



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 07:42 AM JST

PDB ID : 5B66 / pdb\_00005b66  
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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.015 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

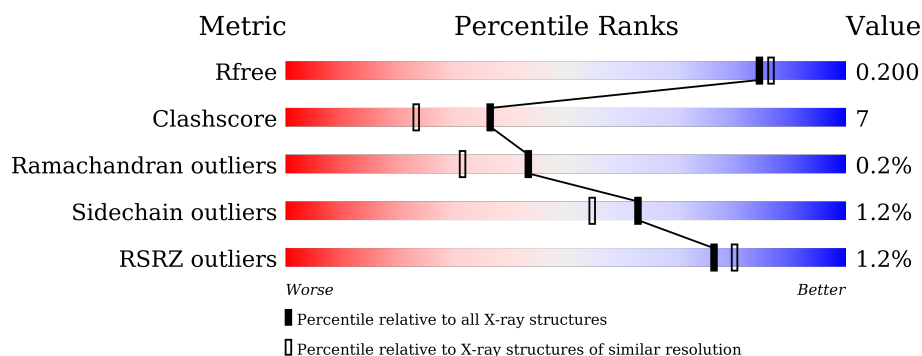
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3428 (1.86-1.86)                                      |
| Clashscore            | 190562                      | 3579 (1.86-1.86)                                      |
| Ramachandran outliers | 187476                      | 3553 (1.86-1.86)                                      |
| Sidechain outliers    | 187428                      | 3553 (1.86-1.86)                                      |
| RSRZ outliers         | 180081                      | 3429 (1.86-1.86)                                      |

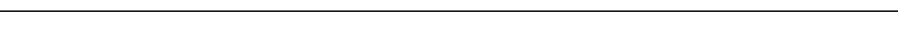
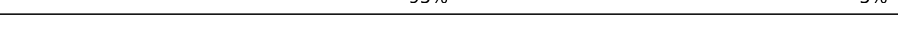
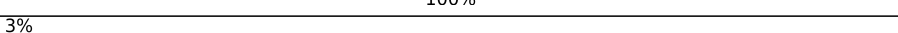
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

| Mol | Chain | Length | Quality of chain                                |
|-----|-------|--------|-------------------------------------------------|
| 1   | A     | 344    | <div> <div>0%</div> <div>87% 10% .</div> </div> |
| 1   | a     | 344    | <div> <div>88% 9% .</div> </div>                |
| 2   | B     | 505    | <div> <div>2%</div> <div>89% 10%</div> </div>   |
| 2   | b     | 505    | <div> <div>3%</div> <div>90% 8% ..</div> </div> |
| 3   | C     | 455    | <div> <div>91% 8% .</div> </div>                |
| 3   | c     | 455    | <div> <div>90% 10%</div> </div>                 |

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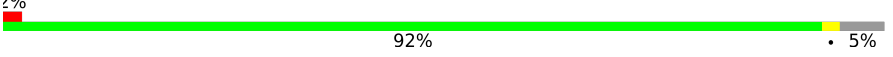
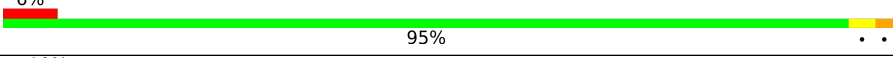
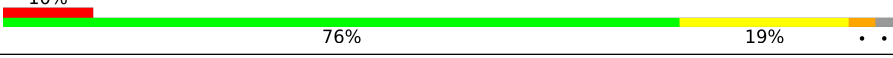


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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 4   | D     | 342    |  90% 9% .       |
| 4   | d     | 342    |  91% 9%         |
| 5   | E     | 83     |  77% 16% . 6%   |
| 5   | e     | 83     |  80% 13% . 6%   |
| 6   | F     | 44     |  64% 11% 25%    |
| 6   | f     | 44     |  59% 14% 27%    |
| 7   | H     | 65     |  91% 6% . .     |
| 7   | h     | 65     |  88% 6% . 5%    |
| 8   | I     | 38     |  82% 8% . 8%    |
| 8   | i     | 38     |  79% 13% . 5%   |
| 9   | J     | 40     |  80% 8% . 10%   |
| 9   | j     | 40     |  95% 5%         |
| 10  | K     | 37     |  89% 11%      |
| 10  | k     | 37     |  81% 16% .    |
| 11  | L     | 37     |  95% 5%       |
| 11  | l     | 37     |  100%         |
| 12  | M     | 36     |  78% 11% . 8% |
| 12  | m     | 36     |  86% 8% 6%    |
| 13  | O     | 244    |  89% 10%      |
| 13  | o     | 244    |  88% 11%      |
| 14  | T     | 32     |  81% . 6% 9%  |
| 14  | t     | 32     |  81% 9% . 6%  |
| 15  | U     | 104    |  82% 12% 7%   |
| 15  | u     | 104    |  87% 7% 7%    |
| 16  | V     | 137    |  96% .        |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 16  | v     | 137    |  |
| 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 |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 26  | UNL  | U     | 901    | -         | -        | X       | -                |
| 28  | DMS  | B     | 635    | -         | -        | X       | -                |
| 28  | DMS  | B     | 642    | -         | -        | X       | -                |
| 28  | DMS  | B     | 644    | -         | -        | X       | -                |
| 28  | DMS  | C     | 531    | -         | -        | X       | -                |
| 28  | DMS  | C     | 532    | -         | -        | X       | -                |
| 28  | DMS  | D     | 414    | -         | -        | X       | -                |
| 28  | DMS  | U     | 903[B] | -         | -        | X       | -                |
| 28  | DMS  | b     | 631    | -         | -        | X       | -                |
| 28  | DMS  | b     | 639    | -         | -        | X       | -                |
| 28  | DMS  | c     | 530    | -         | -        | X       | -                |
| 28  | DMS  | c     | 536    | -         | -        | X       | -                |
| 28  | DMS  | d     | 414    | -         | -        | X       | -                |
| 28  | DMS  | i     | 104    | -         | -        | X       | -                |
| 28  | DMS  | o     | 302    | -         | -        | X       | -                |
| 28  | DMS  | o     | 303    | -         | -        | X       | -                |
| 28  | DMS  | o     | 306    | -         | -        | X       | -                |
| 28  | DMS  | v     | 206    | -         | -        | X       | -                |
| 31  | BCT  | A     | 421    | -         | -        | X       | -                |
| 40  | HEC  | V     | 201    | X         | -        | -       | -                |
| 40  | HEC  | v     | 201    | 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 |         |         |       |

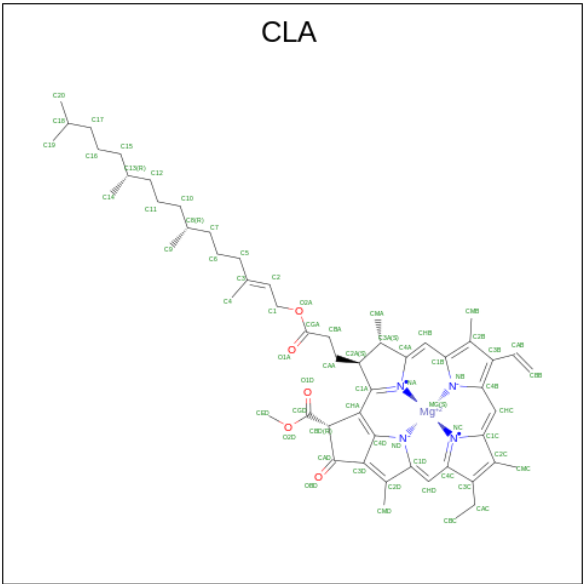
- Molecule 18 is a protein called Photosystem II reaction center protein X.

| 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 (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| 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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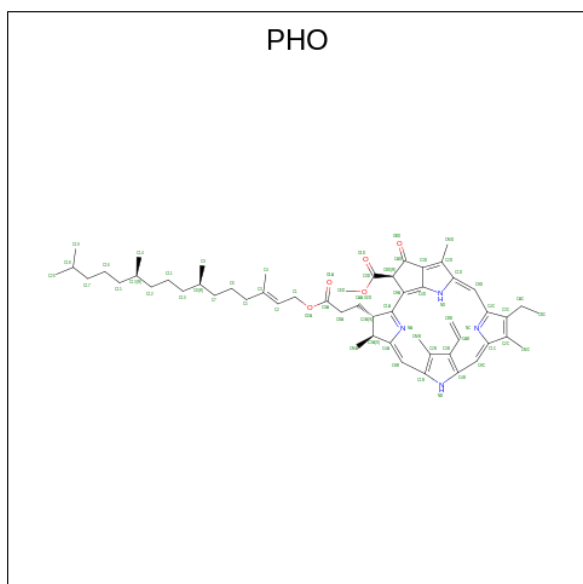
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 20  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 20  | 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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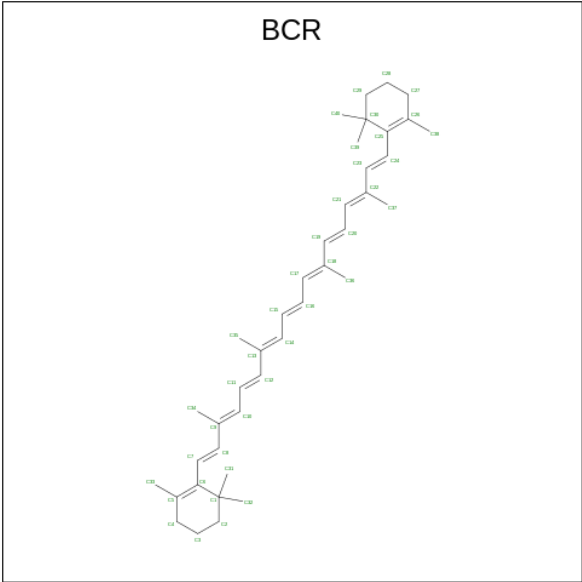
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 20  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 20  | c     | 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 (CCD ID: 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 (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



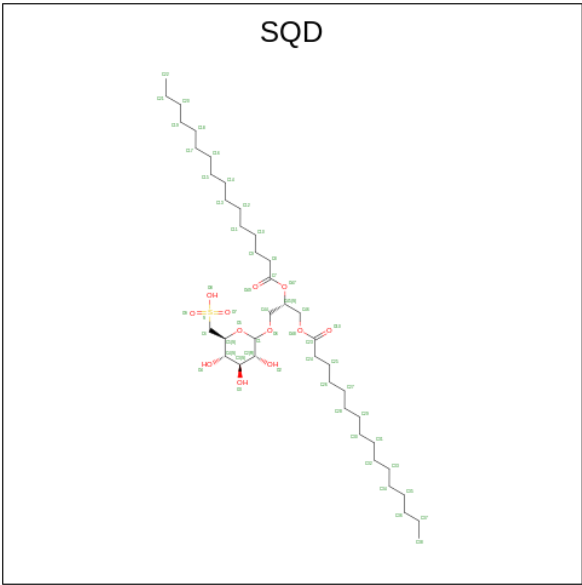
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 22  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 22  | B     | 1        | Total C<br>40 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 (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



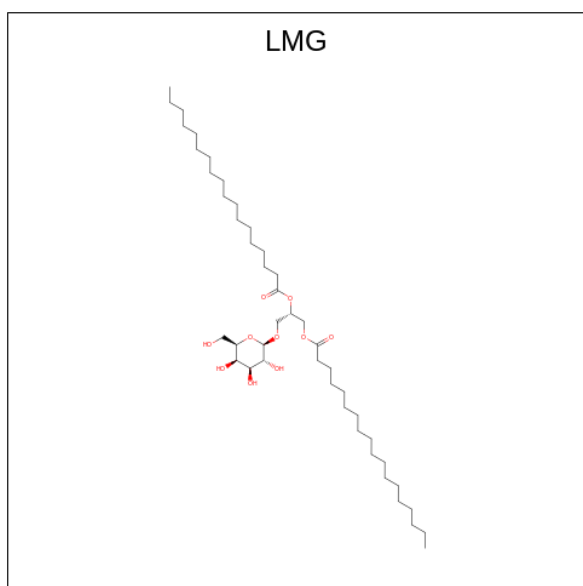
| Mol | Chain | Residues | Atoms                     | ZeroOcc | AltConf |
|-----|-------|----------|---------------------------|---------|---------|
| 23  | A     | 1        | Total C O S<br>54 41 12 1 | 0       | 0       |
| 23  | A     | 1        | Total C O S<br>54 41 12 1 | 0       | 0       |
| 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 (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



| 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 (CCD ID: 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 (CCD ID: UNL) (formula: ).

| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 26  | A     | 2        | Total | C  | O | 0       | 0       |
|     |       |          | 40    | 35 | 5 |         |         |
| 26  | B     | 6        | Total | C  |   | 0       | 0       |
|     |       |          | 84    | 84 |   |         |         |
| 26  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 34    | 29 | 5 |         |         |
| 26  | D     | 2        | Total | C  | O | 0       | 0       |
|     |       |          | 53    | 48 | 5 |         |         |
| 26  | E     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 15    | 15 |   |         |         |
| 26  | H     | 2        | Total | C  |   | 0       | 0       |
|     |       |          | 10    | 10 |   |         |         |
| 26  | I     | 5        | Total | C  |   | 0       | 0       |
|     |       |          | 61    | 61 |   |         |         |
| 26  | J     | 4        | Total | C  |   | 0       | 0       |
|     |       |          | 33    | 33 |   |         |         |
| 26  | L     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 14    | 14 |   |         |         |
| 26  | M     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 12    | 12 |   |         |         |
| 26  | T     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 13    | 13 |   |         |         |
| 26  | U     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 14    | 14 |   |         |         |
| 26  | X     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 16    | 16 |   |         |         |

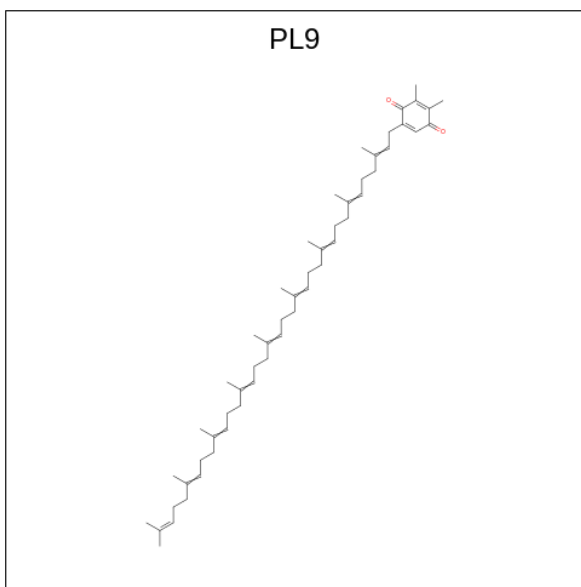
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| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 26  | Z     | 1        | Total C<br>4 4       | 0       | 0       |
| 26  | a     | 3        | Total C O<br>45 40 5 | 0       | 0       |
| 26  | b     | 7        | Total C<br>68 68     | 0       | 0       |
| 26  | c     | 3        | Total C O<br>48 43 5 | 0       | 0       |
| 26  | d     | 3        | Total C O<br>68 63 5 | 0       | 0       |
| 26  | e     | 1        | Total C<br>7 7       | 0       | 0       |
| 26  | h     | 1        | Total C<br>16 16     | 0       | 0       |
| 26  | i     | 3        | Total C<br>38 38     | 0       | 0       |
| 26  | j     | 2        | Total C<br>22 22     | 0       | 0       |
| 26  | t     | 1        | Total C<br>16 16     | 0       | 0       |
| 26  | x     | 1        | Total C<br>9 9       | 0       | 0       |
| 26  | z     | 1        | Total C<br>6 6       | 0       | 0       |

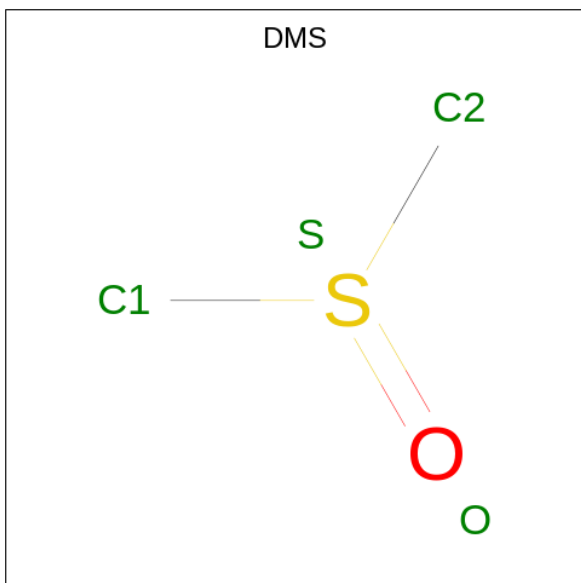
- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).





| 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 (CCD ID: 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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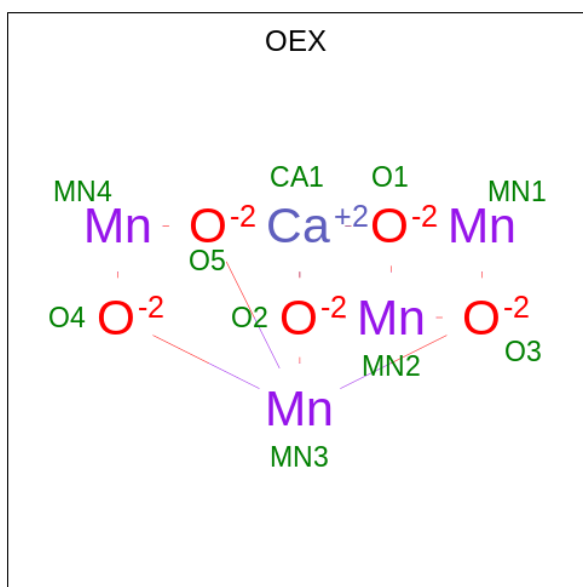
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| Mol | Chain | Residues | Atoms                  | ZeroOcc | AltConf |
|-----|-------|----------|------------------------|---------|---------|
| 28  | u     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 28  | u     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 28  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 28  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 28  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 28  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 28  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 28  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 28  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 28  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

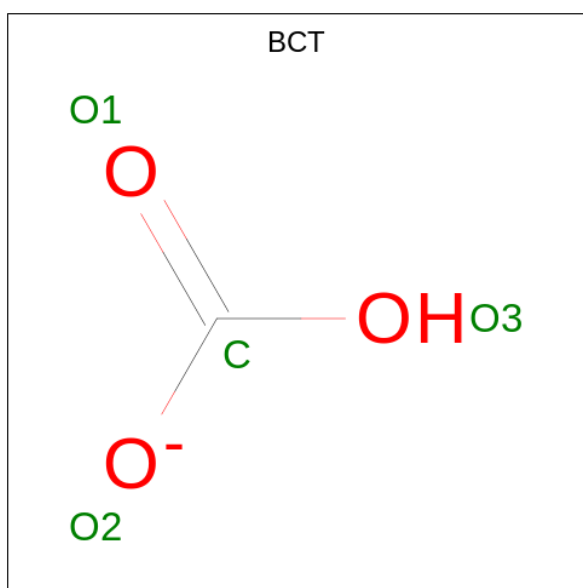
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 29  | A     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 29  | a     | 1        | Total Fe<br>1 1 | 0       | 0       |

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



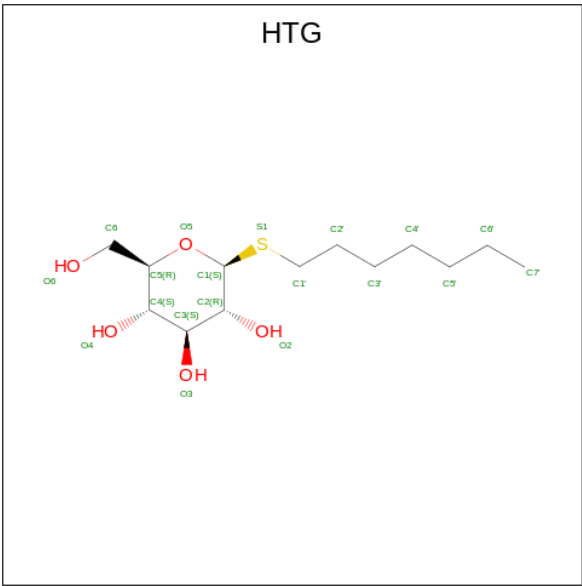
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 30  | A     | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |
| 30  | a     | 1       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

- Molecule 31 is BICARBONATE ION (CCD ID: 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 (CCD ID: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



| 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 |         |         |
| 32  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |

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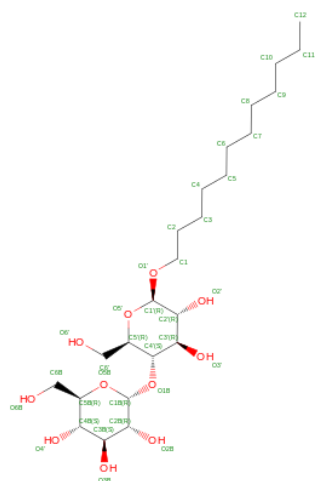
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| Mol | Chain | Residues | Atoms                    | ZeroOcc | AltConf |
|-----|-------|----------|--------------------------|---------|---------|
| 32  | b     | 1        | Total C O S<br>19 13 5 1 | 0       | 0       |
| 32  | b     | 1        | 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  | 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 (CCD ID: CA) (formula: Ca).

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

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

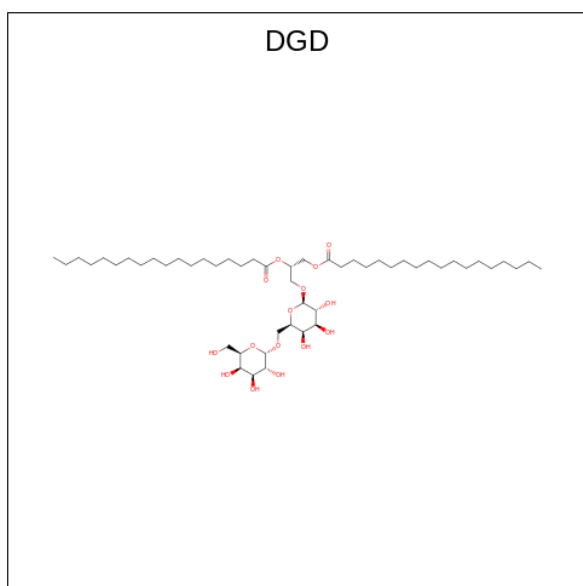


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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 34  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 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) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



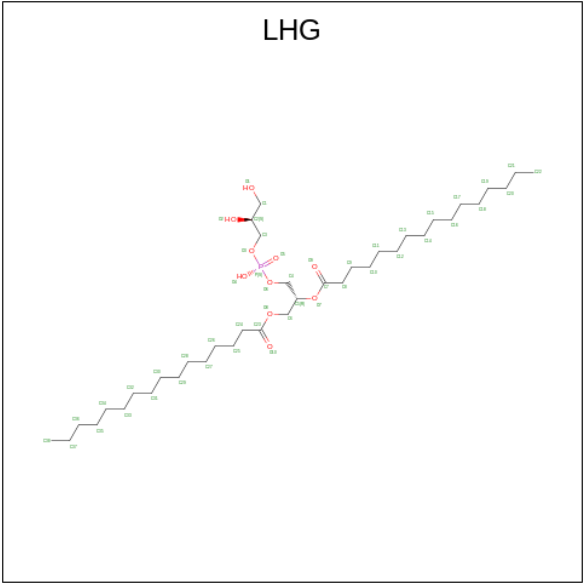
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 35  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 35  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 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 (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>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 |         |         |

- # HEM

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

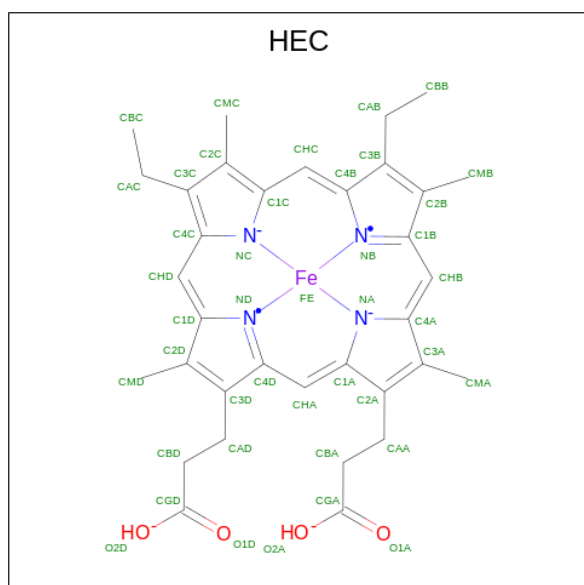
- 
- RRX
- The image shows a chemical structure of a long-chain polyene, specifically a carotenoid derivative. The structure is a zig-zag chain of alternating double and single bonds. At the right end, there is a terminal group consisting of a five-membered ring with a hydroxyl group (OH) attached to one of the ring carbons. The chain is numbered with small black numbers (1 through 22) at various positions along the backbone and on the side groups. The overall structure is drawn in a perspective view, showing the spatial arrangement of the atoms.

| 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 (CCD ID: 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 (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>36</sub>FeN<sub>4</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 40  | 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      |

*Continued on next page...*

*Continued from previous page...*

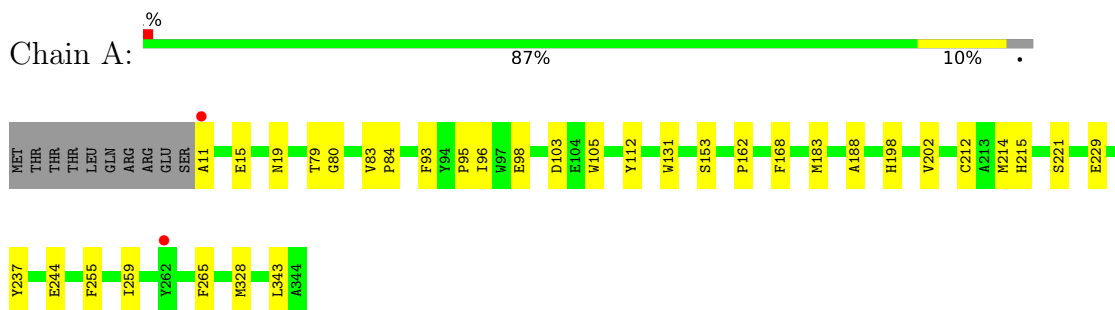
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 41  | d     | 176      | Total<br>182 | O<br>182 | 0       | 6       |
| 41  | e     | 48       | Total<br>49  | O<br>49  | 0       | 1       |
| 41  | f     | 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       |



