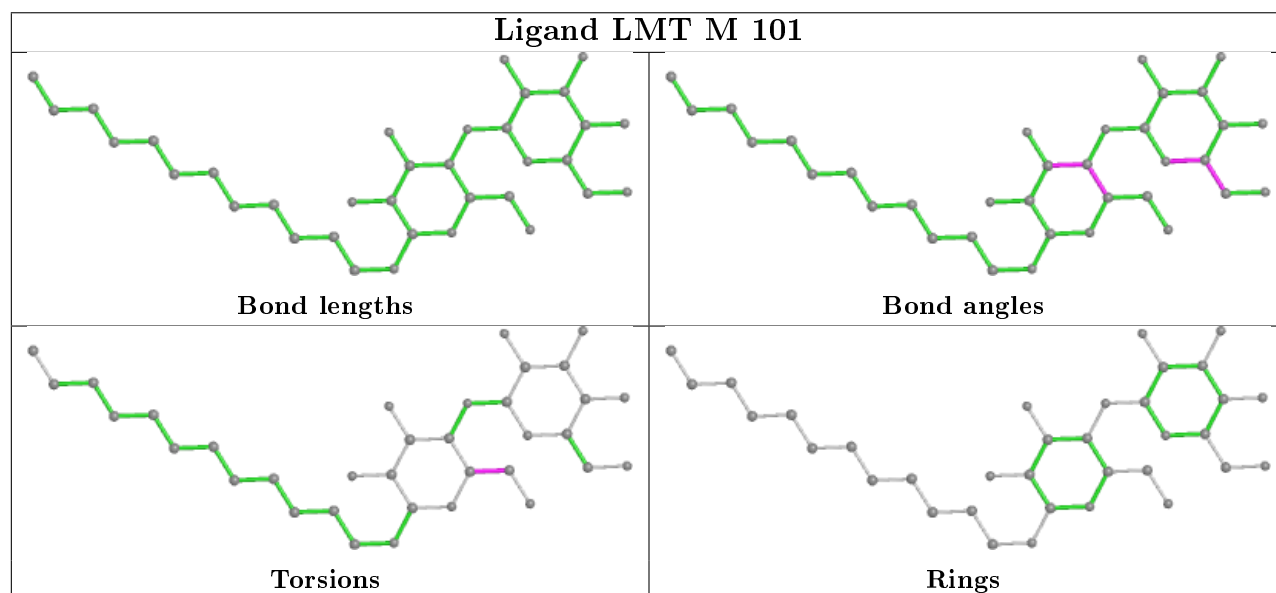
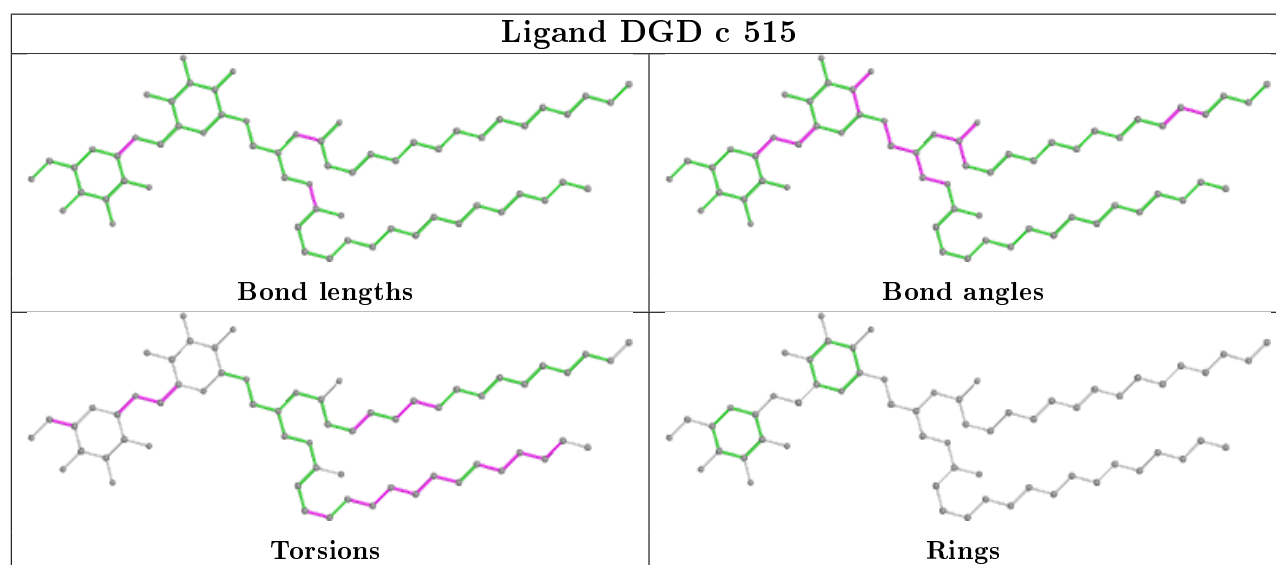
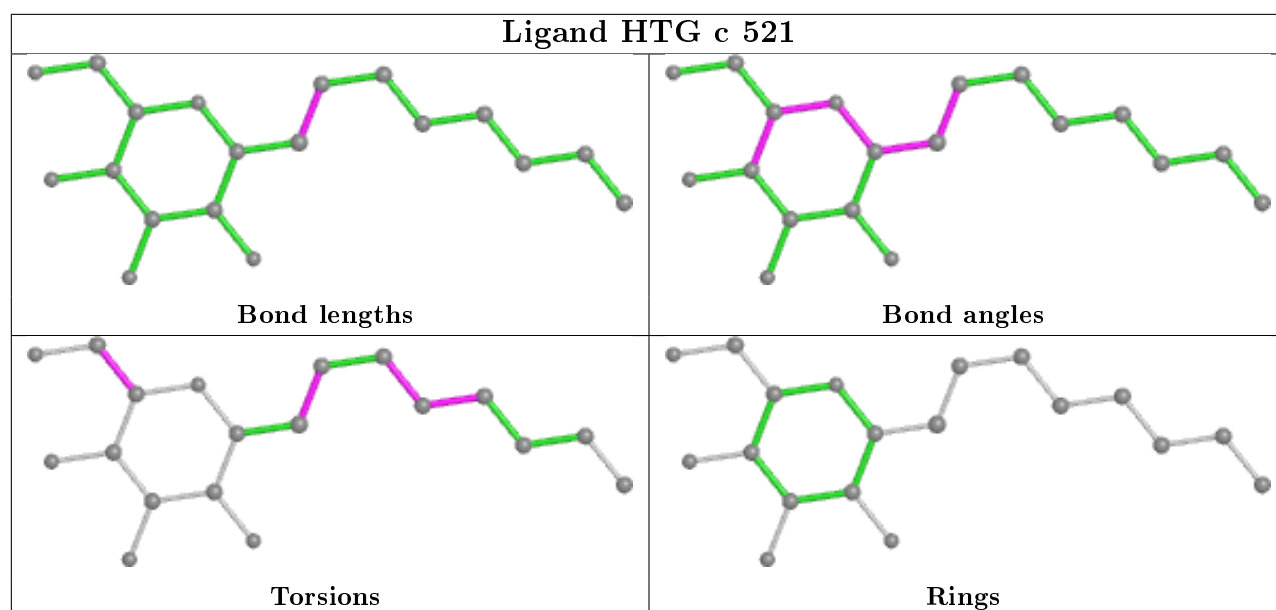




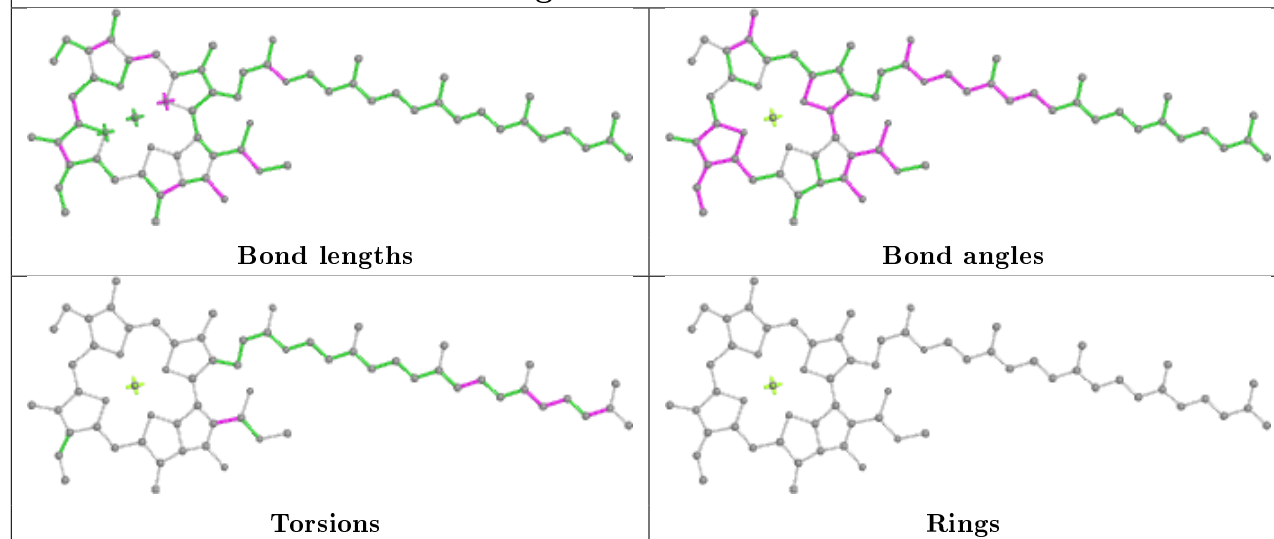
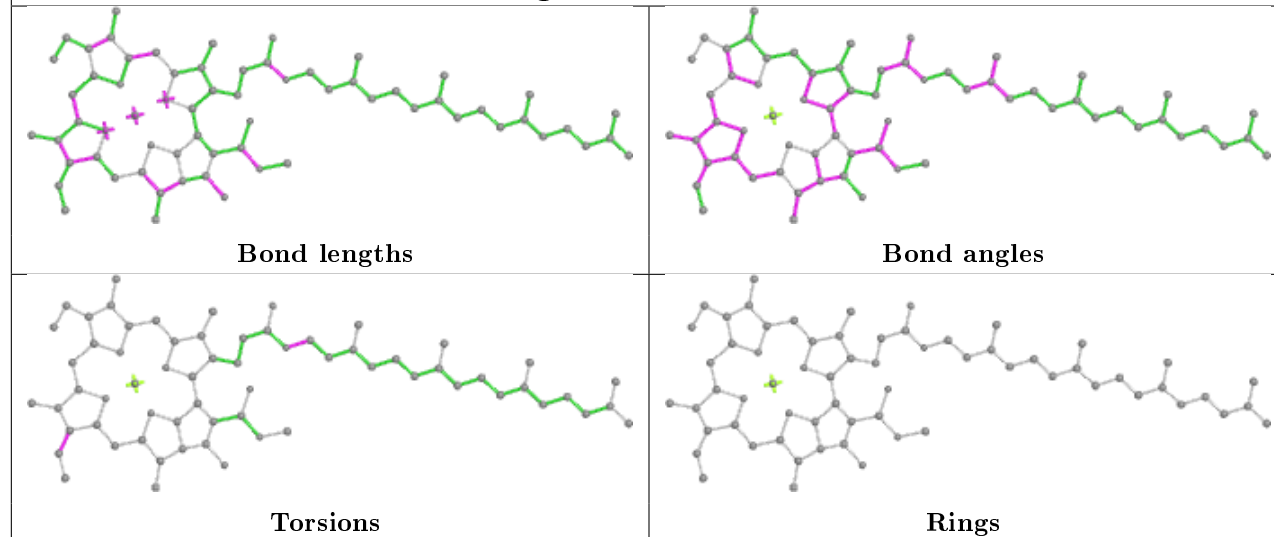


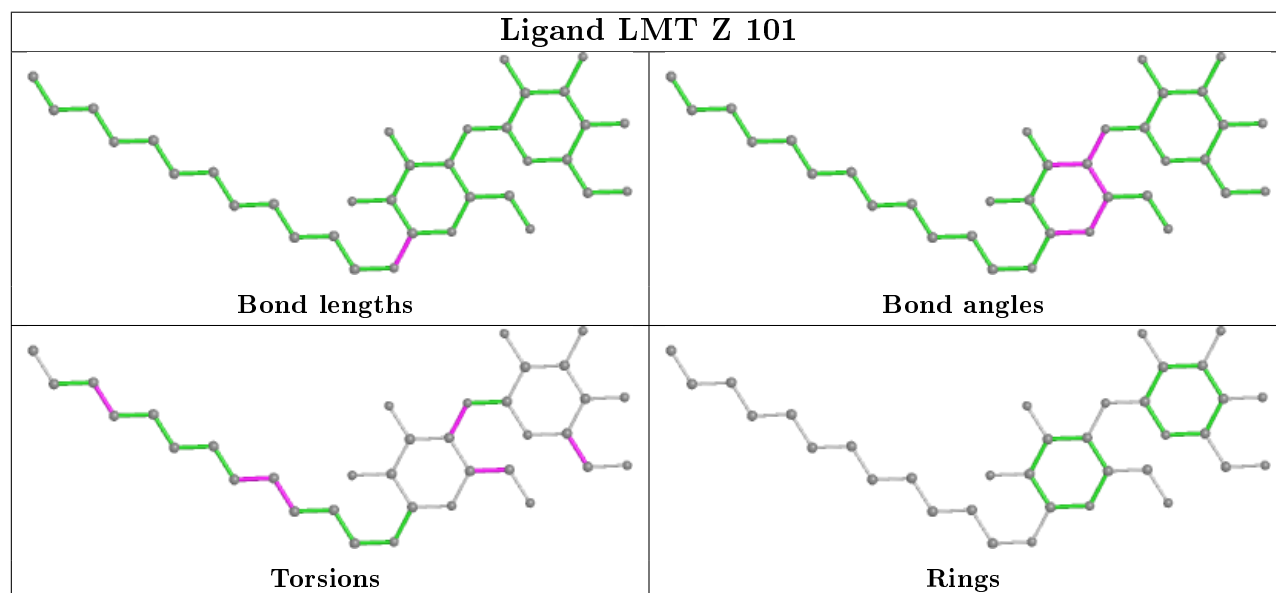
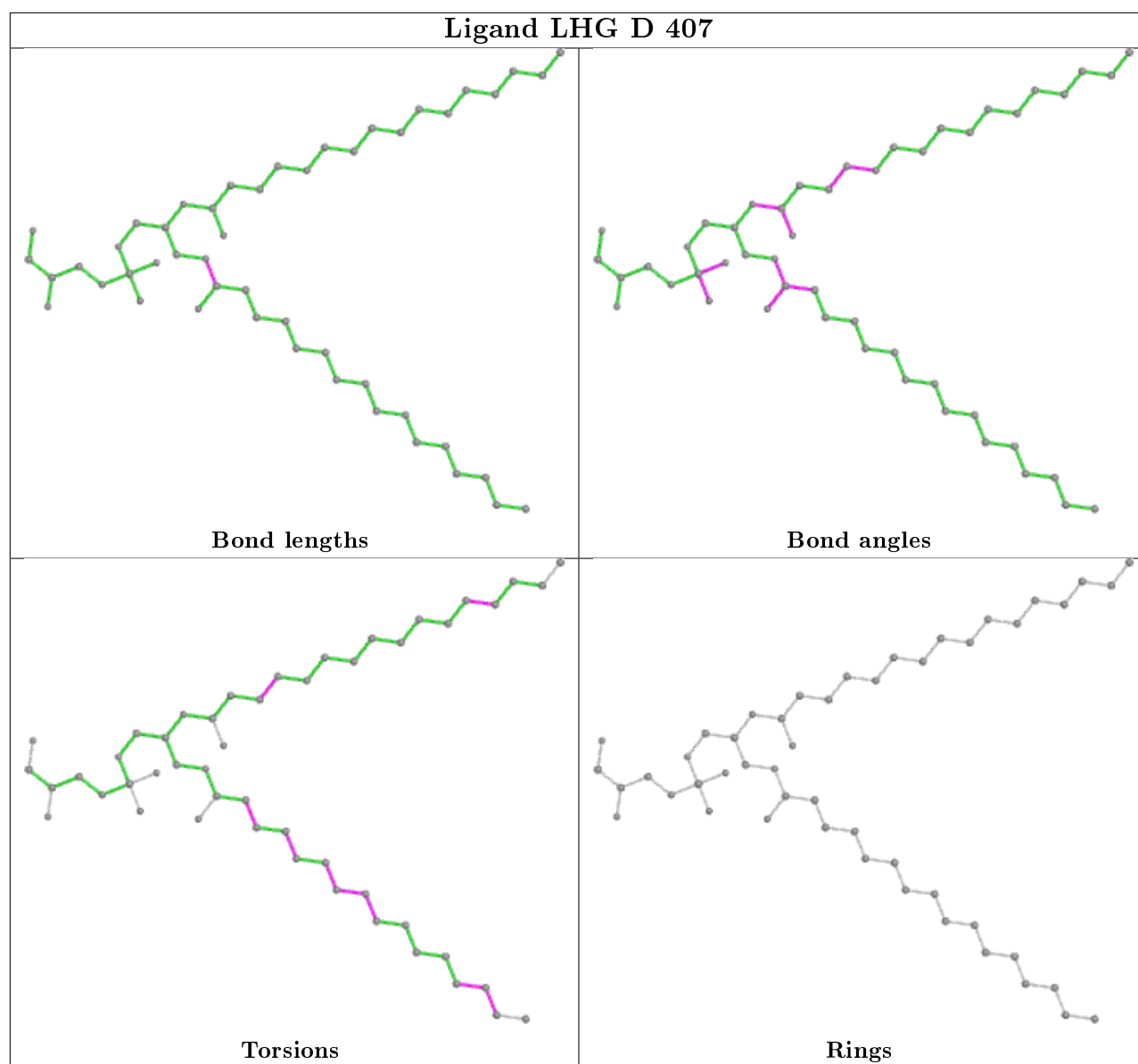
**Ligand CLA B 605****Ligand CLA b 618****Ligand BCR j 102**

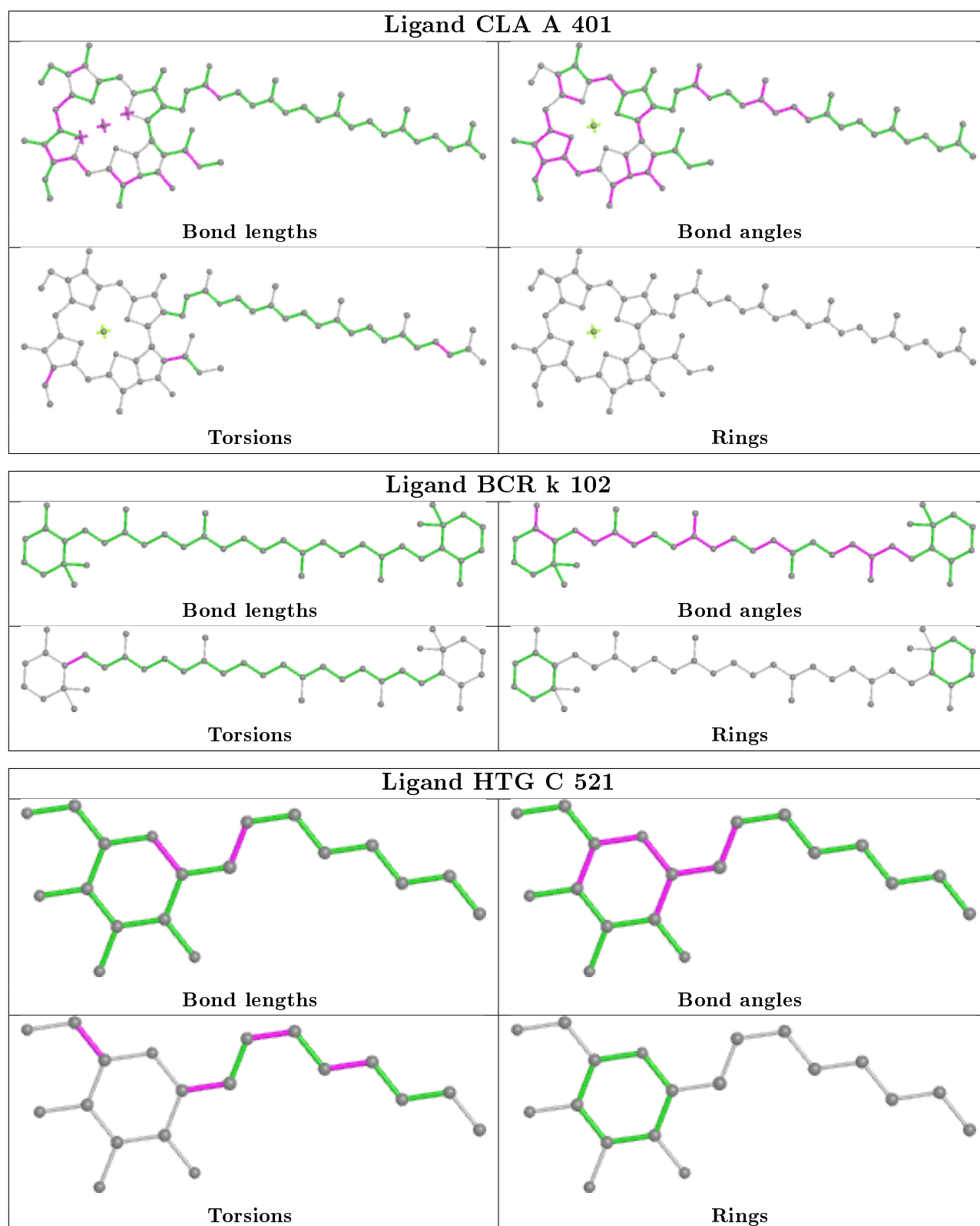




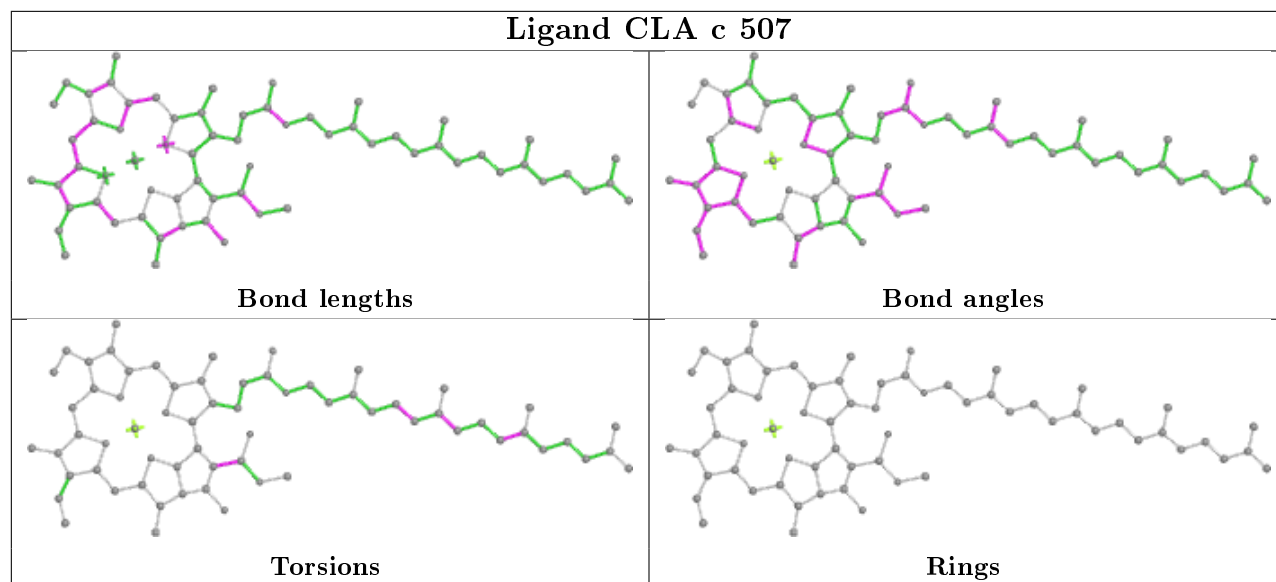


**Ligand CLA b 613****Ligand CLA d 402**

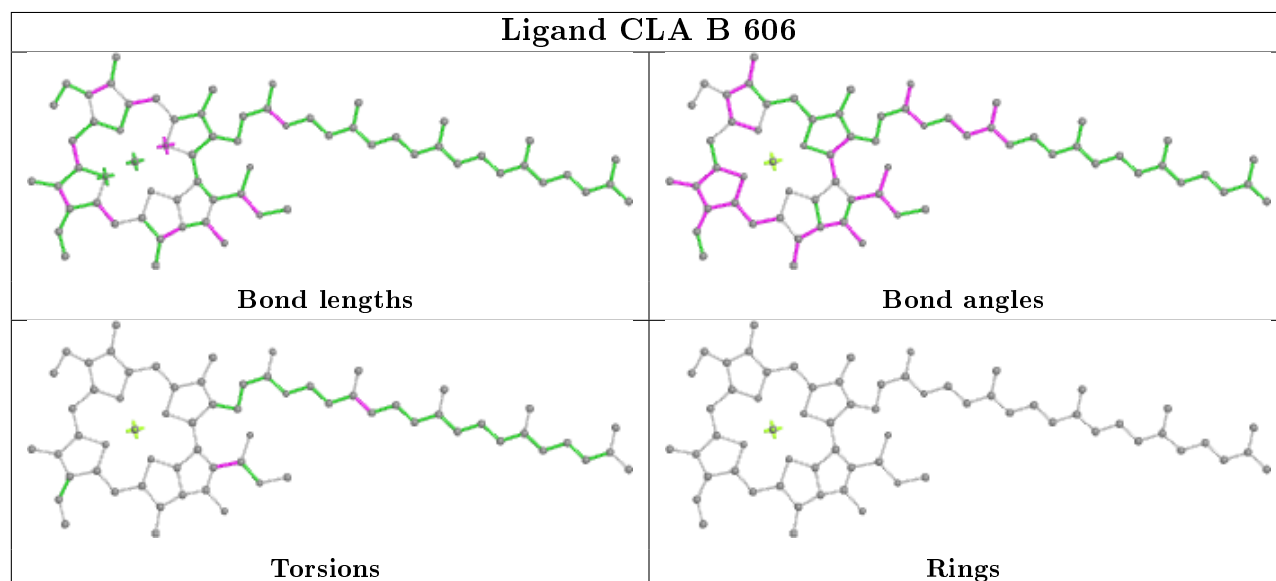




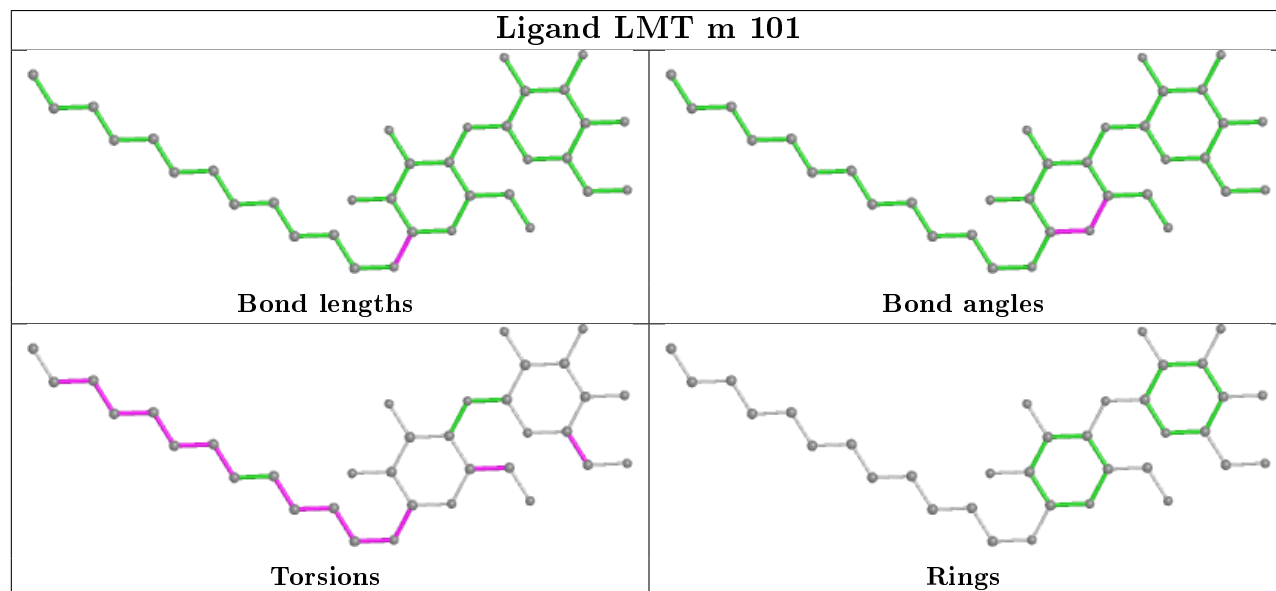
## Ligand CLA c 507

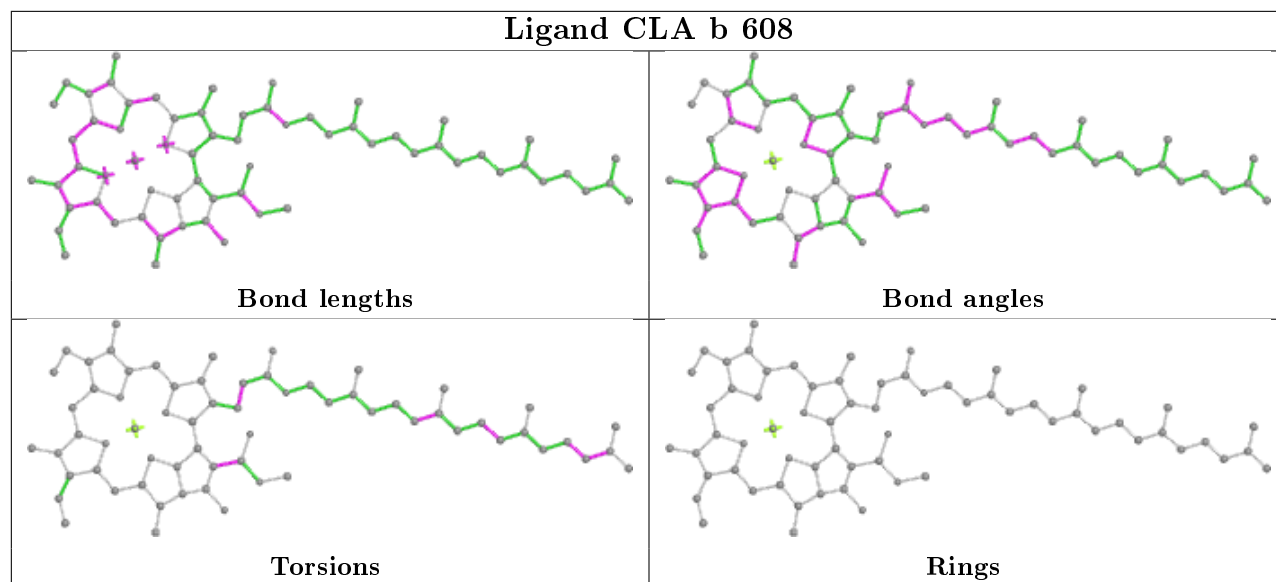
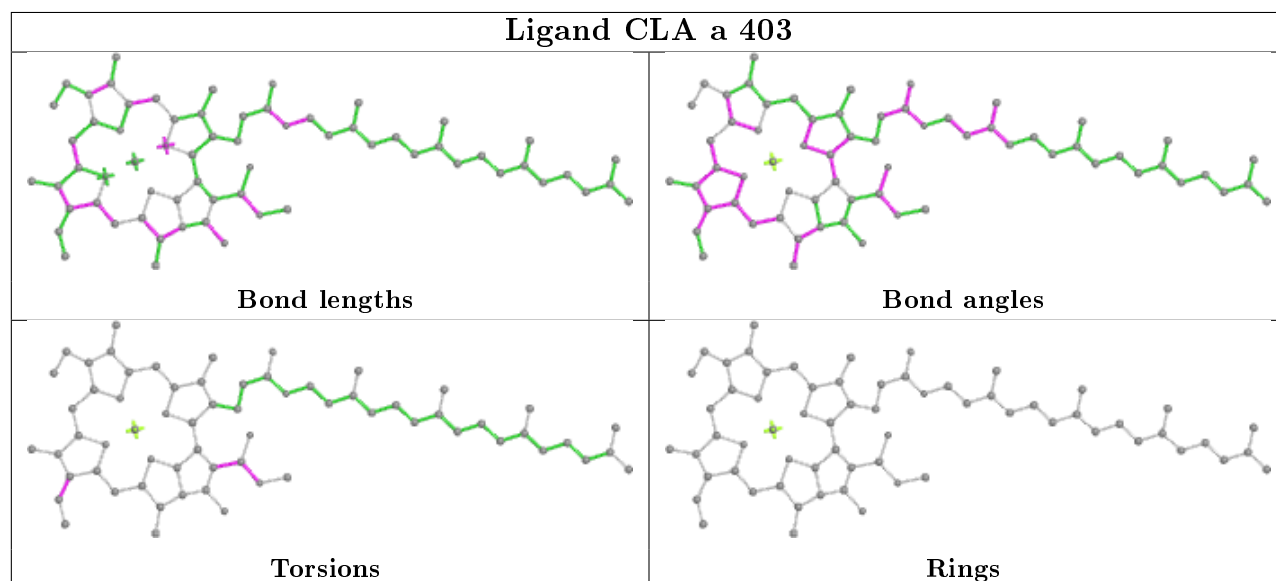
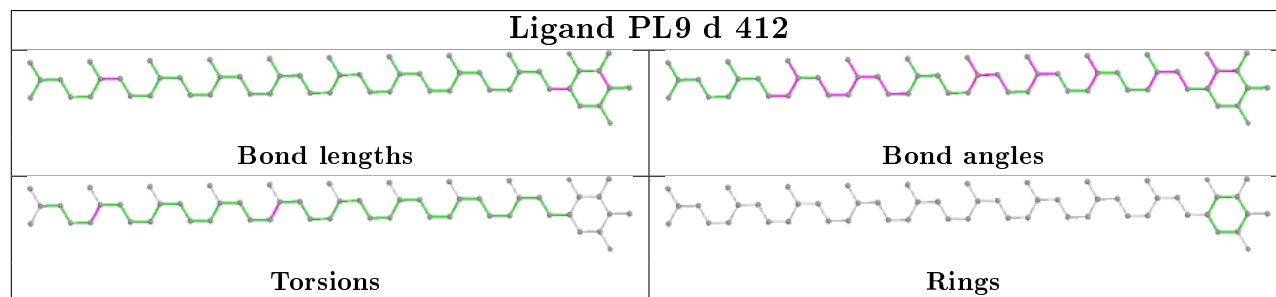


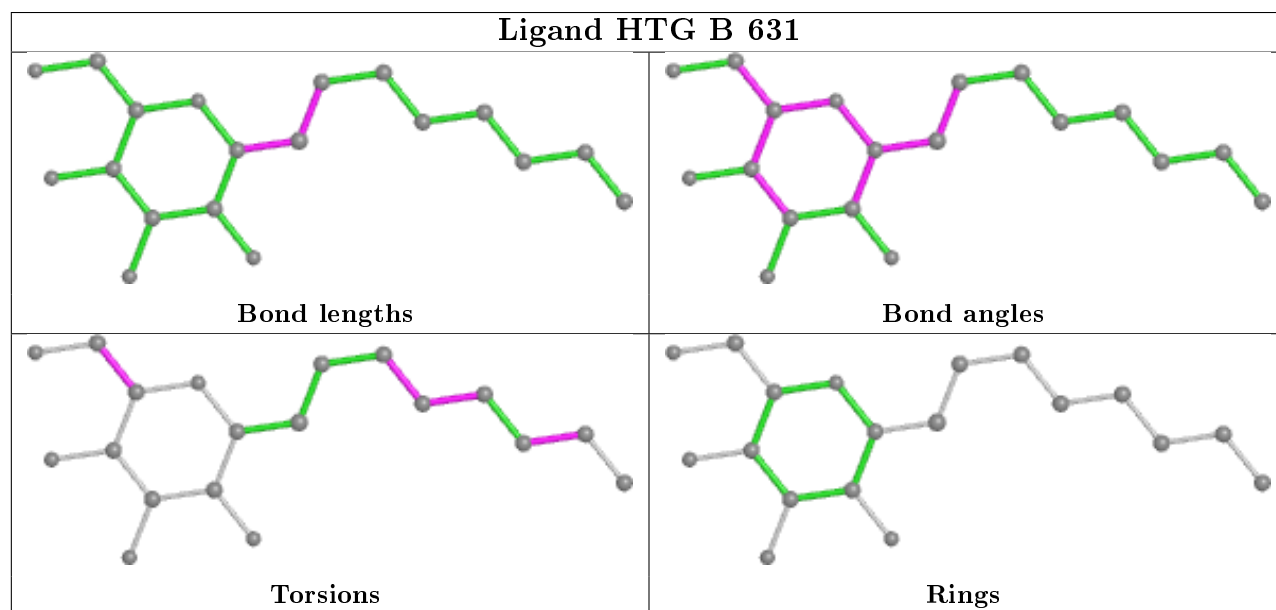
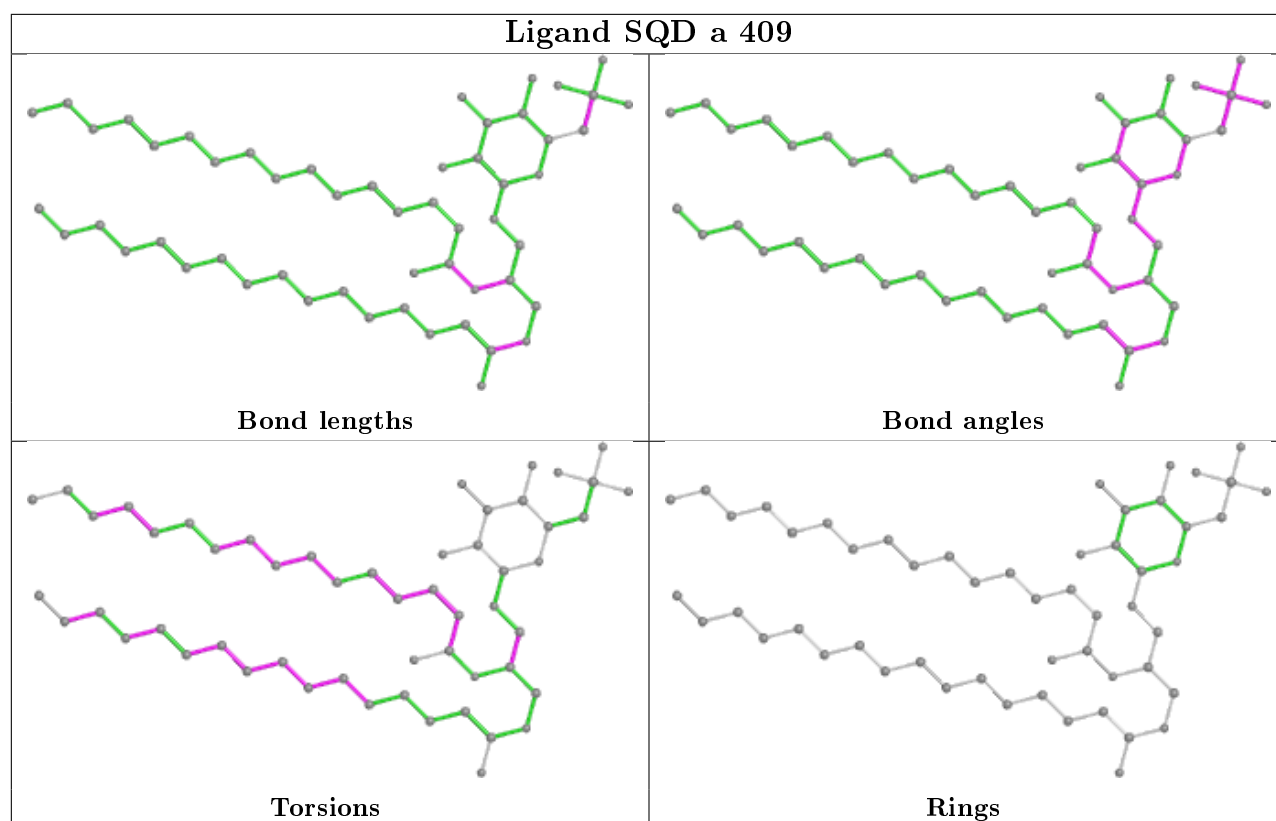
## Ligand CLA B 606

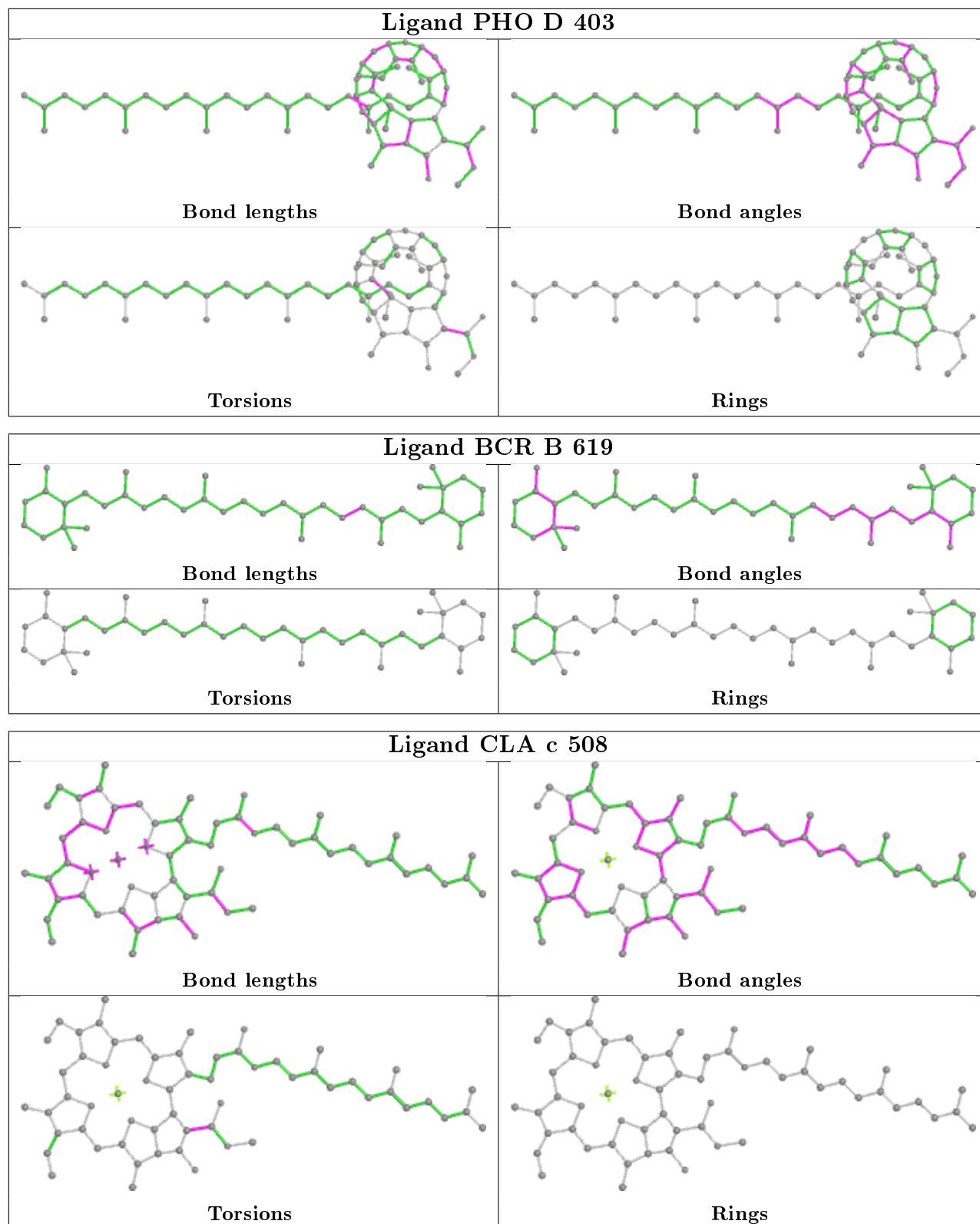


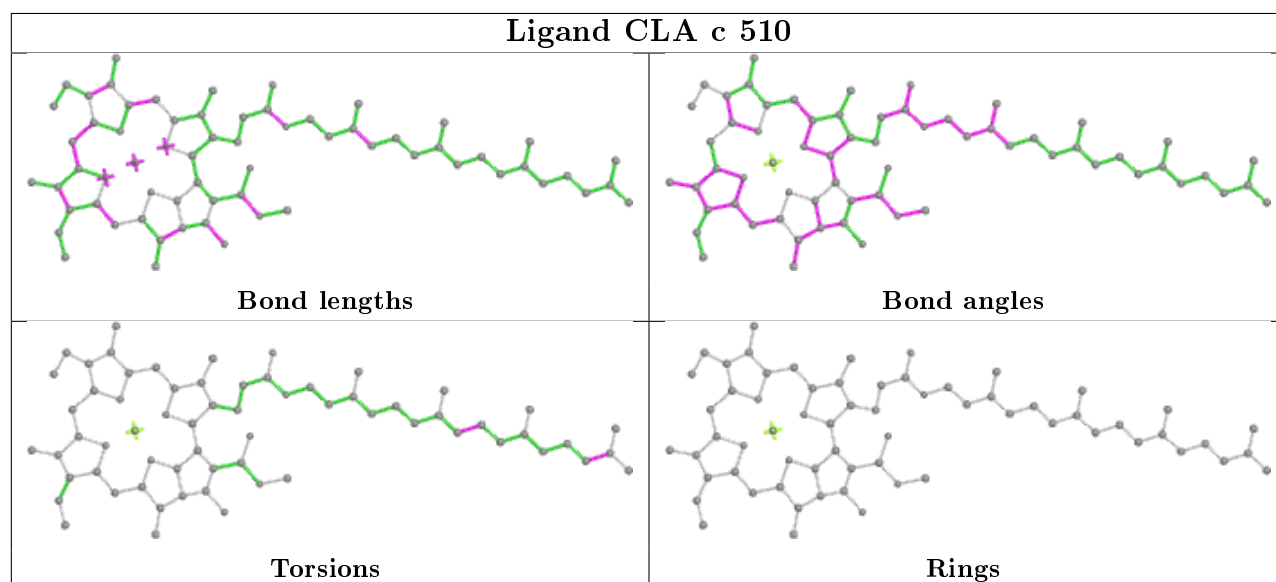
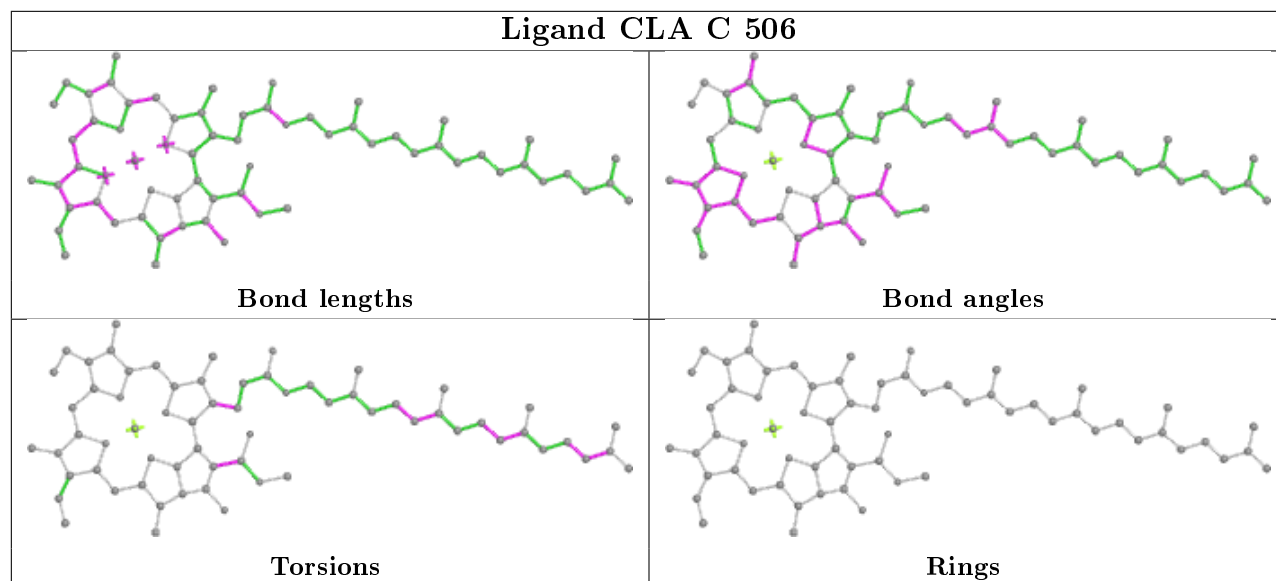
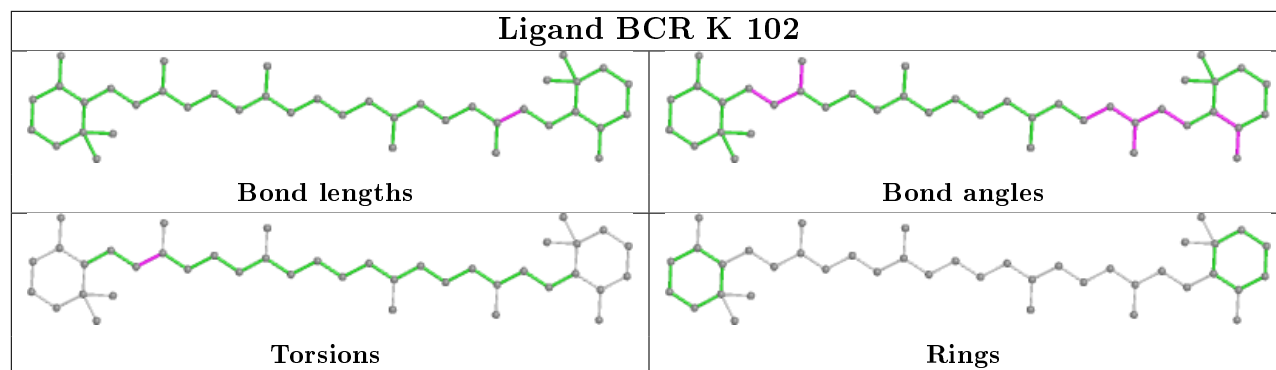
## Ligand LMT m 101



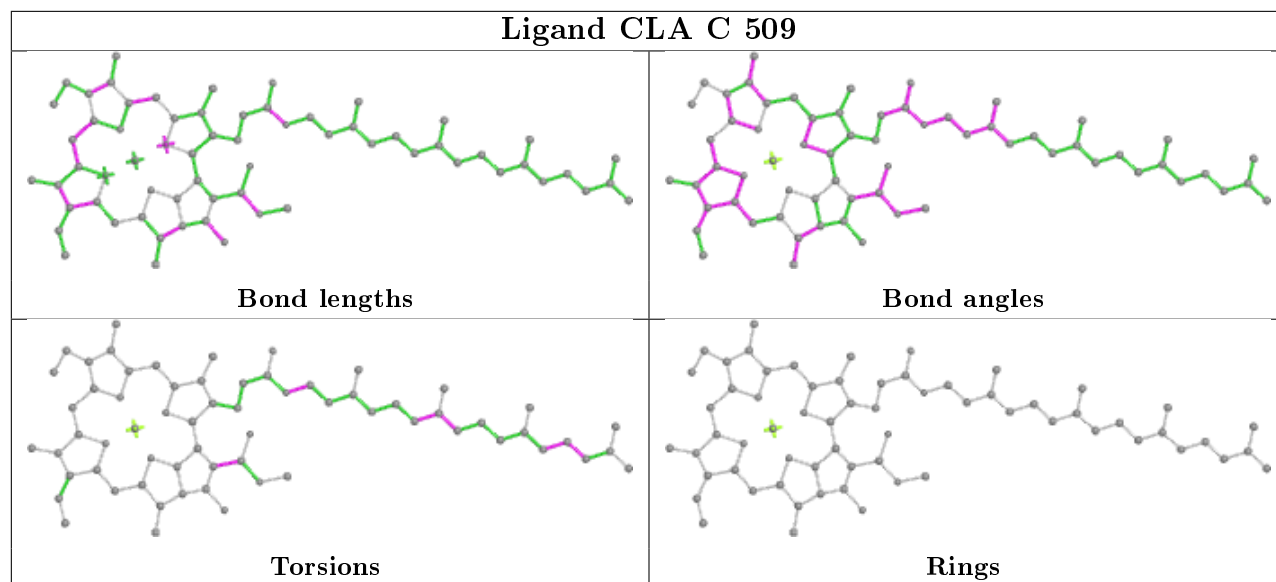
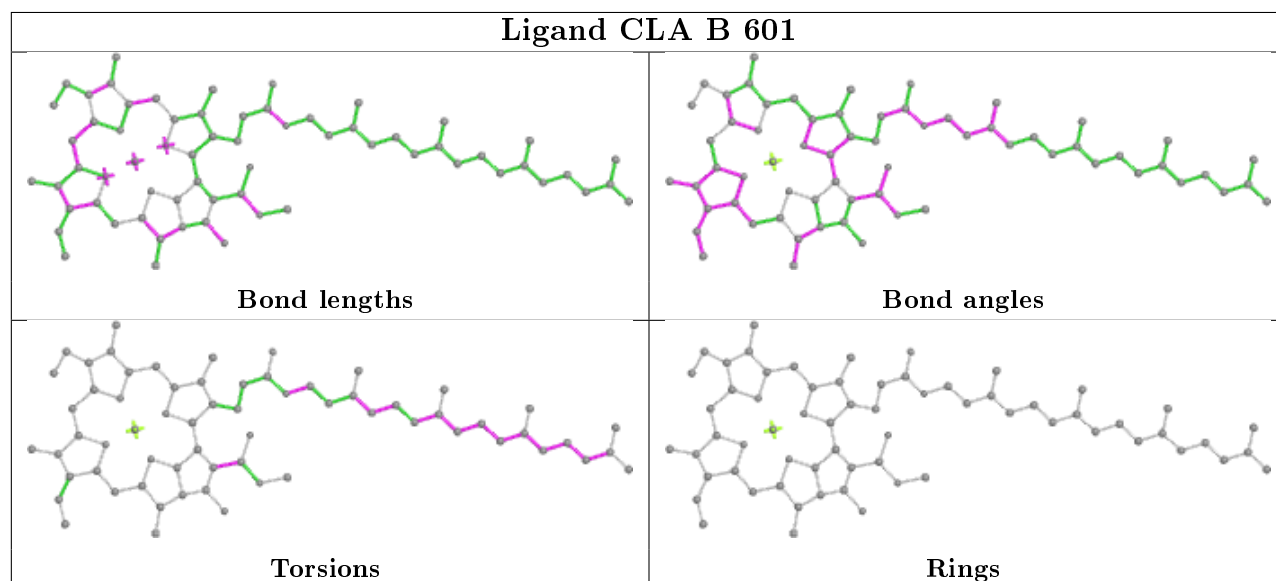
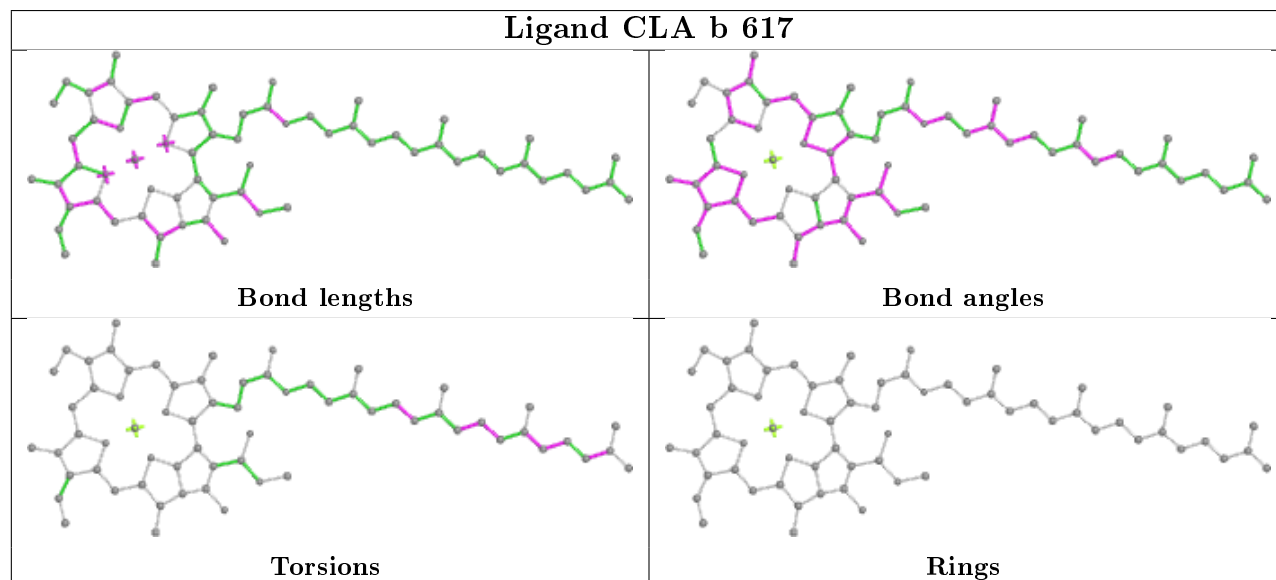
**Ligand CLA b 608****Ligand CLA a 403****Ligand PL9 d 412**

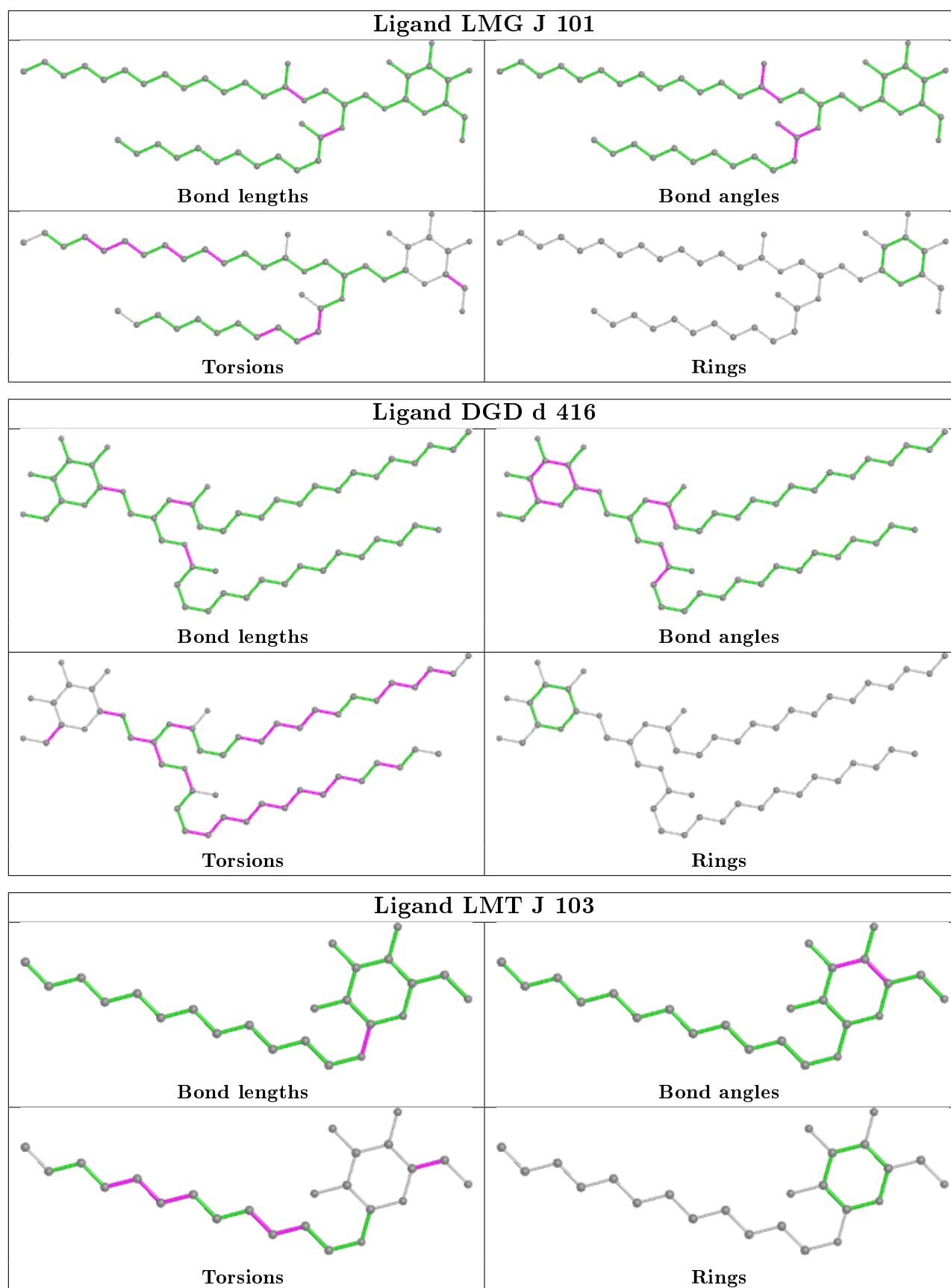


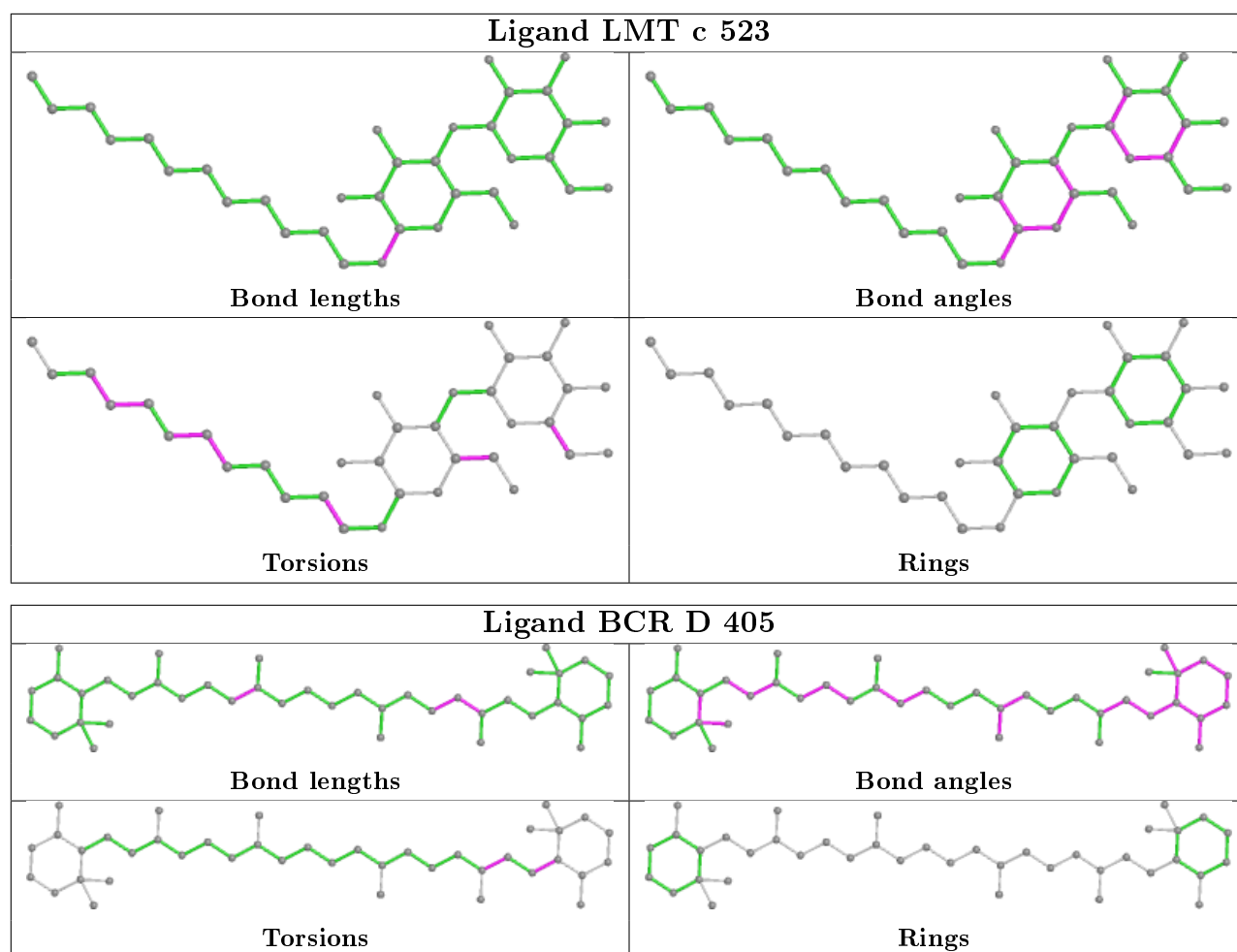


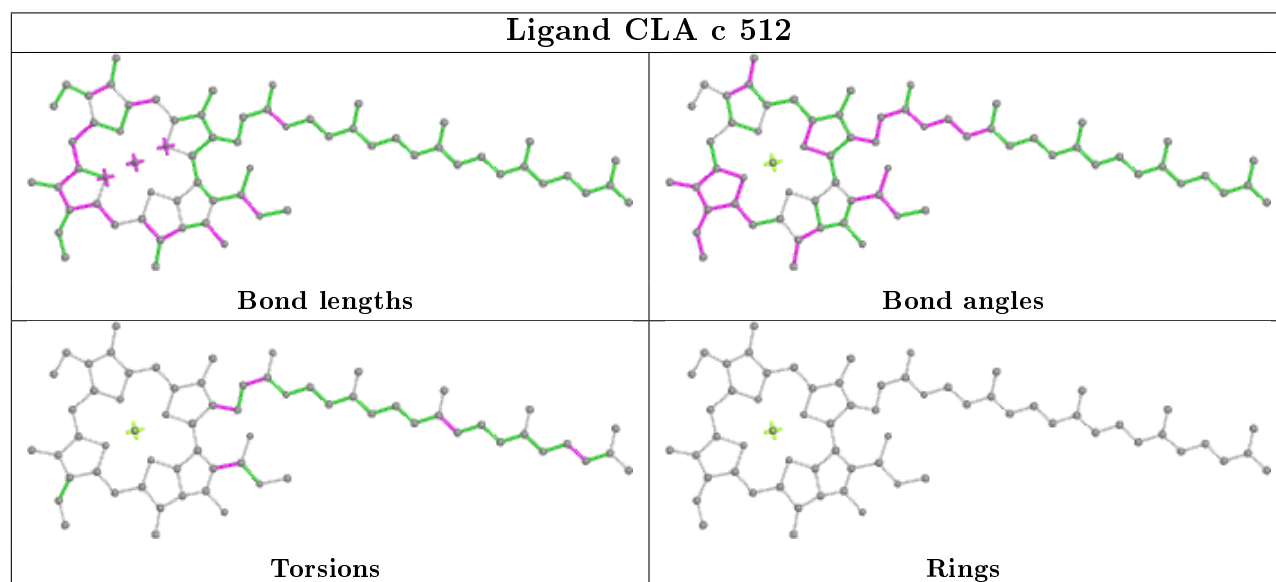
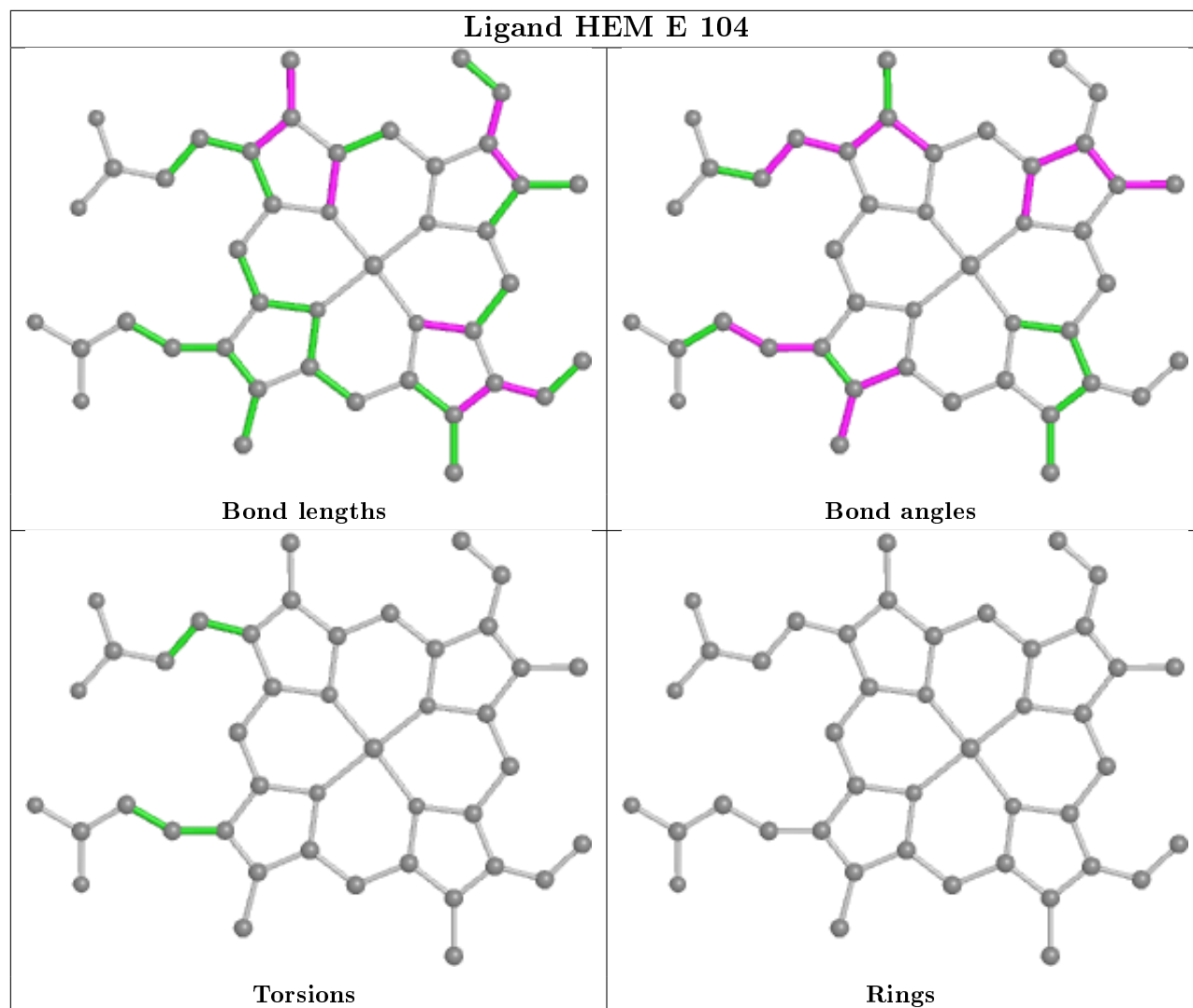




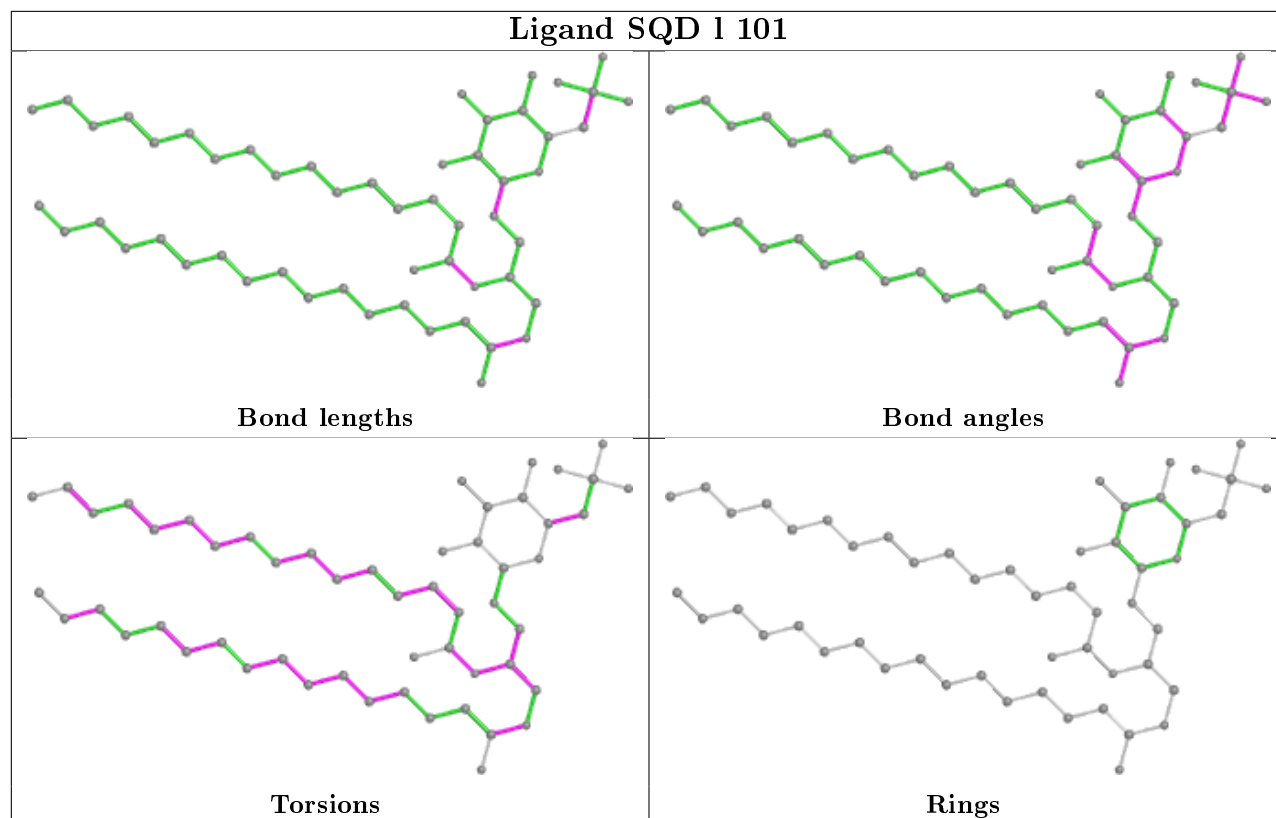
**Ligand CLA C 509****Ligand CLA B 601****Ligand CLA b 617**



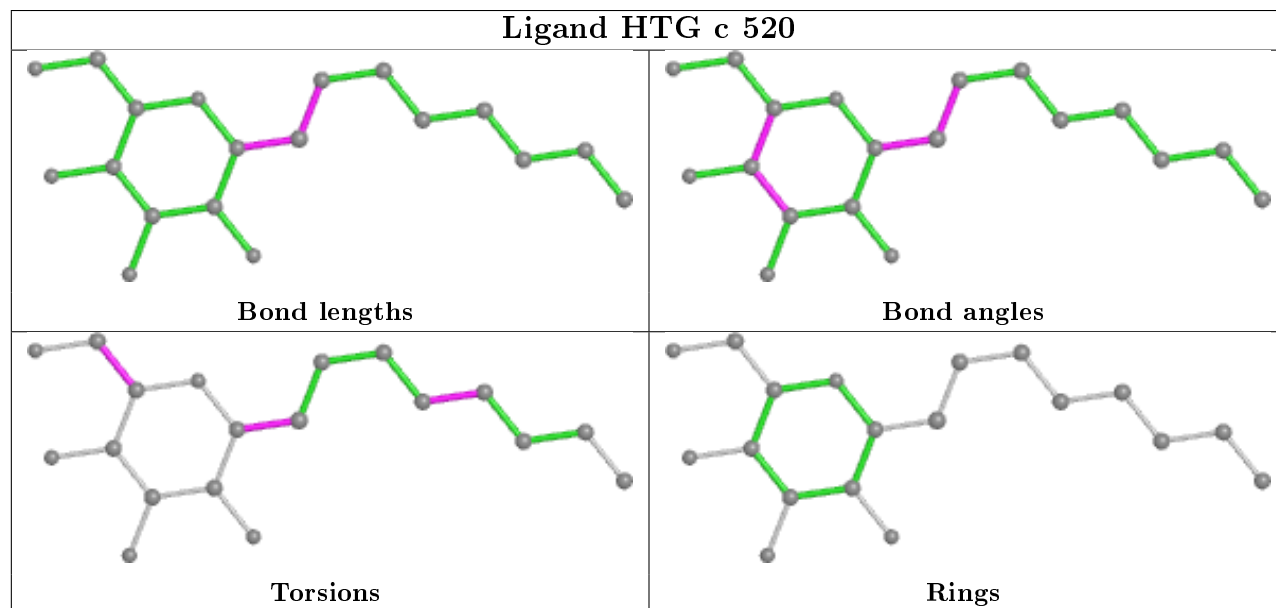


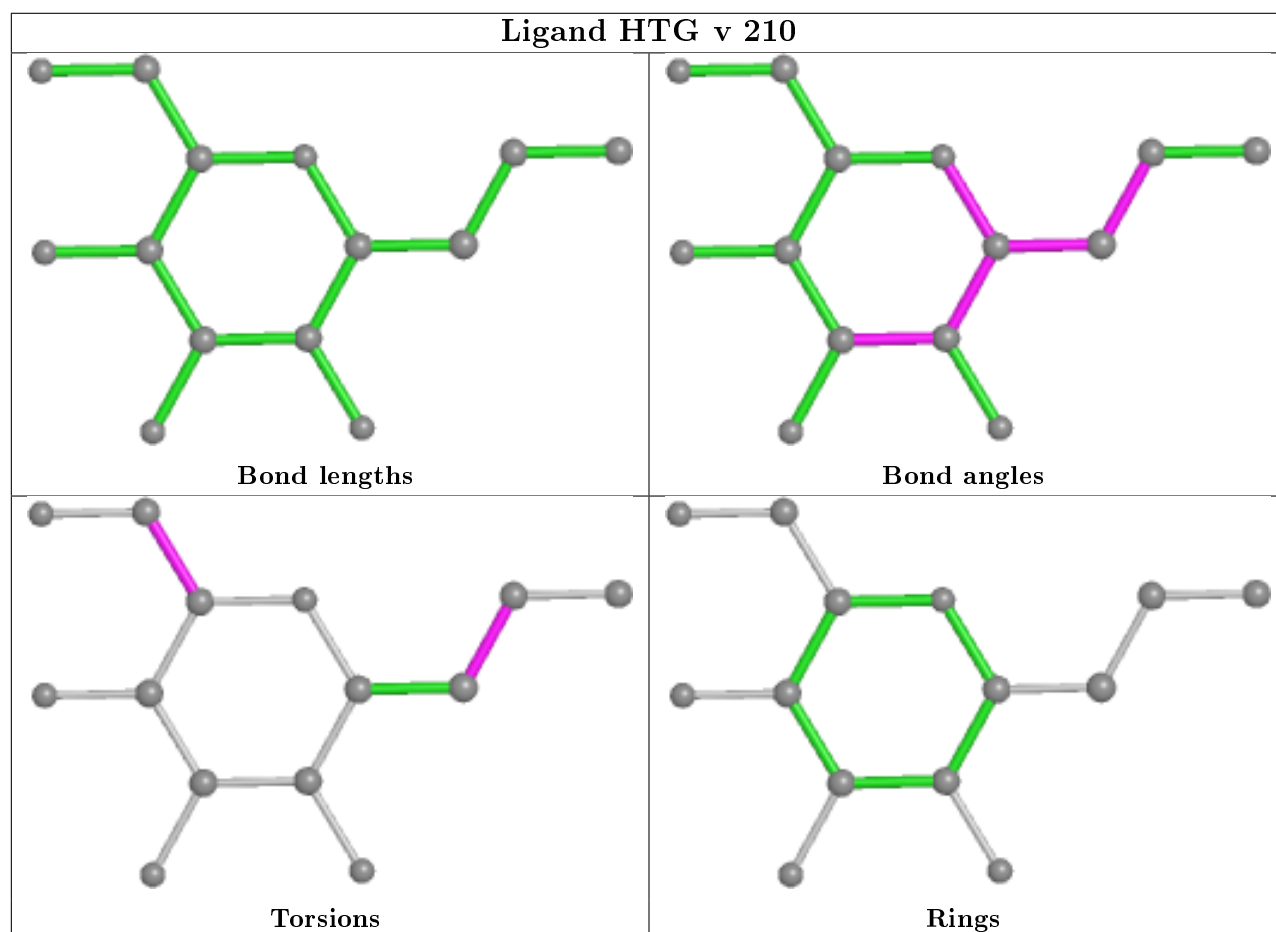
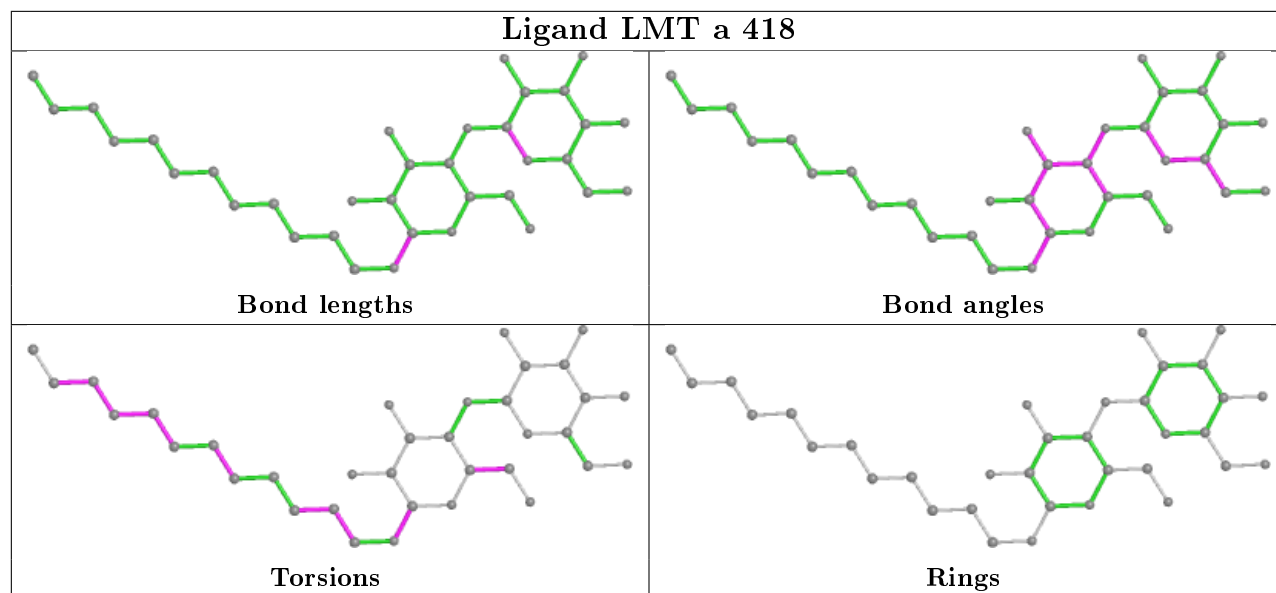