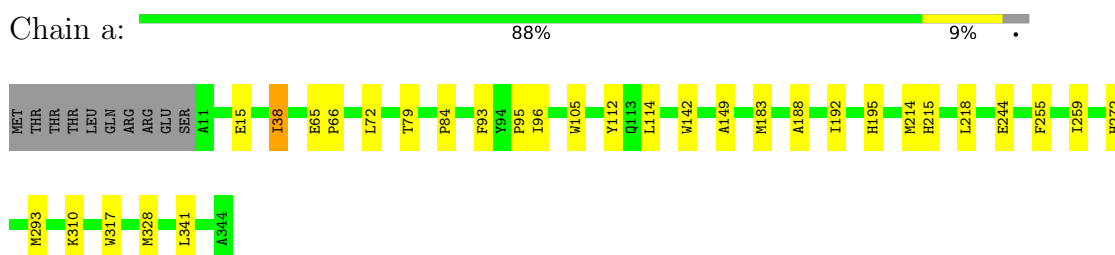
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

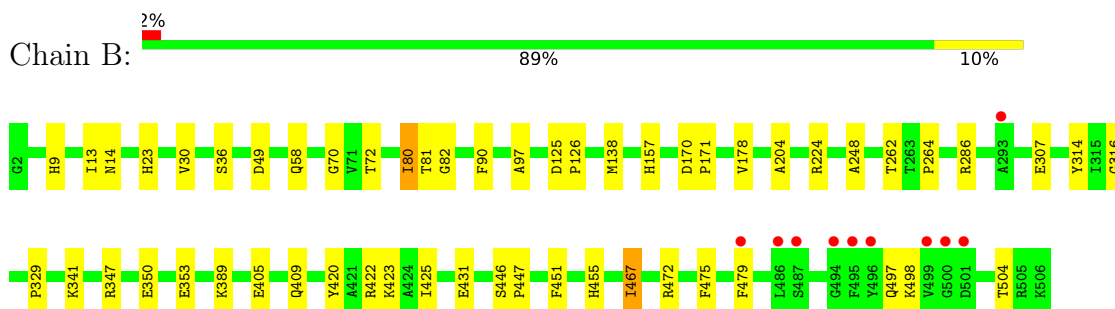
- Molecule 1: Photosystem II protein D1



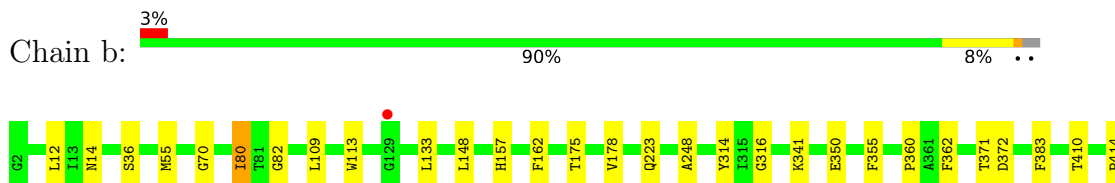
- Molecule 1: Photosystem II protein D1

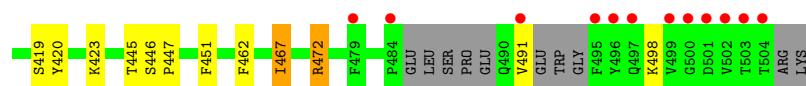


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91% 8%



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 90% 10%



• Molecule 4: Photosystem II D2 protein

Chain D: 90% 9%



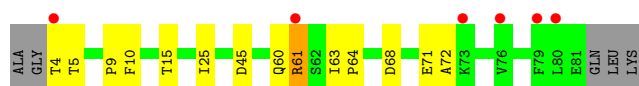
• Molecule 4: Photosystem II D2 protein

Chain d: 91% 9%

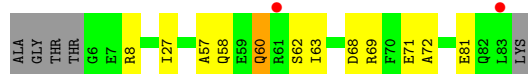
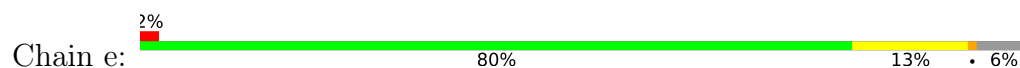


• Molecule 5: Cytochrome b559 subunit alpha

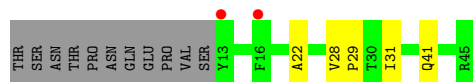
Chain E: 7% 77% 16% 6%



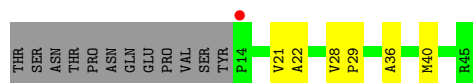
- Molecule 5: Cytochrome b559 subunit alpha



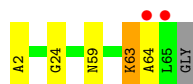
- Molecule 6: Cytochrome b559 subunit beta



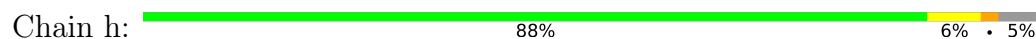
- Molecule 6: Cytochrome b559 subunit beta



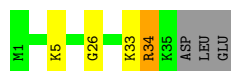
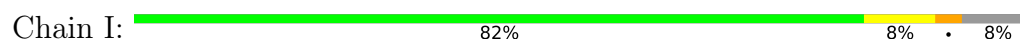
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

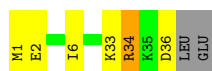


- Molecule 8: Photosystem II reaction center protein I



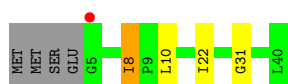
- Molecule 8: Photosystem II reaction center protein I

Chain i:  79% 13% • 5%

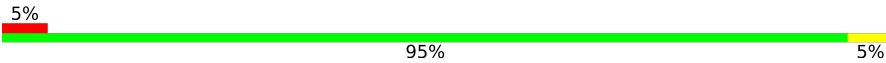


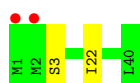
- Molecule 9: Photosystem II reaction center protein J

Chain J:  80% 8% • 10%



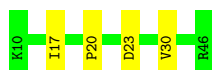
- Molecule 9: Photosystem II reaction center protein J

Chain j:  95% 5% 5%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  89% 11%

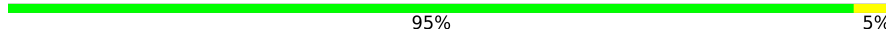


- Molecule 10: Photosystem II reaction center protein K

Chain k:  81% 16% •

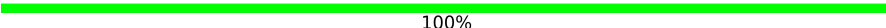


- Molecule 11: Photosystem II reaction center protein L

Chain L:  95% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 11% • 8%



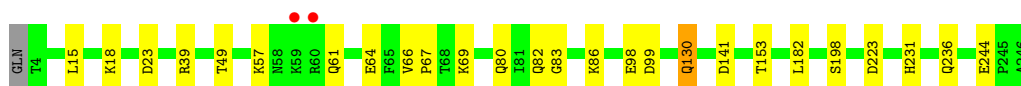
- Molecule 12: Photosystem II reaction center protein M

Chain m: 86% 8% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 89% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 88% 11%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 6% 9%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 81% 9% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 82% 12% 7%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 87% 7% 7%



- Molecule 16: Cytochrome c-550

Chain V: 96% .



- Molecule 16: Cytochrome c-550

Chain v: 91% 9%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 7% 73% 23% .



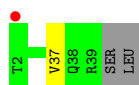
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 83% 13% .



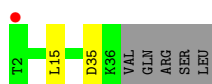
- Molecule 18: Photosystem II reaction center protein X

Chain X: 2% 92% 5%



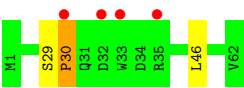
- Molecule 18: Photosystem II reaction center protein X

Chain x: 2% 82% 5% 12%

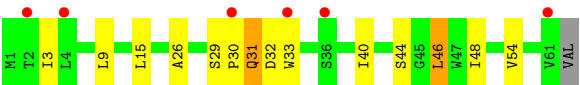
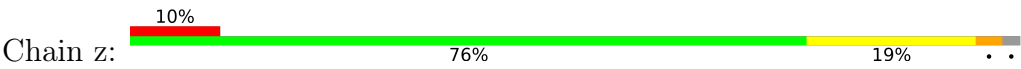


- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 6% 95% . .



● 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>99.9 (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 , 65.1                                                 | 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: HEM, DMS, FME, HEC, BCT, HTG, DGD, BCR, FE2, CL, OEX, RRX, LMG, LMT, CLA, MG, UNL, LHG, SQD, PHO, PL9, CA

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

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 1   | A     | 1.19         | 3/2717 (0.1%) | 0.98        | 2/3707 (0.1%) |
| 1   | a     | 1.15         | 3/2718 (0.1%) | 1.02        | 3/3707 (0.1%) |
| 2   | B     | 1.10         | 4/4181 (0.1%) | 0.96        | 1/5700 (0.0%) |
| 2   | b     | 1.13         | 1/4029 (0.0%) | 0.96        | 1/5490 (0.0%) |
| 3   | C     | 1.06         | 2/3599 (0.1%) | 0.95        | 1/4901 (0.0%) |
| 3   | c     | 1.03         | 1/3640 (0.0%) | 0.96        | 1/4956 (0.0%) |
| 4   | D     | 1.17         | 3/2826 (0.1%) | 0.99        | 6/3850 (0.2%) |
| 4   | d     | 1.15         | 3/2817 (0.1%) | 0.94        | 0/3839        |
| 5   | E     | 0.89         | 0/654         | 0.96        | 0/896         |
| 5   | e     | 0.85         | 0/661         | 0.99        | 2/904 (0.2%)  |
| 6   | F     | 0.93         | 0/278         | 0.82        | 0/379         |
| 6   | f     | 0.98         | 0/265         | 0.93        | 0/360         |
| 7   | H     | 0.95         | 0/524         | 0.94        | 0/715         |
| 7   | h     | 0.97         | 0/517         | 0.91        | 0/704         |
| 8   | I     | 0.86         | 0/281         | 0.93        | 1/380 (0.3%)  |
| 8   | i     | 0.80         | 0/300         | 0.90        | 0/405         |
| 9   | J     | 0.89         | 0/257         | 0.88        | 0/349         |
| 9   | j     | 0.88         | 0/278         | 1.00        | 0/378         |
| 10  | K     | 0.89         | 0/303         | 0.95        | 0/416         |
| 10  | k     | 0.85         | 0/295         | 0.91        | 0/407         |
| 11  | L     | 0.98         | 1/312 (0.3%)  | 0.95        | 0/425         |
| 11  | l     | 1.02         | 0/306         | 1.00        | 0/418         |
| 12  | M     | 0.87         | 0/265         | 1.02        | 0/362         |
| 12  | m     | 0.84         | 0/270         | 0.97        | 0/369         |
| 13  | O     | 0.95         | 0/1919        | 0.98        | 0/2607        |
| 13  | o     | 0.91         | 0/1875        | 0.98        | 0/2548        |
| 14  | T     | 0.92         | 0/259         | 1.11        | 4/352 (1.1%)  |
| 14  | t     | 0.95         | 0/257         | 0.98        | 0/349         |
| 15  | U     | 0.99         | 0/777         | 0.91        | 0/1055        |
| 15  | u     | 0.94         | 0/781         | 0.91        | 0/1059        |
| 16  | V     | 1.05         | 0/1110        | 0.99        | 0/1506        |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 16  | v     | 0.94         | 0/1073          | 0.94        | 1/1461 (0.1%)   |
| 17  | Y     | 0.72         | 0/213           | 0.96        | 0/285           |
| 17  | y     | 0.63         | 0/214           | 0.97        | 0/286           |
| 18  | X     | 0.75         | 0/277           | 1.07        | 0/375           |
| 18  | x     | 0.77         | 0/255           | 0.92        | 0/345           |
| 19  | Z     | 0.78         | 0/461           | 0.95        | 0/632           |
| 19  | z     | 0.68         | 0/444           | 1.03        | 0/611           |
| All | All   | 1.05         | 21/42208 (0.0%) | 0.97        | 23/57488 (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 21 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 343 | LEU  | C-N     | 11.57 | 1.49        | 1.33     |
| 2   | b     | 414 | PRO  | CA-C    | 6.43  | 1.58        | 1.52     |
| 4   | D     | 87  | HIS  | CG-CD2  | 6.31  | 1.42        | 1.35     |
| 4   | d     | 330 | ALA  | C-O     | -6.04 | 1.18        | 1.24     |
| 4   | d     | 117 | HIS  | ND1-CE1 | 5.87  | 1.38        | 1.32     |

The worst 5 of 23 bond angle outliers are listed below:

| Mol | Chain | Res   | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|--------|-------|-------------|----------|
| 4   | D     | 139   | ARG  | CA-C-N | -7.16 | 114.42      | 121.65   |
| 4   | D     | 139   | ARG  | C-N-CA | -7.16 | 114.42      | 121.65   |
| 14  | T     | 25[A] | GLU  | CA-C-N | -6.25 | 113.94      | 120.38   |
| 14  | T     | 25[A] | GLU  | C-N-CA | -6.25 | 113.94      | 120.38   |
| 14  | T     | 25[B] | GLU  | CA-C-N | -6.25 | 113.94      | 120.38   |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2626  | 0        | 2515     | 26      | 0            |
| 1   | a     | 2622  | 0        | 2529     | 25      | 0            |
| 2   | B     | 4012  | 0        | 3860     | 58      | 0            |
| 2   | b     | 3884  | 0        | 3743     | 50      | 0            |
| 3   | C     | 3483  | 0        | 3397     | 33      | 0            |
| 3   | c     | 3523  | 0        | 3439     | 39      | 0            |
| 4   | D     | 2728  | 0        | 2636     | 35      | 0            |
| 4   | d     | 2722  | 0        | 2623     | 27      | 0            |
| 5   | E     | 632   | 0        | 605      | 16      | 0            |
| 5   | e     | 636   | 0        | 612      | 9       | 0            |
| 6   | F     | 269   | 0        | 277      | 4       | 0            |
| 6   | f     | 257   | 0        | 269      | 4       | 0            |
| 7   | H     | 508   | 0        | 524      | 6       | 0            |
| 7   | h     | 501   | 0        | 526      | 4       | 0            |
| 8   | I     | 284   | 0        | 303      | 6       | 0            |
| 8   | i     | 300   | 0        | 320      | 2       | 0            |
| 9   | J     | 251   | 0        | 257      | 3       | 0            |
| 9   | j     | 272   | 0        | 271      | 2       | 0            |
| 10  | K     | 293   | 0        | 305      | 4       | 0            |
| 10  | k     | 285   | 0        | 290      | 4       | 0            |
| 11  | L     | 302   | 0        | 316      | 1       | 0            |
| 11  | l     | 296   | 0        | 305      | 0       | 0            |
| 12  | M     | 259   | 0        | 281      | 32      | 0            |
| 12  | m     | 264   | 0        | 283      | 26      | 0            |
| 13  | O     | 1870  | 0        | 1836     | 29      | 0            |
| 13  | o     | 1838  | 0        | 1789     | 30      | 0            |
| 14  | T     | 257   | 0        | 260      | 1       | 0            |
| 14  | t     | 258   | 0        | 261      | 3       | 0            |
| 15  | U     | 766   | 0        | 758      | 21      | 0            |
| 15  | u     | 770   | 0        | 769      | 6       | 0            |
| 16  | V     | 1080  | 0        | 1097     | 9       | 0            |
| 16  | v     | 1052  | 0        | 1040     | 14      | 0            |
| 17  | Y     | 212   | 0        | 237      | 4       | 0            |
| 17  | y     | 213   | 0        | 239      | 4       | 0            |
| 18  | X     | 274   | 0        | 297      | 1       | 0            |
| 18  | x     | 252   | 0        | 277      | 2       | 0            |
| 19  | Z     | 450   | 0        | 455      | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | z     | 433   | 0        | 422      | 7       | 0            |
| 20  | A     | 189   | 0        | 202      | 8       | 0            |
| 20  | B     | 1040  | 0        | 1152     | 22      | 0            |
| 20  | C     | 830   | 0        | 900      | 25      | 0            |
| 20  | D     | 195   | 0        | 216      | 4       | 0            |
| 20  | a     | 172   | 0        | 166      | 5       | 0            |
| 20  | b     | 1040  | 0        | 1152     | 32      | 0            |
| 20  | c     | 840   | 0        | 923      | 29      | 0            |
| 20  | d     | 195   | 0        | 216      | 4       | 0            |
| 21  | A     | 64    | 0        | 74       | 1       | 0            |
| 21  | D     | 64    | 0        | 74       | 1       | 0            |
| 21  | a     | 128   | 0        | 148      | 2       | 0            |
| 22  | A     | 40    | 0        | 56       | 5       | 0            |
| 22  | B     | 120   | 0        | 168      | 6       | 0            |
| 22  | C     | 80    | 0        | 112      | 3       | 0            |
| 22  | D     | 40    | 0        | 56       | 3       | 0            |
| 22  | K     | 80    | 0        | 112      | 3       | 0            |
| 22  | T     | 40    | 0        | 56       | 4       | 0            |
| 22  | a     | 40    | 0        | 56       | 1       | 0            |
| 22  | b     | 120   | 0        | 168      | 5       | 0            |
| 22  | c     | 40    | 0        | 56       | 1       | 0            |
| 22  | d     | 40    | 0        | 56       | 3       | 0            |
| 22  | j     | 40    | 0        | 56       | 5       | 0            |
| 22  | k     | 80    | 0        | 112      | 6       | 0            |
| 22  | t     | 40    | 0        | 56       | 4       | 0            |
| 23  | A     | 108   | 0        | 156      | 5       | 0            |
| 23  | F     | 35    | 0        | 40       | 1       | 0            |
| 23  | a     | 108   | 0        | 156      | 9       | 0            |
| 23  | b     | 54    | 0        | 78       | 3       | 0            |
| 23  | f     | 40    | 0        | 47       | 2       | 0            |
| 23  | l     | 54    | 0        | 78       | 2       | 0            |
| 24  | A     | 51    | 0        | 72       | 4       | 0            |
| 24  | B     | 51    | 0        | 72       | 0       | 0            |
| 24  | C     | 96    | 0        | 132      | 5       | 0            |
| 24  | J     | 45    | 0        | 60       | 0       | 0            |
| 24  | a     | 51    | 0        | 72       | 4       | 0            |
| 24  | b     | 49    | 0        | 68       | 2       | 0            |
| 24  | c     | 102   | 0        | 144      | 0       | 0            |
| 24  | j     | 45    | 0        | 60       | 0       | 0            |
| 25  | A     | 2     | 0        | 0        | 0       | 0            |
| 25  | a     | 2     | 0        | 0        | 0       | 0            |
| 26  | A     | 40    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26  | B     | 84    | 0        | 0        | 3       | 0            |
| 26  | C     | 34    | 0        | 0        | 0       | 0            |
| 26  | D     | 53    | 0        | 0        | 0       | 0            |
| 26  | E     | 15    | 0        | 0        | 0       | 0            |
| 26  | H     | 10    | 0        | 0        | 0       | 0            |
| 26  | I     | 61    | 0        | 0        | 0       | 0            |
| 26  | J     | 33    | 0        | 0        | 1       | 0            |
| 26  | L     | 14    | 0        | 0        | 0       | 0            |
| 26  | M     | 12    | 0        | 0        | 0       | 0            |
| 26  | T     | 13    | 0        | 0        | 0       | 0            |
| 26  | U     | 14    | 0        | 0        | 3       | 0            |
| 26  | X     | 16    | 0        | 0        | 0       | 0            |
| 26  | Z     | 4     | 0        | 0        | 0       | 0            |
| 26  | a     | 45    | 0        | 0        | 1       | 0            |
| 26  | b     | 68    | 0        | 0        | 2       | 0            |
| 26  | c     | 48    | 0        | 0        | 0       | 0            |
| 26  | d     | 68    | 0        | 0        | 0       | 0            |
| 26  | e     | 7     | 0        | 0        | 0       | 0            |
| 26  | h     | 16    | 0        | 0        | 0       | 0            |
| 26  | i     | 38    | 0        | 0        | 0       | 0            |
| 26  | j     | 22    | 0        | 0        | 0       | 0            |
| 26  | t     | 16    | 0        | 0        | 0       | 0            |
| 26  | x     | 9     | 0        | 0        | 0       | 0            |
| 26  | z     | 6     | 0        | 0        | 0       | 0            |
| 27  | A     | 55    | 0        | 80       | 11      | 0            |
| 27  | D     | 55    | 0        | 80       | 0       | 0            |
| 27  | a     | 55    | 0        | 80       | 10      | 0            |
| 27  | d     | 55    | 0        | 80       | 0       | 0            |
| 28  | A     | 20    | 0        | 30       | 8       | 0            |
| 28  | B     | 48    | 0        | 72       | 24      | 0            |
| 28  | C     | 40    | 0        | 60       | 15      | 0            |
| 28  | D     | 16    | 0        | 24       | 12      | 0            |
| 28  | F     | 4     | 0        | 6        | 3       | 0            |
| 28  | H     | 4     | 0        | 6        | 0       | 0            |
| 28  | O     | 36    | 0        | 54       | 7       | 0            |
| 28  | U     | 16    | 0        | 24       | 16      | 0            |
| 28  | V     | 24    | 0        | 36       | 5       | 0            |
| 28  | b     | 44    | 0        | 66       | 27      | 0            |
| 28  | c     | 40    | 0        | 60       | 16      | 0            |
| 28  | d     | 12    | 0        | 18       | 8       | 0            |
| 28  | h     | 4     | 0        | 6        | 0       | 0            |
| 28  | i     | 4     | 0        | 6        | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | j     | 4     | 0        | 6        | 0       | 0            |
| 28  | o     | 28    | 0        | 42       | 22      | 0            |
| 28  | u     | 12    | 0        | 18       | 3       | 0            |
| 28  | v     | 32    | 0        | 48       | 4       | 0            |
| 29  | A     | 1     | 0        | 0        | 0       | 0            |
| 29  | a     | 1     | 0        | 0        | 0       | 0            |
| 30  | A     | 10    | 0        | 0        | 0       | 0            |
| 30  | a     | 10    | 0        | 0        | 0       | 0            |
| 31  | A     | 4     | 0        | 0        | 5       | 0            |
| 31  | a     | 4     | 0        | 0        | 0       | 0            |
| 32  | B     | 95    | 0        | 130      | 17      | 0            |
| 32  | C     | 76    | 0        | 104      | 2       | 0            |
| 32  | D     | 19    | 0        | 26       | 3       | 0            |
| 32  | O     | 19    | 0        | 26       | 0       | 0            |
| 32  | V     | 13    | 0        | 11       | 0       | 0            |
| 32  | b     | 76    | 0        | 104      | 6       | 0            |
| 32  | c     | 38    | 0        | 52       | 1       | 0            |
| 32  | d     | 19    | 0        | 26       | 0       | 0            |
| 32  | u     | 8     | 0        | 15       | 0       | 0            |
| 32  | v     | 14    | 0        | 13       | 1       | 0            |
| 33  | B     | 1     | 0        | 0        | 0       | 0            |
| 33  | O     | 1     | 0        | 0        | 0       | 0            |
| 33  | V     | 1     | 0        | 0        | 0       | 0            |
| 33  | b     | 1     | 0        | 0        | 0       | 0            |
| 33  | c     | 1     | 0        | 0        | 0       | 0            |
| 33  | o     | 1     | 0        | 0        | 0       | 0            |
| 34  | B     | 64    | 0        | 95       | 4       | 0            |
| 34  | E     | 24    | 0        | 35       | 0       | 0            |
| 34  | I     | 35    | 0        | 46       | 2       | 0            |
| 34  | J     | 24    | 0        | 35       | 1       | 0            |
| 34  | M     | 35    | 0        | 46       | 0       | 0            |
| 34  | T     | 24    | 0        | 35       | 0       | 0            |
| 34  | Z     | 35    | 0        | 46       | 0       | 0            |
| 34  | a     | 35    | 0        | 46       | 10      | 0            |
| 34  | b     | 57    | 0        | 72       | 3       | 0            |
| 34  | c     | 35    | 0        | 46       | 2       | 0            |
| 34  | f     | 24    | 0        | 35       | 0       | 0            |
| 34  | m     | 70    | 0        | 92       | 1       | 0            |
| 34  | z     | 35    | 0        | 46       | 5       | 0            |
| 35  | C     | 179   | 0        | 232      | 0       | 0            |
| 35  | D     | 51    | 0        | 71       | 5       | 0            |
| 35  | H     | 62    | 0        | 82       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | c     | 181   | 0        | 236      | 3       | 0            |
| 35  | d     | 51    | 0        | 71       | 2       | 0            |
| 35  | h     | 62    | 0        | 82       | 1       | 0            |
| 36  | D     | 147   | 0        | 222      | 19      | 0            |
| 36  | E     | 48    | 0        | 71       | 6       | 0            |
| 36  | L     | 49    | 0        | 74       | 0       | 0            |
| 36  | d     | 147   | 0        | 222      | 22      | 0            |
| 36  | l     | 49    | 0        | 74       | 1       | 0            |
| 37  | E     | 43    | 0        | 30       | 1       | 0            |
| 37  | e     | 43    | 0        | 30       | 3       | 0            |
| 38  | H     | 41    | 0        | 56       | 0       | 0            |
| 38  | x     | 41    | 0        | 56       | 3       | 0            |
| 39  | J     | 1     | 0        | 0        | 0       | 0            |
| 39  | j     | 1     | 0        | 0        | 0       | 0            |
| 40  | V     | 43    | 0        | 30       | 0       | 0            |
| 40  | v     | 43    | 0        | 30       | 0       | 0            |
| 41  | A     | 182   | 0        | 0        | 3       | 0            |
| 41  | B     | 473   | 0        | 0        | 18      | 0            |
| 41  | C     | 324   | 0        | 0        | 9       | 0            |
| 41  | D     | 180   | 0        | 0        | 1       | 0            |
| 41  | E     | 66    | 0        | 0        | 1       | 0            |
| 41  | F     | 8     | 0        | 0        | 0       | 0            |
| 41  | H     | 65    | 0        | 0        | 2       | 0            |
| 41  | I     | 16    | 0        | 0        | 1       | 0            |
| 41  | J     | 23    | 0        | 0        | 0       | 0            |
| 41  | K     | 12    | 0        | 0        | 0       | 0            |
| 41  | L     | 21    | 0        | 0        | 0       | 0            |
| 41  | M     | 12    | 0        | 0        | 1       | 0            |
| 41  | O     | 273   | 0        | 0        | 10      | 0            |
| 41  | T     | 20    | 0        | 0        | 0       | 0            |
| 41  | U     | 136   | 0        | 0        | 4       | 0            |
| 41  | V     | 183   | 0        | 0        | 4       | 0            |
| 41  | X     | 22    | 0        | 0        | 1       | 0            |
| 41  | Y     | 7     | 0        | 0        | 0       | 0            |
| 41  | Z     | 5     | 0        | 0        | 0       | 0            |
| 41  | a     | 185   | 0        | 0        | 6       | 0            |
| 41  | b     | 465   | 0        | 0        | 8       | 0            |
| 41  | c     | 374   | 0        | 0        | 4       | 0            |
| 41  | d     | 182   | 0        | 0        | 5       | 0            |
| 41  | e     | 49    | 0        | 0        | 0       | 0            |
| 41  | f     | 16    | 0        | 0        | 0       | 0            |
| 41  | h     | 70    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41  | i     | 21    | 0        | 0        | 2       | 0            |
| 41  | j     | 24    | 0        | 0        | 0       | 0            |
| 41  | k     | 12    | 0        | 0        | 0       | 0            |
| 41  | l     | 24    | 0        | 0        | 1       | 0            |
| 41  | m     | 24    | 0        | 0        | 0       | 0            |
| 41  | o     | 230   | 0        | 0        | 10      | 0            |
| 41  | t     | 20    | 0        | 0        | 0       | 0            |
| 41  | u     | 150   | 0        | 0        | 0       | 0            |
| 41  | v     | 147   | 0        | 0        | 2       | 0            |
| 41  | x     | 26    | 0        | 0        | 1       | 0            |
| 41  | y     | 7     | 0        | 0        | 1       | 0            |
| 41  | z     | 12    | 0        | 0        | 1       | 0            |
| All | All   | 54996 | 0        | 51554    | 741     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 741 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:M:16[B]:LEU:HD11 | 12:m:16[B]:LEU:CD2  | 1.18                     | 1.58              |
| 12:M:16[B]:LEU:CD1  | 12:m:16[B]:LEU:HD22 | 1.43                     | 1.45              |
| 12:M:16[B]:LEU:CD2  | 12:m:16[B]:LEU:HD11 | 1.55                     | 1.32              |
| 12:M:16[B]:LEU:CD1  | 12:m:16[B]:LEU:CD2  | 2.06                     | 1.19              |
| 3:c:362:ARG:HD3     | 28:c:530:DMS:H11    | 1.21                     | 1.19              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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



| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 335/344 (97%)  | 329 (98%) | 5 (2%)  | 1 (0%)   | 36          | 25  |
| 1   | a     | 336/344 (98%)  | 330 (98%) | 5 (2%)  | 1 (0%)   | 36          | 25  |
| 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%)   | 43          | 31  |
| 3   | c     | 454/455 (100%) | 442 (97%) | 11 (2%) | 1 (0%)   | 43          | 31  |
| 4   | D     | 341/342 (100%) | 334 (98%) | 6 (2%)  | 1 (0%)   | 36          | 25  |
| 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 |
| 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%)   | 30          | 17  |
| 13  | o     | 243/244 (100%) | 231 (95%) | 9 (4%)  | 3 (1%)   | 10          | 2   |
| 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 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 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%)   | 7           | 1   |
| 19  | z     | 59/62 (95%)     | 54 (92%)   | 3 (5%)   | 2 (3%)   | 3           | 0   |
| All | All   | 5201/5350 (97%) | 5069 (98%) | 120 (2%) | 12 (0%)  | 43          | 31  |

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%)   | 84          | 82 |
| 1   | a     | 270/279 (97%)  | 269 (100%) | 1 (0%)   | 84          | 82 |
| 2   | B     | 405/403 (100%) | 401 (99%)  | 4 (1%)   | 68          | 60 |
| 2   | b     | 390/403 (97%)  | 385 (99%)  | 5 (1%)   | 61          | 51 |
| 3   | C     | 351/356 (99%)  | 347 (99%)  | 4 (1%)   | 65          | 57 |
| 3   | c     | 356/356 (100%) | 353 (99%)  | 3 (1%)   | 73          | 67 |
| 4   | D     | 277/277 (100%) | 274 (99%)  | 3 (1%)   | 65          | 57 |
| 4   | d     | 276/277 (100%) | 274 (99%)  | 2 (1%)   | 76          | 70 |
| 5   | E     | 68/72 (94%)    | 65 (96%)   | 3 (4%)   | 25          | 10 |
| 5   | e     | 68/72 (94%)    | 64 (94%)   | 4 (6%)   | 18          | 5  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 6   | F     | 27/38 (71%)     | 27 (100%)  | 0        | 100         | 100 |
| 6   | f     | 26/38 (68%)     | 26 (100%)  | 0        | 100         | 100 |
| 7   | H     | 54/54 (100%)    | 53 (98%)   | 1 (2%)   | 50          | 38  |
| 7   | h     | 54/54 (100%)    | 53 (98%)   | 1 (2%)   | 50          | 38  |
| 8   | I     | 30/34 (88%)     | 30 (100%)  | 0        | 100         | 100 |
| 8   | i     | 32/34 (94%)     | 28 (88%)   | 4 (12%)  | 4           | 0   |
| 9   | J     | 23/28 (82%)     | 21 (91%)   | 2 (9%)   | 9           | 2   |
| 9   | j     | 24/28 (86%)     | 24 (100%)  | 0        | 100         | 100 |
| 10  | K     | 30/30 (100%)    | 29 (97%)   | 1 (3%)   | 33          | 18  |
| 10  | k     | 28/30 (93%)     | 26 (93%)   | 2 (7%)   | 13          | 3   |
| 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%)   | 33          | 18  |
| 12  | m     | 30/33 (91%)     | 30 (100%)  | 0        | 100         | 100 |
| 13  | O     | 207/207 (100%)  | 204 (99%)  | 3 (1%)   | 59          | 49  |
| 13  | o     | 199/207 (96%)   | 199 (100%) | 0        | 100         | 100 |
| 14  | T     | 26/28 (93%)     | 23 (88%)   | 3 (12%)  | 5           | 1   |
| 14  | t     | 26/28 (93%)     | 25 (96%)   | 1 (4%)   | 29          | 14  |
| 15  | U     | 82/89 (92%)     | 82 (100%)  | 0        | 100         | 100 |
| 15  | u     | 83/89 (93%)     | 82 (99%)   | 1 (1%)   | 63          | 55  |
| 16  | V     | 120/117 (103%)  | 119 (99%)  | 1 (1%)   | 73          | 67  |
| 16  | v     | 114/117 (97%)   | 113 (99%)  | 1 (1%)   | 70          | 64  |
| 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%)   | 44          | 30  |
| 19  | z     | 39/52 (75%)     | 37 (95%)   | 2 (5%)   | 21          | 7   |
| All | All   | 4223/4376 (96%) | 4166 (99%) | 57 (1%)  | 63          | 51  |

5 of 57 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | Y     | 30  | ILE  |
| 19  | z     | 29  | SER  |
| 2   | b     | 472 | ARG  |
| 16  | v     | 6   | GLU  |
| 8   | i     | 36  | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 53  | ASN  |
| 15  | u     | 73  | GLN  |
| 2   | b     | 331 | ASN  |
| 16  | v     | 118 | HIS  |
| 13  | o     | 82  | 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 | $\# Z  > 2$ |
| 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%)     |
| 8   | FME  | I     | 1   | 8    | 8,9,10       | 0.69 | 0           | 7,9,11      | 1.11 | 0           |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 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 | -     |
| 8   | FME  | I     | 1   | 8    | -       | 2/7/9/11 | -     |

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 349 ligands modelled in this entry, 14 are monoatomic and 55 are unknown - 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 | $\# Z  > 2$ |
| 20  | CLA  | a     | 404    | 41   | 64,68,73     | 1.94 | 17 (26%)    | 77,107,113  | 2.44 | 27 (35%)    |
| 22  | BCR  | K     | 101    | -    | 41,41,41     | 0.83 | 1 (2%)      | 56,56,56    | 1.48 | 13 (23%)    |
| 28  | DMS  | U     | 903[B] | -    | 3,3,3        | 2.44 | 1 (33%)     | 3,3,3       | 0.17 | 0           |
| 28  | DMS  | b     | 635    | -    | 3,3,3        | 2.68 | 1 (33%)     | 3,3,3       | 0.75 | 0           |
| 23  | SQD  | A     | 412    | -    | 53,54,54     | 1.02 | 3 (5%)      | 62,65,65    | 1.71 | 10 (16%)    |
| 28  | DMS  | b     | 633    | -    | 3,3,3        | 2.55 | 1 (33%)     | 3,3,3       | 1.05 | 0           |
| 20  | CLA  | b     | 605    | 2    | 69,73,73     | 2.13 | 20 (28%)    | 83,113,113  | 2.37 | 31 (37%)    |
| 23  | SQD  | l     | 101    | -    | 53,54,54     | 1.08 | 4 (7%)      | 62,65,65    | 1.68 | 8 (12%)     |
| 20  | CLA  | c     | 501    | 3    | 69,73,73     | 2.13 | 17 (24%)    | 83,113,113  | 2.95 | 29 (34%)    |
| 28  | DMS  | B     | 641    | -    | 3,3,3        | 2.65 | 1 (33%)     | 3,3,3       | 0.64 | 0           |
| 32  | HTG  | c     | 521    | -    | 19,19,19     | 0.96 | 1 (5%)      | 23,24,24    | 2.03 | 3 (13%)     |
| 20  | CLA  | b     | 616    | 2    | 69,73,73     | 2.02 | 15 (21%)    | 83,113,113  | 2.67 | 34 (40%)    |
| 28  | DMS  | V     | 207    | -    | 3,3,3        | 2.58 | 1 (33%)     | 3,3,3       | 0.47 | 0           |
| 21  | PHO  | A     | 403    | -    | 58,69,69     | 2.32 | 12 (20%)    | 56,99,99    | 3.15 | 13 (23%)    |
| 22  | BCR  | b     | 621    | -    | 41,41,41     | 0.80 | 1 (2%)      | 56,56,56    | 1.47 | 8 (14%)     |
| 22  | BCR  | c     | 514    | -    | 41,41,41     | 0.85 | 1 (2%)      | 56,56,56    | 1.49 | 7 (12%)     |
| 28  | DMS  | D     | 413    | -    | 3,3,3        | 2.73 | 1 (33%)     | 3,3,3       | 0.66 | 0           |
| 32  | HTG  | C     | 534    | -    | 19,19,19     | 1.08 | 1 (5%)      | 23,24,24    | 1.47 | 5 (21%)     |
| 20  | CLA  | C     | 501    | 3    | 69,73,73     | 2.09 | 19 (27%)    | 83,113,113  | 2.28 | 22 (26%)    |
| 20  | CLA  | B     | 611    | 41   | 69,73,73     | 2.26 | 18 (26%)    | 83,113,113  | 2.49 | 28 (33%)    |
| 21  | PHO  | D     | 403    | -    | 58,69,69     | 2.60 | 12 (20%)    | 56,99,99    | 2.95 | 17 (30%)    |
| 32  | HTG  | D     | 417    | -    | 19,19,19     | 1.05 | 1 (5%)      | 23,24,24    | 1.49 | 3 (13%)     |
| 28  | DMS  | o     | 305    | -    | 3,3,3        | 2.73 | 1 (33%)     | 3,3,3       | 0.77 | 0           |
| 34  | LMT  | m     | 101    | -    | 36,36,36     | 0.61 | 1 (2%)      | 47,47,47    | 0.96 | 1 (2%)      |
| 28  | DMS  | u     | 203    | -    | 3,3,3        | 2.57 | 1 (33%)     | 3,3,3       | 0.78 | 0           |
| 20  | CLA  | a     | 407    | 1    | 51,55,73     | 2.37 | 17 (33%)    | 61,91,113   | 2.64 | 27 (44%)    |
| 28  | DMS  | B     | 634    | -    | 3,3,3        | 1.94 | 1 (33%)     | 3,3,3       | 0.29 | 0           |
| 20  | CLA  | c     | 502    | 3    | 69,73,73     | 2.19 | 19 (27%)    | 83,113,113  | 2.55 | 30 (36%)    |
| 28  | DMS  | h     | 102    | -    | 3,3,3        | 2.75 | 1 (33%)     | 3,3,3       | 0.56 | 0           |
| 24  | LMG  | c     | 519    | -    | 51,51,55     | 1.01 | 3 (5%)      | 59,59,63    | 1.17 | 7 (11%)     |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | CLA  | b     | 607    | 2    | 69,73,73     | 2.09 | 19 (27%) | 83,113,113  | 2.40 | 23 (27%) |
| 28  | DMS  | A     | 418    | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.73 | 0        |
| 36  | LHG  | D     | 407    | -    | 48,48,48     | 0.86 | 1 (2%)   | 51,54,54    | 1.26 | 5 (9%)   |
| 27  | PL9  | d     | 412    | -    | 55,55,55     | 1.09 | 3 (5%)   | 68,69,69    | 1.59 | 16 (23%) |
| 32  | HTG  | O     | 302    | -    | 19,19,19     | 1.29 | 2 (10%)  | 23,24,24    | 1.18 | 2 (8%)   |
| 20  | CLA  | B     | 614    | 2    | 69,73,73     | 1.90 | 17 (24%) | 83,113,113  | 2.22 | 24 (28%) |
| 20  | CLA  | A     | 404    | 1    | 69,73,73     | 2.02 | 19 (27%) | 83,113,113  | 2.75 | 30 (36%) |
| 21  | PHO  | a     | 405    | -    | 58,69,69     | 2.26 | 14 (24%) | 56,99,99    | 2.61 | 14 (25%) |
| 22  | BCR  | b     | 619    | -    | 41,41,41     | 0.95 | 0        | 56,56,56    | 1.77 | 11 (19%) |
| 28  | DMS  | V     | 209    | -    | 3,3,3        | 2.61 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 28  | DMS  | c     | 529    | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 28  | DMS  | i     | 104    | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.33 | 0        |
| 20  | CLA  | d     | 402    | 4    | 69,73,73     | 1.88 | 20 (28%) | 83,113,113  | 2.02 | 25 (30%) |
| 36  | LHG  | D     | 409    | -    | 48,48,48     | 0.95 | 2 (4%)   | 51,54,54    | 1.05 | 3 (5%)   |
| 32  | HTG  | C     | 521    | -    | 19,19,19     | 0.98 | 2 (10%)  | 23,24,24    | 1.97 | 4 (17%)  |
| 28  | DMS  | C     | 530    | -    | 3,3,3        | 2.61 | 1 (33%)  | 3,3,3       | 1.00 | 0        |
| 28  | DMS  | b     | 632    | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 28  | DMS  | v     | 203    | -    | 3,3,3        | 2.59 | 1 (33%)  | 3,3,3       | 0.85 | 0        |
| 20  | CLA  | B     | 606    | 2    | 69,73,73     | 1.93 | 16 (23%) | 83,113,113  | 2.49 | 30 (36%) |
| 20  | CLA  | b     | 614    | 2    | 69,73,73     | 2.04 | 20 (28%) | 83,113,113  | 2.37 | 28 (33%) |
| 24  | LMG  | c     | 518    | -    | 51,51,55     | 1.11 | 3 (5%)   | 59,59,63    | 1.31 | 7 (11%)  |
| 27  | PL9  | A     | 411    | -    | 55,55,55     | 0.83 | 3 (5%)   | 68,69,69    | 1.69 | 18 (26%) |
| 28  | DMS  | v     | 205    | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 20  | CLA  | B     | 608    | 41   | 69,73,73     | 1.95 | 14 (20%) | 83,113,113  | 2.22 | 23 (27%) |
| 28  | DMS  | c     | 532    | -    | 3,3,3        | 2.60 | 1 (33%)  | 3,3,3       | 0.47 | 0        |
| 31  | BCT  | A     | 421    | 29   | 2,3,3        | 0.47 | 0        | 2,3,3       | 1.14 | 0        |
| 32  | HTG  | b     | 624    | -    | 19,19,19     | 1.15 | 2 (10%)  | 23,24,24    | 1.60 | 2 (8%)   |
| 28  | DMS  | A     | 416    | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 24  | LMG  | a     | 410    | -    | 51,51,55     | 0.89 | 2 (3%)   | 59,59,63    | 1.08 | 2 (3%)   |
| 28  | DMS  | U     | 903[A] | -    | 3,3,3        | 2.56 | 1 (33%)  | 3,3,3       | 0.75 | 0        |
| 28  | DMS  | c     | 530    | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 1.01 | 0        |
| 28  | DMS  | v     | 204    | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 22  | BCR  | t     | 101    | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.74 | 19 (33%) |
| 28  | DMS  | B     | 638    | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.82 | 0        |
| 38  | RRX  | x     | 101    | -    | 42,42,42     | 0.82 | 0        | 57,58,58    | 1.22 | 6 (10%)  |

| Mol | Type | Chain | Res | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | BCR  | D     | 405 | -      | 41,41,41     | 1.03 | 3 (7%)   | 56,56,56    | 1.73 | 13 (23%) |
| 28  | DMS  | o     | 302 | -      | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.90 | 0        |
| 28  | DMS  | B     | 639 | -      | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.63 | 0        |
| 24  | LMG  | j     | 101 | 39     | 45,45,55     | 1.00 | 3 (6%)   | 53,53,63    | 1.02 | 6 (11%)  |
| 20  | CLA  | C     | 510 | 3      | 69,73,73     | 2.20 | 20 (28%) | 83,113,113  | 2.33 | 27 (32%) |
| 35  | DGD  | H     | 102 | -      | 63,63,67     | 1.04 | 3 (4%)   | 77,77,81    | 1.27 | 8 (10%)  |
| 20  | CLA  | C     | 503 | 3      | 69,73,73     | 2.41 | 21 (30%) | 83,113,113  | 2.20 | 27 (32%) |
| 28  | DMS  | B     | 640 | -      | 3,3,3        | 2.55 | 1 (33%)  | 3,3,3       | 0.97 | 0        |
| 22  | BCR  | C     | 515 | -      | 41,41,41     | 0.97 | 0        | 56,56,56    | 1.19 | 6 (10%)  |
| 28  | DMS  | b     | 639 | -      | 3,3,3        | 2.81 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 32  | HTG  | C     | 522 | -      | 19,19,19     | 1.06 | 2 (10%)  | 23,24,24    | 1.56 | 1 (4%)   |
| 34  | LMT  | B     | 626 | -      | 24,24,36     | 0.54 | 0        | 29,29,47    | 1.14 | 3 (10%)  |
| 28  | DMS  | C     | 532 | -      | 3,3,3        | 3.28 | 1 (33%)  | 3,3,3       | 1.29 | 1 (33%)  |
| 20  | CLA  | c     | 505 | 3      | 69,73,73     | 2.22 | 21 (30%) | 83,113,113  | 2.16 | 23 (27%) |
| 28  | DMS  | b     | 640 | -      | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 1.38 | 1 (33%)  |
| 28  | DMS  | c     | 531 | -      | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 28  | DMS  | d     | 413 | -      | 3,3,3        | 2.57 | 1 (33%)  | 3,3,3       | 0.91 | 0        |
| 32  | HTG  | C     | 520 | -      | 19,19,19     | 0.89 | 1 (5%)   | 23,24,24    | 1.46 | 1 (4%)   |
| 22  | BCR  | k     | 102 | -      | 41,41,41     | 0.79 | 0        | 56,56,56    | 1.29 | 9 (16%)  |
| 28  | DMS  | u     | 202 | -      | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 1.29 | 0        |
| 36  | LHG  | E     | 103 | -      | 46,46,48     | 1.03 | 2 (4%)   | 49,50,54    | 1.14 | 5 (10%)  |
| 36  | LHG  | d     | 408 | -      | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 0.99 | 5 (9%)   |
| 34  | LMT  | M     | 101 | -      | 36,36,36     | 0.64 | 0        | 47,47,47    | 0.93 | 2 (4%)   |
| 30  | OEX  | a     | 419 | 3,41,1 | 0,14,14      | -    | -        | -           | -    | -        |
| 22  | BCR  | B     | 617 | -      | 41,41,41     | 0.98 | 0        | 56,56,56    | 1.62 | 11 (19%) |
| 20  | CLA  | C     | 502 | 3      | 69,73,73     | 2.23 | 18 (26%) | 83,113,113  | 2.33 | 29 (34%) |
| 28  | DMS  | B     | 637 | -      | 3,3,3        | 2.56 | 1 (33%)  | 3,3,3       | 0.73 | 0        |
| 28  | DMS  | V     | 205 | -      | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 24  | LMG  | B     | 620 | -      | 51,51,55     | 1.02 | 2 (3%)   | 59,59,63    | 1.31 | 5 (8%)   |
| 28  | DMS  | v     | 208 | -      | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.66 | 0        |
| 32  | HTG  | d     | 401 | -      | 19,19,19     | 1.08 | 1 (5%)   | 23,24,24    | 2.36 | 4 (17%)  |
| 20  | CLA  | b     | 610 | 2      | 69,73,73     | 2.25 | 18 (26%) | 83,113,113  | 2.27 | 24 (28%) |
| 28  | DMS  | A     | 415 | -      | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 1.01 | 0        |
| 20  | CLA  | B     | 610 | 2      | 69,73,73     | 2.30 | 19 (27%) | 83,113,113  | 2.22 | 27 (32%) |
| 28  | DMS  | o     | 303 | -      | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.50 | 0        |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | LHG  | D     | 408 | -    | 48,48,48     | 0.82 | 2 (4%)   | 51,54,54    | 1.03 | 1 (1%)   |
| 20  | CLA  | c     | 510 | 3    | 69,73,73     | 1.99 | 20 (28%) | 83,113,113  | 2.37 | 32 (38%) |
| 28  | DMS  | C     | 529 | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 20  | CLA  | b     | 606 | 2    | 69,73,73     | 2.02 | 19 (27%) | 83,113,113  | 2.40 | 26 (31%) |
| 34  | LMT  | E     | 101 | -    | 24,24,36     | 0.62 | 1 (4%)   | 29,29,47    | 1.01 | 3 (10%)  |
| 20  | CLA  | B     | 601 | 2    | 69,73,73     | 2.07 | 18 (26%) | 83,113,113  | 2.37 | 29 (34%) |
| 20  | CLA  | C     | 511 | 3    | 69,73,73     | 2.32 | 21 (30%) | 83,113,113  | 2.57 | 30 (36%) |
| 28  | DMS  | d     | 415 | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 32  | HTG  | B     | 632 | -    | 19,19,19     | 1.02 | 1 (5%)   | 23,24,24    | 1.26 | 2 (8%)   |
| 28  | DMS  | U     | 902 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 1.63 | 1 (33%)  |
| 34  | LMT  | B     | 627 | -    | 15,15,36     | 0.48 | 0        | 14,14,47    | 0.67 | 0        |
| 20  | CLA  | C     | 507 | 41   | 69,73,73     | 2.40 | 21 (30%) | 83,113,113  | 2.43 | 26 (31%) |
| 20  | CLA  | C     | 512 | 3    | 59,63,73     | 2.76 | 24 (40%) | 71,101,113  | 2.50 | 27 (38%) |
| 20  | CLA  | b     | 618 | 2    | 69,73,73     | 2.18 | 21 (30%) | 83,113,113  | 2.36 | 28 (33%) |
| 28  | DMS  | c     | 533 | -    | 3,3,3        | 2.74 | 1 (33%)  | 3,3,3       | 0.83 | 0        |
| 28  | DMS  | D     | 415 | -    | 3,3,3        | 2.92 | 1 (33%)  | 3,3,3       | 0.73 | 0        |
| 20  | CLA  | a     | 403 | 1    | 69,73,73     | 1.85 | 15 (21%) | 83,113,113  | 2.22 | 27 (32%) |
| 28  | DMS  | c     | 528 | -    | 3,3,3        | 2.57 | 1 (33%)  | 3,3,3       | 0.44 | 0        |
| 20  | CLA  | C     | 508 | 3    | 64,68,73     | 2.49 | 19 (29%) | 77,107,113  | 2.50 | 27 (35%) |
| 23  | SQD  | b     | 622 | -    | 53,54,54     | 1.10 | 3 (5%)   | 62,65,65    | 1.55 | 11 (17%) |
| 23  | SQD  | f     | 101 | -    | 39,40,54     | 1.37 | 3 (7%)   | 48,51,65    | 3.70 | 12 (25%) |
| 20  | CLA  | C     | 506 | 3    | 69,73,73     | 2.39 | 22 (31%) | 83,113,113  | 2.35 | 23 (27%) |
| 20  | CLA  | B     | 612 | 2    | 69,73,73     | 1.85 | 14 (20%) | 83,113,113  | 2.39 | 29 (34%) |
| 28  | DMS  | O     | 311 | -    | 3,3,3        | 2.87 | 1 (33%)  | 3,3,3       | 0.92 | 0        |
| 28  | DMS  | j     | 105 | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.85 | 0        |
| 32  | HTG  | u     | 201 | -    | 7,7,19       | 0.43 | 0        | 6,6,24      | 0.70 | 0        |
| 20  | CLA  | D     | 404 | 4    | 69,73,73     | 2.11 | 22 (31%) | 83,113,113  | 2.43 | 32 (38%) |
| 28  | DMS  | O     | 307 | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.42 | 0        |
| 34  | LMT  | z     | 102 | -    | 36,36,36     | 0.76 | 1 (2%)   | 47,47,47    | 1.49 | 8 (17%)  |
| 22  | BCR  | B     | 619 | -    | 41,41,41     | 1.06 | 1 (2%)   | 56,56,56    | 1.58 | 9 (16%)  |
| 28  | DMS  | V     | 204 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 32  | HTG  | b     | 601 | -    | 19,19,19     | 1.04 | 2 (10%)  | 23,24,24    | 1.27 | 2 (8%)   |
| 20  | CLA  | c     | 506 | 3    | 69,73,73     | 2.38 | 20 (28%) | 83,113,113  | 2.41 | 28 (33%) |
| 22  | BCR  | K     | 102 | -    | 41,41,41     | 0.92 | 1 (2%)   | 56,56,56    | 1.48 | 6 (10%)  |
| 35  | DGD  | C     | 518 | -    | 63,63,67     | 0.86 | 2 (3%)   | 77,77,81    | 1.04 | 3 (3%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | DMS  | O     | 305 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.79 | 0        |
| 20  | CLA  | C     | 504 | 41   | 69,73,73     | 2.23 | 17 (24%) | 83,113,113  | 2.33 | 24 (28%) |
| 28  | DMS  | o     | 306 | -    | 3,3,3        | 2.79 | 1 (33%)  | 3,3,3       | 1.03 | 0        |
| 28  | DMS  | O     | 310 | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.70 | 0        |
| 32  | HTG  | B     | 622 | -    | 19,19,19     | 1.34 | 3 (15%)  | 23,24,24    | 1.93 | 6 (26%)  |
| 20  | CLA  | b     | 608 | 2    | 69,73,73     | 2.33 | 18 (26%) | 83,113,113  | 2.26 | 25 (30%) |
| 22  | BCR  | j     | 102 | -    | 41,41,41     | 0.85 | 0        | 56,56,56    | 1.38 | 9 (16%)  |
| 28  | DMS  | O     | 304 | -    | 3,3,3        | 2.61 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 28  | DMS  | v     | 207 | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 28  | DMS  | O     | 306 | -    | 3,3,3        | 2.53 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 34  | LMT  | B     | 625 | -    | 24,24,36     | 0.53 | 0        | 29,29,47    | 1.26 | 4 (13%)  |
| 20  | CLA  | A     | 402 | 41   | 63,67,73     | 1.85 | 18 (28%) | 75,105,113  | 2.96 | 31 (41%) |
| 20  | CLA  | D     | 402 | 41   | 69,73,73     | 1.96 | 20 (28%) | 83,113,113  | 2.27 | 23 (27%) |
| 28  | DMS  | C     | 528 | -    | 3,3,3        | 2.31 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 20  | CLA  | c     | 511 | 3    | 69,73,73     | 2.48 | 19 (27%) | 83,113,113  | 2.38 | 24 (28%) |
| 32  | HTG  | v     | 210 | -    | 14,14,19     | 0.62 | 0        | 18,19,24    | 2.19 | 4 (22%)  |
| 22  | BCR  | B     | 618 | -    | 41,41,41     | 1.05 | 0        | 56,56,56    | 1.26 | 7 (12%)  |
| 28  | DMS  | b     | 637 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 40  | HEC  | V     | 201 | 16   | 50,50,50     | 1.82 | 10 (20%) | 68,82,82    | 1.59 | 11 (16%) |
| 32  | HTG  | b     | 625 | -    | 19,19,19     | 1.21 | 2 (10%)  | 23,24,24    | 1.34 | 4 (17%)  |
| 20  | CLA  | C     | 505 | 3    | 69,73,73     | 2.38 | 21 (30%) | 83,113,113  | 2.11 | 23 (27%) |
| 32  | HTG  | B     | 621 | -    | 19,19,19     | 1.45 | 3 (15%)  | 23,24,24    | 1.79 | 6 (26%)  |
| 28  | DMS  | A     | 417 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.45 | 0        |
| 28  | DMS  | O     | 303 | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 28  | DMS  | d     | 414 | -    | 3,3,3        | 2.50 | 1 (33%)  | 3,3,3       | 0.24 | 0        |
| 28  | DMS  | B     | 636 | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.78 | 0        |
| 35  | DGD  | D     | 406 | -    | 51,51,67     | 1.11 | 2 (3%)   | 59,59,81    | 1.21 | 5 (8%)   |
| 22  | BCR  | b     | 620 | -    | 41,41,41     | 1.08 | 1 (2%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 20  | CLA  | D     | 401 | 4    | 69,73,73     | 1.93 | 20 (28%) | 83,113,113  | 2.41 | 29 (34%) |
| 24  | LMG  | J     | 101 | 39   | 45,45,55     | 1.01 | 2 (4%)   | 53,53,63    | 0.98 | 3 (5%)   |
| 22  | BCR  | k     | 101 | -    | 41,41,41     | 0.94 | 0        | 56,56,56    | 1.12 | 6 (10%)  |
| 28  | DMS  | D     | 414 | -    | 3,3,3        | 2.53 | 1 (33%)  | 3,3,3       | 0.25 | 0        |
| 28  | DMS  | b     | 636 | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.75 | 0        |
| 28  | DMS  | o     | 307 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.85 | 0        |
| 34  | LMT  | b     | 627 | -    | 33,33,36     | 0.88 | 1 (3%)   | 44,44,47    | 1.80 | 10 (22%) |