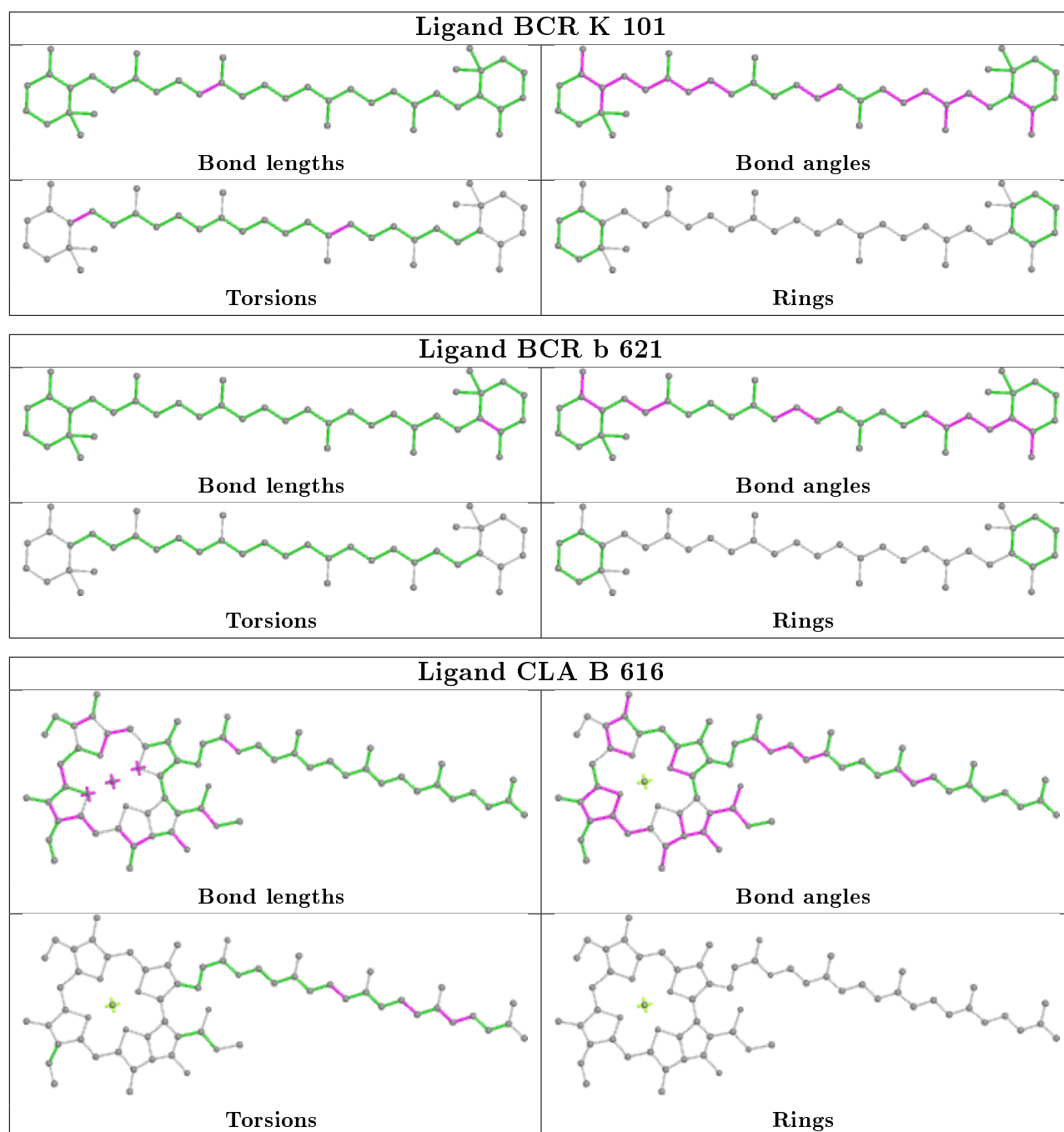
## Ligand SQD 1 101

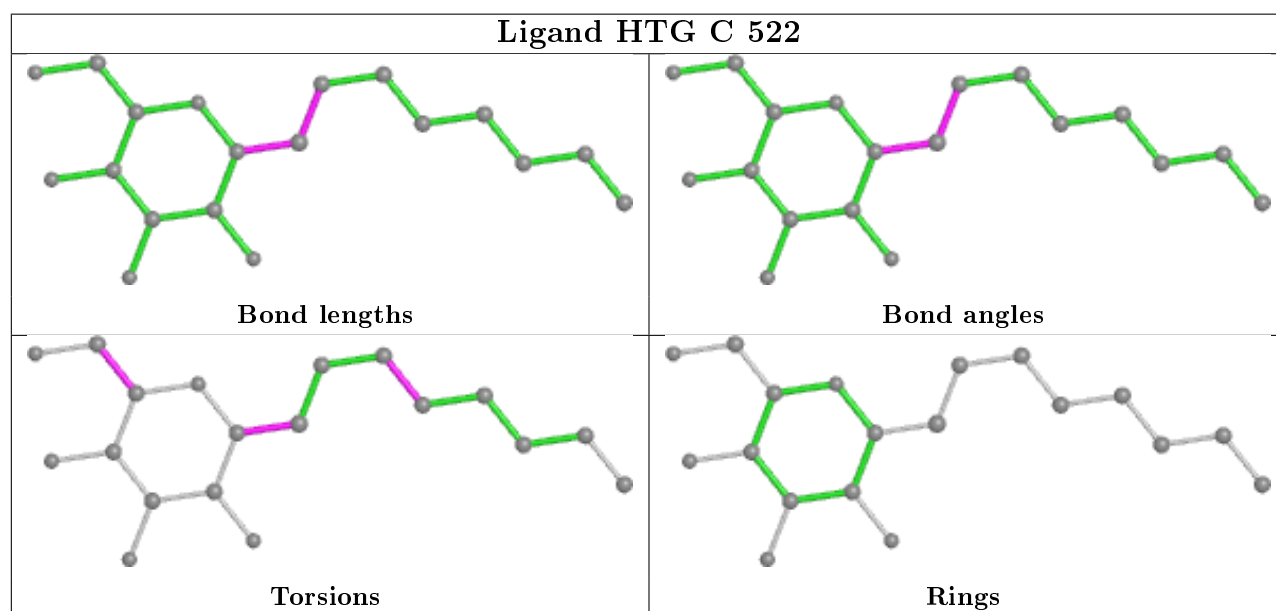
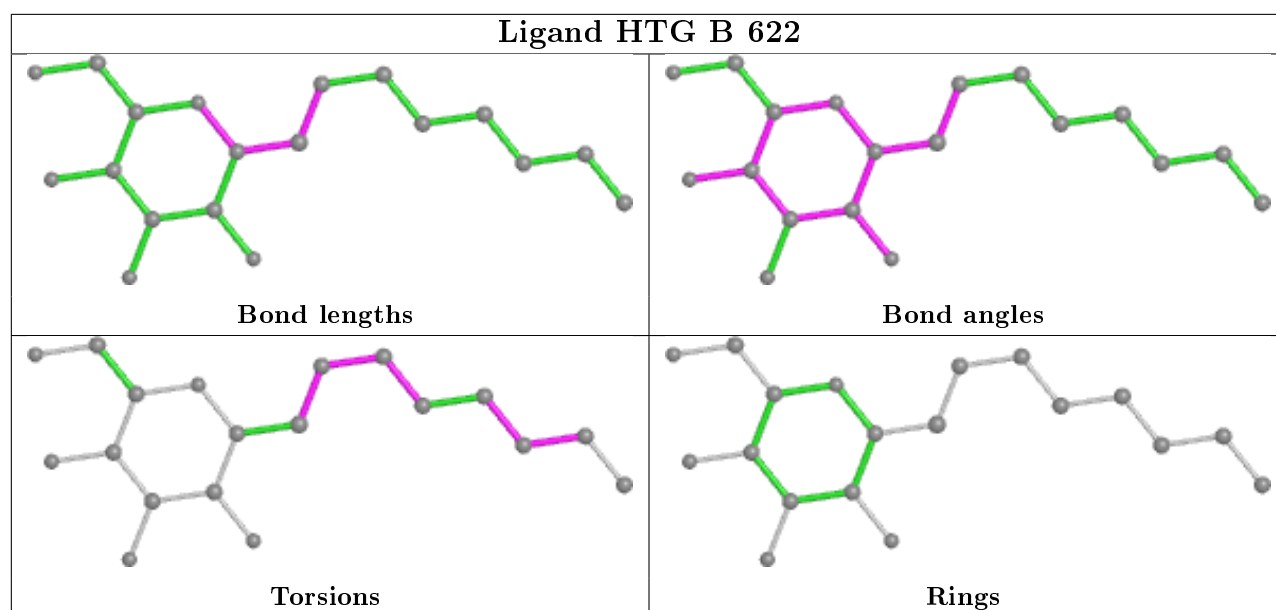


## Ligand HTG c 520

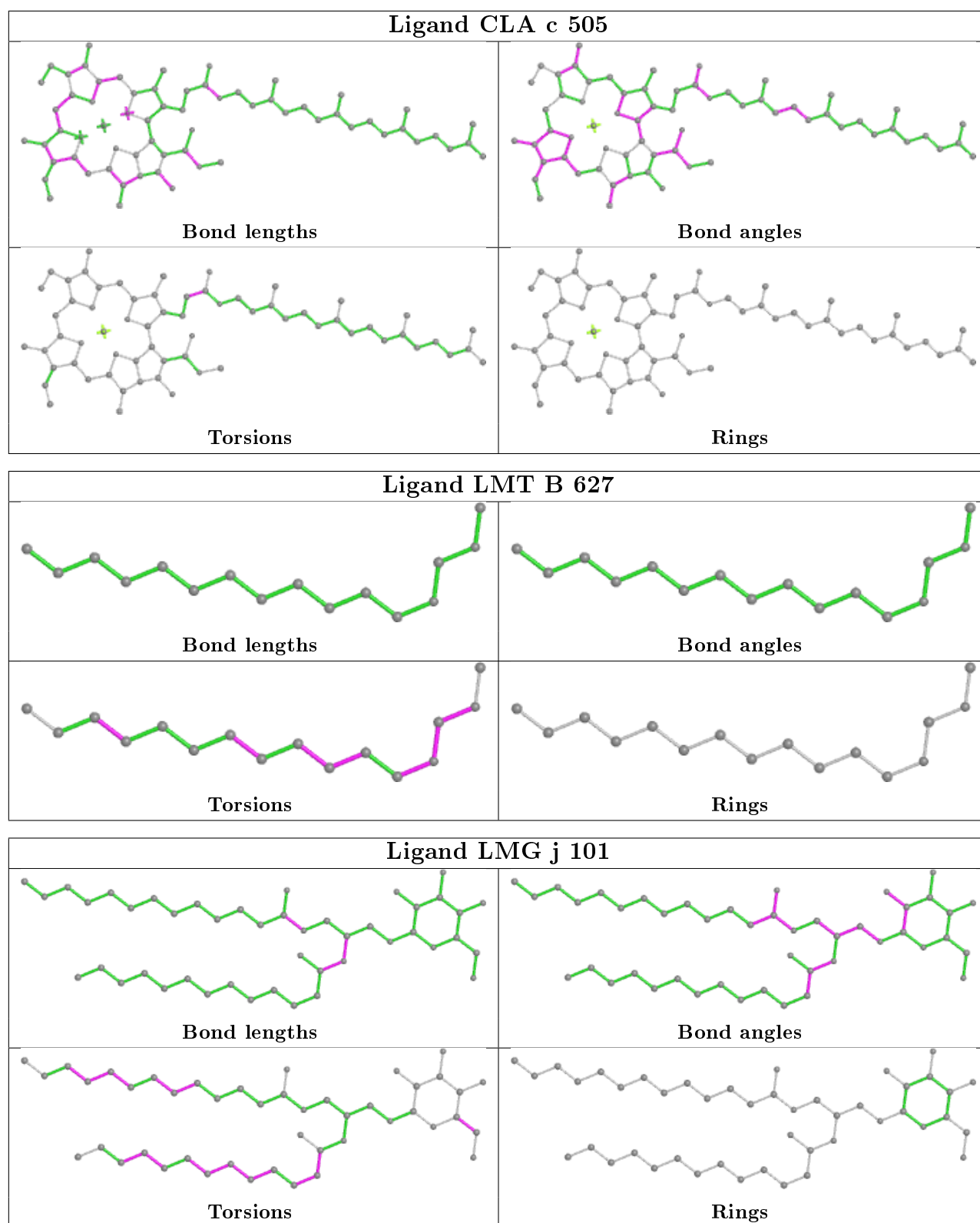


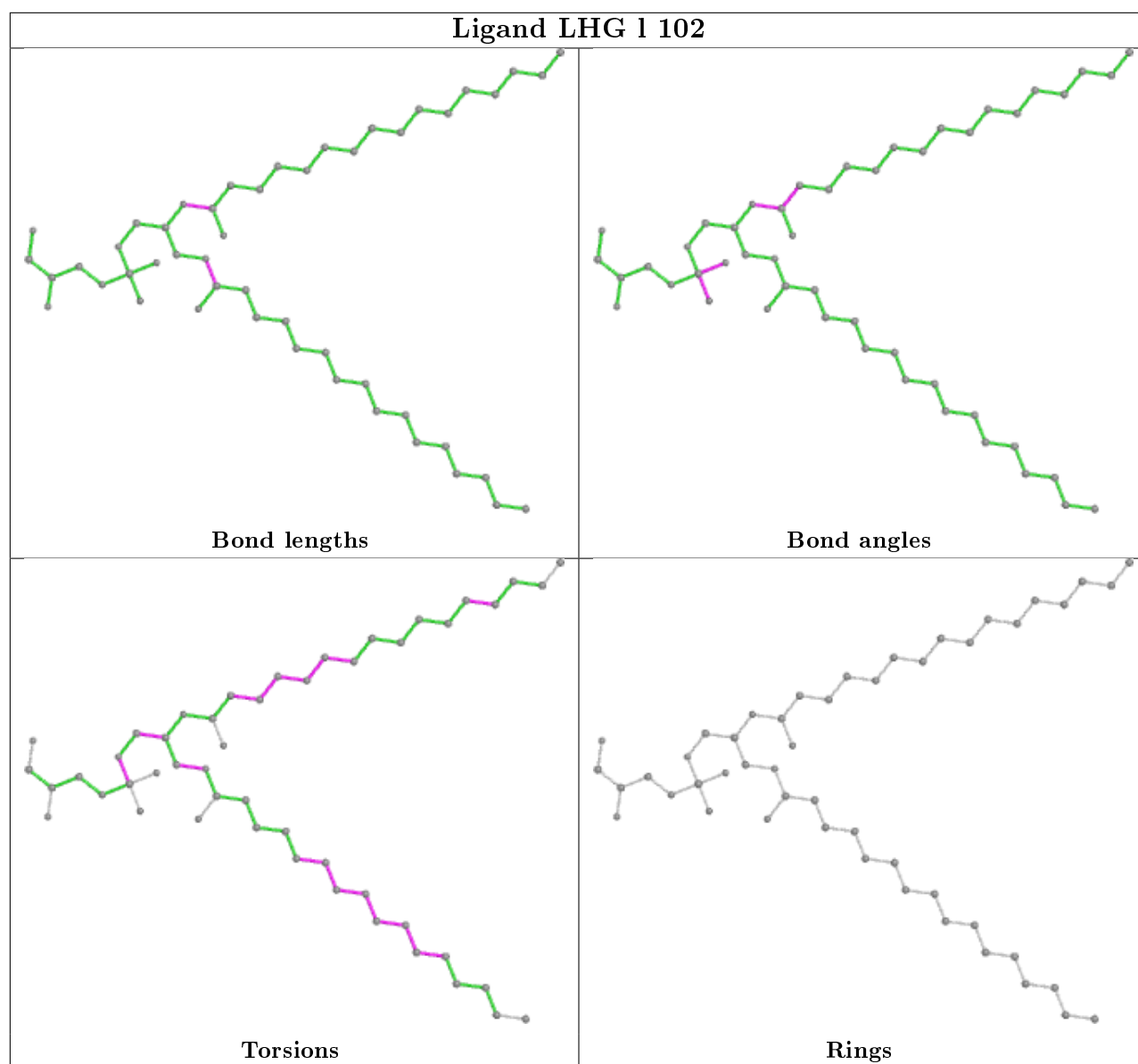


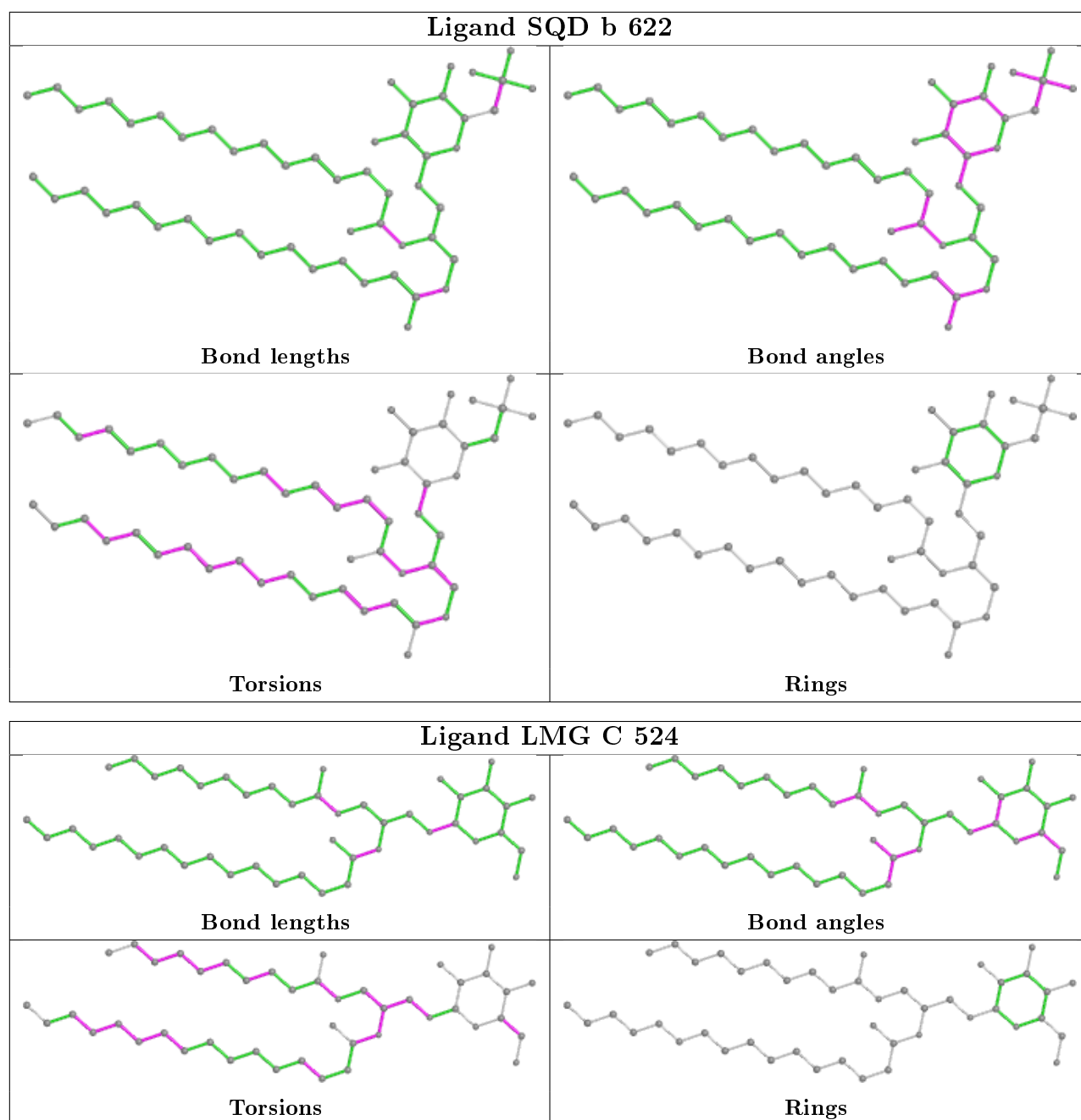


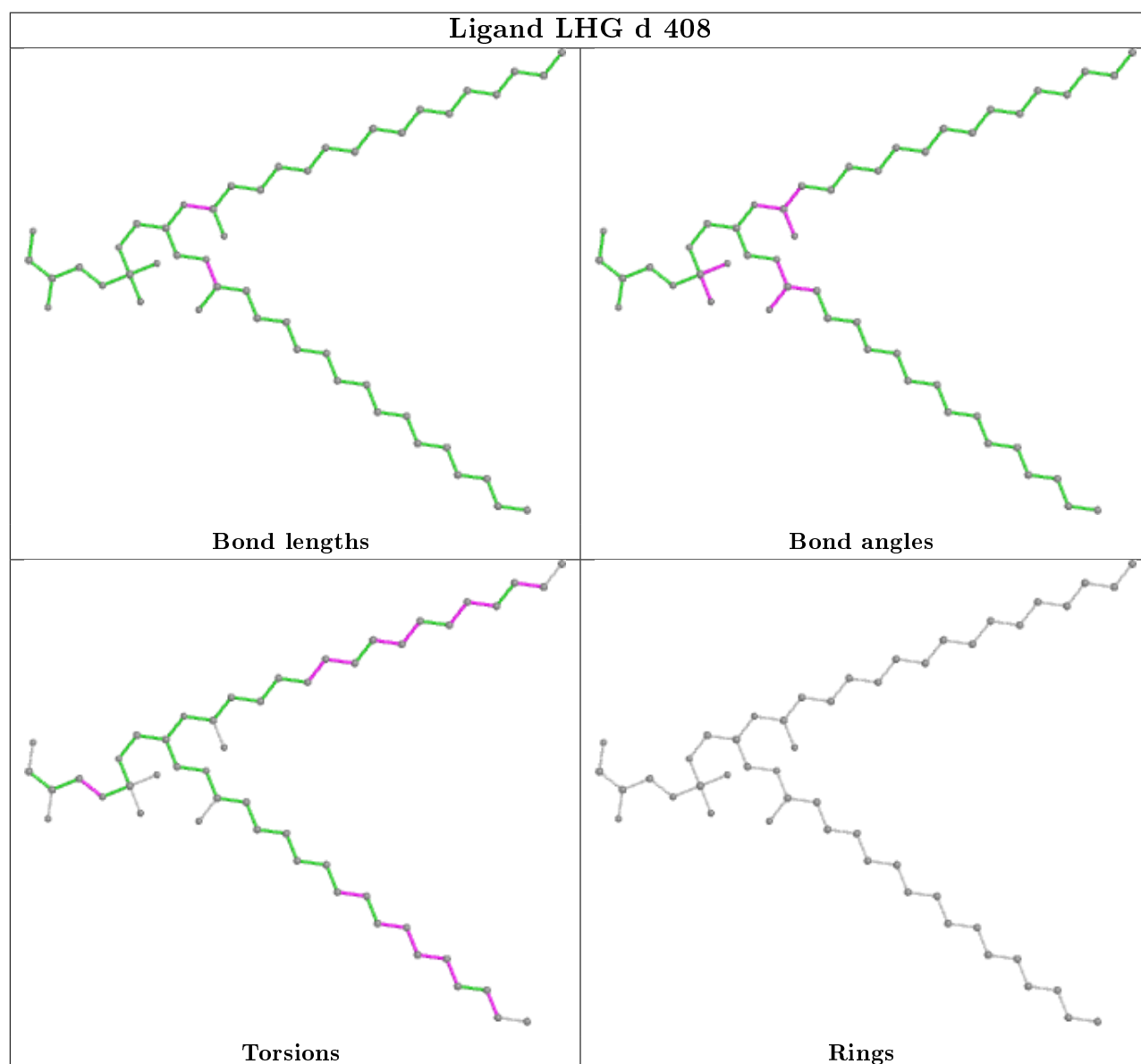
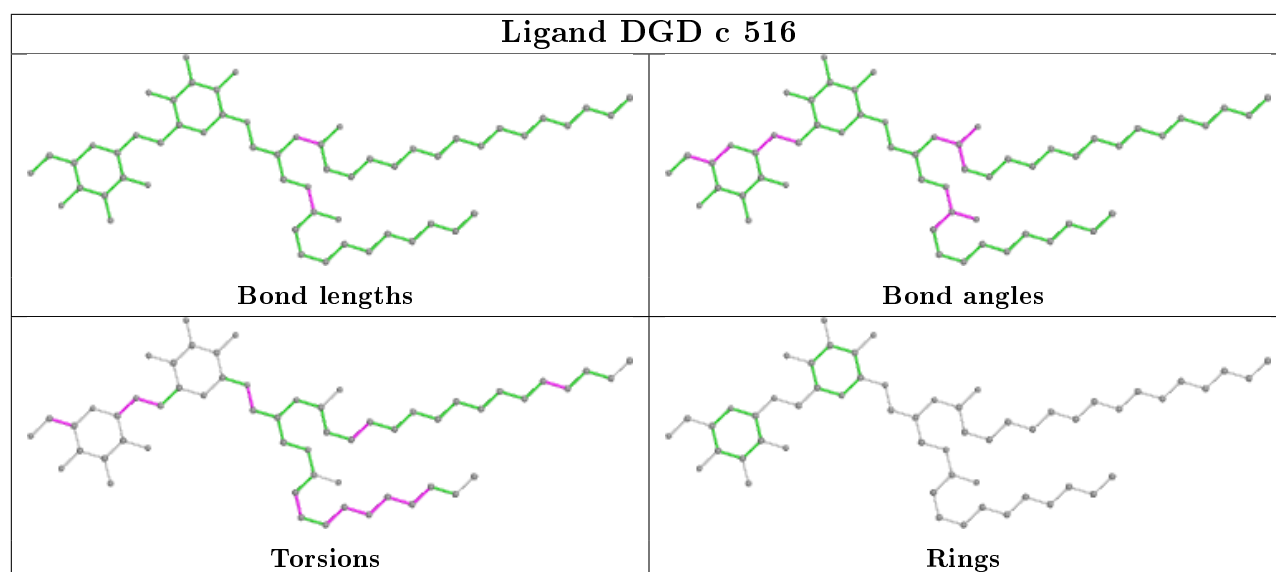


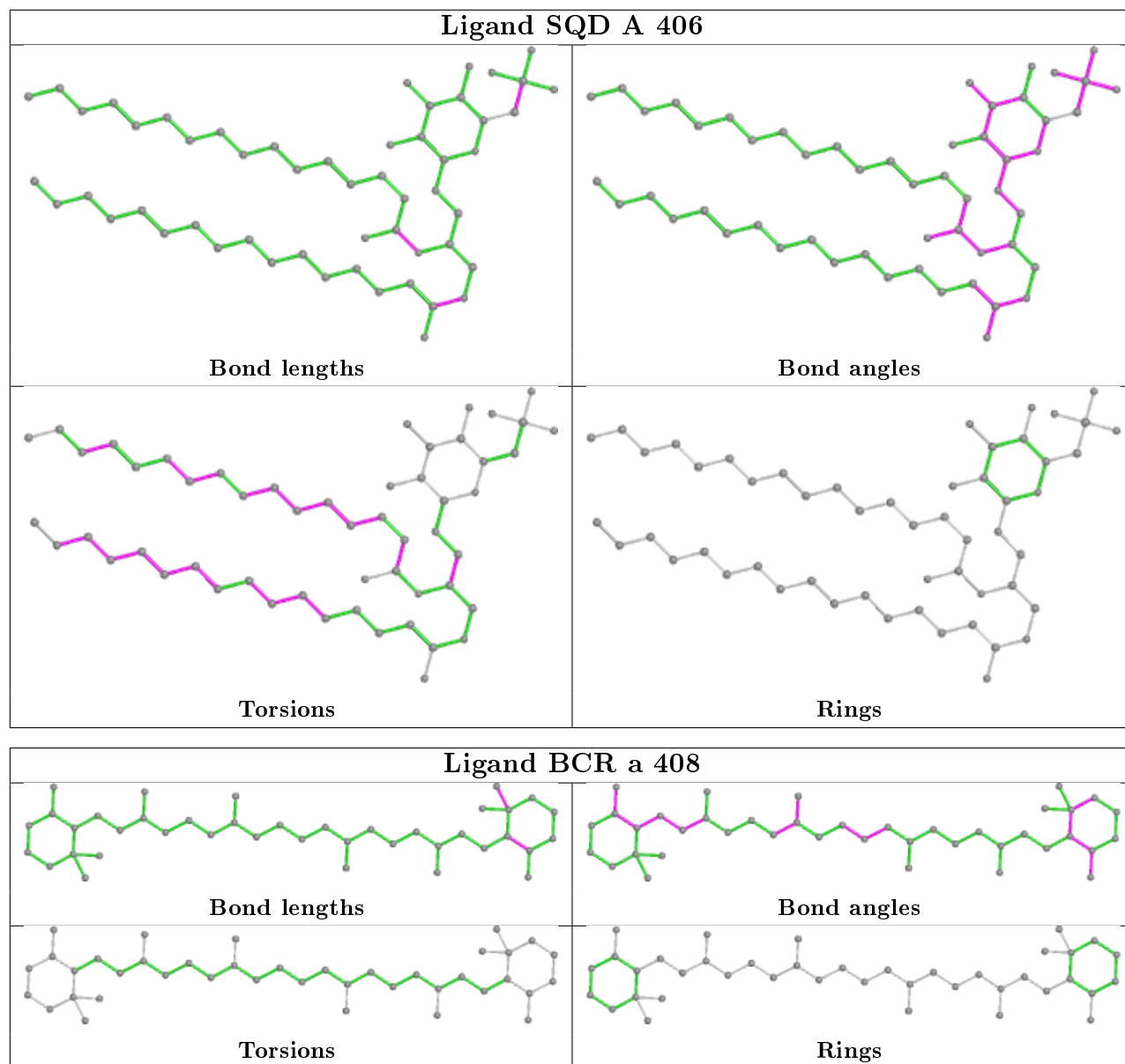


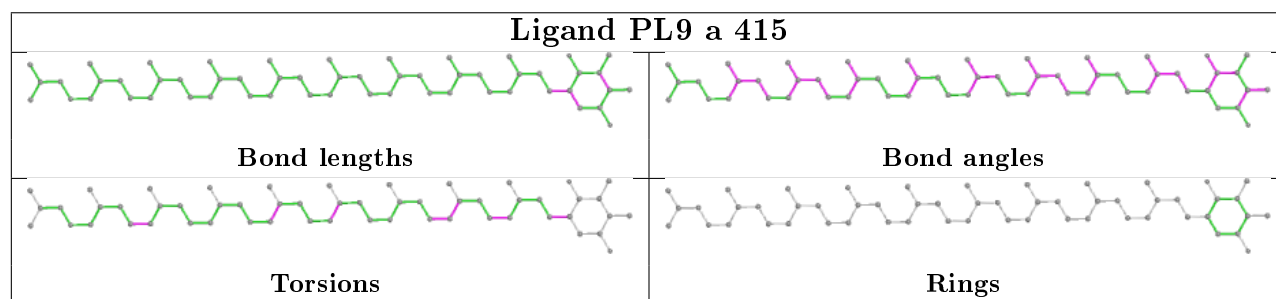
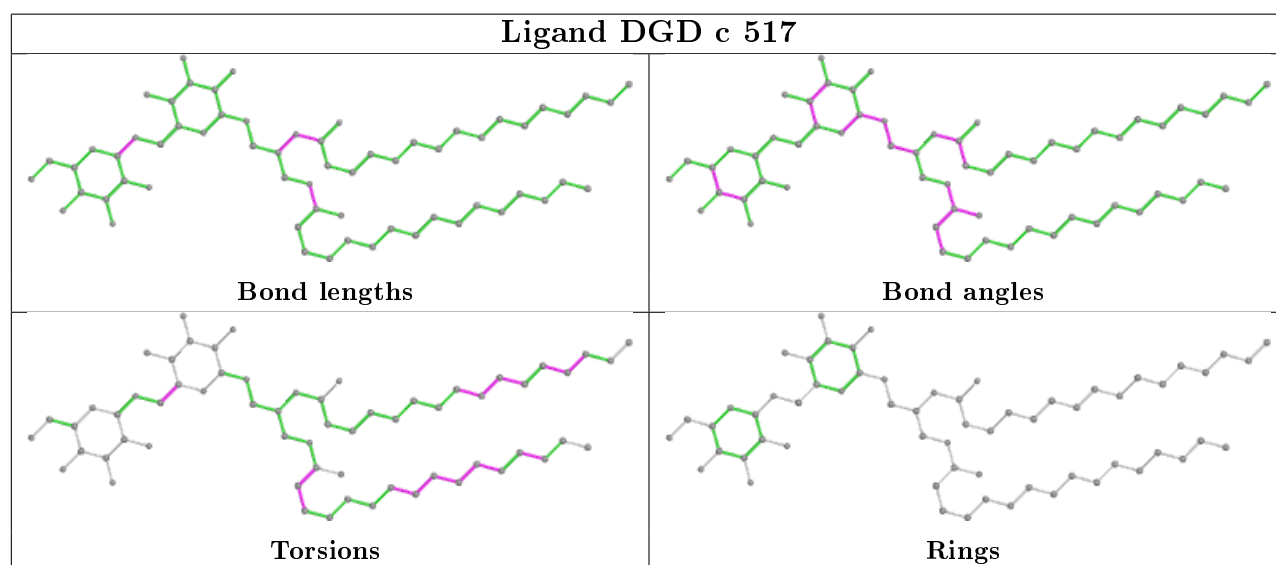
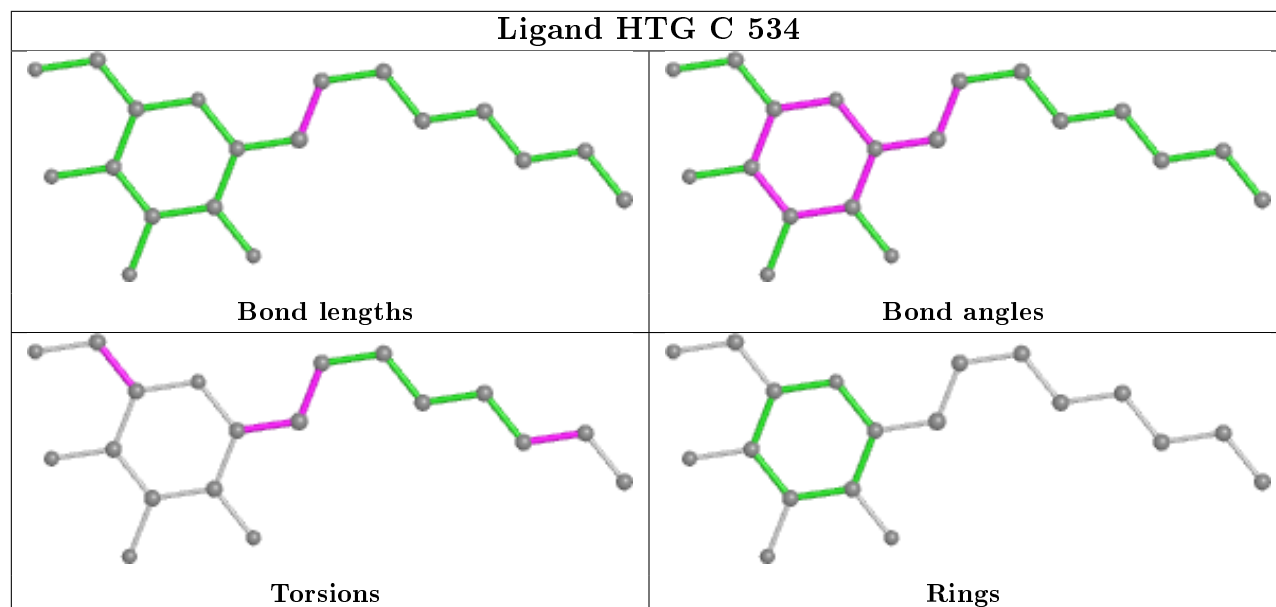


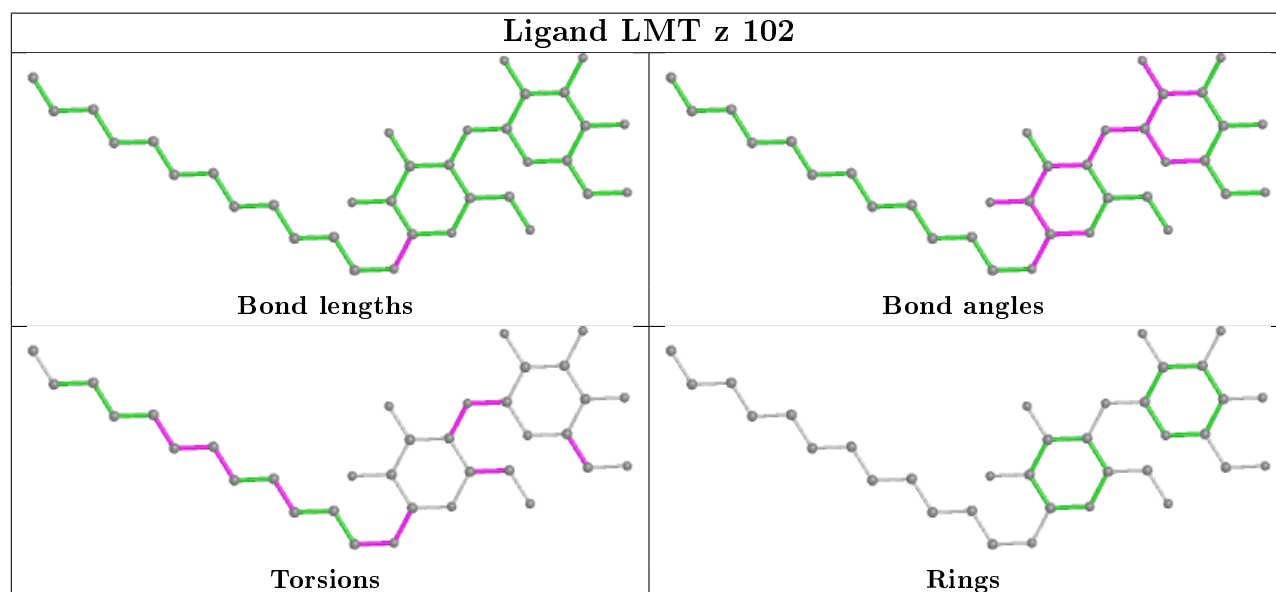
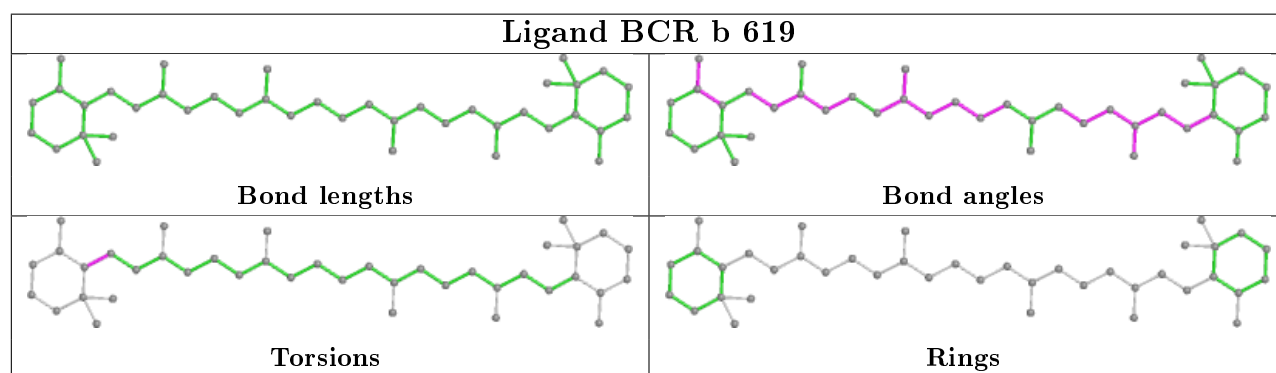
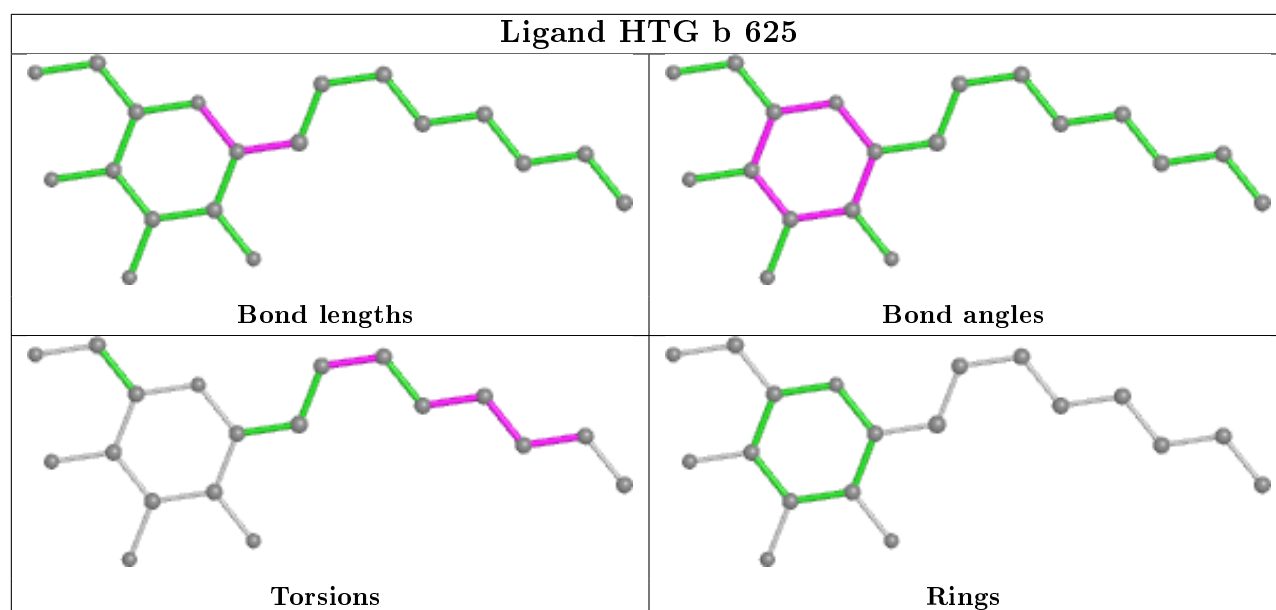


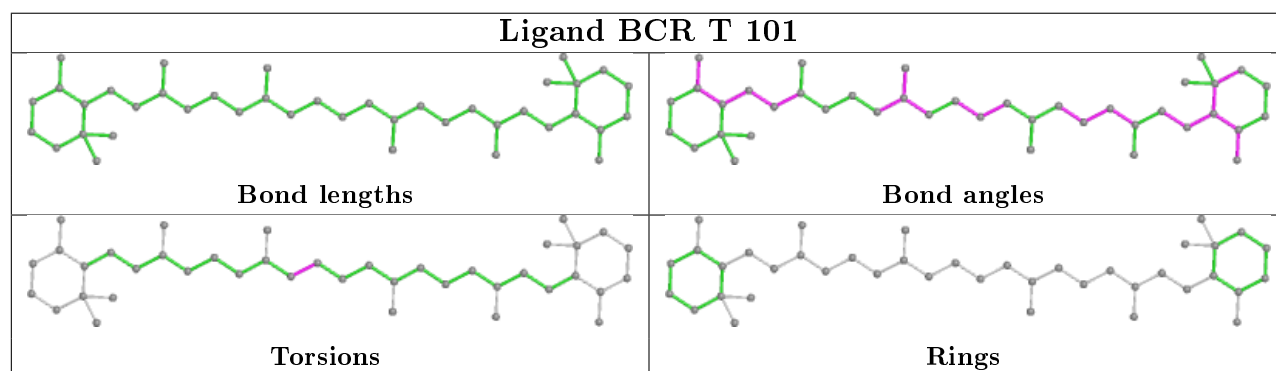
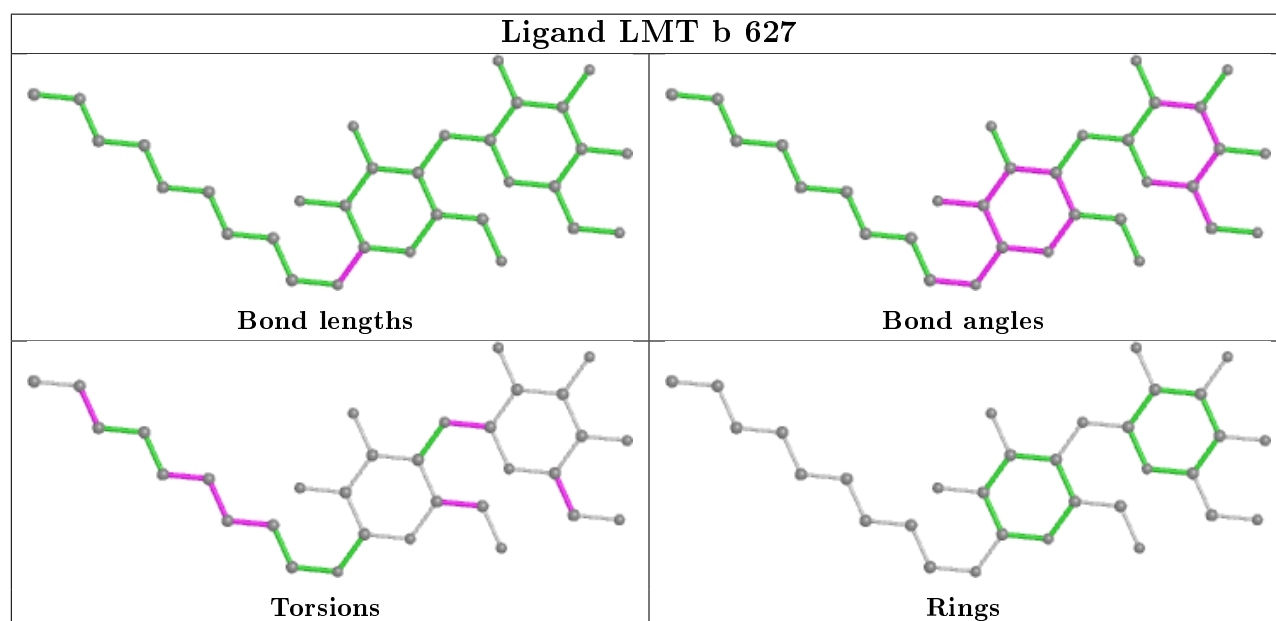
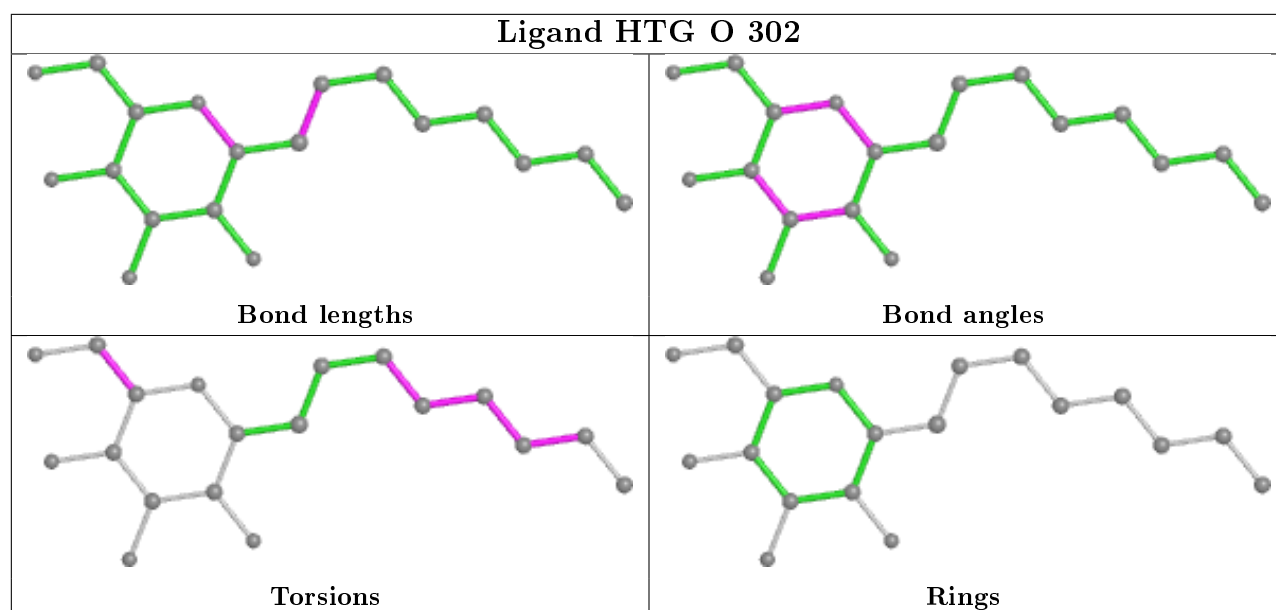






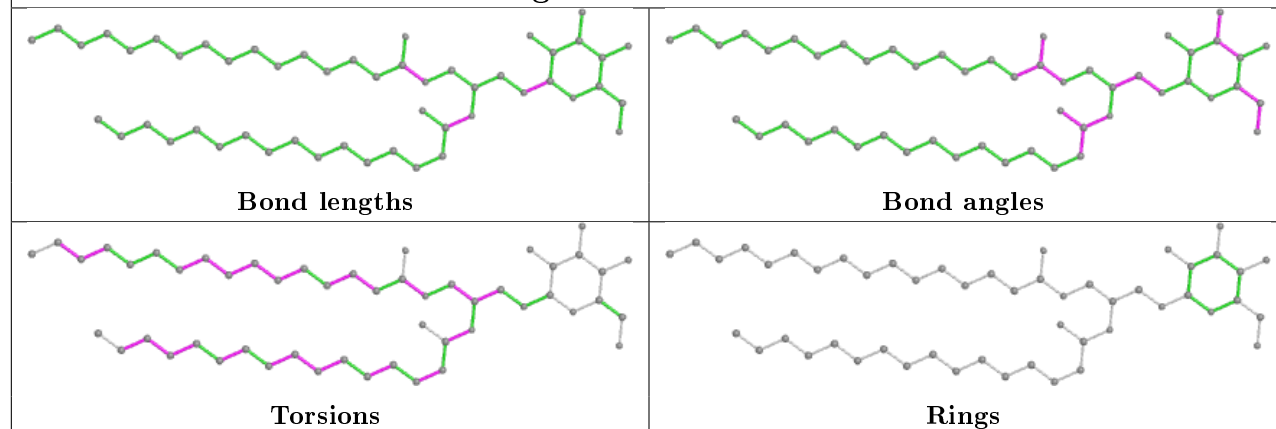




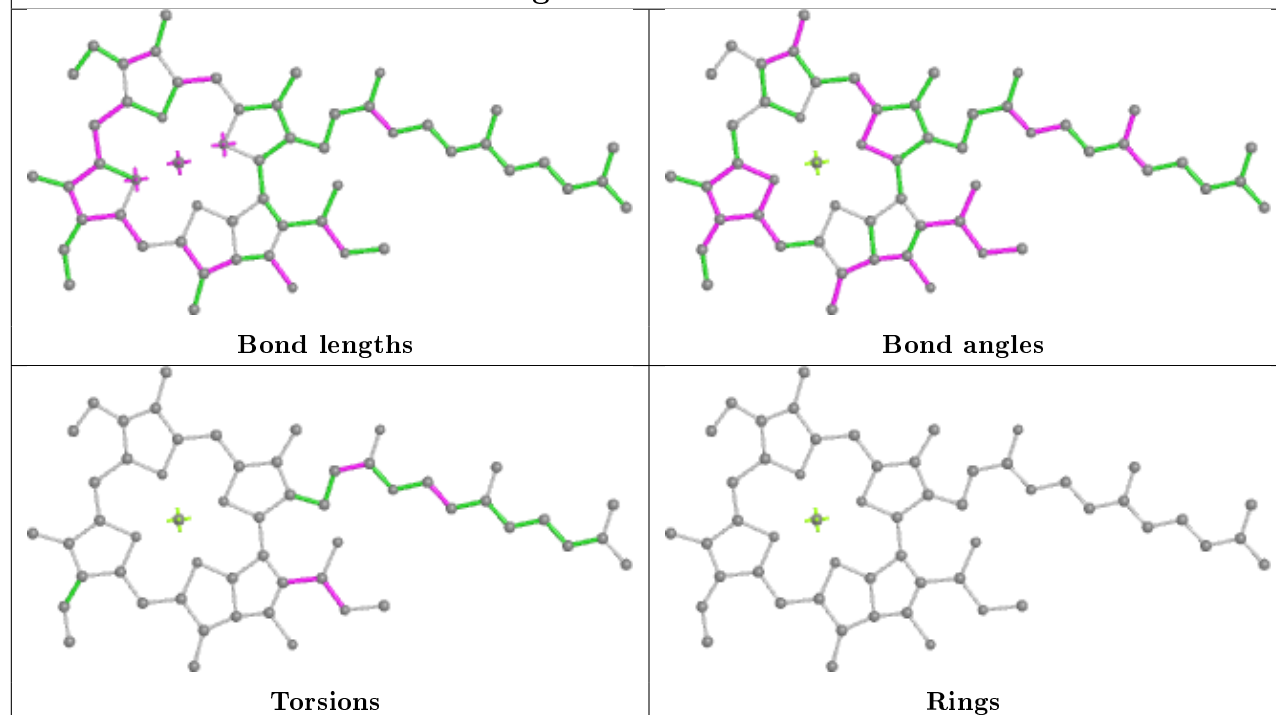




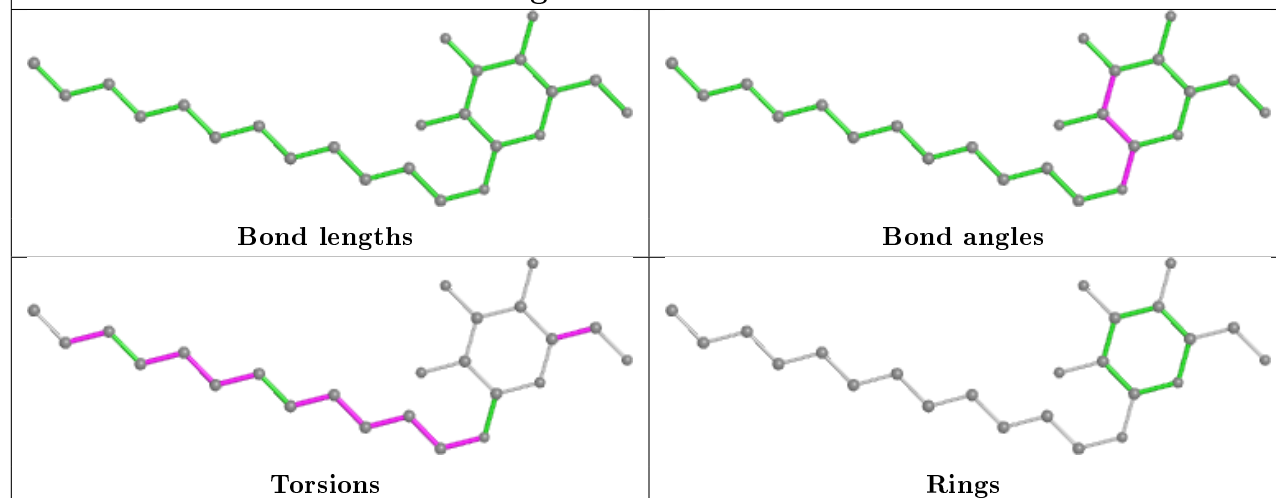
## Ligand LMG c 519

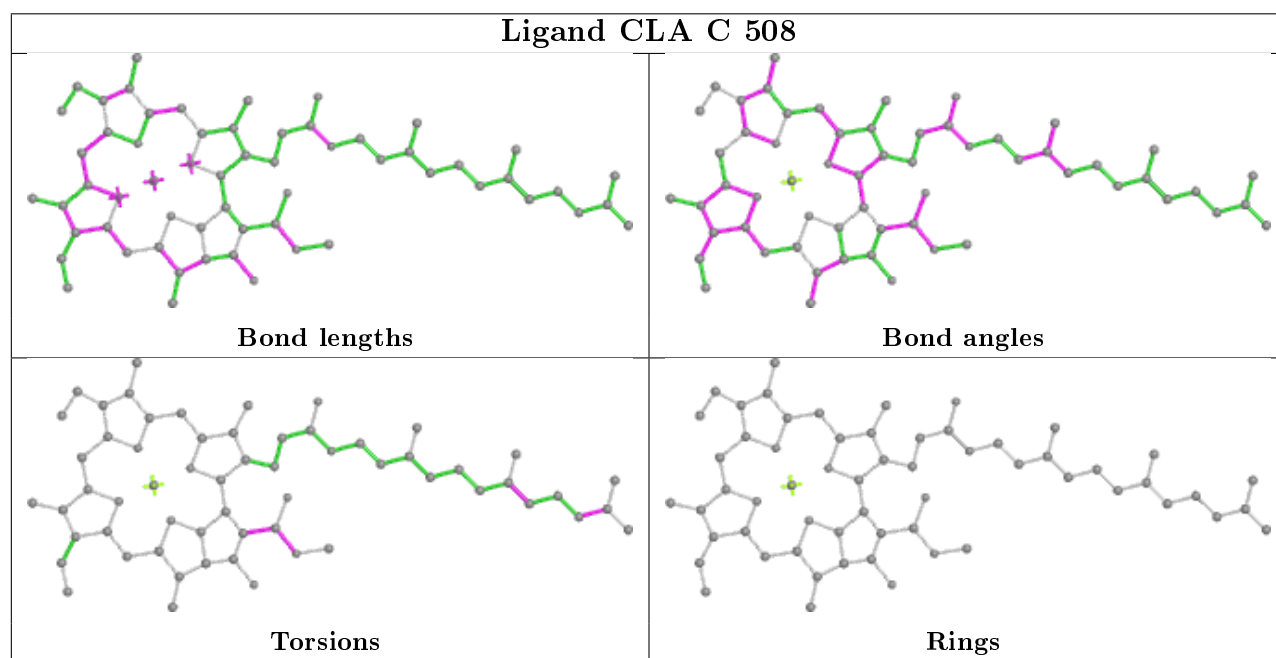
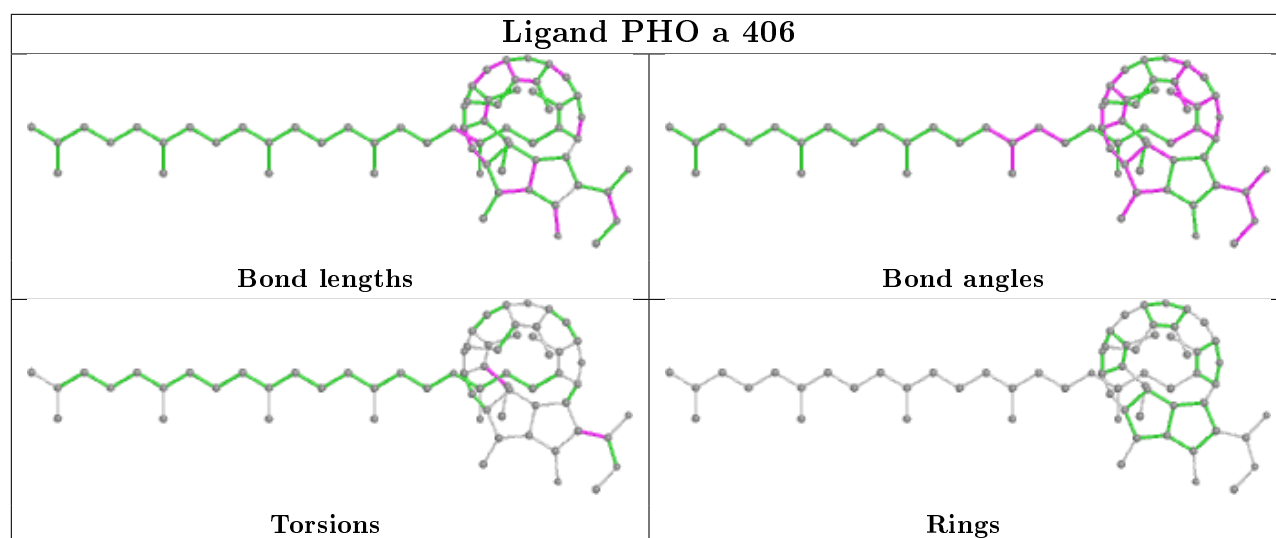


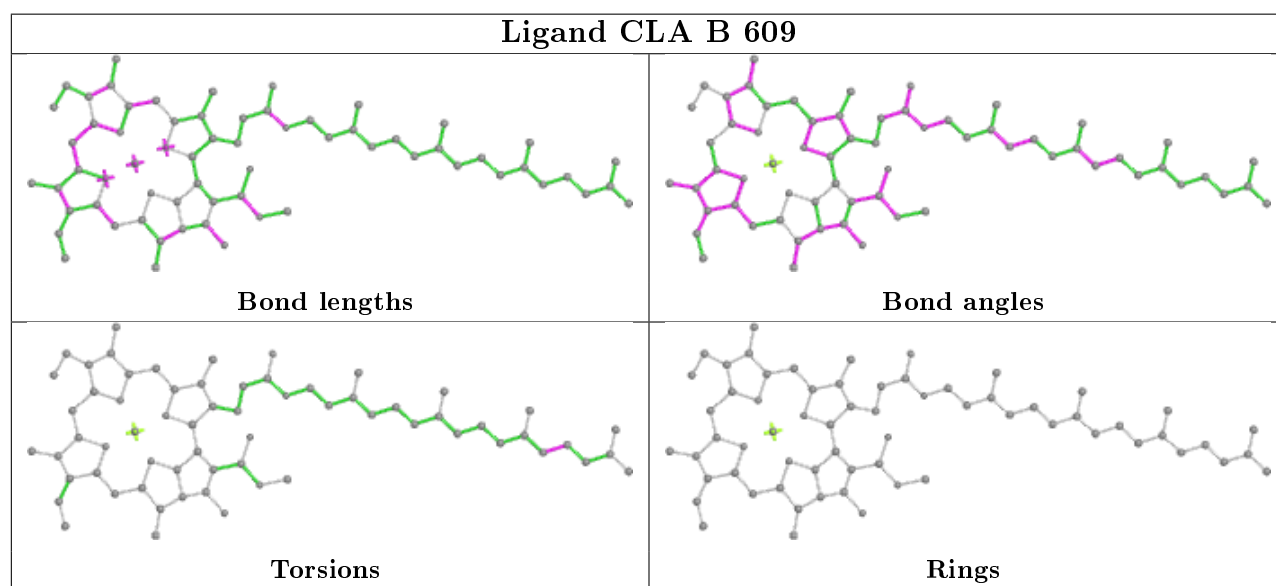
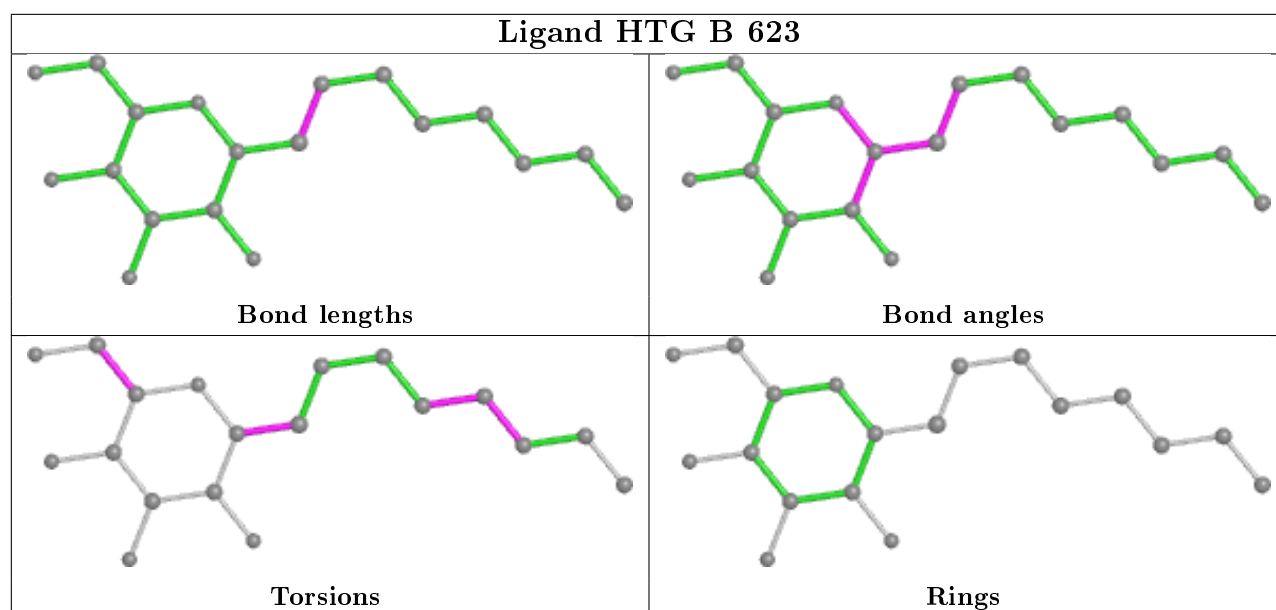
## Ligand CLA C 512

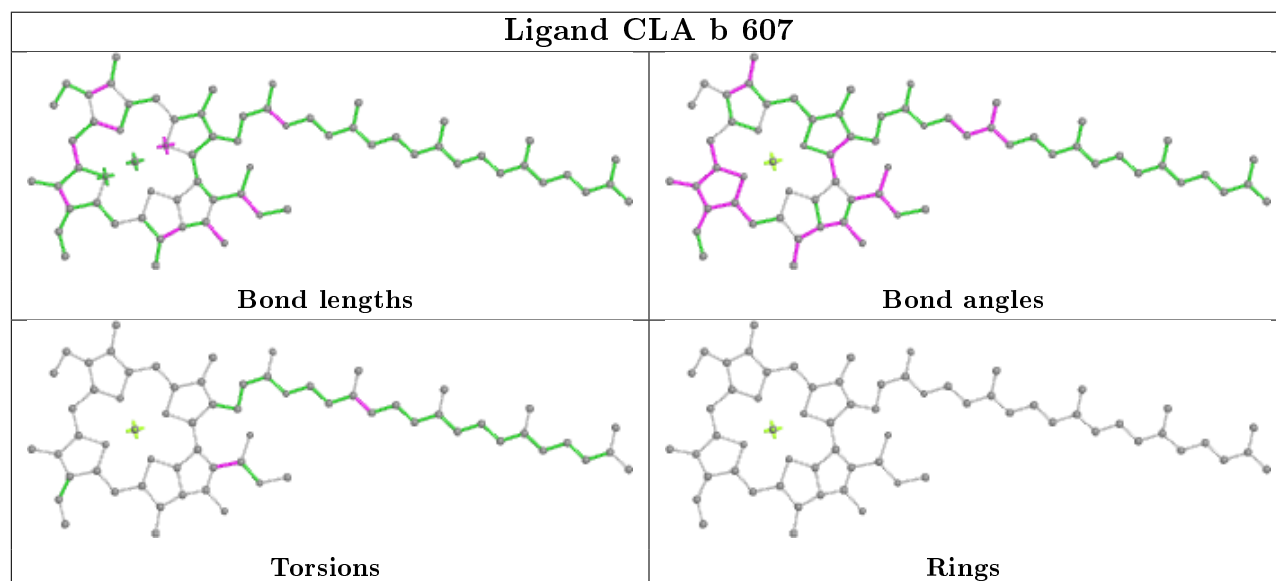
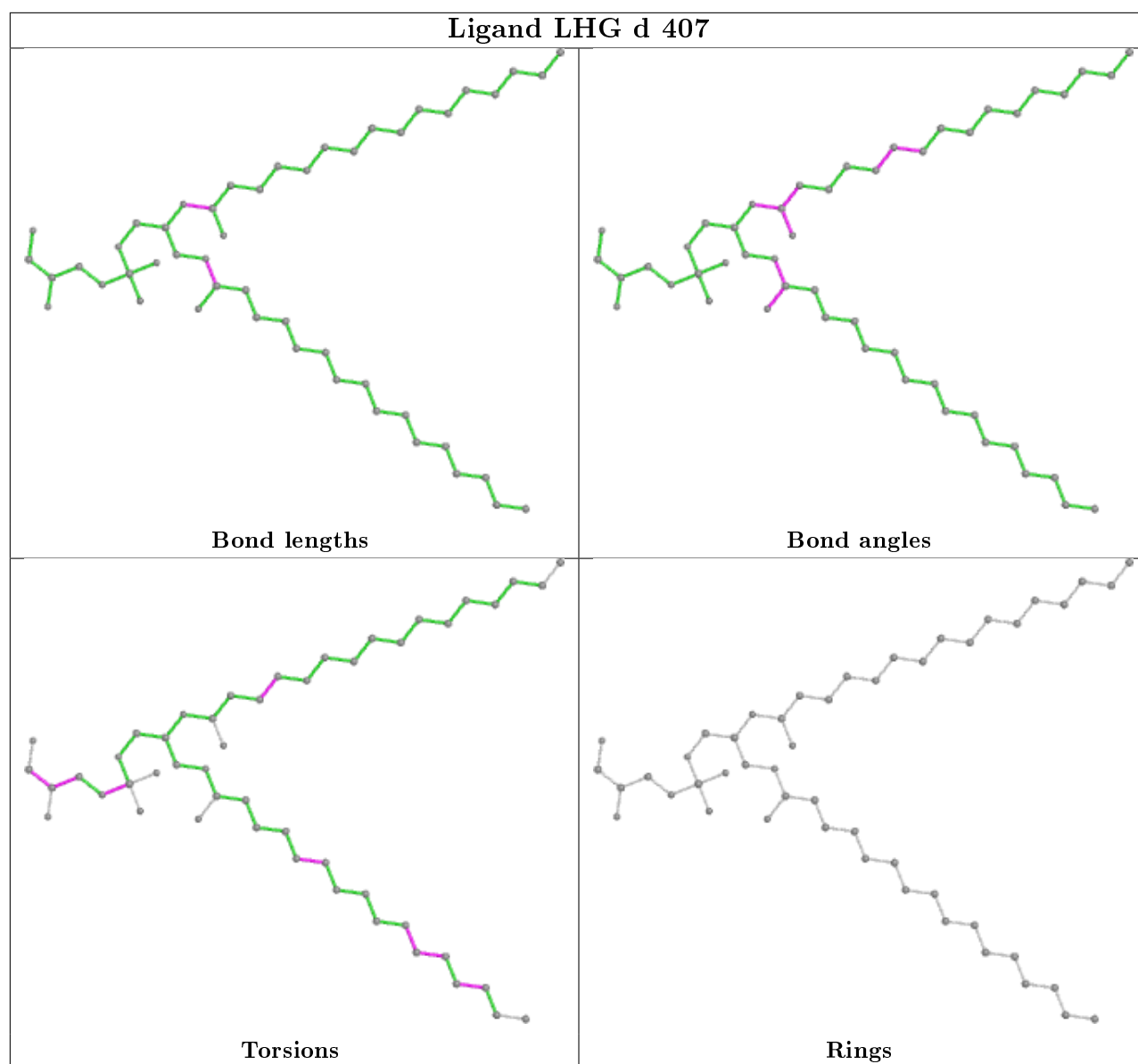


## Ligand LMT T 102

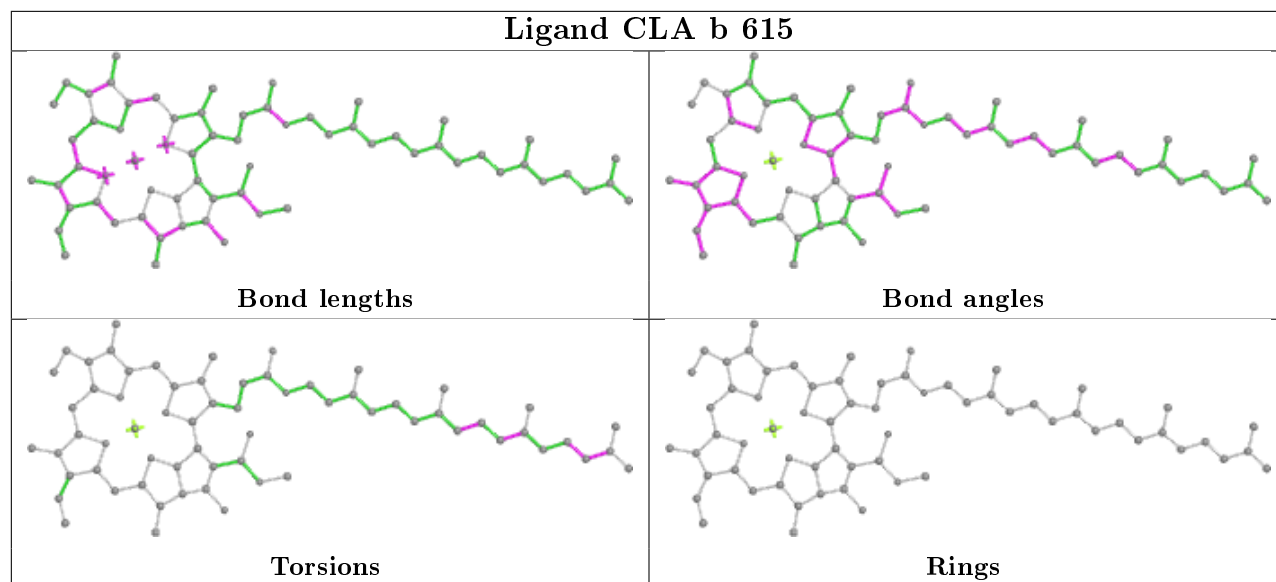




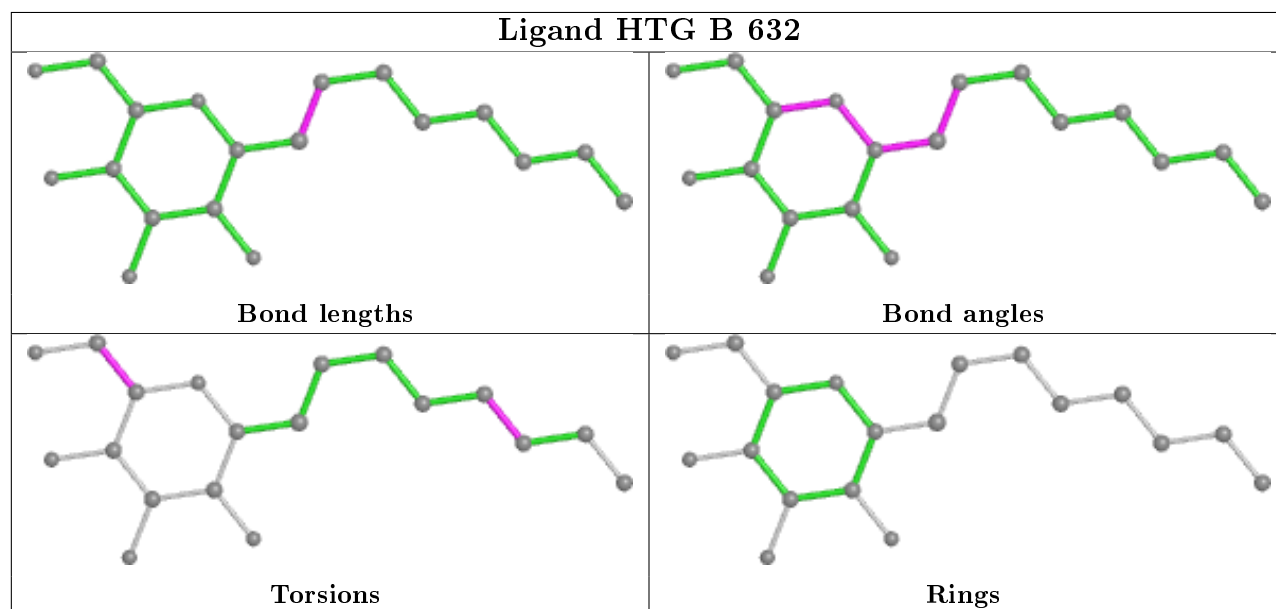




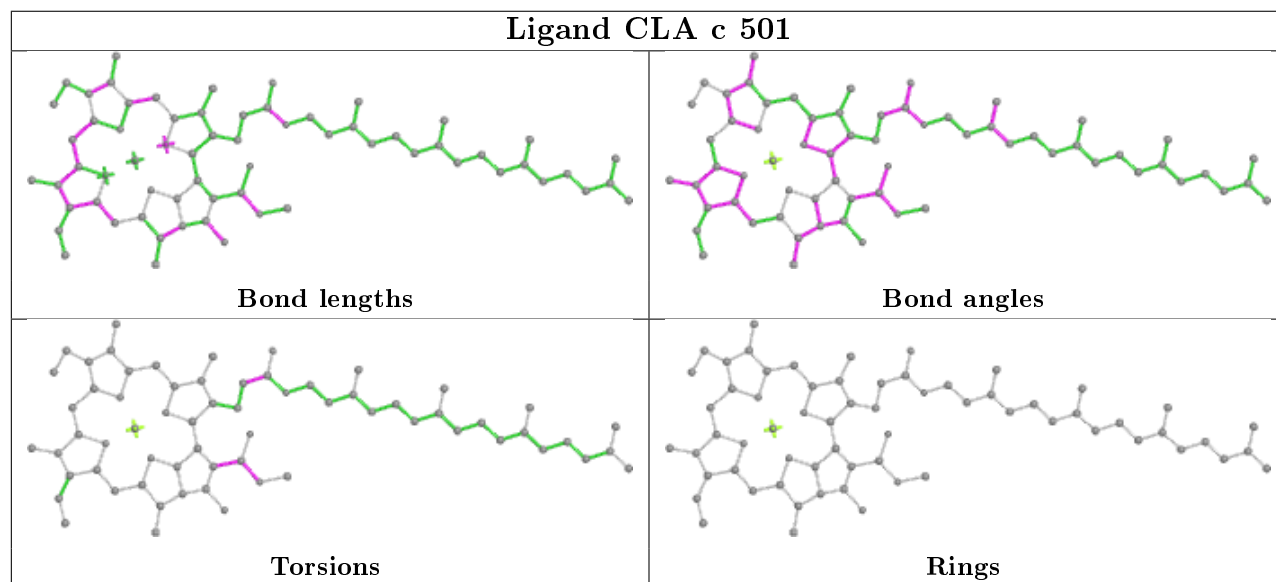
## Ligand CLA b 615

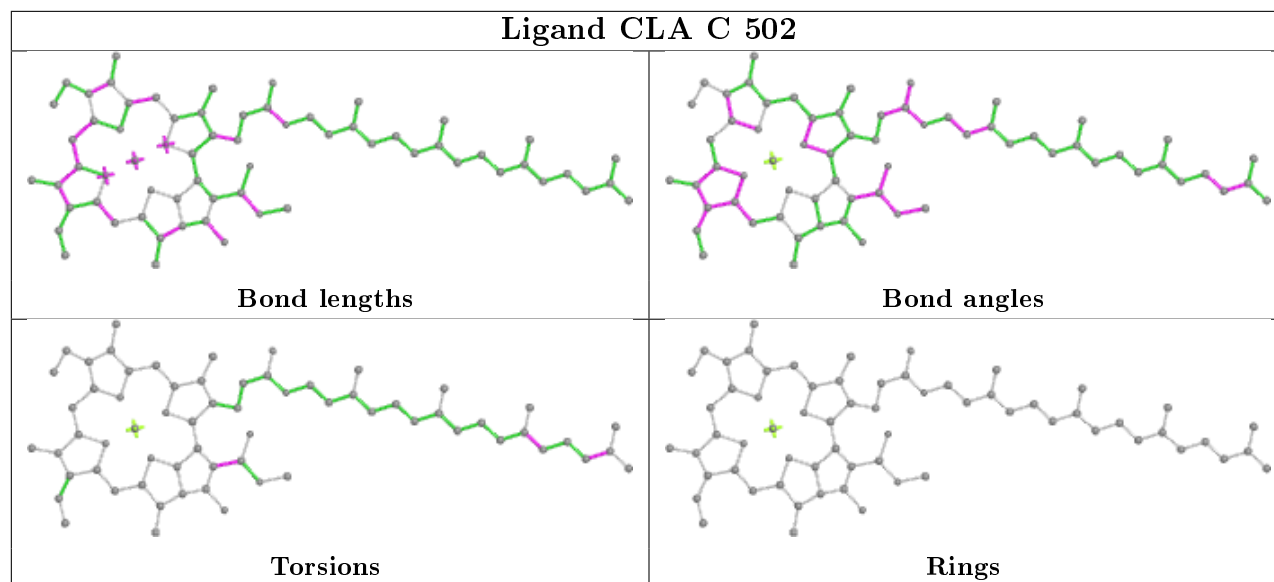
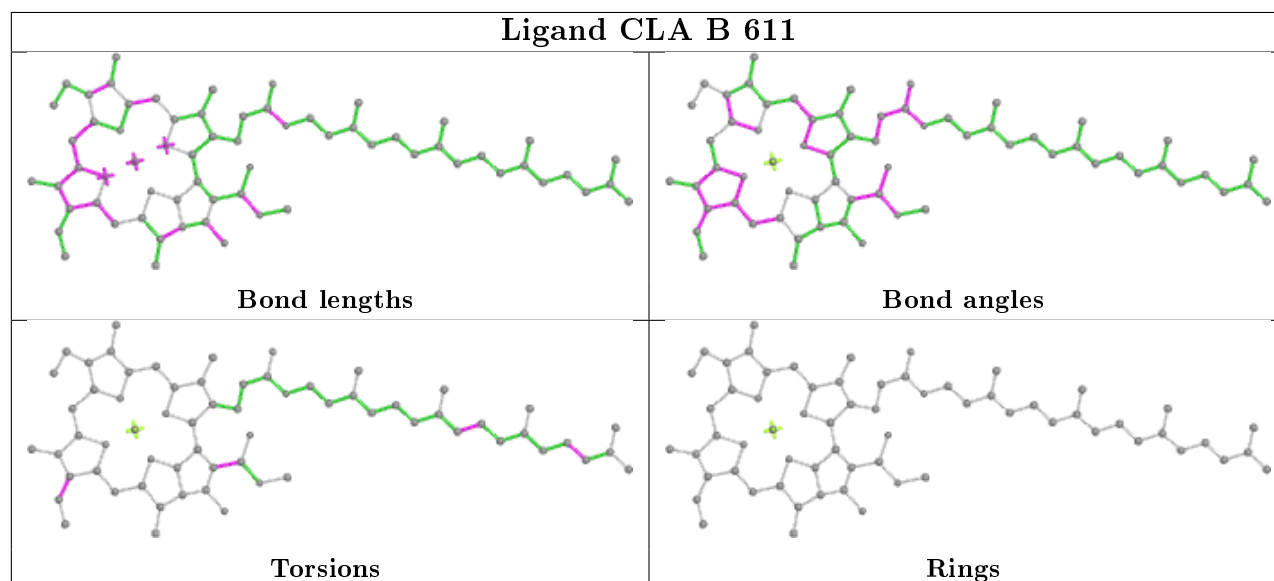
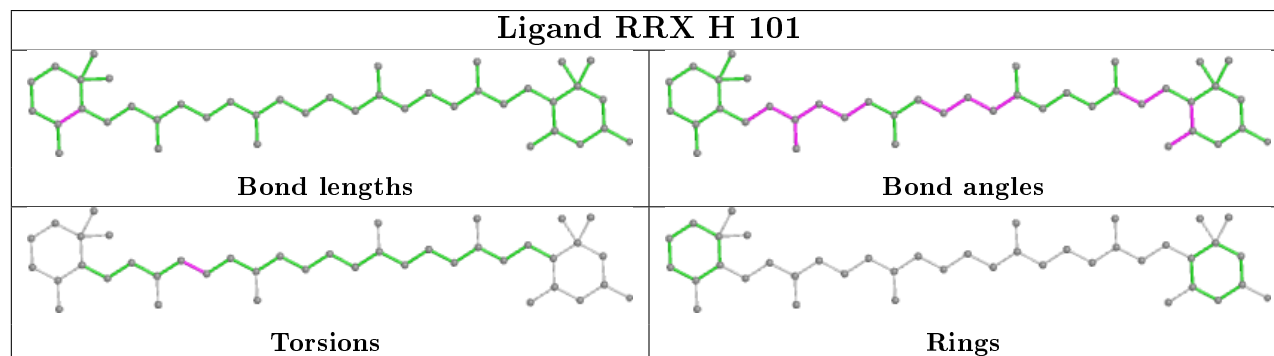