| Mol | Type | Chain | Res | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | CLA  | B     | 615 | 2      | 69,73,73     | 2.08 | 19 (27%) | 83,113,113  | 2.68 | 32 (38%) |
| 32  | HTG  | B     | 631 | -      | 19,19,19     | 0.94 | 2 (10%)  | 23,24,24    | 2.09 | 6 (26%)  |
| 30  | OEX  | A     | 420 | 3,41,1 | 0,14,14      | -    | -        | -           |      |          |
| 34  | LMT  | a     | 418 | -      | 36,36,36     | 0.68 | 2 (5%)   | 47,47,47    | 1.54 | 6 (12%)  |
| 28  | DMS  | v     | 202 | -      | 3,3,3        | 2.50 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 32  | HTG  | B     | 623 | -      | 19,19,19     | 0.96 | 1 (5%)   | 23,24,24    | 1.56 | 2 (8%)   |
| 34  | LMT  | T     | 102 | -      | 24,24,36     | 0.45 | 0        | 29,29,47    | 1.15 | 2 (6%)   |
| 22  | BCR  | a     | 408 | -      | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.44 | 7 (12%)  |
| 34  | LMT  | I     | 101 | -      | 36,36,36     | 0.65 | 1 (2%)   | 47,47,47    | 1.28 | 6 (12%)  |
| 40  | HEC  | v     | 201 | 16     | 50,50,50     | 1.85 | 13 (26%) | 68,82,82    | 1.55 | 13 (19%) |
| 20  | CLA  | b     | 612 | 41     | 69,73,73     | 2.10 | 20 (28%) | 83,113,113  | 2.38 | 27 (32%) |
| 28  | DMS  | V     | 208 | -      | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.74 | 0        |
| 22  | BCR  | C     | 514 | -      | 41,41,41     | 0.85 | 0        | 56,56,56    | 1.31 | 7 (12%)  |
| 28  | DMS  | v     | 206 | -      | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.66 | 0        |
| 36  | LHG  | l     | 102 | -      | 48,48,48     | 0.78 | 2 (4%)   | 51,54,54    | 1.00 | 2 (3%)   |
| 20  | CLA  | c     | 507 | 41     | 69,73,73     | 2.28 | 16 (23%) | 83,113,113  | 2.52 | 27 (32%) |
| 28  | DMS  | b     | 634 | -      | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.68 | 0        |
| 28  | DMS  | b     | 631 | -      | 3,3,3        | 2.88 | 1 (33%)  | 3,3,3       | 1.24 | 0        |
| 20  | CLA  | B     | 602 | 41     | 69,73,73     | 2.58 | 20 (28%) | 83,113,113  | 2.67 | 30 (36%) |
| 20  | CLA  | B     | 603 | 2      | 69,73,73     | 2.16 | 19 (27%) | 83,113,113  | 2.29 | 25 (30%) |
| 20  | CLA  | c     | 503 | 3      | 69,73,73     | 2.49 | 22 (31%) | 83,113,113  | 2.39 | 26 (31%) |
| 28  | DMS  | v     | 209 | -      | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 35  | DGD  | d     | 416 | -      | 51,51,67     | 1.11 | 3 (5%)   | 59,59,81    | 1.20 | 6 (10%)  |
| 24  | LMG  | C     | 524 | -      | 45,45,55     | 1.10 | 3 (6%)   | 53,53,63    | 1.36 | 5 (9%)   |
| 34  | LMT  | f     | 102 | -      | 24,24,36     | 0.79 | 1 (4%)   | 29,29,47    | 0.96 | 2 (6%)   |
| 28  | DMS  | c     | 527 | -      | 3,3,3        | 2.31 | 1 (33%)  | 3,3,3       | 0.49 | 0        |
| 38  | RRX  | H     | 101 | -      | 42,42,42     | 0.77 | 1 (2%)   | 57,58,58    | 1.49 | 8 (14%)  |
| 34  | LMT  | c     | 523 | -      | 36,36,36     | 0.81 | 1 (2%)   | 47,47,47    | 1.60 | 6 (12%)  |
| 20  | CLA  | B     | 605 | 2      | 69,73,73     | 2.12 | 19 (27%) | 83,113,113  | 2.07 | 26 (31%) |
| 34  | LMT  | b     | 628 | -      | 25,25,36     | 0.55 | 0        | 30,30,47    | 1.20 | 2 (6%)   |
| 23  | SQD  | a     | 401 | -      | 53,54,54     | 1.12 | 3 (5%)   | 62,65,65    | 1.40 | 7 (11%)  |
| 28  | DMS  | b     | 638 | -      | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.94 | 0        |
| 20  | CLA  | b     | 611 | 2      | 69,73,73     | 2.66 | 21 (30%) | 83,113,113  | 2.00 | 24 (28%) |
| 20  | CLA  | b     | 613 | 2      | 69,73,73     | 2.02 | 13 (18%) | 83,113,113  | 2.34 | 29 (34%) |
| 20  | CLA  | B     | 609 | 2      | 69,73,73     | 1.94 | 18 (26%) | 83,113,113  | 2.47 | 28 (33%) |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | DMS  | c     | 534    | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.76 | 0        |
| 35  | DGD  | C     | 517    | -    | 56,56,67     | 0.98 | 2 (3%)   | 70,70,81    | 0.93 | 4 (5%)   |
| 22  | BCR  | A     | 405    | -    | 41,41,41     | 0.95 | 3 (7%)   | 56,56,56    | 1.27 | 7 (12%)  |
| 28  | DMS  | C     | 525[A] | -    | 3,3,3        | 2.80 | 1 (33%)  | 3,3,3       | 0.85 | 0        |
| 37  | HEM  | e     | 102    | 5,6  | 50,50,50     | 1.97 | 10 (20%) | 66,82,82    | 1.54 | 8 (12%)  |
| 20  | CLA  | b     | 609    | 41   | 69,73,73     | 2.10 | 21 (30%) | 83,113,113  | 2.17 | 30 (36%) |
| 22  | BCR  | d     | 405    | -    | 41,41,41     | 0.94 | 0        | 56,56,56    | 1.84 | 11 (19%) |
| 31  | BCT  | a     | 413    | 29   | 2,3,3        | 0.65 | 0        | 2,3,3       | 1.47 | 0        |
| 20  | CLA  | C     | 509    | 3    | 69,73,73     | 2.22 | 17 (24%) | 83,113,113  | 2.57 | 28 (33%) |
| 24  | LMG  | C     | 519    | -    | 51,51,55     | 1.03 | 2 (3%)   | 59,59,63    | 1.23 | 8 (13%)  |
| 28  | DMS  | U     | 904    | -    | 3,3,3        | 2.85 | 1 (33%)  | 3,3,3       | 0.70 | 0        |
| 34  | LMT  | m     | 102    | -    | 36,36,36     | 0.58 | 0        | 47,47,47    | 1.14 | 4 (8%)   |
| 32  | HTG  | V     | 202    | -    | 12,13,19     | 0.76 | 1 (8%)   | 16,18,24    | 2.50 | 6 (37%)  |
| 32  | HTG  | c     | 520    | -    | 19,19,19     | 0.89 | 2 (10%)  | 23,24,24    | 1.32 | 2 (8%)   |
| 20  | CLA  | b     | 604    | 2    | 69,73,73     | 2.14 | 20 (28%) | 83,113,113  | 2.34 | 32 (38%) |
| 36  | LHG  | d     | 406    | -    | 48,48,48     | 0.94 | 2 (4%)   | 51,54,54    | 1.16 | 5 (9%)   |
| 36  | LHG  | d     | 407    | -    | 48,48,48     | 0.73 | 2 (4%)   | 51,54,54    | 0.99 | 4 (7%)   |
| 28  | DMS  | c     | 535    | -    | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.79 | 0        |
| 20  | CLA  | B     | 607    | 2    | 69,73,73     | 2.36 | 20 (28%) | 83,113,113  | 2.60 | 29 (34%) |
| 28  | DMS  | C     | 527    | -    | 3,3,3        | 2.56 | 1 (33%)  | 3,3,3       | 0.49 | 0        |
| 28  | DMS  | F     | 102    | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.61 | 0        |
| 35  | DGD  | h     | 101    | -    | 63,63,67     | 0.98 | 3 (4%)   | 77,77,81    | 1.04 | 4 (5%)   |
| 28  | DMS  | A     | 414    | -    | 3,3,3        | 1.97 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 28  | DMS  | C     | 533    | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 28  | DMS  | B     | 643    | -    | 3,3,3        | 2.78 | 1 (33%)  | 3,3,3       | 0.74 | 0        |
| 20  | CLA  | c     | 512    | 3    | 69,73,73     | 2.37 | 22 (31%) | 83,113,113  | 2.44 | 25 (30%) |
| 20  | CLA  | A     | 401    | 1    | 69,73,73     | 1.94 | 19 (27%) | 83,113,113  | 2.16 | 24 (28%) |
| 28  | DMS  | C     | 525[B] | -    | 3,3,3        | 2.59 | 1 (33%)  | 3,3,3       | 0.79 | 0        |
| 28  | DMS  | O     | 309    | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 1.16 | 0        |
| 28  | DMS  | V     | 206    | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.67 | 0        |
| 20  | CLA  | B     | 616    | 2    | 69,73,73     | 2.15 | 18 (26%) | 83,113,113  | 2.30 | 25 (30%) |
| 20  | CLA  | C     | 513    | 3    | 69,73,73     | 2.53 | 20 (28%) | 83,113,113  | 2.32 | 22 (26%) |
| 35  | DGD  | C     | 516    | -    | 63,63,67     | 0.89 | 2 (3%)   | 77,77,81    | 1.20 | 7 (9%)   |
| 28  | DMS  | C     | 531    | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.97 | 0        |
| 28  | DMS  | B     | 642    | -    | 3,3,3        | 2.79 | 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 |
| 28  | DMS  | C     | 526 | -    | 3,3,3        | 2.56 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 32  | HTG  | b     | 602 | -    | 19,19,19     | 1.00 | 2 (10%)  | 23,24,24    | 1.15 | 1 (4%)   |
| 28  | DMS  | H     | 103 | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.63 | 0        |
| 28  | DMS  | o     | 308 | -    | 3,3,3        | 2.85 | 1 (33%)  | 3,3,3       | 0.81 | 0        |
| 20  | CLA  | B     | 604 | 2    | 69,73,73     | 2.08 | 21 (30%) | 83,113,113  | 2.57 | 28 (33%) |
| 20  | CLA  | b     | 603 | 41   | 69,73,73     | 2.88 | 20 (28%) | 83,113,113  | 2.50 | 29 (34%) |
| 24  | LMG  | A     | 407 | -    | 51,51,55     | 0.95 | 2 (3%)   | 59,59,63    | 1.06 | 3 (5%)   |
| 28  | DMS  | B     | 645 | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.93 | 0        |
| 28  | DMS  | o     | 304 | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.65 | 0        |
| 20  | CLA  | b     | 617 | 2    | 69,73,73     | 2.14 | 18 (26%) | 83,113,113  | 2.31 | 25 (30%) |
| 35  | DGD  | c     | 517 | -    | 63,63,67     | 1.04 | 4 (6%)   | 77,77,81    | 1.19 | 8 (10%)  |
| 20  | CLA  | c     | 508 | 3    | 64,68,73     | 2.32 | 17 (26%) | 77,107,113  | 2.49 | 28 (36%) |
| 28  | DMS  | B     | 644 | -    | 3,3,3        | 2.87 | 1 (33%)  | 3,3,3       | 1.26 | 0        |
| 35  | DGD  | c     | 515 | -    | 63,63,67     | 0.85 | 3 (4%)   | 77,77,81    | 1.19 | 8 (10%)  |
| 23  | SQD  | a     | 409 | -    | 53,54,54     | 1.01 | 4 (7%)   | 62,65,65    | 2.11 | 11 (17%) |
| 20  | CLA  | c     | 509 | 3    | 69,73,73     | 2.22 | 19 (27%) | 83,113,113  | 2.54 | 31 (37%) |
| 20  | CLA  | b     | 615 | 2    | 69,73,73     | 1.95 | 19 (27%) | 83,113,113  | 2.43 | 27 (32%) |
| 27  | PL9  | a     | 415 | -    | 55,55,55     | 0.83 | 3 (5%)   | 68,69,69    | 1.67 | 16 (23%) |
| 28  | DMS  | b     | 641 | -    | 3,3,3        | 2.79 | 1 (33%)  | 3,3,3       | 1.11 | 0        |
| 23  | SQD  | A     | 406 | -    | 53,54,54     | 1.00 | 3 (5%)   | 62,65,65    | 1.75 | 14 (22%) |
| 20  | CLA  | B     | 613 | 2    | 69,73,73     | 2.13 | 18 (26%) | 83,113,113  | 2.37 | 28 (33%) |
| 20  | CLA  | c     | 513 | 3    | 69,73,73     | 2.53 | 19 (27%) | 83,113,113  | 2.35 | 26 (31%) |
| 27  | PL9  | D     | 412 | -    | 55,55,55     | 1.06 | 3 (5%)   | 68,69,69    | 1.51 | 12 (17%) |
| 35  | DGD  | c     | 516 | -    | 58,58,67     | 0.86 | 2 (3%)   | 72,72,81    | 1.13 | 6 (8%)   |
| 34  | LMT  | J     | 103 | -    | 24,24,36     | 0.65 | 1 (4%)   | 29,29,47    | 1.12 | 1 (3%)   |
| 28  | DMS  | D     | 416 | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 20  | CLA  | c     | 504 | 41   | 69,73,73     | 2.14 | 22 (31%) | 83,113,113  | 2.80 | 29 (34%) |
| 23  | SQD  | F     | 101 | -    | 34,35,54     | 1.01 | 2 (5%)   | 42,45,65    | 1.59 | 7 (16%)  |
| 28  | DMS  | O     | 308 | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.79 | 0        |
| 28  | DMS  | u     | 204 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.49 | 0        |
| 20  | CLA  | d     | 404 | 4    | 69,73,73     | 2.00 | 19 (27%) | 83,113,113  | 2.58 | 30 (36%) |
| 37  | HEM  | E     | 104 | 5,6  | 50,50,50     | 2.19 | 9 (18%)  | 66,82,82    | 1.75 | 10 (15%) |
| 22  | BCR  | T     | 101 | -    | 41,41,41     | 0.81 | 0        | 56,56,56    | 1.50 | 11 (19%) |
| 28  | DMS  | B     | 635 | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.46 | 0        |
| 36  | LHG  | L     | 101 | -    | 48,48,48     | 0.90 | 3 (6%)   | 51,54,54    | 0.90 | 1 (1%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | LMT  | Z     | 101 | -    | 36,36,36     | 0.68 | 1 (2%)   | 47,47,47    | 0.98 | 3 (6%)   |
| 28  | DMS  | c     | 536 | -    | 3,3,3        | 2.84 | 1 (33%)  | 3,3,3       | 1.23 | 0        |
| 20  | CLA  | d     | 403 | 41   | 69,73,73     | 2.01 | 18 (26%) | 83,113,113  | 2.29 | 24 (28%) |
| 24  | LMG  | b     | 623 | -    | 49,49,55     | 0.96 | 2 (4%)   | 57,57,63    | 1.31 | 6 (10%)  |
| 21  | PHO  | a     | 406 | -    | 58,69,69     | 2.55 | 13 (22%) | 56,99,99    | 2.84 | 16 (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   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 20  | CLA  | a     | 404 | 41   | -       | 7/33/109/115  | -       |
| 22  | BCR  | K     | 101 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 23  | SQD  | A     | 412 | -    | -       | 24/49/69/69   | 0/1/1/1 |
| 20  | CLA  | b     | 605 | 2    | -       | 1/39/115/115  | -       |
| 23  | SQD  | l     | 101 | -    | -       | 28/49/69/69   | 0/1/1/1 |
| 20  | CLA  | c     | 501 | 3    | -       | 3/39/115/115  | -       |
| 32  | HTG  | c     | 521 | -    | -       | 5/10/30/30    | 0/1/1/1 |
| 20  | CLA  | b     | 616 | 2    | -       | 18/39/115/115 | -       |
| 21  | PHO  | A     | 403 | -    | -       | 2/37/103/103  | 0/5/6/6 |
| 22  | BCR  | b     | 621 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 22  | BCR  | c     | 514 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 32  | HTG  | C     | 534 | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 20  | CLA  | C     | 501 | 3    | -       | 5/39/115/115  | -       |
| 20  | CLA  | B     | 611 | 41   | -       | 4/39/115/115  | -       |
| 21  | PHO  | D     | 403 | -    | -       | 3/37/103/103  | 0/5/6/6 |
| 32  | HTG  | D     | 417 | -    | -       | 5/10/30/30    | 0/1/1/1 |
| 34  | LMT  | m     | 101 | -    | -       | 15/21/61/61   | 0/2/2/2 |
| 20  | CLA  | a     | 407 | 1    | -       | 0/18/94/115   | -       |
| 20  | CLA  | c     | 502 | 3    | -       | 6/39/115/115  | -       |
| 24  | LMG  | c     | 519 | -    | -       | 26/46/66/70   | 0/1/1/1 |
| 20  | CLA  | b     | 607 | 2    | -       | 4/39/115/115  | -       |
| 36  | LHG  | D     | 407 | -    | -       | 9/53/53/53    | -       |
| 27  | PL9  | d     | 412 | -    | -       | 3/53/73/73    | 0/1/1/1 |
| 20  | CLA  | B     | 614 | 2    | -       | 6/39/115/115  | -       |
| 21  | PHO  | a     | 405 | -    | -       | 4/37/103/103  | 0/5/6/6 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 20  | CLA  | A     | 404 | 1    | -       | 10/39/115/115 | -       |
| 22  | BCR  | b     | 619 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 36  | LHG  | D     | 409 | -    | -       | 14/53/53/53   | -       |
| 20  | CLA  | d     | 402 | 4    | -       | 5/39/115/115  | -       |
| 32  | HTG  | C     | 521 | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 32  | HTG  | O     | 302 | -    | -       | 5/10/30/30    | 0/1/1/1 |
| 20  | CLA  | B     | 606 | 2    | -       | 4/39/115/115  | -       |
| 20  | CLA  | b     | 614 | 2    | -       | 4/39/115/115  | -       |
| 24  | LMG  | c     | 518 | -    | -       | 8/46/66/70    | 0/1/1/1 |
| 27  | PL9  | A     | 411 | -    | -       | 10/53/73/73   | 0/1/1/1 |
| 32  | HTG  | b     | 624 | -    | -       | 0/10/30/30    | 0/1/1/1 |
| 20  | CLA  | B     | 608 | 41   | -       | 1/39/115/115  | -       |
| 24  | LMG  | a     | 410 | -    | -       | 18/46/66/70   | 0/1/1/1 |
| 22  | BCR  | t     | 101 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 38  | RRX  | x     | 101 | -    | -       | 3/29/65/65    | 0/2/2/2 |
| 22  | BCR  | D     | 405 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 24  | LMG  | j     | 101 | 39   | -       | 15/40/60/70   | 0/1/1/1 |
| 20  | CLA  | C     | 510 | 3    | -       | 2/39/115/115  | -       |
| 35  | DGD  | H     | 102 | -    | -       | 15/51/91/95   | 0/2/2/2 |
| 20  | CLA  | C     | 503 | 3    | -       | 4/39/115/115  | -       |
| 22  | BCR  | C     | 515 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 32  | HTG  | C     | 522 | -    | -       | 4/10/30/30    | 0/1/1/1 |
| 34  | LMT  | B     | 626 | -    | -       | 7/15/35/61    | 0/1/1/2 |
| 20  | CLA  | c     | 505 | 3    | -       | 1/39/115/115  | -       |
| 36  | LHG  | E     | 103 | -    | -       | 27/45/45/53   | -       |
| 32  | HTG  | C     | 520 | -    | -       | 4/10/30/30    | 0/1/1/1 |
| 22  | BCR  | k     | 102 | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 36  | LHG  | d     | 408 | -    | -       | 14/53/53/53   | -       |
| 34  | LMT  | M     | 101 | -    | -       | 1/21/61/61    | 0/2/2/2 |
| 22  | BCR  | B     | 617 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 20  | CLA  | C     | 502 | 3    | -       | 7/39/115/115  | -       |
| 32  | HTG  | d     | 401 | -    | -       | 9/10/30/30    | 0/1/1/1 |
| 24  | LMG  | B     | 620 | -    | -       | 19/46/66/70   | 0/1/1/1 |
| 36  | LHG  | D     | 408 | -    | -       | 10/53/53/53   | -       |
| 20  | CLA  | b     | 610 | 2    | -       | 1/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 20  | CLA  | B     | 610 | 2    | -       | 3/39/115/115  | -       |
| 20  | CLA  | c     | 510 | 3    | -       | 3/39/115/115  | -       |
| 20  | CLA  | b     | 606 | 2    | -       | 3/39/115/115  | -       |
| 34  | LMT  | E     | 101 | -    | -       | 8/15/35/61    | 0/1/1/2 |
| 20  | CLA  | B     | 601 | 2    | -       | 18/39/115/115 | -       |
| 20  | CLA  | C     | 511 | 3    | -       | 0/39/115/115  | -       |
| 32  | HTG  | B     | 632 | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 34  | LMT  | B     | 627 | -    | -       | 7/13/13/61    | -       |
| 20  | CLA  | C     | 507 | 41   | -       | 11/39/115/115 | -       |
| 20  | CLA  | C     | 512 | 3    | -       | 6/27/103/115  | -       |
| 20  | CLA  | b     | 618 | 2    | -       | 17/39/115/115 | -       |
| 20  | CLA  | a     | 403 | 1    | -       | 4/39/115/115  | -       |
| 20  | CLA  | C     | 508 | 3    | -       | 6/33/109/115  | -       |
| 23  | SQD  | b     | 622 | -    | -       | 23/49/69/69   | 0/1/1/1 |
| 23  | SQD  | f     | 101 | -    | -       | 16/34/54/69   | 0/1/1/1 |
| 20  | CLA  | C     | 506 | 3    | -       | 12/39/115/115 | -       |
| 20  | CLA  | B     | 612 | 2    | -       | 3/39/115/115  | -       |
| 32  | HTG  | u     | 201 | -    | -       | 1/5/5/30      | -       |
| 20  | CLA  | D     | 404 | 4    | -       | 13/39/115/115 | -       |
| 34  | LMT  | z     | 102 | -    | -       | 13/21/61/61   | 0/2/2/2 |
| 22  | BCR  | B     | 619 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 32  | HTG  | b     | 601 | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 20  | CLA  | c     | 506 | 3    | -       | 10/39/115/115 | -       |
| 22  | BCR  | K     | 102 | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 35  | DGD  | C     | 518 | -    | -       | 12/51/91/95   | 0/2/2/2 |
| 32  | HTG  | B     | 622 | -    | -       | 5/10/30/30    | 0/1/1/1 |
| 20  | CLA  | C     | 504 | 41   | -       | 11/39/115/115 | -       |
| 20  | CLA  | b     | 608 | 2    | -       | 9/39/115/115  | -       |
| 22  | BCR  | j     | 102 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 34  | LMT  | B     | 625 | -    | -       | 4/15/35/61    | 0/1/1/2 |
| 20  | CLA  | A     | 402 | 41   | -       | 3/32/108/115  | -       |
| 20  | CLA  | D     | 402 | 41   | -       | 5/39/115/115  | -       |
| 20  | CLA  | c     | 511 | 3    | -       | 0/39/115/115  | -       |
| 32  | HTG  | v     | 210 | -    | -       | 3/5/25/30     | 0/1/1/1 |
| 22  | BCR  | B     | 618 | -    | -       | 0/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 40  | HEC  | V     | 201 | 16   | 1/1/3/7 | 5/14/54/54    | -       |
| 32  | HTG  | b     | 625 | -    | -       | 4/10/30/30    | 0/1/1/1 |
| 20  | CLA  | C     | 505 | 3    | -       | 1/39/115/115  | -       |
| 32  | HTG  | B     | 621 | -    | -       | 5/10/30/30    | 0/1/1/1 |
| 35  | DGD  | D     | 406 | -    | -       | 26/46/66/95   | 0/1/1/2 |
| 22  | BCR  | b     | 620 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 20  | CLA  | D     | 401 | 4    | -       | 7/39/115/115  | -       |
| 24  | LMG  | J     | 101 | 39   | -       | 9/40/60/70    | 0/1/1/1 |
| 22  | BCR  | k     | 101 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 34  | LMT  | b     | 627 | -    | -       | 10/18/58/61   | 0/2/2/2 |
| 20  | CLA  | B     | 615 | 2    | -       | 10/39/115/115 | -       |
| 32  | HTG  | B     | 631 | -    | -       | 5/10/30/30    | 0/1/1/1 |
| 34  | LMT  | a     | 418 | -    | -       | 11/21/61/61   | 0/2/2/2 |
| 32  | HTG  | B     | 623 | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 34  | LMT  | T     | 102 | -    | -       | 11/15/35/61   | 0/1/1/2 |
| 22  | BCR  | a     | 408 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 34  | LMT  | I     | 101 | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 40  | HEC  | v     | 201 | 16   | 1/1/3/7 | 6/14/54/54    | -       |
| 20  | CLA  | b     | 612 | 41   | -       | 5/39/115/115  | -       |
| 22  | BCR  | C     | 514 | -    | -       | 5/29/63/63    | 0/2/2/2 |
| 36  | LHG  | l     | 102 | -    | -       | 19/53/53/53   | -       |
| 20  | CLA  | c     | 507 | 41   | -       | 6/39/115/115  | -       |
| 20  | CLA  | B     | 602 | 41   | -       | 23/39/115/115 | -       |
| 20  | CLA  | B     | 603 | 2    | -       | 3/39/115/115  | -       |
| 20  | CLA  | c     | 503 | 3    | -       | 3/39/115/115  | -       |
| 35  | DGD  | d     | 416 | -    | -       | 30/46/66/95   | 0/1/1/2 |
| 24  | LMG  | C     | 524 | -    | -       | 22/40/60/70   | 0/1/1/1 |
| 34  | LMT  | f     | 102 | -    | -       | 8/15/35/61    | 0/1/1/2 |
| 38  | RRX  | H     | 101 | -    | -       | 1/29/65/65    | 0/2/2/2 |
| 34  | LMT  | c     | 523 | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 20  | CLA  | B     | 605 | 2    | -       | 8/39/115/115  | -       |
| 34  | LMT  | b     | 628 | -    | -       | 9/17/37/61    | 0/1/1/2 |
| 23  | SQD  | a     | 401 | -    | -       | 20/49/69/69   | 0/1/1/1 |
| 20  | CLA  | b     | 611 | 2    | -       | 0/39/115/115  | -       |
| 20  | CLA  | b     | 613 | 2    | -       | 7/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 20  | CLA  | B     | 609 | 2    | -       | 1/39/115/115  | -       |
| 35  | DGD  | C     | 517 | -    | -       | 14/44/84/95   | 0/2/2/2 |
| 22  | BCR  | A     | 405 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 37  | HEM  | e     | 102 | 5,6  | -       | 4/14/54/54    | -       |
| 20  | CLA  | b     | 609 | 41   | -       | 3/39/115/115  | -       |
| 22  | BCR  | d     | 405 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 20  | CLA  | C     | 509 | 3    | -       | 8/39/115/115  | -       |
| 24  | LMG  | C     | 519 | -    | -       | 19/46/66/70   | 0/1/1/1 |
| 34  | LMT  | m     | 102 | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 32  | HTG  | V     | 202 | -    | -       | 1/4/24/30     | 0/1/1/1 |
| 32  | HTG  | c     | 520 | -    | -       | 5/10/30/30    | 0/1/1/1 |
| 20  | CLA  | b     | 604 | 2    | -       | 7/39/115/115  | -       |
| 36  | LHG  | d     | 406 | -    | -       | 11/53/53/53   | -       |
| 36  | LHG  | d     | 407 | -    | -       | 11/53/53/53   | -       |
| 20  | CLA  | B     | 607 | 2    | -       | 11/39/115/115 | -       |
| 35  | DGD  | h     | 101 | -    | -       | 15/51/91/95   | 0/2/2/2 |
| 20  | CLA  | c     | 512 | 3    | -       | 9/39/115/115  | -       |
| 20  | CLA  | A     | 401 | 1    | -       | 4/39/115/115  | -       |
| 20  | CLA  | B     | 616 | 2    | -       | 5/39/115/115  | -       |
| 20  | CLA  | C     | 513 | 3    | -       | 10/39/115/115 | -       |
| 35  | DGD  | C     | 516 | -    | -       | 18/51/91/95   | 0/2/2/2 |
| 32  | HTG  | b     | 602 | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 20  | CLA  | B     | 604 | 2    | -       | 3/39/115/115  | -       |
| 20  | CLA  | b     | 603 | 41   | -       | 18/39/115/115 | -       |
| 24  | LMG  | A     | 407 | -    | -       | 28/46/66/70   | 0/1/1/1 |
| 20  | CLA  | b     | 617 | 2    | -       | 8/39/115/115  | -       |
| 35  | DGD  | c     | 517 | -    | -       | 14/51/91/95   | 0/2/2/2 |
| 20  | CLA  | c     | 508 | 3    | -       | 2/33/109/115  | -       |
| 35  | DGD  | c     | 515 | -    | -       | 18/51/91/95   | 0/2/2/2 |
| 23  | SQD  | a     | 409 | -    | -       | 20/49/69/69   | 0/1/1/1 |
| 20  | CLA  | c     | 509 | 3    | -       | 10/39/115/115 | -       |
| 20  | CLA  | b     | 615 | 2    | -       | 6/39/115/115  | -       |
| 27  | PL9  | a     | 415 | -    | -       | 11/53/73/73   | 0/1/1/1 |
| 23  | SQD  | A     | 406 | -    | -       | 21/49/69/69   | 0/1/1/1 |
| 20  | CLA  | B     | 613 | 2    | -       | 0/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 20  | CLA  | c     | 513 | 3    | -       | 15/39/115/115 | -       |
| 27  | PL9  | D     | 412 | -    | -       | 3/53/73/73    | 0/1/1/1 |
| 35  | DGD  | c     | 516 | -    | -       | 13/46/86/95   | 0/2/2/2 |
| 34  | LMT  | J     | 103 | -    | -       | 7/15/35/61    | 0/1/1/2 |
| 20  | CLA  | c     | 504 | 41   | -       | 5/39/115/115  | -       |
| 23  | SQD  | F     | 101 | -    | -       | 17/28/48/69   | 0/1/1/1 |
| 37  | HEM  | E     | 104 | 5,6  | -       | 7/14/54/54    | -       |
| 20  | CLA  | d     | 404 | 4    | -       | 8/39/115/115  | -       |
| 22  | BCR  | T     | 101 | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 36  | LHG  | L     | 101 | -    | -       | 17/53/53/53   | -       |
| 34  | LMT  | Z     | 101 | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 20  | CLA  | d     | 403 | 41   | -       | 5/39/115/115  | -       |
| 24  | LMG  | b     | 623 | -    | -       | 14/44/64/70   | 0/1/1/1 |
| 21  | PHO  | a     | 406 | -    | -       | 2/37/103/103  | 0/5/6/6 |

The worst 5 of 1682 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 2619 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   |
| 21  | A     | 403 | PHO  | C2D-C1D-ND | 11.02  | 117.13      | 109.53   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 40  | V     | 201 | HEC  | NA   |
| 40  | v     | 201 | HEC  | NA   |

5 of 1416 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | B     | 601 | CLA  | C11-C10-C8-C9   |
| 20  | B     | 602 | CLA  | CBA-CGA-O2A-C1  |
| 20  | B     | 602 | CLA  | O1A-CGA-O2A-C1  |
| 20  | B     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 20  | B     | 602 | CLA  | CHA-CBD-CGD-O2D |

There are no ring outliers.

186 monomers are involved in 488 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 20  | a     | 404    | CLA  | 1       | 0            |
| 22  | K     | 101    | BCR  | 2       | 0            |
| 28  | U     | 903[B] | DMS  | 10      | 0            |
| 28  | b     | 635    | DMS  | 1       | 0            |
| 23  | A     | 412    | SQD  | 2       | 0            |
| 20  | b     | 605    | CLA  | 2       | 0            |
| 23  | l     | 101    | SQD  | 2       | 0            |
| 20  | c     | 501    | CLA  | 3       | 0            |
| 28  | B     | 641    | DMS  | 3       | 0            |
| 20  | b     | 616    | CLA  | 1       | 0            |
| 21  | A     | 403    | PHO  | 1       | 0            |
| 22  | b     | 621    | BCR  | 4       | 0            |
| 22  | c     | 514    | BCR  | 1       | 0            |
| 28  | D     | 413    | DMS  | 2       | 0            |
| 32  | C     | 534    | HTG  | 1       | 0            |
| 20  | C     | 501    | CLA  | 3       | 0            |
| 20  | B     | 611    | CLA  | 4       | 0            |
| 21  | D     | 403    | PHO  | 1       | 0            |
| 32  | D     | 417    | HTG  | 3       | 0            |
| 28  | u     | 203    | DMS  | 1       | 0            |
| 20  | c     | 502    | CLA  | 3       | 0            |
| 20  | b     | 607    | CLA  | 4       | 0            |
| 28  | A     | 418    | DMS  | 3       | 0            |
| 20  | B     | 614    | CLA  | 1       | 0            |
| 21  | a     | 405    | PHO  | 1       | 0            |
| 28  | i     | 104    | DMS  | 4       | 0            |
| 36  | D     | 409    | LHG  | 19      | 0            |
| 28  | C     | 530    | DMS  | 1       | 0            |
| 28  | b     | 632    | DMS  | 2       | 0            |
| 20  | B     | 606    | CLA  | 6       | 0            |
| 20  | b     | 614    | CLA  | 1       | 0            |

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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 27  | A     | 411    | PL9  | 11      | 0            |
| 31  | A     | 421    | BCT  | 5       | 0            |
| 28  | A     | 416    | DMS  | 3       | 0            |
| 24  | a     | 410    | LMG  | 4       | 0            |
| 28  | U     | 903[A] | DMS  | 2       | 0            |
| 28  | c     | 530    | DMS  | 7       | 0            |
| 22  | t     | 101    | BCR  | 4       | 0            |
| 38  | x     | 101    | RRX  | 3       | 0            |
| 22  | D     | 405    | BCR  | 3       | 0            |
| 28  | o     | 302    | DMS  | 9       | 0            |
| 20  | C     | 510    | CLA  | 3       | 0            |
| 35  | H     | 102    | DGD  | 2       | 0            |
| 20  | C     | 503    | CLA  | 2       | 0            |
| 22  | C     | 515    | BCR  | 1       | 0            |
| 28  | b     | 639    | DMS  | 9       | 0            |
| 34  | B     | 626    | LMT  | 2       | 0            |
| 28  | C     | 532    | DMS  | 6       | 0            |
| 20  | c     | 505    | CLA  | 1       | 0            |
| 28  | b     | 640    | DMS  | 3       | 0            |
| 28  | d     | 413    | DMS  | 3       | 0            |
| 32  | C     | 520    | HTG  | 1       | 0            |
| 22  | k     | 102    | BCR  | 3       | 0            |
| 28  | u     | 202    | DMS  | 2       | 0            |
| 36  | E     | 103    | LHG  | 6       | 0            |
| 36  | d     | 408    | LHG  | 20      | 0            |
| 20  | C     | 502    | CLA  | 2       | 0            |
| 28  | B     | 637    | DMS  | 1       | 0            |
| 28  | V     | 205    | DMS  | 1       | 0            |
| 20  | b     | 610    | CLA  | 1       | 0            |
| 28  | A     | 415    | DMS  | 2       | 0            |
| 28  | o     | 303    | DMS  | 4       | 0            |
| 20  | c     | 510    | CLA  | 2       | 0            |
| 20  | b     | 606    | CLA  | 3       | 0            |
| 20  | B     | 601    | CLA  | 4       | 0            |
| 20  | C     | 511    | CLA  | 1       | 0            |
| 32  | B     | 632    | HTG  | 2       | 0            |
| 28  | U     | 902    | DMS  | 1       | 0            |
| 34  | B     | 627    | LMT  | 1       | 0            |
| 20  | C     | 507    | CLA  | 2       | 0            |
| 20  | b     | 618    | CLA  | 5       | 0            |
| 28  | c     | 533    | DMS  | 1       | 0            |
| 28  | D     | 415    | DMS  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 20  | a     | 403 | CLA  | 4       | 0            |
| 20  | C     | 508 | CLA  | 3       | 0            |
| 23  | b     | 622 | SQD  | 3       | 0            |
| 23  | f     | 101 | SQD  | 2       | 0            |
| 20  | C     | 506 | CLA  | 2       | 0            |
| 20  | B     | 612 | CLA  | 1       | 0            |
| 28  | O     | 307 | DMS  | 2       | 0            |
| 34  | z     | 102 | LMT  | 5       | 0            |
| 22  | B     | 619 | BCR  | 3       | 0            |
| 28  | V     | 204 | DMS  | 1       | 0            |
| 20  | c     | 506 | CLA  | 4       | 0            |
| 22  | K     | 102 | BCR  | 1       | 0            |
| 28  | O     | 305 | DMS  | 1       | 0            |
| 20  | C     | 504 | CLA  | 3       | 0            |
| 28  | o     | 306 | DMS  | 5       | 0            |
| 28  | O     | 310 | DMS  | 2       | 0            |
| 32  | B     | 622 | HTG  | 8       | 0            |
| 20  | b     | 608 | CLA  | 4       | 0            |
| 22  | j     | 102 | BCR  | 5       | 0            |
| 28  | O     | 306 | DMS  | 1       | 0            |
| 34  | B     | 625 | LMT  | 1       | 0            |
| 20  | A     | 402 | CLA  | 2       | 0            |
| 20  | D     | 402 | CLA  | 3       | 0            |
| 20  | c     | 511 | CLA  | 1       | 0            |
| 32  | v     | 210 | HTG  | 1       | 0            |
| 22  | B     | 618 | BCR  | 3       | 0            |
| 32  | b     | 625 | HTG  | 6       | 0            |
| 32  | B     | 621 | HTG  | 6       | 0            |
| 28  | A     | 417 | DMS  | 1       | 0            |
| 28  | d     | 414 | DMS  | 5       | 0            |
| 35  | D     | 406 | DGD  | 5       | 0            |
| 22  | b     | 620 | BCR  | 1       | 0            |
| 20  | D     | 401 | CLA  | 1       | 0            |
| 22  | k     | 101 | BCR  | 3       | 0            |
| 28  | D     | 414 | DMS  | 8       | 0            |
| 28  | o     | 307 | DMS  | 3       | 0            |
| 34  | b     | 627 | LMT  | 2       | 0            |
| 32  | B     | 631 | HTG  | 1       | 0            |
| 34  | a     | 418 | LMT  | 10      | 0            |
| 22  | a     | 408 | BCR  | 1       | 0            |
| 34  | I     | 101 | LMT  | 2       | 0            |
| 20  | b     | 612 | CLA  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 28  | V     | 208 | DMS  | 1       | 0            |
| 22  | C     | 514 | BCR  | 2       | 0            |
| 28  | v     | 206 | DMS  | 4       | 0            |
| 36  | l     | 102 | LHG  | 1       | 0            |
| 20  | c     | 507 | CLA  | 3       | 0            |
| 28  | b     | 634 | DMS  | 2       | 0            |
| 28  | b     | 631 | DMS  | 6       | 0            |
| 20  | B     | 602 | CLA  | 2       | 0            |
| 20  | B     | 603 | CLA  | 1       | 0            |
| 20  | c     | 503 | CLA  | 2       | 0            |
| 35  | d     | 416 | DGD  | 2       | 0            |
| 24  | C     | 524 | LMG  | 2       | 0            |
| 34  | c     | 523 | LMT  | 2       | 0            |
| 20  | B     | 605 | CLA  | 2       | 0            |
| 34  | b     | 628 | LMT  | 1       | 0            |
| 23  | a     | 401 | SQD  | 4       | 0            |
| 28  | b     | 638 | DMS  | 3       | 0            |
| 20  | b     | 611 | CLA  | 2       | 0            |
| 20  | b     | 613 | CLA  | 1       | 0            |
| 22  | A     | 405 | BCR  | 5       | 0            |
| 37  | e     | 102 | HEM  | 3       | 0            |
| 20  | b     | 609 | CLA  | 2       | 0            |
| 22  | d     | 405 | BCR  | 3       | 0            |
| 20  | C     | 509 | CLA  | 5       | 0            |
| 24  | C     | 519 | LMG  | 3       | 0            |
| 28  | U     | 904 | DMS  | 3       | 0            |
| 34  | m     | 102 | LMT  | 1       | 0            |
| 32  | c     | 520 | HTG  | 1       | 0            |
| 20  | b     | 604 | CLA  | 3       | 0            |
| 36  | d     | 406 | LHG  | 2       | 0            |
| 20  | B     | 607 | CLA  | 1       | 0            |
| 28  | C     | 527 | DMS  | 3       | 0            |
| 28  | F     | 102 | DMS  | 3       | 0            |
| 35  | h     | 101 | DGD  | 1       | 0            |
| 28  | B     | 643 | DMS  | 1       | 0            |
| 20  | c     | 512 | CLA  | 3       | 0            |
| 20  | A     | 401 | CLA  | 6       | 0            |
| 28  | V     | 206 | DMS  | 2       | 0            |
| 20  | B     | 616 | CLA  | 2       | 0            |
| 20  | C     | 513 | CLA  | 2       | 0            |
| 28  | C     | 531 | DMS  | 5       | 0            |
| 28  | B     | 642 | DMS  | 8       | 0            |

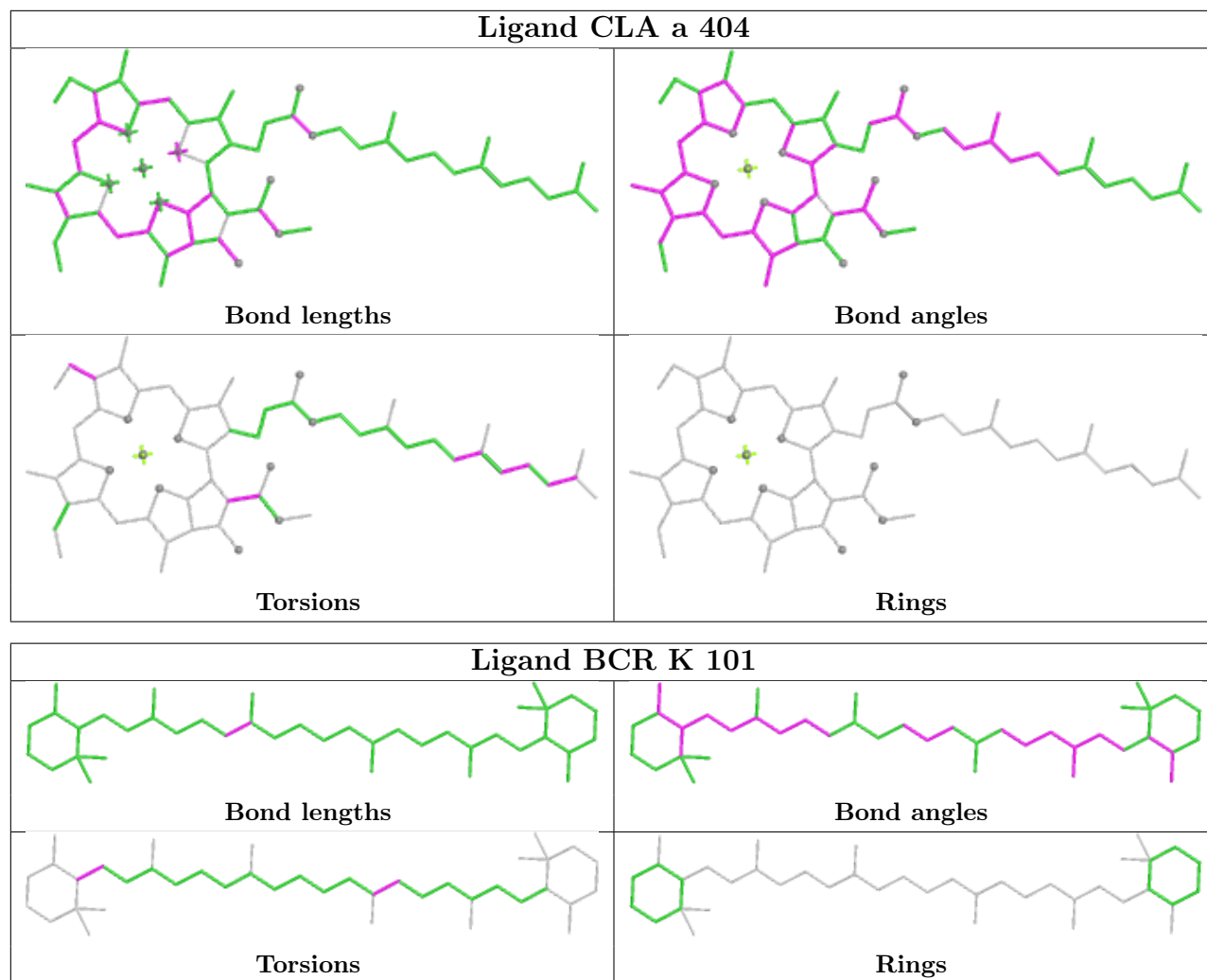
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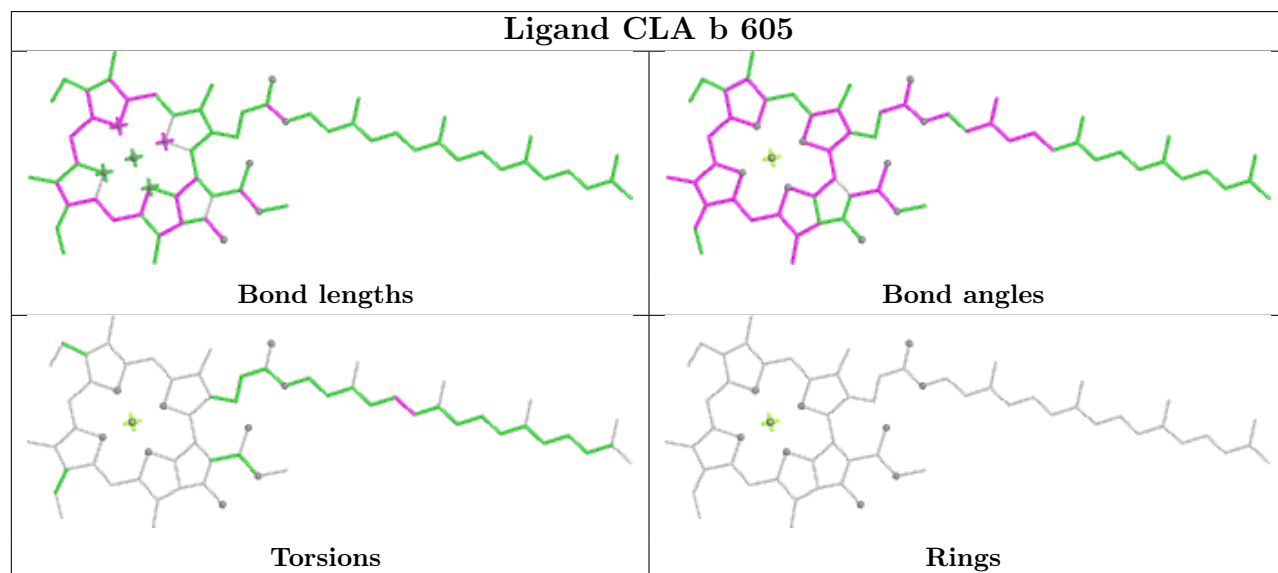
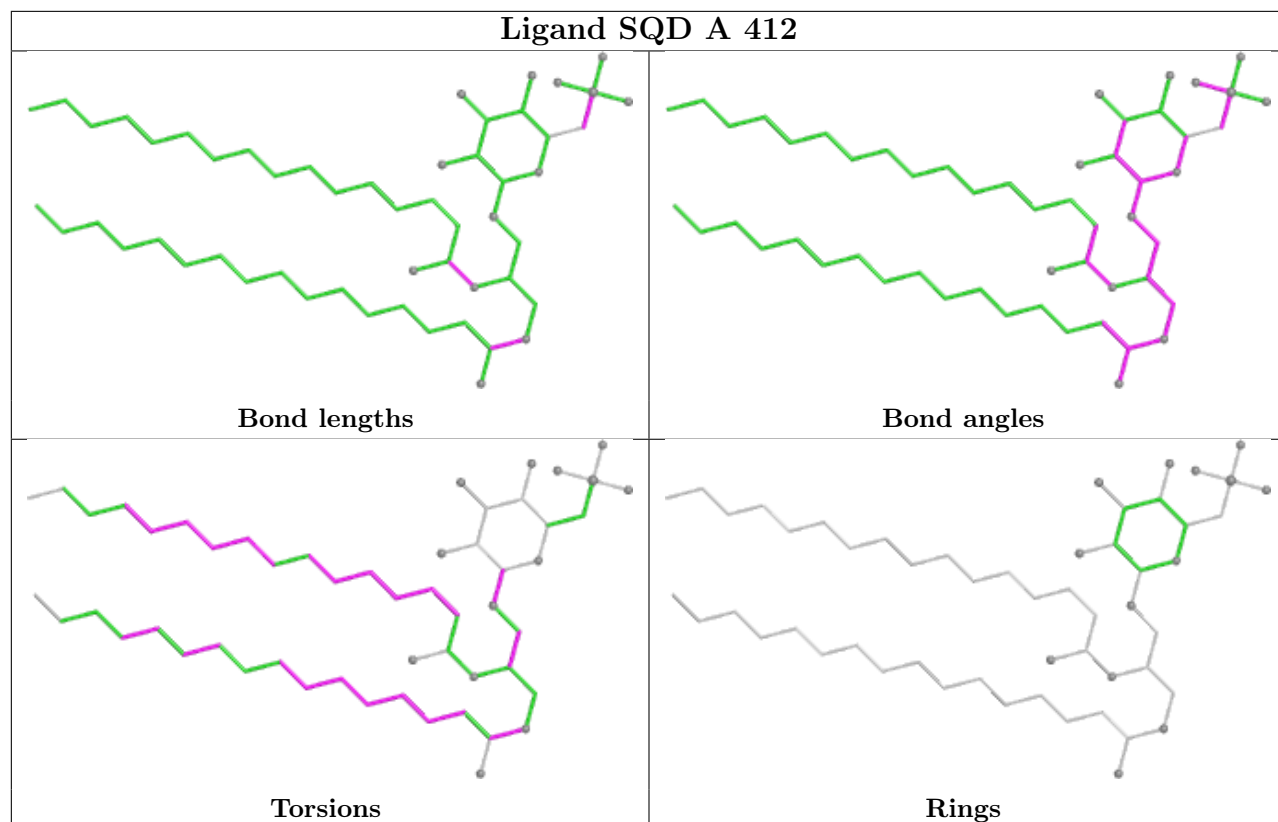
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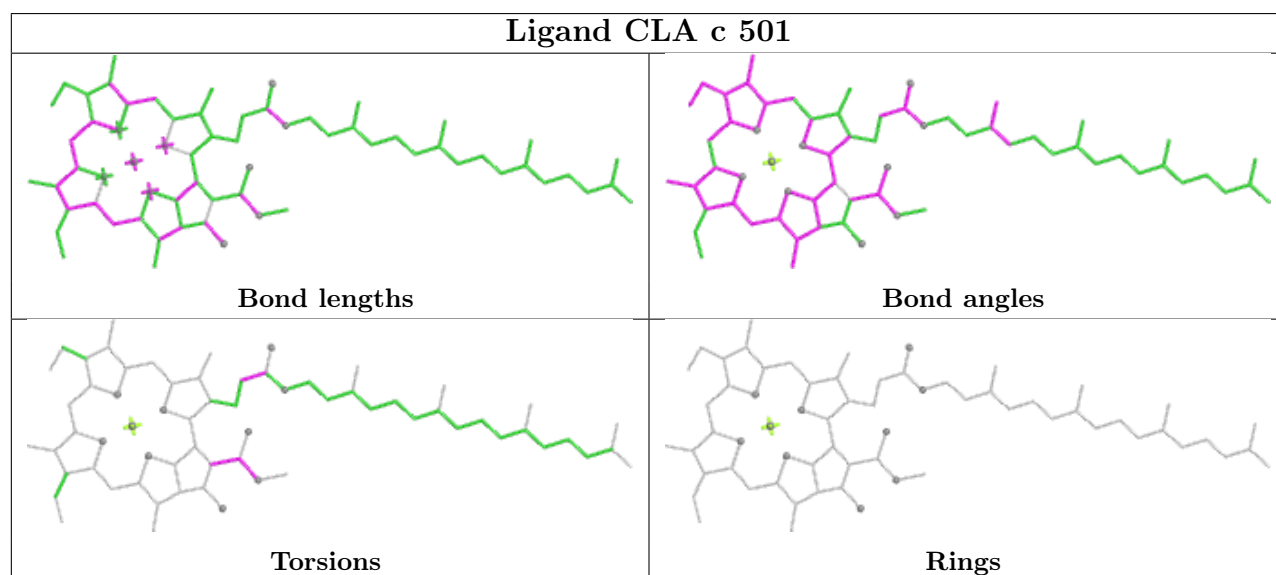
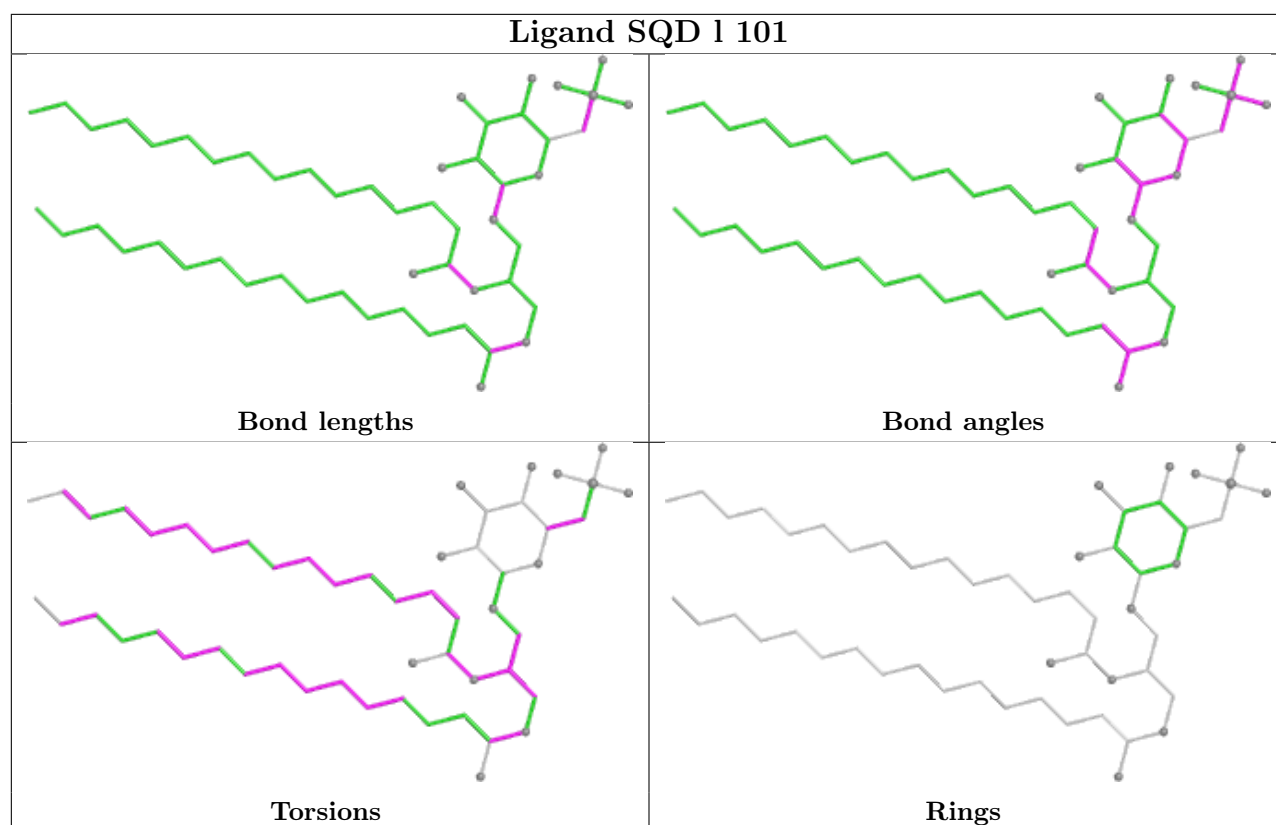
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 28  | o     | 308 | DMS  | 1       | 0            |
| 20  | B     | 604 | CLA  | 2       | 0            |
| 20  | b     | 603 | CLA  | 1       | 0            |
| 24  | A     | 407 | LMG  | 4       | 0            |
| 28  | B     | 645 | DMS  | 2       | 0            |
| 20  | b     | 617 | CLA  | 2       | 0            |
| 35  | c     | 517 | DGD  | 2       | 0            |
| 20  | c     | 508 | CLA  | 6       | 0            |
| 28  | B     | 644 | DMS  | 5       | 0            |
| 23  | a     | 409 | SQD  | 5       | 0            |
| 20  | c     | 509 | CLA  | 2       | 0            |
| 20  | b     | 615 | CLA  | 2       | 0            |
| 27  | a     | 415 | PL9  | 10      | 0            |
| 28  | b     | 641 | DMS  | 2       | 0            |
| 23  | A     | 406 | SQD  | 3       | 0            |
| 20  | c     | 513 | CLA  | 3       | 0            |
| 35  | c     | 516 | DGD  | 2       | 0            |
| 34  | J     | 103 | LMT  | 1       | 0            |
| 20  | c     | 504 | CLA  | 3       | 0            |
| 23  | F     | 101 | SQD  | 1       | 0            |
| 28  | O     | 308 | DMS  | 1       | 0            |
| 20  | d     | 404 | CLA  | 2       | 0            |
| 37  | E     | 104 | HEM  | 1       | 0            |
| 22  | T     | 101 | BCR  | 4       | 0            |
| 28  | B     | 635 | DMS  | 4       | 0            |
| 28  | c     | 536 | DMS  | 8       | 0            |
| 20  | d     | 403 | CLA  | 2       | 0            |
| 24  | b     | 623 | LMG  | 2       | 0            |
| 21  | a     | 406 | PHO  | 1       | 0            |