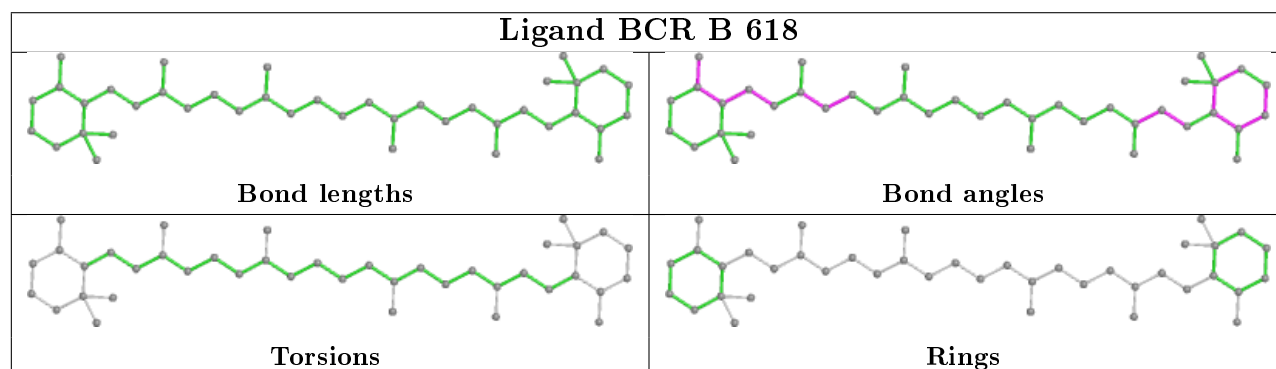
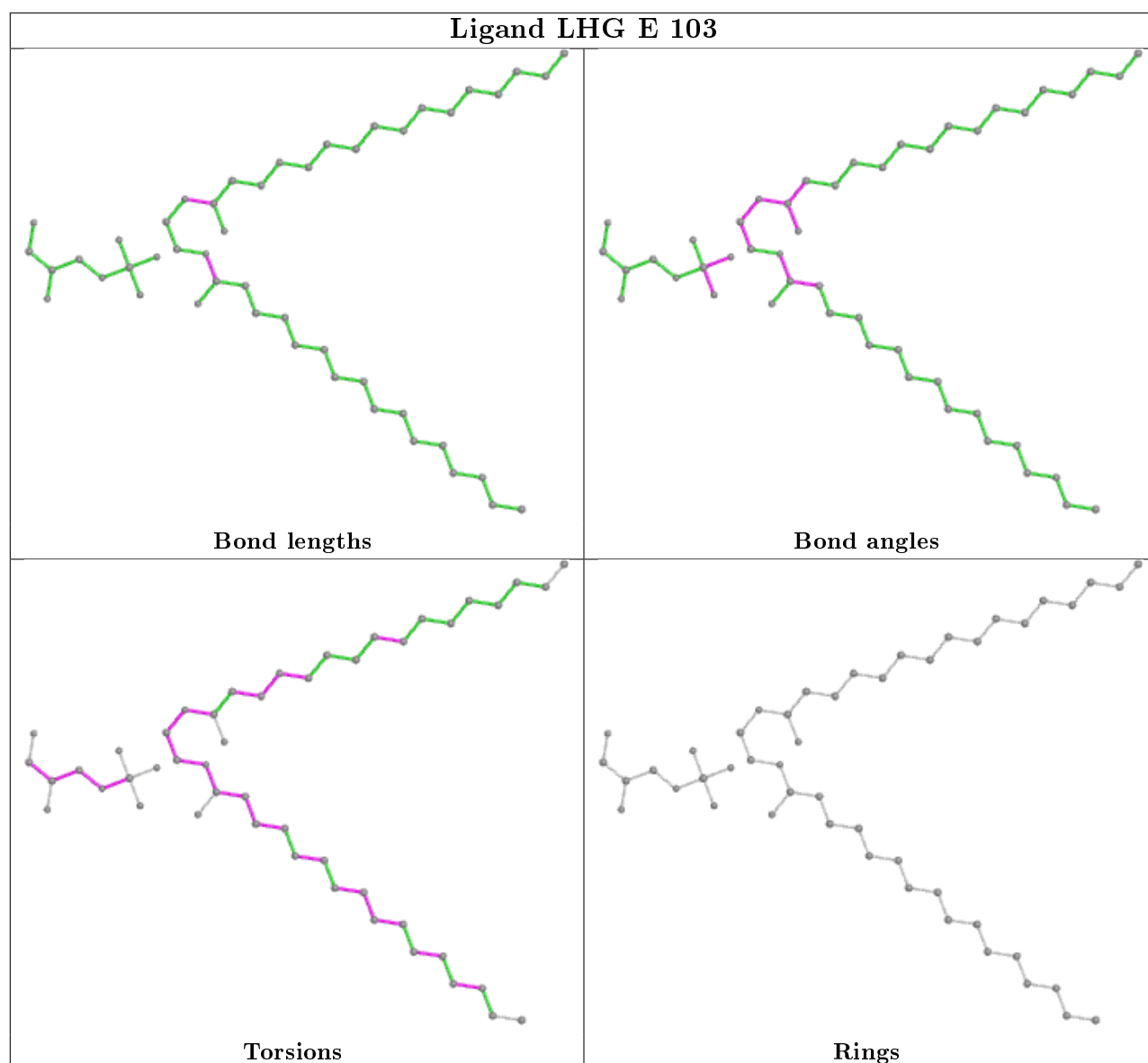
## Ligand HTG B 632

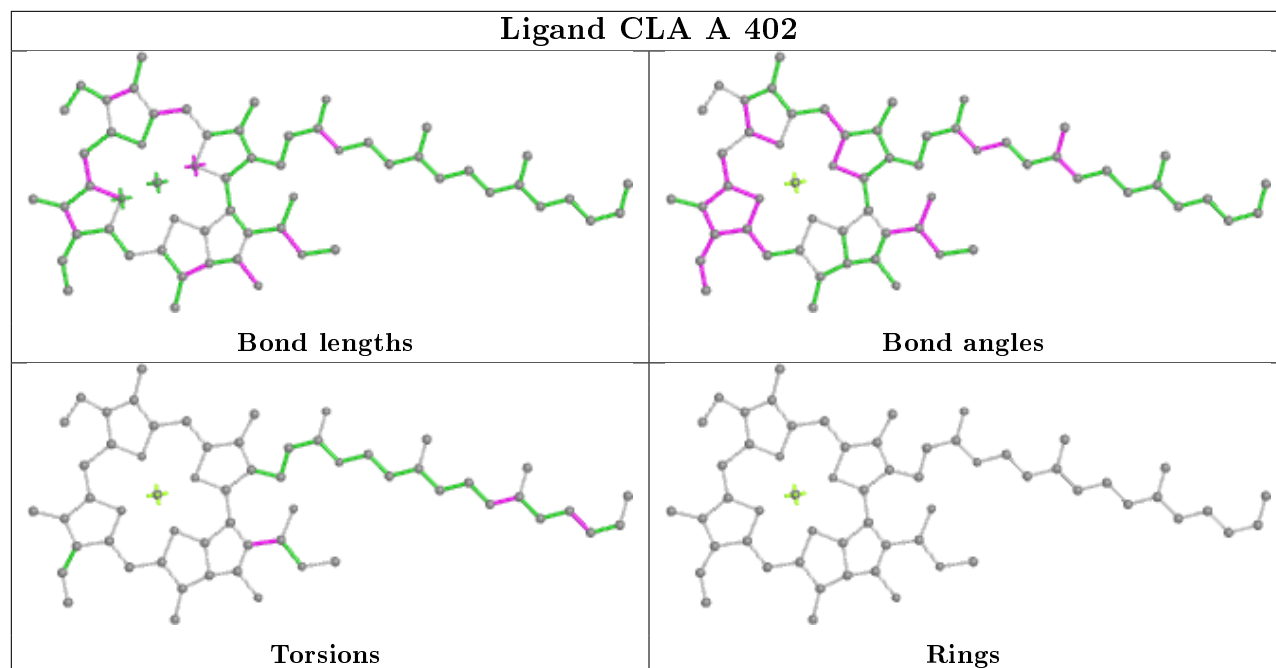
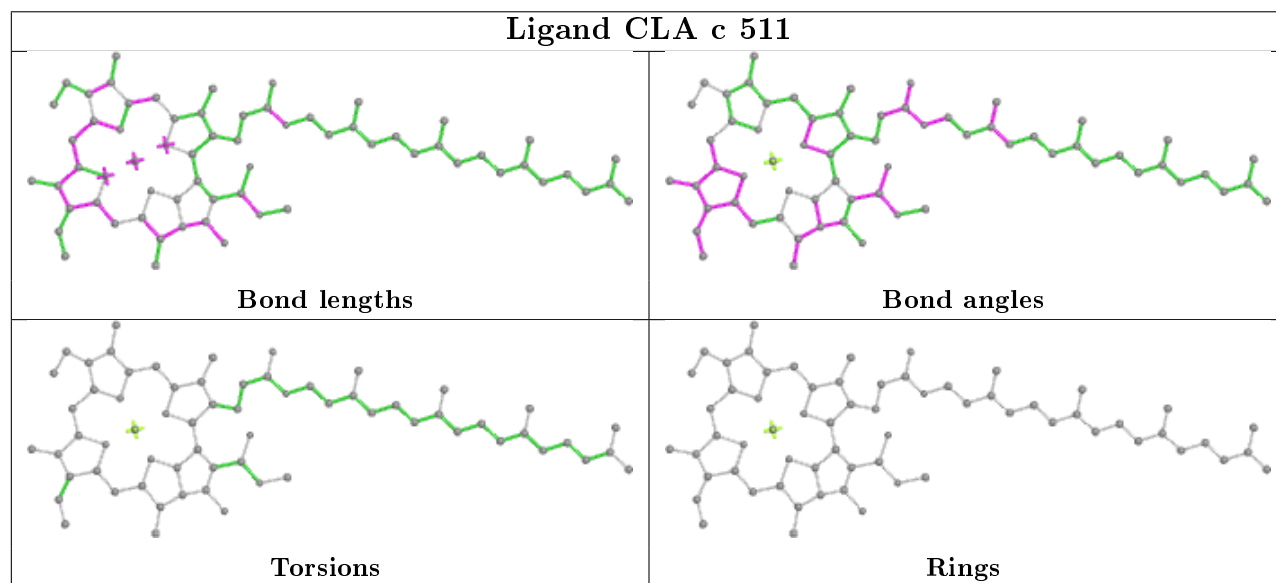
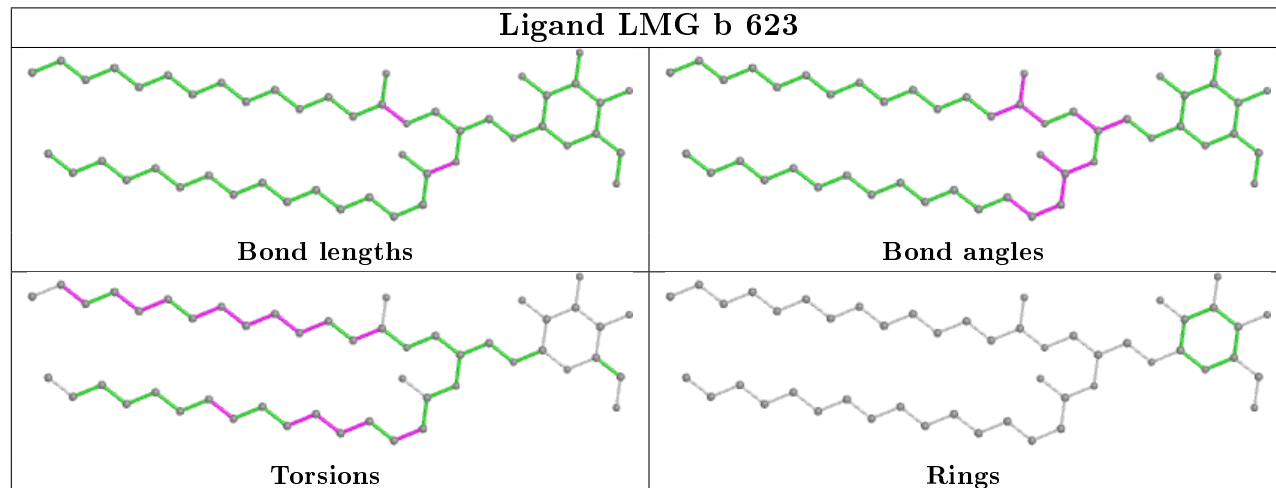


## Ligand CLA c 501

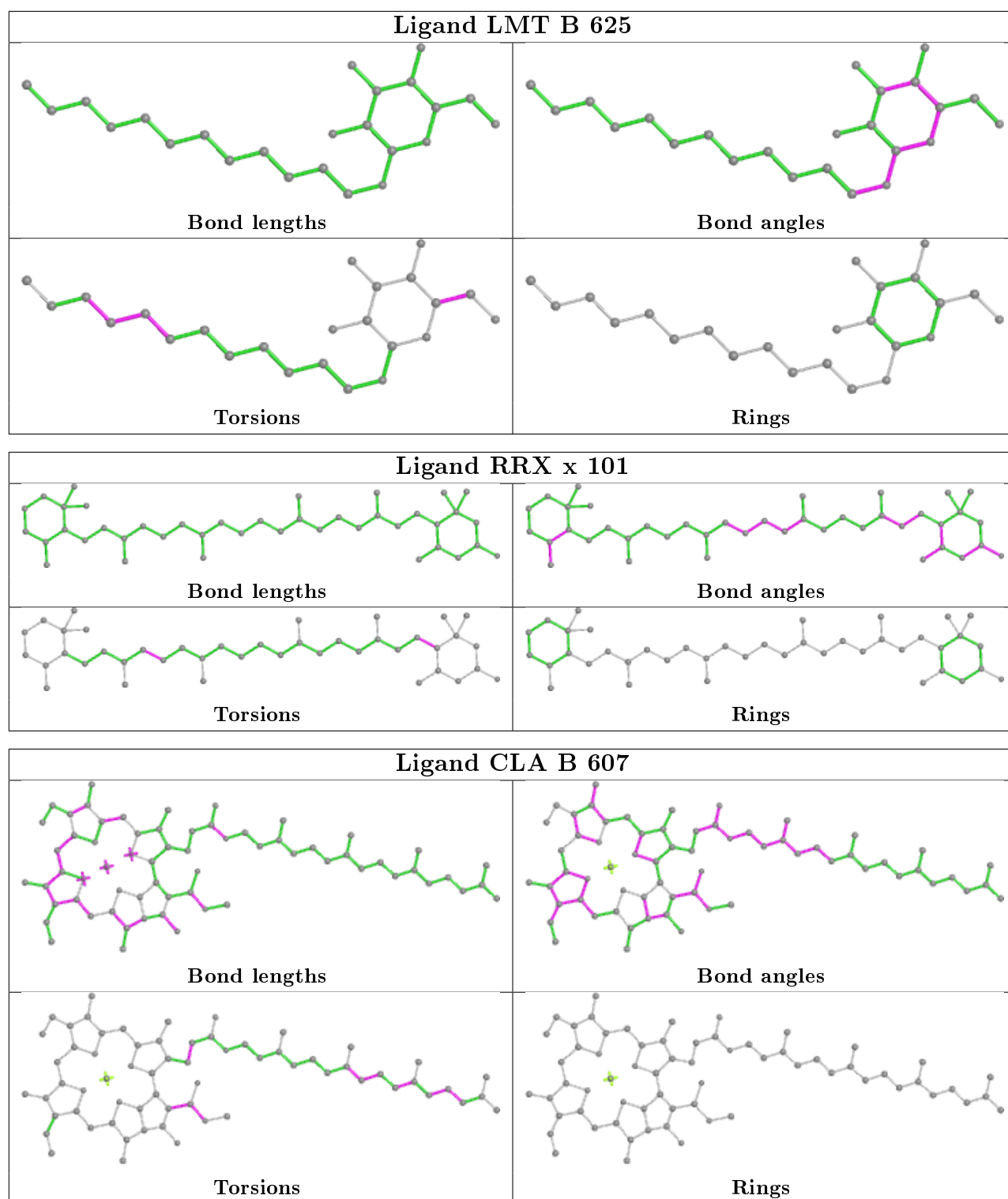


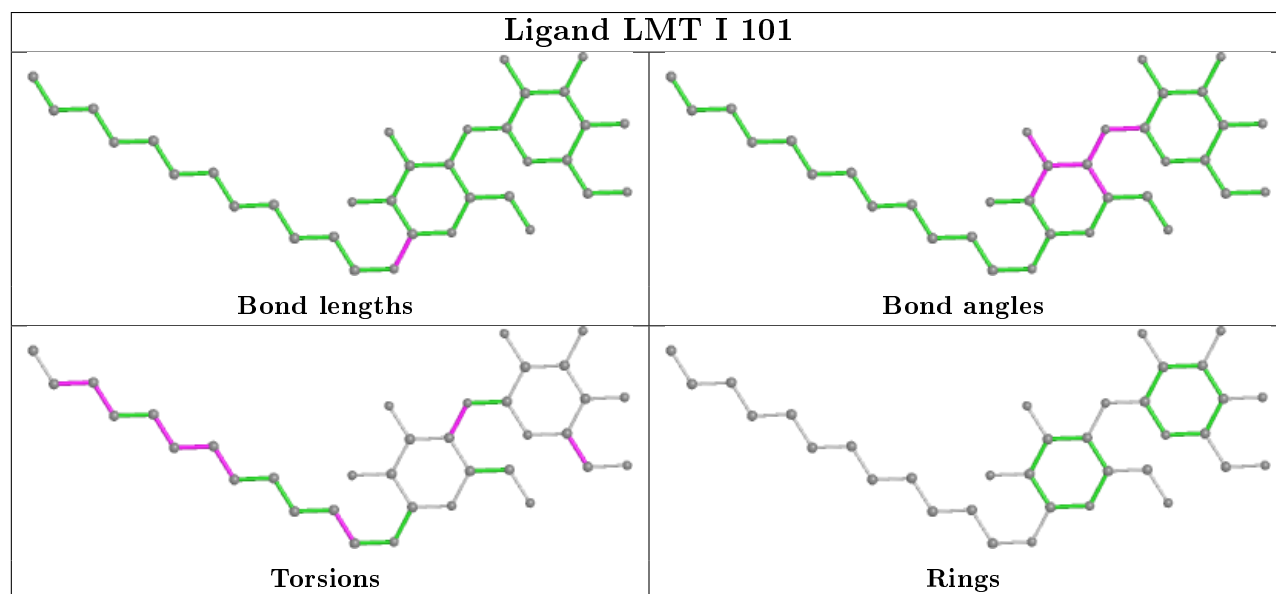
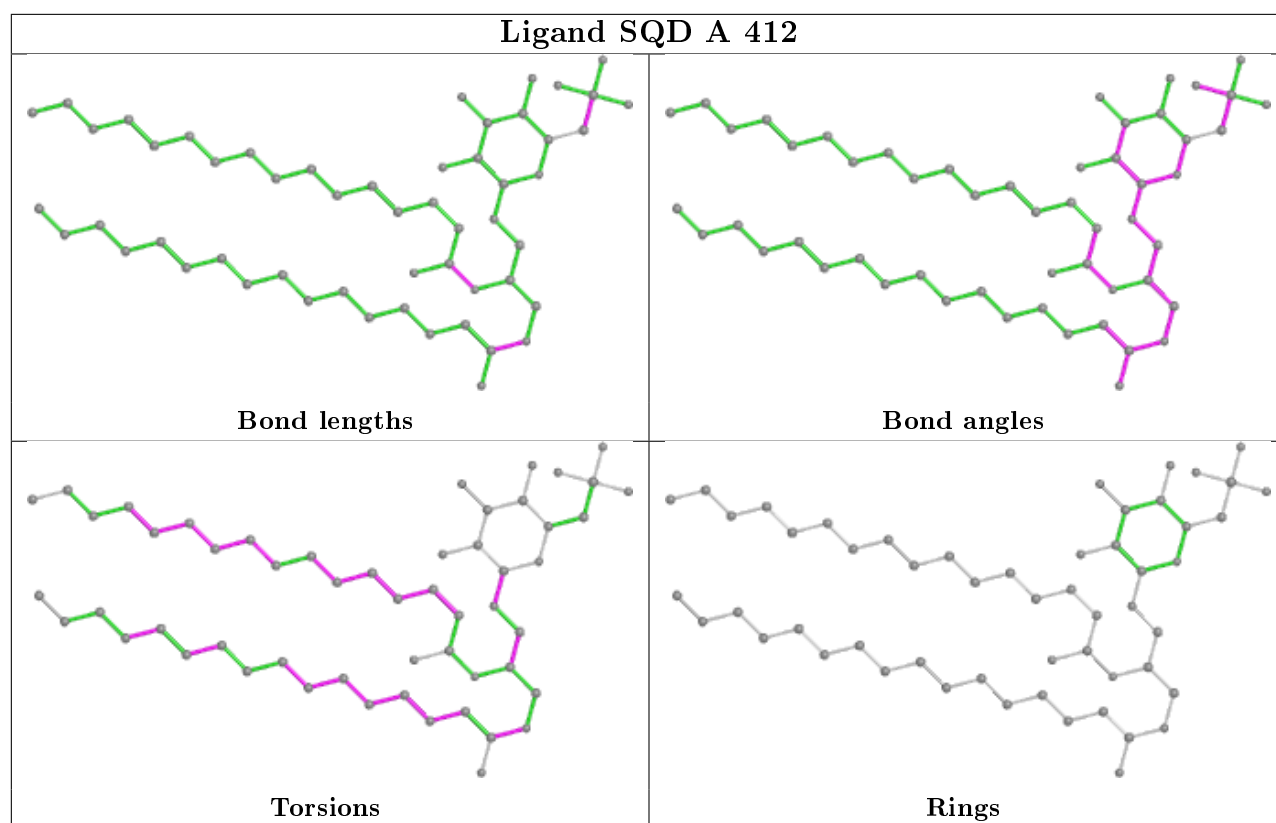
**Ligand CLA C 502****Ligand CLA B 611****Ligand RRX H 101**



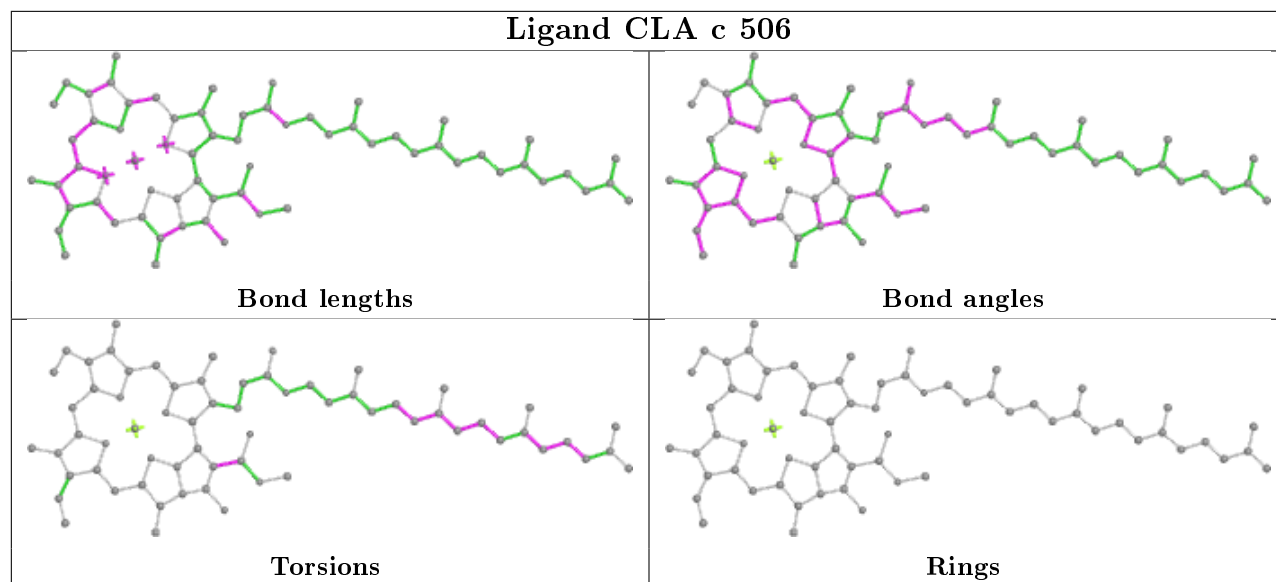
**Ligand CLA A 402****Ligand CLA c 511****Ligand LMG b 623**



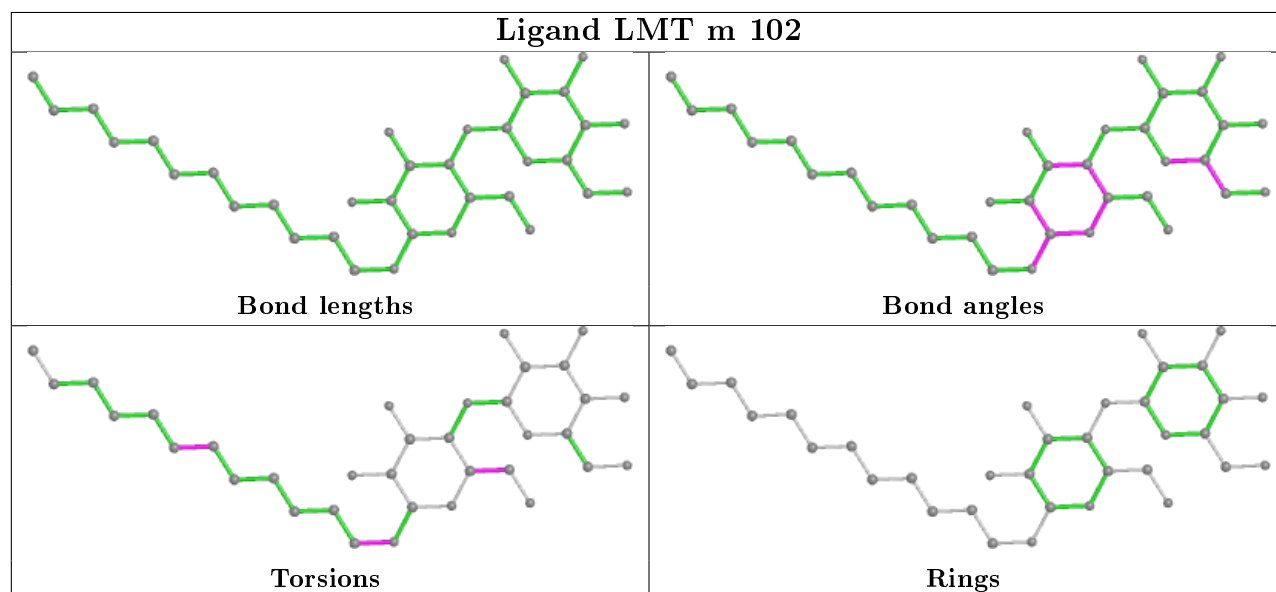




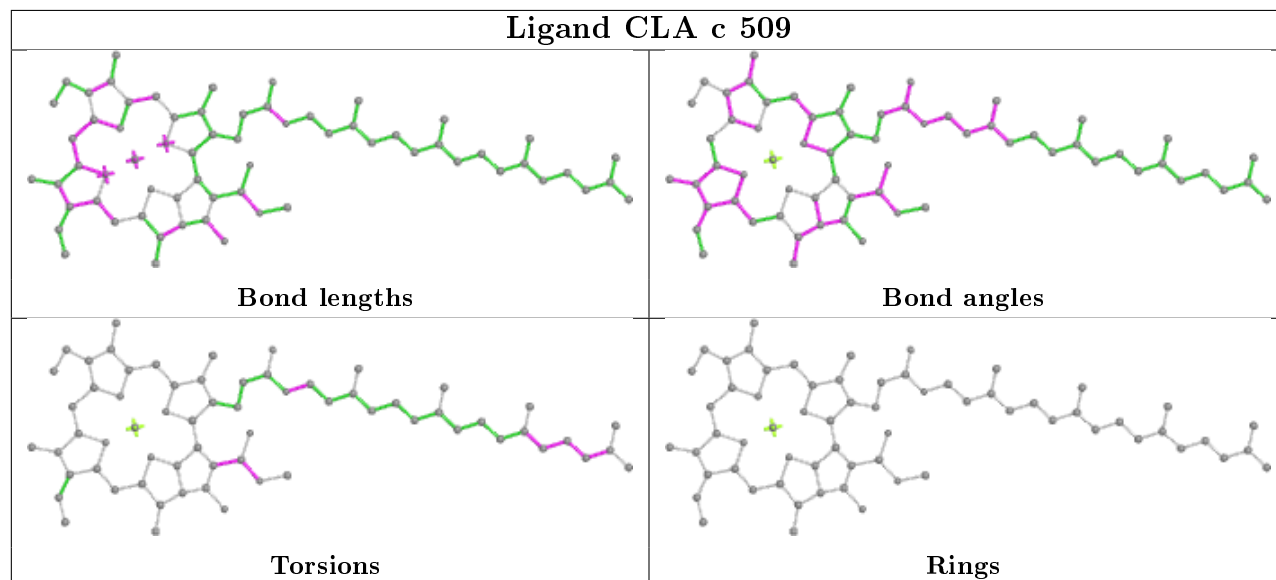
## Ligand CLA c 506

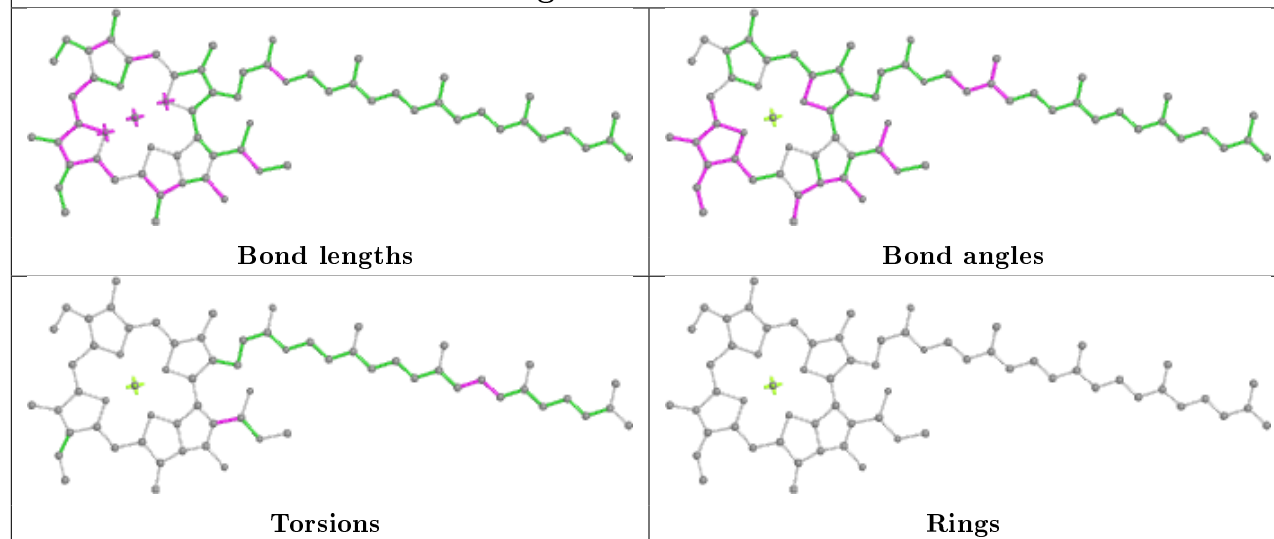
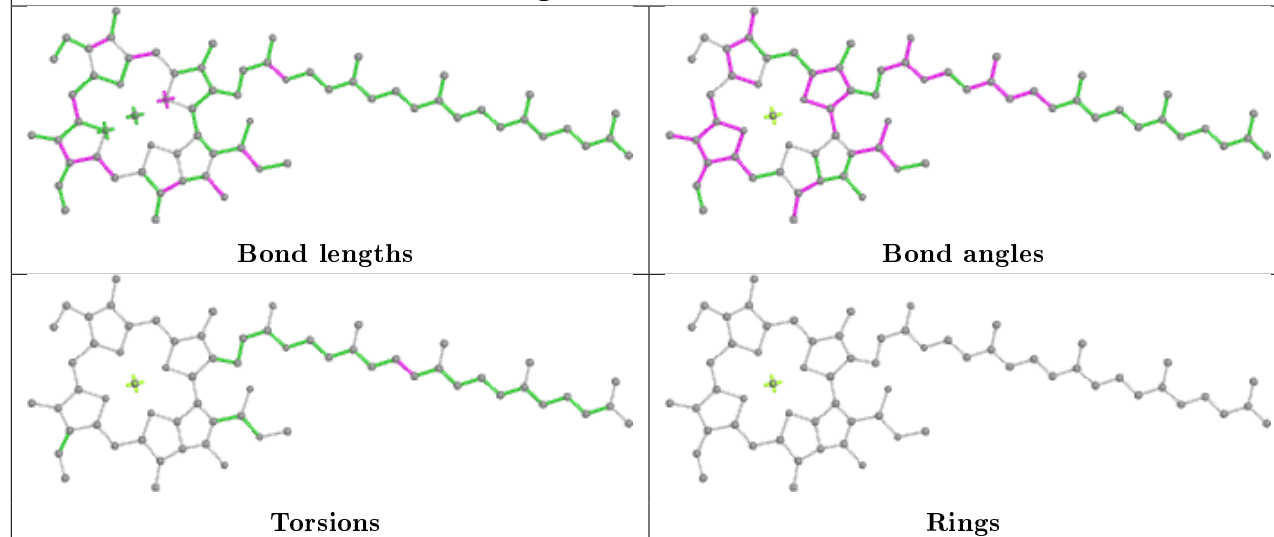


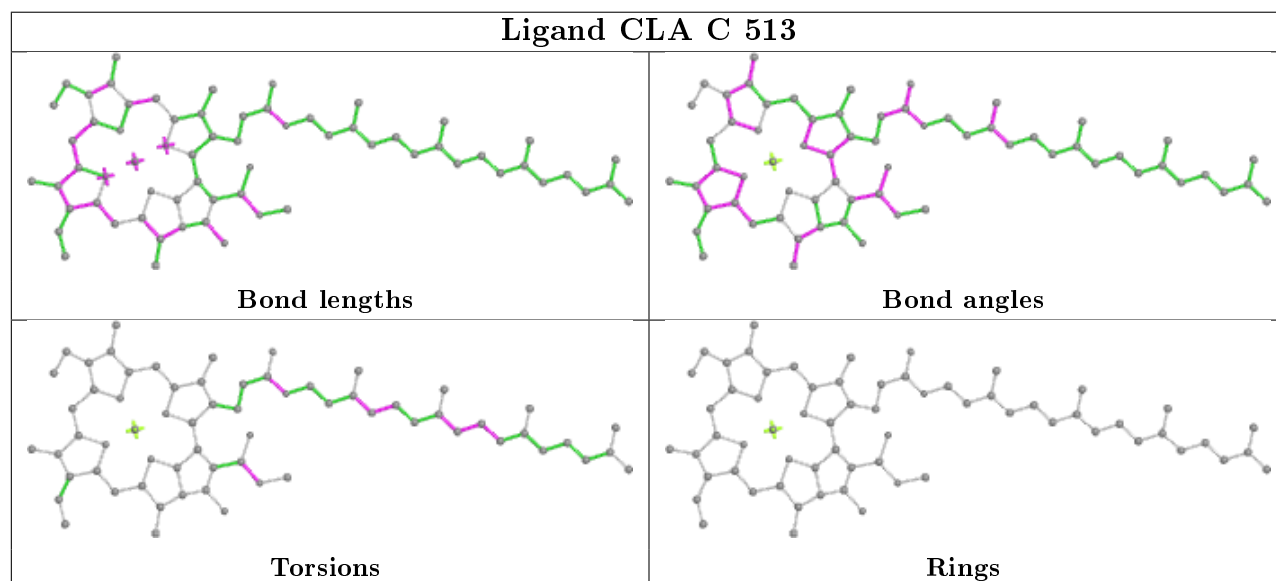
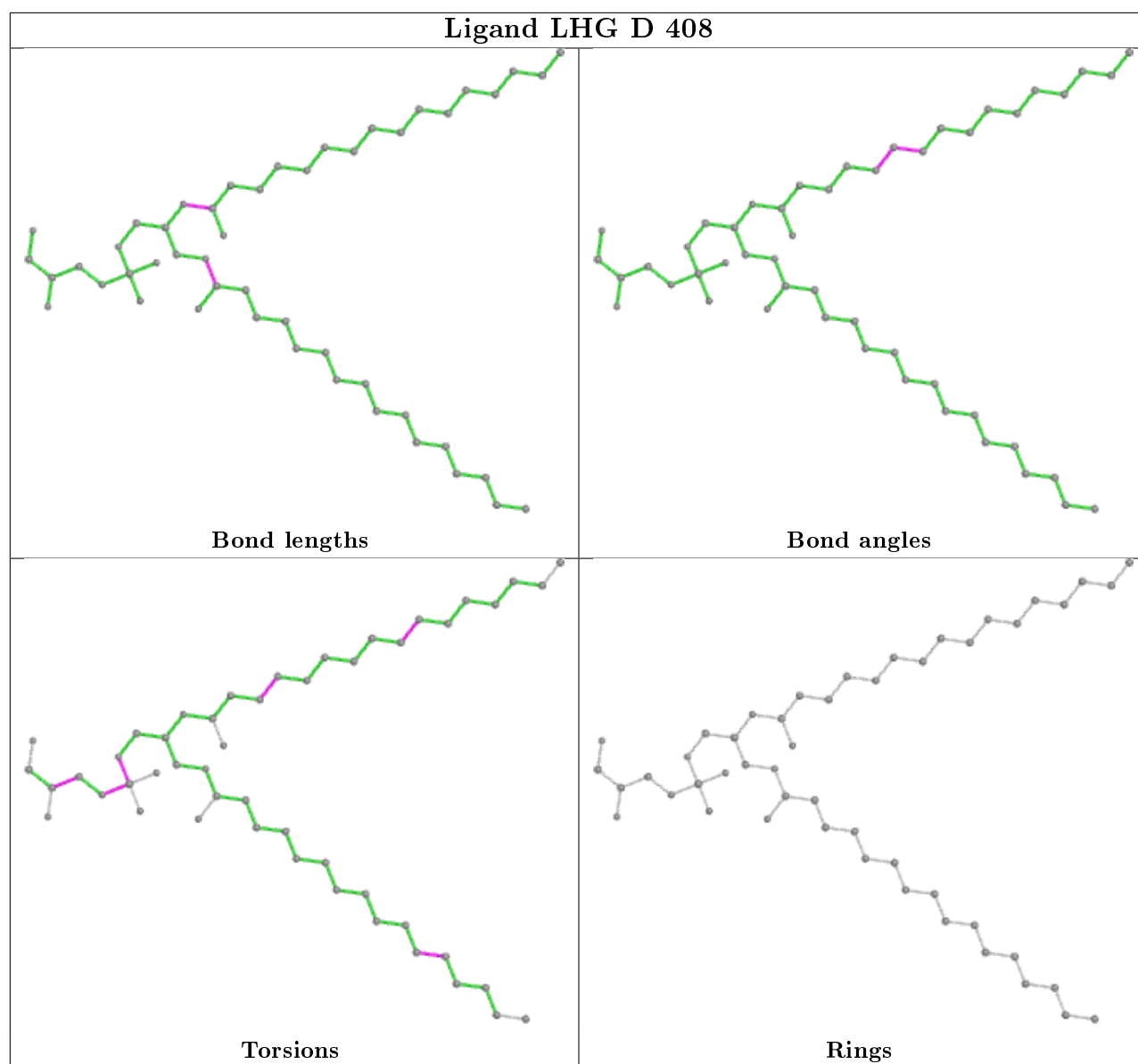
## Ligand LMT m 102

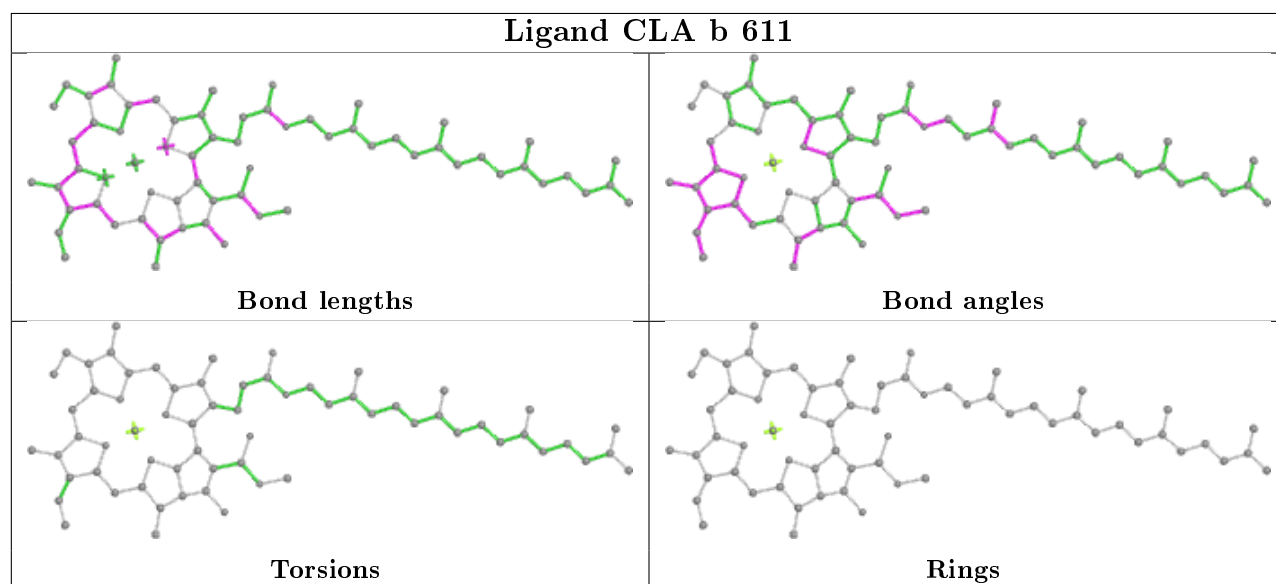
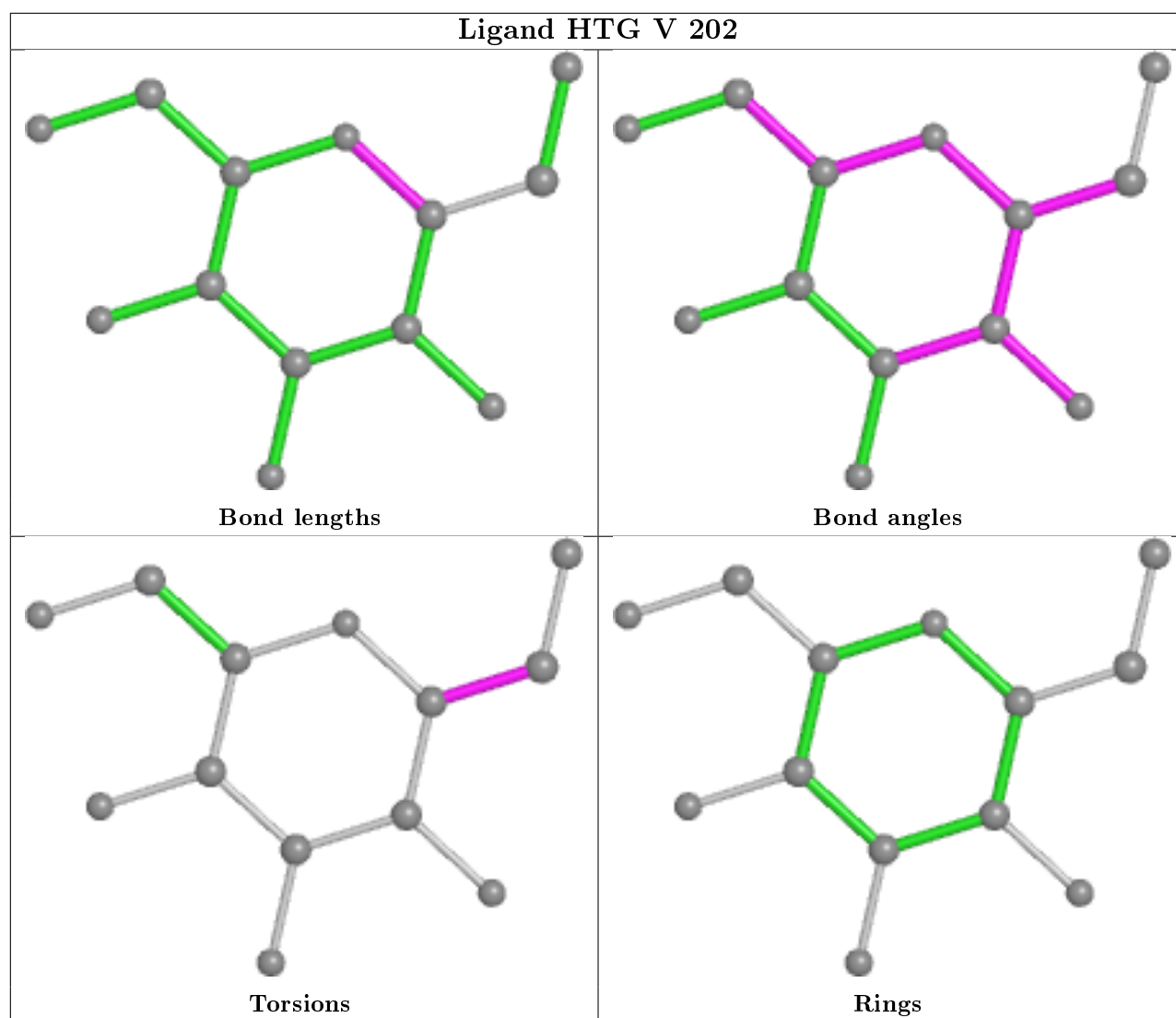


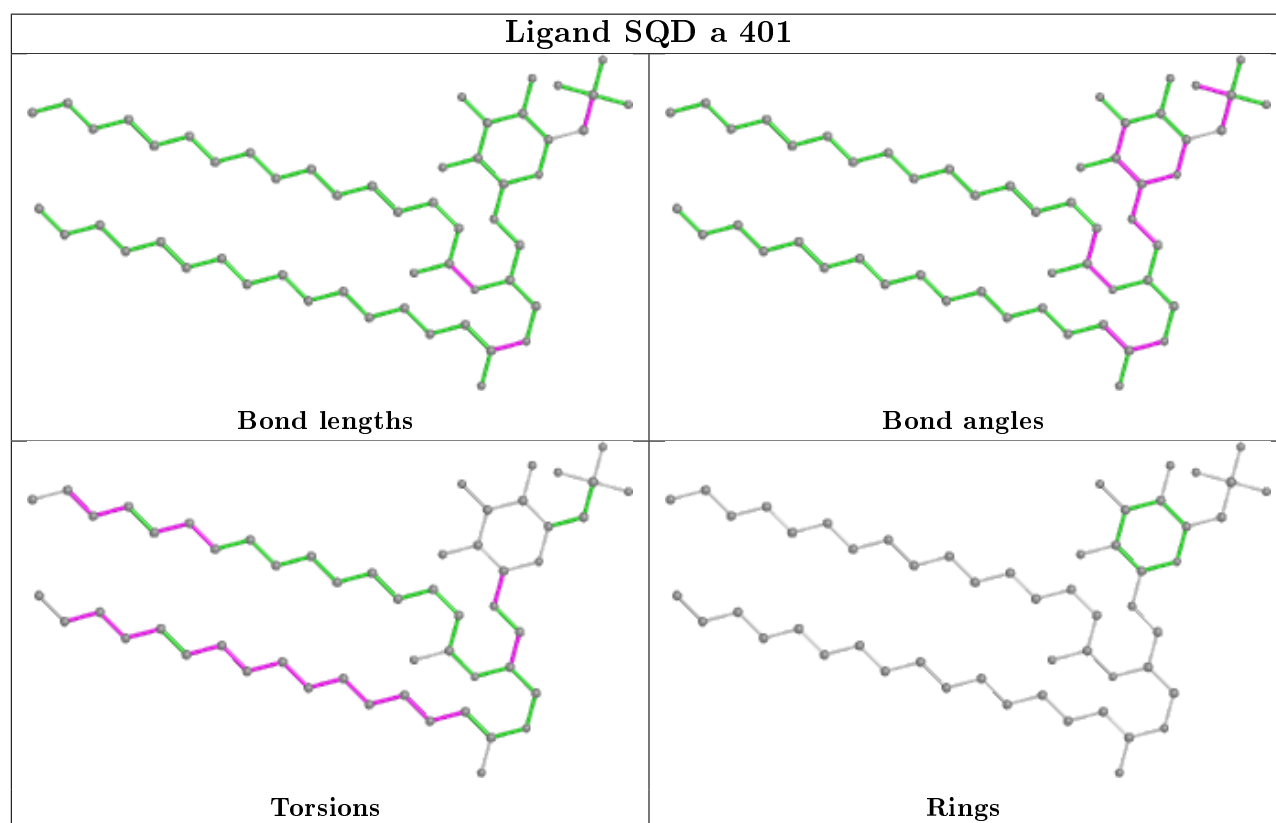
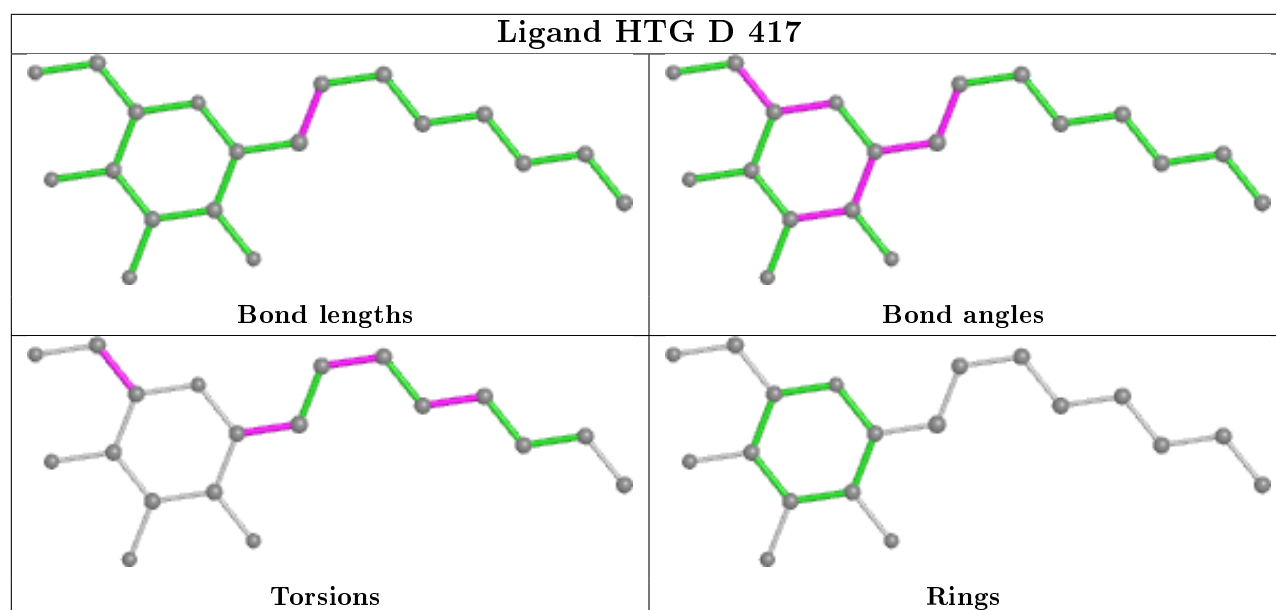
## Ligand CLA c 509

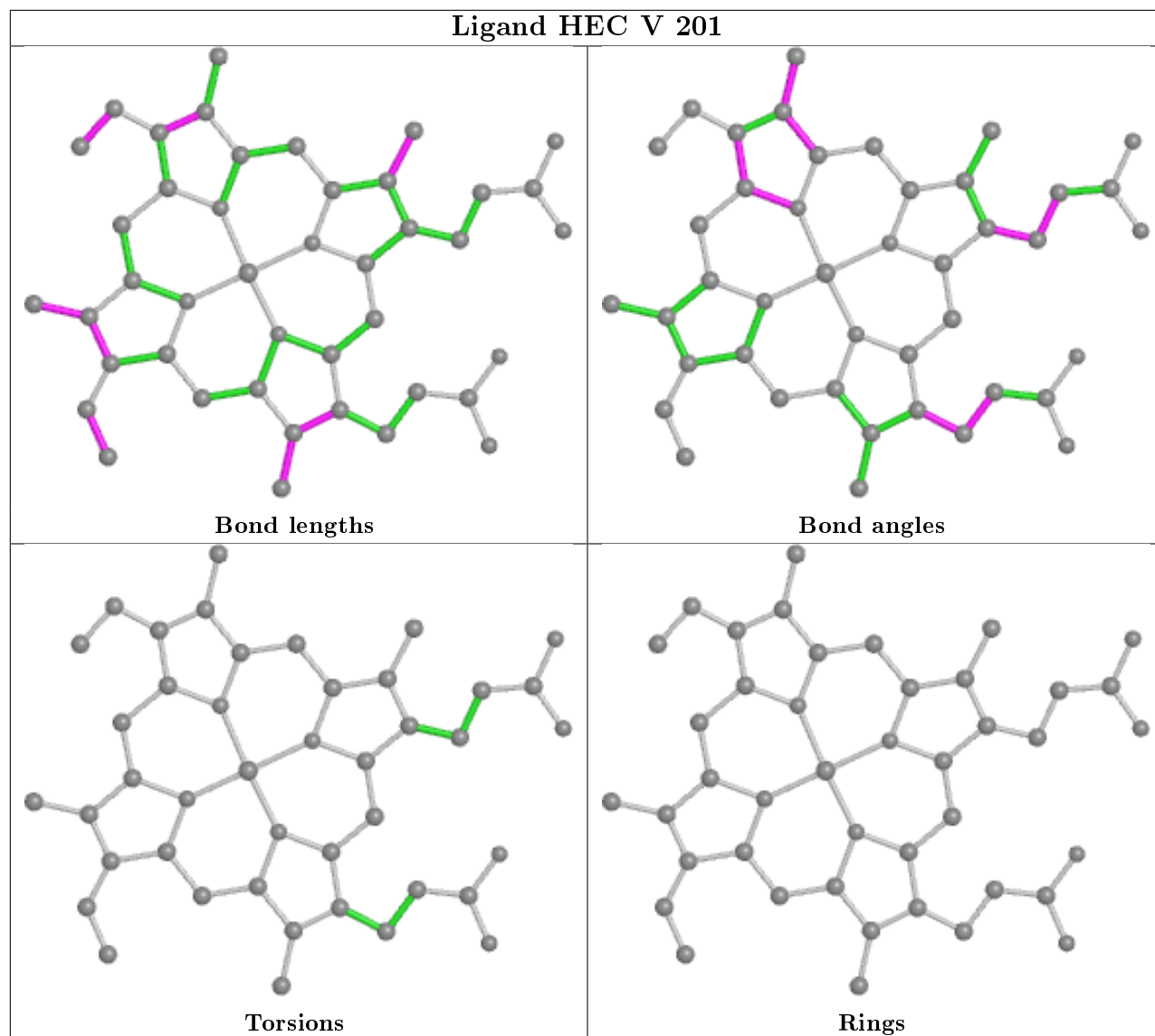
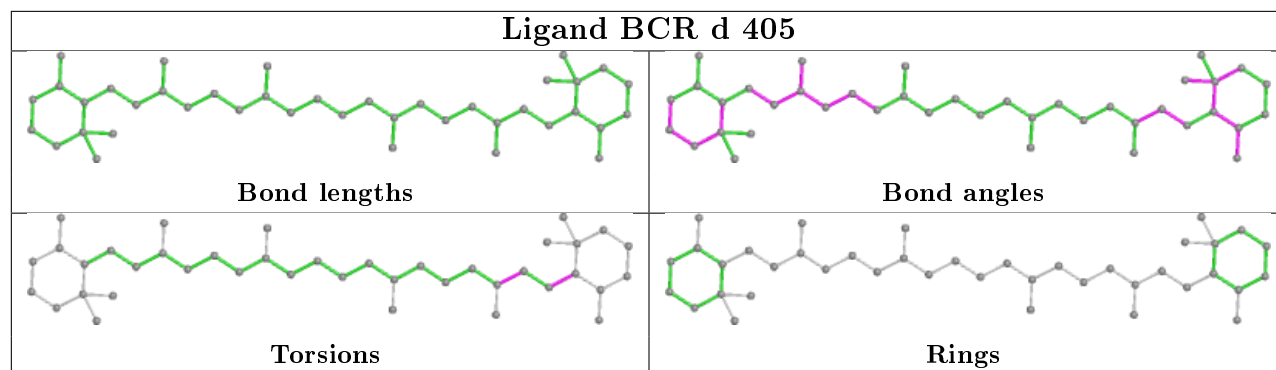


**Ligand CLA c 503****Ligand CLA b 605**

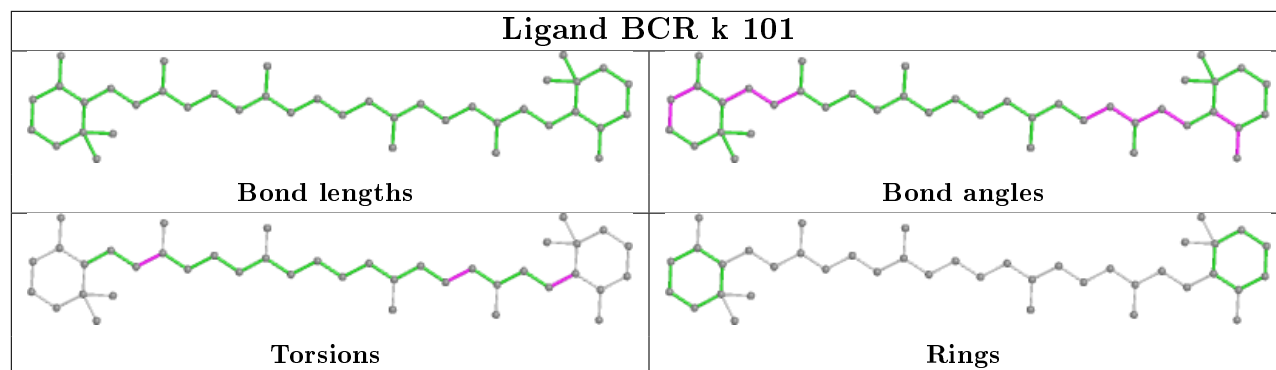
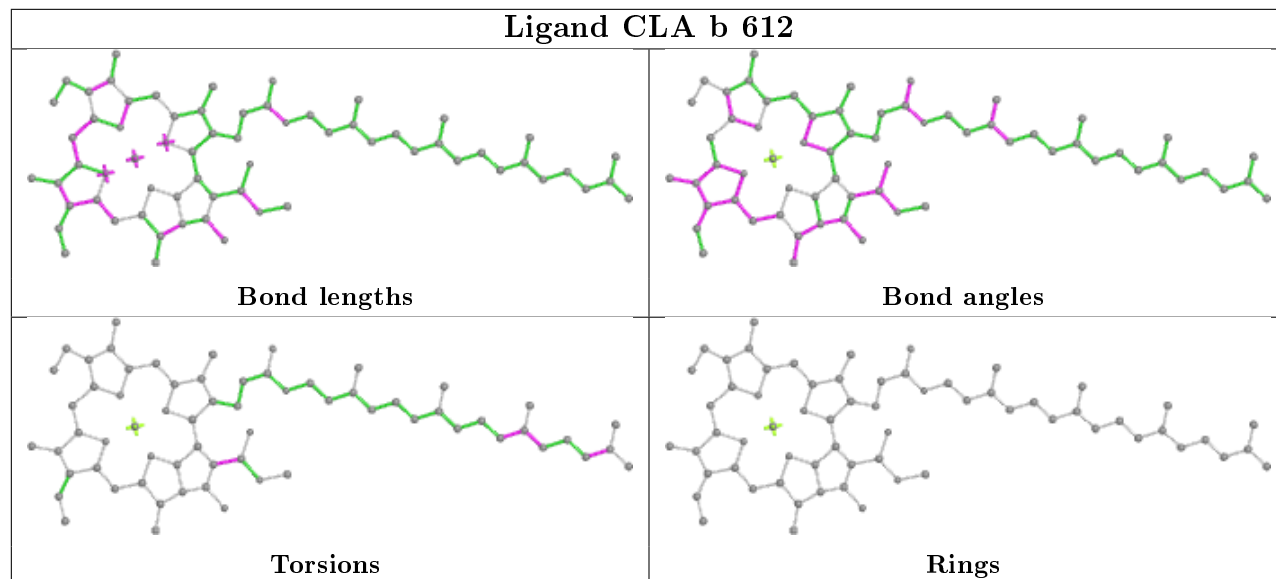
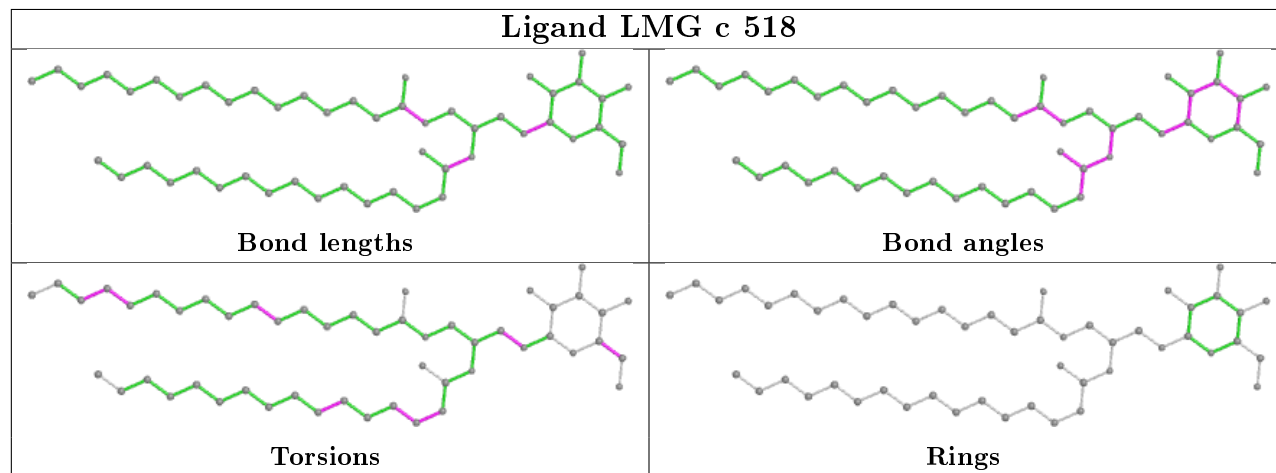


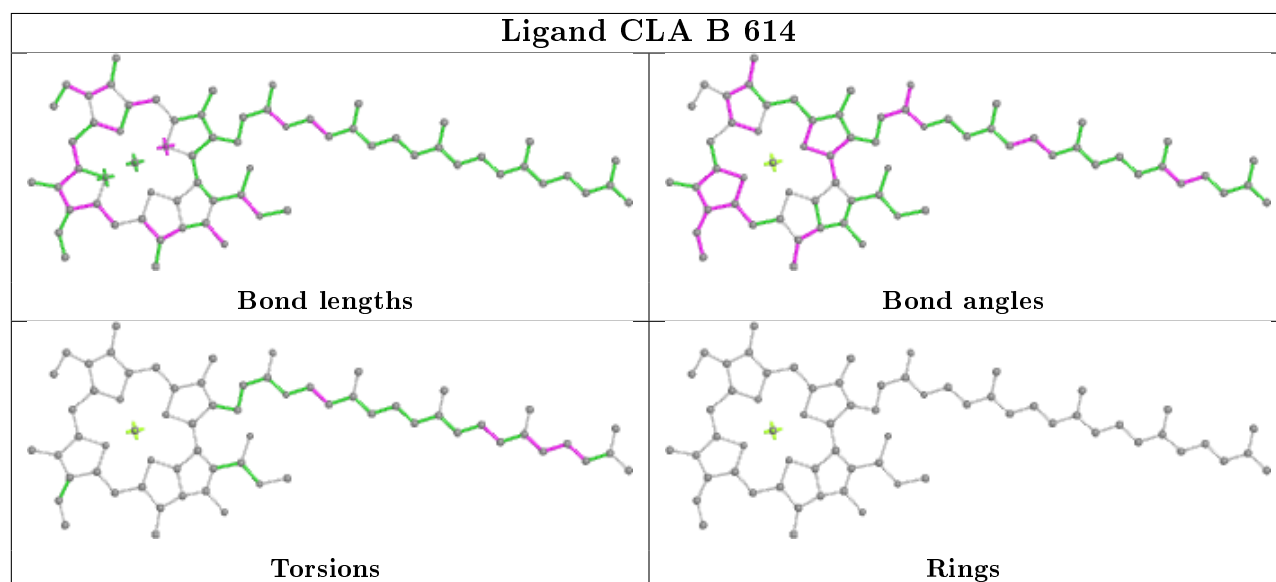
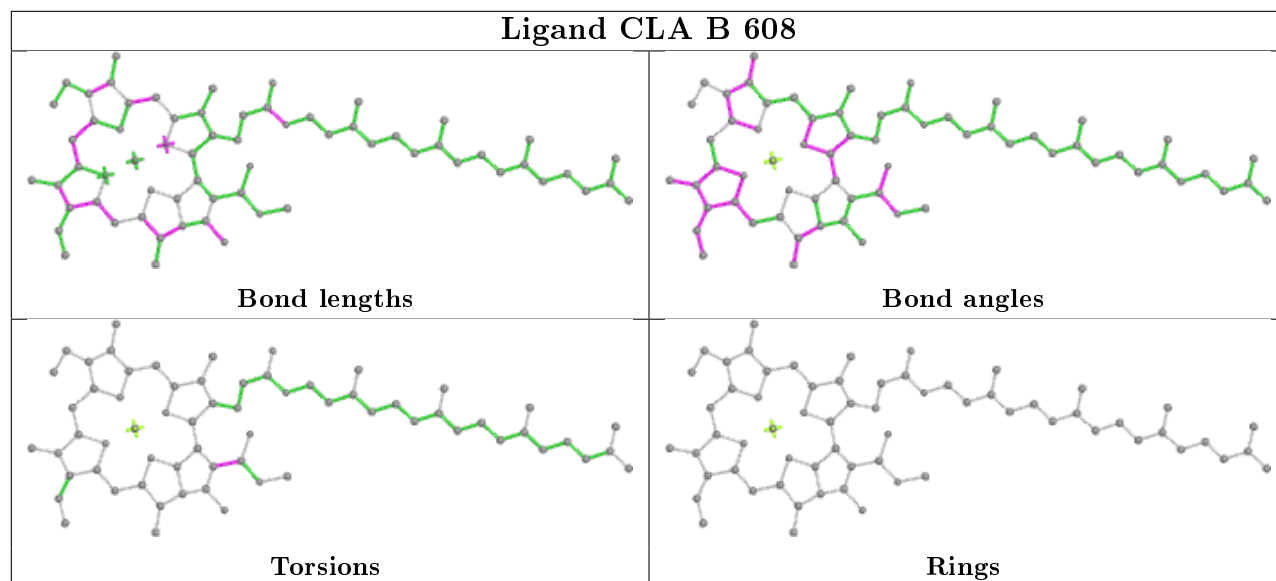
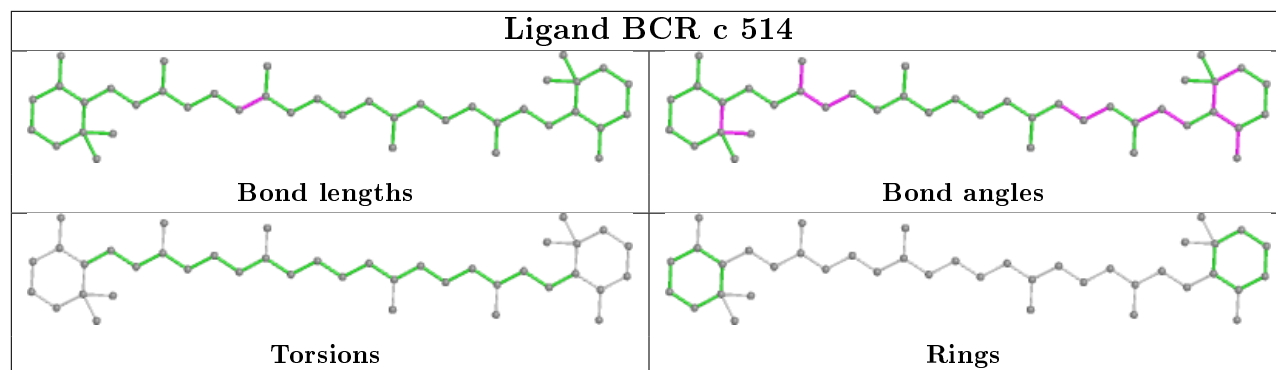


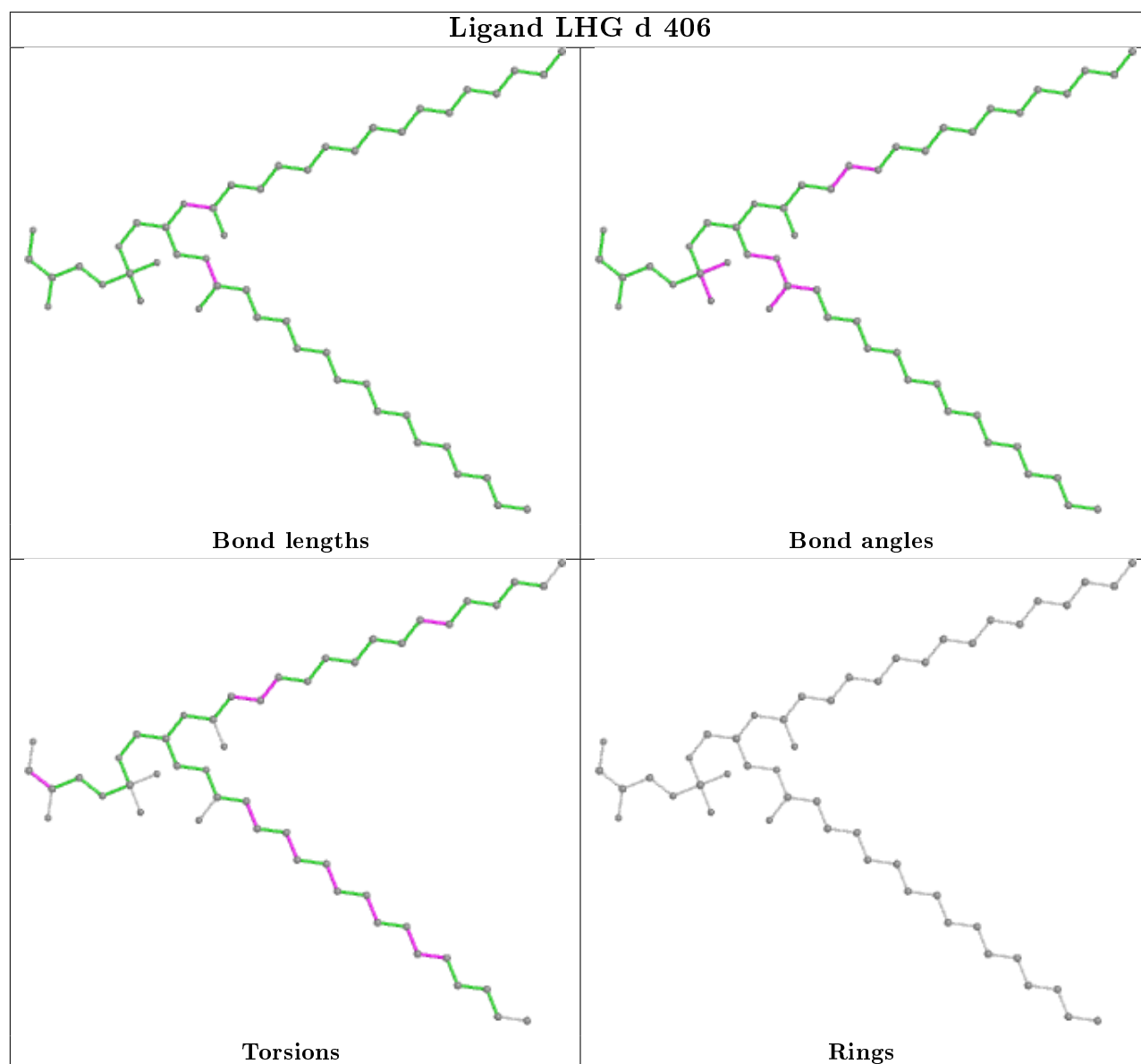
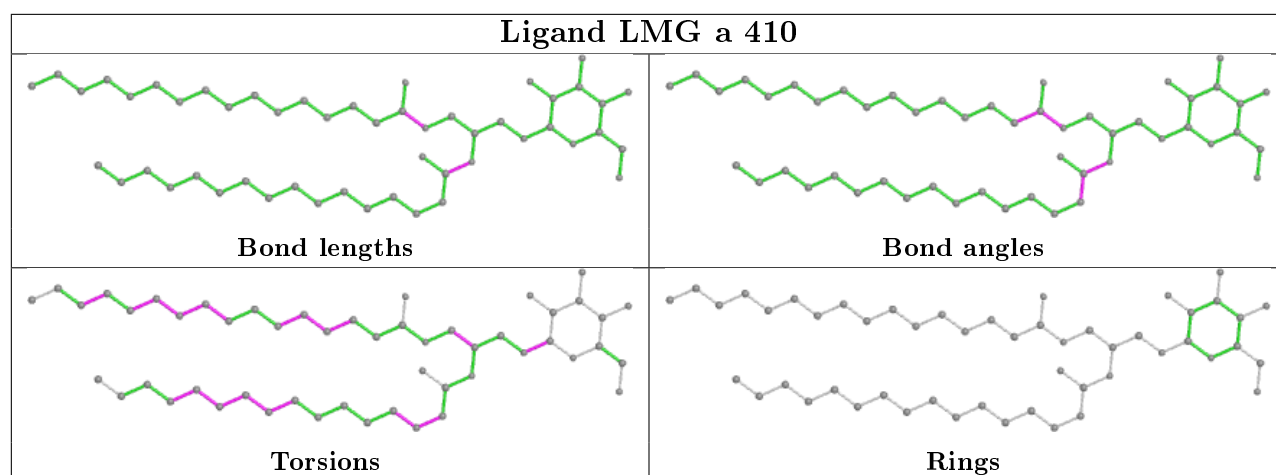