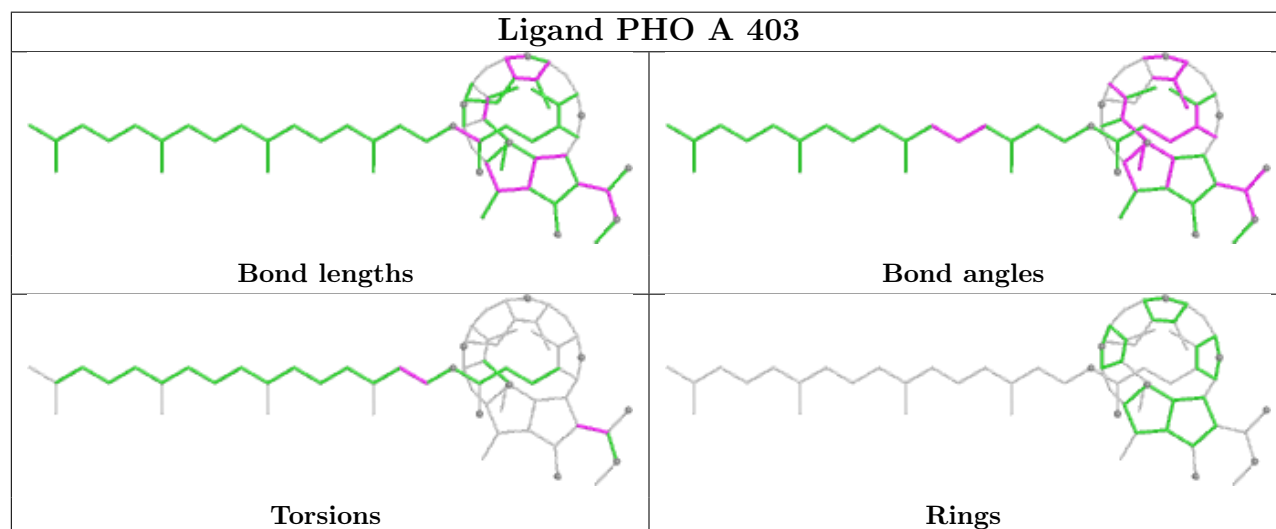
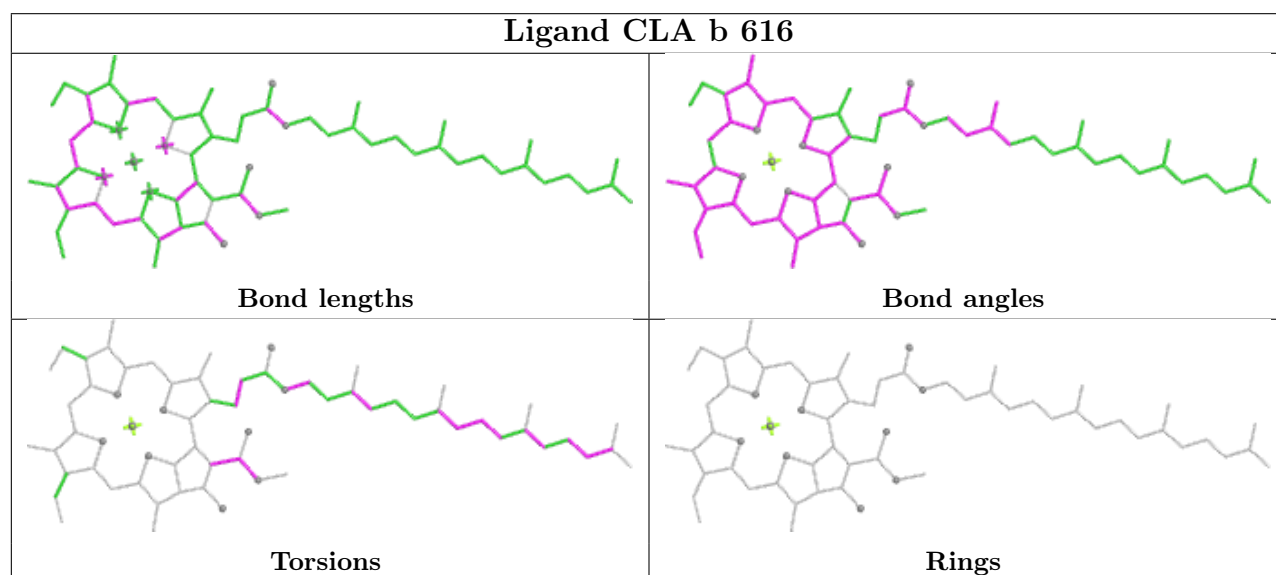
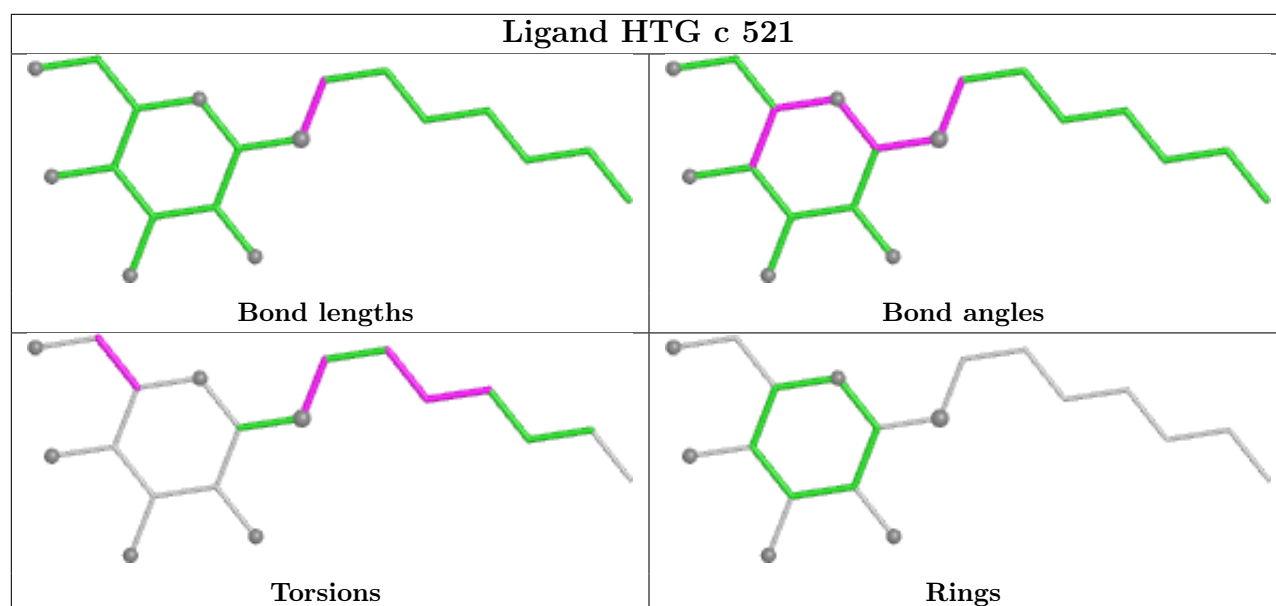
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

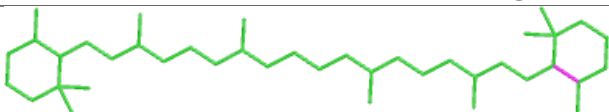
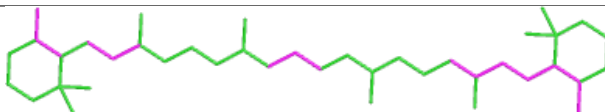
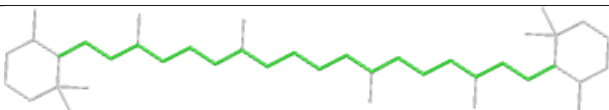
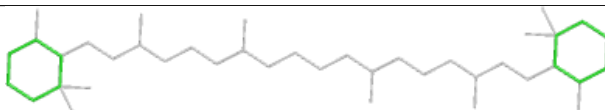


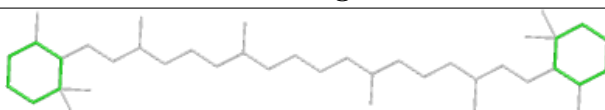


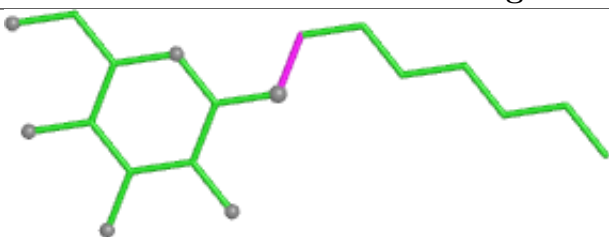
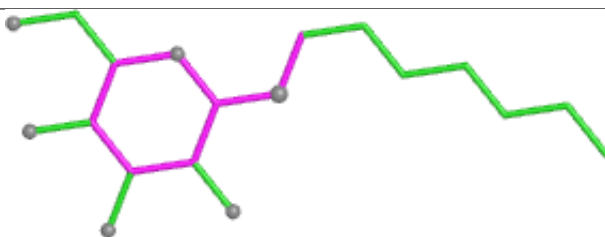
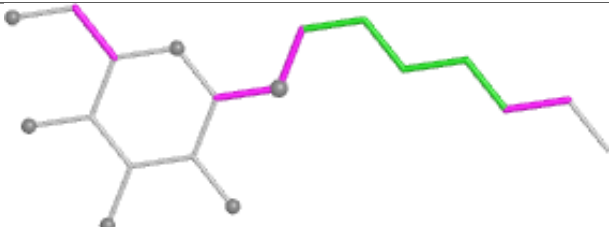
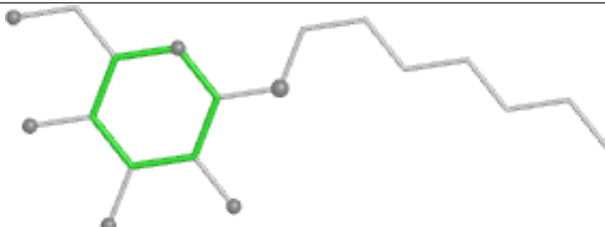


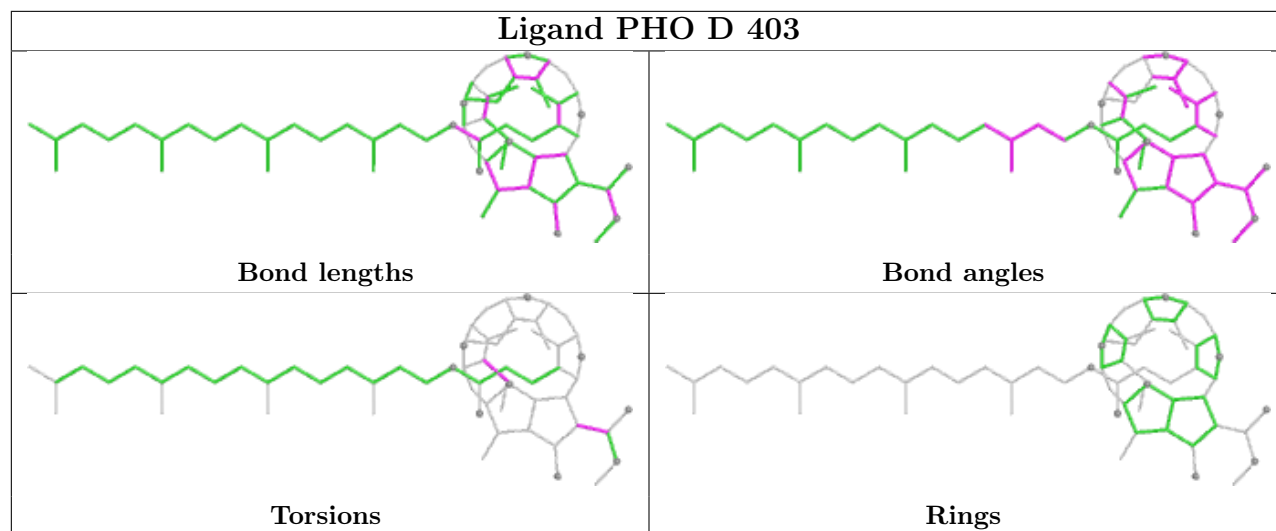
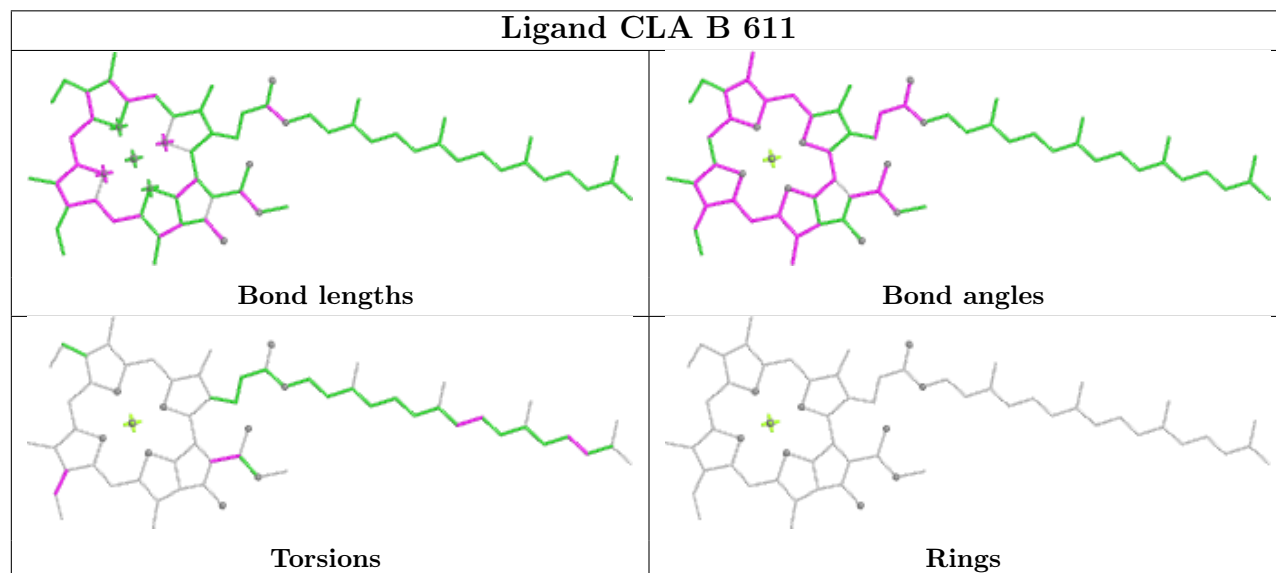
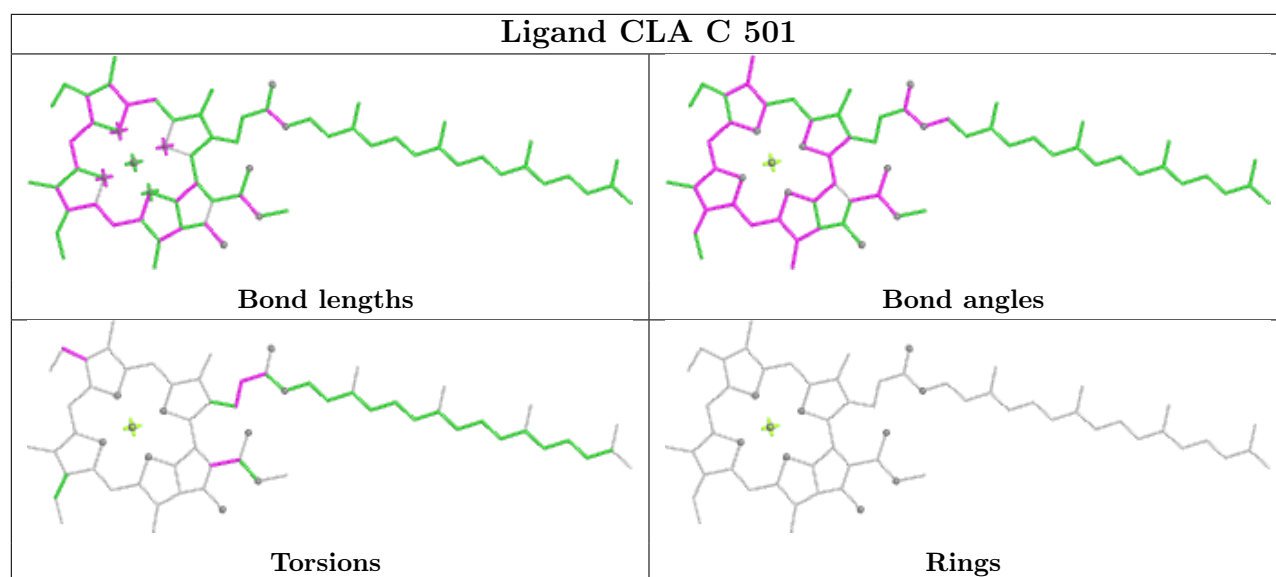


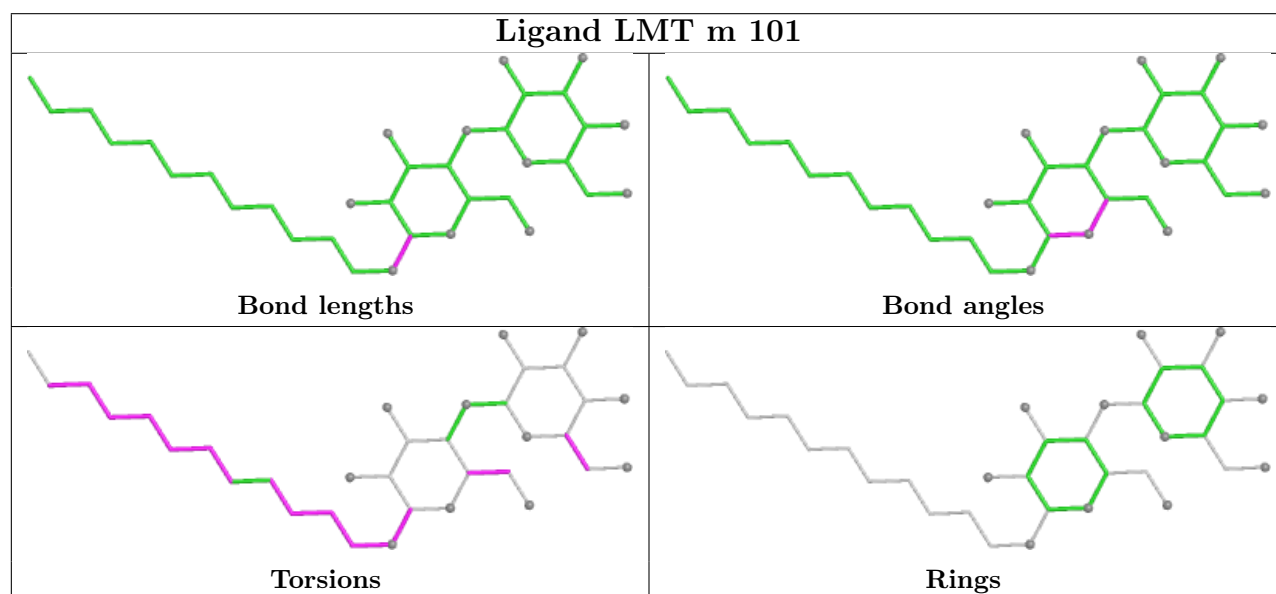
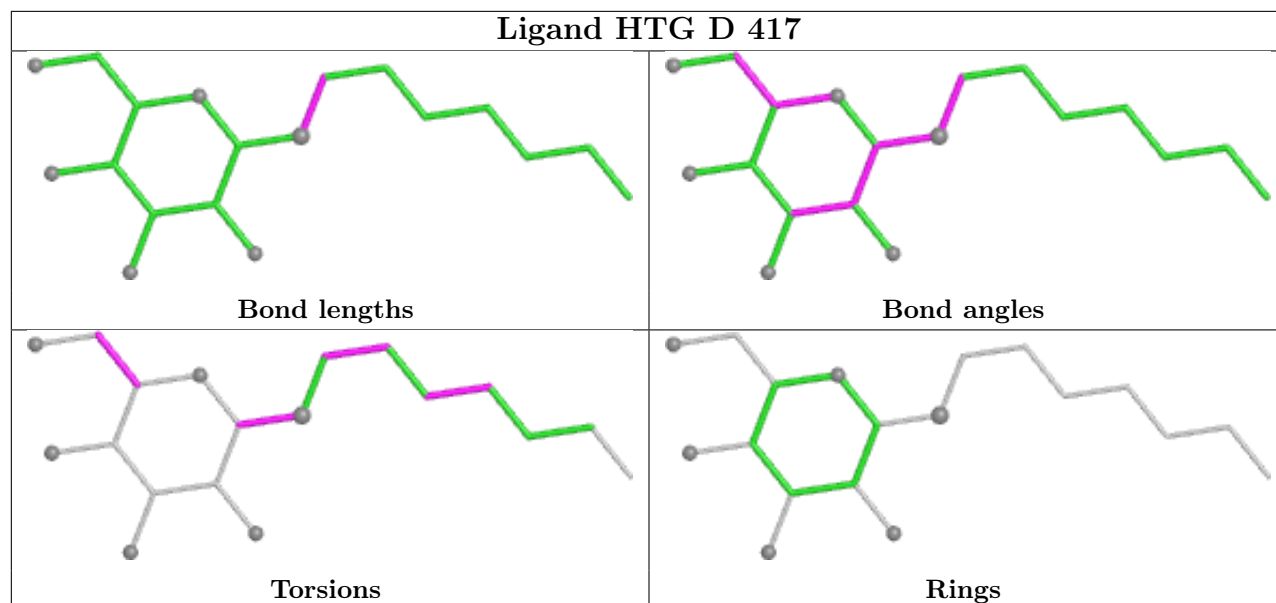


| Ligand BCR b 621                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

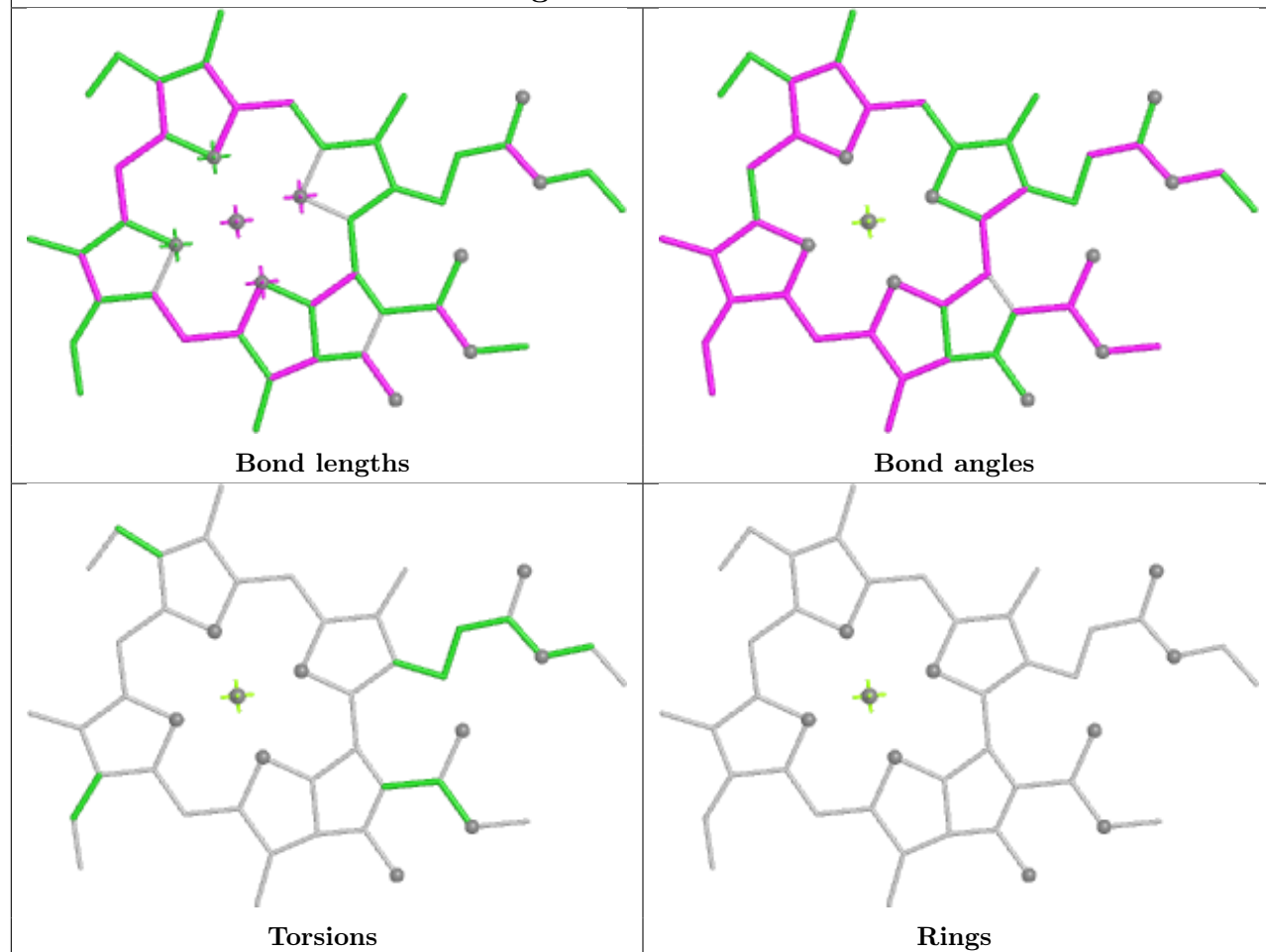
| Ligand BCR c 514                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand HTG C 534                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

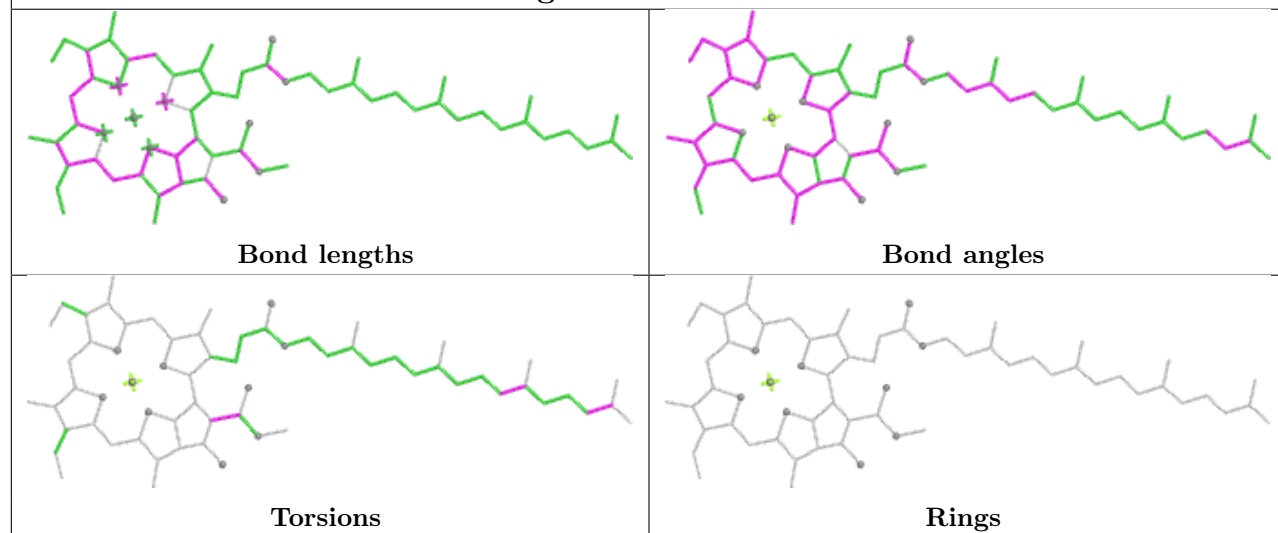




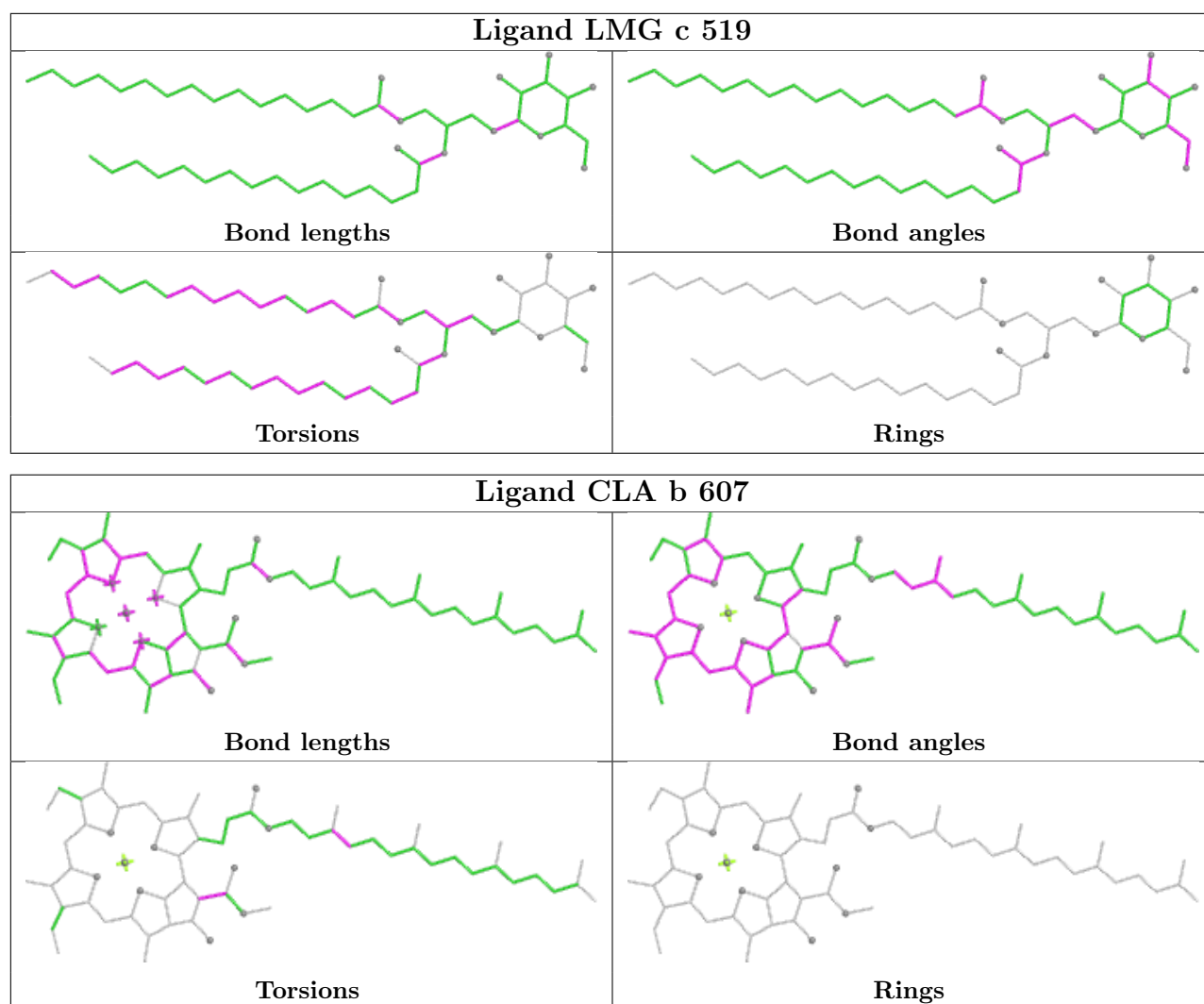
## Ligand CLA a 407

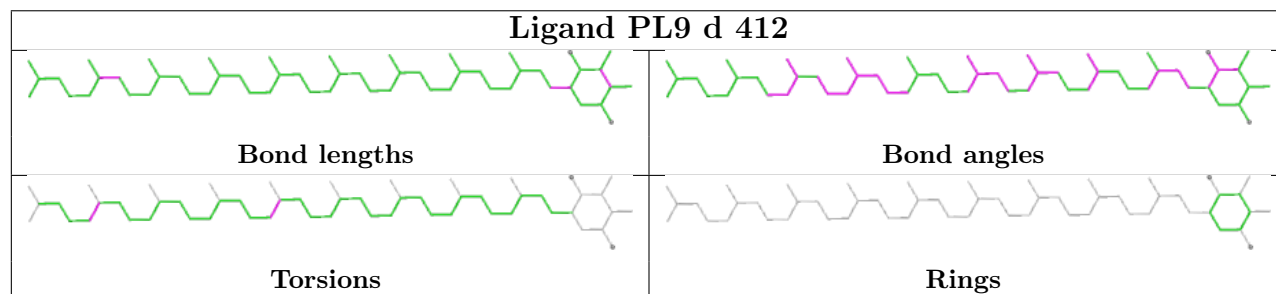
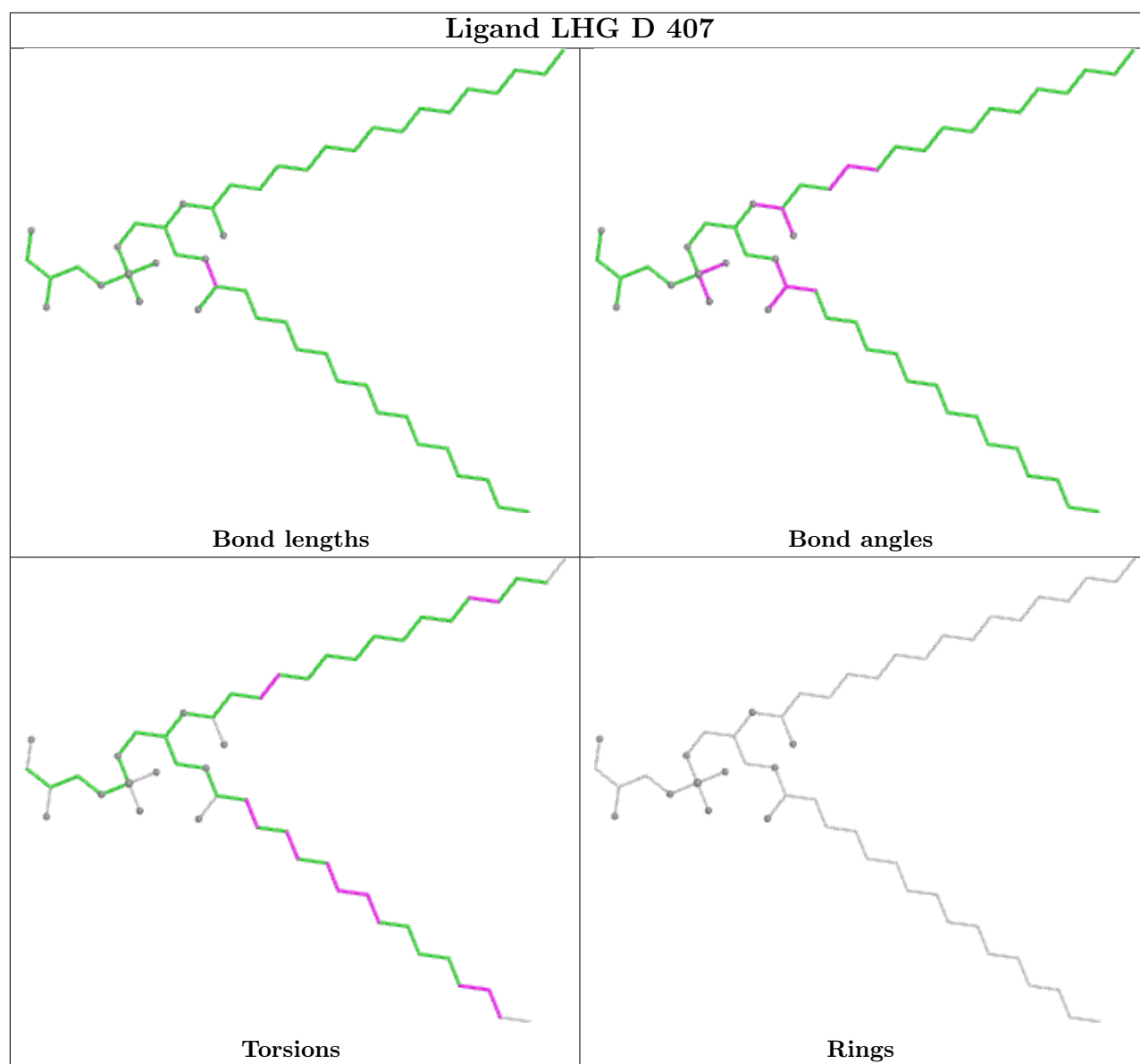


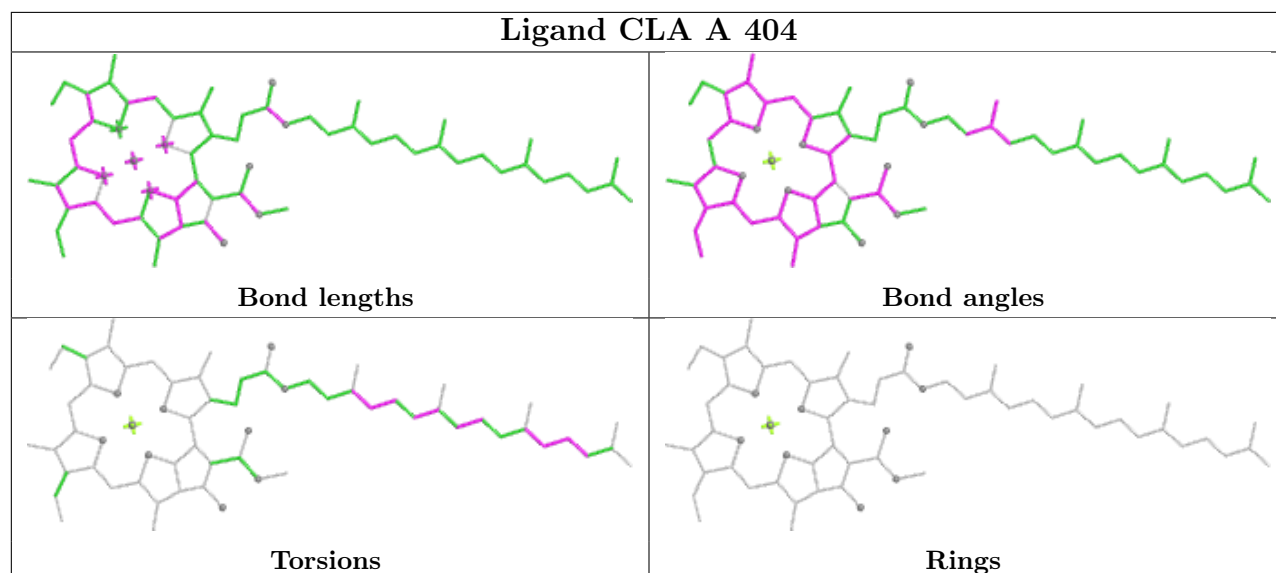
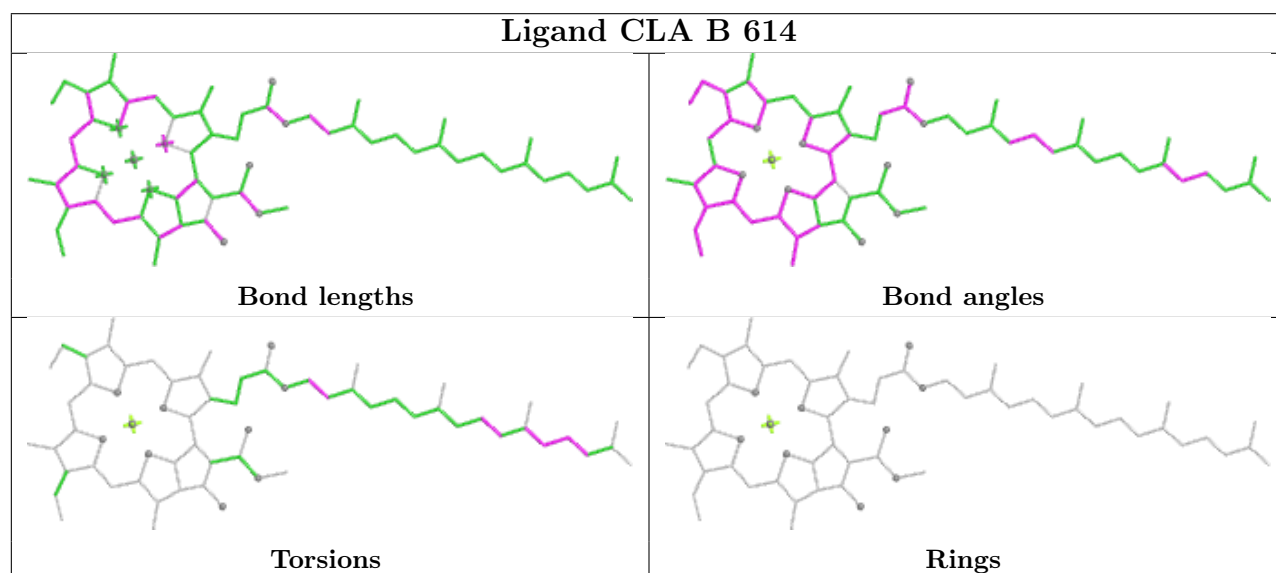
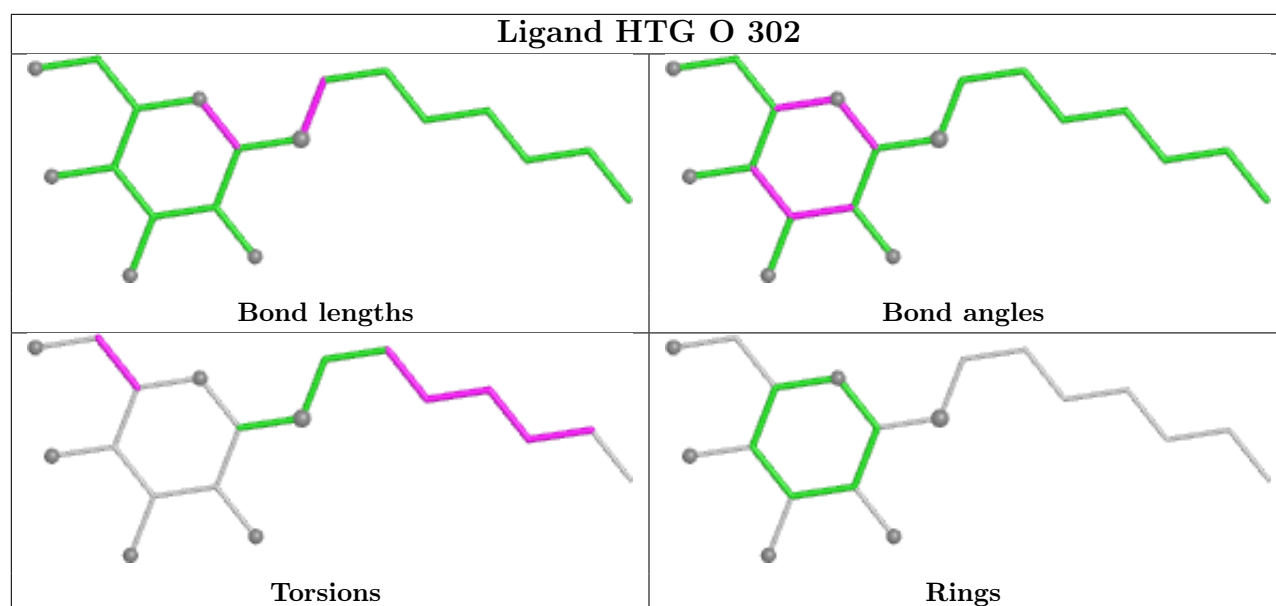
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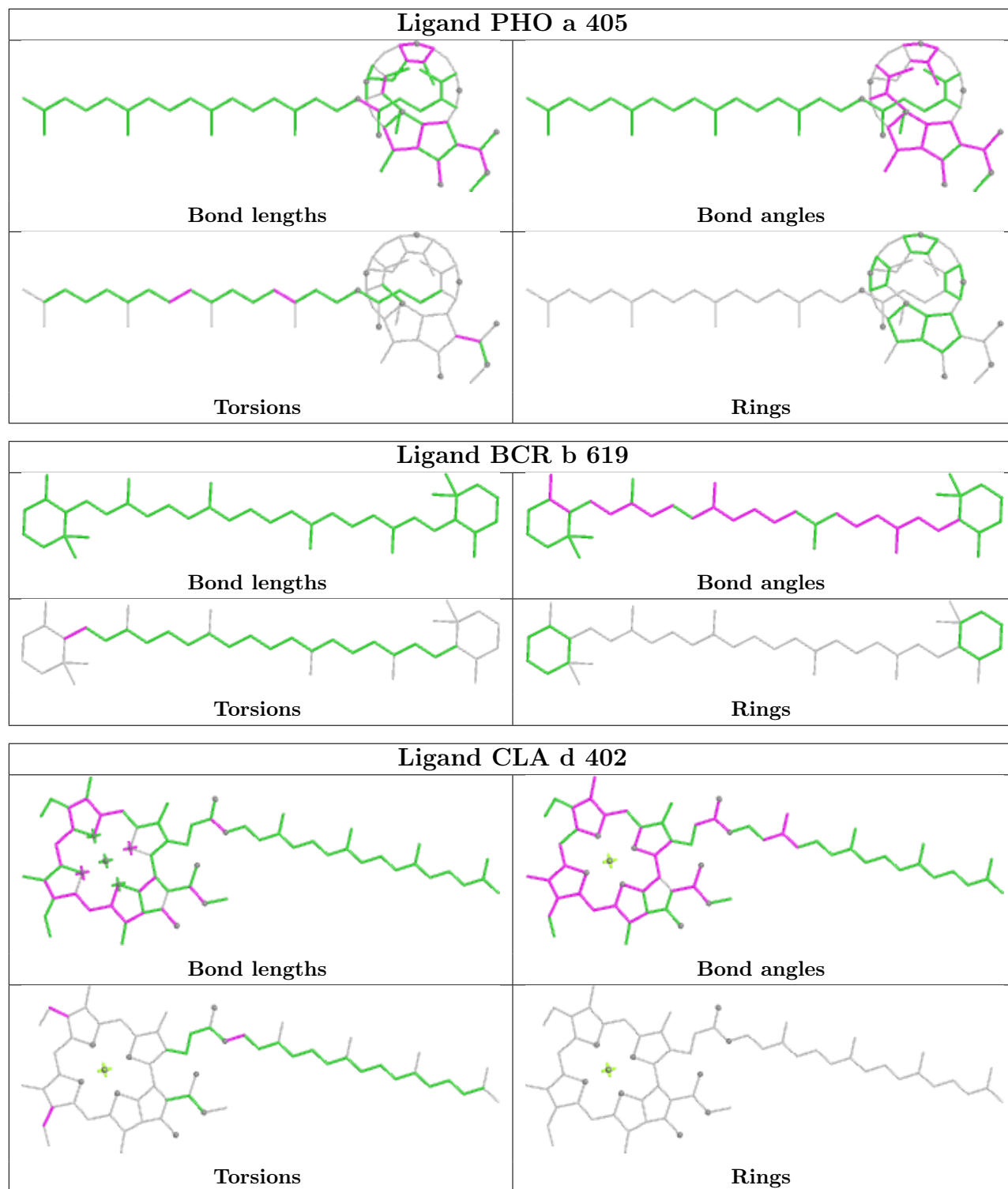