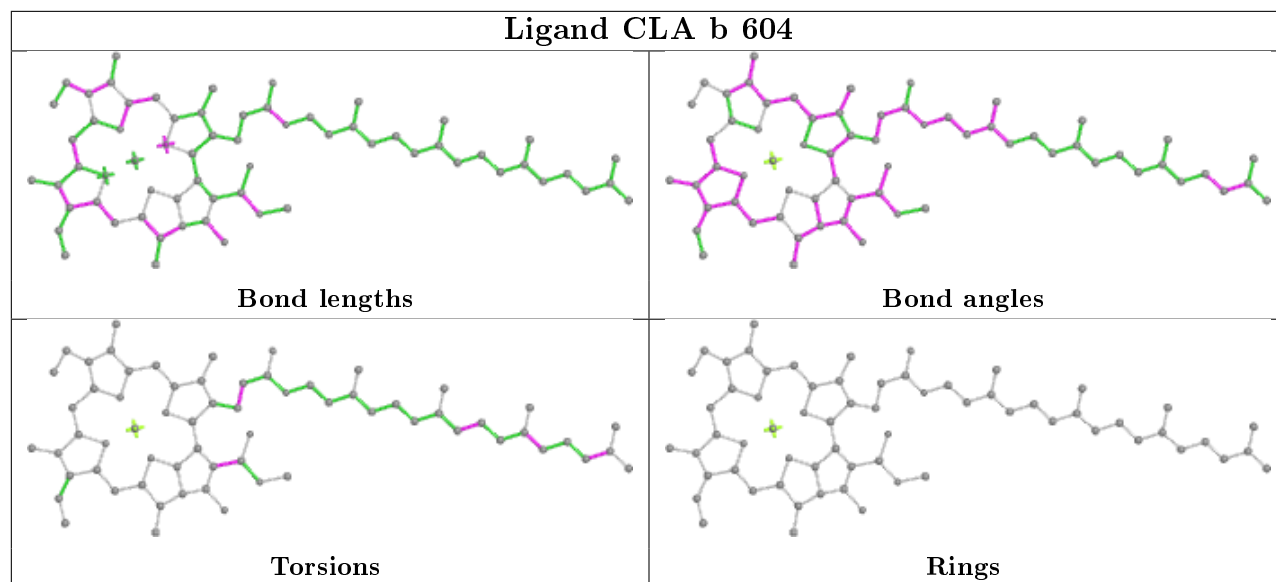


**Ligand BCR k 101****Ligand CLA b 612****Ligand LMG c 518**

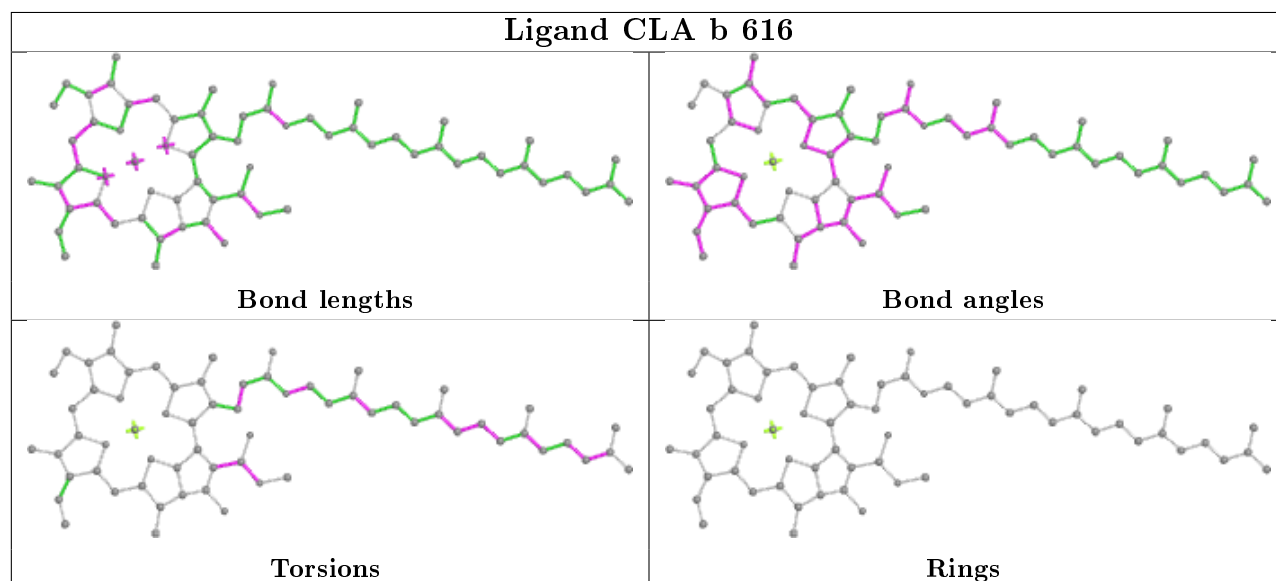




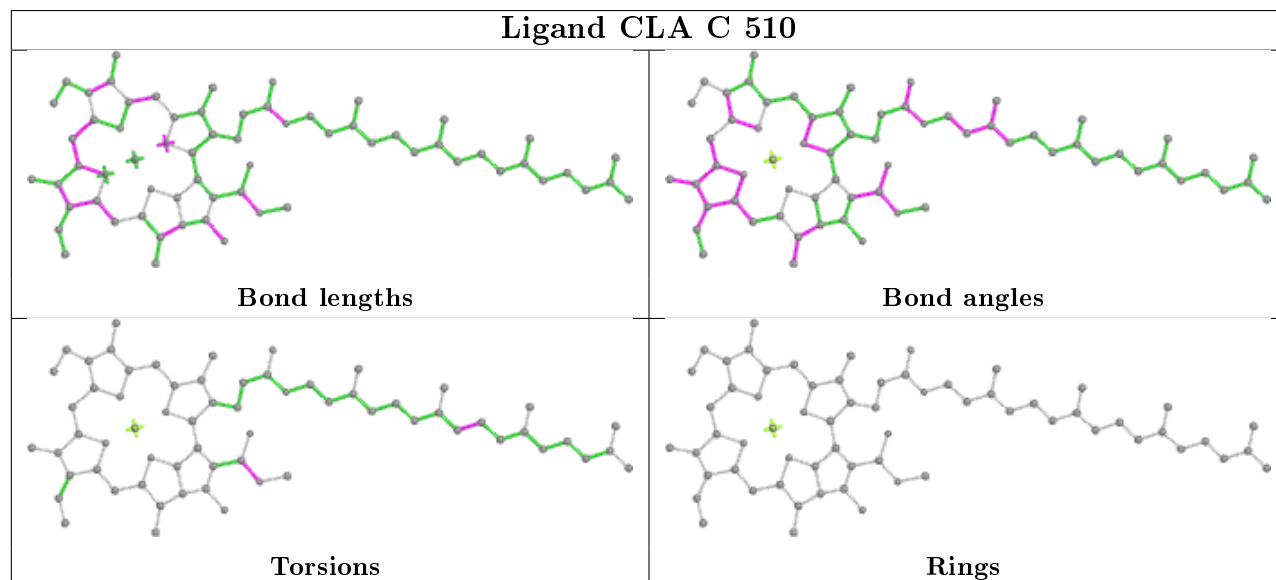
## Ligand CLA b 604

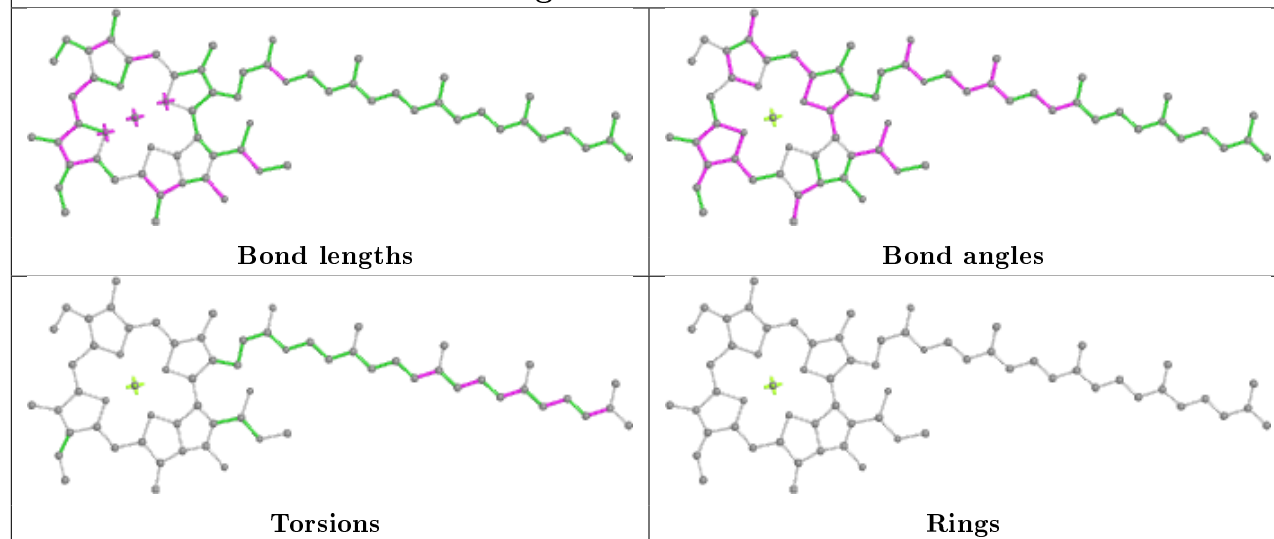
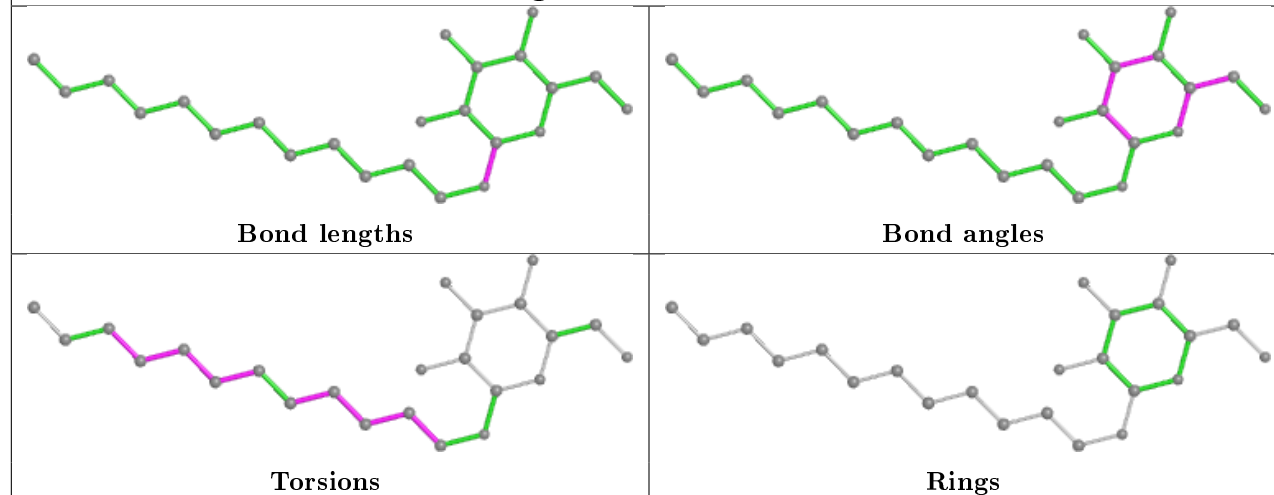
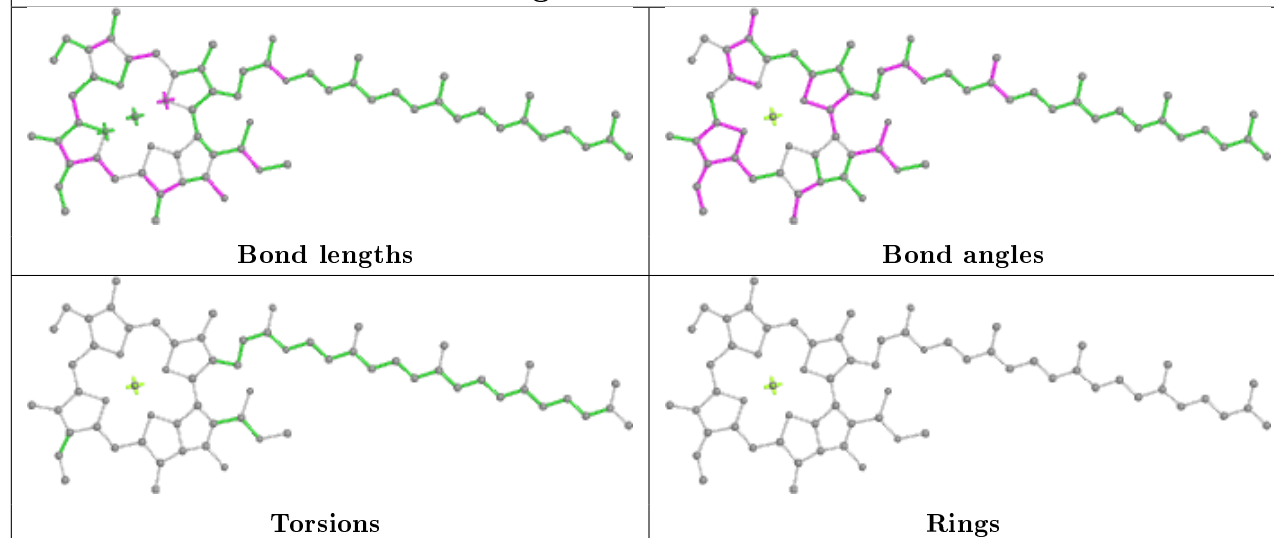


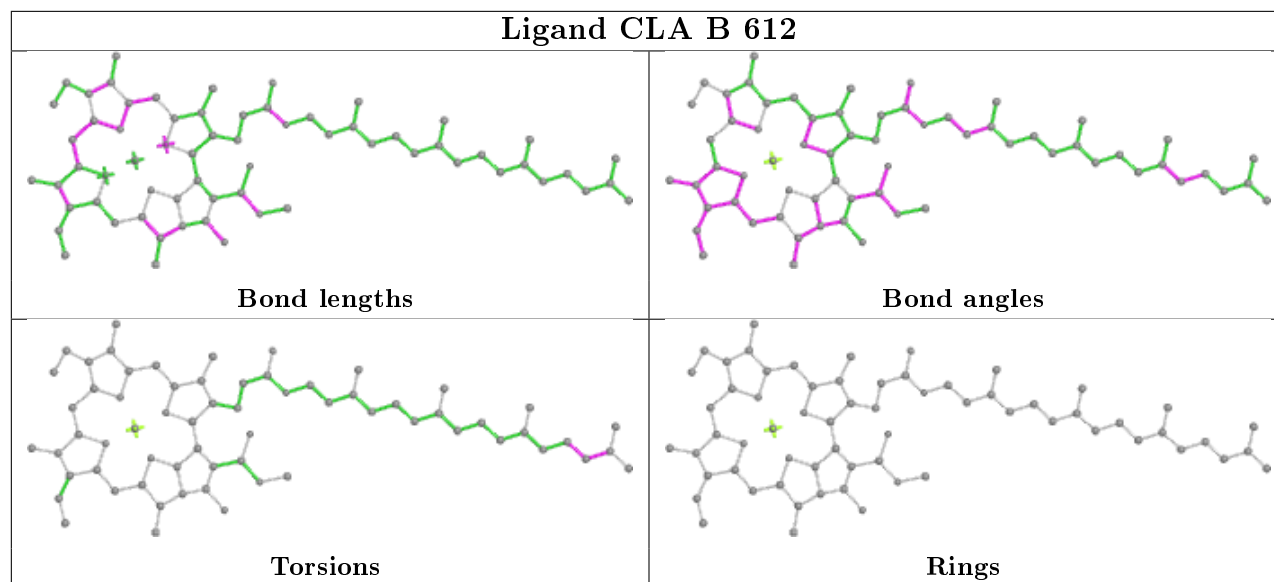
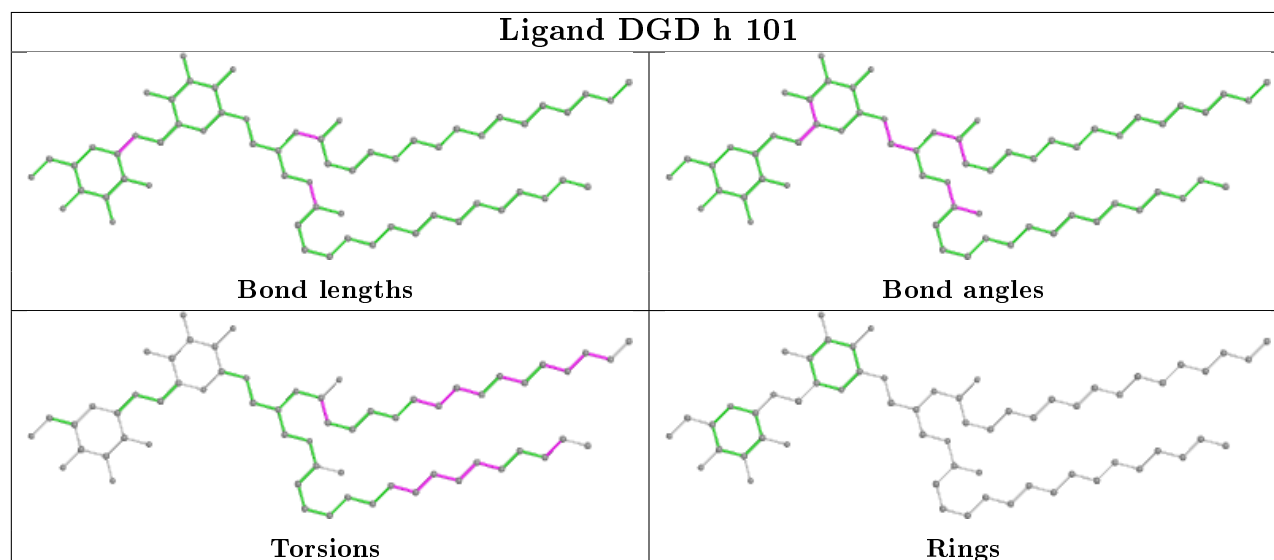
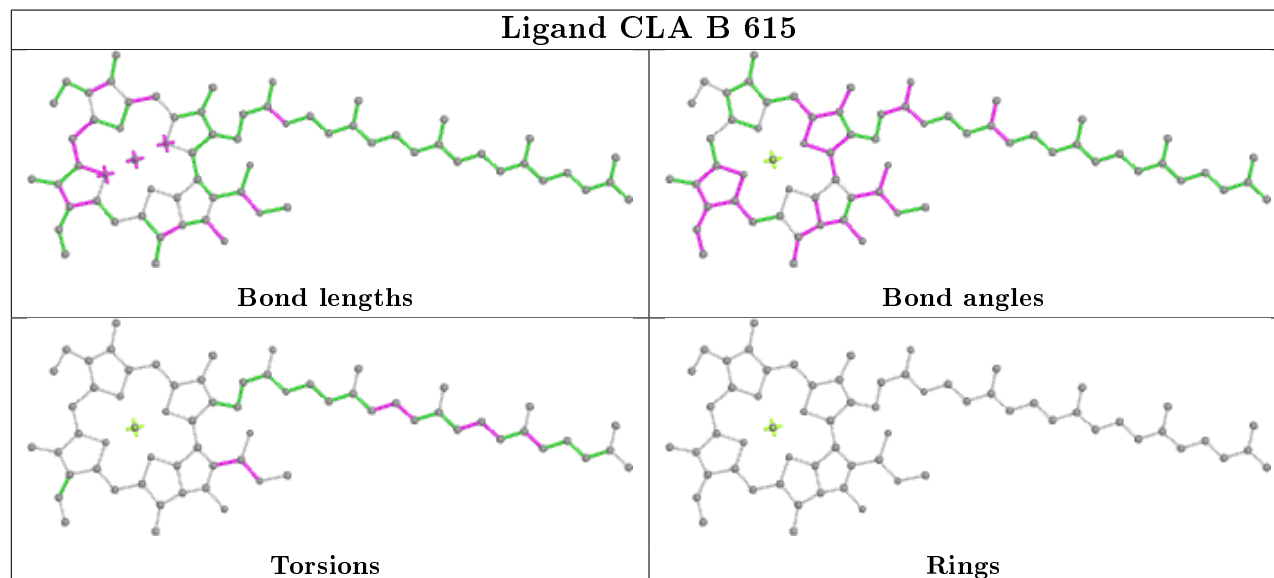
## Ligand CLA b 616

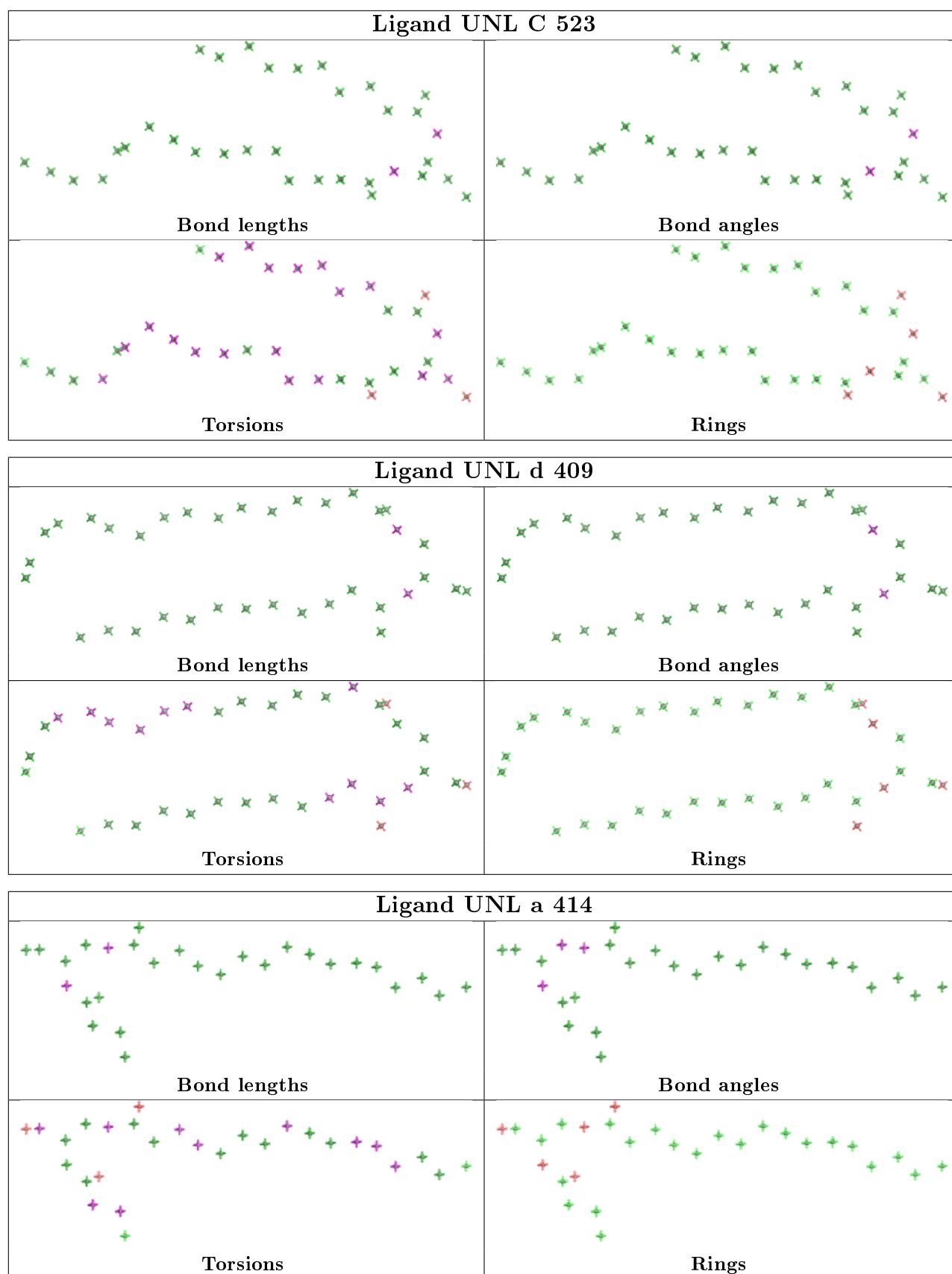


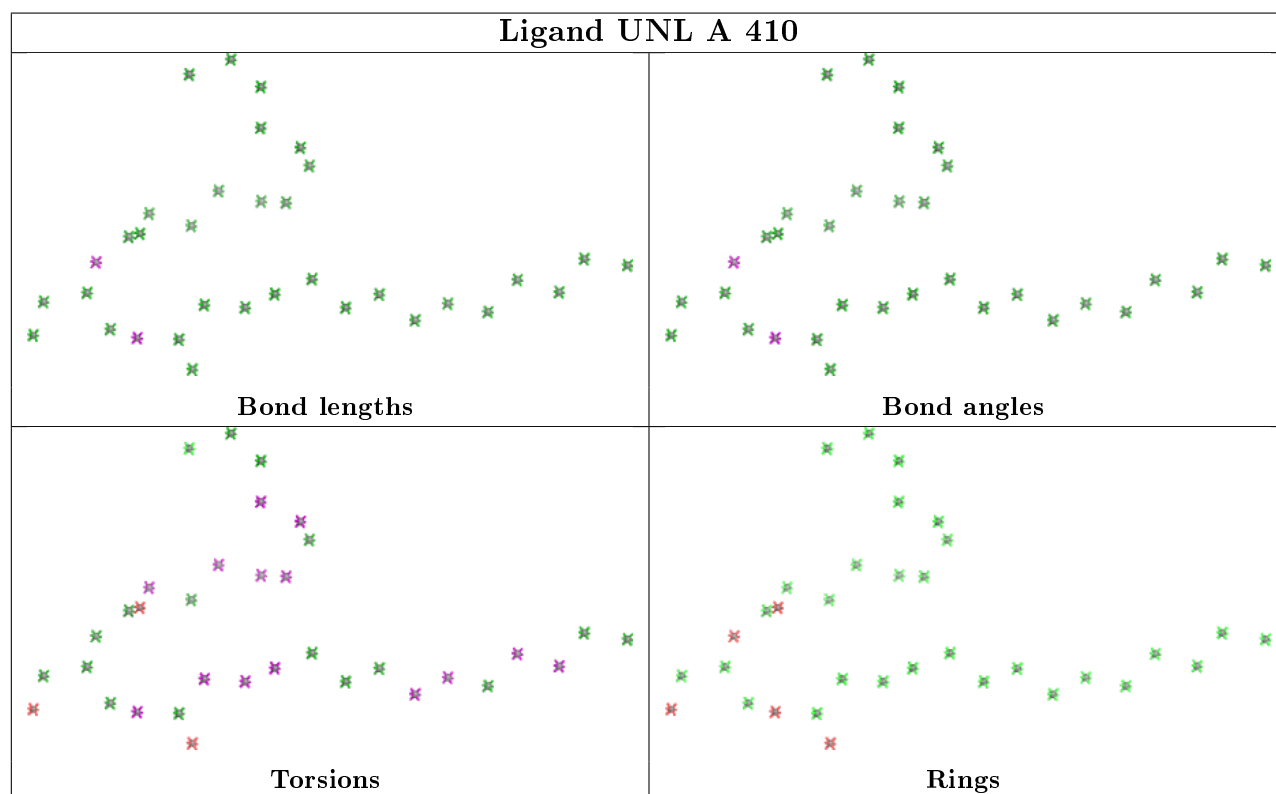
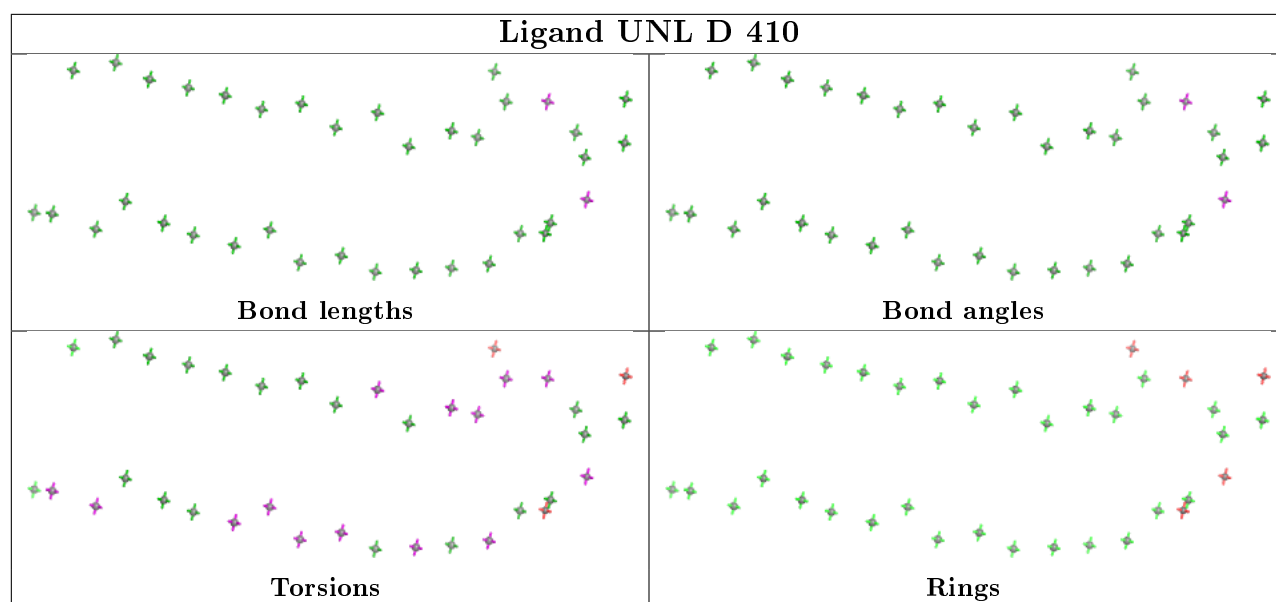
## Ligand CLA C 510



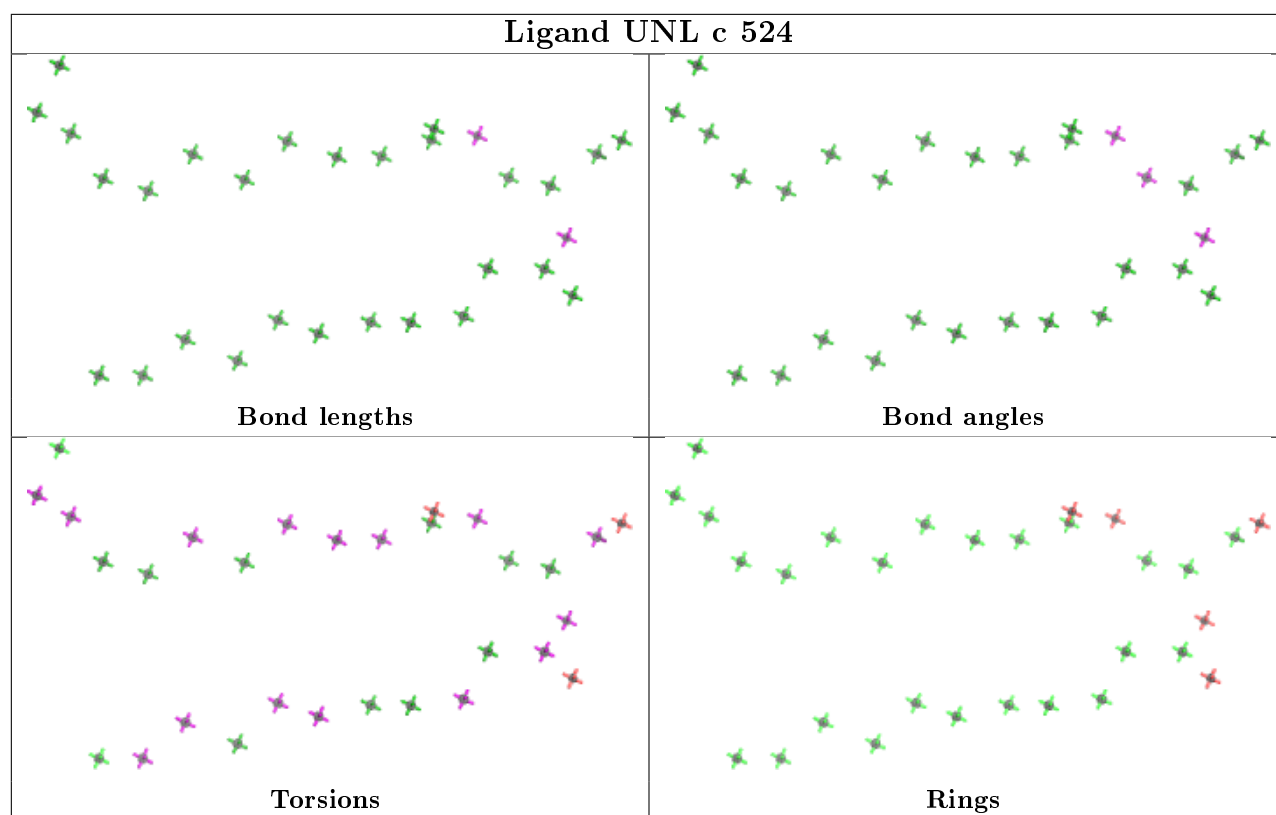
**Ligand CLA d 404****Ligand LMT E 101****Ligand CLA B 613**

**Ligand CLA B 612****Ligand DGD h 101****Ligand CLA B 615**









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 334/344 (97%)  | -0.70  | 3 (0%) 84 84  | 16, 23, 46, 68        | 0     |
| 1   | a     | 334/344 (97%)  | -0.63  | 7 (2%) 63 63  | 18, 23, 48, 78        | 0     |
| 2   | B     | 505/505 (100%) | -0.47  | 19 (3%) 40 38 | 19, 28, 54, 85        | 0     |
| 2   | b     | 495/505 (98%)  | -0.40  | 20 (4%) 38 36 | 19, 28, 53, 95        | 0     |
| 3   | C     | 451/455 (99%)  | -0.45  | 8 (1%) 68 68  | 21, 33, 49, 83        | 0     |
| 3   | c     | 455/455 (100%) | -0.47  | 6 (1%) 77 78  | 22, 33, 46, 79        | 0     |
| 4   | D     | 342/342 (100%) | -0.67  | 4 (1%) 79 79  | 17, 24, 44, 90        | 0     |
| 4   | d     | 342/342 (100%) | -0.73  | 5 (1%) 73 74  | 18, 25, 42, 86        | 0     |
| 5   | E     | 78/83 (93%)    | 0.76   | 19 (24%) 0 0  | 28, 47, 75, 87        | 0     |
| 5   | e     | 78/83 (93%)    | 0.64   | 16 (20%) 1 1  | 29, 44, 67, 81        | 0     |
| 6   | F     | 33/44 (75%)    | -0.09  | 4 (12%) 4 4   | 28, 36, 63, 66        | 0     |
| 6   | f     | 32/44 (72%)    | -0.04  | 3 (9%) 8 8    | 28, 34, 72, 90        | 0     |
| 7   | H     | 64/65 (98%)    | 0.08   | 3 (4%) 31 30  | 26, 37, 50, 78        | 0     |
| 7   | h     | 62/65 (95%)    | -0.24  | 0 100 100     | 25, 36, 48, 58        | 0     |
| 8   | I     | 34/38 (89%)    | -0.11  | 3 (8%) 10 9   | 29, 36, 60, 78        | 0     |
| 8   | i     | 35/38 (92%)    | -0.15  | 2 (5%) 23 23  | 29, 34, 52, 85        | 0     |
| 9   | J     | 36/40 (90%)    | -0.04  | 2 (5%) 24 23  | 26, 41, 74, 90        | 0     |
| 9   | j     | 40/40 (100%)   | -0.03  | 3 (7%) 14 14  | 27, 39, 56, 65        | 0     |
| 10  | K     | 37/37 (100%)   | -0.27  | 2 (5%) 25 24  | 33, 40, 52, 59        | 0     |
| 10  | k     | 37/37 (100%)   | -0.22  | 1 (2%) 54 53  | 32, 40, 56, 64        | 0     |
| 11  | L     | 37/37 (100%)   | -0.36  | 3 (8%) 12 12  | 18, 22, 65, 81        | 0     |
| 11  | l     | 37/37 (100%)   | -0.22  | 3 (8%) 12 12  | 18, 22, 76, 91        | 0     |
| 12  | M     | 33/36 (91%)    | -0.65  | 1 (3%) 50 48  | 21, 25, 39, 57        | 0     |
| 12  | m     | 34/36 (94%)    | -0.55  | 3 (8%) 10 9   | 20, 26, 53, 74        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13  | O     | 243/244 (99%)   | -0.23  | 8 (3%) 46 44   | 18, 32, 56, 85        | 0     |
| 13  | o     | 243/244 (99%)   | -0.09  | 19 (7%) 13 13  | 19, 35, 67, 89        | 0     |
| 14  | T     | 28/32 (87%)     | -0.69  | 1 (3%) 42 40   | 19, 24, 37, 54        | 0     |
| 14  | t     | 29/32 (90%)     | -0.36  | 2 (6%) 16 16   | 20, 23, 49, 74        | 0     |
| 15  | U     | 97/104 (93%)    | -0.34  | 2 (2%) 63 63   | 22, 29, 49, 67        | 0     |
| 15  | u     | 97/104 (93%)    | -0.36  | 1 (1%) 82 82   | 24, 29, 44, 75        | 0     |
| 16  | V     | 137/137 (100%)  | -0.62  | 0 100 100      | 22, 28, 43, 60        | 0     |
| 16  | v     | 137/137 (100%)  | -0.25  | 5 (3%) 42 40   | 25, 36, 53, 74        | 0     |
| 17  | Y     | 29/30 (96%)     | 1.08   | 6 (20%) 1 0    | 41, 51, 72, 79        | 0     |
| 17  | y     | 29/30 (96%)     | 0.76   | 4 (13%) 2 3    | 41, 50, 66, 70        | 0     |
| 18  | X     | 38/40 (95%)     | 0.26   | 5 (13%) 3 3    | 32, 42, 68, 72        | 0     |
| 18  | x     | 35/40 (87%)     | -0.09  | 2 (5%) 23 23   | 33, 40, 63, 67        | 0     |
| 19  | Z     | 62/62 (100%)    | 0.66   | 13 (20%) 1 0   | 38, 48, 86, 98        | 0     |
| 19  | z     | 61/62 (98%)     | 0.71   | 12 (19%) 1 1   | 45, 54, 86, 96        | 0     |
| All | All   | 5230/5350 (97%) | -0.37  | 220 (4%) 36 34 | 16, 30, 57, 98        | 0     |

The worst 5 of 220 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | b     | 496 | TYR  | 9.7  |
| 2   | b     | 495 | PHE  | 9.2  |
| 2   | b     | 503 | THR  | 8.4  |
| 13  | o     | 246 | ALA  | 8.3  |
| 2   | b     | 502 | VAL  | 7.4  |

## 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 14  | FME  | T     | 1   | 10/11 | 0.97 | 0.07 | 23,29,48,51                | 0     |
| 14  | FME  | t     | 1   | 10/11 | 0.97 | 0.06 | 23,27,49,50                | 0     |
| 8   | FME  | i     | 1   | 10/11 | 0.98 | 0.09 | 30,31,34,35                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 8   | FME  | I     | 1   | 10/11 | 0.98 | 0.07 | 26,32,36,37                 | 0     |

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 32  | HTG  | C     | 534 | 19/19 | 0.39 | 0.39 | 68,110,128,130              | 0     |
| 24  | LMG  | C     | 524 | 45/55 | 0.52 | 0.32 | 22,46,51,56                 | 45    |
| 26  | UNL  | Z     | 102 | 4/-   | 0.52 | 0.17 | 59,61,62,63                 | 0     |
| 32  | HTG  | D     | 417 | 19/19 | 0.53 | 0.31 | 67,105,119,120              | 0     |
| 28  | DMS  | U     | 904 | 4/4   | 0.55 | 0.22 | 58,66,66,83                 | 0     |
| 32  | HTG  | c     | 521 | 19/19 | 0.56 | 0.35 | 57,85,102,105               | 0     |
| 26  | UNL  | b     | 642 | 13/-  | 0.57 | 0.22 | 71,80,87,90                 | 0     |
| 32  | HTG  | d     | 401 | 19/19 | 0.58 | 0.29 | 58,99,111,120               | 0     |
| 26  | UNL  | b     | 645 | 6/-   | 0.58 | 0.24 | 57,65,76,76                 | 0     |
| 32  | HTG  | B     | 623 | 19/19 | 0.59 | 0.35 | 53,88,93,94                 | 0     |
| 34  | LMT  | f     | 102 | 24/35 | 0.59 | 0.26 | 62,77,94,98                 | 0     |
| 35  | DGD  | D     | 406 | 51/66 | 0.59 | 0.30 | 57,74,100,108               | 0     |
| 26  | UNL  | J     | 104 | 14/-  | 0.60 | 0.24 | 67,77,80,81                 | 0     |
| 34  | LMT  | J     | 103 | 24/35 | 0.60 | 0.23 | 53,61,81,85                 | 0     |
| 28  | DMS  | H     | 103 | 4/4   | 0.61 | 0.40 | 84,101,109,112              | 0     |
| 28  | DMS  | B     | 636 | 4/4   | 0.61 | 0.40 | 77,86,90,96                 | 0     |
| 34  | LMT  | m     | 101 | 35/35 | 0.63 | 0.25 | 48,94,110,114               | 0     |
| 26  | UNL  | A     | 410 | 36/-  | 0.64 | 0.25 | 57,78,84,91                 | 0     |
| 34  | LMT  | b     | 628 | 25/35 | 0.64 | 0.22 | 54,79,95,96                 | 0     |
| 35  | DGD  | d     | 416 | 51/66 | 0.64 | 0.27 | 56,75,96,103                | 0     |
| 32  | HTG  | B     | 632 | 19/19 | 0.65 | 0.23 | 51,97,108,114               | 0     |
| 36  | LHG  | E     | 103 | 48/49 | 0.66 | 0.29 | 44,99,108,119               | 0     |
| 28  | DMS  | v     | 207 | 4/4   | 0.67 | 0.20 | 53,66,72,87                 | 0     |
| 26  | UNL  | a     | 414 | 28/-  | 0.67 | 0.23 | 59,68,84,87                 | 0     |
| 32  | HTG  | C     | 521 | 19/19 | 0.67 | 0.26 | 46,78,89,90                 | 0     |
| 26  | UNL  | B     | 646 | 16/-  | 0.68 | 0.24 | 85,89,93,94                 | 0     |
| 26  | UNL  | b     | 643 | 9/-   | 0.68 | 0.18 | 67,67,74,74                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 26  | UNL  | E     | 102 | 15/-  | 0.68 | 0.28 | 55,62,76,77                 | 0     |
| 28  | DMS  | O     | 305 | 4/4   | 0.69 | 0.30 | 64,66,77,86                 | 0     |
| 28  | DMS  | j     | 105 | 4/4   | 0.69 | 0.19 | 70,74,75,88                 | 0     |
| 26  | UNL  | T     | 103 | 13/-  | 0.69 | 0.17 | 64,68,72,72                 | 0     |
| 32  | HTG  | v     | 210 | 14/19 | 0.69 | 0.27 | 60,80,92,100                | 0     |
| 26  | UNL  | a     | 402 | 6/-   | 0.69 | 0.17 | 50,57,62,63                 | 0     |
| 26  | UNL  | B     | 630 | 14/-  | 0.70 | 0.20 | 67,74,83,84                 | 0     |
| 34  | LMT  | Z     | 101 | 35/35 | 0.70 | 0.23 | 44,90,107,109               | 0     |
| 32  | HTG  | b     | 602 | 19/19 | 0.70 | 0.20 | 51,103,117,118              | 0     |
| 34  | LMT  | b     | 627 | 32/35 | 0.71 | 0.24 | 42,67,84,87                 | 0     |
| 24  | LMG  | c     | 518 | 51/55 | 0.72 | 0.21 | 37,72,84,87                 | 0     |
| 26  | UNL  | B     | 629 | 10/-  | 0.72 | 0.27 | 54,69,74,74                 | 0     |
| 26  | UNL  | c     | 524 | 30/-  | 0.72 | 0.19 | 59,74,86,87                 | 0     |
| 26  | UNL  | J     | 107 | 3/-   | 0.73 | 0.21 | 61,61,63,64                 | 0     |
| 34  | LMT  | a     | 418 | 35/35 | 0.73 | 0.21 | 45,69,78,81                 | 0     |
| 26  | UNL  | U     | 901 | 14/-  | 0.74 | 0.27 | 40,49,59,59                 | 0     |
| 26  | UNL  | h     | 103 | 16/-  | 0.74 | 0.29 | 61,69,73,76                 | 0     |
| 34  | LMT  | B     | 626 | 24/35 | 0.74 | 0.20 | 37,54,86,95                 | 0     |
| 32  | HTG  | u     | 201 | 8/19  | 0.74 | 0.21 | 45,52,69,89                 | 0     |
| 34  | LMT  | m     | 102 | 35/35 | 0.74 | 0.20 | 34,53,58,59                 | 0     |
| 28  | DMS  | b     | 638 | 4/4   | 0.75 | 0.28 | 67,75,77,86                 | 0     |
| 23  | SQD  | l     | 101 | 54/54 | 0.75 | 0.20 | 47,68,101,106               | 0     |
| 26  | UNL  | a     | 416 | 11/-  | 0.75 | 0.16 | 66,68,76,78                 | 0     |
| 34  | LMT  | M     | 101 | 35/35 | 0.75 | 0.20 | 34,53,63,64                 | 0     |
| 26  | UNL  | C     | 523 | 34/-  | 0.75 | 0.22 | 59,80,92,101                | 0     |
| 26  | UNL  | I     | 106 | 11/-  | 0.76 | 0.19 | 61,73,81,81                 | 0     |
| 34  | LMT  | B     | 625 | 24/35 | 0.76 | 0.16 | 48,67,86,89                 | 0     |
| 28  | DMS  | b     | 640 | 4/4   | 0.76 | 0.27 | 49,58,71,73                 | 0     |
| 26  | UNL  | B     | 647 | 13/-  | 0.76 | 0.24 | 71,81,90,91                 | 0     |
| 27  | PL9  | a     | 415 | 55/55 | 0.77 | 0.23 | 52,67,89,94                 | 0     |
| 28  | DMS  | B     | 642 | 4/4   | 0.77 | 0.31 | 43,51,68,71                 | 0     |
| 34  | LMT  | I     | 101 | 35/35 | 0.77 | 0.24 | 67,82,91,92                 | 0     |
| 28  | DMS  | O     | 308 | 4/4   | 0.77 | 0.24 | 66,74,76,87                 | 0     |
| 26  | UNL  | t     | 102 | 16/-  | 0.77 | 0.17 | 61,71,80,80                 | 0     |
| 32  | HTG  | c     | 520 | 19/19 | 0.78 | 0.21 | 77,88,99,100                | 0     |
| 26  | UNL  | c     | 526 | 8/-   | 0.78 | 0.15 | 54,59,64,65                 | 0     |
| 34  | LMT  | z     | 102 | 35/35 | 0.78 | 0.19 | 46,85,99,101                | 0     |
| 26  | UNL  | H     | 105 | 6/-   | 0.78 | 0.14 | 51,55,63,65                 | 0     |
| 26  | UNL  | J     | 105 | 12/-  | 0.79 | 0.23 | 63,67,71,71                 | 0     |
| 26  | UNL  | d     | 409 | 36/-  | 0.79 | 0.18 | 36,60,91,102                | 0     |
| 27  | PL9  | A     | 411 | 55/55 | 0.79 | 0.20 | 43,67,89,92                 | 0     |
| 26  | UNL  | B     | 633 | 16/-  | 0.80 | 0.25 | 53,61,69,70                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 26  | UNL  | i     | 102 | 11/-  | 0.80 | 0.16 | 48,54,64,65                 | 0     |
| 23  | SQD  | b     | 622 | 54/54 | 0.80 | 0.17 | 46,63,95,100                | 0     |
| 32  | HTG  | C     | 522 | 19/19 | 0.80 | 0.27 | 66,83,104,107               | 0     |
| 34  | LMT  | T     | 102 | 24/35 | 0.80 | 0.19 | 36,53,78,85                 | 0     |
| 23  | SQD  | a     | 401 | 54/54 | 0.81 | 0.16 | 39,58,82,86                 | 0     |
| 34  | LMT  | E     | 101 | 24/35 | 0.81 | 0.26 | 64,78,84,90                 | 0     |
| 28  | DMS  | V     | 205 | 4/4   | 0.81 | 0.25 | 67,76,77,79                 | 0     |
| 32  | HTG  | b     | 624 | 19/19 | 0.81 | 0.23 | 49,74,80,85                 | 0     |
| 26  | UNL  | b     | 630 | 11/-  | 0.81 | 0.21 | 55,60,67,68                 | 0     |
| 28  | DMS  | O     | 309 | 4/4   | 0.81 | 0.23 | 58,65,72,73                 | 0     |
| 34  | LMT  | c     | 523 | 35/35 | 0.81 | 0.23 | 67,77,83,85                 | 0     |
| 26  | UNL  | X     | 101 | 16/-  | 0.81 | 0.17 | 37,40,59,59                 | 0     |
| 26  | UNL  | d     | 410 | 16/-  | 0.82 | 0.18 | 33,45,63,63                 | 0     |
| 34  | LMT  | B     | 627 | 16/35 | 0.82 | 0.18 | 52,60,78,78                 | 0     |
| 23  | SQD  | A     | 412 | 54/54 | 0.82 | 0.16 | 41,60,78,81                 | 0     |
| 26  | UNL  | j     | 106 | 6/-   | 0.82 | 0.19 | 52,55,58,59                 | 0     |
| 28  | DMS  | O     | 303 | 4/4   | 0.82 | 0.29 | 63,72,77,78                 | 0     |
| 26  | UNL  | e     | 101 | 7/-   | 0.82 | 0.24 | 54,58,64,65                 | 0     |
| 26  | UNL  | J     | 106 | 4/-   | 0.83 | 0.16 | 57,60,61,67                 | 0     |
| 26  | UNL  | I     | 104 | 11/-  | 0.83 | 0.18 | 53,56,59,62                 | 0     |
| 28  | DMS  | u     | 204 | 4/4   | 0.83 | 0.20 | 71,78,83,86                 | 0     |
| 26  | UNL  | D     | 410 | 37/-  | 0.83 | 0.15 | 42,57,93,98                 | 0     |
| 23  | SQD  | f     | 101 | 40/54 | 0.83 | 0.25 | 57,86,102,107               | 0     |
| 26  | UNL  | x     | 102 | 9/-   | 0.83 | 0.28 | 56,68,72,72                 | 0     |
| 28  | DMS  | b     | 641 | 4/4   | 0.83 | 0.17 | 63,65,75,80                 | 0     |
| 28  | DMS  | o     | 308 | 4/4   | 0.83 | 0.21 | 60,61,62,63                 | 0     |
| 26  | UNL  | c     | 525 | 10/-  | 0.84 | 0.15 | 58,65,66,67                 | 0     |
| 26  | UNL  | I     | 105 | 10/-  | 0.84 | 0.15 | 60,66,71,72                 | 0     |
| 32  | HTG  | B     | 622 | 19/19 | 0.84 | 0.16 | 28,46,54,54                 | 0     |
| 26  | UNL  | M     | 102 | 12/-  | 0.84 | 0.22 | 49,53,95,98                 | 0     |
| 28  | DMS  | O     | 310 | 4/4   | 0.84 | 0.32 | 76,78,82,94                 | 0     |
| 28  | DMS  | o     | 306 | 4/4   | 0.84 | 0.25 | 55,58,65,77                 | 0     |
| 26  | UNL  | I     | 102 | 16/-  | 0.85 | 0.19 | 38,47,63,64                 | 0     |
| 26  | UNL  | L     | 102 | 14/-  | 0.85 | 0.22 | 56,60,84,84                 | 0     |
| 28  | DMS  | D     | 415 | 4/4   | 0.85 | 0.25 | 57,58,63,65                 | 0     |
| 28  | DMS  | c     | 533 | 4/4   | 0.85 | 0.27 | 73,75,77,87                 | 0     |
| 26  | UNL  | i     | 101 | 16/-  | 0.85 | 0.18 | 41,45,65,65                 | 0     |
| 32  | HTG  | b     | 625 | 19/19 | 0.85 | 0.20 | 30,44,66,70                 | 0     |
| 23  | SQD  | F     | 101 | 35/54 | 0.86 | 0.23 | 51,76,89,90                 | 0     |
| 28  | DMS  | B     | 635 | 4/4   | 0.86 | 0.24 | 90,94,95,96                 | 0     |
| 26  | UNL  | b     | 646 | 6/-   | 0.86 | 0.14 | 54,58,60,62                 | 0     |
| 26  | UNL  | B     | 628 | 15/-  | 0.86 | 0.15 | 45,50,60,66                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 32  | HTG  | V     | 202 | 13/19 | 0.86 | 0.21 | 45,49,70,82                 | 0     |
| 28  | DMS  | o     | 304 | 4/4   | 0.86 | 0.32 | 68,79,82,83                 | 0     |
| 28  | DMS  | v     | 209 | 4/4   | 0.86 | 0.31 | 71,78,79,79                 | 0     |
| 26  | UNL  | A     | 413 | 4/-   | 0.86 | 0.19 | 64,64,64,66                 | 0     |
| 32  | HTG  | C     | 520 | 19/19 | 0.86 | 0.21 | 64,70,76,79                 | 0     |
| 28  | DMS  | B     | 644 | 4/4   | 0.87 | 0.32 | 52,53,61,69                 | 0     |
| 28  | DMS  | b     | 637 | 4/4   | 0.87 | 0.17 | 77,79,84,93                 | 0     |
| 32  | HTG  | b     | 601 | 19/19 | 0.87 | 0.15 | 45,61,67,80                 | 0     |
| 24  | LMG  | B     | 620 | 51/55 | 0.87 | 0.12 | 33,43,55,58                 | 0     |
| 20  | CLA  | C     | 513 | 65/65 | 0.87 | 0.14 | 40,48,72,77                 | 0     |
| 28  | DMS  | C     | 532 | 4/4   | 0.87 | 0.19 | 33,40,41,48                 | 0     |
| 24  | LMG  | A     | 407 | 51/55 | 0.87 | 0.13 | 40,55,70,78                 | 0     |
| 28  | DMS  | B     | 638 | 4/4   | 0.87 | 0.19 | 53,61,63,68                 | 0     |
| 26  | UNL  | H     | 104 | 4/-   | 0.88 | 0.20 | 60,62,65,67                 | 0     |
| 32  | HTG  | B     | 631 | 19/19 | 0.88 | 0.12 | 41,57,69,73                 | 0     |
| 24  | LMG  | a     | 410 | 51/55 | 0.88 | 0.15 | 44,55,65,67                 | 0     |
| 33  | CA   | V     | 203 | 1/1   | 0.88 | 0.11 | 63,63,63,63                 | 0     |
| 28  | DMS  | U     | 902 | 4/4   | 0.88 | 0.23 | 35,44,49,58                 | 0     |
| 20  | CLA  | B     | 602 | 65/65 | 0.88 | 0.14 | 29,42,77,81                 | 0     |
| 26  | UNL  | I     | 103 | 13/-  | 0.88 | 0.13 | 47,53,84,87                 | 0     |
| 24  | LMG  | C     | 519 | 51/55 | 0.89 | 0.15 | 31,67,83,84                 | 0     |
| 28  | DMS  | O     | 306 | 4/4   | 0.89 | 0.29 | 66,73,73,75                 | 0     |
| 26  | UNL  | D     | 411 | 16/-  | 0.89 | 0.16 | 39,45,58,62                 | 0     |
| 22  | BCR  | d     | 405 | 40/40 | 0.89 | 0.12 | 24,30,56,58                 | 0     |
| 26  | UNL  | j     | 104 | 16/-  | 0.89 | 0.11 | 49,58,64,66                 | 0     |
| 24  | LMG  | c     | 519 | 51/55 | 0.89 | 0.13 | 29,59,86,88                 | 0     |
| 28  | DMS  | C     | 527 | 4/4   | 0.89 | 0.17 | 73,76,79,87                 | 0     |
| 20  | CLA  | b     | 603 | 65/65 | 0.89 | 0.15 | 30,45,75,82                 | 0     |
| 24  | LMG  | b     | 623 | 49/55 | 0.89 | 0.12 | 33,42,54,61                 | 0     |
| 26  | UNL  | b     | 644 | 7/-   | 0.90 | 0.18 | 64,65,70,70                 | 0     |
| 28  | DMS  | b     | 632 | 4/4   | 0.90 | 0.15 | 55,58,66,70                 | 0     |
| 26  | UNL  | z     | 101 | 6/-   | 0.90 | 0.13 | 49,55,55,57                 | 0     |
| 28  | DMS  | c     | 534 | 4/4   | 0.90 | 0.24 | 70,71,75,81                 | 0     |
| 28  | DMS  | O     | 311 | 4/4   | 0.90 | 0.26 | 57,65,69,72                 | 0     |
| 28  | DMS  | A     | 418 | 4/4   | 0.90 | 0.31 | 68,74,80,85                 | 0     |
| 28  | DMS  | b     | 636 | 4/4   | 0.90 | 0.14 | 66,71,72,79                 | 0     |
| 22  | BCR  | D     | 405 | 40/40 | 0.90 | 0.11 | 26,30,58,60                 | 0     |
| 22  | BCR  | C     | 514 | 40/40 | 0.90 | 0.10 | 36,45,49,50                 | 0     |
| 28  | DMS  | B     | 639 | 4/4   | 0.90 | 0.24 | 65,70,71,76                 | 0     |
| 28  | DMS  | V     | 204 | 4/4   | 0.91 | 0.32 | 58,64,64,72                 | 0     |
| 28  | DMS  | c     | 535 | 4/4   | 0.91 | 0.18 | 58,59,65,68                 | 0     |
| 26  | UNL  | b     | 629 | 16/-  | 0.91 | 0.14 | 41,48,60,60                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 26  | UNL  | i     | 103 | 11/-  | 0.91 | 0.27 | 58,61,65,66                 | 0     |
| 28  | DMS  | u     | 203 | 4/4   | 0.91 | 0.29 | 47,55,56,65                 | 0     |
| 28  | DMS  | d     | 415 | 4/4   | 0.91 | 0.26 | 68,71,71,72                 | 0     |
| 28  | DMS  | A     | 416 | 4/4   | 0.91 | 0.23 | 59,60,69,77                 | 0     |
| 28  | DMS  | V     | 209 | 4/4   | 0.91 | 0.20 | 57,73,77,81                 | 0     |
| 28  | DMS  | o     | 305 | 4/4   | 0.91 | 0.23 | 73,75,77,87                 | 0     |
| 28  | DMS  | b     | 634 | 4/4   | 0.91 | 0.29 | 59,67,67,75                 | 0     |
| 20  | CLA  | b     | 618 | 65/65 | 0.91 | 0.13 | 23,33,92,98                 | 0     |
| 28  | DMS  | u     | 202 | 4/4   | 0.91 | 0.18 | 40,46,52,54                 | 0     |
| 28  | DMS  | v     | 208 | 4/4   | 0.91 | 0.26 | 89,92,92,95                 | 0     |
| 28  | DMS  | o     | 303 | 4/4   | 0.92 | 0.38 | 66,69,75,79                 | 0     |
| 26  | UNL  | d     | 411 | 16/-  | 0.92 | 0.12 | 33,42,55,55                 | 0     |
| 28  | DMS  | b     | 635 | 4/4   | 0.92 | 0.27 | 58,62,69,73                 | 0     |
| 28  | DMS  | c     | 536 | 4/4   | 0.92 | 0.15 | 33,33,45,46                 | 0     |
| 20  | CLA  | c     | 512 | 65/65 | 0.92 | 0.11 | 28,41,70,72                 | 0     |
| 20  | CLA  | C     | 506 | 65/65 | 0.92 | 0.10 | 32,45,86,87                 | 0     |
| 38  | RRX  | x     | 101 | 41/41 | 0.92 | 0.09 | 26,32,47,58                 | 0     |
| 28  | DMS  | O     | 304 | 4/4   | 0.92 | 0.28 | 63,68,72,73                 | 0     |
| 22  | BCR  | K     | 101 | 40/40 | 0.92 | 0.10 | 33,37,42,45                 | 0     |
| 20  | CLA  | c     | 513 | 65/65 | 0.92 | 0.11 | 36,46,81,87                 | 0     |
| 22  | BCR  | K     | 102 | 40/40 | 0.92 | 0.13 | 31,36,40,41                 | 0     |
| 28  | DMS  | C     | 529 | 4/4   | 0.92 | 0.19 | 70,73,74,74                 | 0     |
| 28  | DMS  | B     | 640 | 4/4   | 0.93 | 0.33 | 45,48,49,50                 | 0     |
| 28  | DMS  | O     | 307 | 4/4   | 0.93 | 0.16 | 69,76,77,88                 | 0     |
| 32  | HTG  | B     | 621 | 19/19 | 0.93 | 0.12 | 36,41,48,52                 | 0     |
| 28  | DMS  | A     | 417 | 4/4   | 0.93 | 0.17 | 70,72,77,81                 | 0     |
| 20  | CLA  | B     | 601 | 65/65 | 0.93 | 0.12 | 23,29,82,86                 | 0     |
| 35  | DGD  | H     | 102 | 62/66 | 0.93 | 0.11 | 25,33,40,43                 | 0     |
| 28  | DMS  | c     | 529 | 4/4   | 0.93 | 0.23 | 79,82,86,87                 | 0     |
| 28  | DMS  | C     | 531 | 4/4   | 0.93 | 0.24 | 53,54,58,74                 | 0     |
| 22  | BCR  | k     | 102 | 40/40 | 0.93 | 0.09 | 41,46,51,51                 | 0     |
| 28  | DMS  | v     | 204 | 4/4   | 0.93 | 0.15 | 48,54,57,69                 | 0     |
| 20  | CLA  | C     | 512 | 55/65 | 0.93 | 0.09 | 37,44,49,54                 | 0     |
| 20  | CLA  | c     | 506 | 65/65 | 0.93 | 0.10 | 24,39,71,74                 | 0     |
| 35  | DGD  | h     | 101 | 62/66 | 0.93 | 0.10 | 25,34,41,49                 | 0     |
| 28  | DMS  | v     | 203 | 4/4   | 0.93 | 0.16 | 67,69,76,79                 | 0     |
| 38  | RRX  | H     | 101 | 41/41 | 0.93 | 0.10 | 27,31,41,46                 | 0     |
| 28  | DMS  | D     | 416 | 4/4   | 0.93 | 0.17 | 83,87,89,91                 | 0     |
| 23  | SQD  | A     | 406 | 54/54 | 0.93 | 0.13 | 34,59,71,76                 | 0     |
| 24  | LMG  | j     | 101 | 45/55 | 0.94 | 0.09 | 27,32,60,64                 | 0     |
| 20  | CLA  | d     | 404 | 65/65 | 0.94 | 0.10 | 24,29,78,87                 | 0     |
| 32  | HTG  | O     | 302 | 19/19 | 0.94 | 0.10 | 34,42,50,53                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 23  | SQD  | a     | 409 | 54/54 | 0.94 | 0.12 | 33,56,75,78                 | 0     |
| 28  | DMS  | v     | 206 | 4/4   | 0.94 | 0.20 | 52,53,61,66                 | 0     |
| 28  | DMS  | B     | 643 | 4/4   | 0.94 | 0.14 | 51,53,62,71                 | 0     |
| 28  | DMS  | c     | 531 | 4/4   | 0.94 | 0.15 | 73,78,85,86                 | 0     |
| 33  | CA   | O     | 301 | 1/1   | 0.94 | 0.06 | 47,47,47,47                 | 0     |
| 33  | CA   | o     | 301 | 1/1   | 0.94 | 0.07 | 48,48,48,48                 | 0     |
| 24  | LMG  | J     | 101 | 45/55 | 0.94 | 0.10 | 27,32,64,70                 | 0     |
| 28  | DMS  | A     | 415 | 4/4   | 0.94 | 0.20 | 55,58,65,71                 | 0     |
| 28  | DMS  | c     | 532 | 4/4   | 0.94 | 0.23 | 65,70,76,77                 | 0     |
| 28  | DMS  | C     | 533 | 4/4   | 0.94 | 0.28 | 72,73,73,74                 | 0     |
| 20  | CLA  | B     | 607 | 65/65 | 0.95 | 0.09 | 22,29,55,62                 | 0     |
| 22  | BCR  | t     | 101 | 40/40 | 0.95 | 0.07 | 22,29,41,43                 | 0     |
| 28  | DMS  | B     | 641 | 4/4   | 0.95 | 0.31 | 68,69,75,80                 | 0     |
| 20  | CLA  | D     | 404 | 65/65 | 0.95 | 0.10 | 26,29,77,81                 | 0     |
| 31  | BCT  | A     | 421 | 4/4   | 0.95 | 0.10 | 31,34,40,44                 | 0     |
| 28  | DMS  | V     | 208 | 4/4   | 0.95 | 0.12 | 75,77,82,85                 | 0     |
| 28  | DMS  | d     | 413 | 4/4   | 0.95 | 0.17 | 47,53,55,57                 | 0     |
| 35  | DGD  | c     | 517 | 62/66 | 0.95 | 0.09 | 23,30,56,71                 | 0     |
| 22  | BCR  | B     | 619 | 40/40 | 0.95 | 0.07 | 22,30,42,44                 | 0     |
| 28  | DMS  | b     | 639 | 4/4   | 0.95 | 0.20 | 46,49,49,50                 | 0     |
| 35  | DGD  | C     | 517 | 55/66 | 0.95 | 0.07 | 26,34,59,62                 | 0     |
| 33  | CA   | b     | 626 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 36  | LHG  | D     | 409 | 49/49 | 0.95 | 0.12 | 27,33,81,83                 | 0     |
| 28  | DMS  | o     | 307 | 4/4   | 0.95 | 0.16 | 53,58,63,65                 | 0     |
| 22  | BCR  | k     | 101 | 40/40 | 0.95 | 0.09 | 28,36,41,42                 | 0     |
| 20  | CLA  | b     | 608 | 65/65 | 0.95 | 0.09 | 24,31,59,63                 | 0     |
| 20  | CLA  | c     | 511 | 65/65 | 0.95 | 0.09 | 27,33,40,43                 | 0     |
| 20  | CLA  | C     | 503 | 65/65 | 0.95 | 0.08 | 28,33,37,42                 | 0     |
| 20  | CLA  | C     | 507 | 65/65 | 0.95 | 0.09 | 28,37,52,57                 | 0     |
| 28  | DMS  | d     | 414 | 4/4   | 0.95 | 0.16 | 57,62,64,68                 | 0     |
| 22  | BCR  | C     | 515 | 40/40 | 0.95 | 0.09 | 31,37,43,45                 | 0     |
| 20  | CLA  | C     | 511 | 65/65 | 0.95 | 0.08 | 30,37,42,45                 | 0     |
| 22  | BCR  | j     | 102 | 40/40 | 0.95 | 0.09 | 30,35,42,45                 | 0     |
| 35  | DGD  | c     | 515 | 62/66 | 0.95 | 0.10 | 23,32,71,75                 | 0     |
| 22  | BCR  | c     | 514 | 40/40 | 0.96 | 0.07 | 28,36,39,39                 | 0     |
| 20  | CLA  | b     | 611 | 65/65 | 0.96 | 0.09 | 24,30,34,41                 | 0     |
| 36  | LHG  | D     | 407 | 49/49 | 0.96 | 0.09 | 28,37,44,52                 | 0     |
| 27  | PL9  | d     | 412 | 55/55 | 0.96 | 0.08 | 18,23,29,35                 | 0     |
| 20  | CLA  | b     | 604 | 65/65 | 0.96 | 0.08 | 23,27,33,35                 | 0     |
| 20  | CLA  | C     | 509 | 65/65 | 0.96 | 0.09 | 29,34,52,55                 | 0     |
| 35  | DGD  | c     | 516 | 57/66 | 0.96 | 0.08 | 27,32,62,68                 | 0     |
| 31  | BCT  | a     | 413 | 4/4   | 0.96 | 0.07 | 32,32,38,42                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 35  | DGD  | C     | 518 | 62/66 | 0.96 | 0.09 | 24,30,62,73                 | 0     |
| 20  | CLA  | C     | 504 | 65/65 | 0.96 | 0.08 | 27,30,59,61                 | 0     |
| 28  | DMS  | V     | 206 | 4/4   | 0.96 | 0.21 | 59,61,63,65                 | 0     |
| 22  | BCR  | T     | 101 | 40/40 | 0.96 | 0.07 | 24,32,43,45                 | 0     |
| 20  | CLA  | B     | 610 | 65/65 | 0.96 | 0.10 | 26,31,35,38                 | 0     |
| 20  | CLA  | A     | 404 | 65/65 | 0.96 | 0.10 | 20,25,88,90                 | 0     |
| 22  | BCR  | b     | 620 | 40/40 | 0.96 | 0.07 | 22,27,43,46                 | 0     |
| 20  | CLA  | C     | 510 | 65/65 | 0.96 | 0.08 | 26,31,38,44                 | 0     |
| 20  | CLA  | B     | 603 | 65/65 | 0.96 | 0.08 | 23,28,35,39                 | 0     |
| 37  | HEM  | E     | 104 | 43/43 | 0.96 | 0.10 | 39,44,52,56                 | 0     |
| 20  | CLA  | C     | 508 | 60/65 | 0.96 | 0.07 | 23,31,47,51                 | 0     |
| 20  | CLA  | C     | 501 | 65/65 | 0.96 | 0.08 | 27,33,45,52                 | 0     |
| 28  | DMS  | h     | 102 | 4/4   | 0.96 | 0.17 | 50,51,53,62                 | 0     |
| 28  | DMS  | c     | 528 | 4/4   | 0.96 | 0.18 | 58,62,63,65                 | 0     |
| 20  | CLA  | c     | 501 | 65/65 | 0.96 | 0.08 | 26,30,41,48                 | 0     |
| 28  | DMS  | v     | 205 | 4/4   | 0.96 | 0.18 | 67,70,72,73                 | 0     |
| 22  | BCR  | B     | 618 | 40/40 | 0.96 | 0.08 | 21,28,42,45                 | 0     |
| 28  | DMS  | B     | 637 | 4/4   | 0.96 | 0.17 | 53,53,54,60                 | 0     |
| 20  | CLA  | c     | 509 | 65/65 | 0.96 | 0.09 | 25,30,53,58                 | 0     |
| 20  | CLA  | b     | 616 | 65/65 | 0.96 | 0.09 | 20,26,73,80                 | 0     |
| 28  | DMS  | V     | 207 | 4/4   | 0.96 | 0.10 | 62,63,63,70                 | 0     |
| 22  | BCR  | a     | 408 | 40/40 | 0.96 | 0.07 | 21,25,30,31                 | 0     |
| 20  | CLA  | a     | 404 | 60/65 | 0.96 | 0.09 | 18,22,66,75                 | 0     |
| 20  | CLA  | c     | 503 | 65/65 | 0.96 | 0.08 | 25,35,40,43                 | 0     |
| 28  | DMS  | D     | 413 | 4/4   | 0.96 | 0.11 | 50,56,60,61                 | 0     |
| 28  | DMS  | B     | 645 | 4/4   | 0.96 | 0.11 | 56,59,64,71                 | 0     |
| 20  | CLA  | b     | 612 | 65/65 | 0.96 | 0.08 | 21,27,36,41                 | 0     |
| 20  | CLA  | C     | 505 | 65/65 | 0.96 | 0.08 | 28,33,44,48                 | 0     |
| 28  | DMS  | C     | 530 | 4/4   | 0.96 | 0.16 | 44,44,46,50                 | 0     |
| 20  | CLA  | b     | 609 | 65/65 | 0.97 | 0.07 | 19,22,33,37                 | 0     |
| 28  | DMS  | i     | 104 | 4/4   | 0.97 | 0.21 | 63,66,67,71                 | 0     |
| 20  | CLA  | c     | 510 | 65/65 | 0.97 | 0.07 | 23,29,39,42                 | 0     |
| 20  | CLA  | B     | 608 | 65/65 | 0.97 | 0.07 | 18,21,34,39                 | 0     |
| 22  | BCR  | A     | 405 | 40/40 | 0.97 | 0.08 | 21,26,32,35                 | 0     |
| 20  | CLA  | b     | 613 | 65/65 | 0.97 | 0.07 | 20,22,38,44                 | 0     |
| 21  | PHO  | a     | 405 | 64/64 | 0.97 | 0.07 | 17,20,22,25                 | 0     |
| 20  | CLA  | a     | 407 | 47/65 | 0.97 | 0.08 | 19,22,41,48                 | 0     |
| 37  | HEM  | e     | 102 | 43/43 | 0.97 | 0.09 | 34,41,56,68                 | 0     |
| 20  | CLA  | b     | 617 | 65/65 | 0.97 | 0.07 | 23,30,44,50                 | 0     |
| 28  | DMS  | b     | 631 | 4/4   | 0.97 | 0.10 | 23,24,27,35                 | 0     |
| 20  | CLA  | c     | 508 | 60/65 | 0.97 | 0.07 | 24,28,52,54                 | 0     |
| 20  | CLA  | b     | 605 | 65/65 | 0.97 | 0.07 | 21,25,34,37                 | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 28  | DMS  | b     | 633    | 4/4   | 0.97 | 0.13 | 45,48,49,53                 | 0     |
| 36  | LHG  | d     | 406    | 49/49 | 0.97 | 0.10 | 29,36,43,48                 | 0     |
| 20  | CLA  | c     | 504    | 65/65 | 0.97 | 0.07 | 25,29,55,60                 | 0     |
| 28  | DMS  | C     | 525[B] | 4/4   | 0.97 | 0.19 | 32,33,35,35                 | 4     |
| 20  | CLA  | b     | 614    | 65/65 | 0.97 | 0.07 | 21,25,31,37                 | 0     |
| 28  | DMS  | C     | 525[A] | 4/4   | 0.97 | 0.19 | 48,49,51,57                 | 4     |
| 28  | DMS  | D     | 414    | 4/4   | 0.97 | 0.14 | 55,56,57,58                 | 0     |
| 28  | DMS  | c     | 530    | 4/4   | 0.97 | 0.16 | 36,43,45,49                 | 0     |
| 20  | CLA  | A     | 402    | 59/65 | 0.97 | 0.07 | 18,22,52,58                 | 0     |
| 22  | BCR  | b     | 621    | 40/40 | 0.97 | 0.07 | 27,32,42,44                 | 0     |
| 20  | CLA  | c     | 505    | 65/65 | 0.97 | 0.06 | 25,30,46,50                 | 0     |
| 20  | CLA  | B     | 604    | 65/65 | 0.97 | 0.07 | 21,24,33,39                 | 0     |
| 28  | DMS  | U     | 903[B] | 4/4   | 0.97 | 0.17 | 26,28,29,32                 | 4     |
| 36  | LHG  | d     | 408    | 49/49 | 0.97 | 0.10 | 24,31,83,88                 | 0     |
| 28  | DMS  | U     | 903[A] | 4/4   | 0.97 | 0.17 | 32,34,40,41                 | 4     |
| 20  | CLA  | c     | 507    | 65/65 | 0.97 | 0.08 | 25,30,49,57                 | 0     |
| 39  | MG   | J     | 102    | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 28  | DMS  | F     | 102    | 4/4   | 0.97 | 0.11 | 51,52,56,64                 | 0     |
| 28  | DMS  | C     | 526    | 4/4   | 0.97 | 0.15 | 59,60,63,65                 | 0     |
| 36  | LHG  | L     | 101    | 49/49 | 0.97 | 0.09 | 24,31,49,53                 | 0     |
| 20  | CLA  | B     | 611    | 65/65 | 0.97 | 0.08 | 21,26,34,40                 | 0     |
| 36  | LHG  | l     | 102    | 49/49 | 0.97 | 0.08 | 22,30,51,54                 | 0     |
| 22  | BCR  | b     | 619    | 40/40 | 0.97 | 0.07 | 23,26,32,35                 | 0     |
| 36  | LHG  | d     | 407    | 49/49 | 0.97 | 0.12 | 22,27,46,50                 | 0     |
| 20  | CLA  | B     | 616    | 65/65 | 0.97 | 0.07 | 25,29,48,52                 | 0     |
| 22  | BCR  | B     | 617    | 40/40 | 0.97 | 0.07 | 22,26,32,33                 | 0     |
| 20  | CLA  | c     | 502    | 65/65 | 0.97 | 0.07 | 22,26,39,48                 | 0     |
| 20  | CLA  | C     | 502    | 65/65 | 0.97 | 0.07 | 24,29,41,48                 | 0     |
| 35  | DGD  | C     | 516    | 62/66 | 0.97 | 0.09 | 22,32,74,79                 | 0     |
| 20  | CLA  | a     | 403    | 65/65 | 0.97 | 0.09 | 17,20,29,38                 | 0     |
| 20  | CLA  | b     | 610    | 65/65 | 0.97 | 0.07 | 20,26,31,33                 | 0     |
| 20  | CLA  | B     | 605    | 65/65 | 0.97 | 0.08 | 19,23,55,58                 | 0     |
| 21  | PHO  | D     | 403    | 64/64 | 0.97 | 0.07 | 18,24,29,35                 | 0     |
| 20  | CLA  | B     | 615    | 65/65 | 0.97 | 0.08 | 20,24,70,79                 | 0     |
| 27  | PL9  | D     | 412    | 55/55 | 0.97 | 0.08 | 19,23,29,34                 | 0     |
| 20  | CLA  | b     | 606    | 65/65 | 0.97 | 0.07 | 20,24,54,59                 | 0     |
| 20  | CLA  | b     | 607    | 65/65 | 0.98 | 0.08 | 20,24,33,35                 | 0     |
| 36  | LHG  | D     | 408    | 49/49 | 0.98 | 0.09 | 23,30,44,49                 | 0     |
| 20  | CLA  | B     | 609    | 65/65 | 0.98 | 0.07 | 22,25,31,33                 | 0     |
| 20  | CLA  | b     | 615    | 65/65 | 0.98 | 0.06 | 18,22,53,59                 | 0     |
| 21  | PHO  | A     | 403    | 64/64 | 0.98 | 0.07 | 18,22,24,25                 | 0     |
| 33  | CA   | c     | 522    | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |

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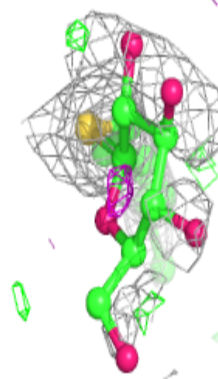
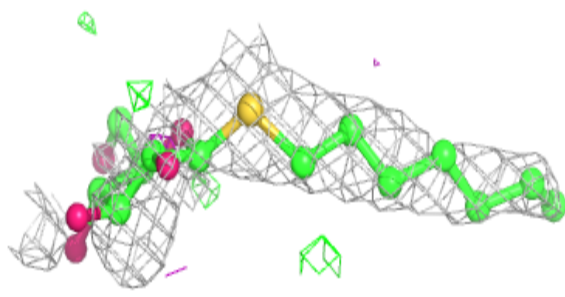
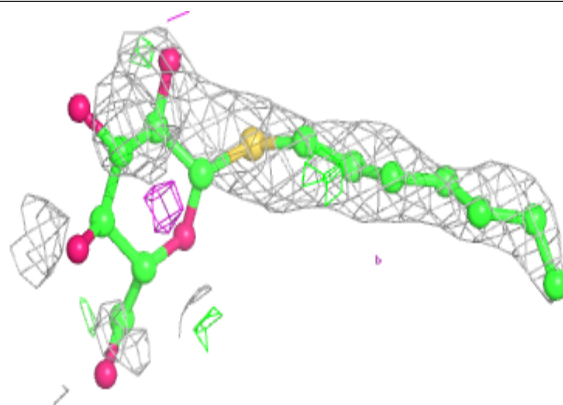
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 20  | CLA  | B     | 614 | 65/65 | 0.98 | 0.06 | 19,22,48,53                | 0     |
| 40  | HEC  | v     | 201 | 43/43 | 0.98 | 0.08 | 25,29,34,37                | 0     |
| 28  | DMS  | v     | 202 | 4/4   | 0.98 | 0.15 | 50,51,53,55                | 0     |
| 20  | CLA  | D     | 401 | 65/65 | 0.98 | 0.08 | 16,20,35,41                | 0     |
| 21  | PHO  | a     | 406 | 64/64 | 0.98 | 0.08 | 19,24,29,32                | 0     |
| 28  | DMS  | B     | 634 | 4/4   | 0.98 | 0.08 | 23,24,25,26                | 0     |
| 20  | CLA  | B     | 613 | 65/65 | 0.98 | 0.07 | 21,25,30,34                | 0     |
| 20  | CLA  | B     | 606 | 65/65 | 0.98 | 0.09 | 19,24,35,37                | 0     |
| 20  | CLA  | d     | 402 | 65/65 | 0.98 | 0.08 | 16,20,35,41                | 0     |
| 20  | CLA  | A     | 401 | 65/65 | 0.98 | 0.08 | 16,19,30,36                | 0     |
| 28  | DMS  | o     | 302 | 4/4   | 0.98 | 0.07 | 20,28,31,36                | 0     |
| 20  | CLA  | D     | 402 | 65/65 | 0.98 | 0.06 | 15,19,30,36                | 0     |
| 20  | CLA  | d     | 403 | 65/65 | 0.98 | 0.07 | 17,19,27,34                | 0     |
| 20  | CLA  | B     | 612 | 65/65 | 0.98 | 0.07 | 19,22,36,42                | 0     |
| 29  | FE2  | A     | 419 | 1/1   | 0.99 | 0.03 | 29,29,29,29                | 0     |
| 28  | DMS  | C     | 528 | 4/4   | 0.99 | 0.09 | 33,37,39,41                | 0     |
| 33  | CA   | B     | 624 | 1/1   | 0.99 | 0.16 | 43,43,43,43                | 0     |
| 40  | HEC  | V     | 201 | 43/43 | 0.99 | 0.08 | 21,23,27,31                | 0     |
| 29  | FE2  | a     | 417 | 1/1   | 0.99 | 0.05 | 27,27,27,27                | 0     |
| 25  | CL   | a     | 412 | 1/1   | 0.99 | 0.06 | 24,24,24,24                | 0     |
| 28  | DMS  | A     | 414 | 4/4   | 0.99 | 0.07 | 25,28,28,29                | 0     |
| 28  | DMS  | c     | 527 | 4/4   | 0.99 | 0.05 | 33,33,34,38                | 0     |
| 25  | CL   | A     | 409 | 1/1   | 0.99 | 0.03 | 22,22,22,22                | 0     |
| 25  | CL   | A     | 408 | 1/1   | 1.00 | 0.05 | 22,22,22,22                | 0     |
| 30  | OEX  | A     | 420 | 10/10 | 1.00 | 0.04 | 21,23,24,24                | 0     |
| 25  | CL   | a     | 411 | 1/1   | 1.00 | 0.02 | 22,22,22,22                | 0     |
| 30  | OEX  | a     | 419 | 10/10 | 1.00 | 0.04 | 21,24,26,26                | 0     |
| 39  | MG   | j     | 103 | 1/1   | 1.00 | 0.08 | 31,31,31,31                | 0     |

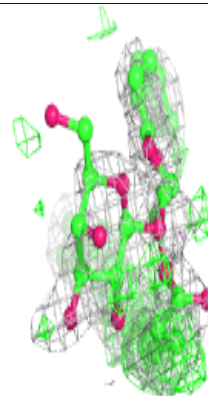
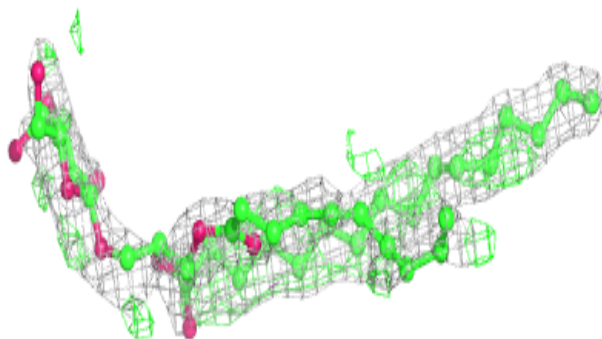
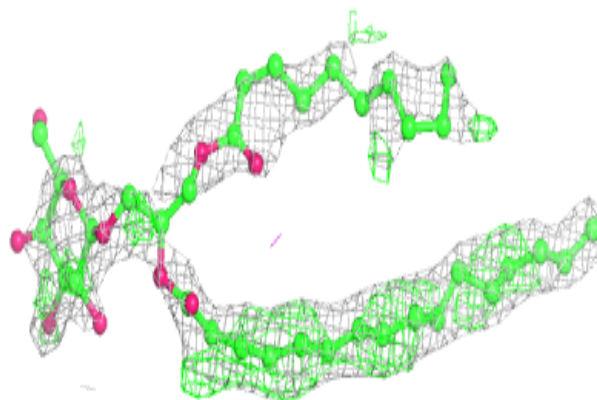
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HTG C 534:**

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

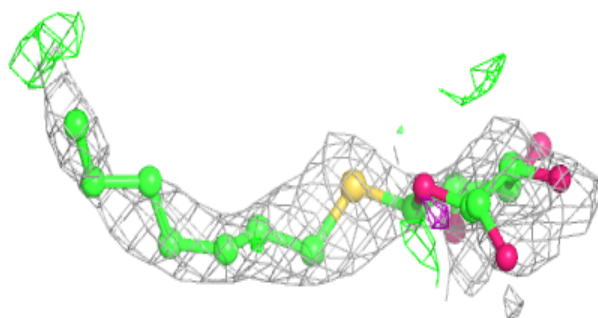
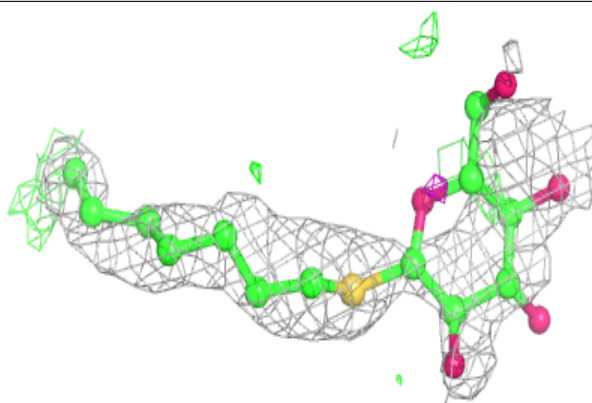
**Electron density around LMG C 524:**

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

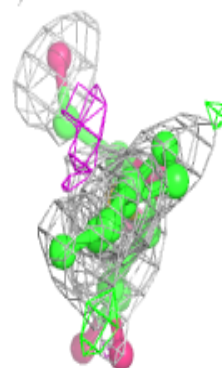
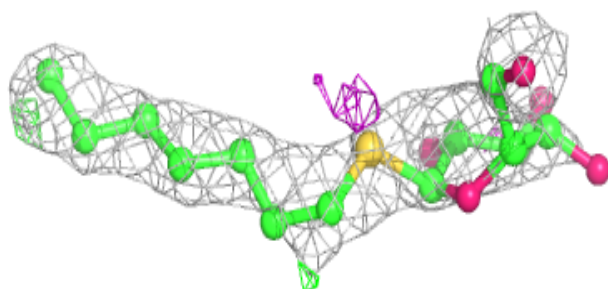
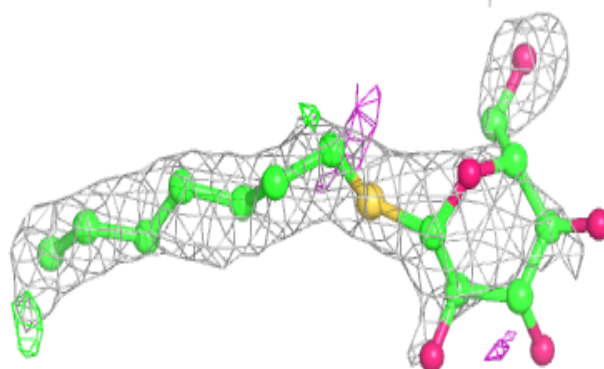


**Electron density around HTG D 417:**

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

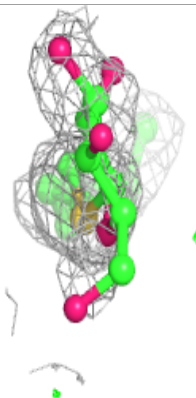
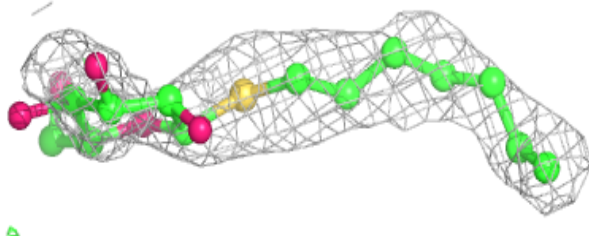
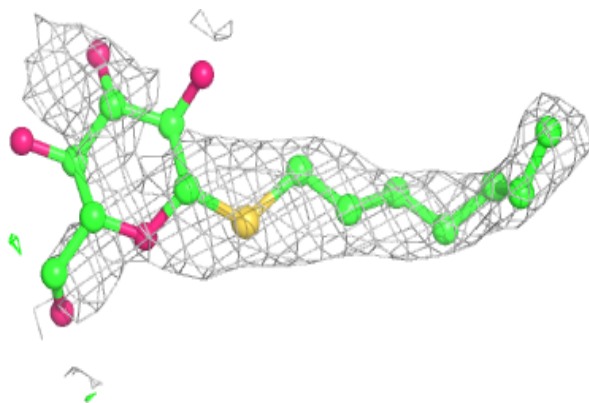
**Electron density around HTG c 521:**

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

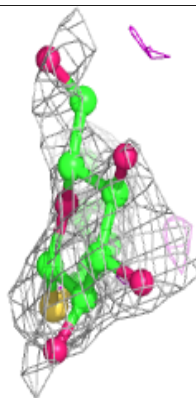
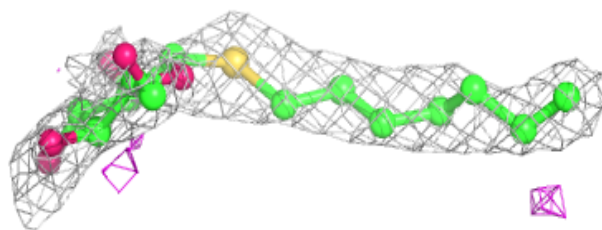
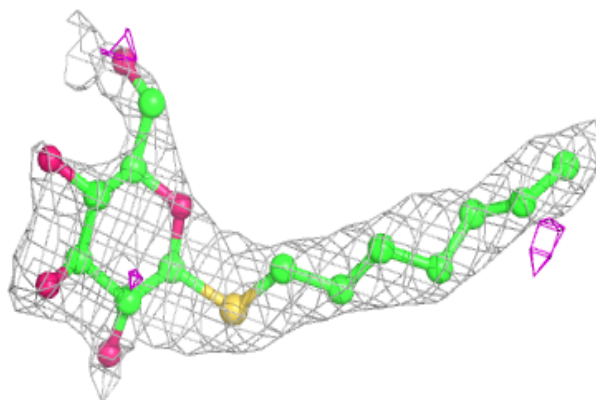


**Electron density around HTG d 401:**

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

**Electron density around HTG B 623:**

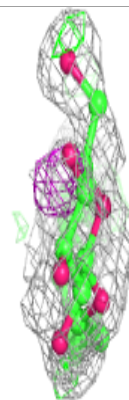
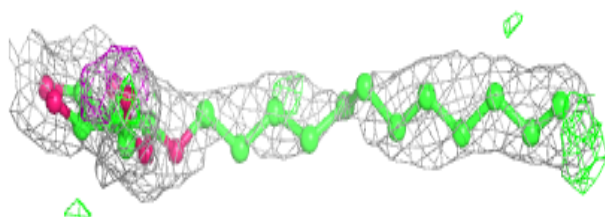
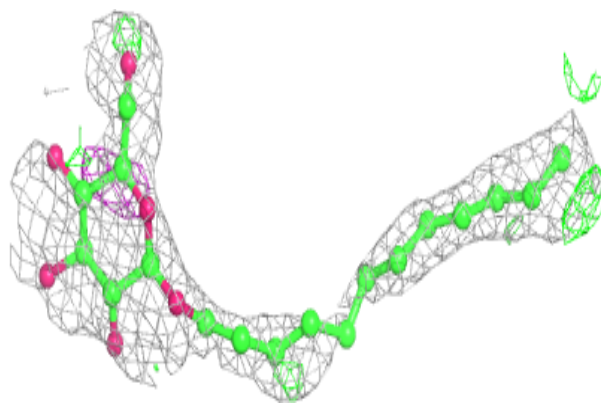
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



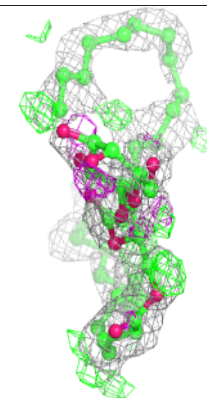
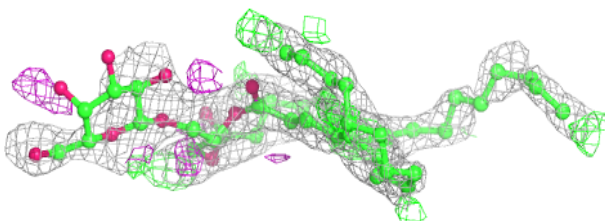
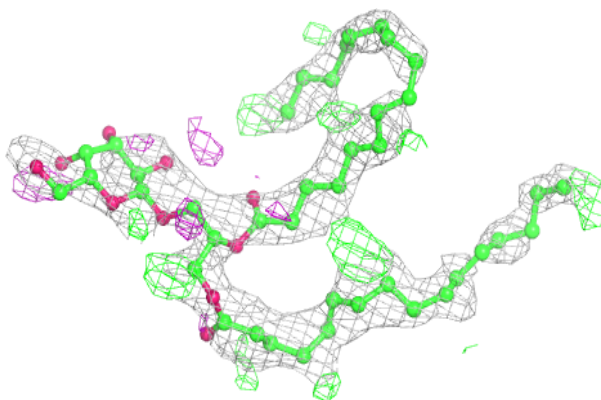


**Electron density around LMT f 102:**

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

**Electron density around DGD D 406:**

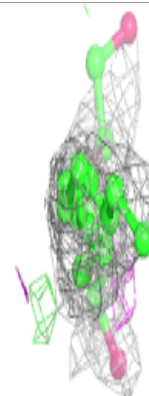
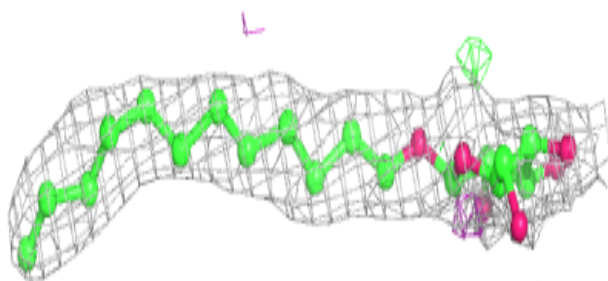
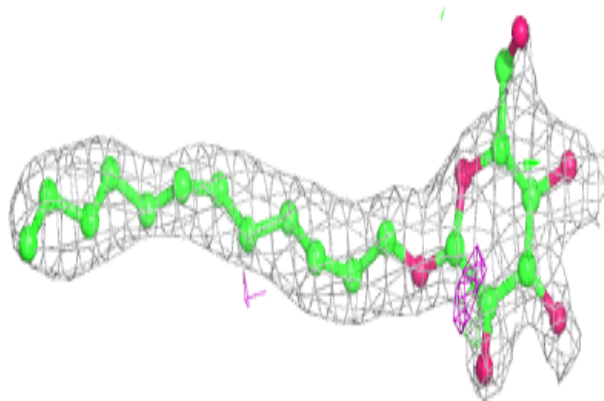
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



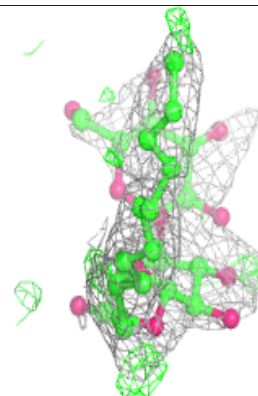
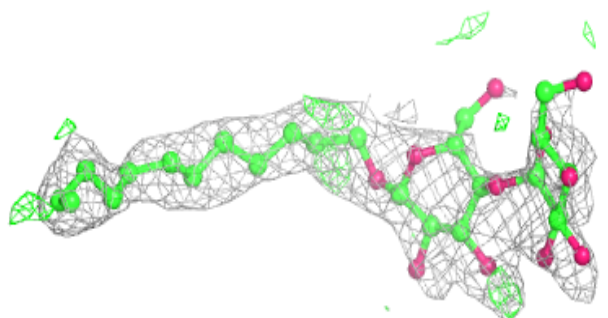
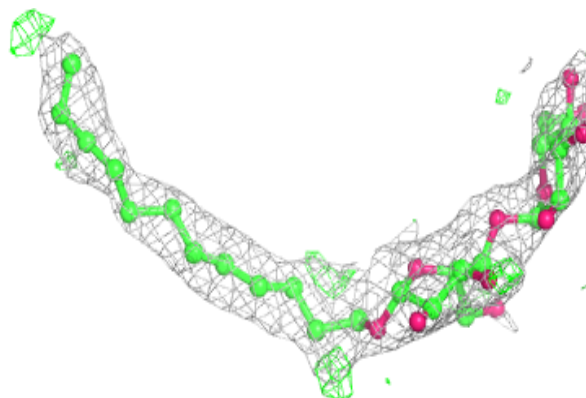


**Electron density around LMT J 103:**

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

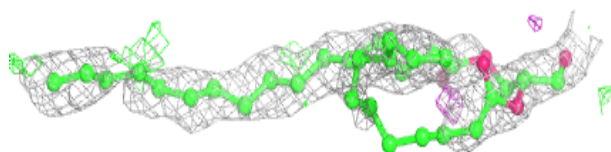
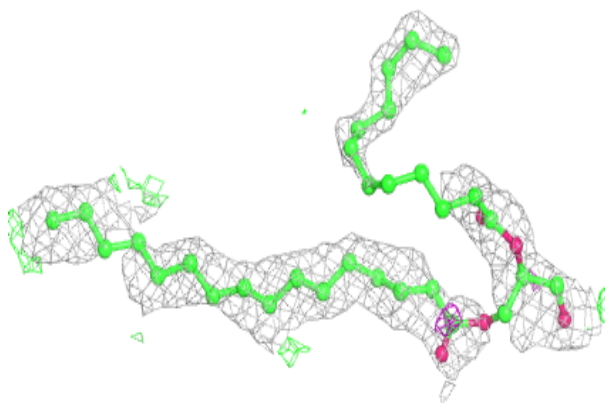
**Electron density around LMT m 101:**

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

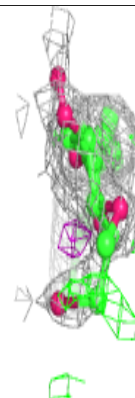
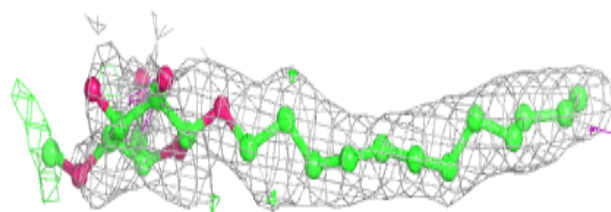
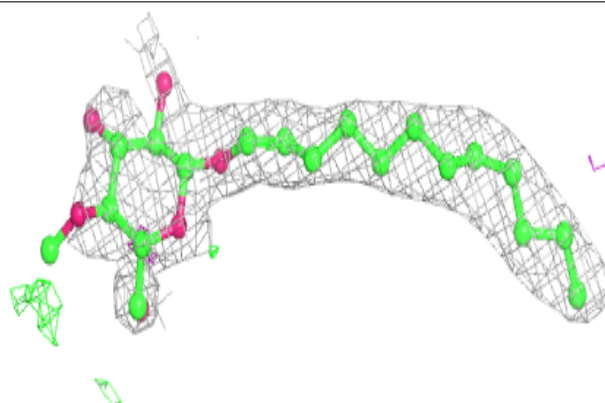


**Electron density around UNL A 410:**

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

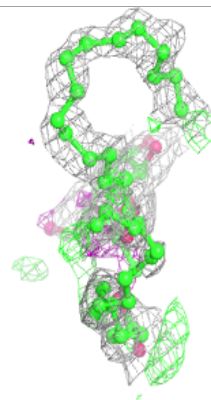
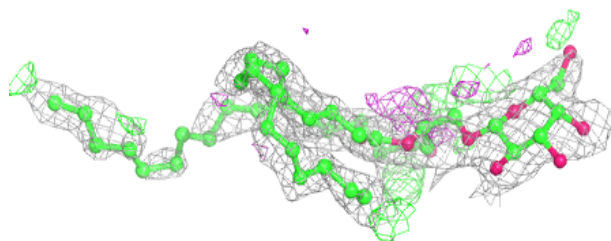
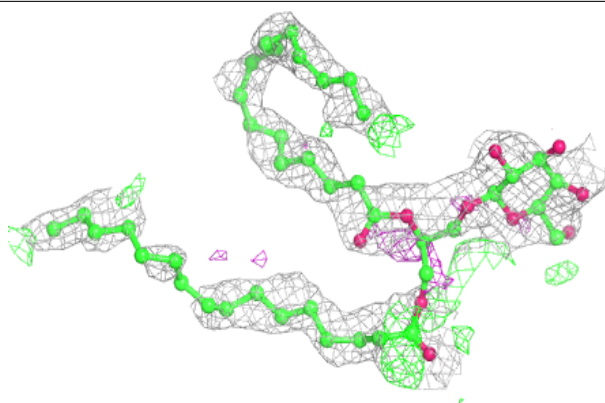
**Electron density around LMT b 628:**

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

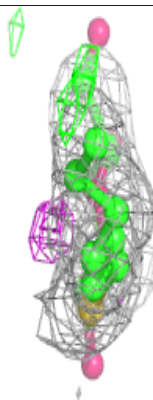
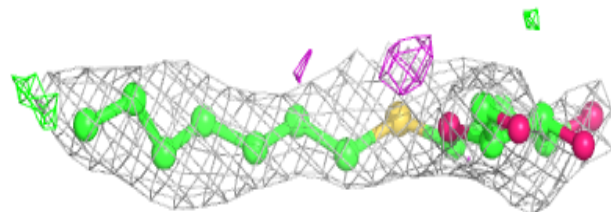
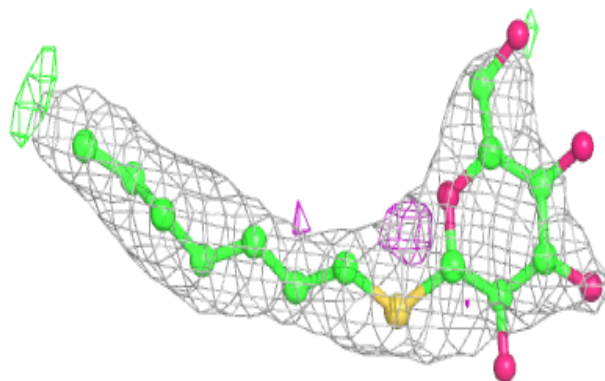


**Electron density around DGD d 416:**

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

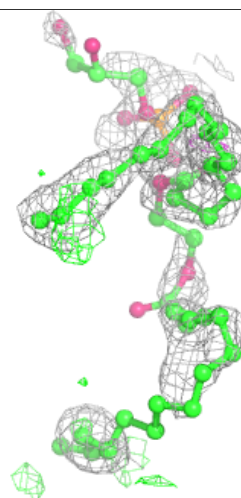
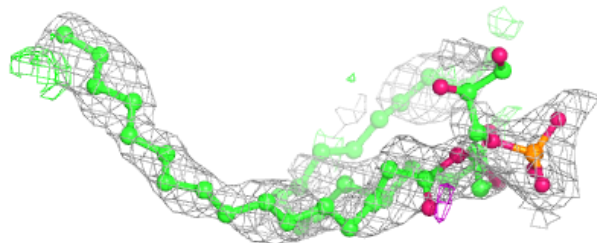
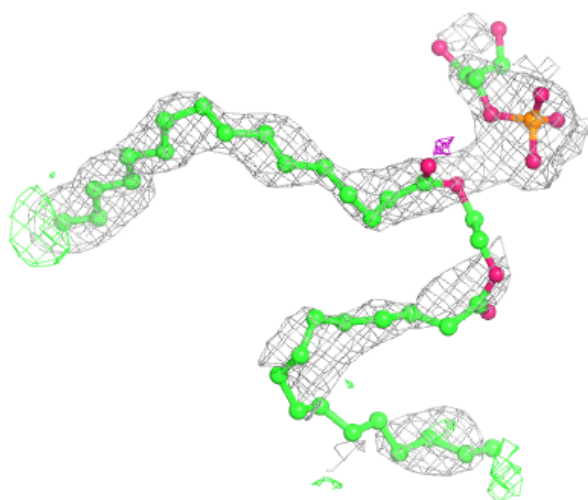
**Electron density around HTG B 632:**

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



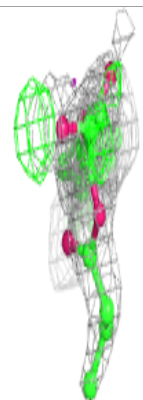
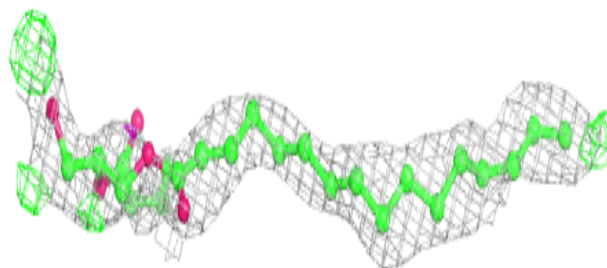
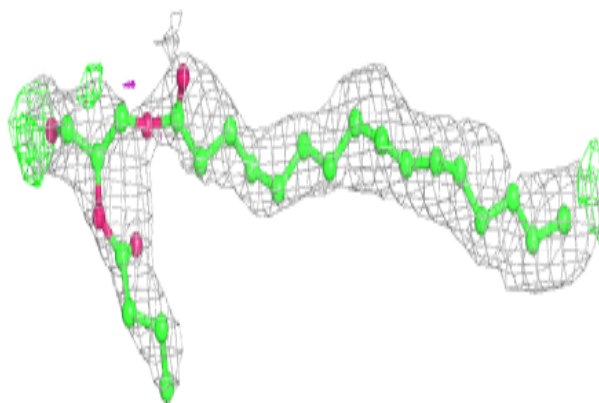
**Electron density around LHG E 103:**

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

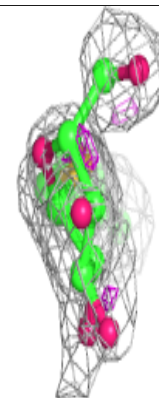
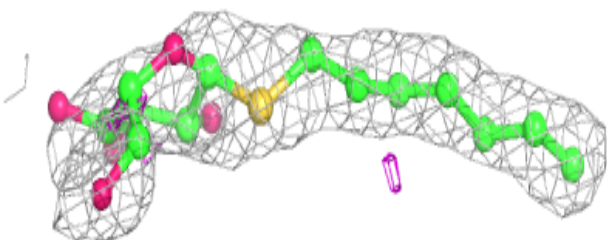
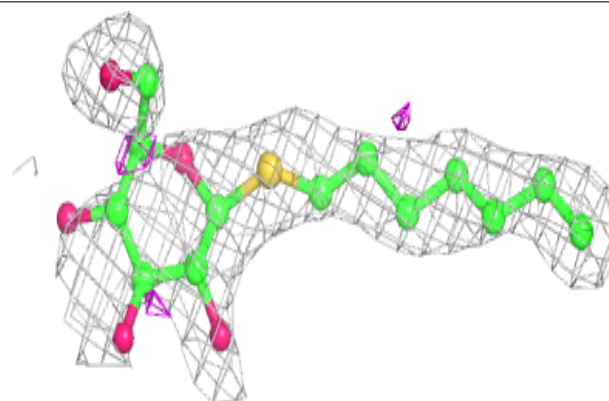


**Electron density around UNL a 414:**

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

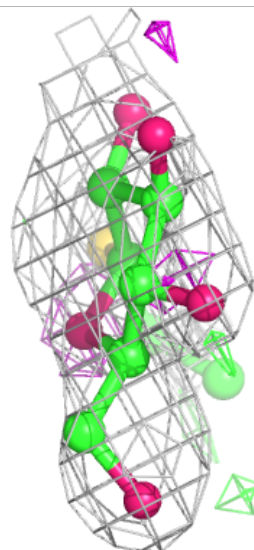
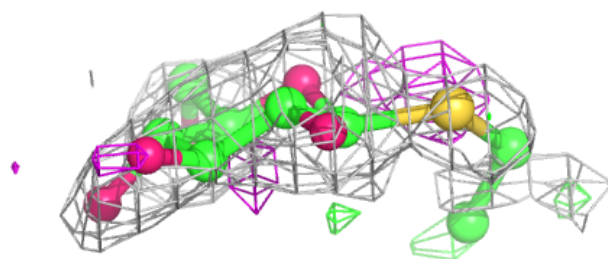
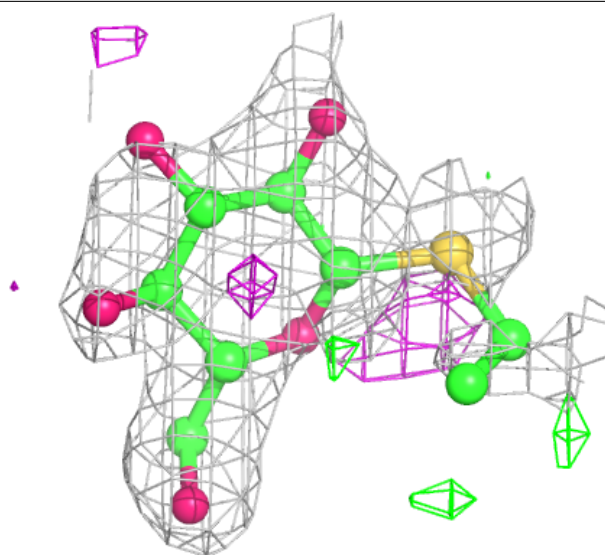
**Electron density around HTG C 521:**

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



**Electron density around HTG v 210:**

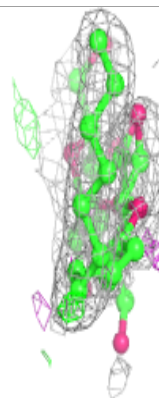
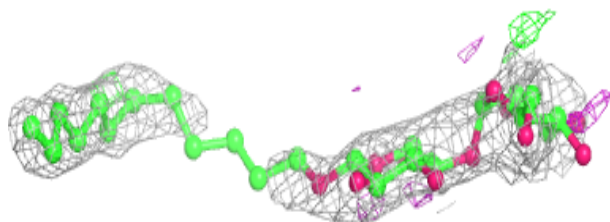
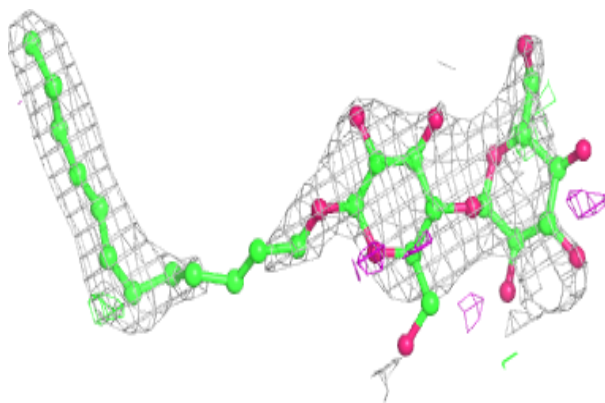
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



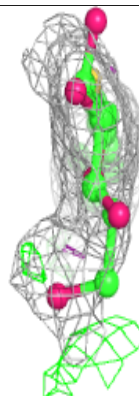
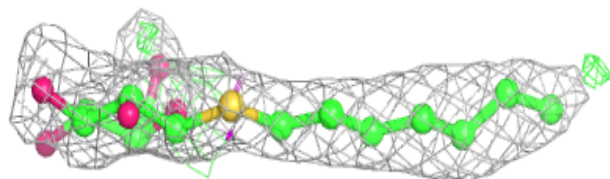
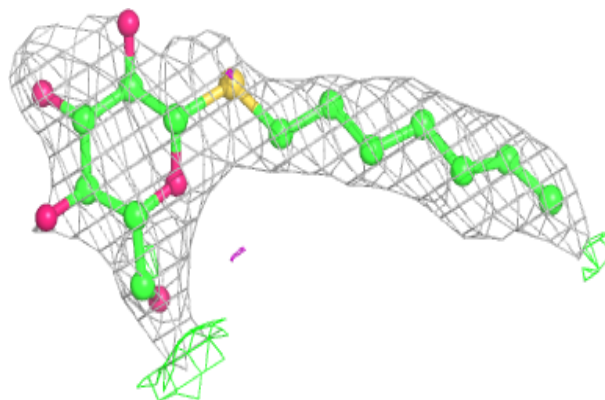


**Electron density around LMT Z 101:**

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

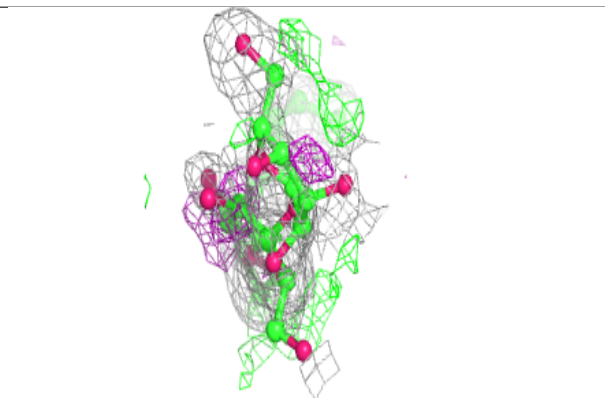
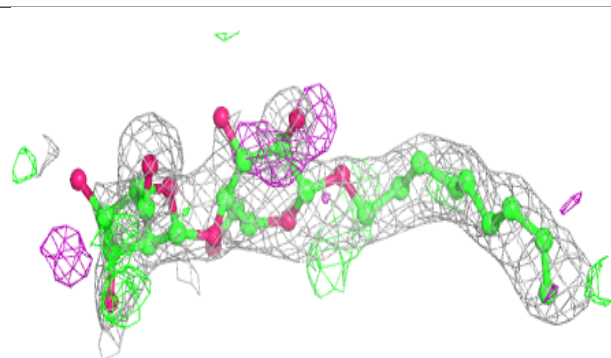
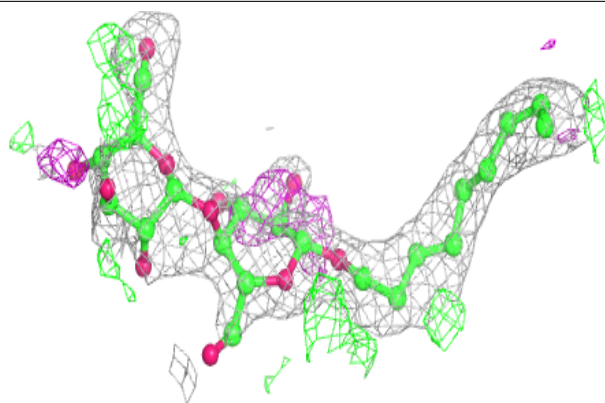
**Electron density around HTG b 602:**

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

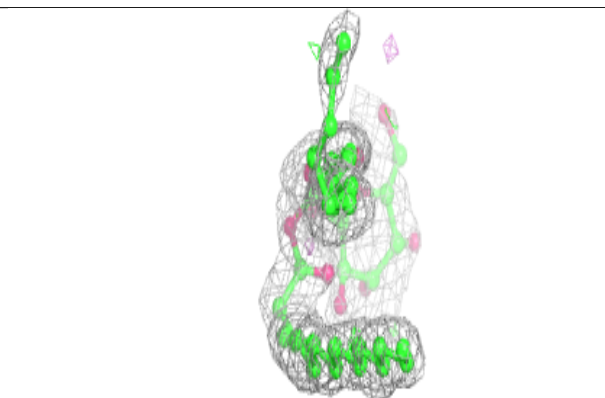
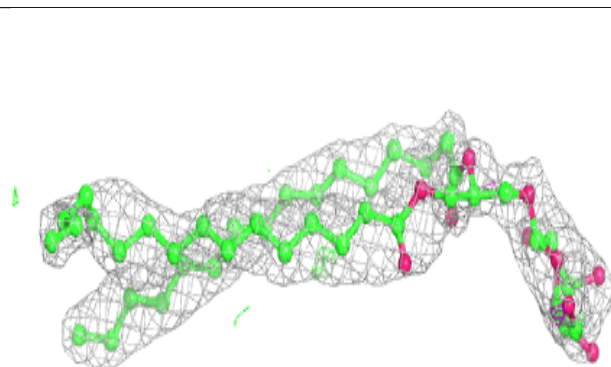
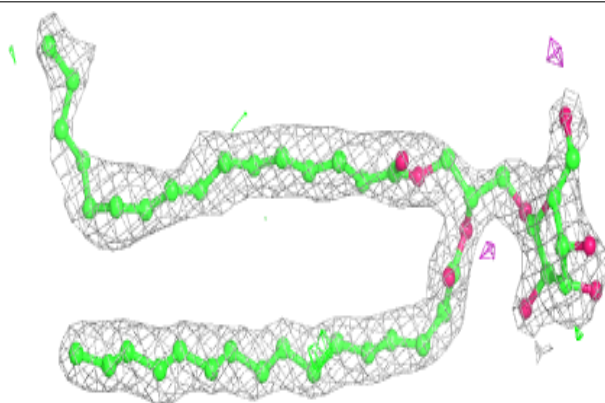


**Electron density around LMT b 627:**

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

**Electron density around LMG c 518:**

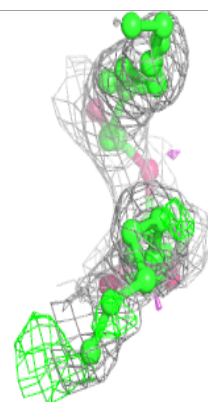
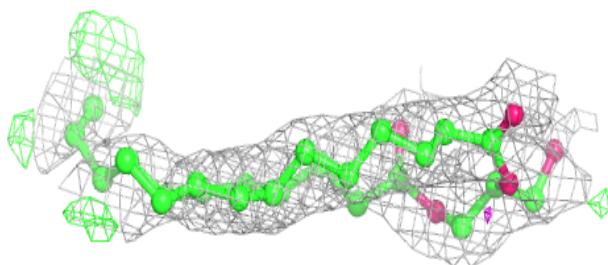
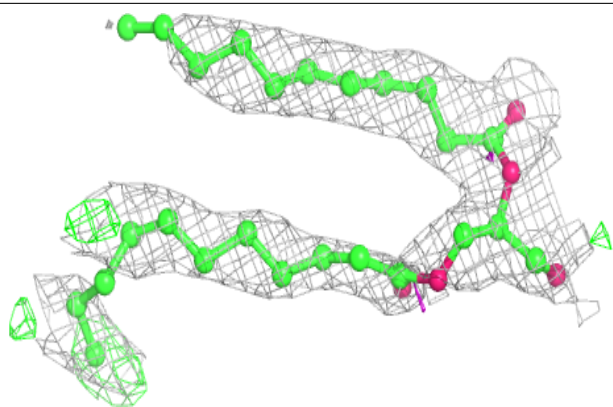
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



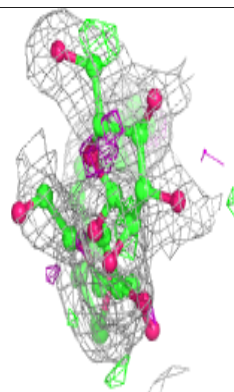
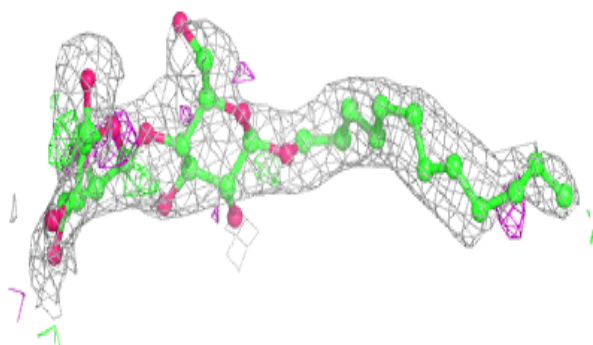
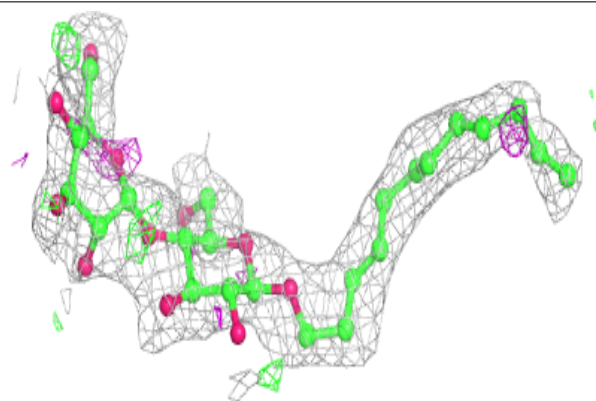


**Electron density around UNL c 524:**

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

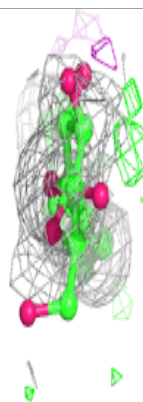
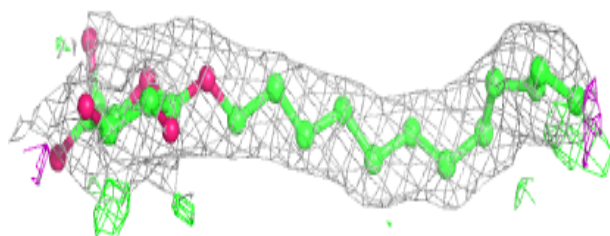
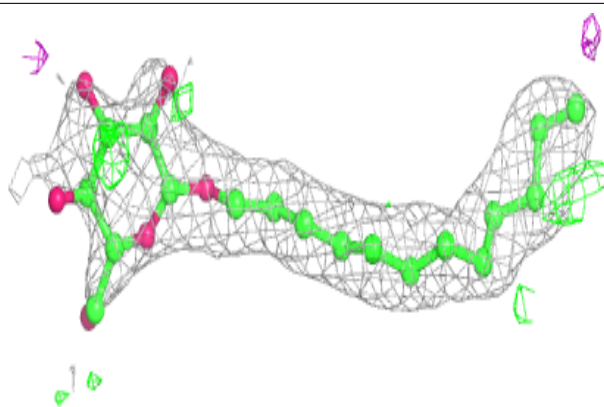
**Electron density around LMT a 418:**

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

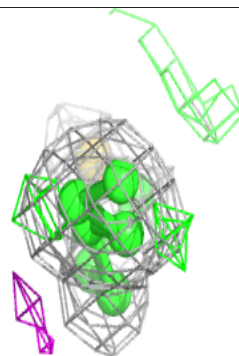
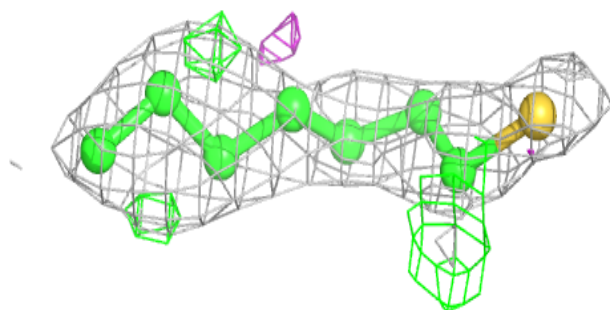
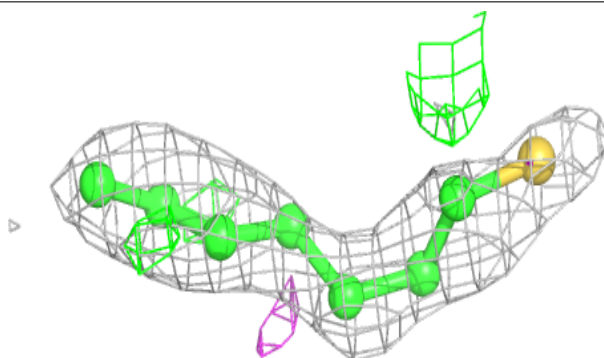


**Electron density around LMT B 626:**

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

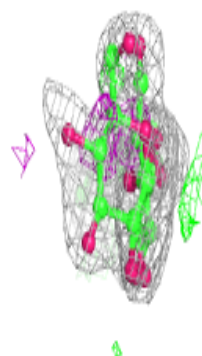
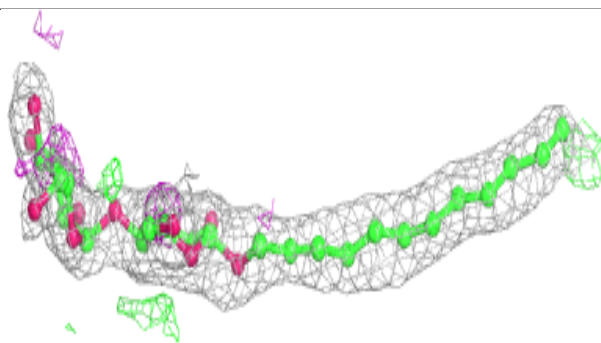
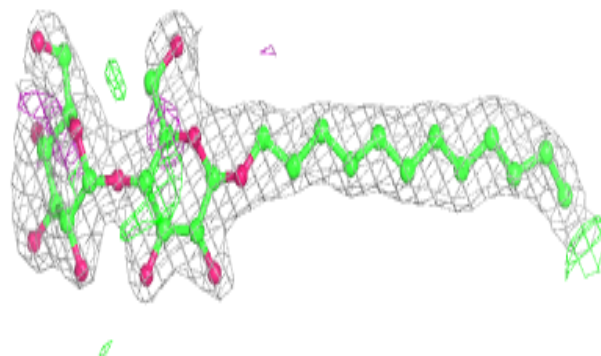
**Electron density around HTG u 201:**

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

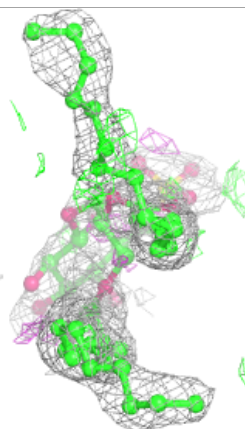
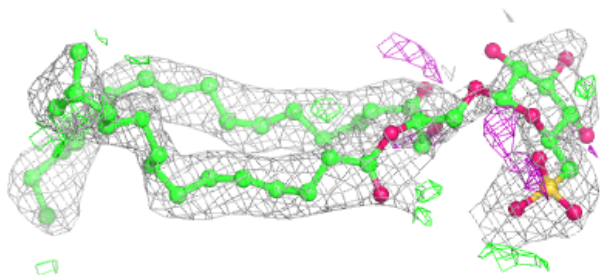
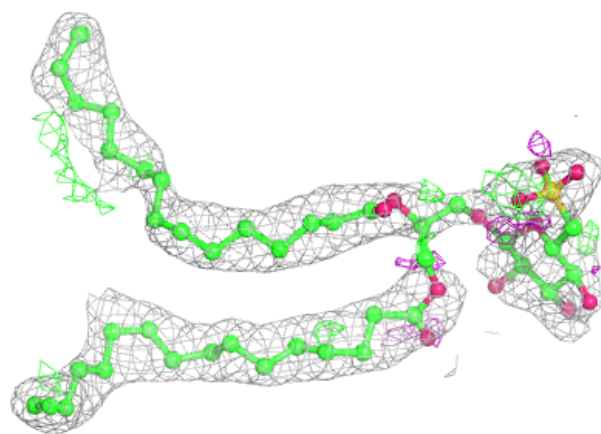


**Electron density around LMT m 102:**

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

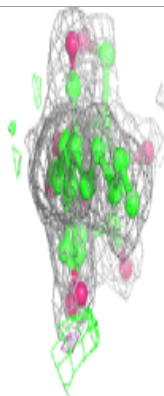
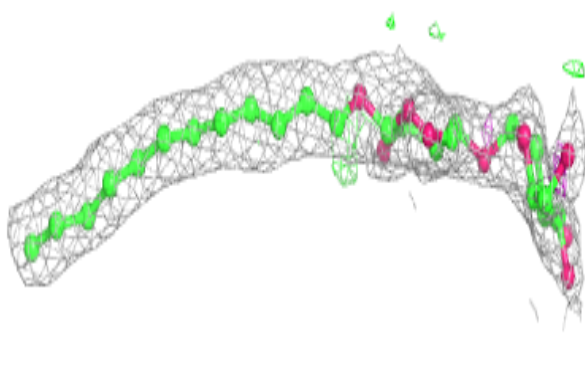
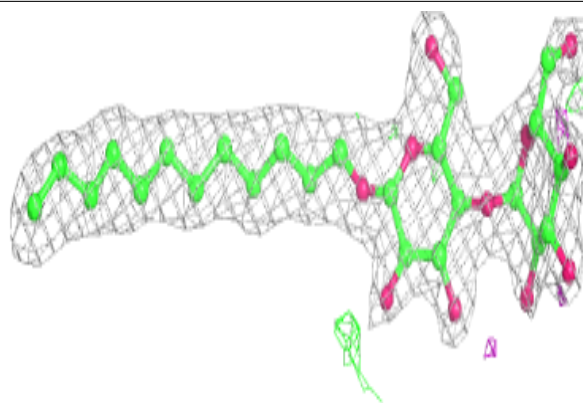
**Electron density around SQD l 101:**

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

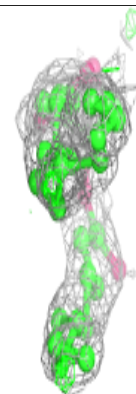
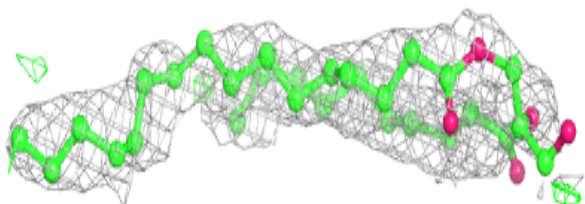
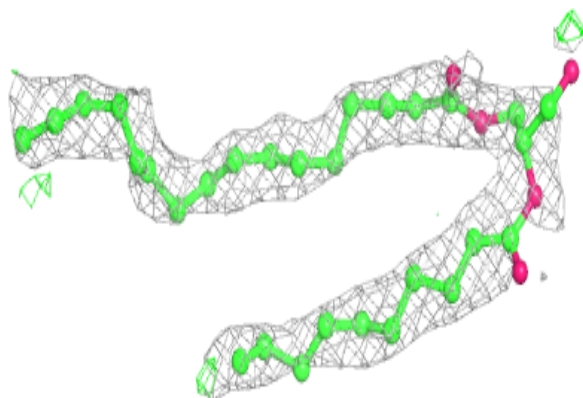


**Electron density around LMT M 101:**

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

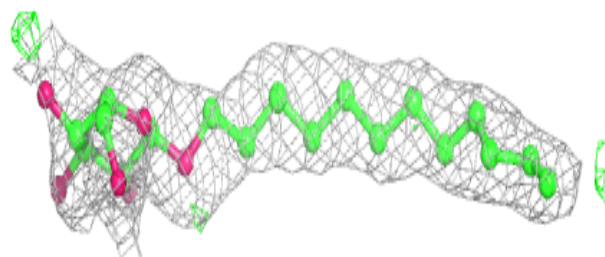
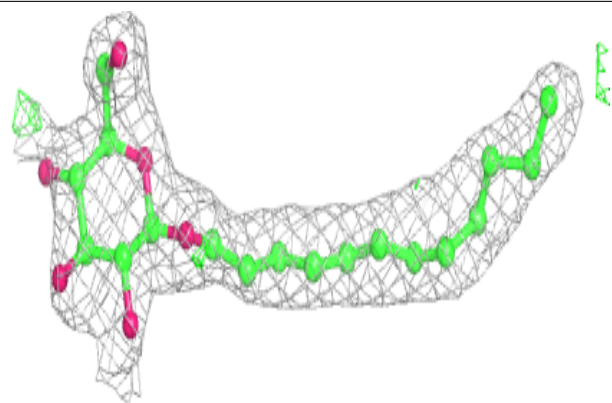
**Electron density around UNL C 523:**

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

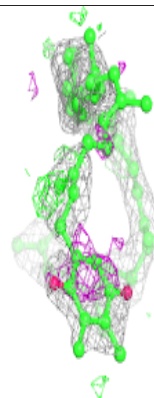
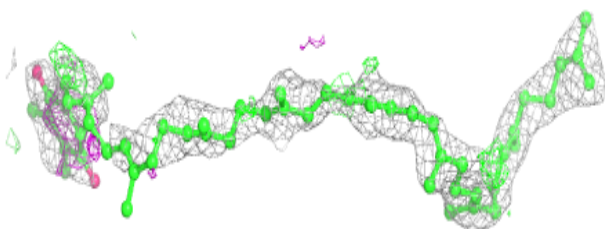
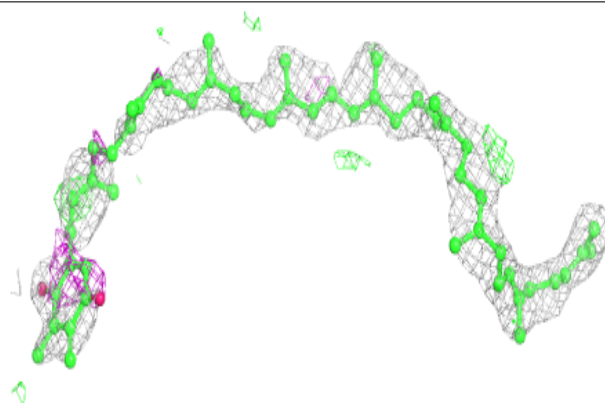


**Electron density around LMT B 625:**

$2mF_o-DF_c$  (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:**

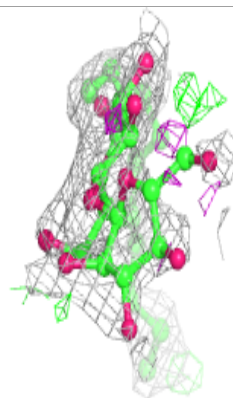
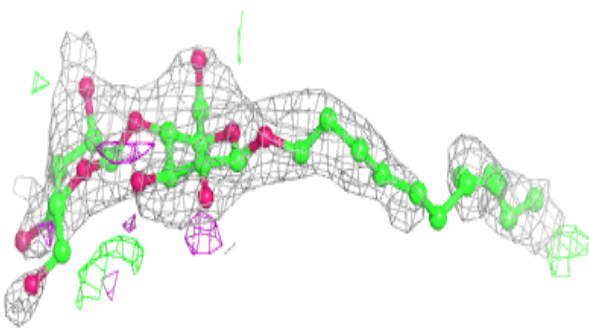
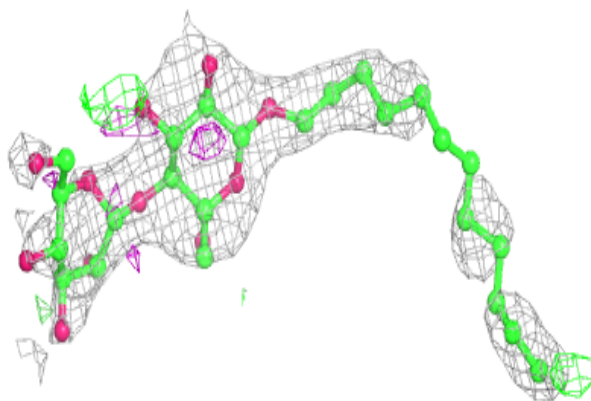
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



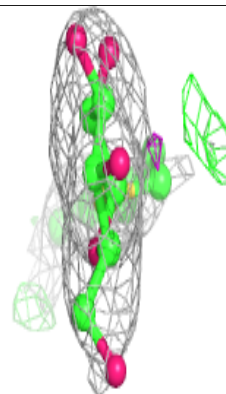
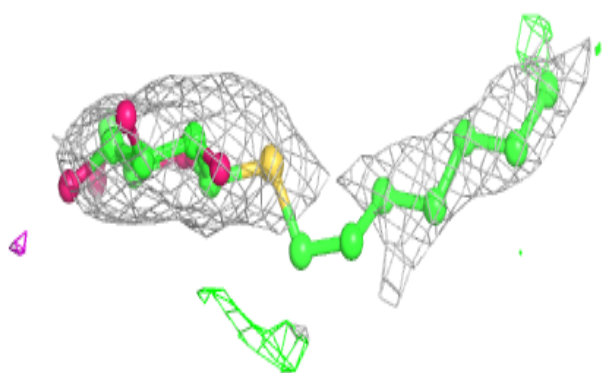
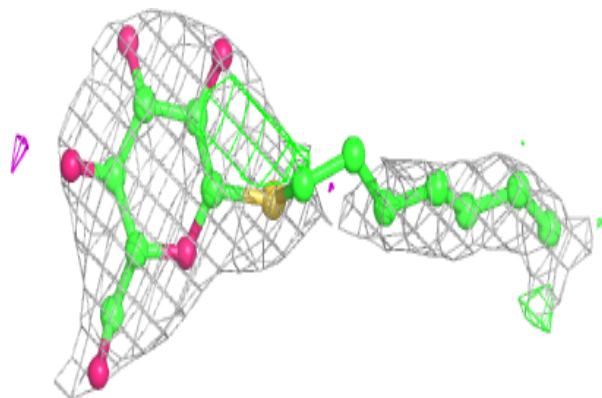


**Electron density around LMT I 101:**

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

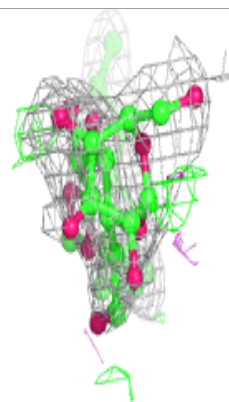
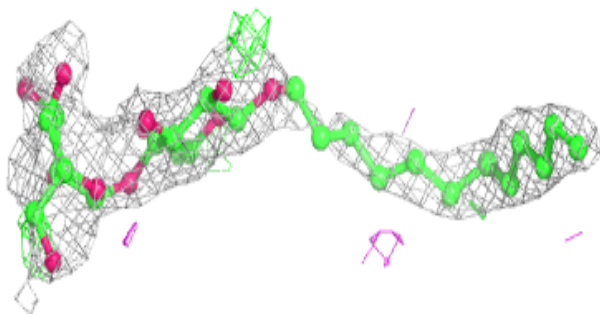
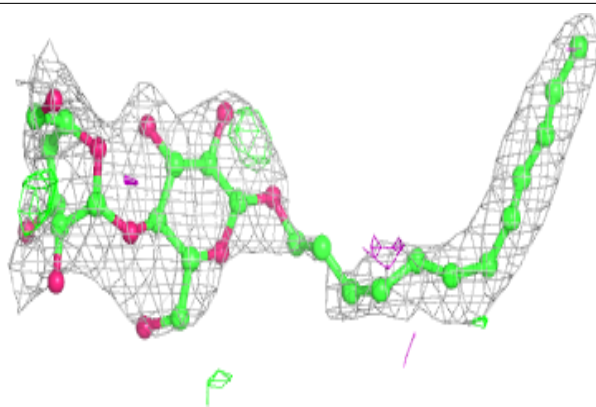
**Electron density around HTG c 520:**

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

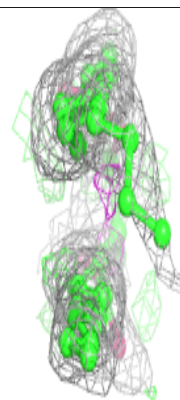
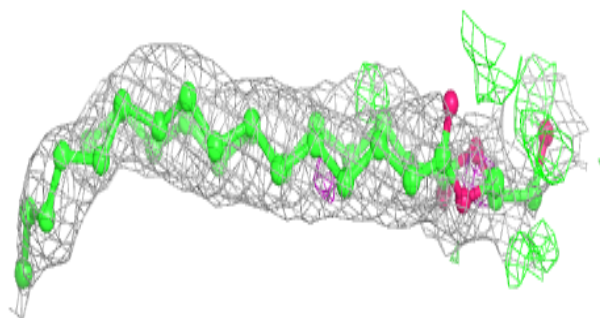
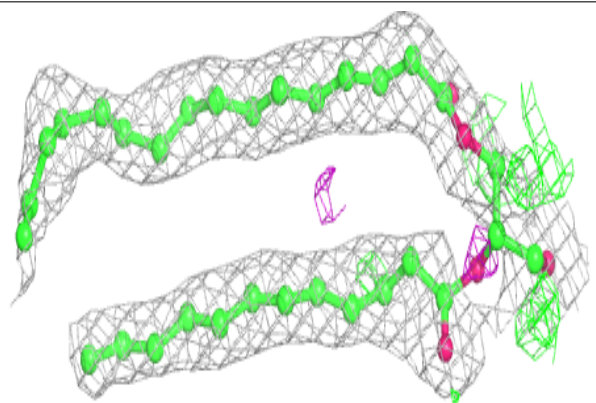


**Electron density around LMT z 102:**

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

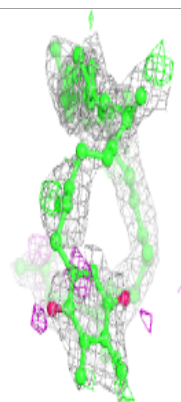
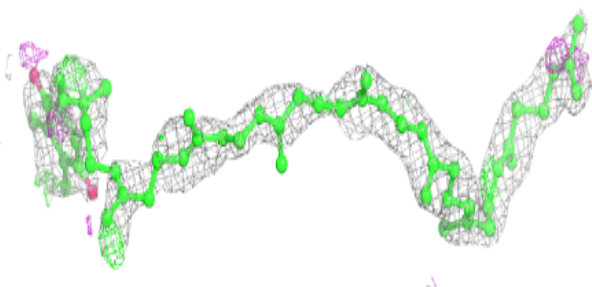
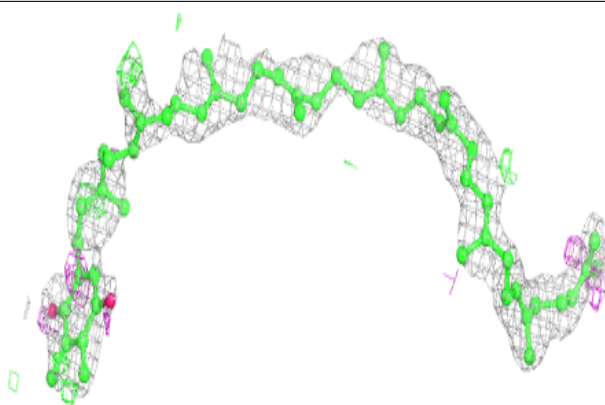
**Electron density around UNL d 409:**

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

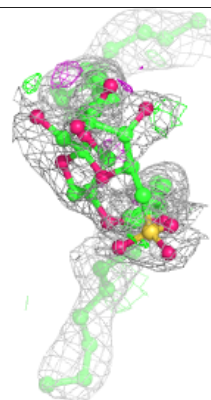
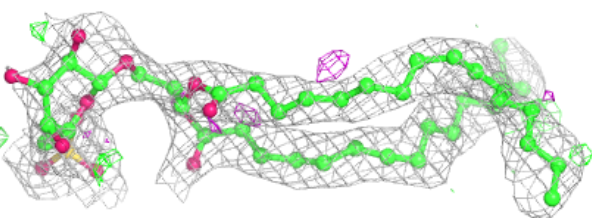
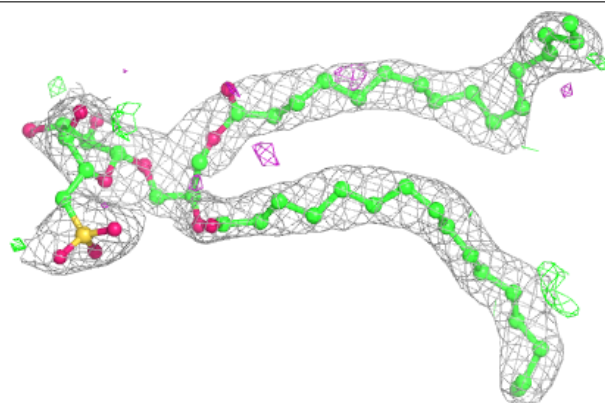


**Electron density around PL9 A 411:**

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

**Electron density around SQD b 622:**

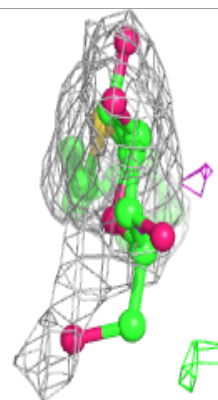
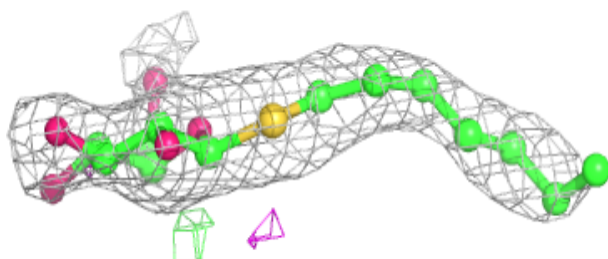
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



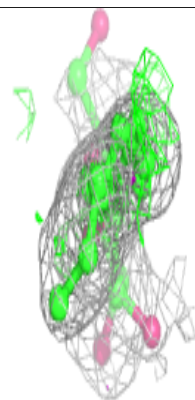
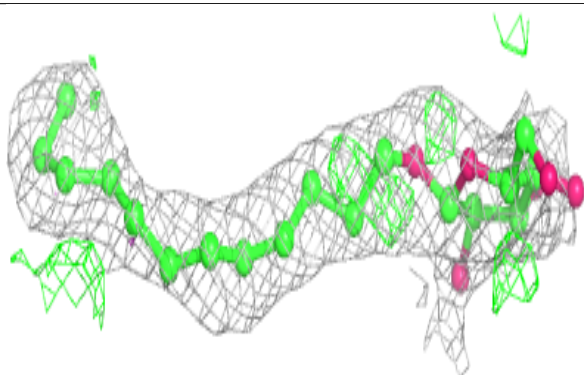
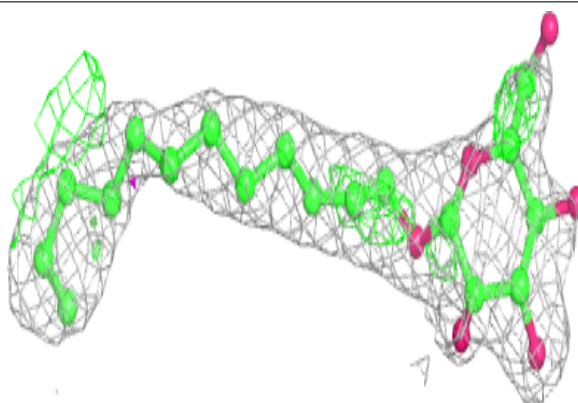


**Electron density around HTG C 522:**

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

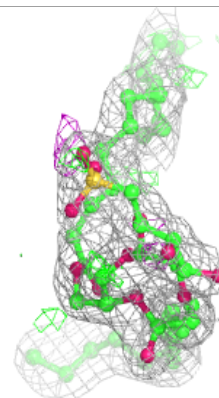
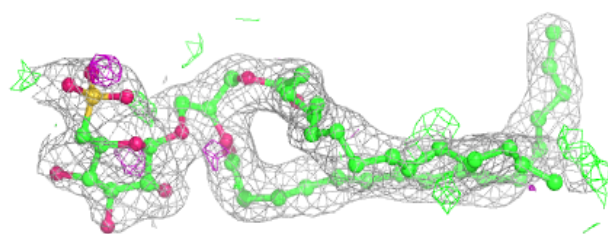
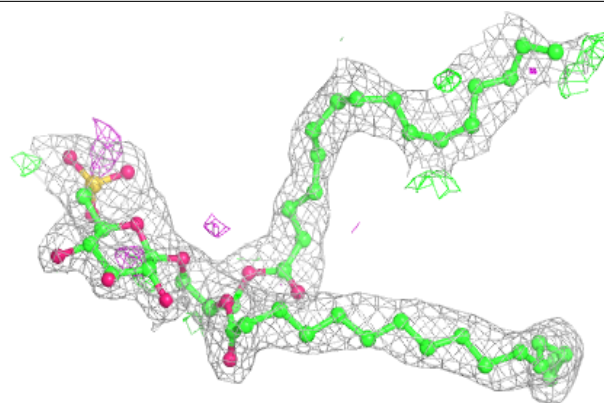
**Electron density around LMT T 102:**

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

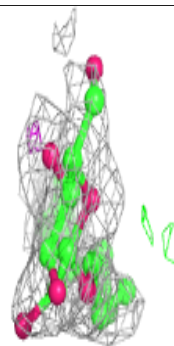
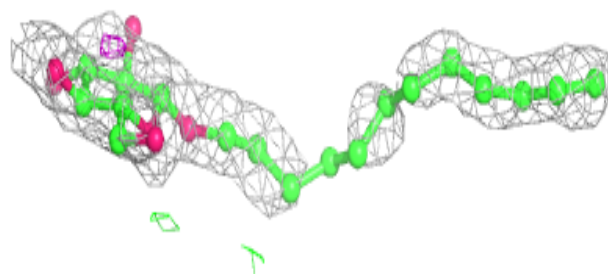
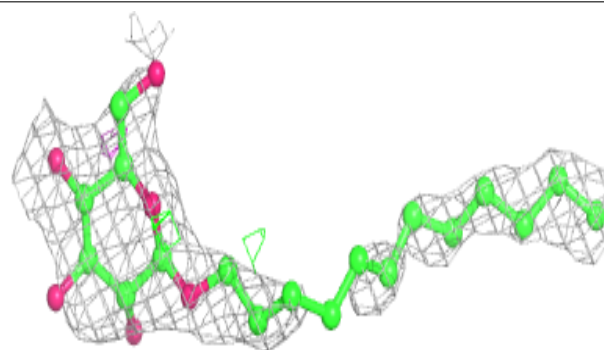


**Electron density around SQD a 401:**

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

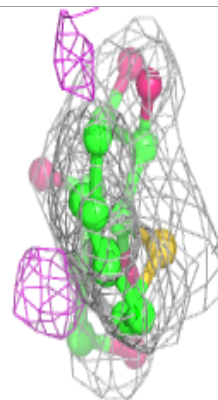
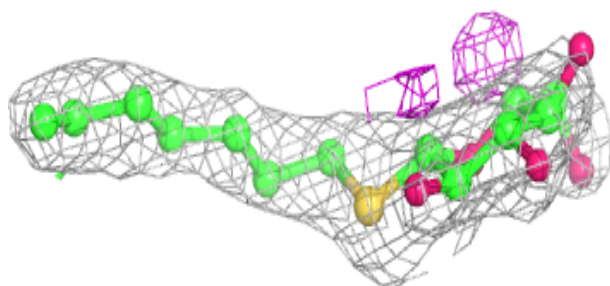
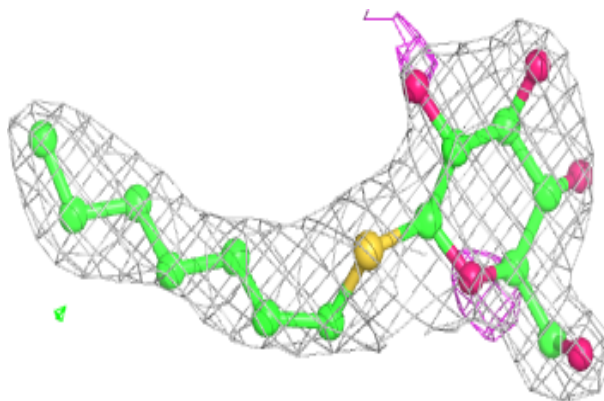
**Electron density around LMT E 101:**

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

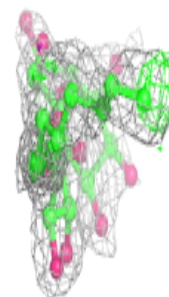
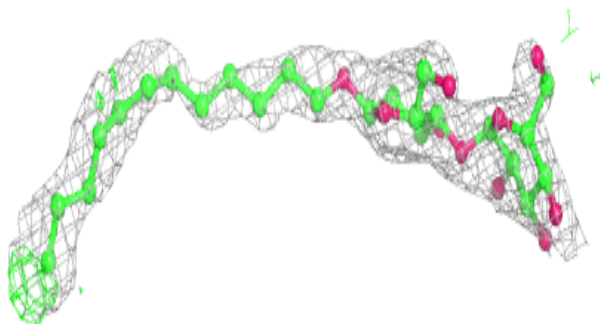
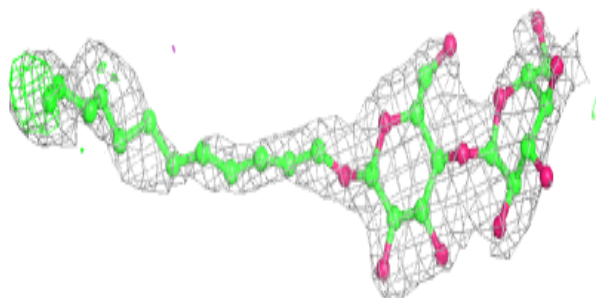


**Electron density around HTG b 624:**

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

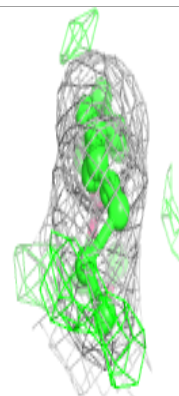
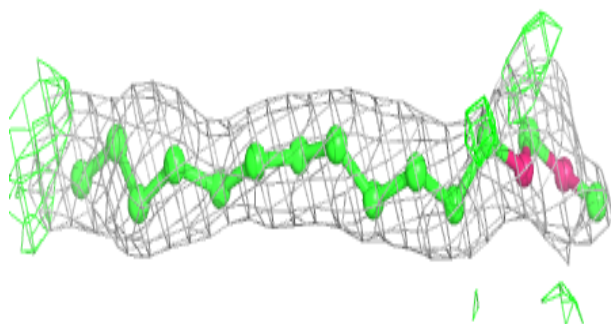
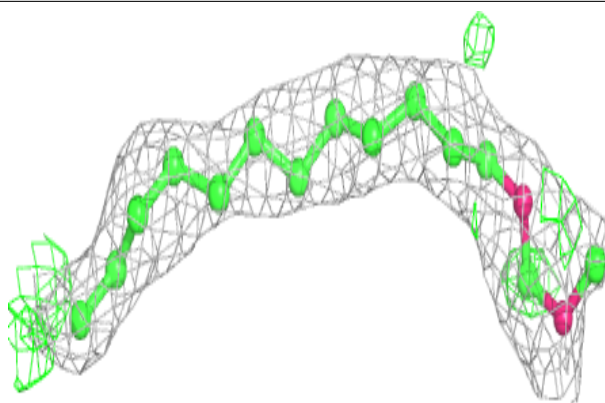
**Electron density around LMT c 523:**

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

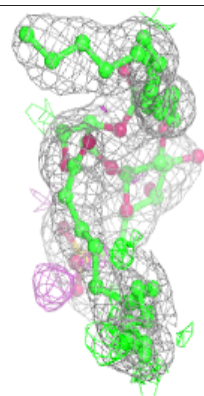
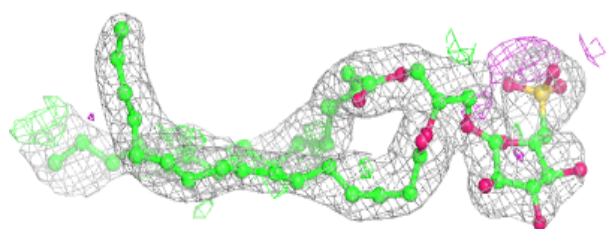
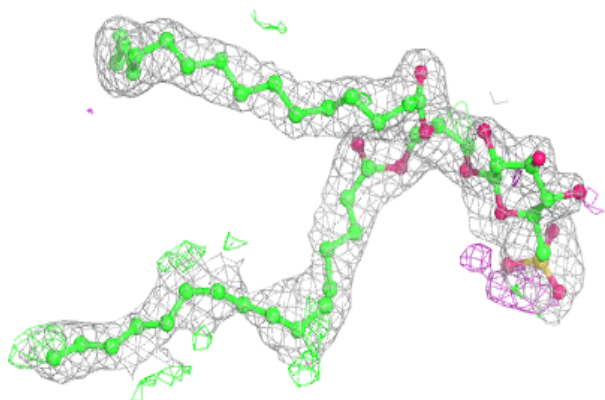


**Electron density around LMT B 627:**

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

**Electron density around SQD A 412:**

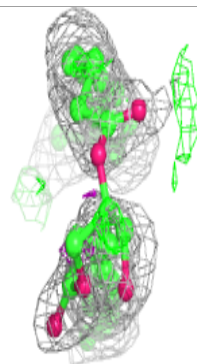
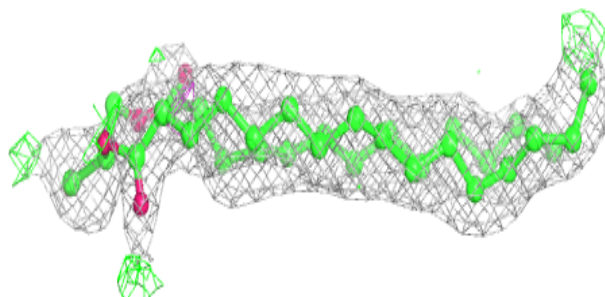
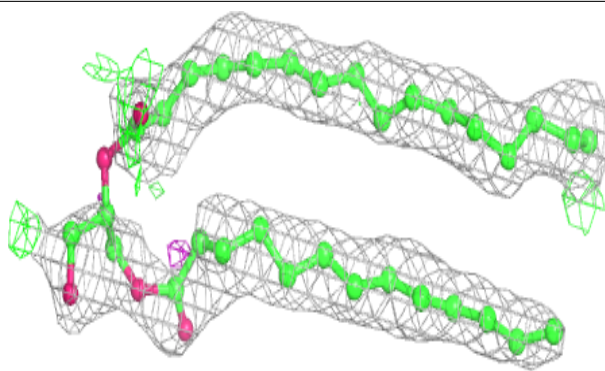
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



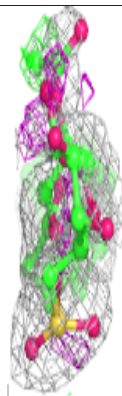
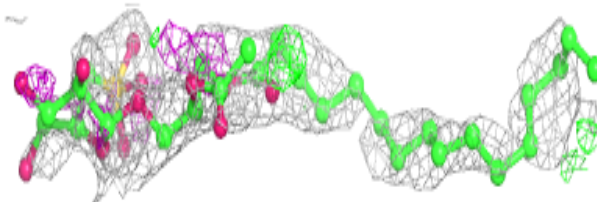
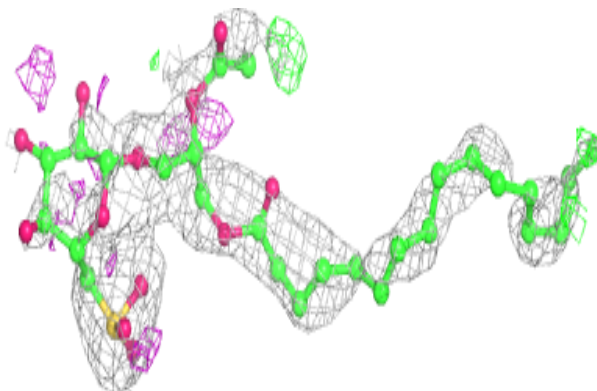


**Electron density around UNL D 410:**

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

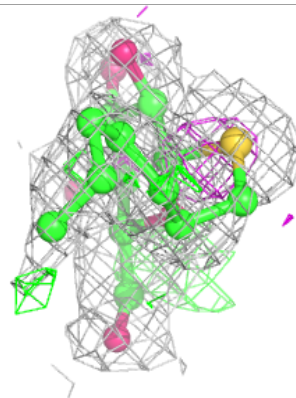
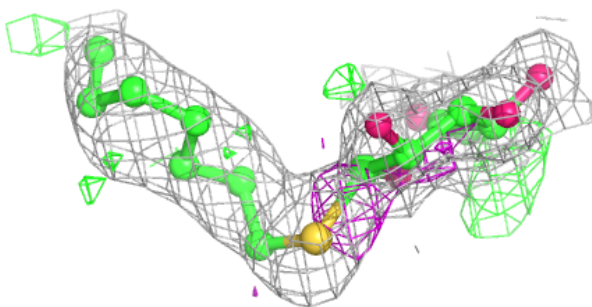
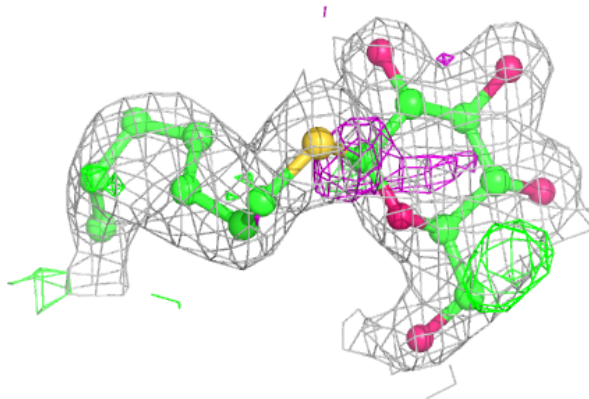
**Electron density around SQD f 101:**

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

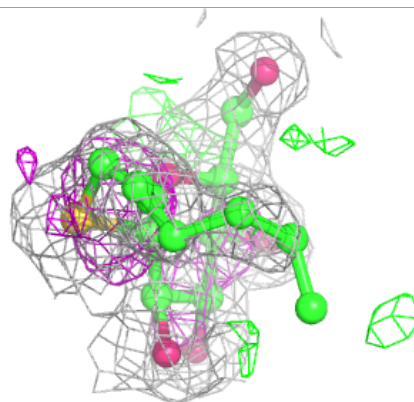
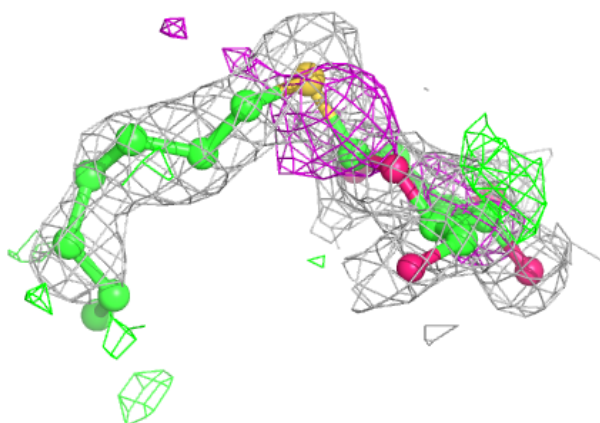
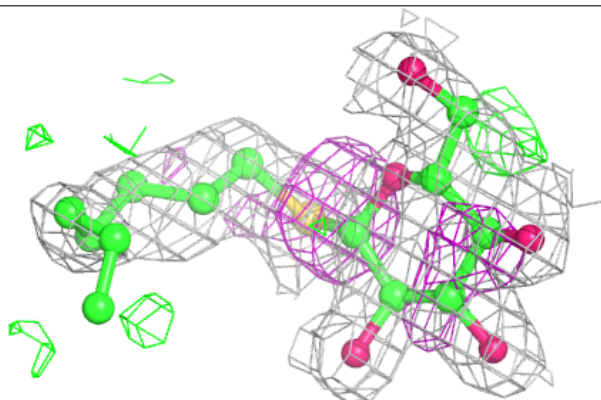


**Electron density around HTG B 622:**

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

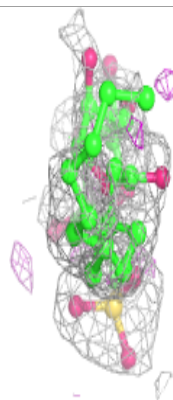
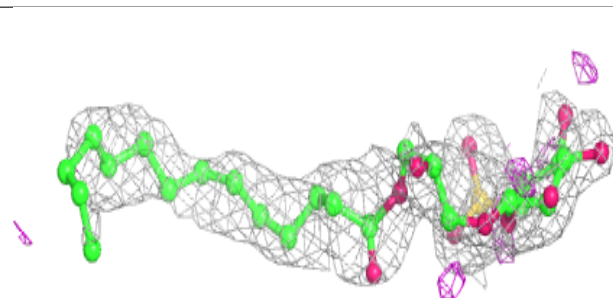
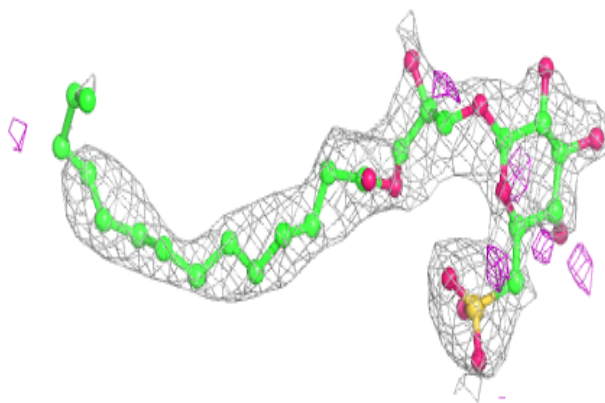
**Electron density around HTG b 625:**

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



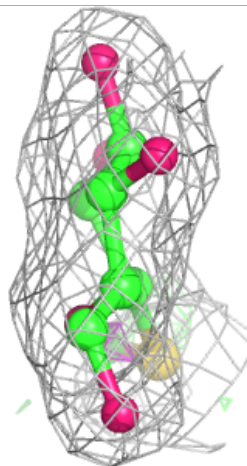
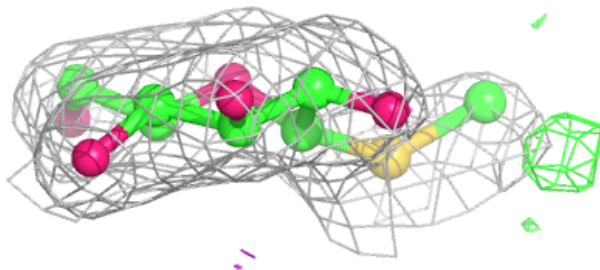
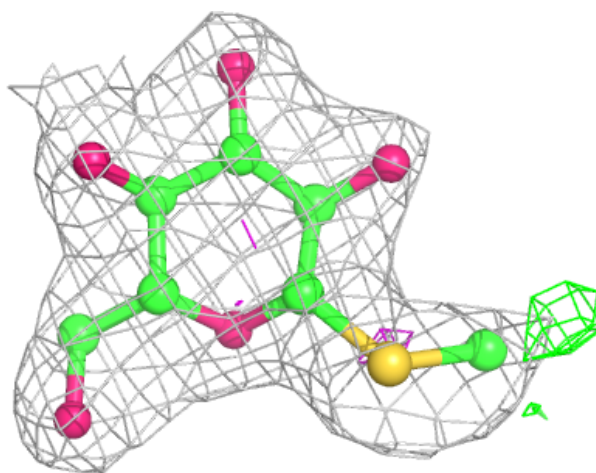
**Electron density around SQD F 101:**

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



**Electron density around HTG V 202:**

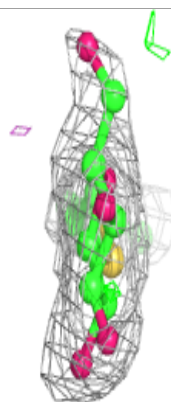
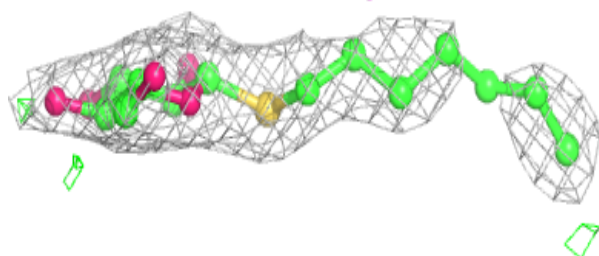
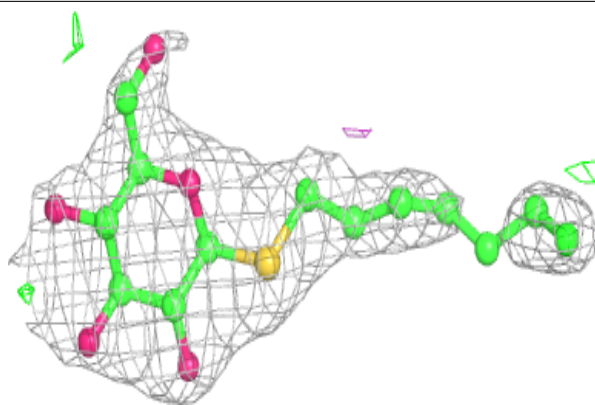
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



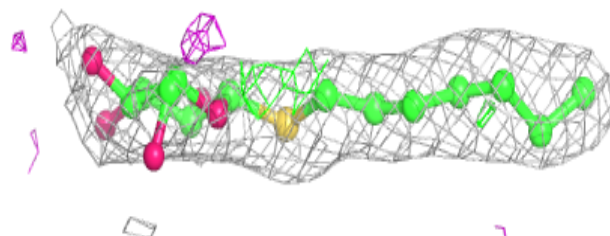
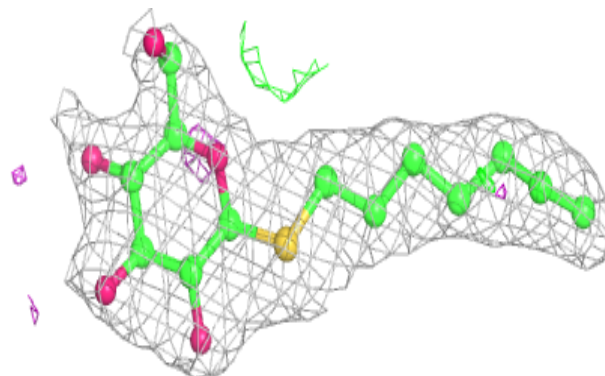


**Electron density around HTG C 520:**

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

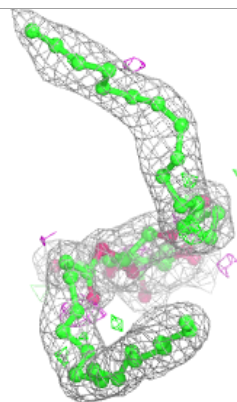
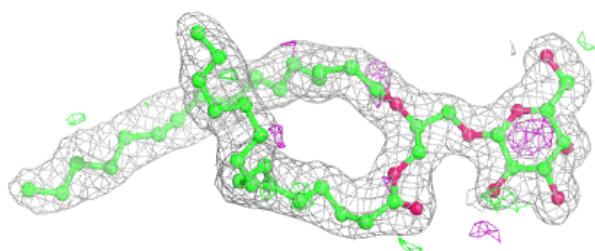
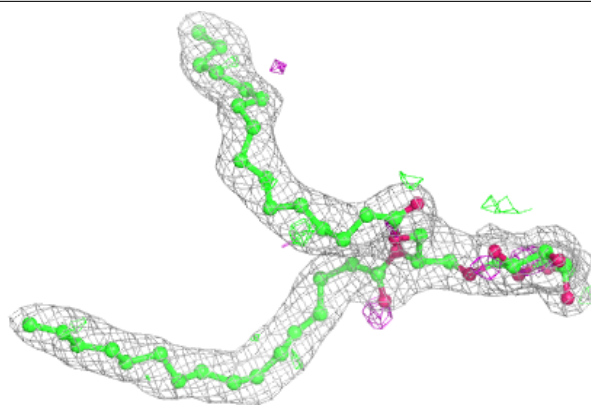
**Electron density around HTG b 601:**

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

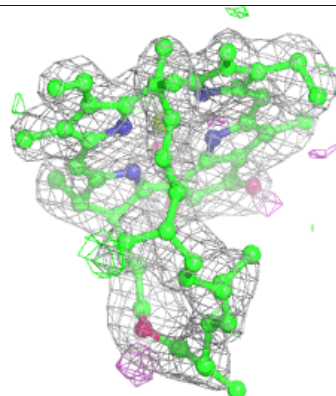
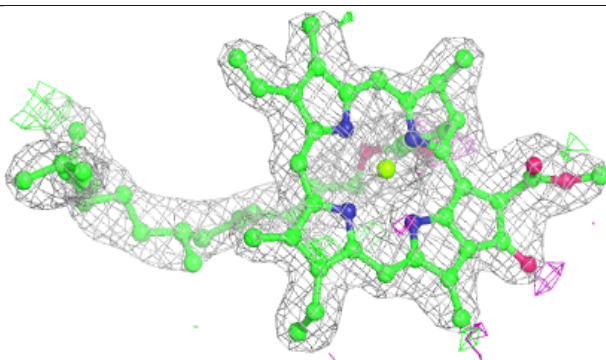
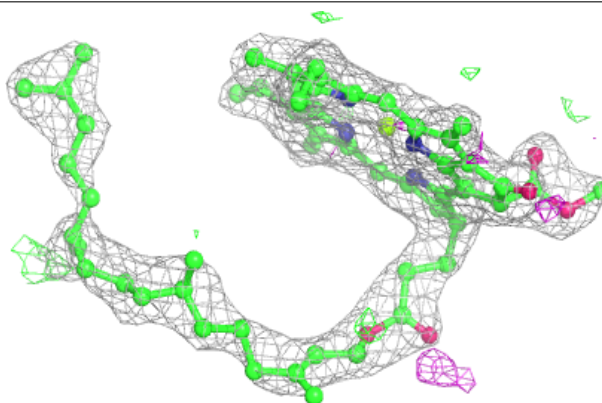


**Electron density around LMG B 620:**

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

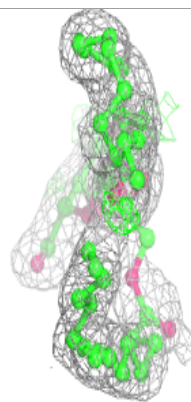
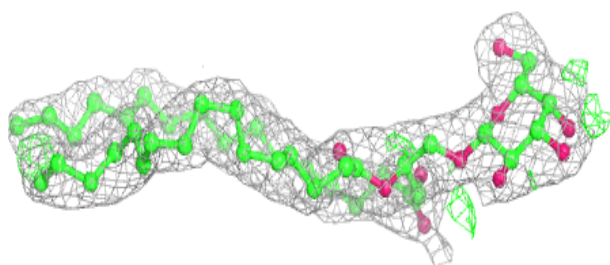
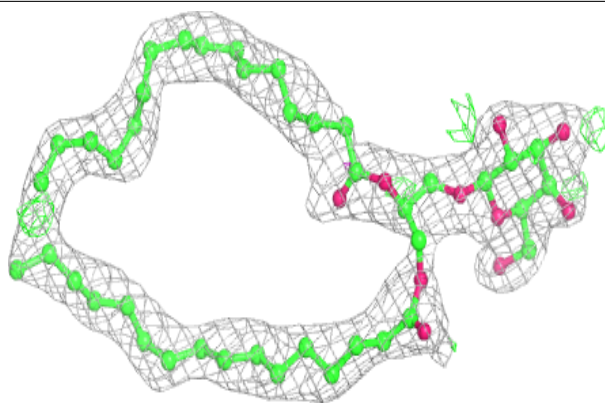
**Electron density around CLA C 513:**

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

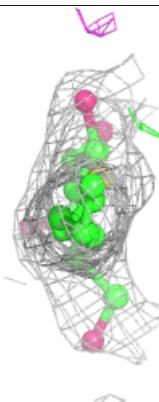
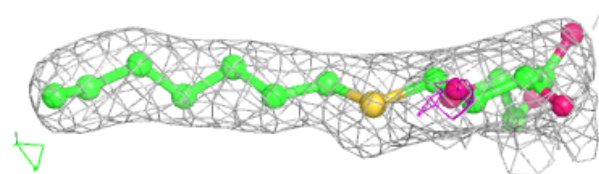
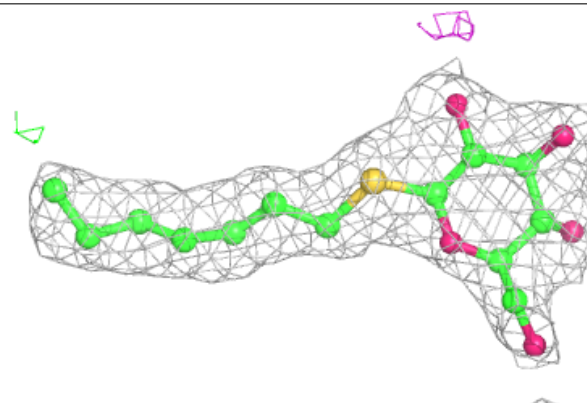


**Electron density around LMG A 407:**

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

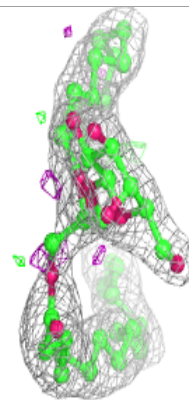
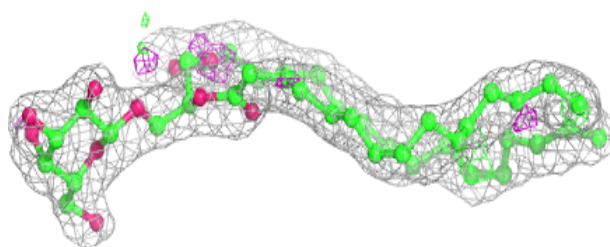
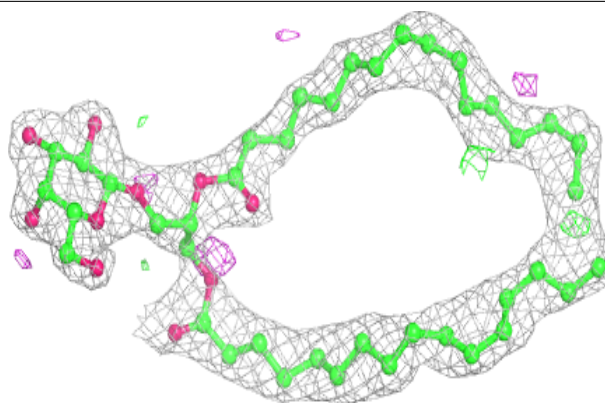
**Electron density around HTG B 631:**

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

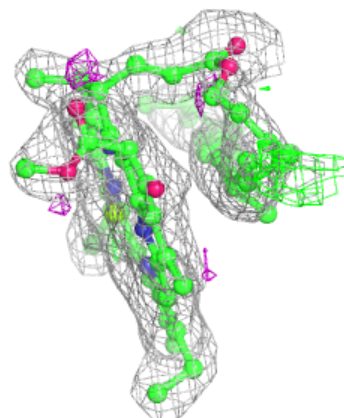
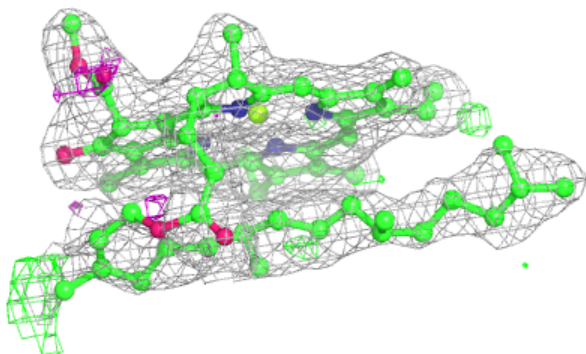
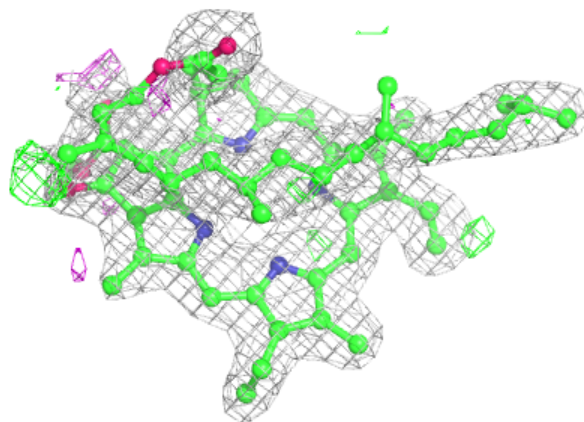


**Electron density around LMG a 410:**

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

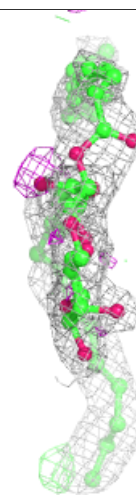
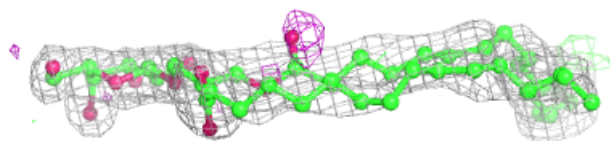
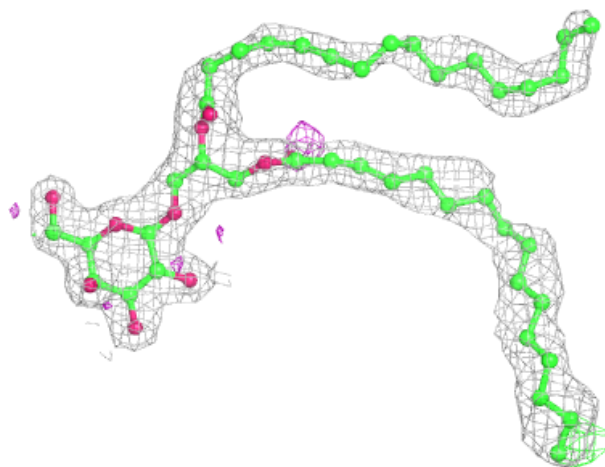
**Electron density around CLA B 602:**

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



**Electron density around LMG C 519:**

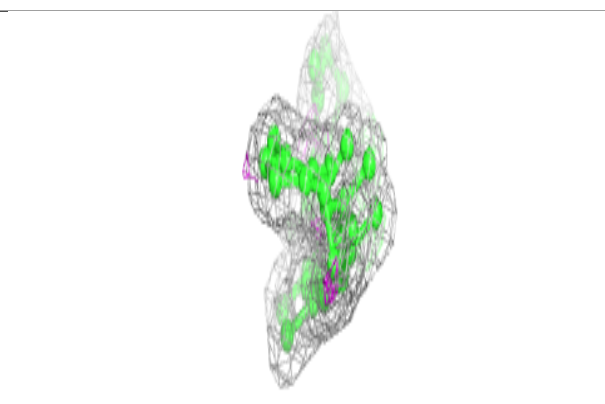
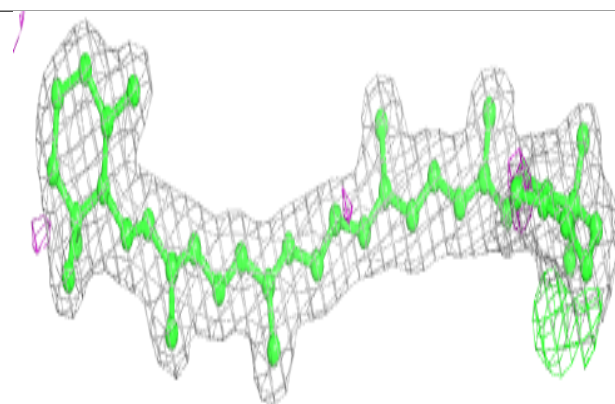
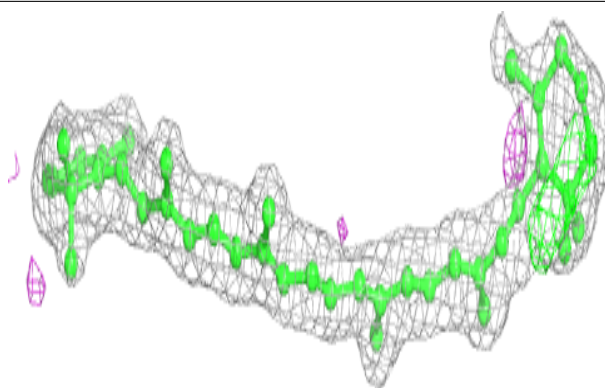
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



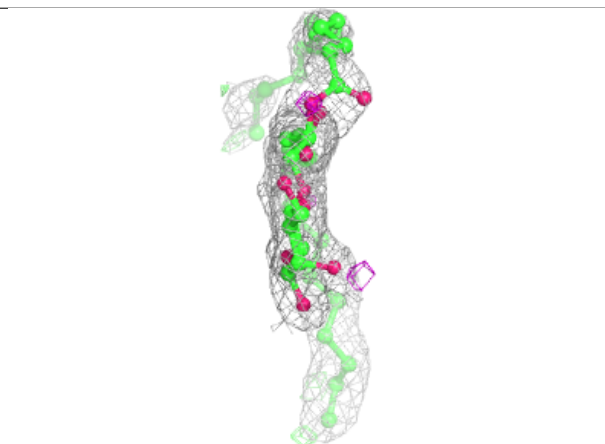
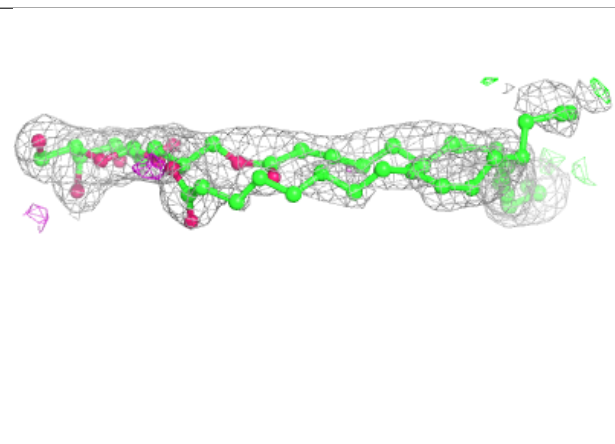
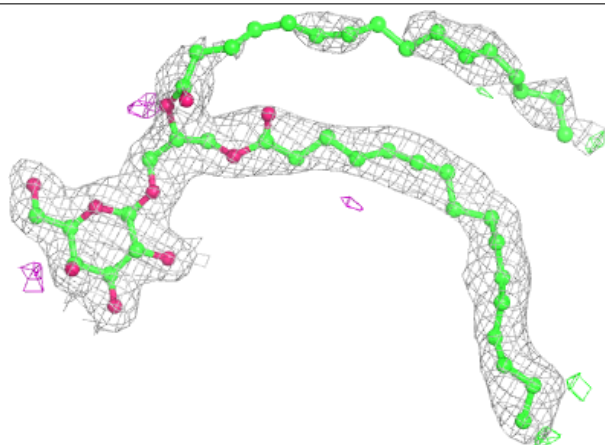


**Electron density around BCR d 405:**

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

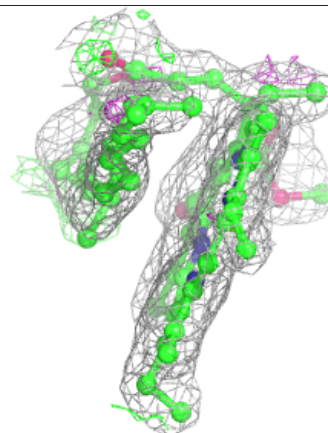
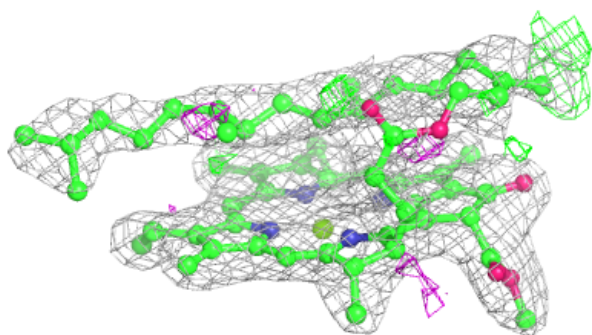
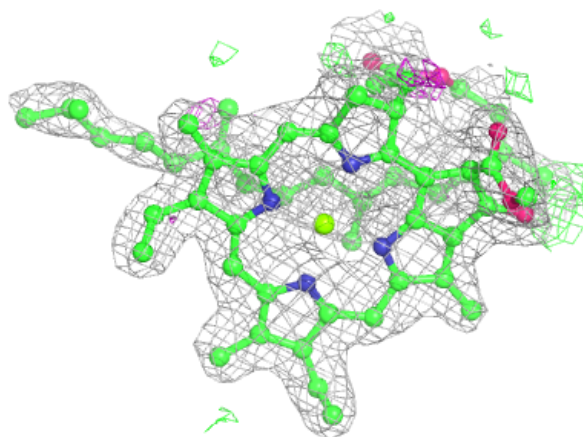
**Electron density around LMG c 519:**

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

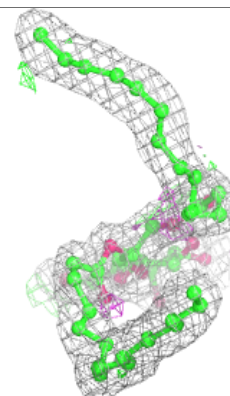
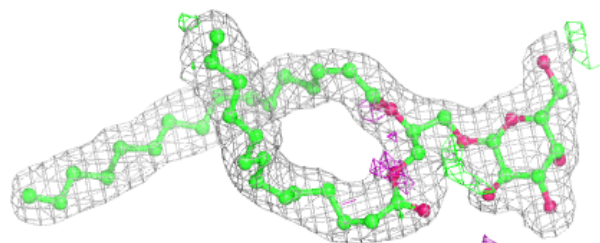
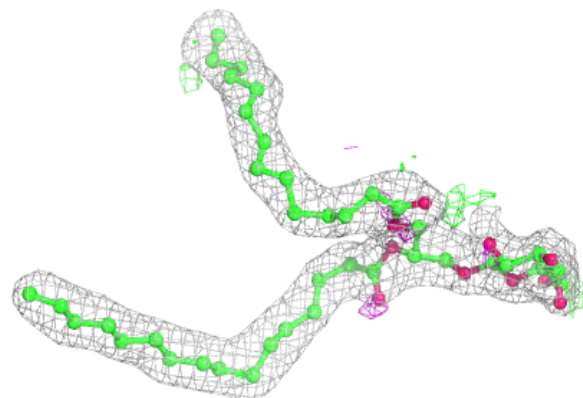


**Electron density around CLA b 603:**

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

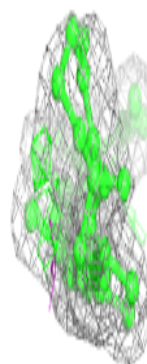
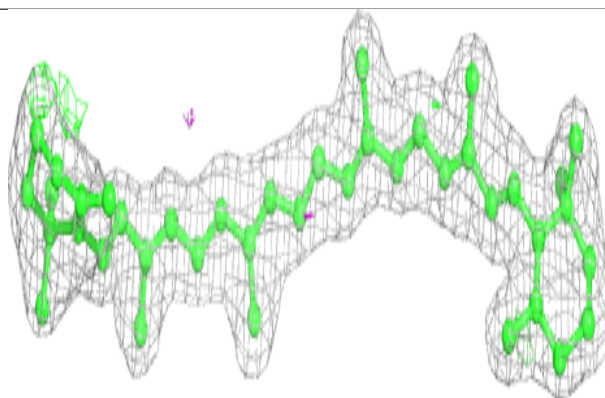
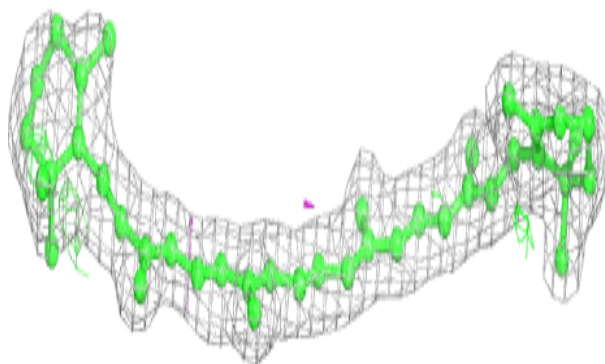
**Electron density around LMG b 623:**

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

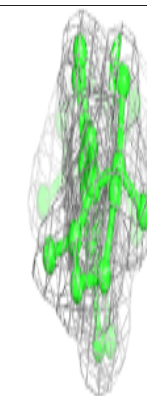
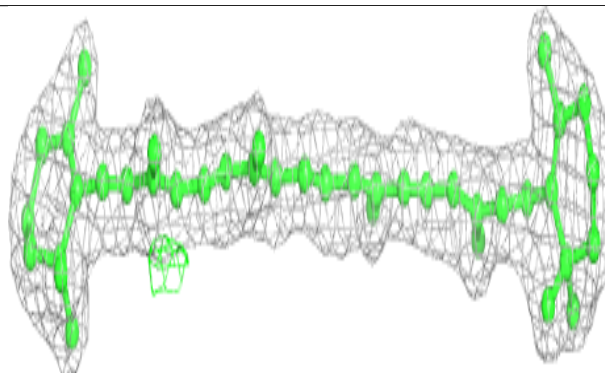
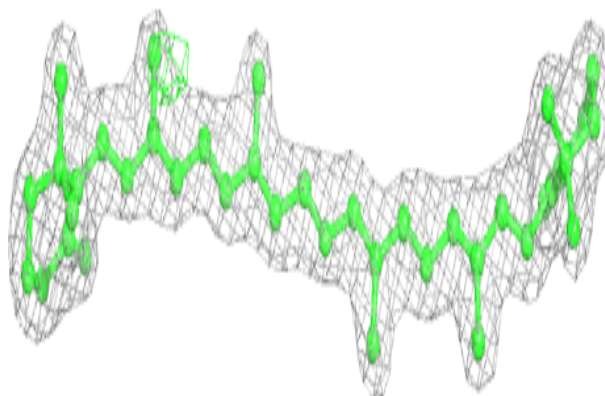


**Electron density around BCR D 405:**

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

**Electron density around BCR C 514:**

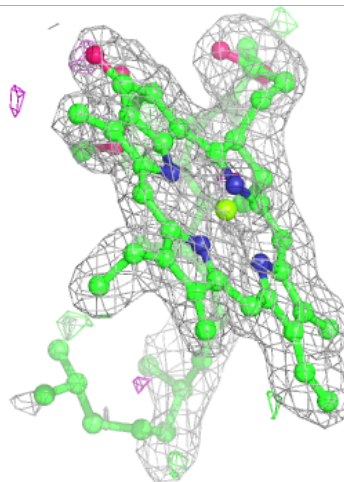
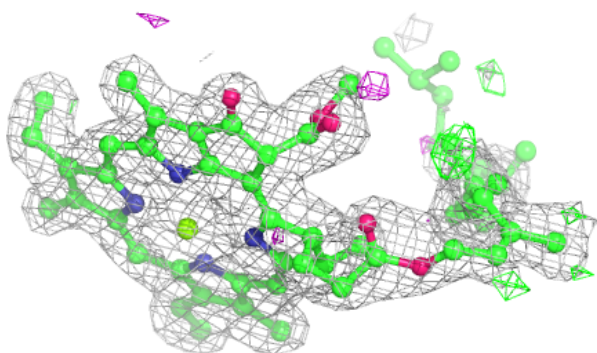
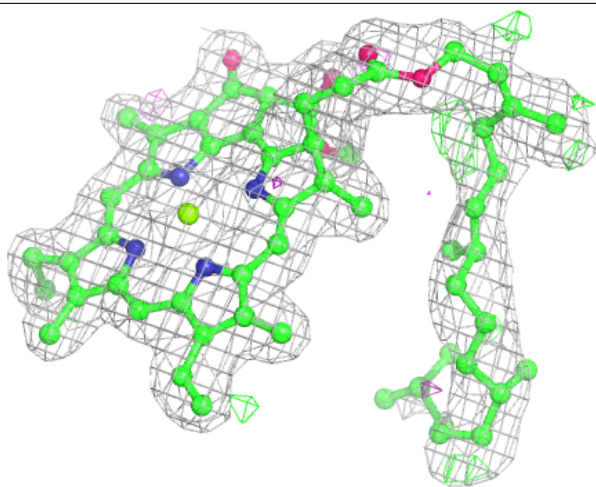
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





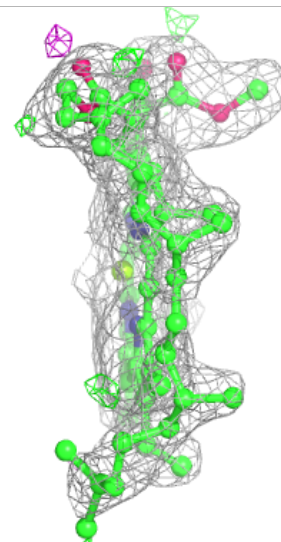
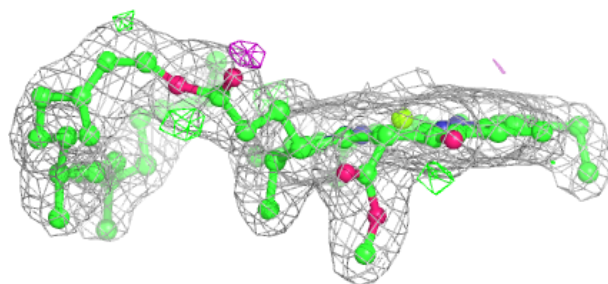
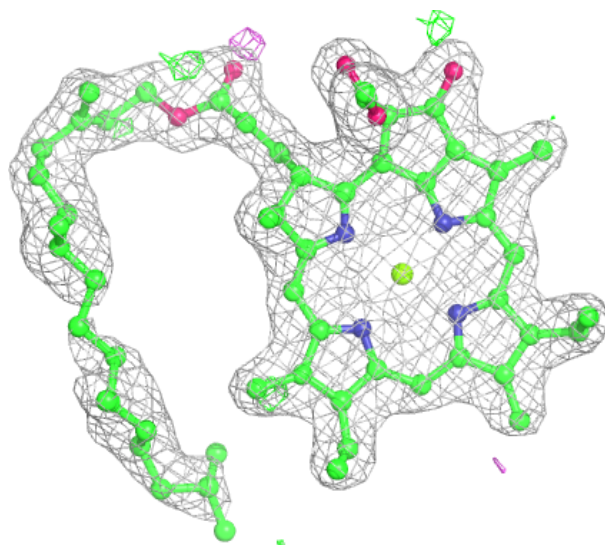
**Electron density around CLA b 618:**

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



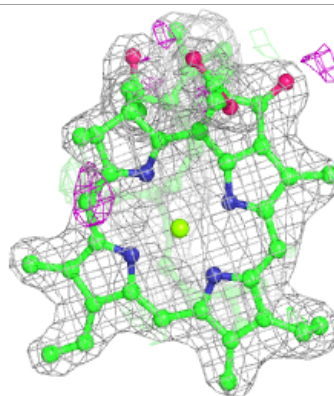
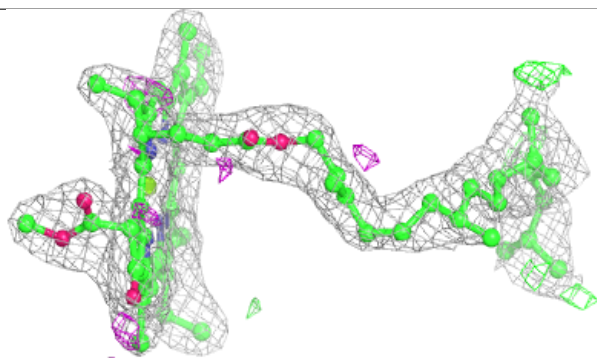
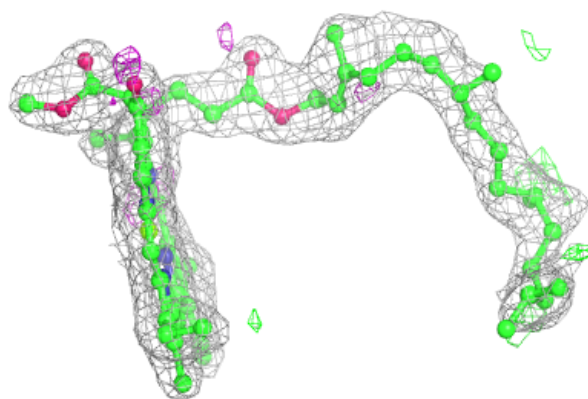
**Electron density around CLA c 512:**

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

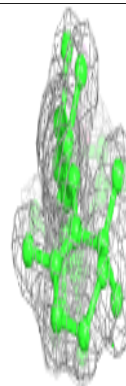
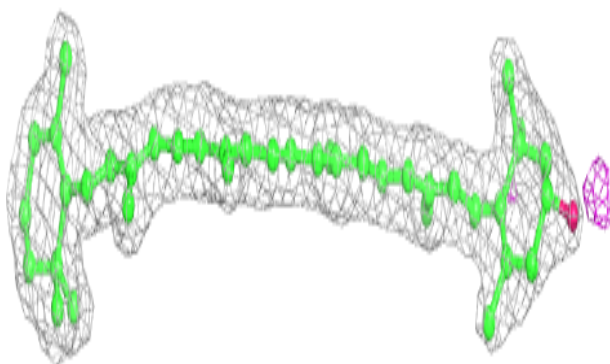
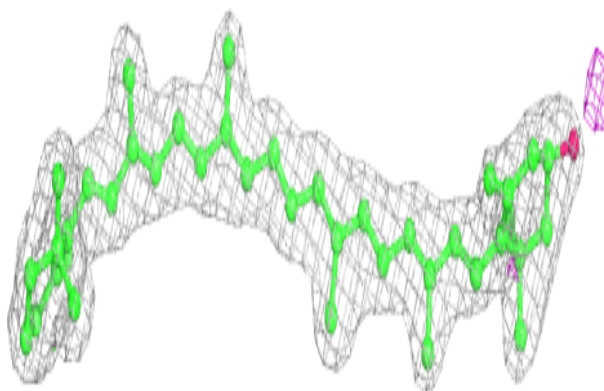


**Electron density around CLA C 506:**

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

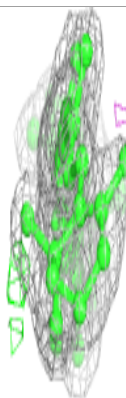
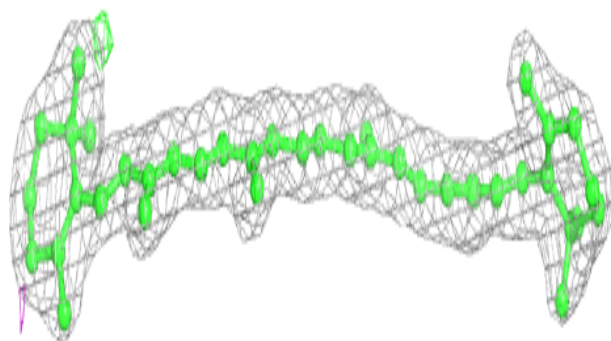
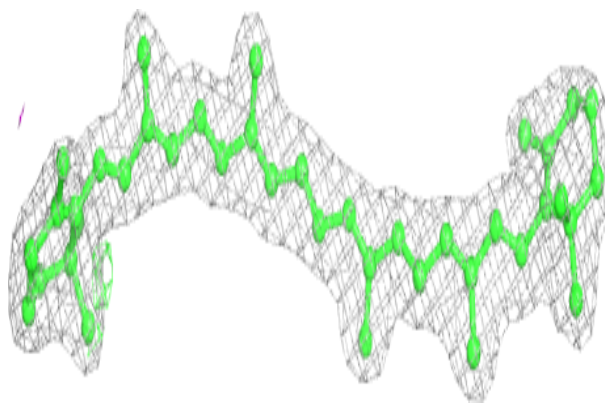
**Electron density around RRX x 101:**

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

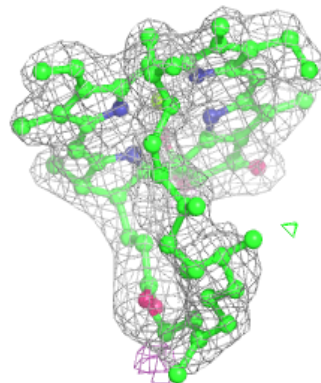
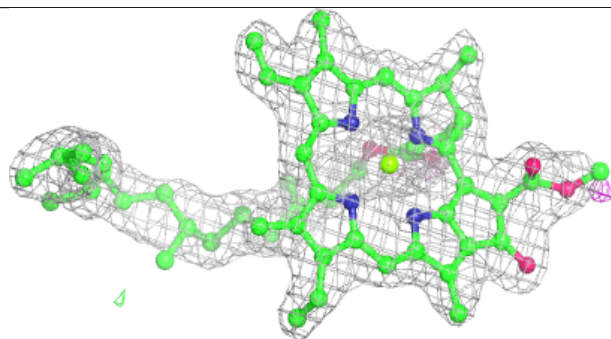
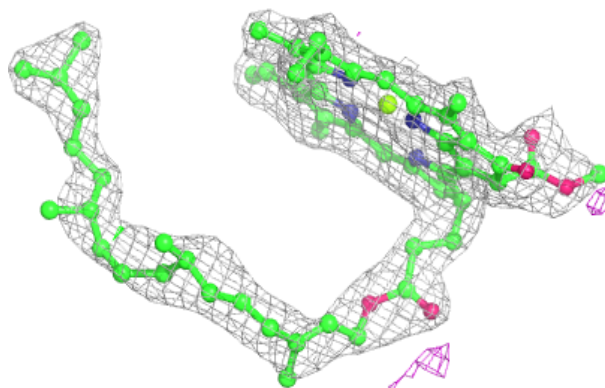


**Electron density around BCR K 101:**

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

**Electron density around CLA c 513:**

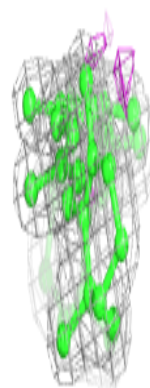
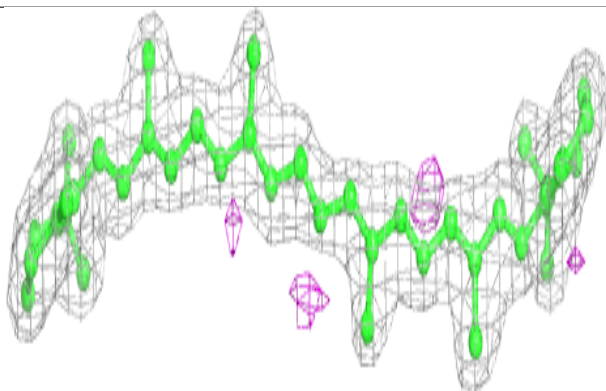
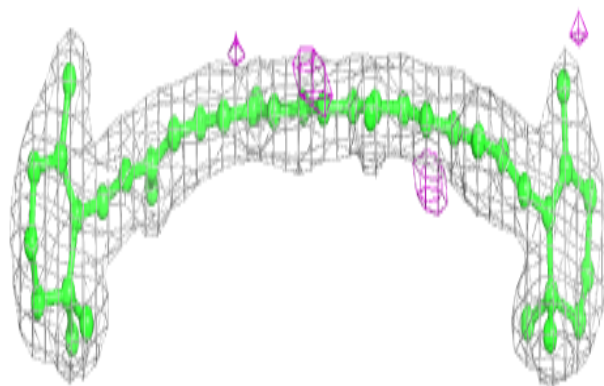
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



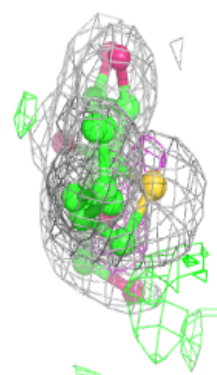
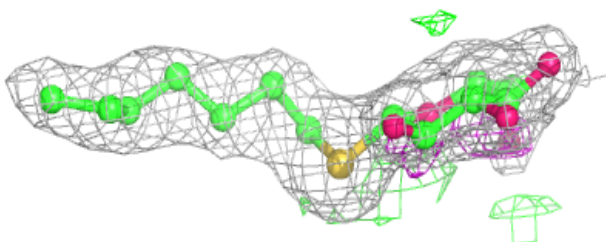
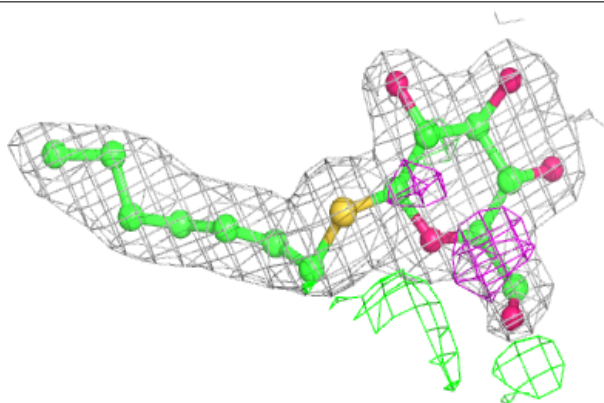


**Electron density around BCR K 102:**

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

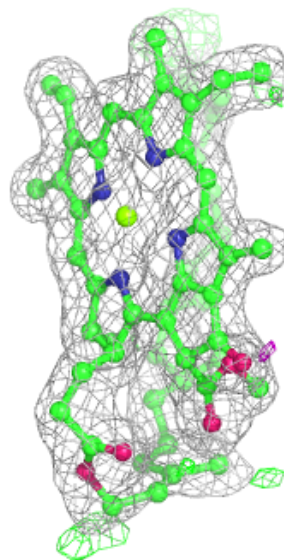
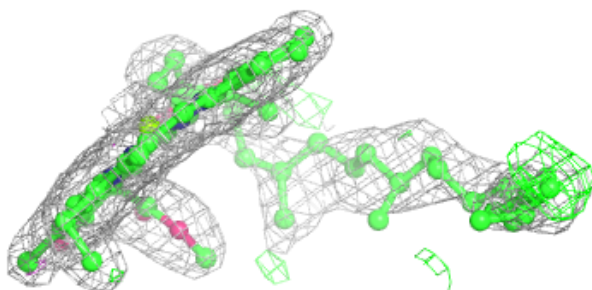
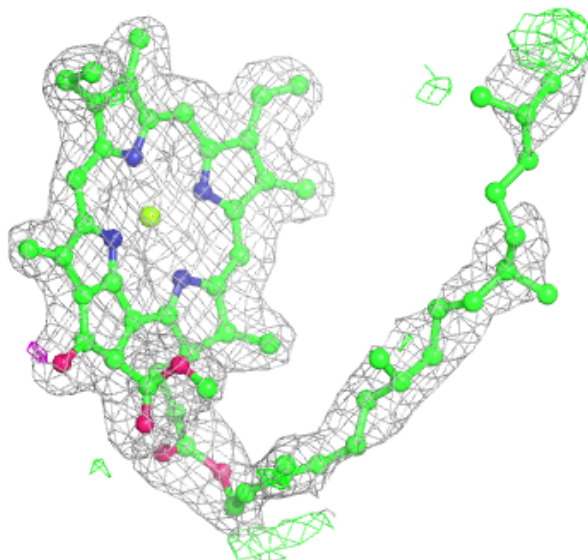
**Electron density around HTG B 621:**

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



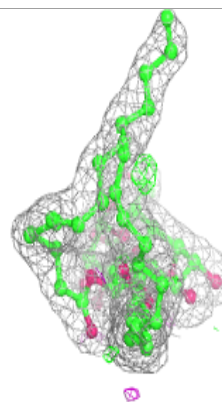
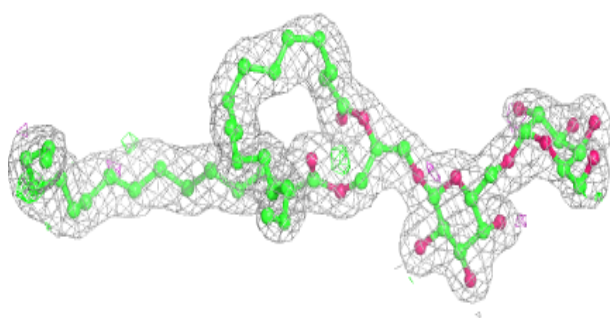
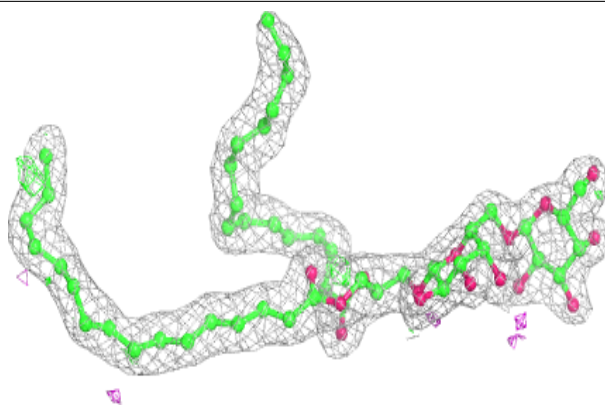
**Electron density around CLA B 601:**

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

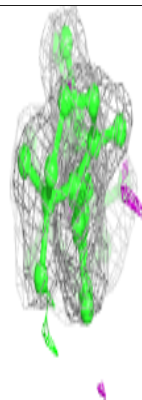
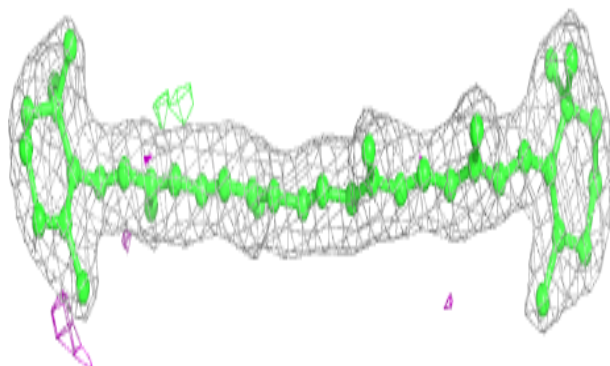
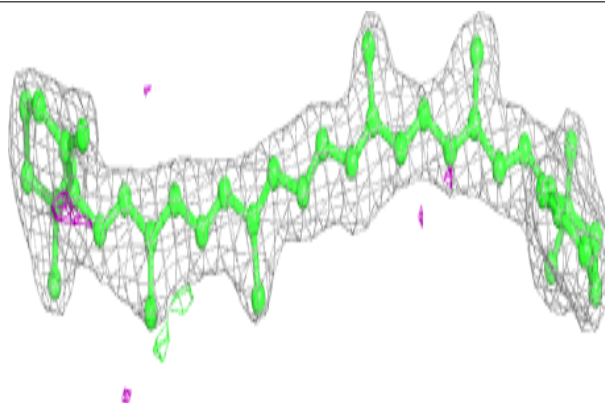


**Electron density around DGD H 102:**

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

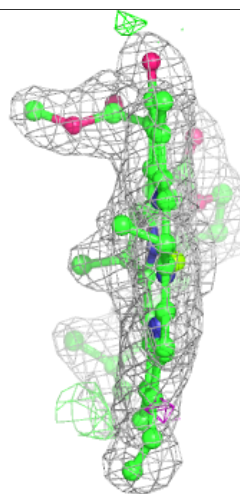
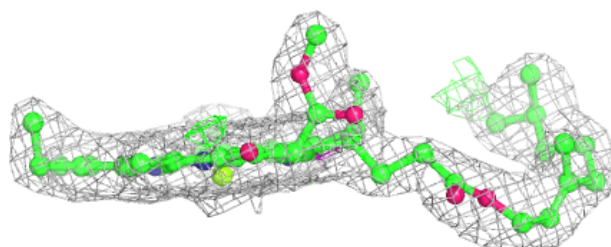
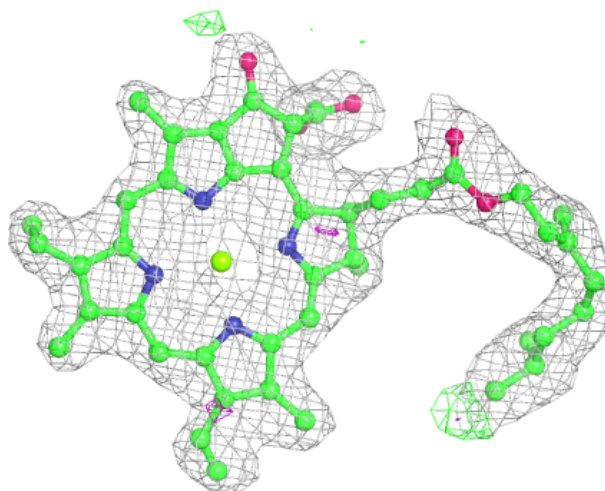
**Electron density around BCR k 102:**

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



**Electron density around CLA C 512:**

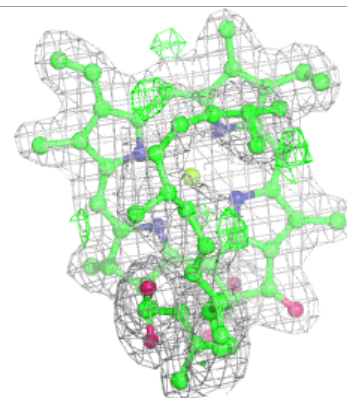
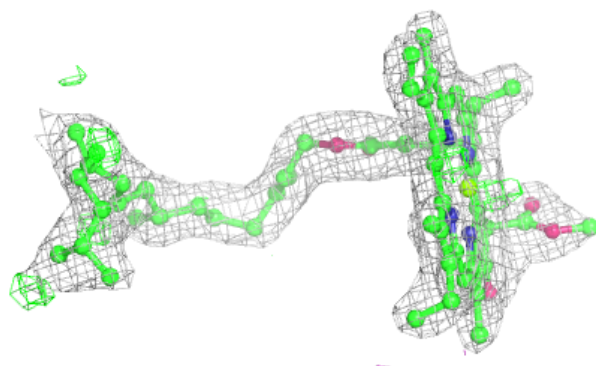
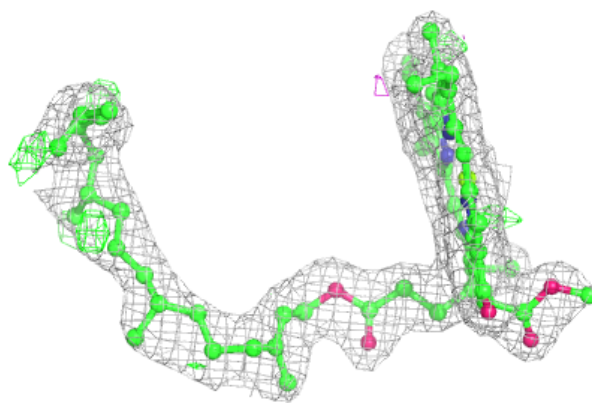
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



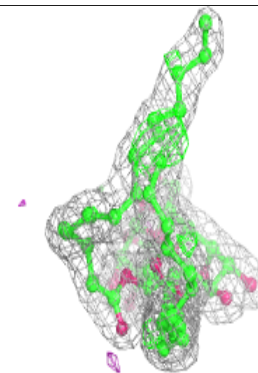
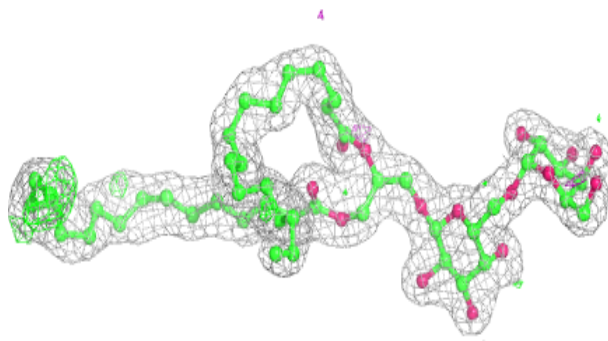
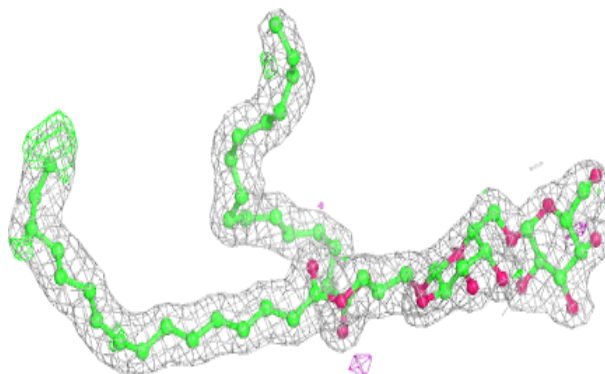


**Electron density around CLA c 506:**

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

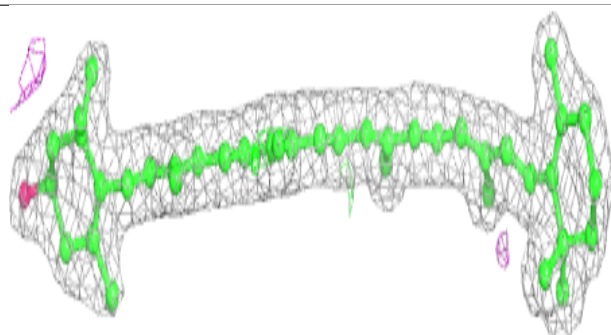
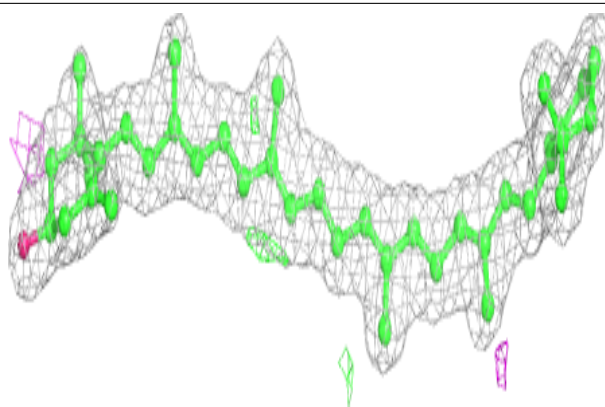
**Electron density around DGD h 101:**

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



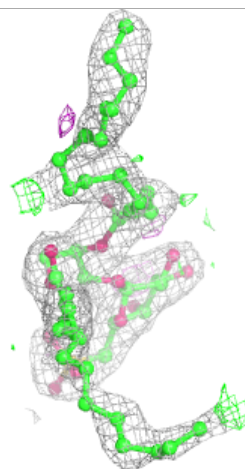
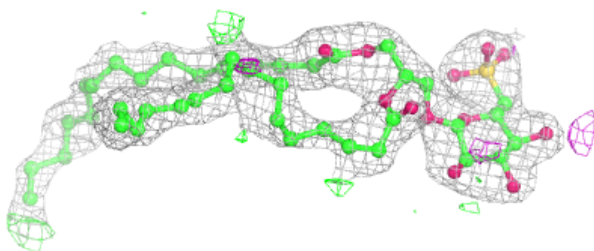
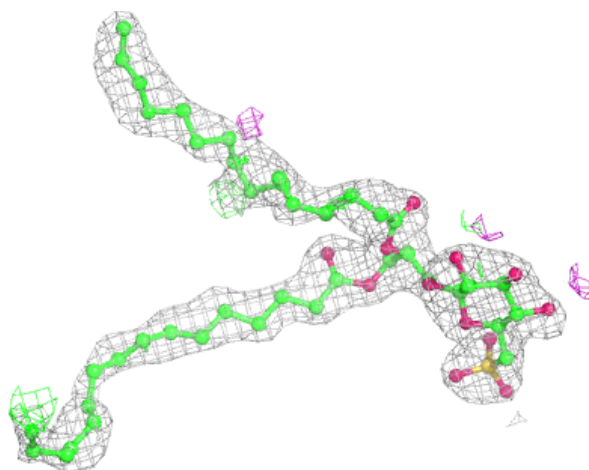
**Electron density around RRX H 101:**

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



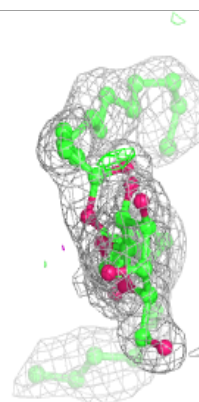
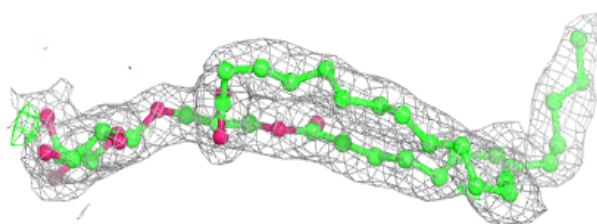
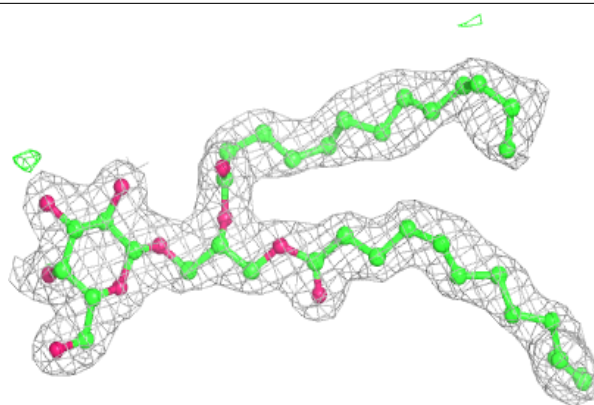
**Electron density around SQD A 406:**

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

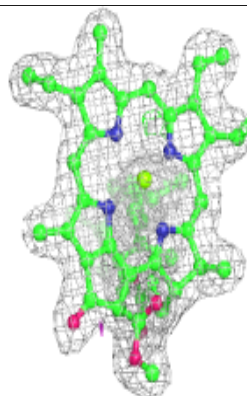
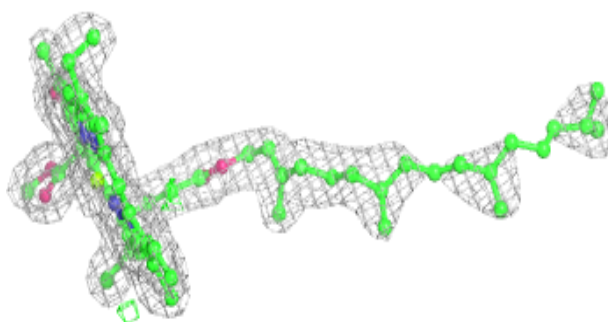
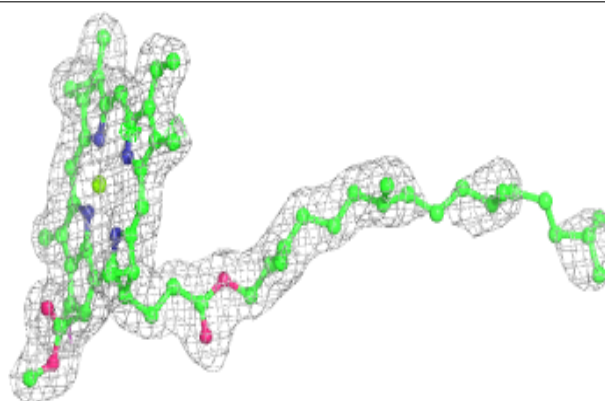


**Electron density around LMG j 101:**

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

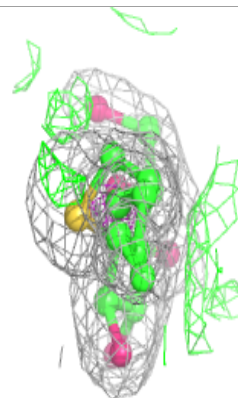
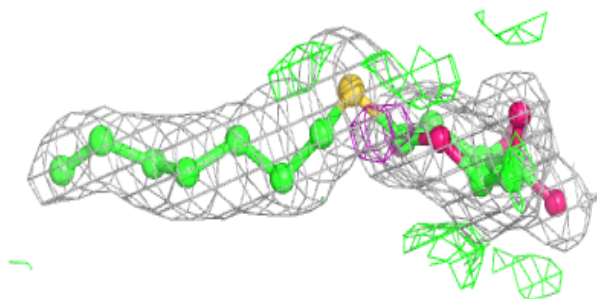
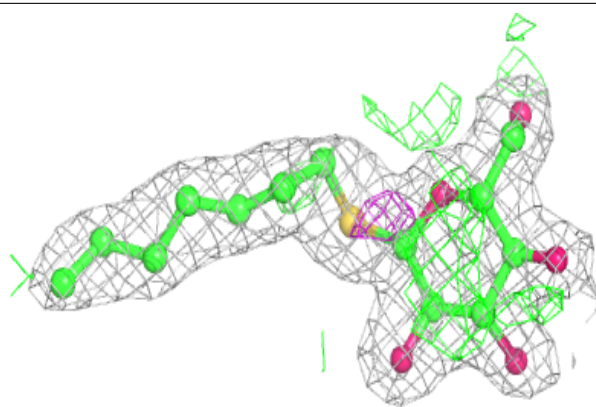
**Electron density around CLA d 404:**

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



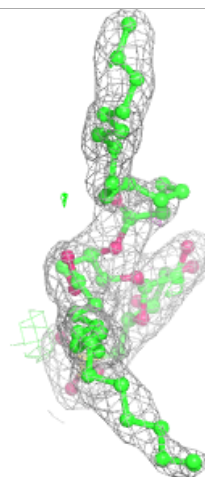
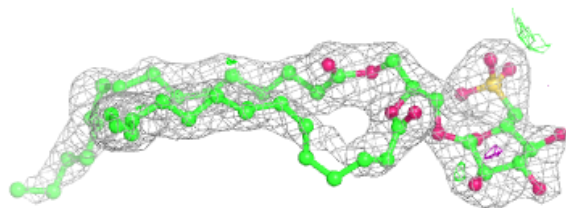
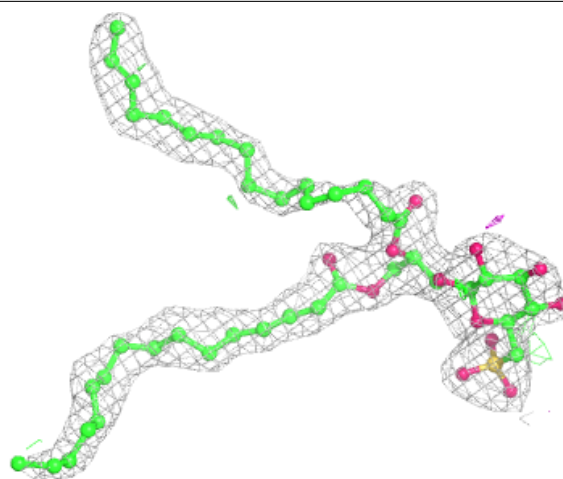
**Electron density around HTG O 302:**

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



**Electron density around SQD a 409:**

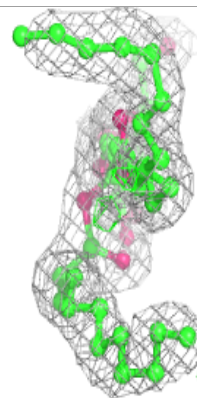
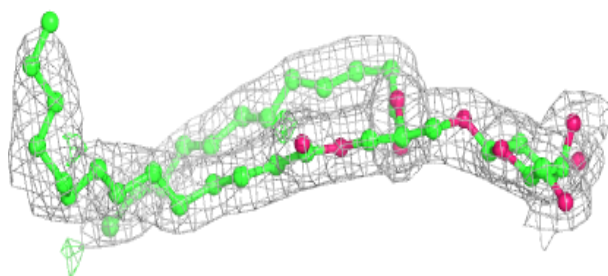
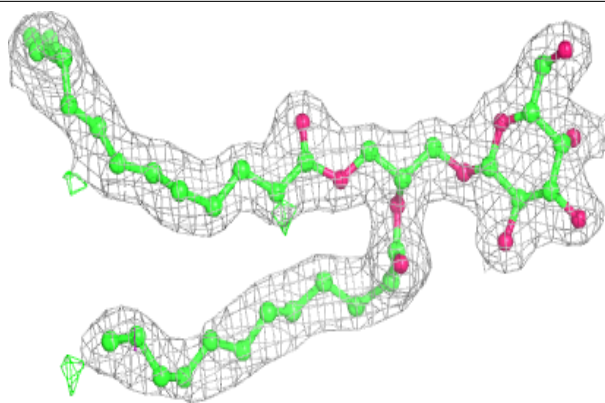
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



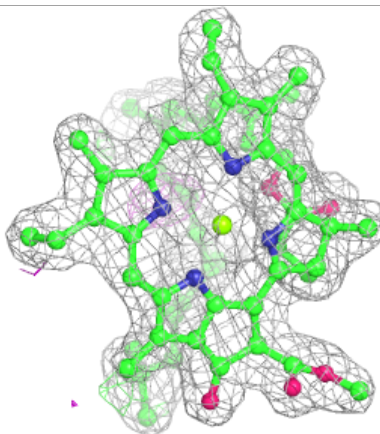
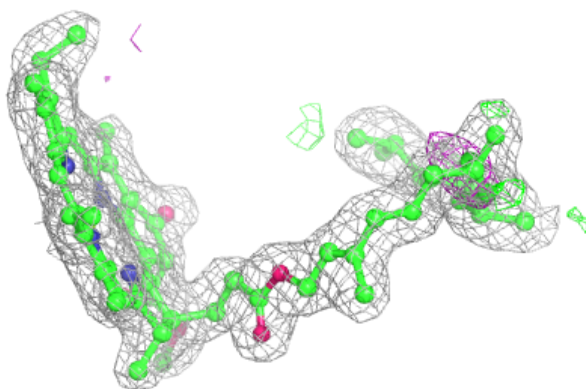
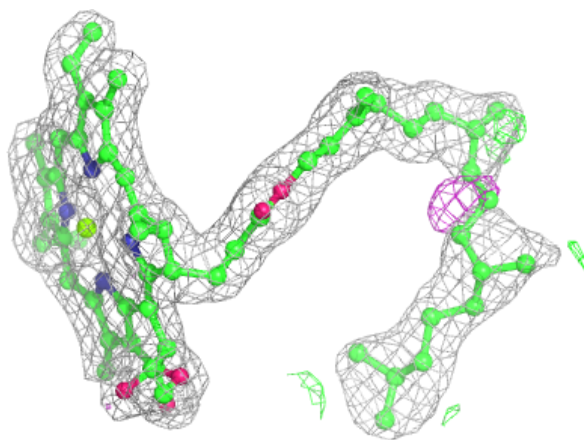


**Electron density around LMG J 101:**

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

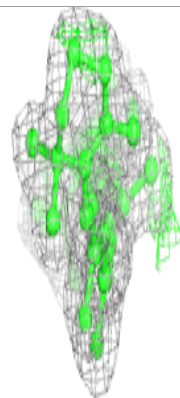
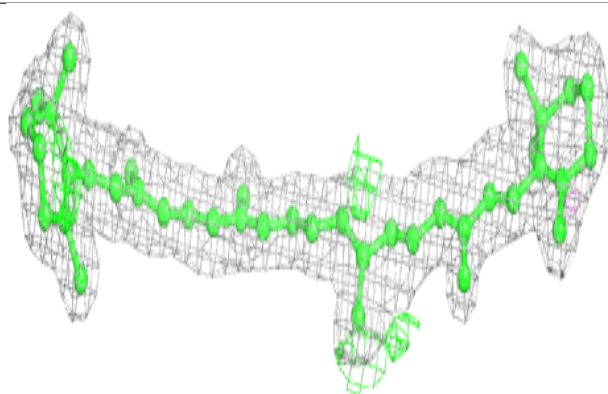
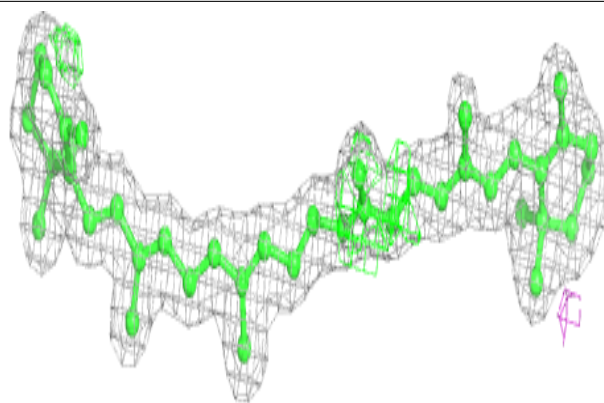
**Electron density around CLA B 607:**

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



**Electron density around BCR t 101:**

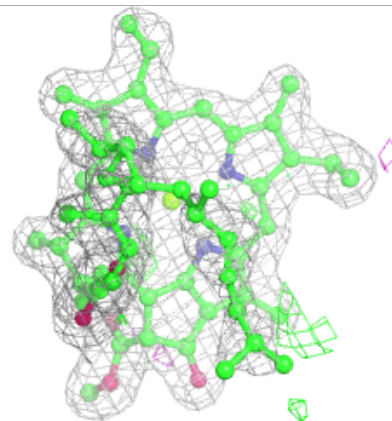
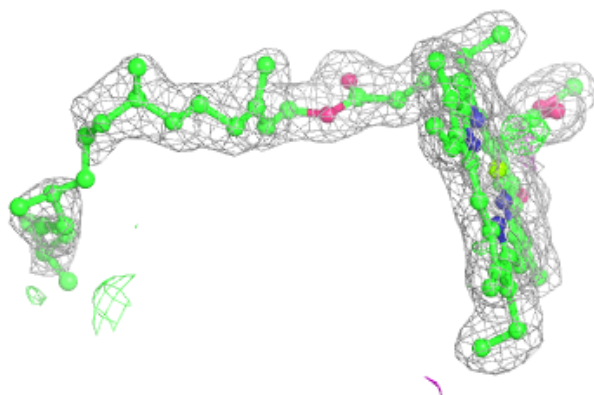
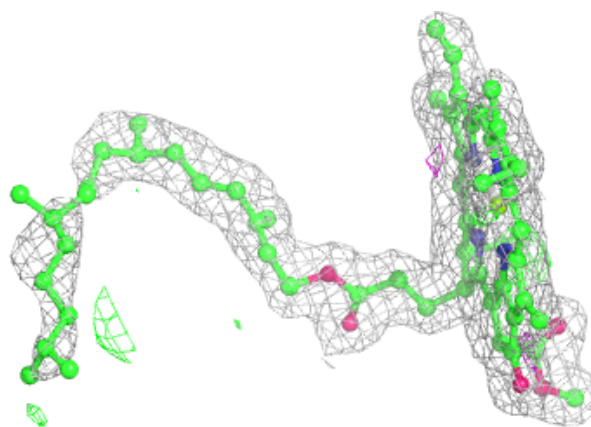
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





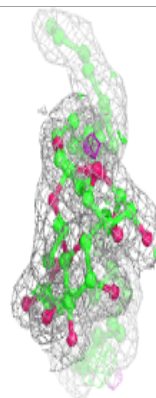
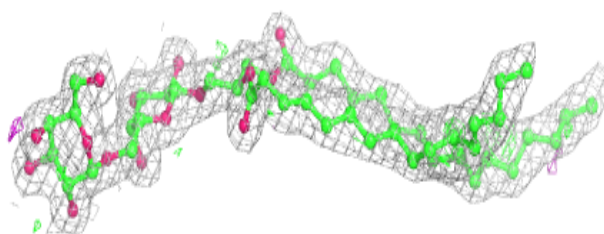
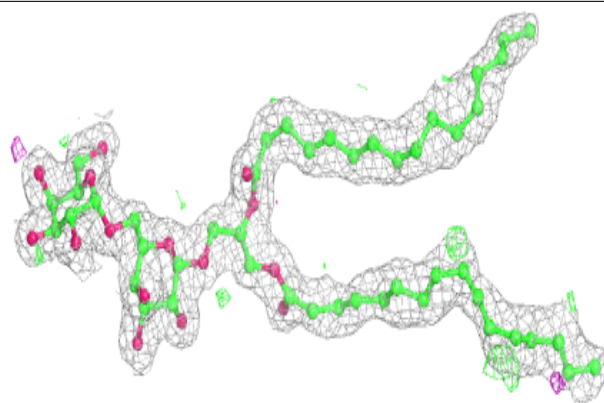
**Electron density around CLA D 404:**

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

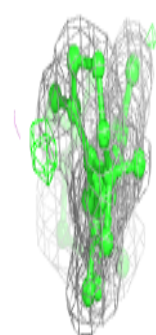
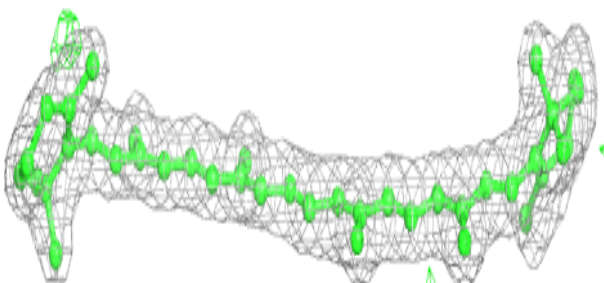
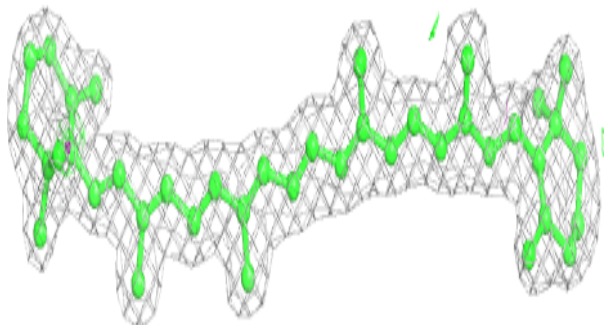


**Electron density around DGD c 517:**

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

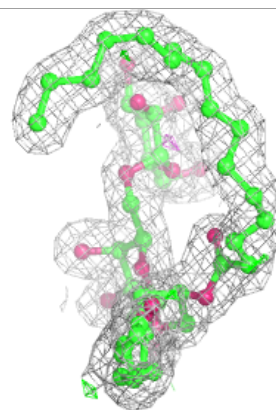
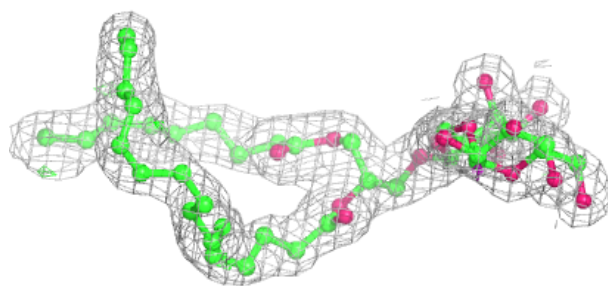
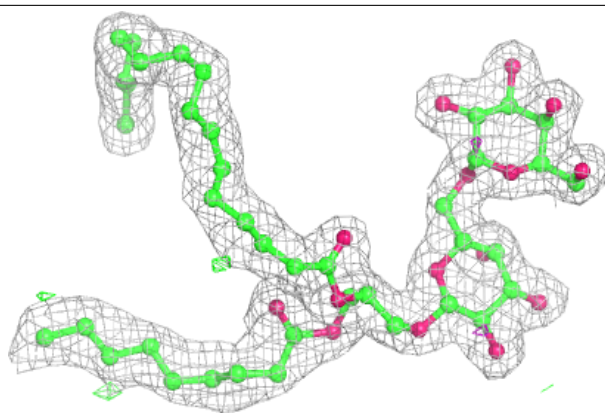
**Electron density around BCR B 619:**

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

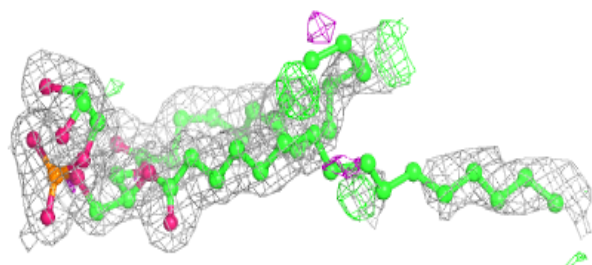
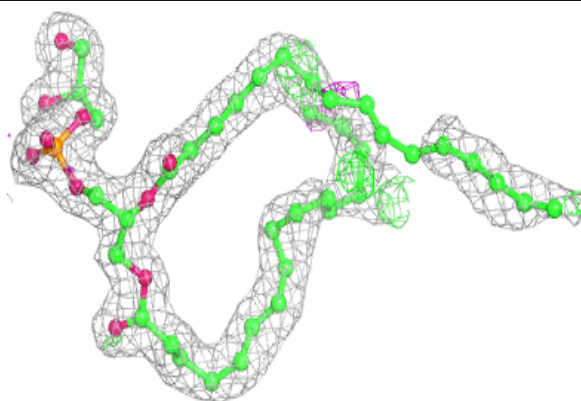


**Electron density around DGD C 517:**

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

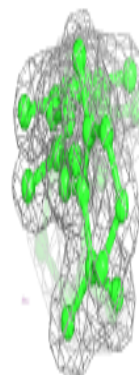
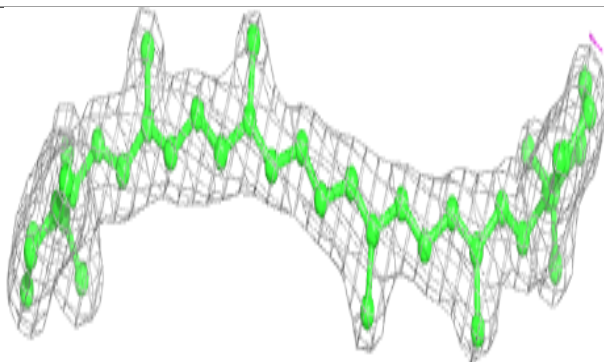
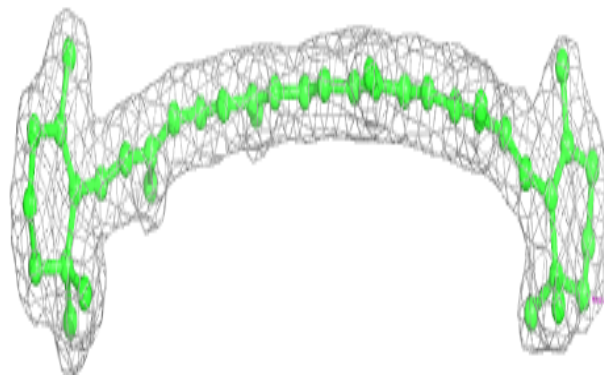
**Electron density around LHG D 409:**

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



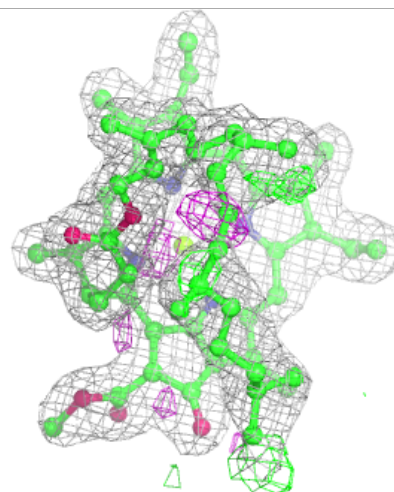
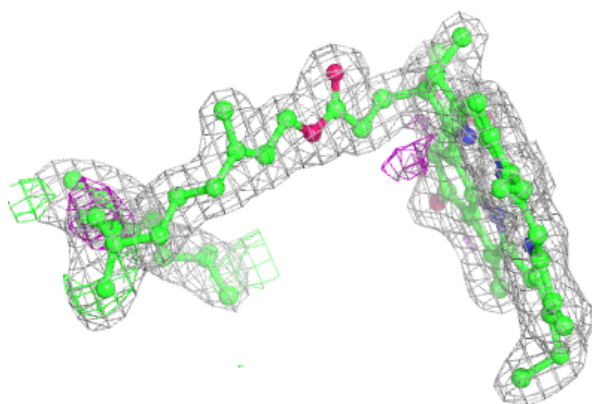
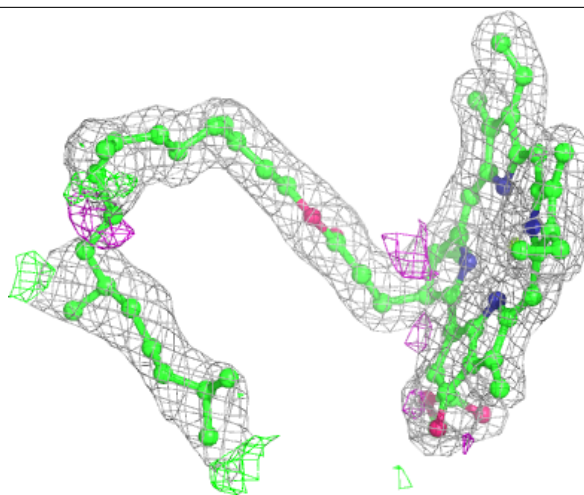
**Electron density around BCR k 101:**

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



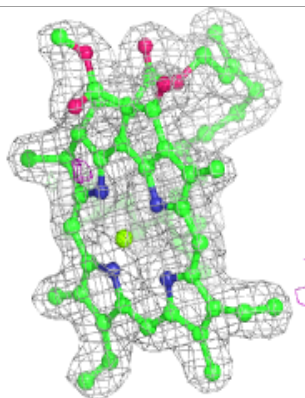
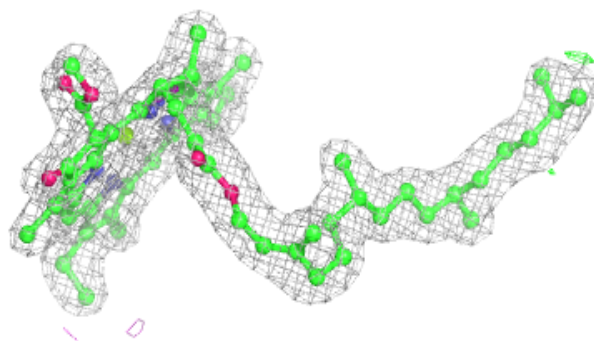
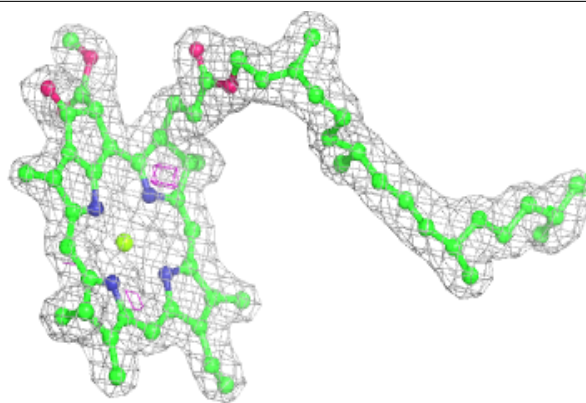
**Electron density around CLA b 608:**

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



**Electron density around CLA c 511:**

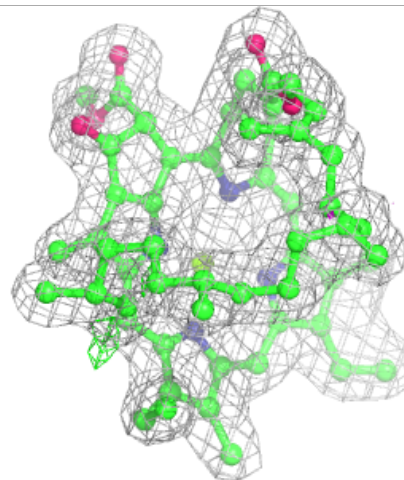
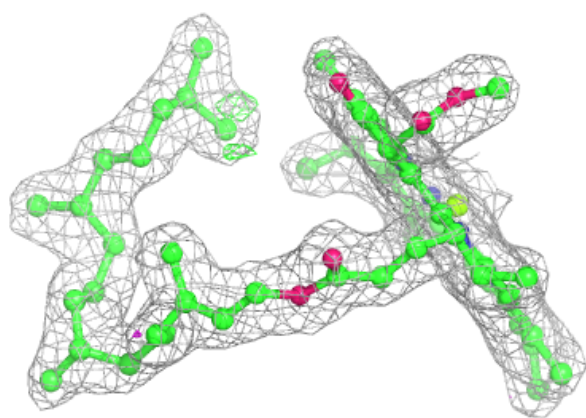
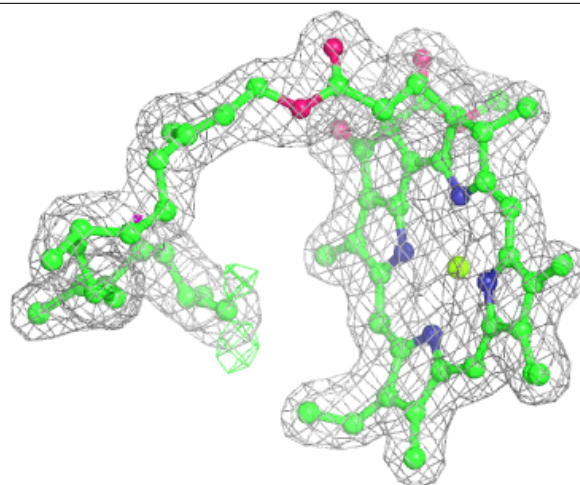
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





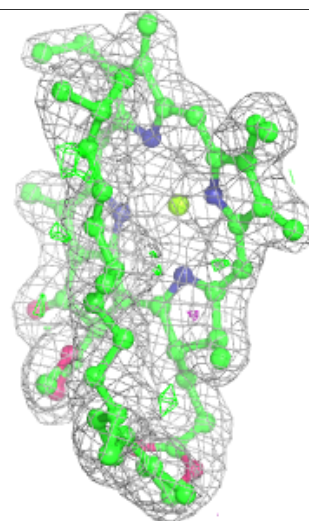
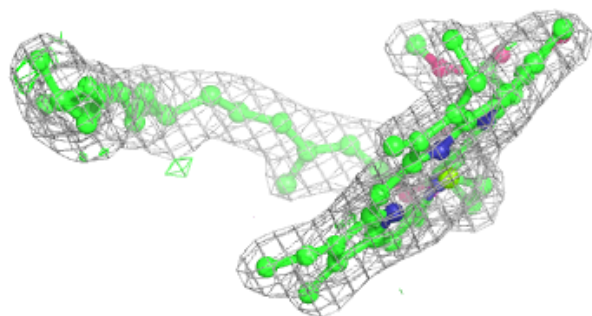
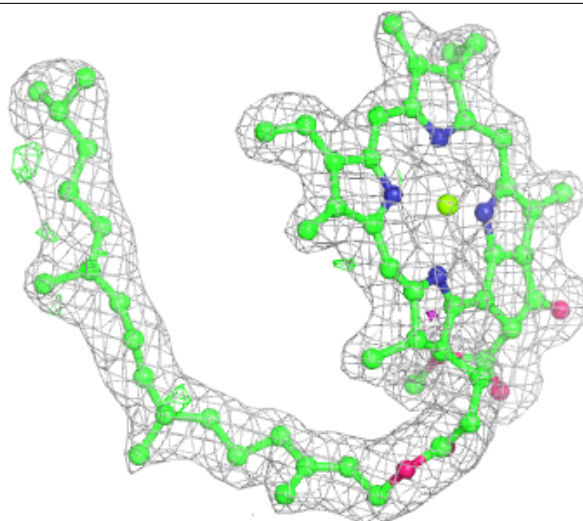
**Electron density around CLA C 503:**

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



**Electron density around CLA C 507:**

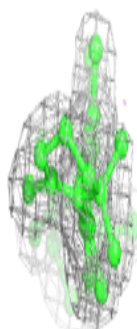
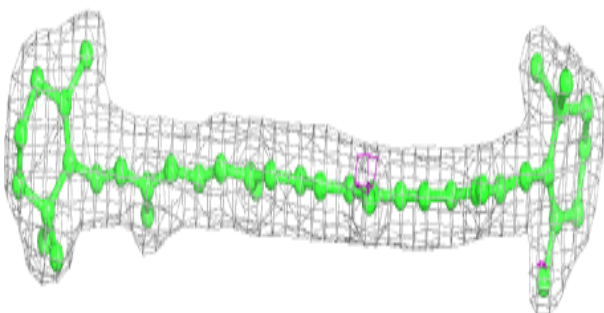
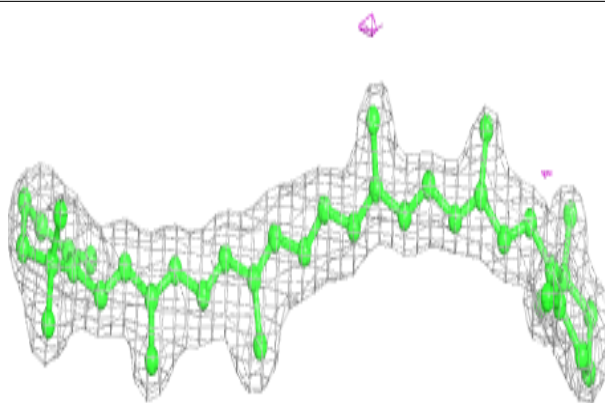
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



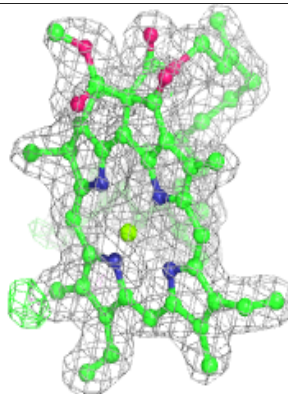
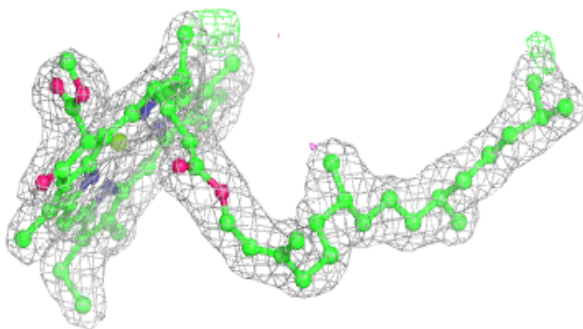
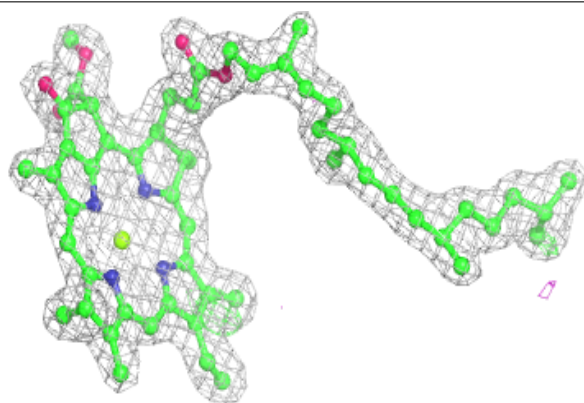


**Electron density around BCR C 515:**

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

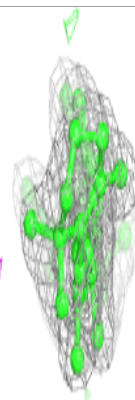
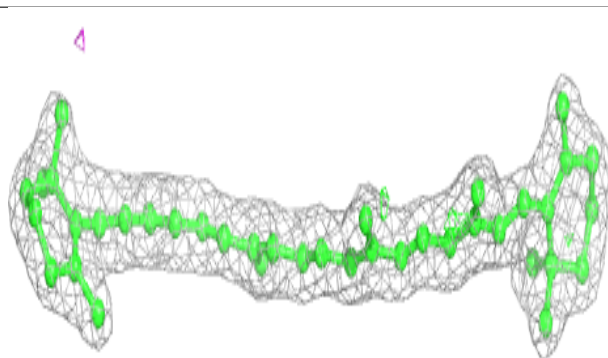
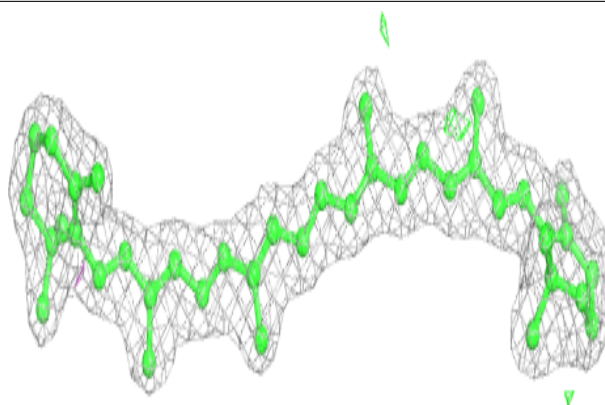
**Electron density around CLA C 511:**

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

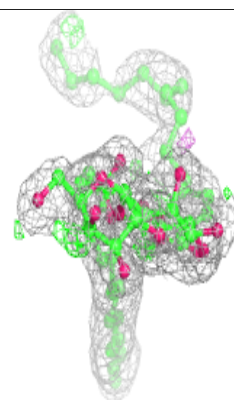
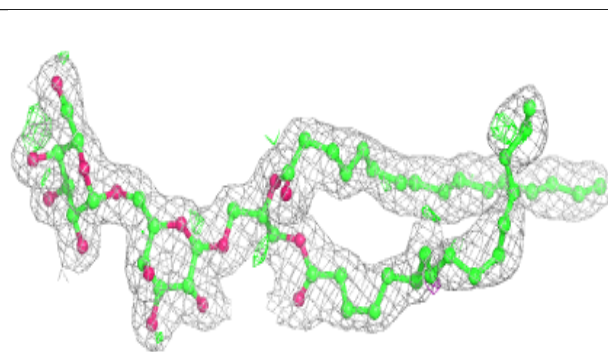
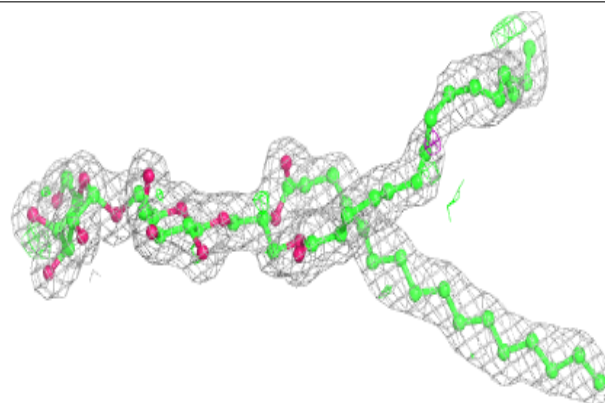


**Electron density around BCR j 102:**

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

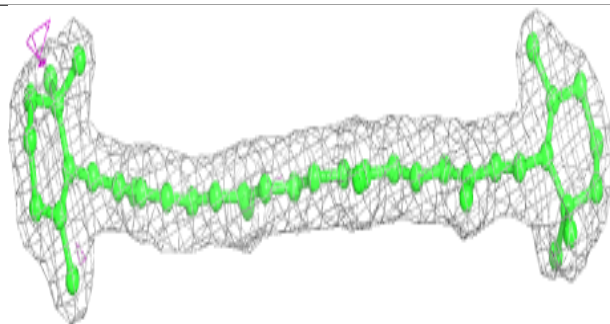
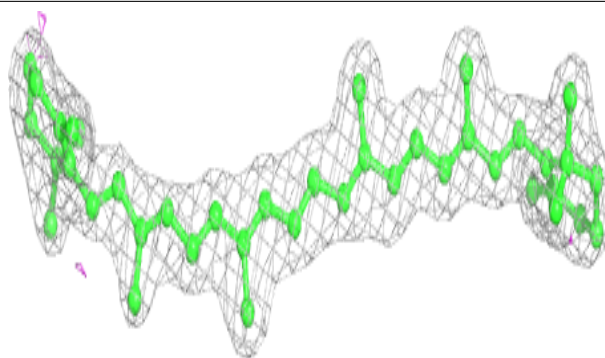
**Electron density around DGD c 515:**

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

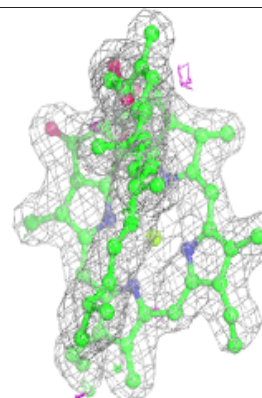
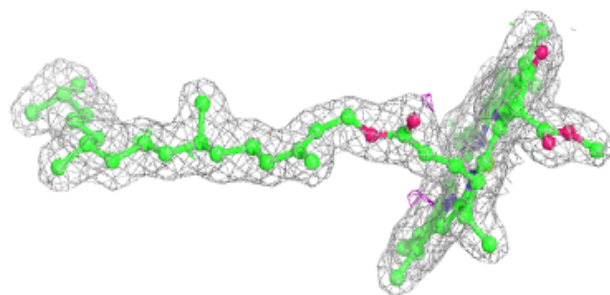
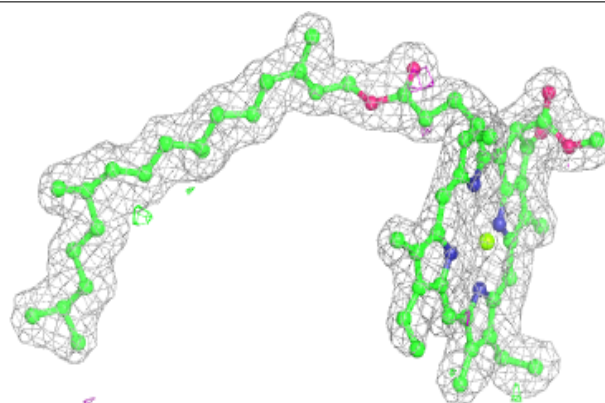


**Electron density around BCR c 514:**

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

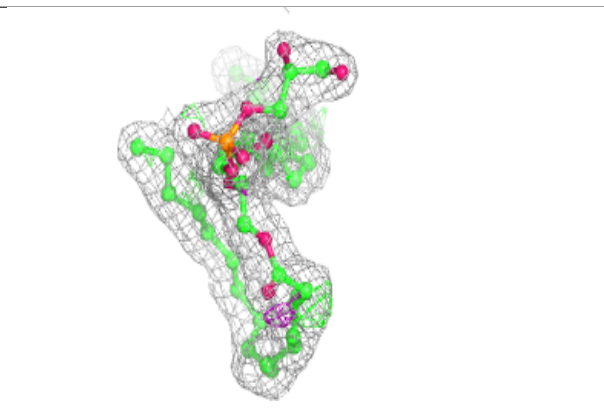
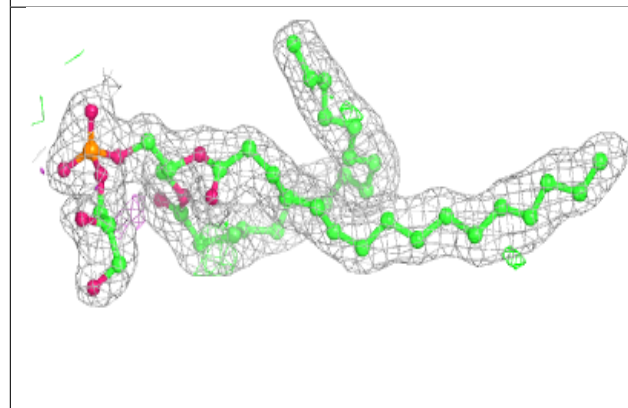
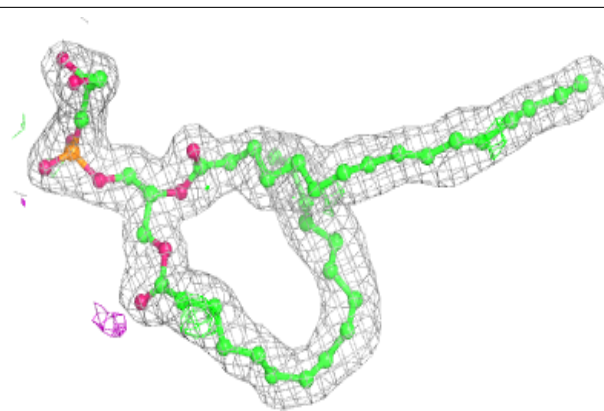
**Electron density around CLA b 611:**

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

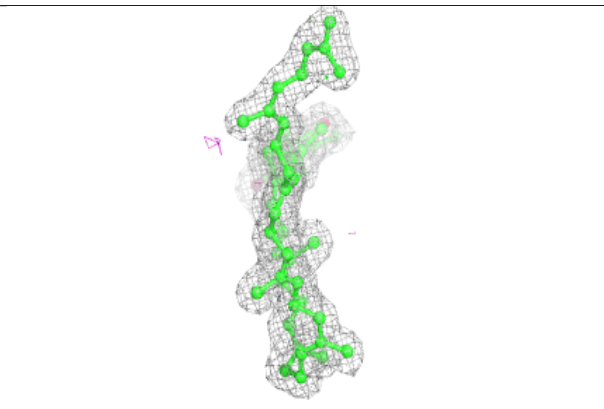
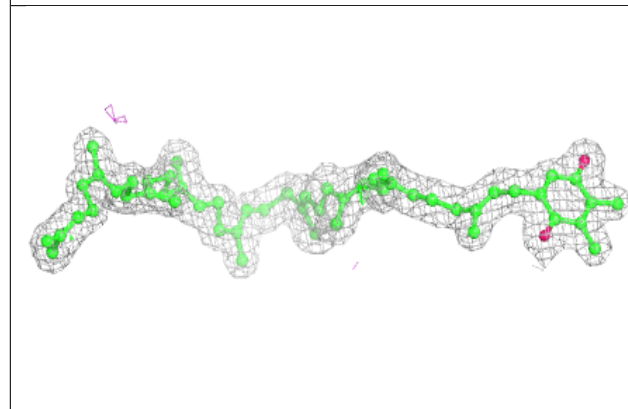
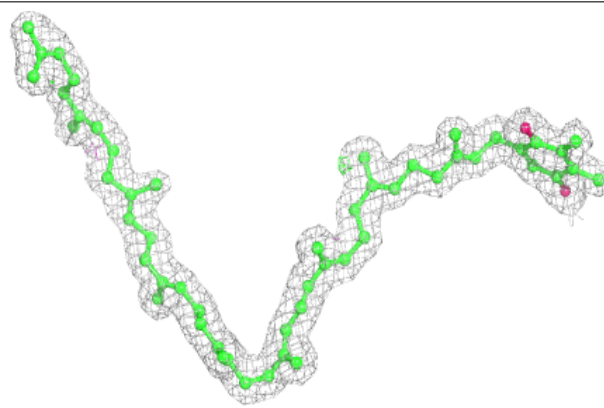


**Electron density around LHG D 407:**

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

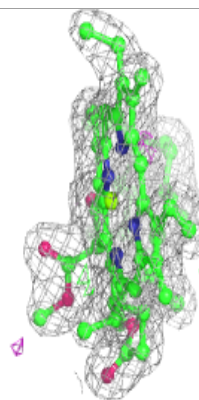
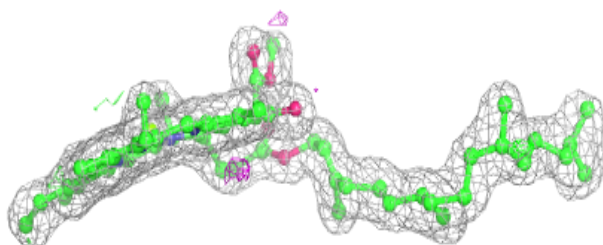
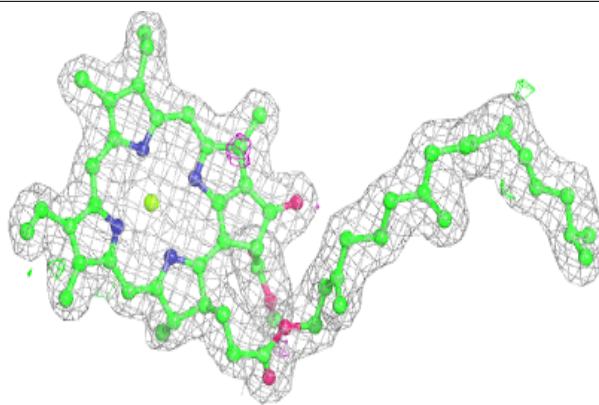
**Electron density around PL9 d 412:**

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



**Electron density around CLA b 604:**

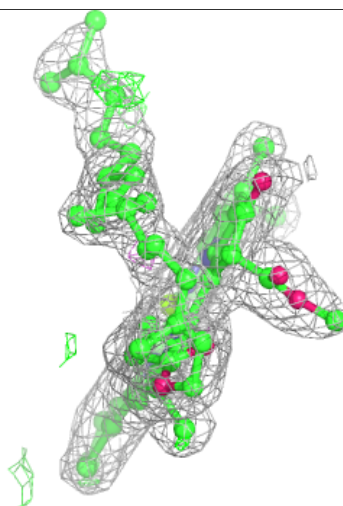
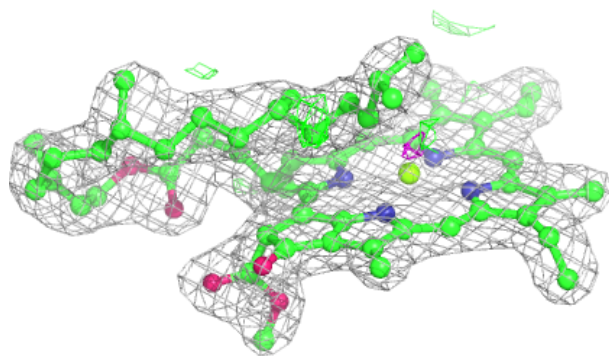
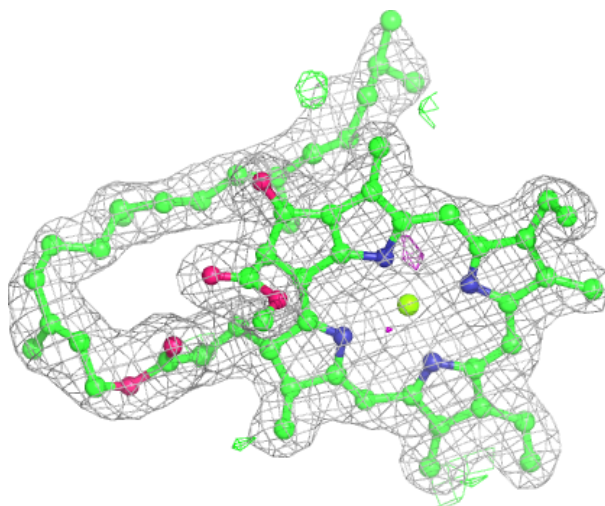
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





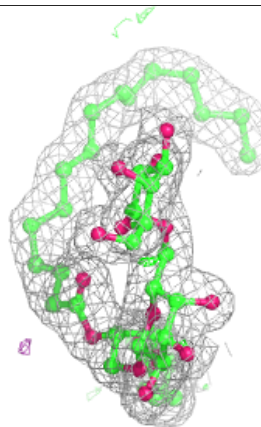
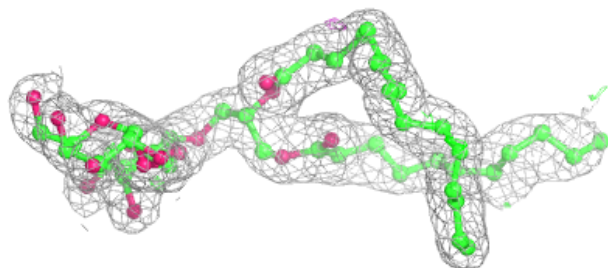
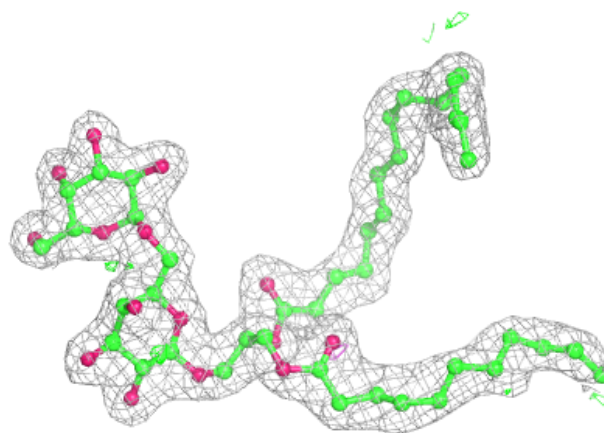
**Electron density around CLA C 509:**

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

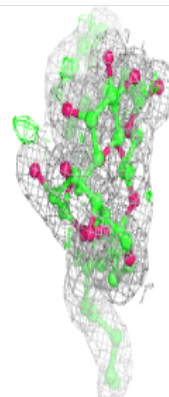
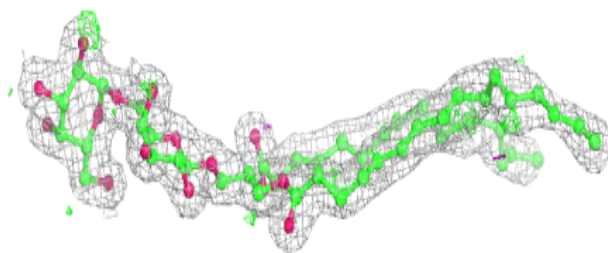
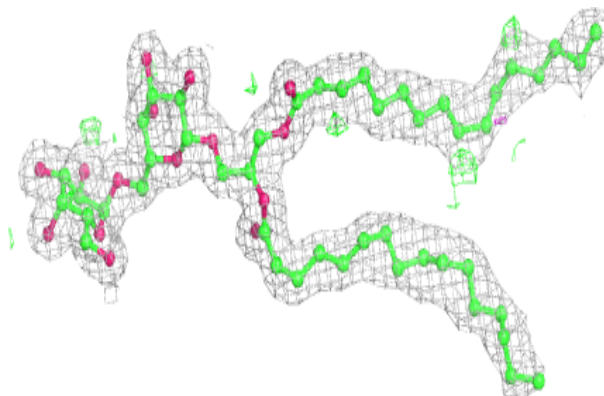


**Electron density around DGD c 516:**

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

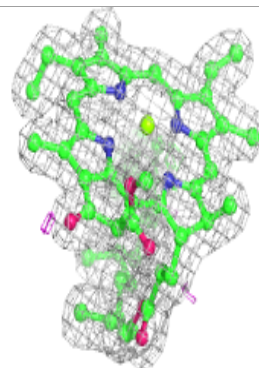
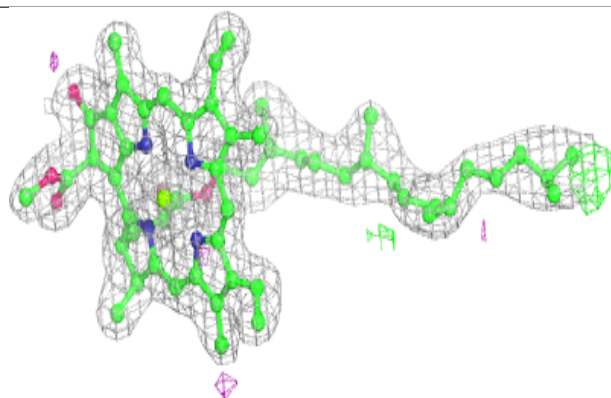
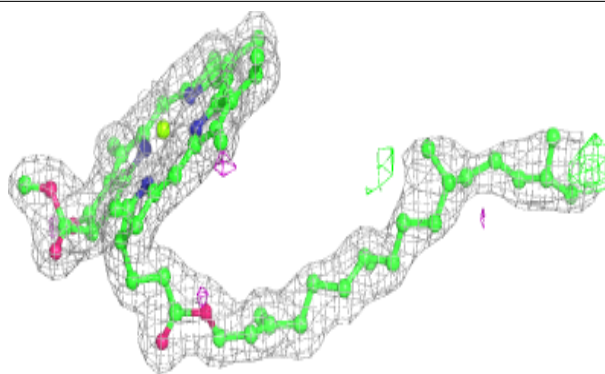
**Electron density around DGD C 518:**

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

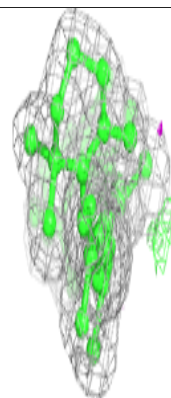
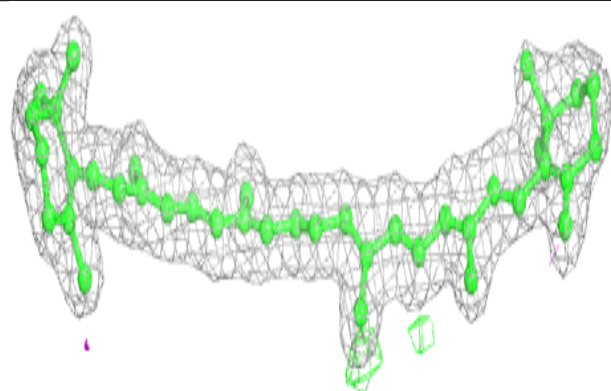
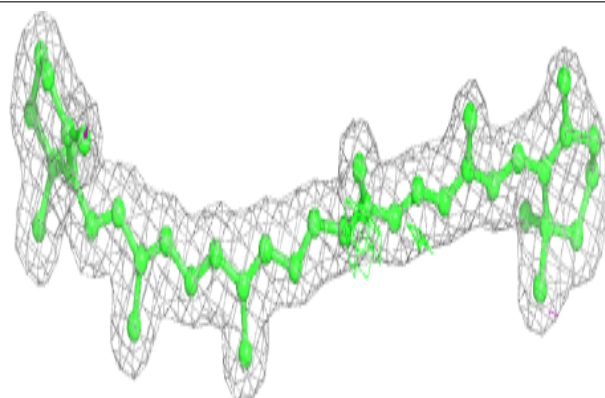


**Electron density around CLA C 504:**

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

**Electron density around BCR T 101:**

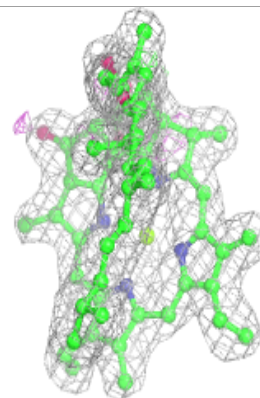
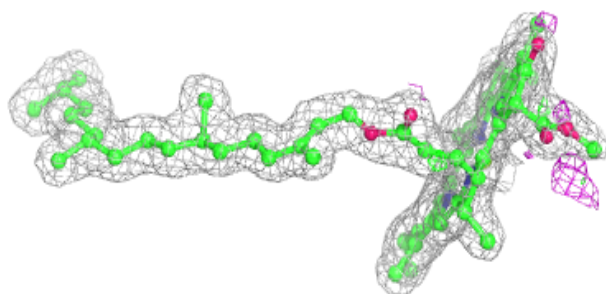
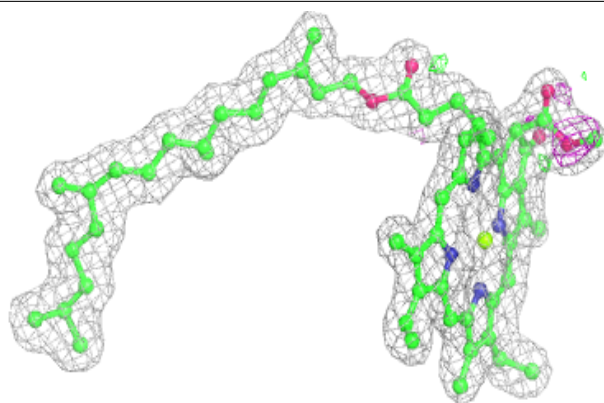
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



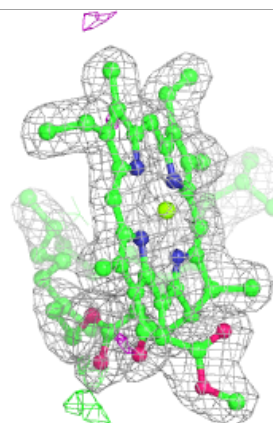
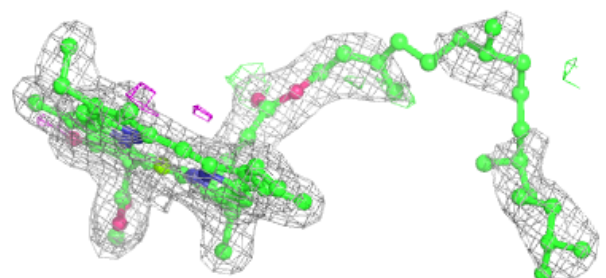
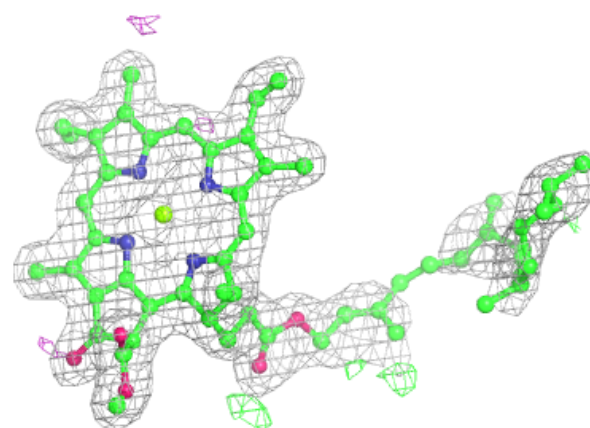


**Electron density around CLA B 610:**

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

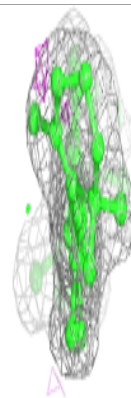
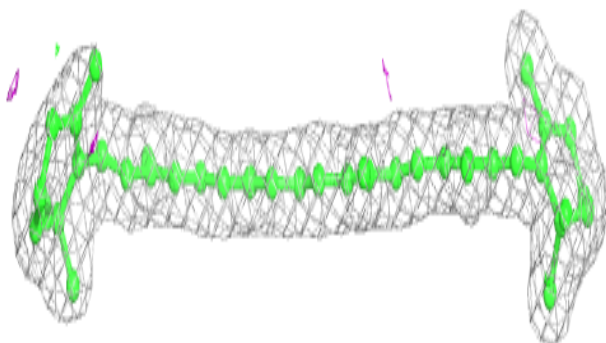
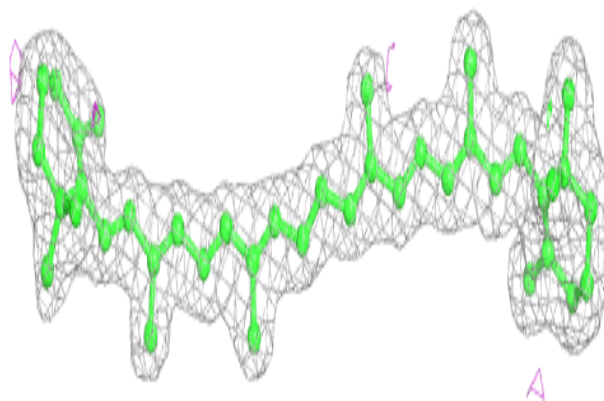
**Electron density around CLA A 404:**

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



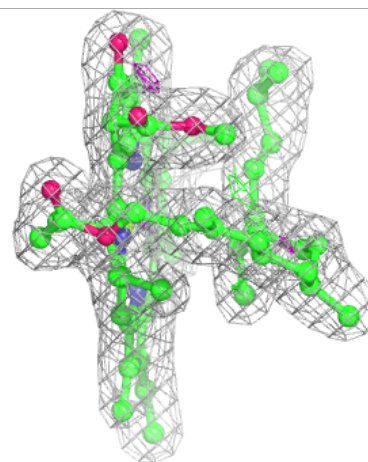
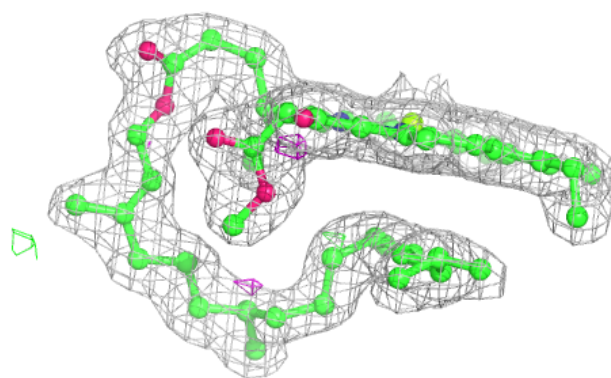
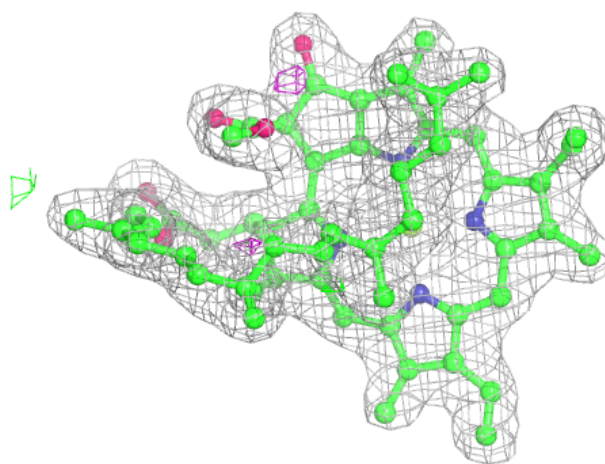
**Electron density around BCR b 620:**

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



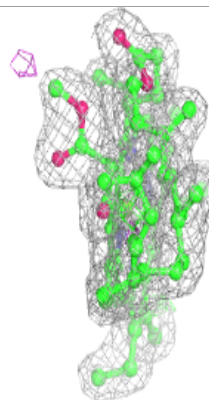
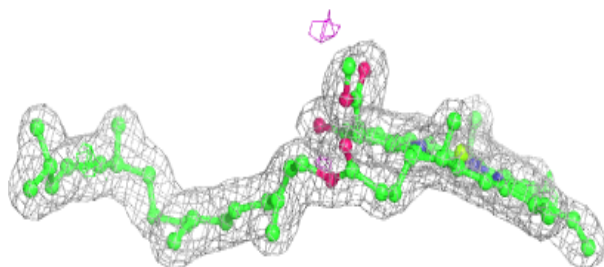
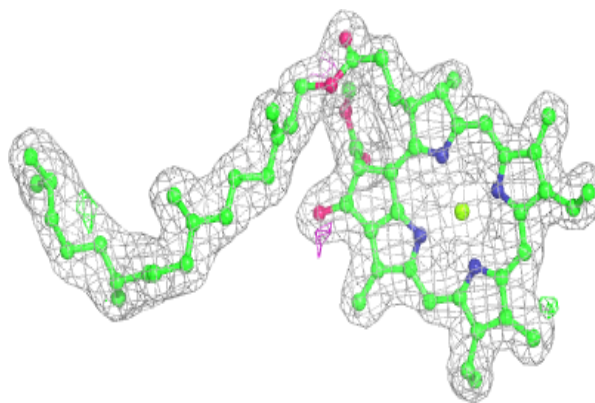
**Electron density around CLA C 510:**

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



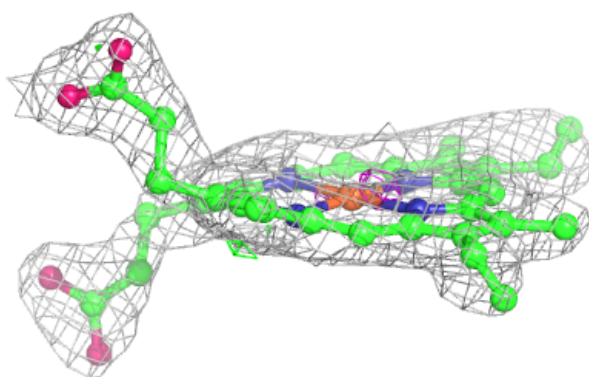
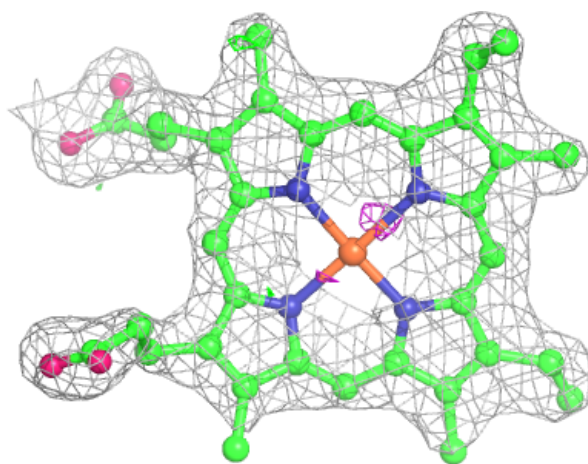
**Electron density around CLA B 603:**

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



**Electron density around HEM E 104:**

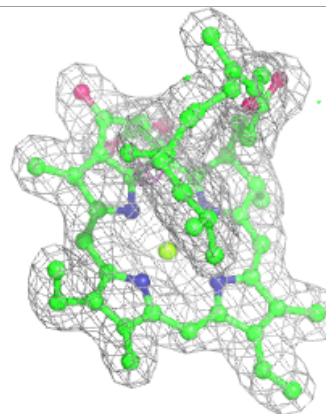
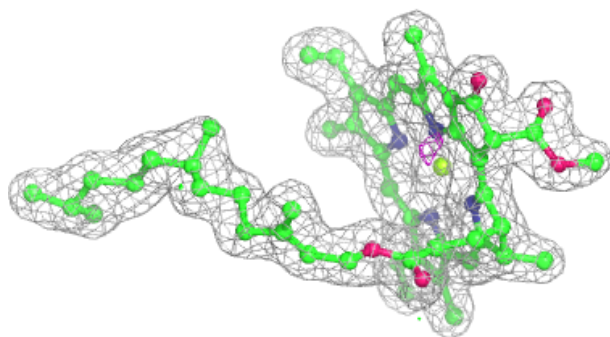
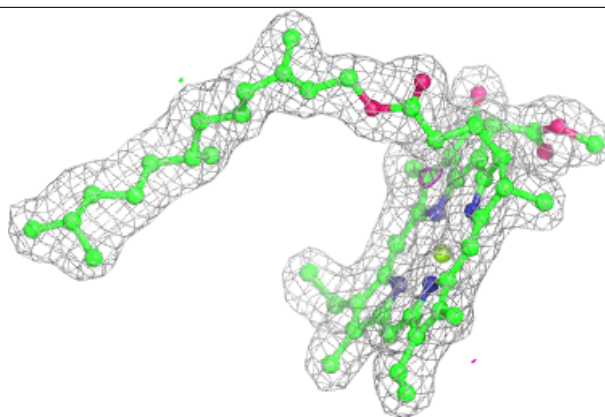
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



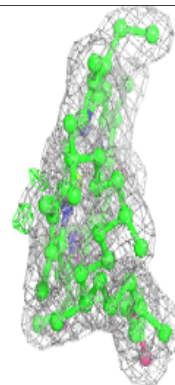
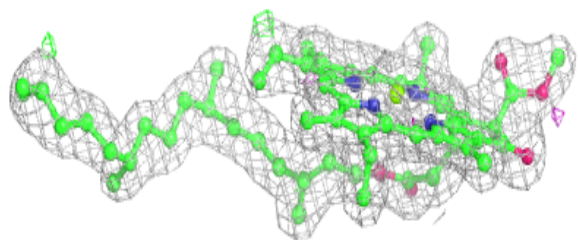
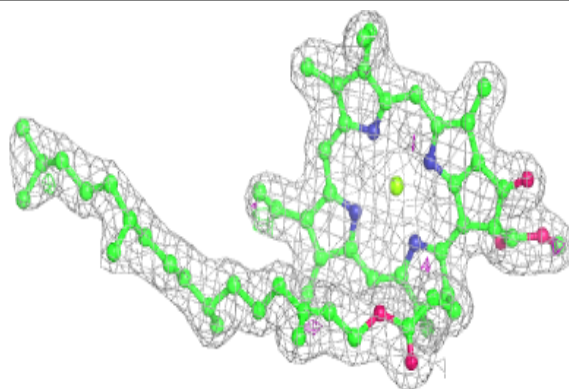


**Electron density around CLA C 508:**

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

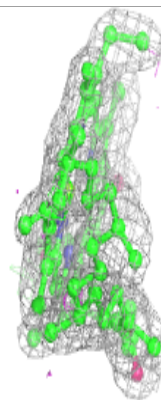
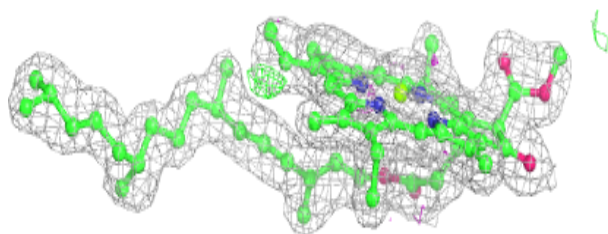
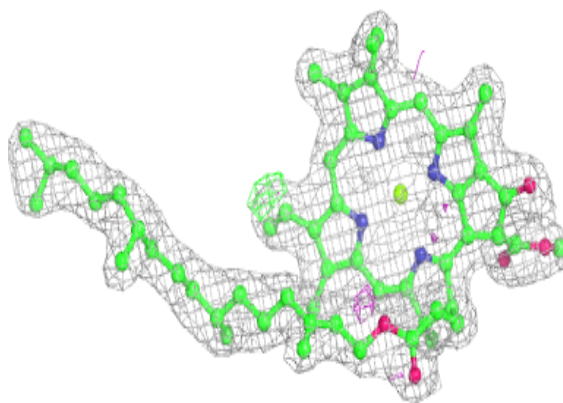
**Electron density around CLA C 501:**

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

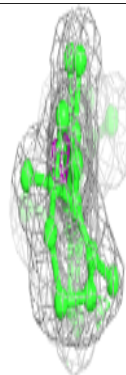
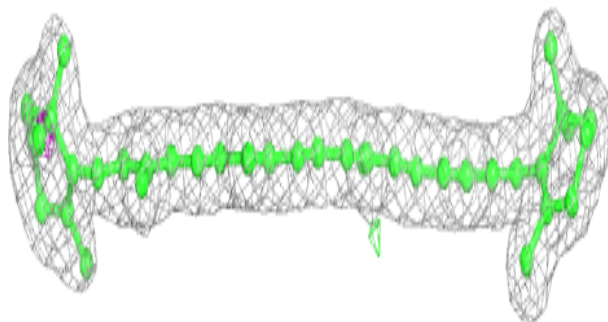
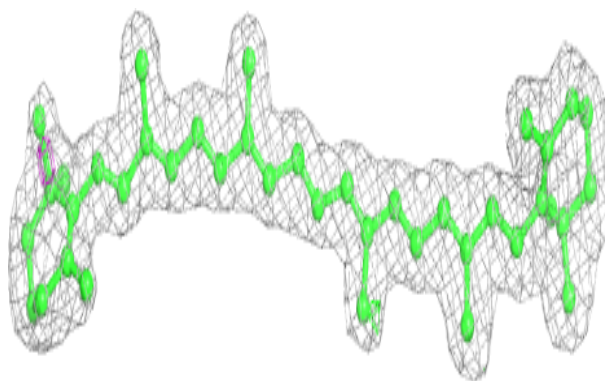


**Electron density around CLA c 501:**

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

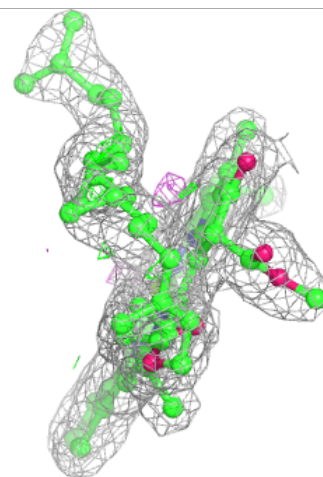
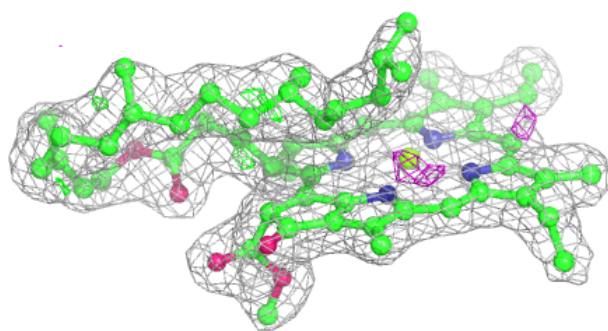
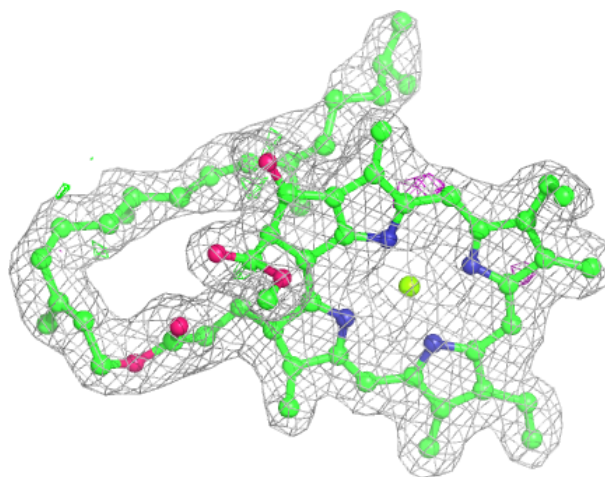
**Electron density around BCR B 618:**

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



**Electron density around CLA c 509:**

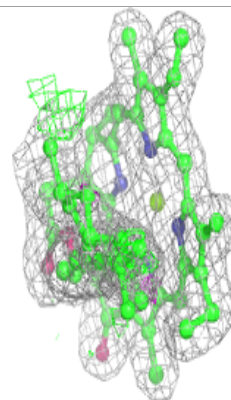
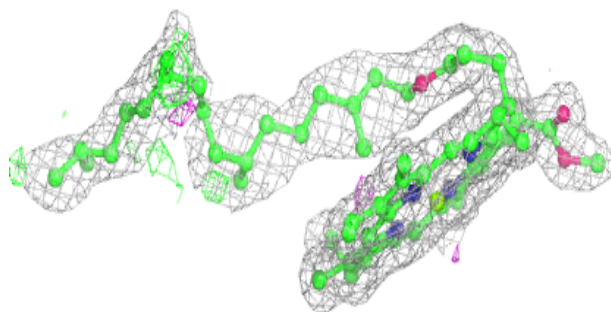
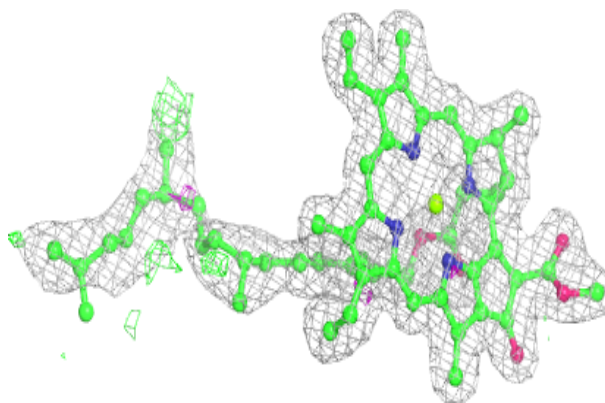
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



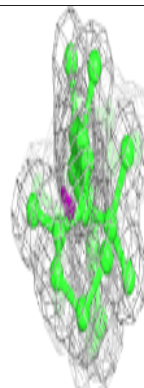
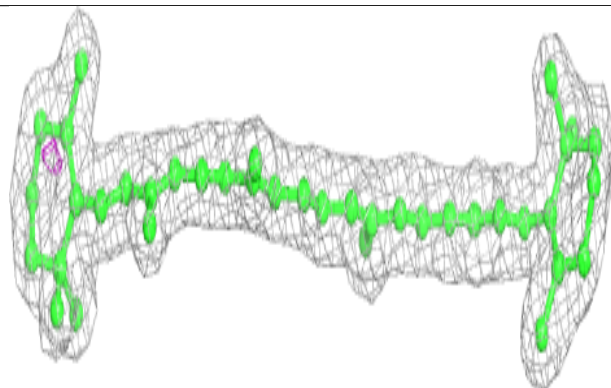
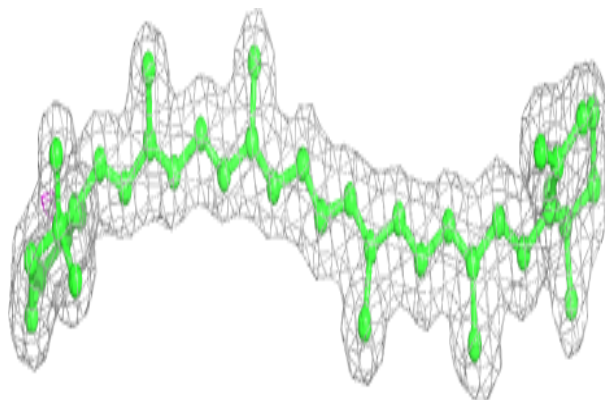


**Electron density around CLA b 616:**

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

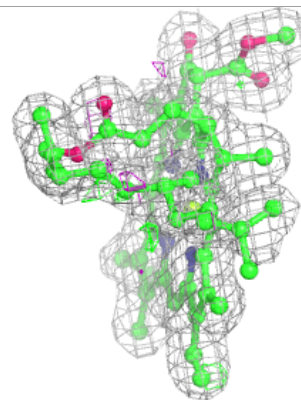
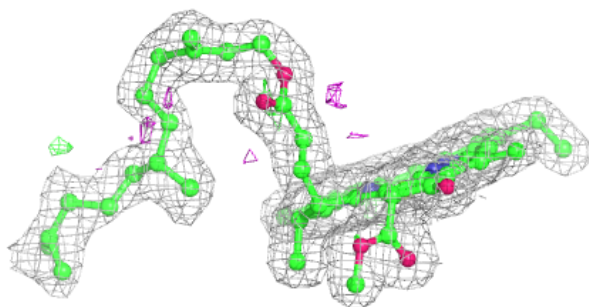
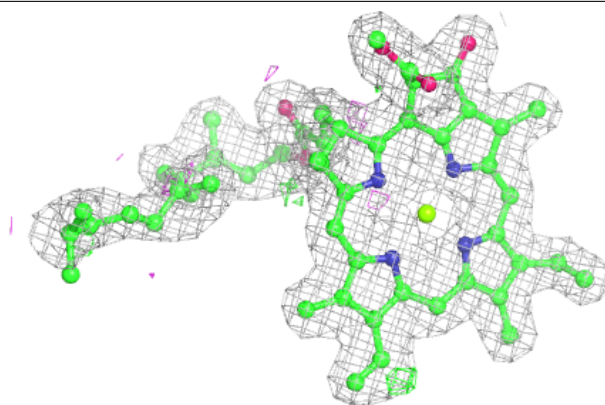
**Electron density around BCR a 408:**

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



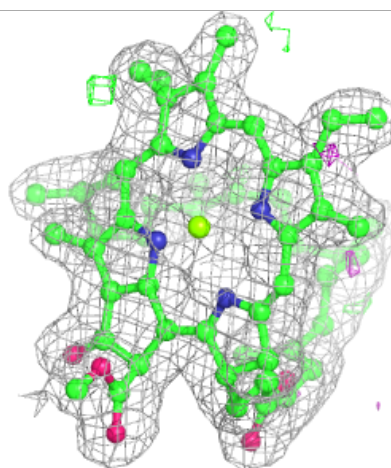
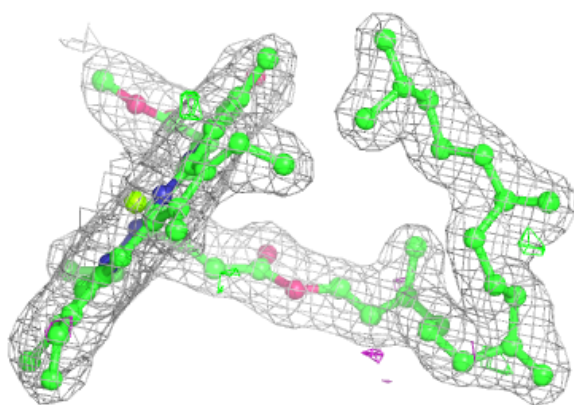
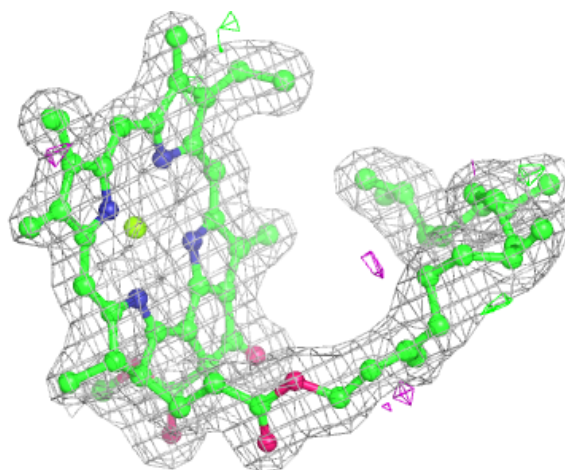
**Electron density around CLA a 404:**

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



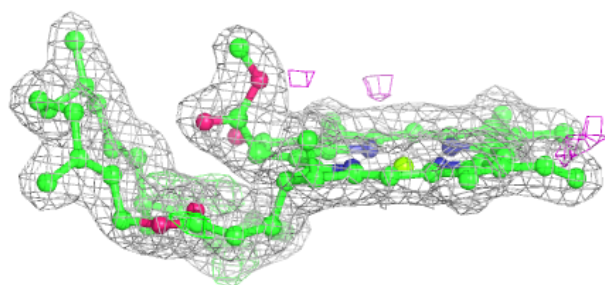
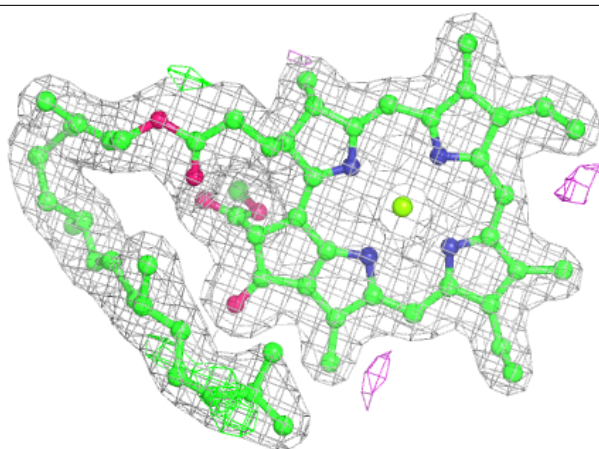
**Electron density around CLA c 503:**

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

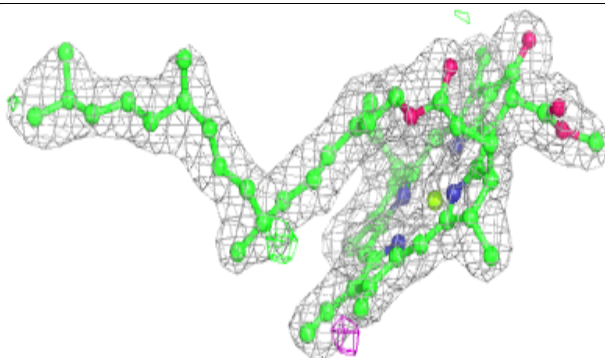
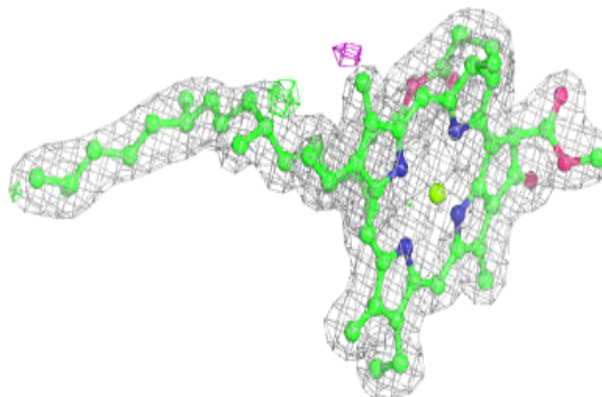


**Electron density around CLA b 612:**

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

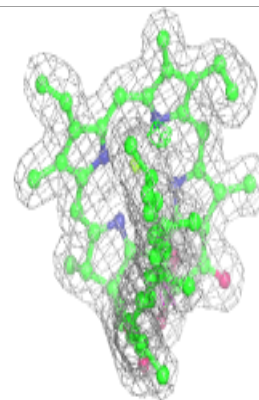
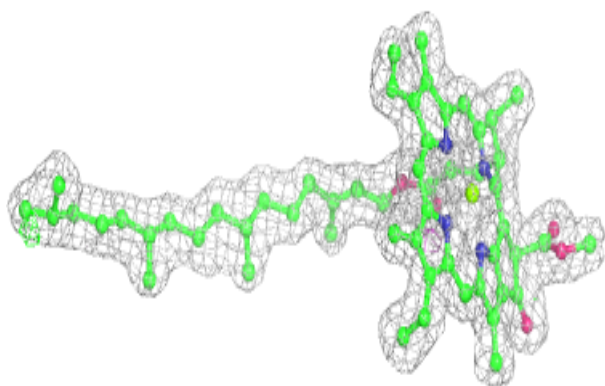
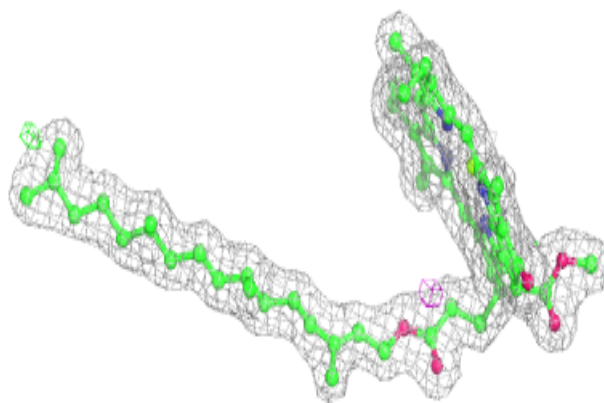
**Electron density around CLA C 505:**

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



**Electron density around CLA b 609:**

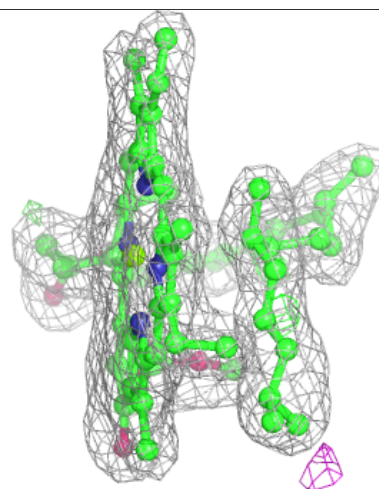
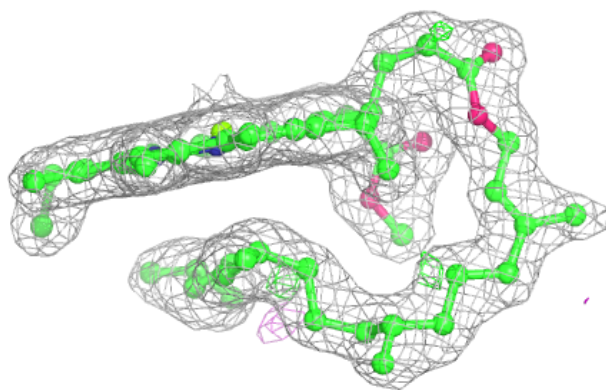
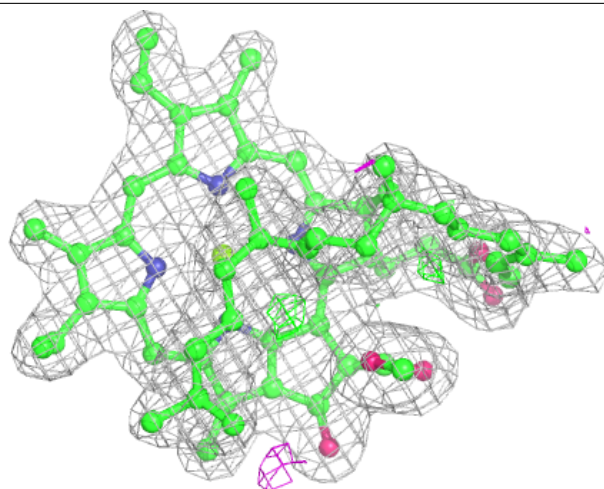
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





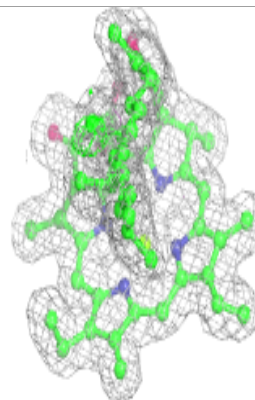
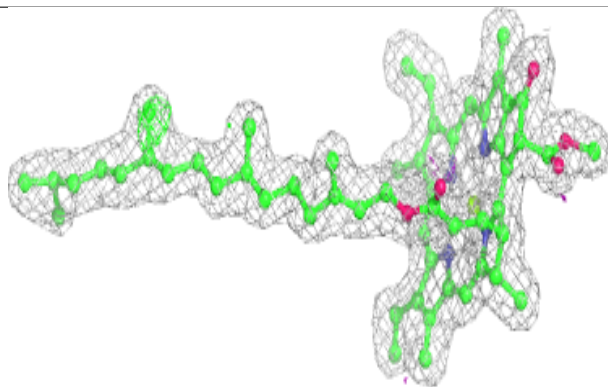
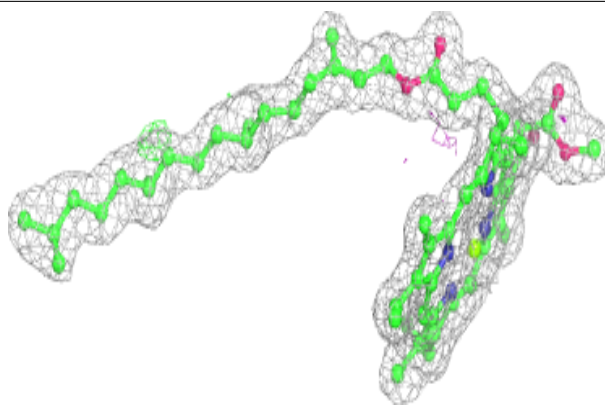
**Electron density around CLA c 510:**

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

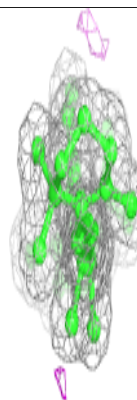
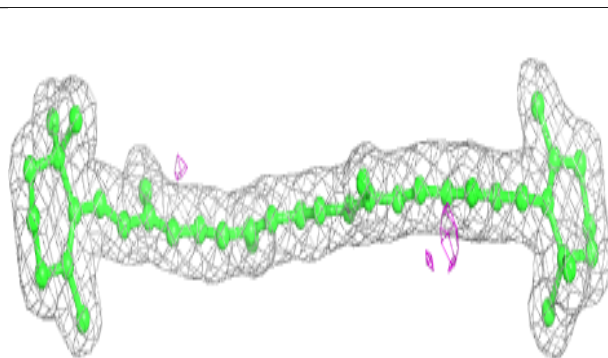
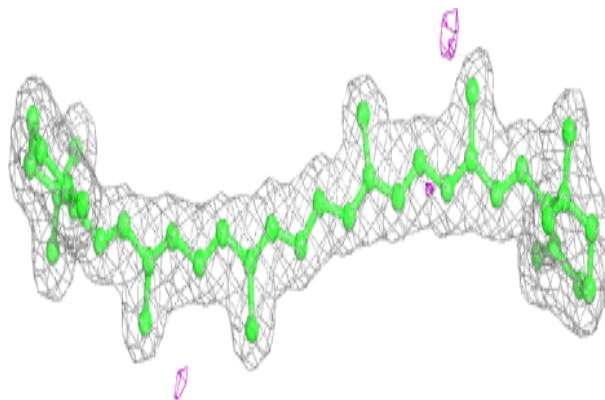


**Electron density around CLA B 608:**

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

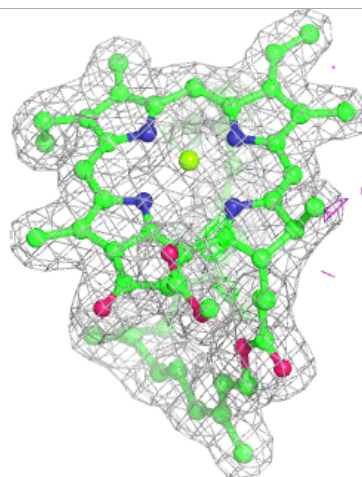
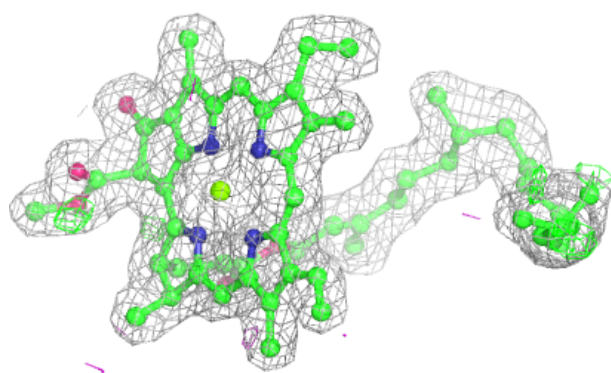
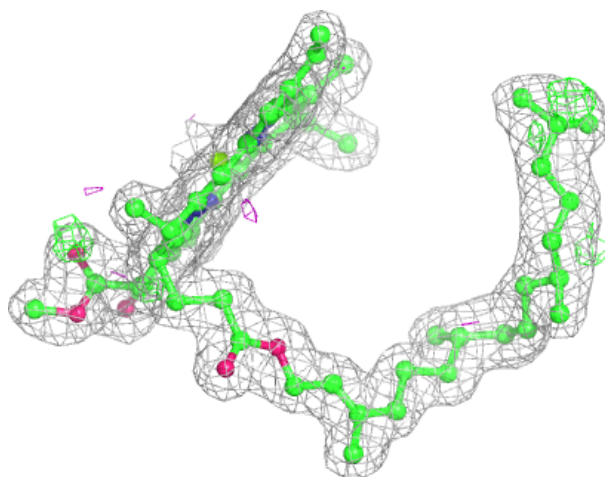
**Electron density around BCR A 405:**

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



**Electron density around CLA b 613:**

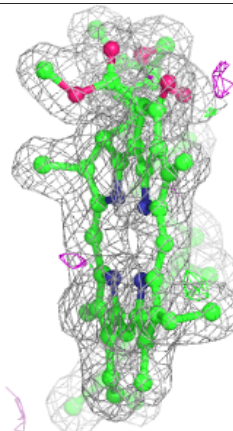
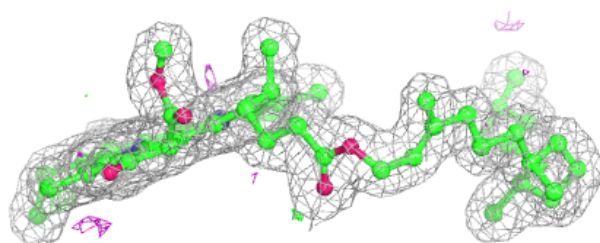
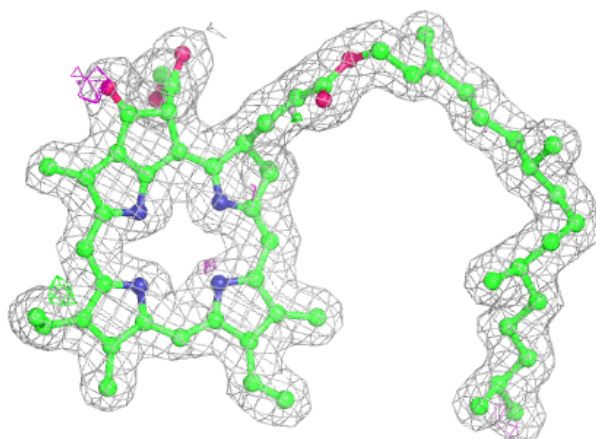
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





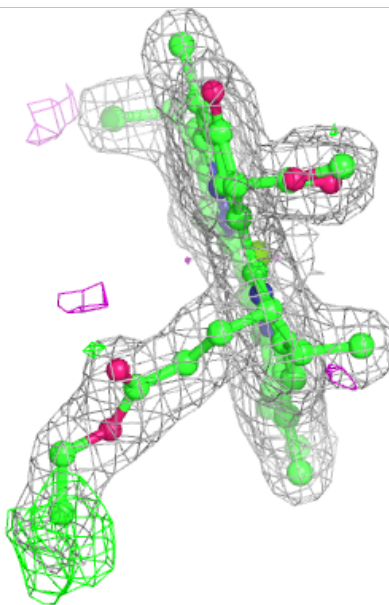
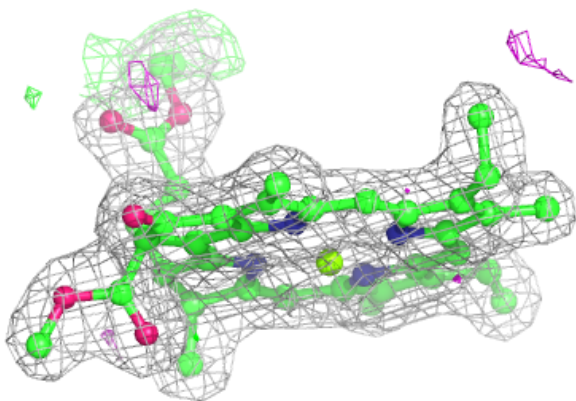
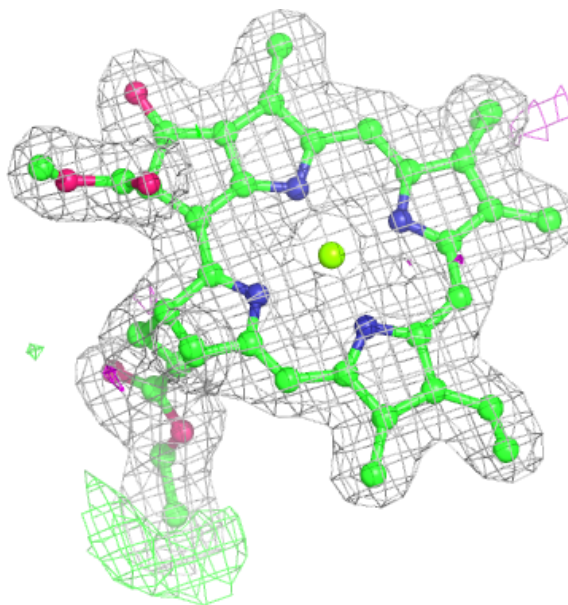
**Electron density around PHO a 405:**

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



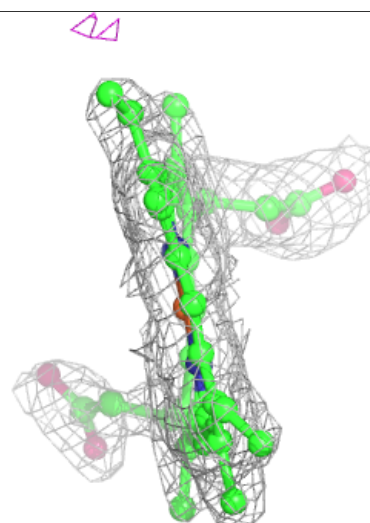
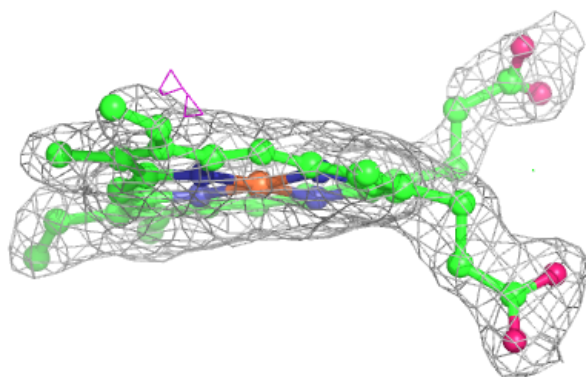
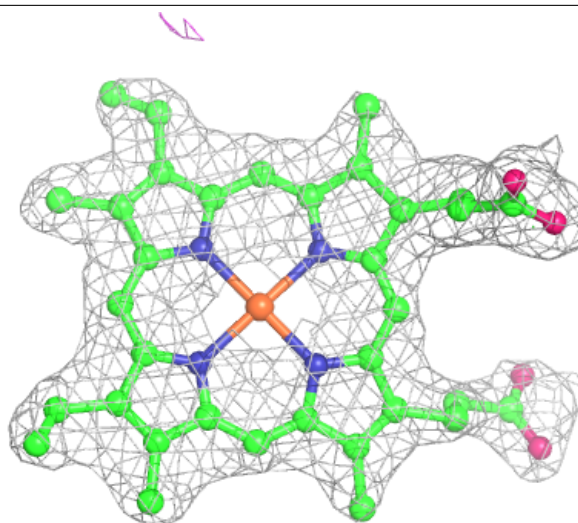
**Electron density around CLA a 407:**

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



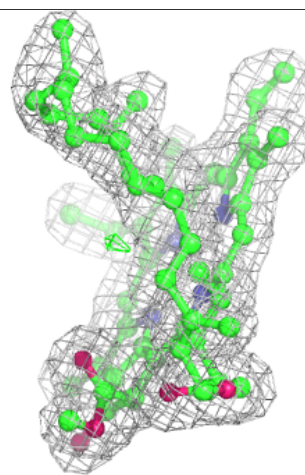
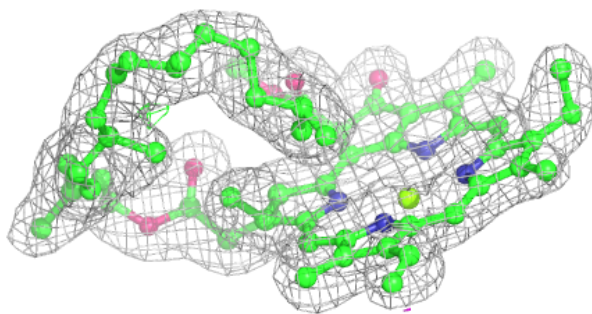
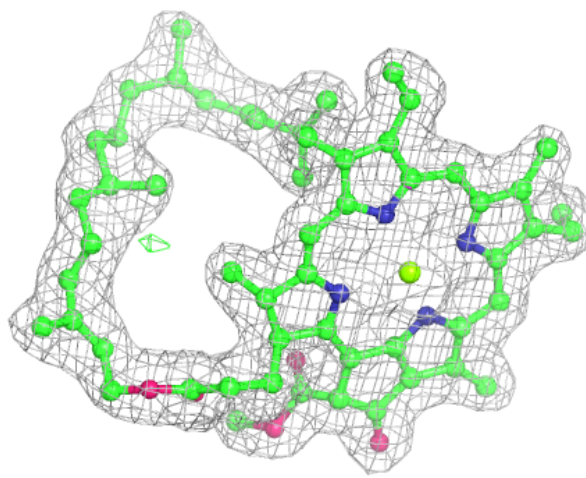
**Electron density around HEM e 102:**

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



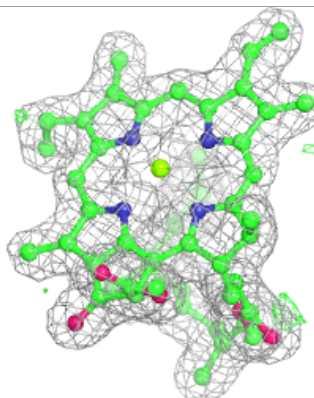
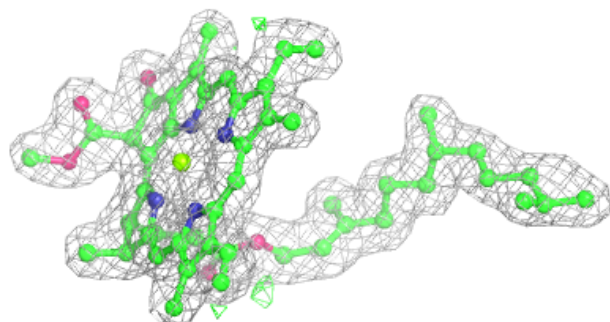
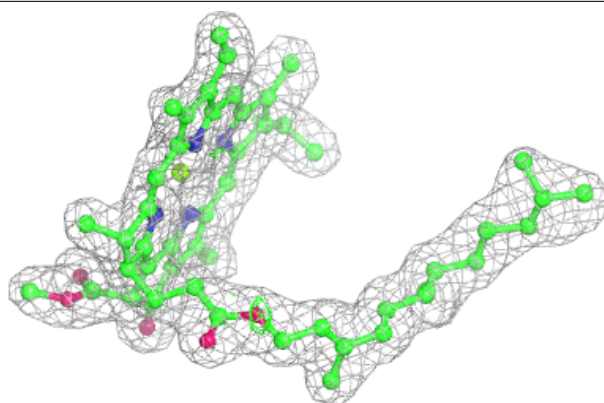
**Electron density around CLA b 617:**

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

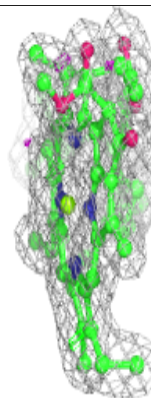
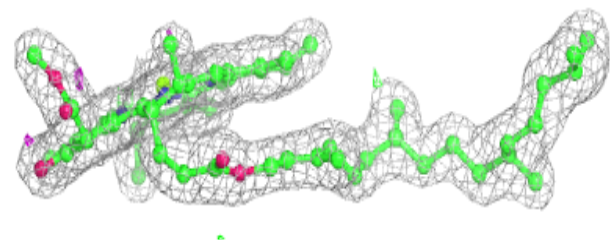
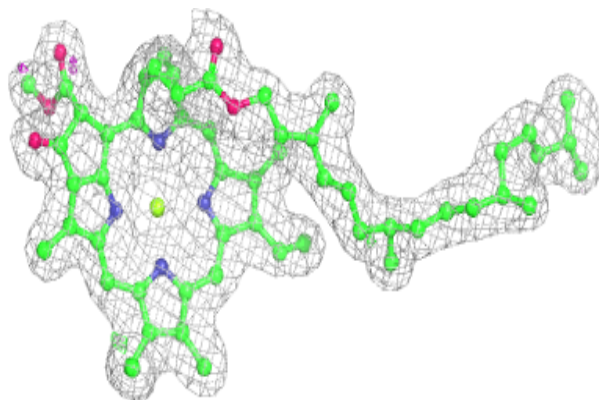


**Electron density around CLA c 508:**

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

**Electron density around CLA b 605:**

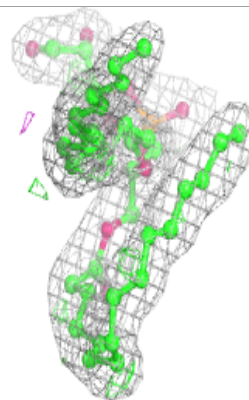
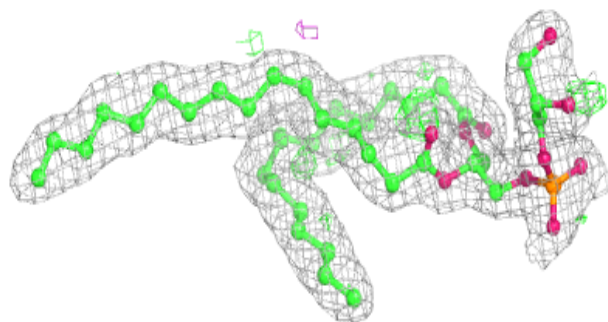
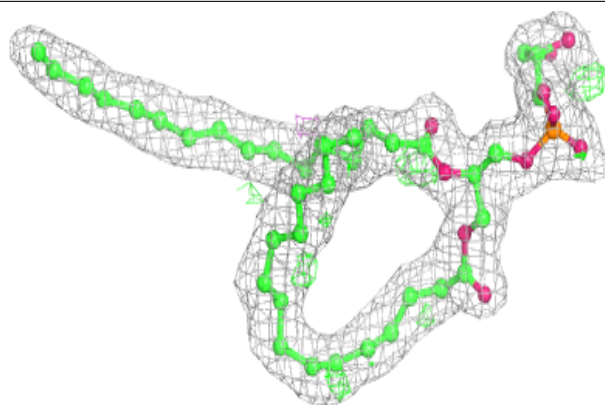
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



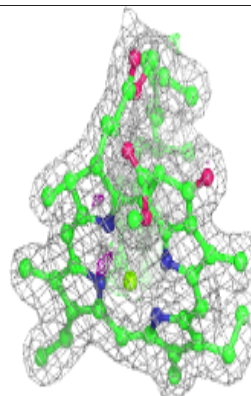
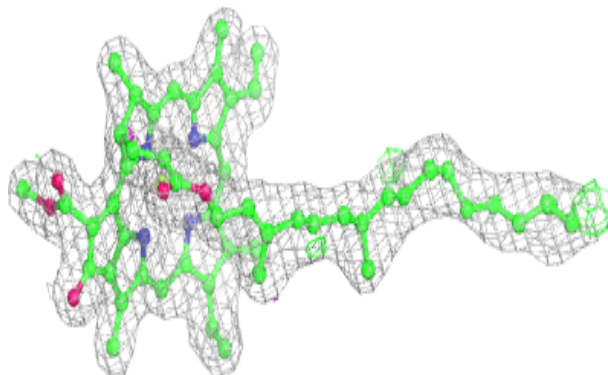
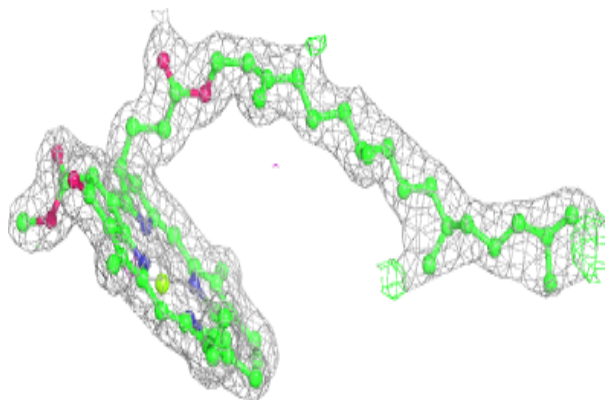


**Electron density around LHG d 406:**

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

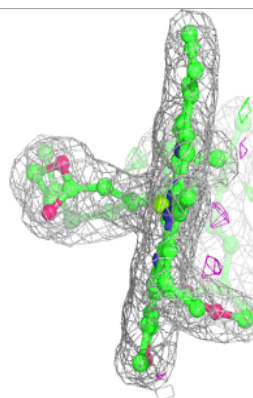
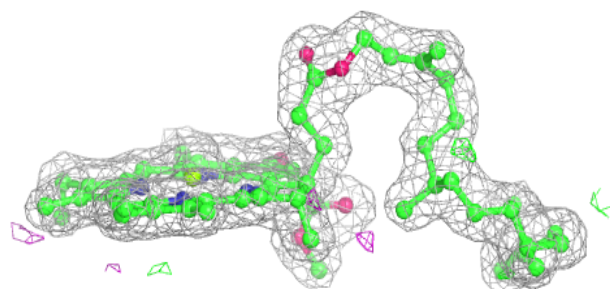
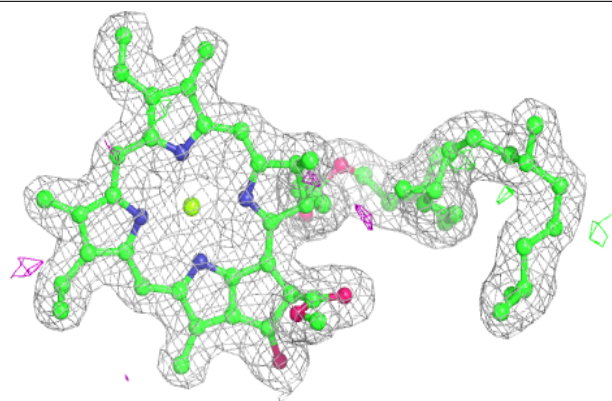
**Electron density around CLA c 504:**

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

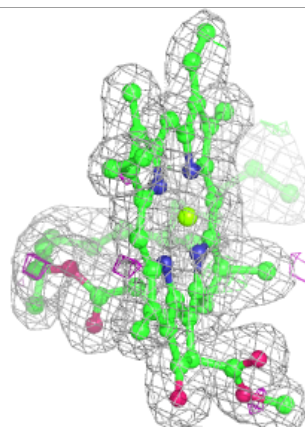
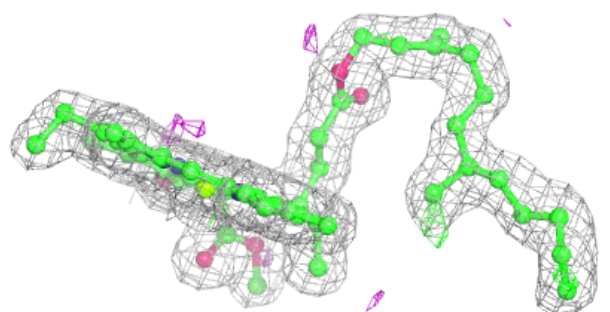
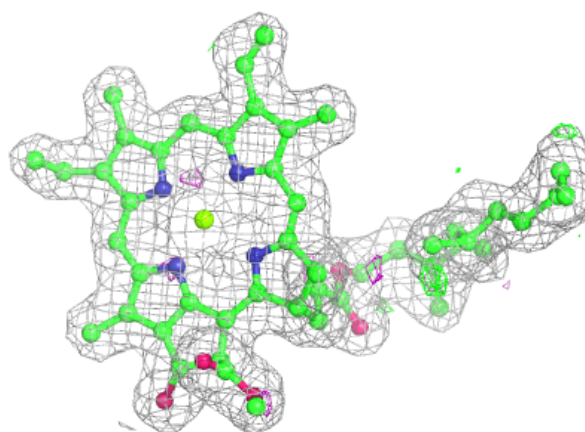


**Electron density around CLA b 614:**

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

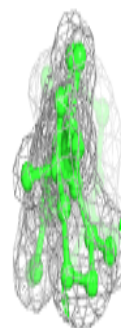
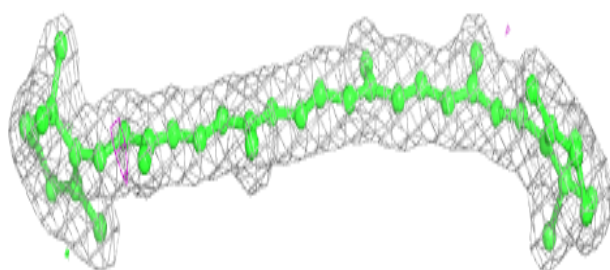
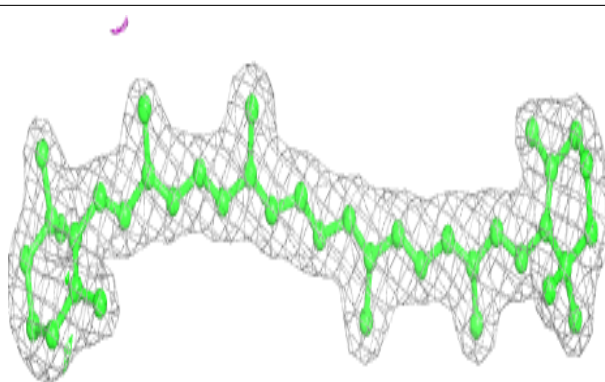
**Electron density around CLA A 402:**

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

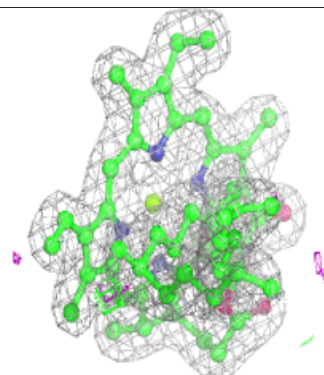
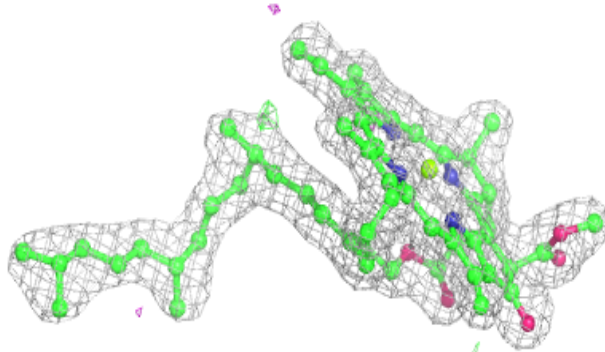
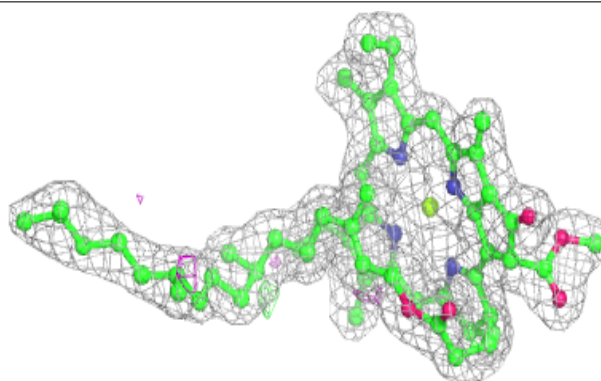


**Electron density around BCR b 621:**

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

**Electron density around CLA c 505:**

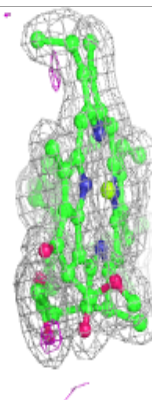
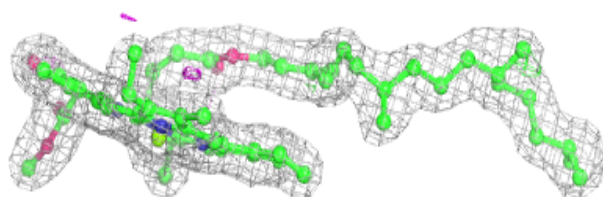
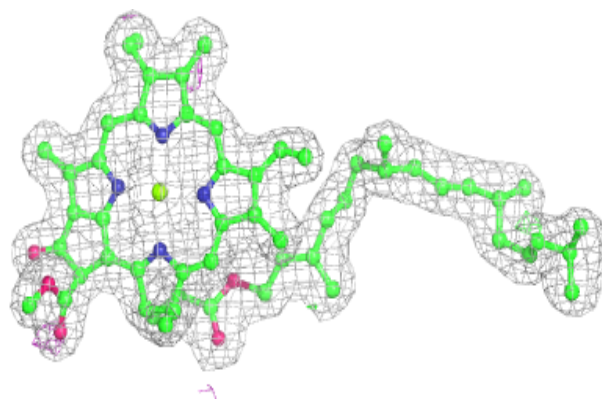
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



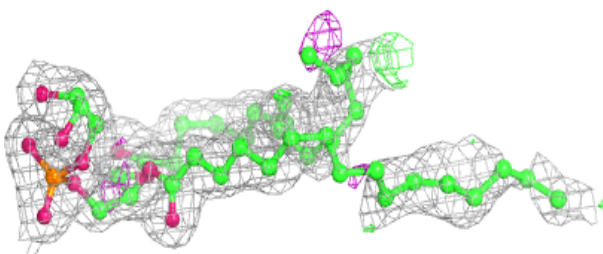
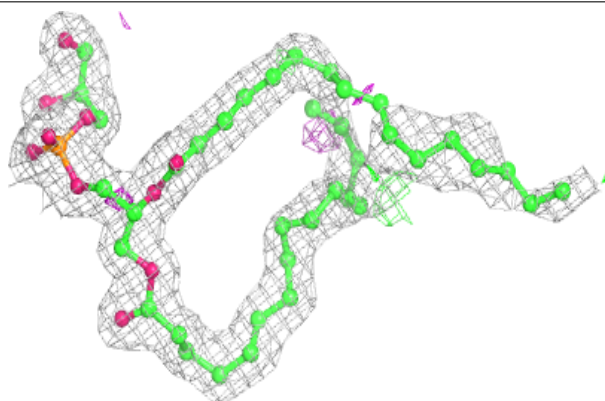


**Electron density around CLA B 604:**

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

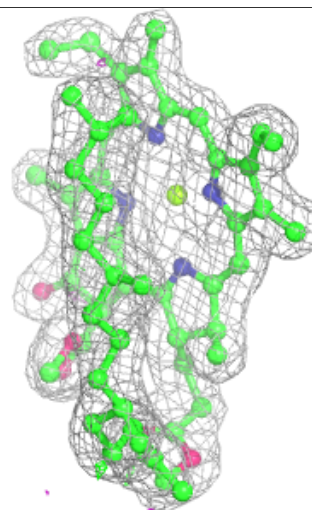
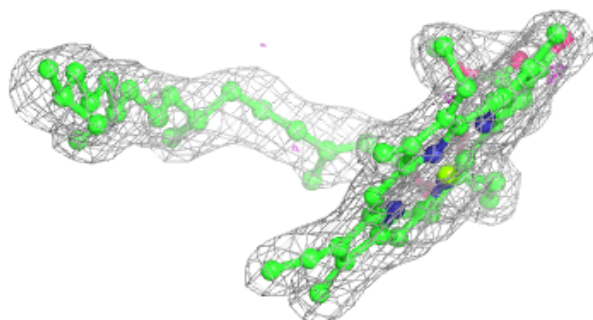
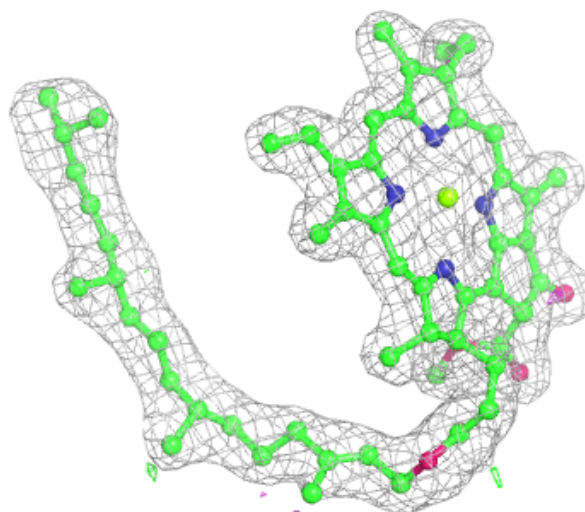
**Electron density around LHG d 408:**

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



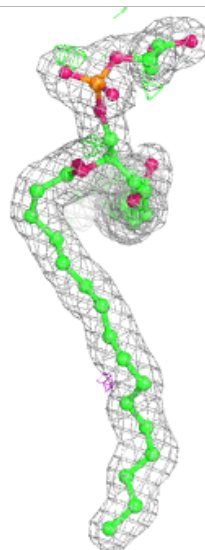
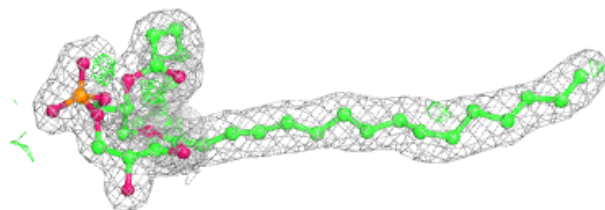
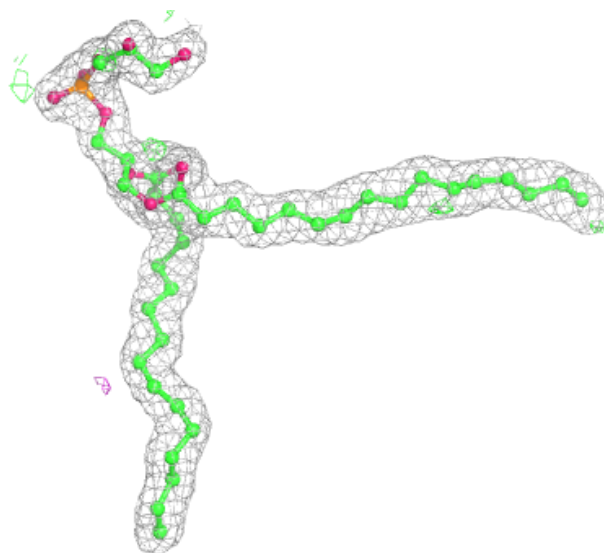
**Electron density around CLA c 507:**

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



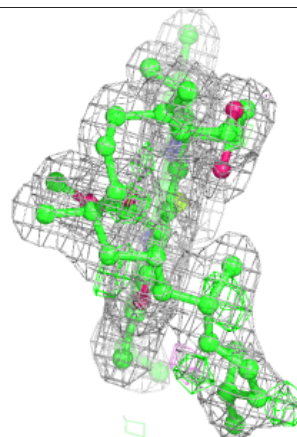
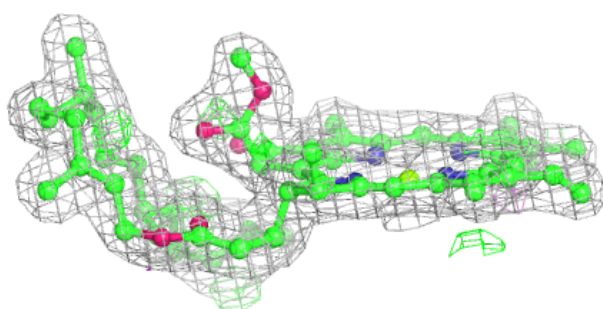
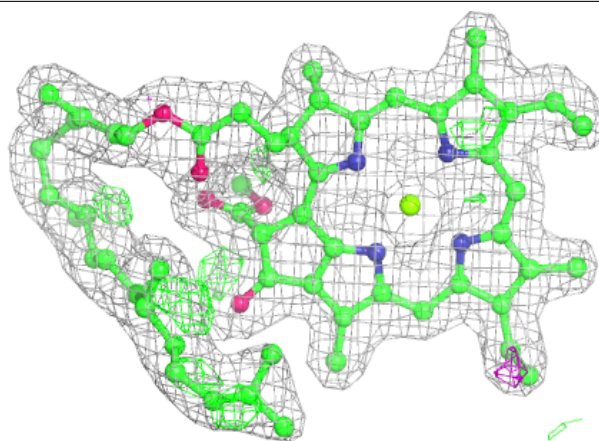
**Electron density around LHG L 101:**

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



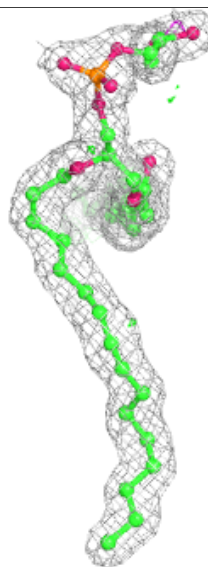
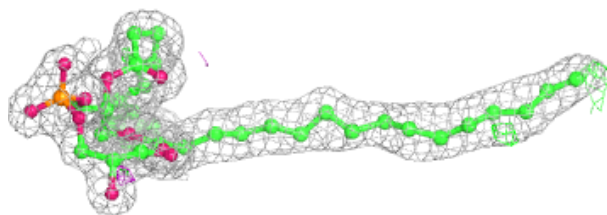
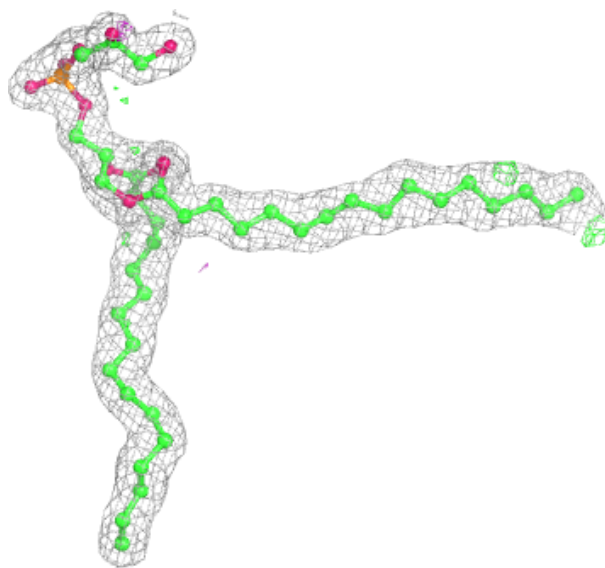
**Electron density around CLA B 611:**

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



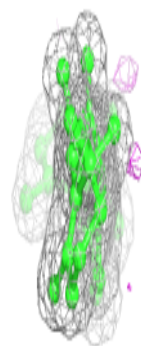
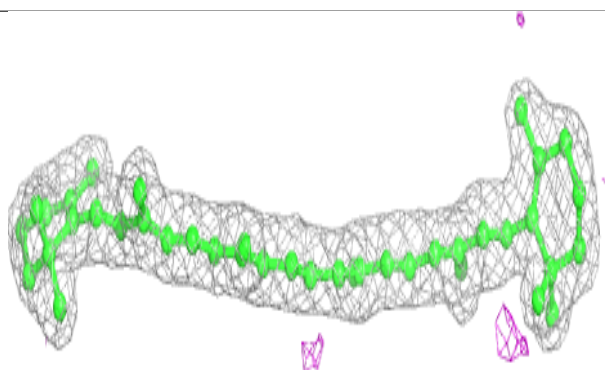
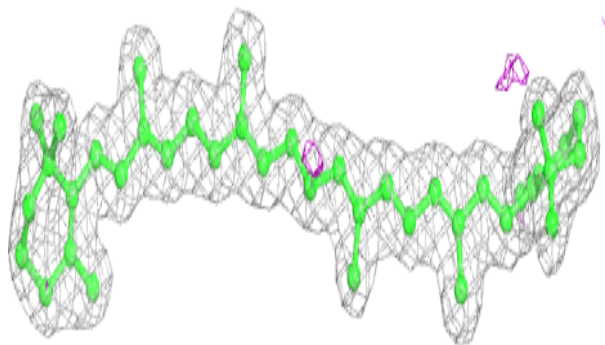
**Electron density around LHG 1 102:**

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

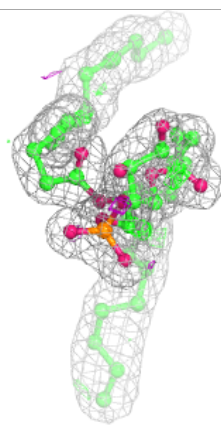
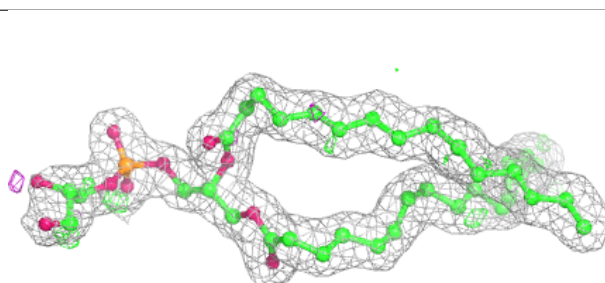
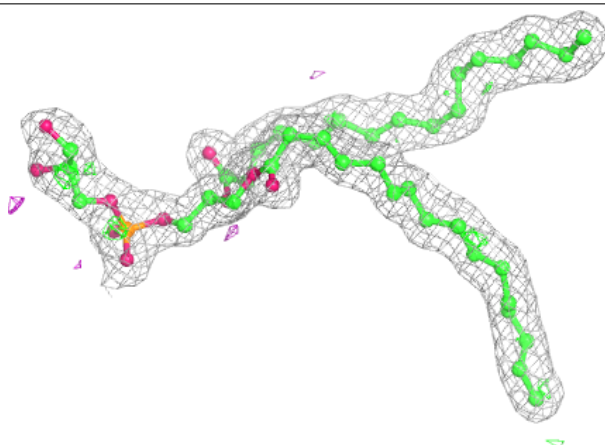


**Electron density around BCR b 619:**

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

**Electron density around LHG d 407:**

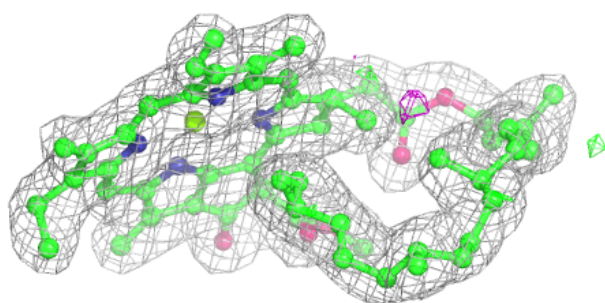
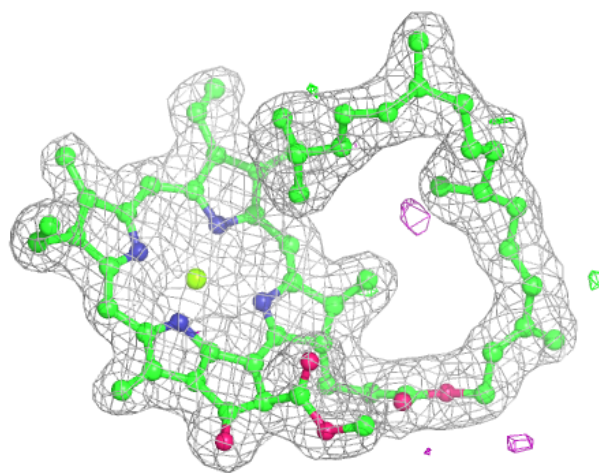
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





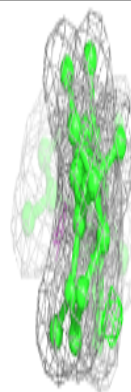
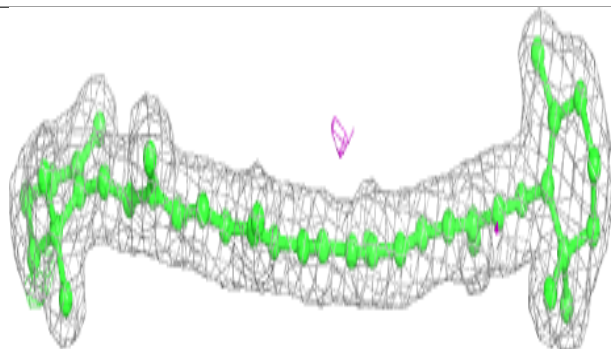
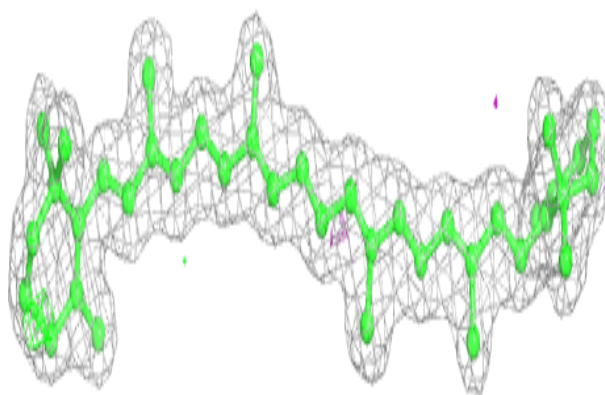
**Electron density around CLA B 616:**

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

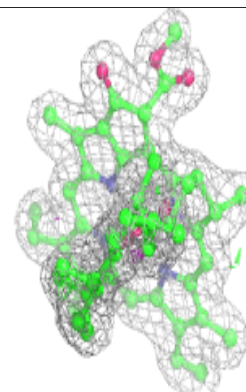
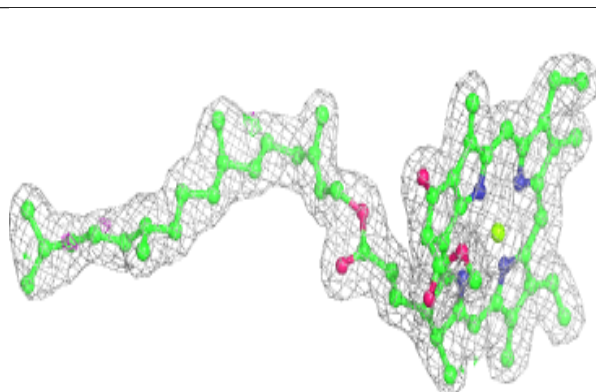
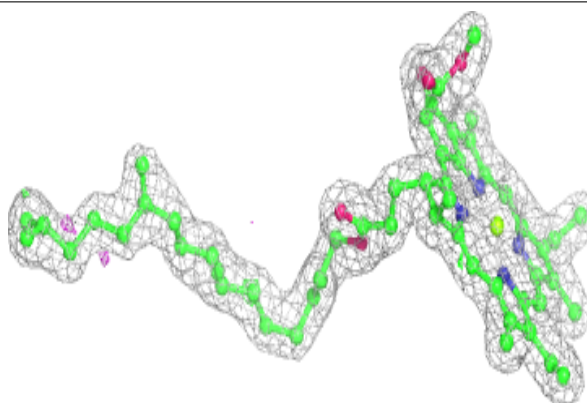


**Electron density around BCR B 617:**

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

**Electron density around CLA c 502:**

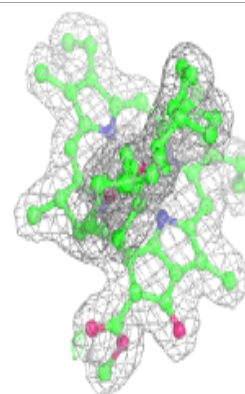
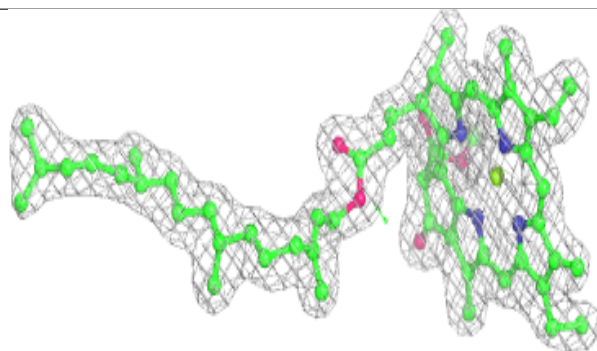
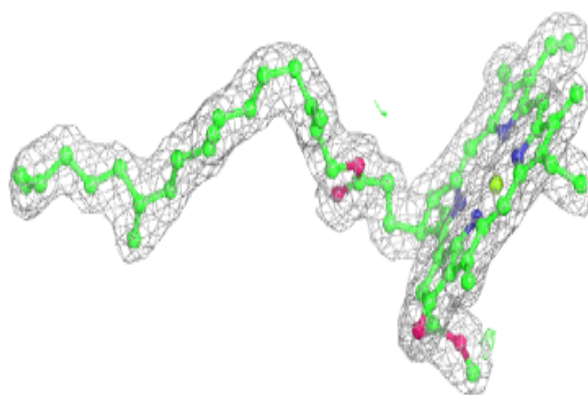
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



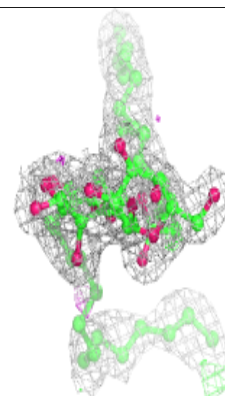
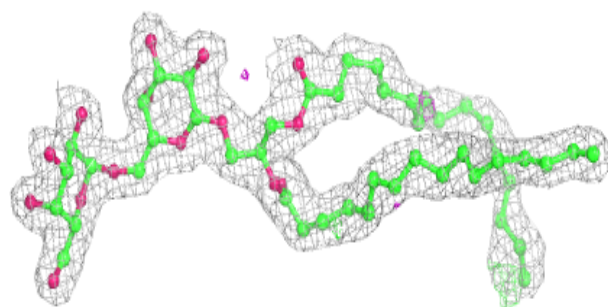
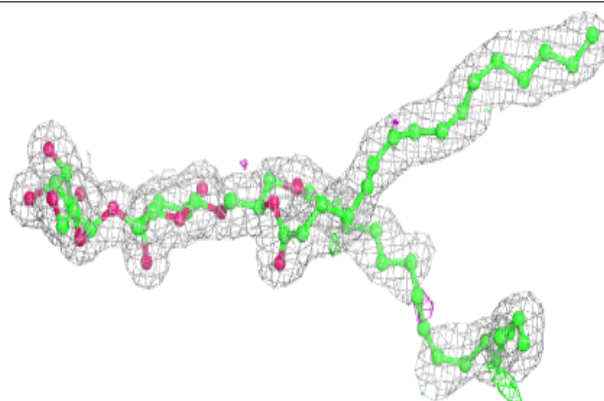


**Electron density around CLA C 502:**

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

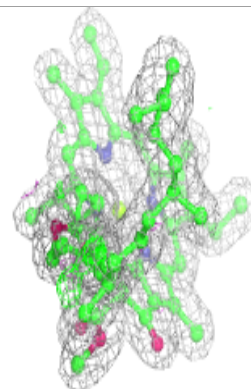
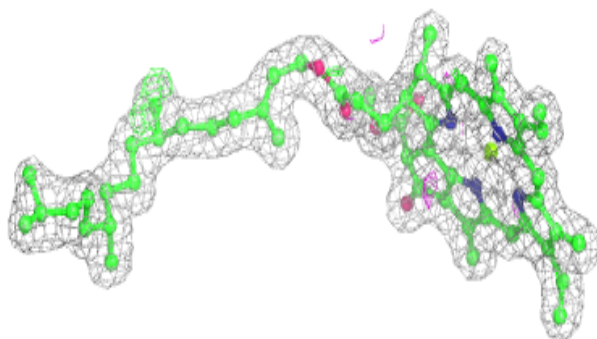
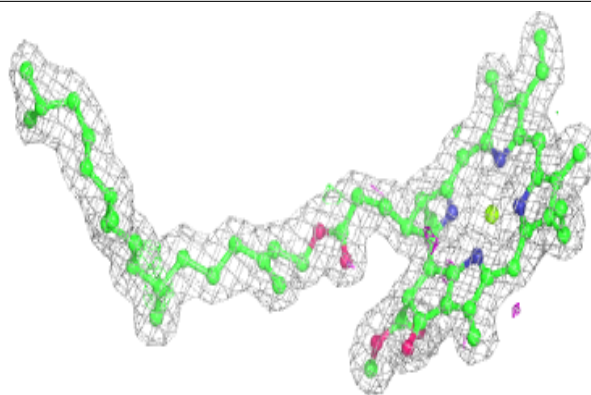
**Electron density around DGD C 516:**

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

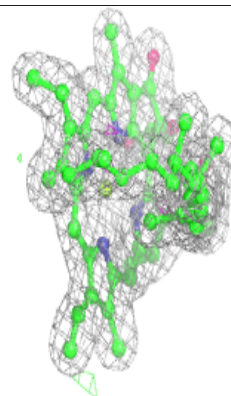
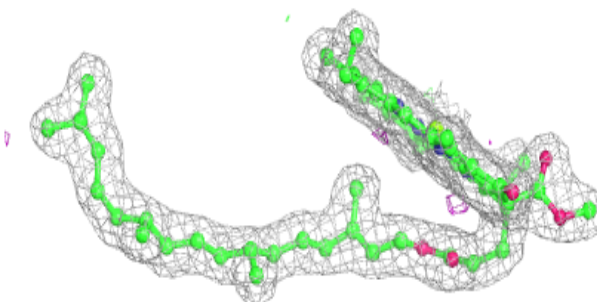
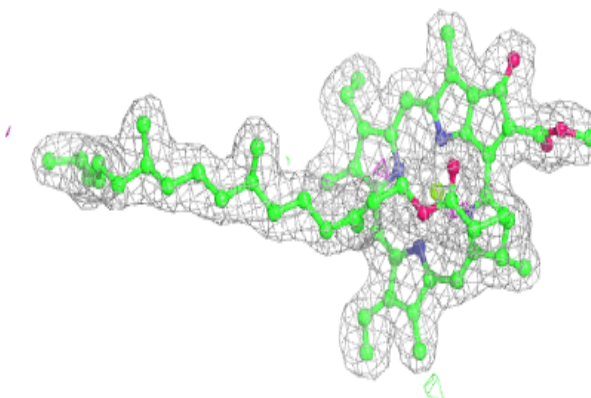


**Electron density around CLA a 403:**

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

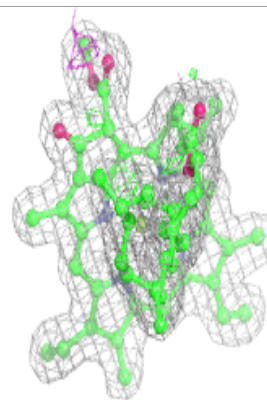
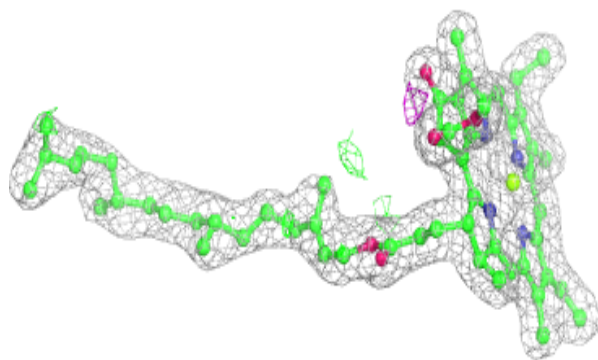
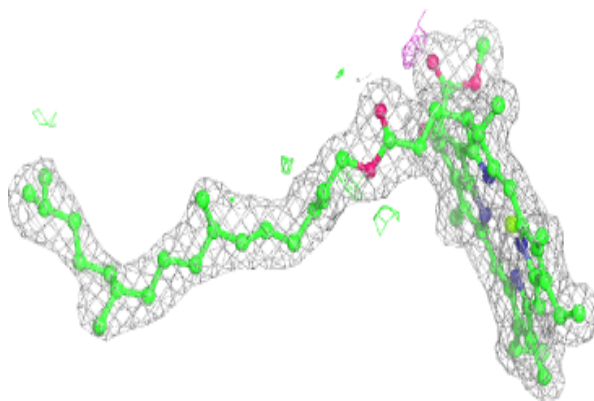
**Electron density around CLA b 610:**

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



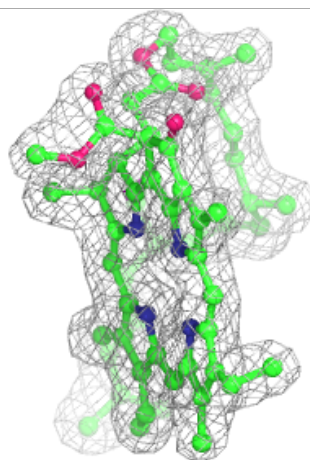
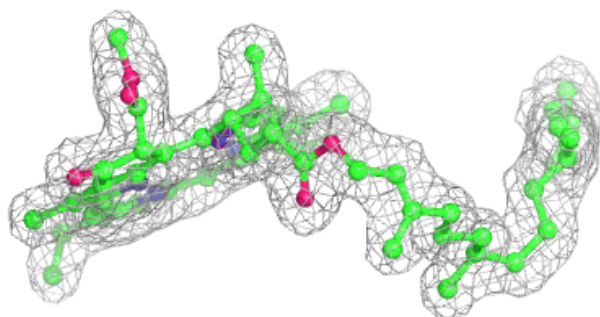
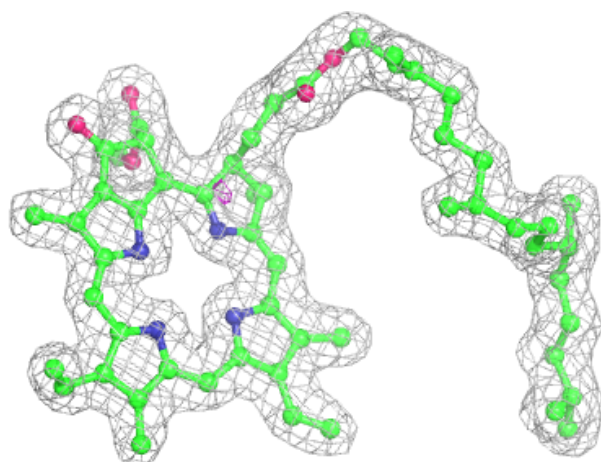
**Electron density around CLA B 605:**

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



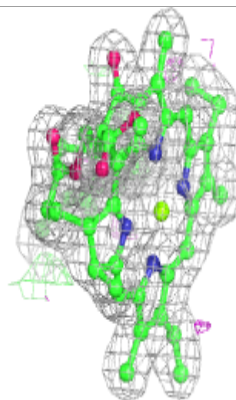
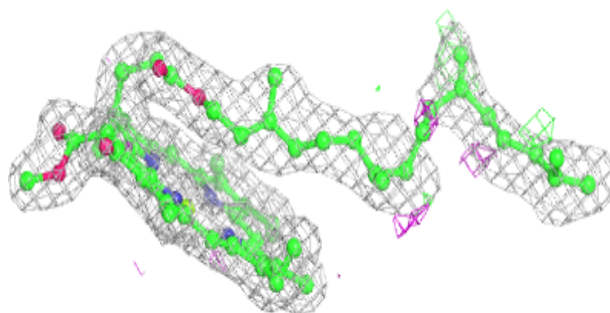
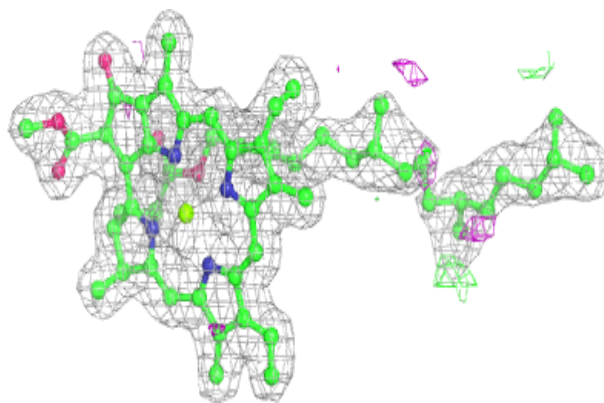
**Electron density around PHO D 403:**

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

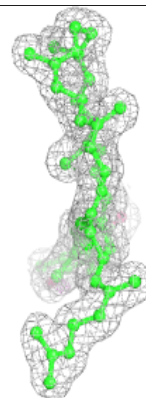
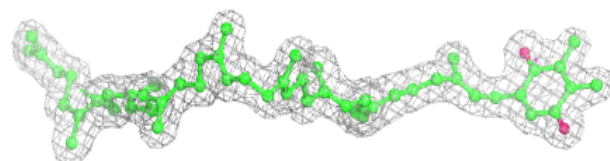
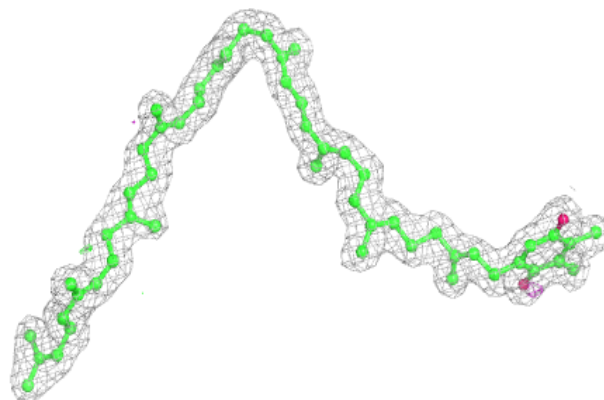


**Electron density around CLA B 615:**

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

**Electron density around PL9 D 412:**

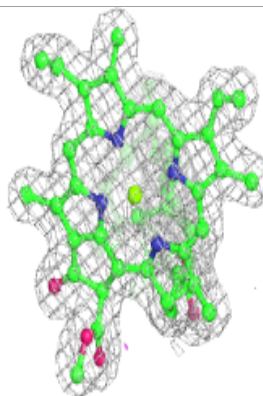
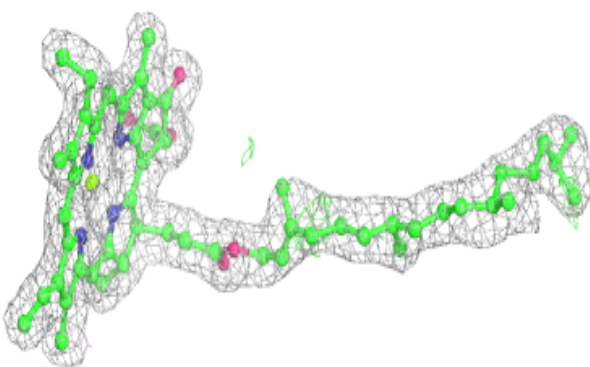
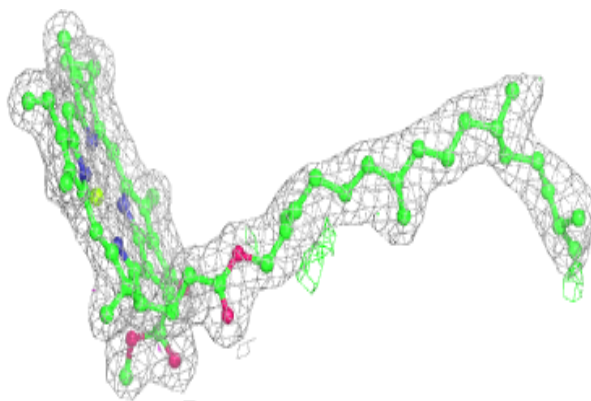
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



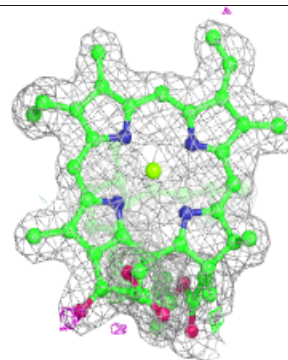
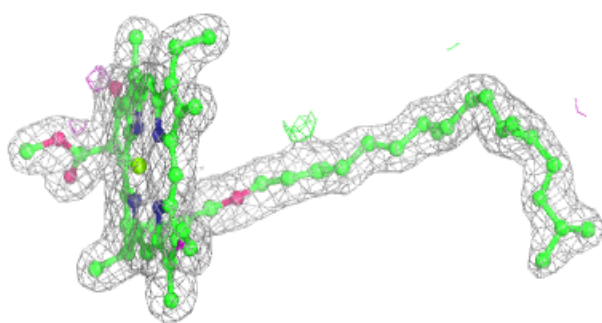
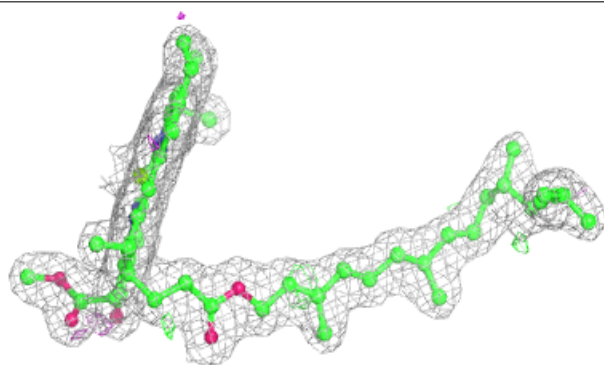


**Electron density around CLA b 606:**

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

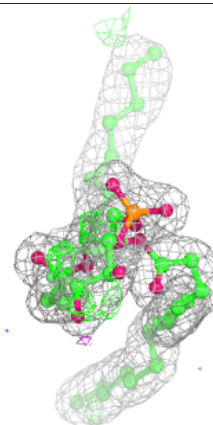
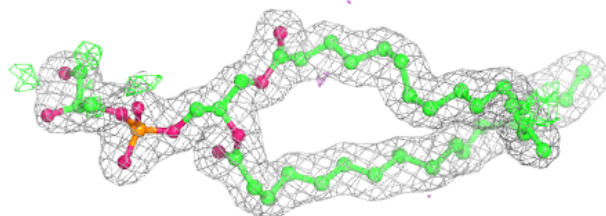
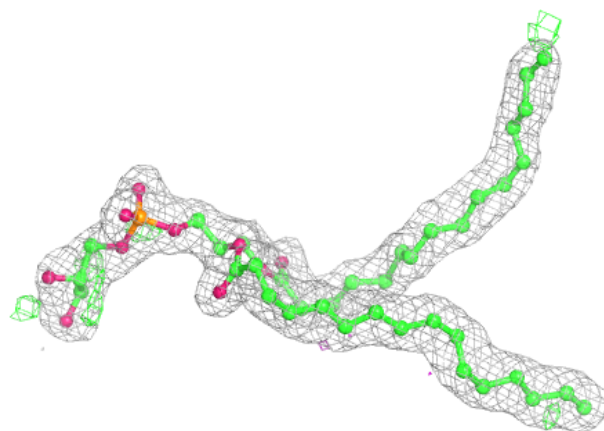
**Electron density around CLA b 607:**

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

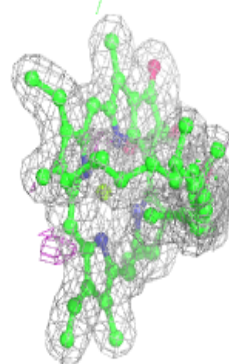
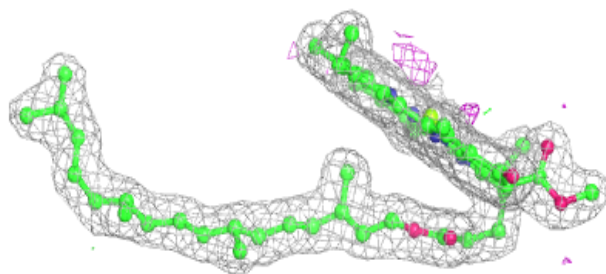
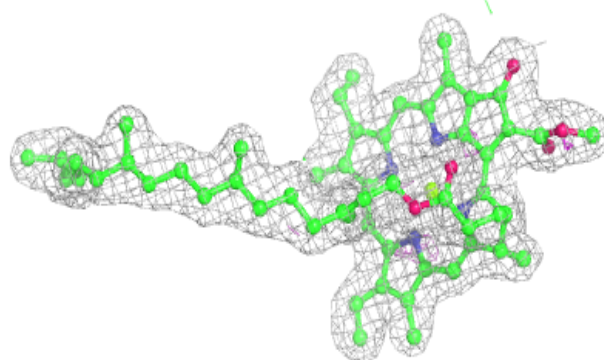


**Electron density around LHG D 408:**

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

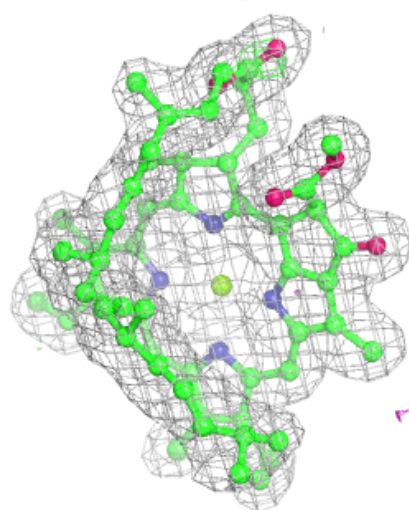
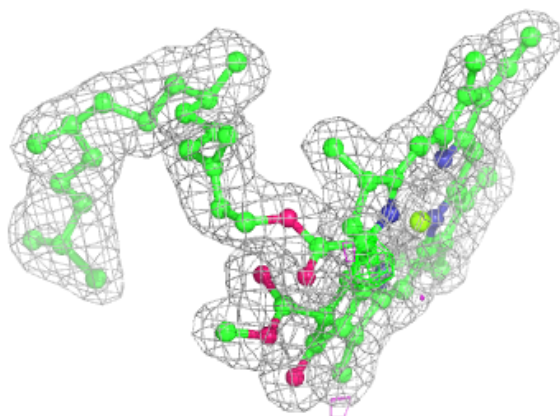
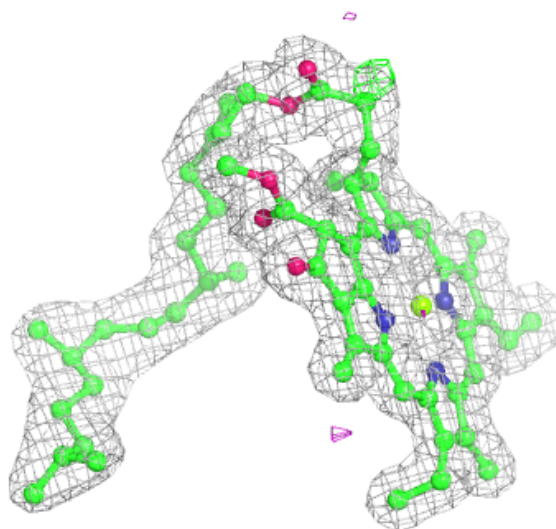
**Electron density around CLA B 609:**

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



**Electron density around CLA b 615:**

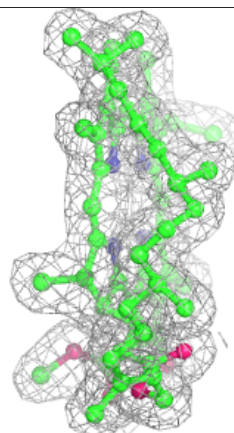
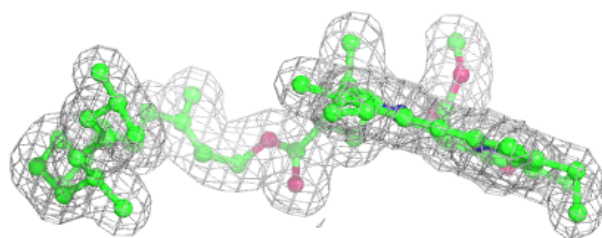
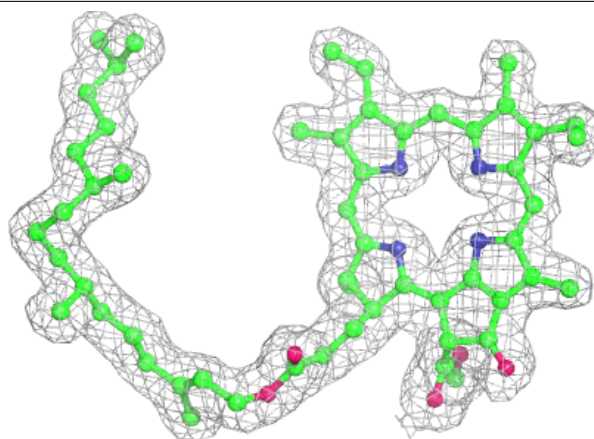
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





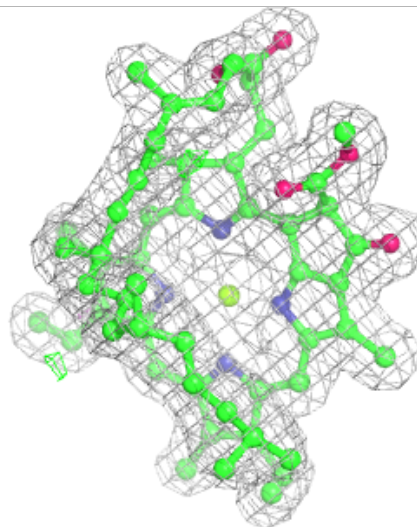
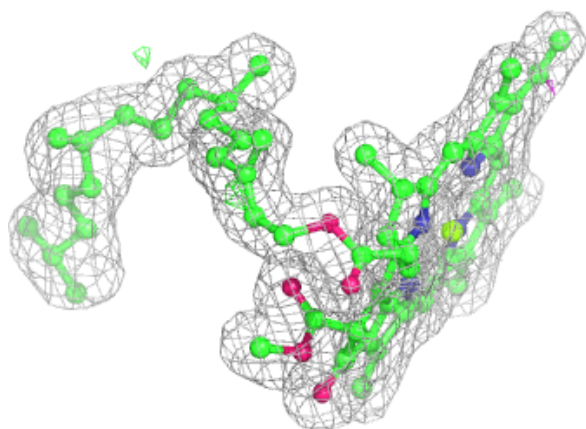
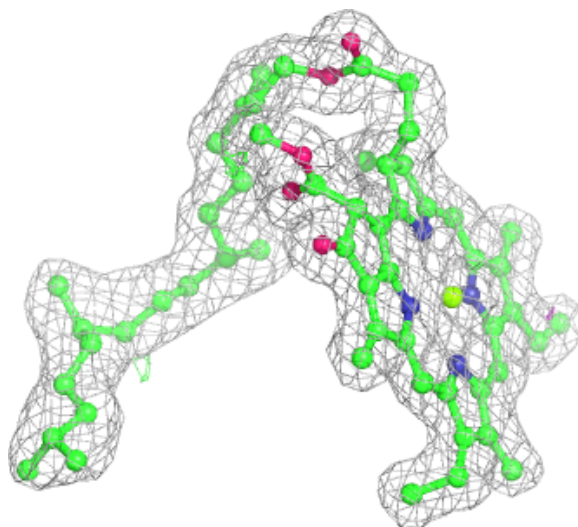
**Electron density around PHO A 403:**

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



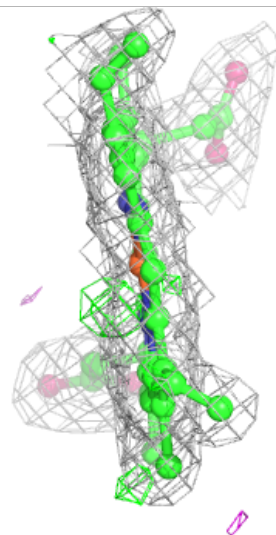
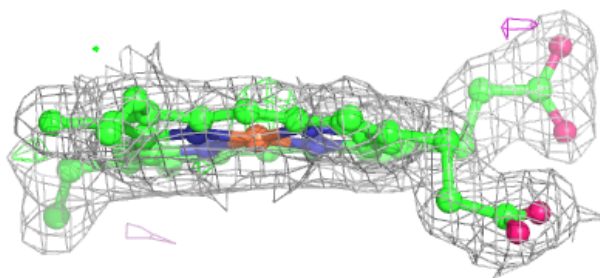
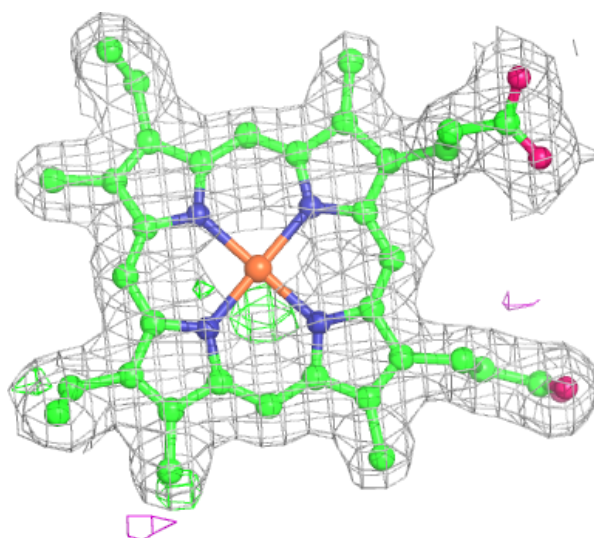
**Electron density around CLA B 614:**

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



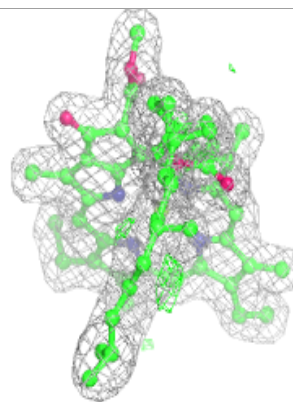
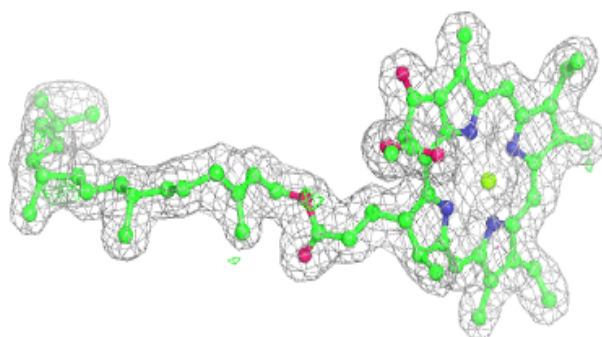
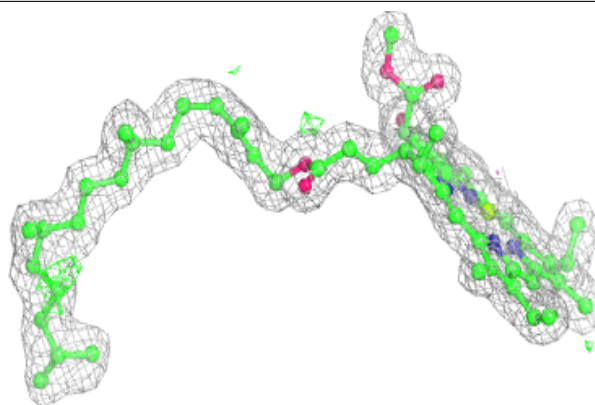
**Electron density around HEC v 201:**

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



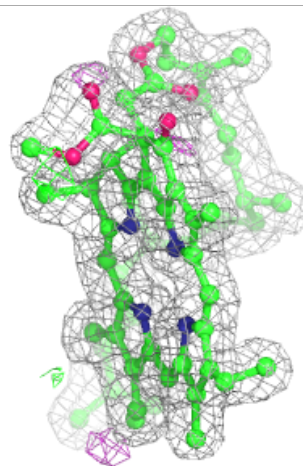
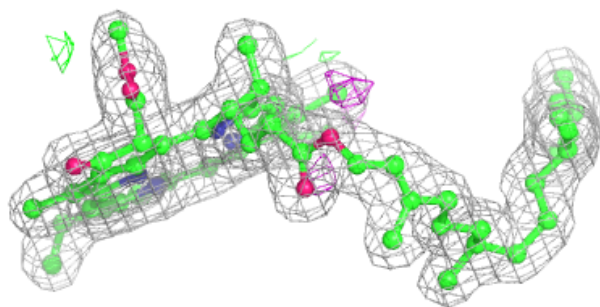
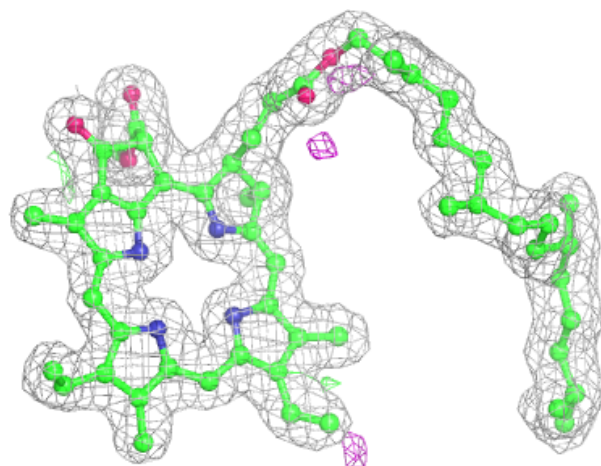
**Electron density around CLA D 401:**

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



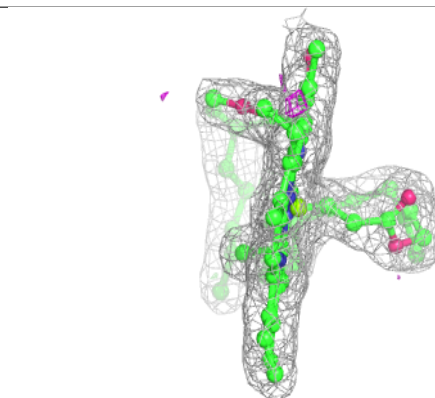
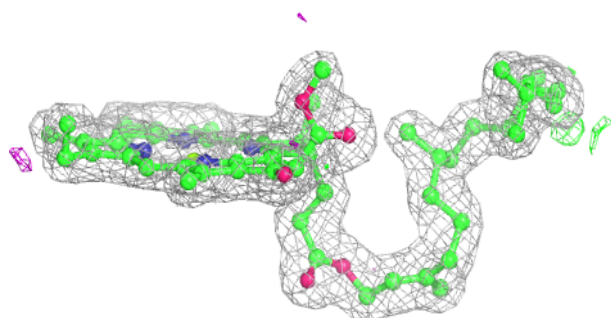
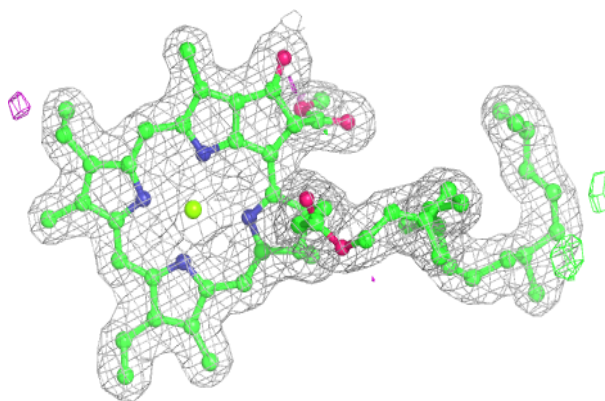
**Electron density around PHO a 406:**

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

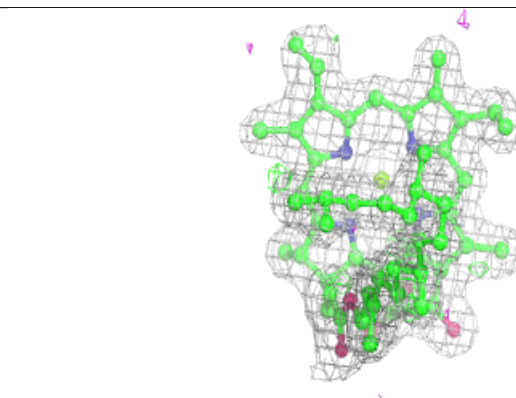
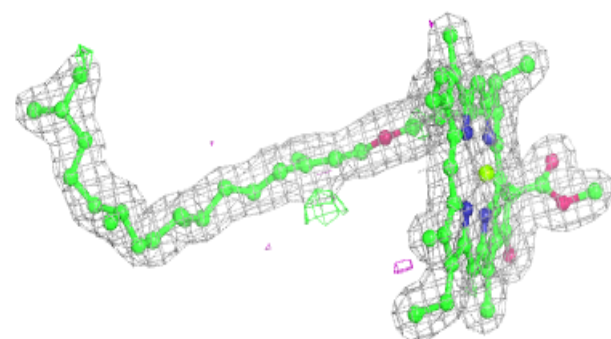
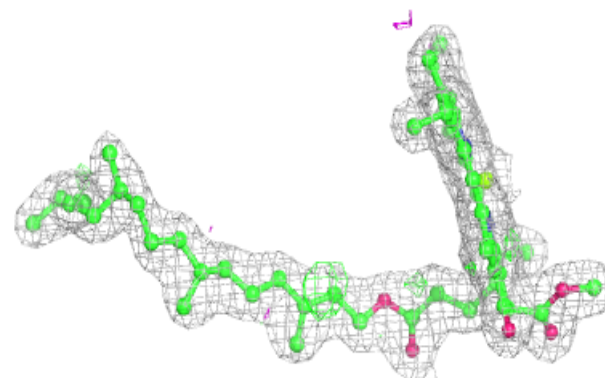


**Electron density around CLA B 613:**

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

**Electron density around CLA B 606:**

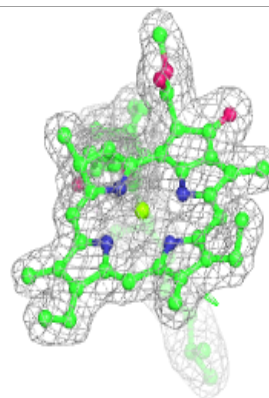
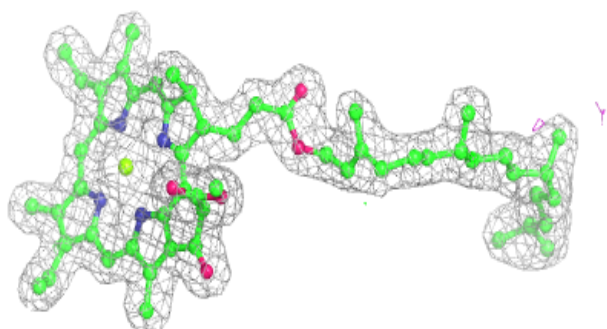
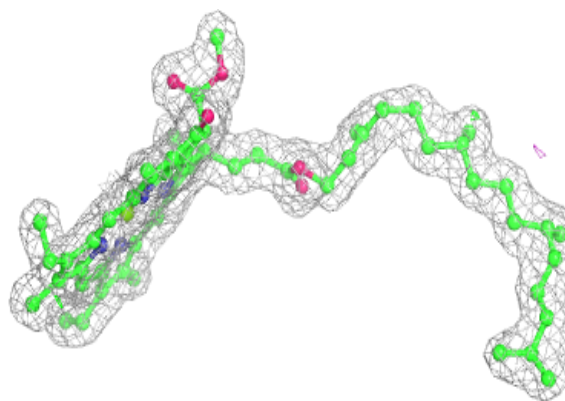
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



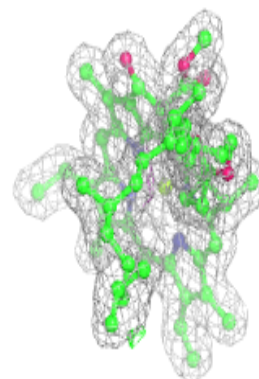
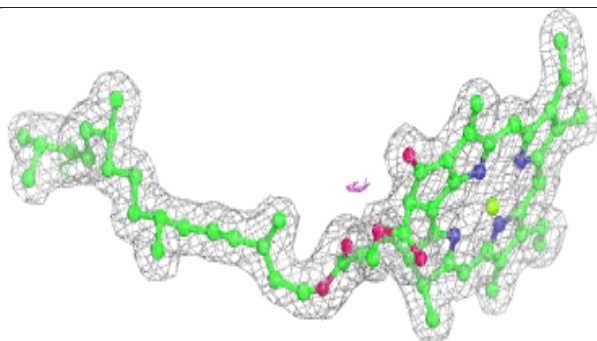
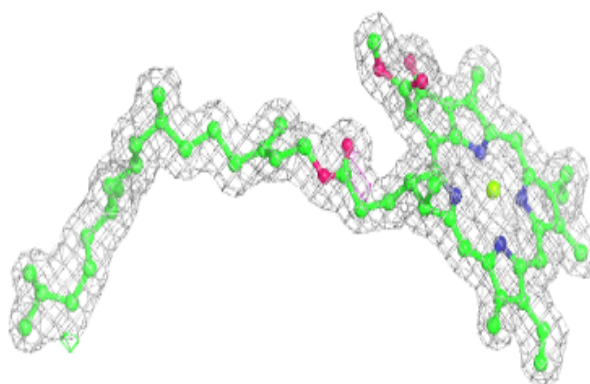


**Electron density around CLA d 402:**

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

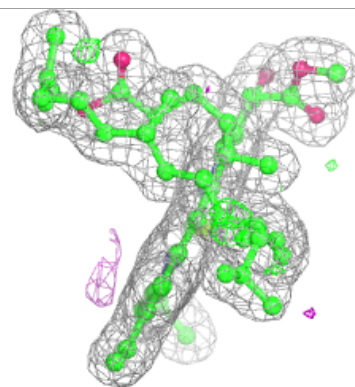
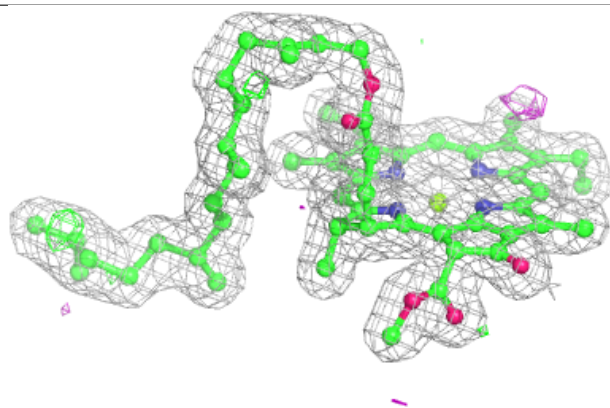
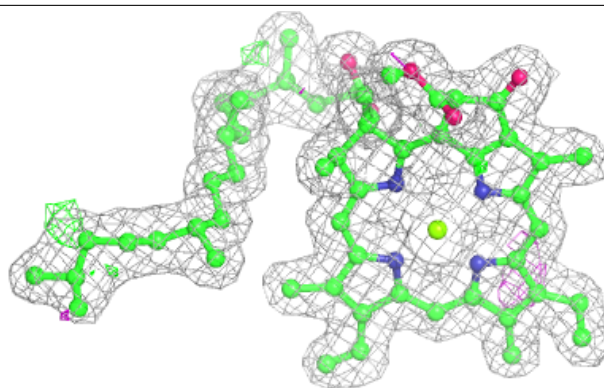
**Electron density around CLA A 401:**

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

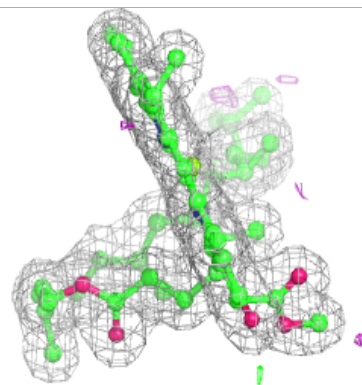
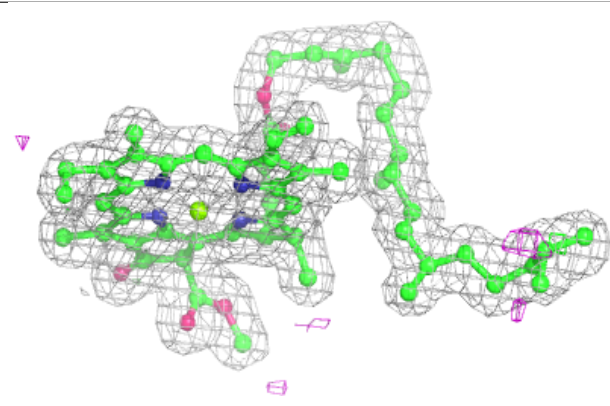
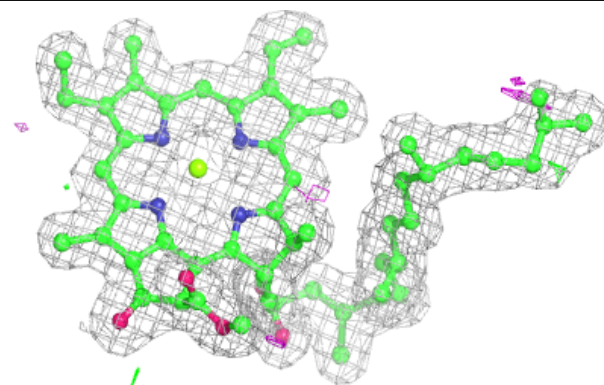


**Electron density around CLA D 402:**

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

**Electron density around CLA d 403:**

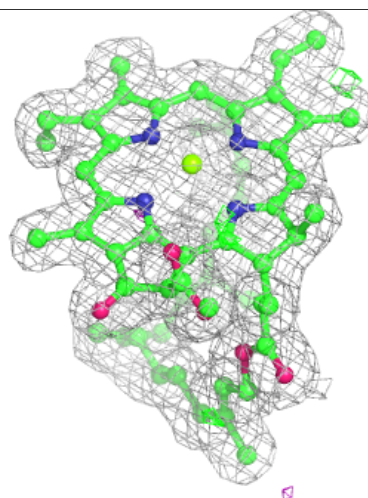
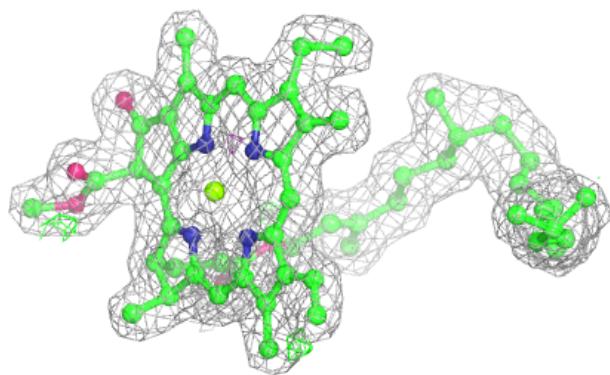
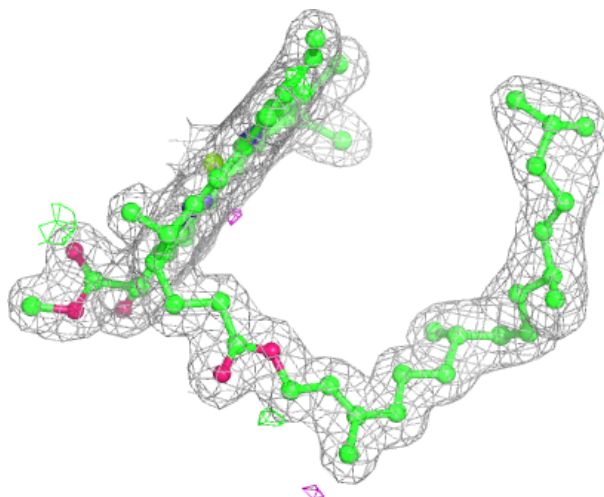
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

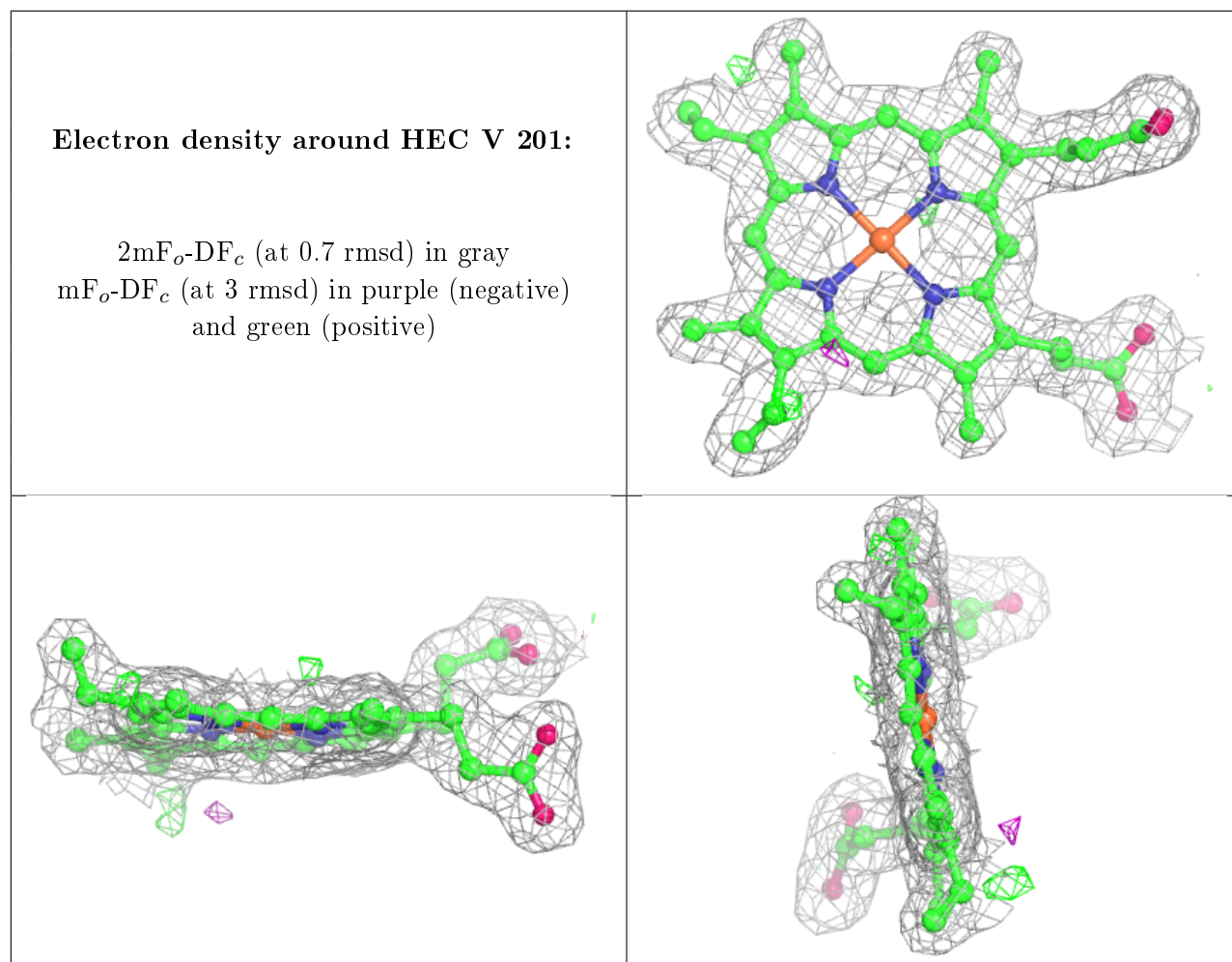




**Electron density around CLA B 612:**

$2mF_o-DF_c$  (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.