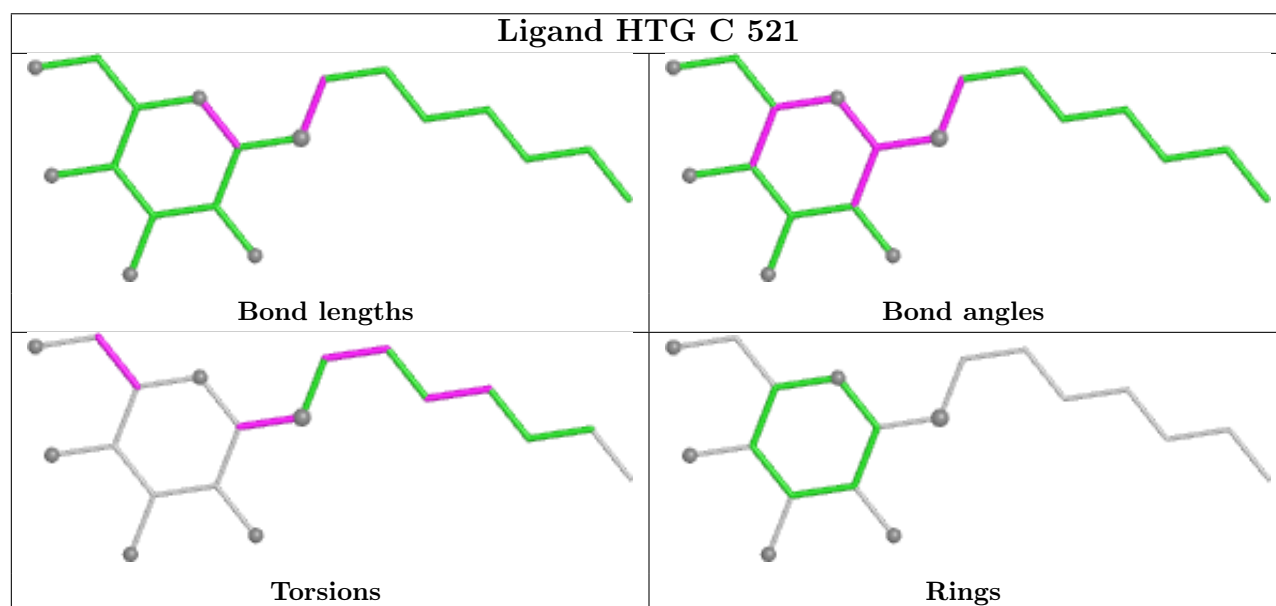
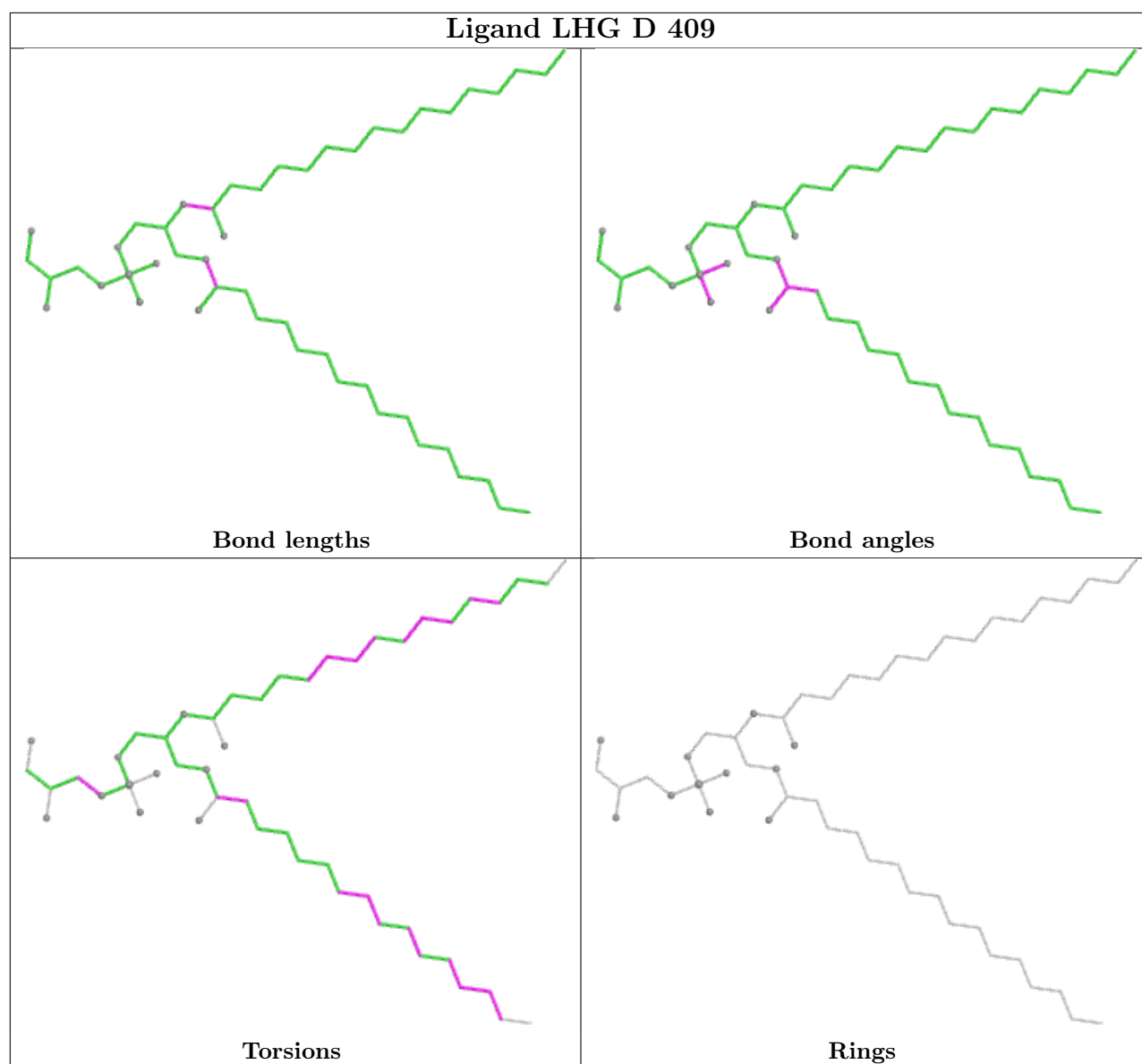


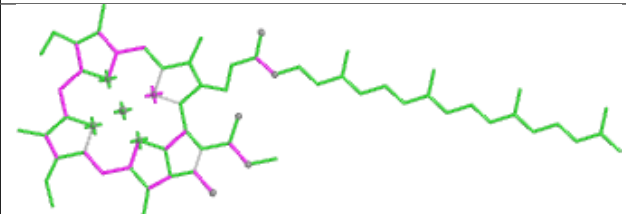
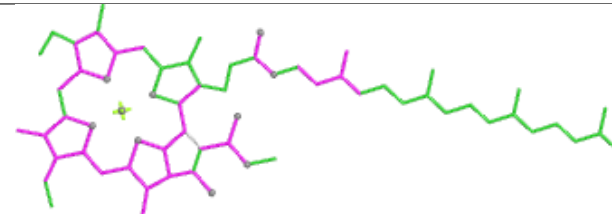
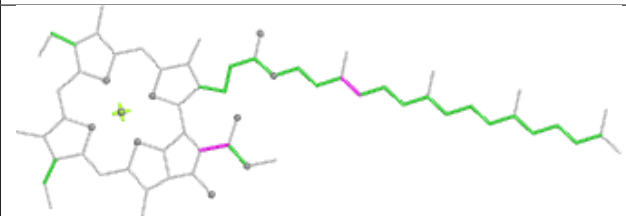
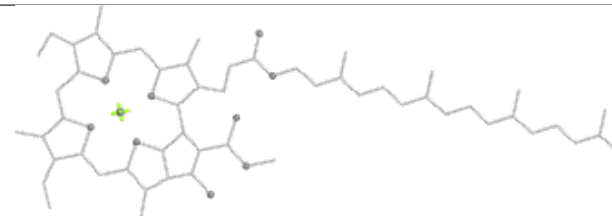


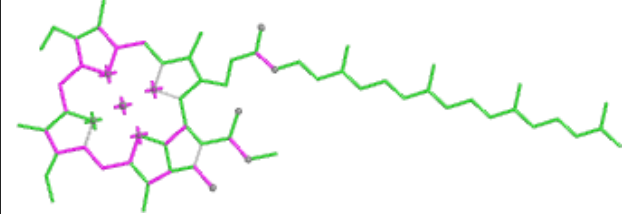
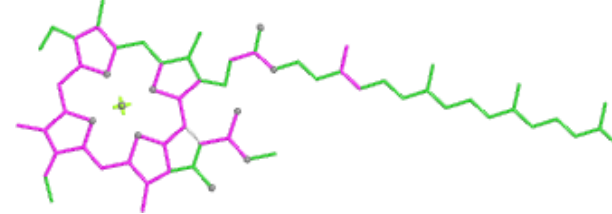
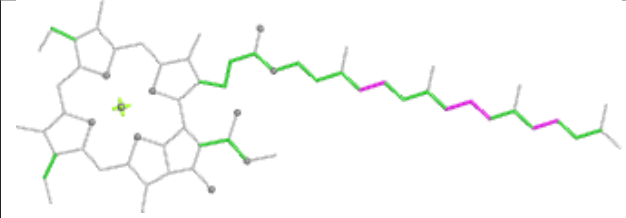
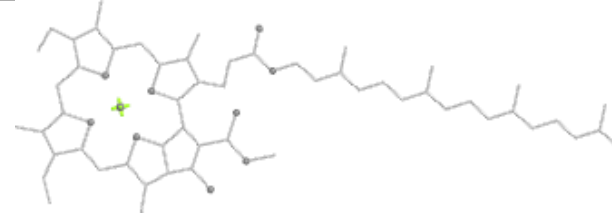


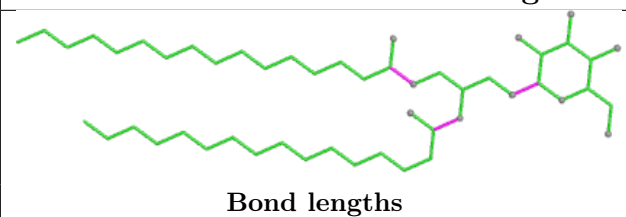
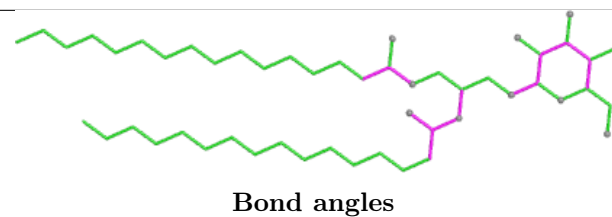
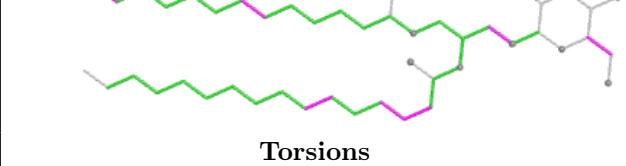


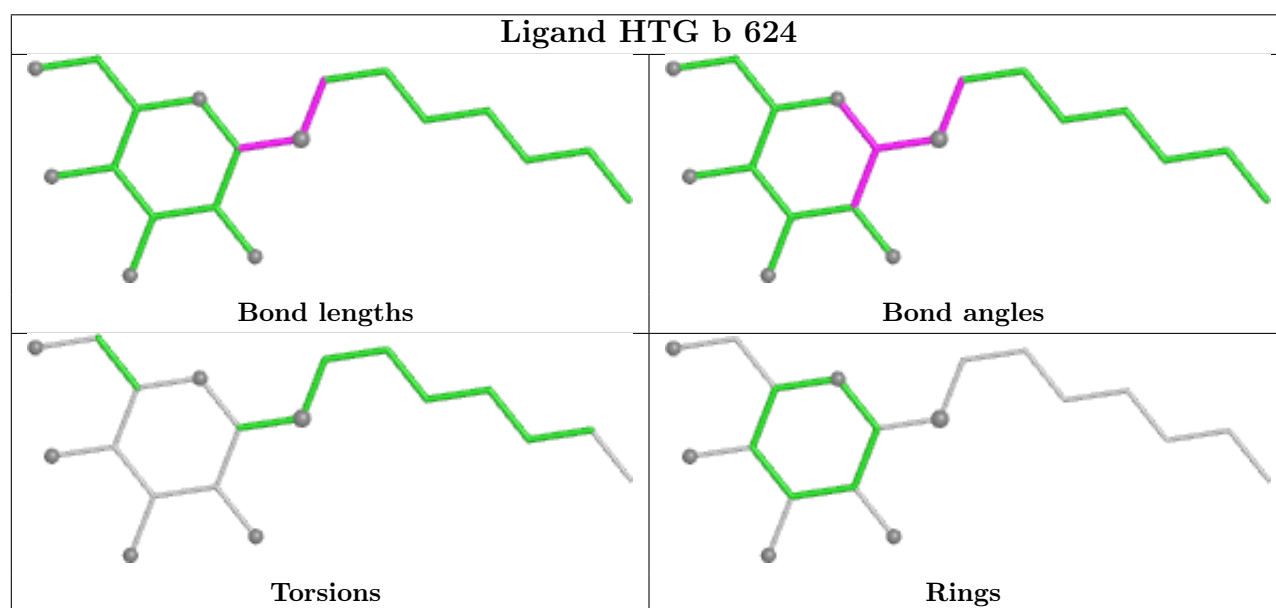
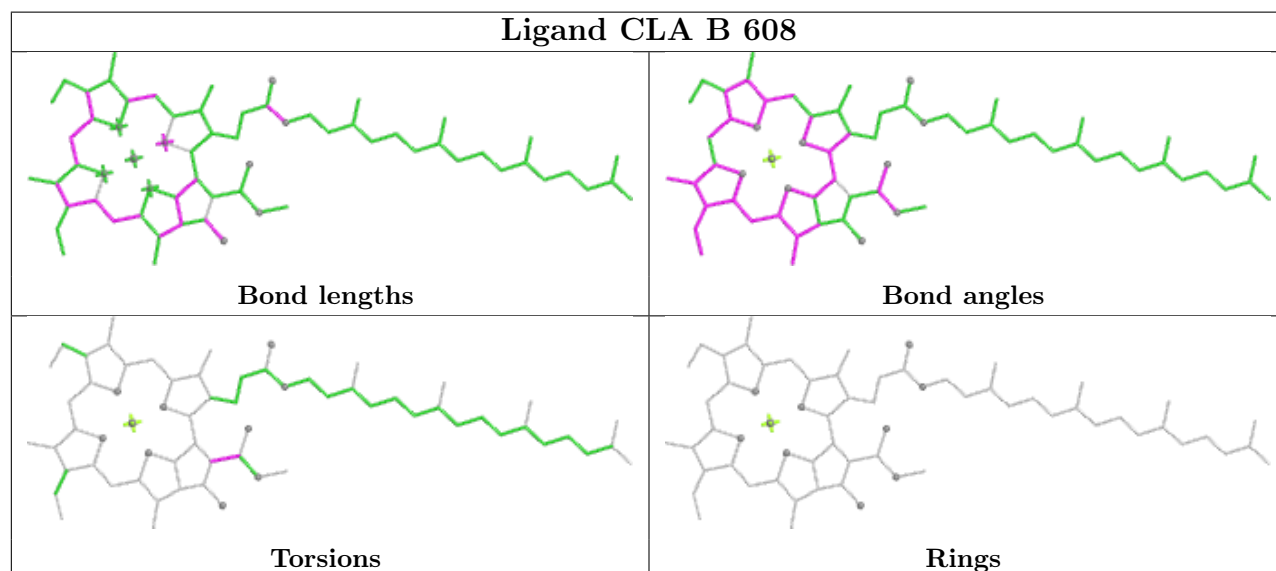
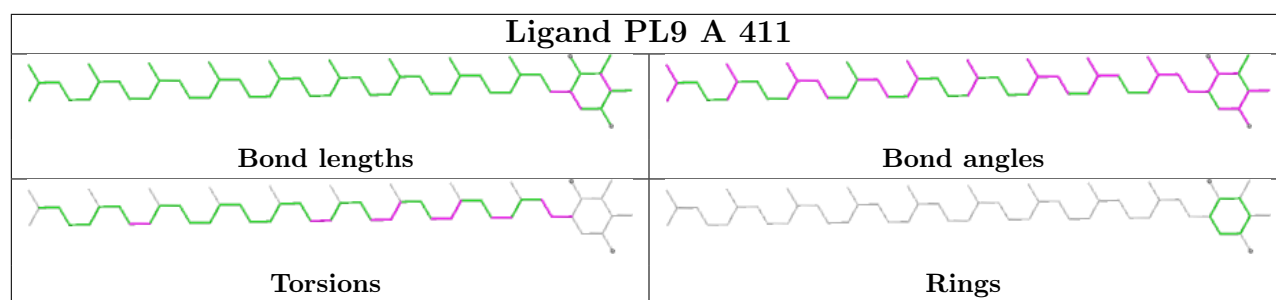


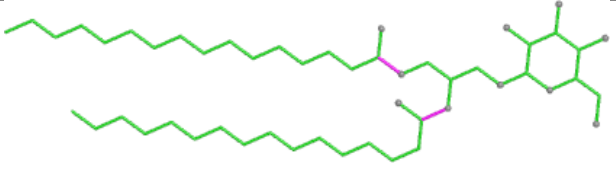
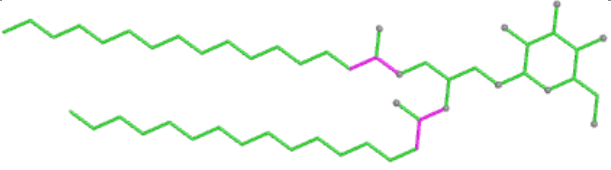
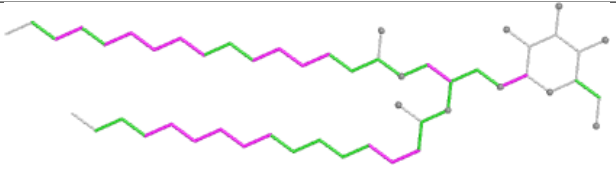
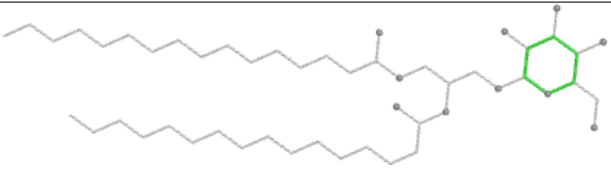


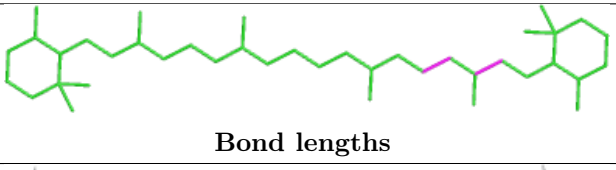
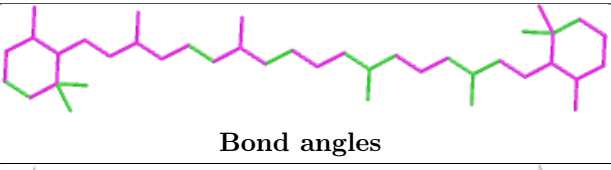
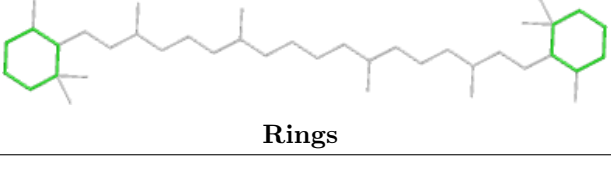
| Ligand CLA B 606                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

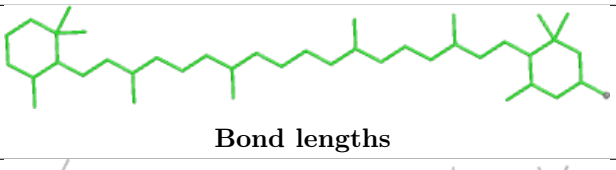
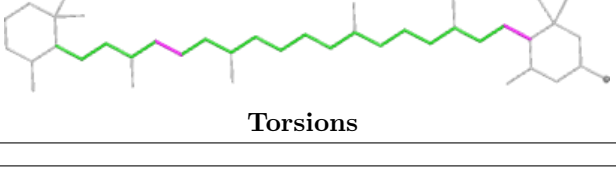
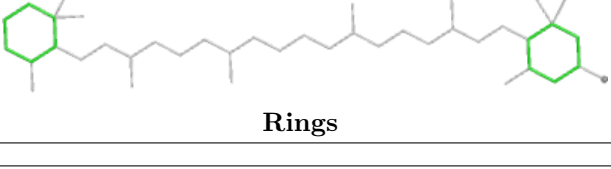
| Ligand CLA b 614                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

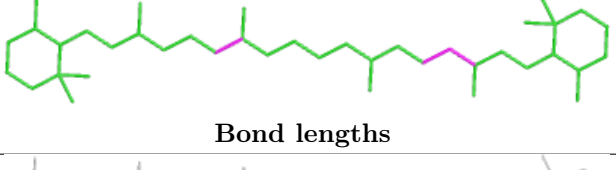
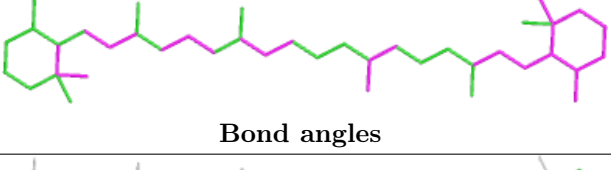
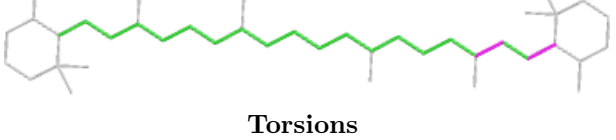
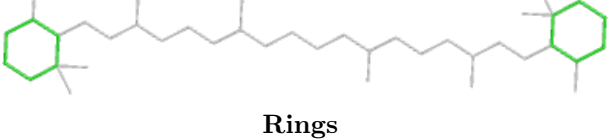
| Ligand LMG c 518                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



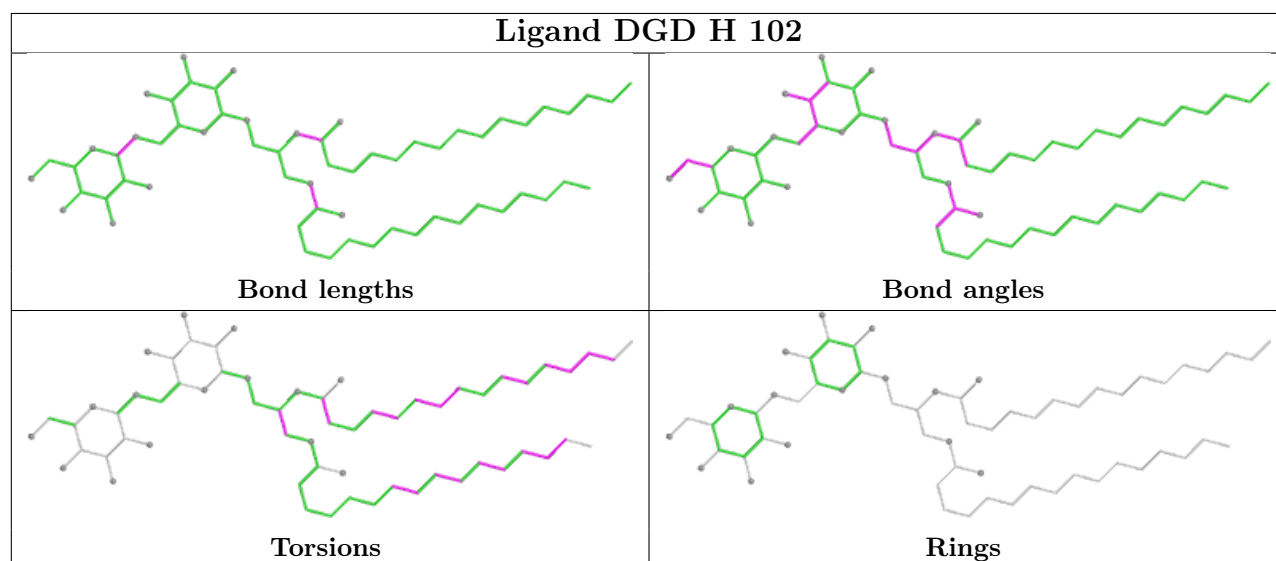
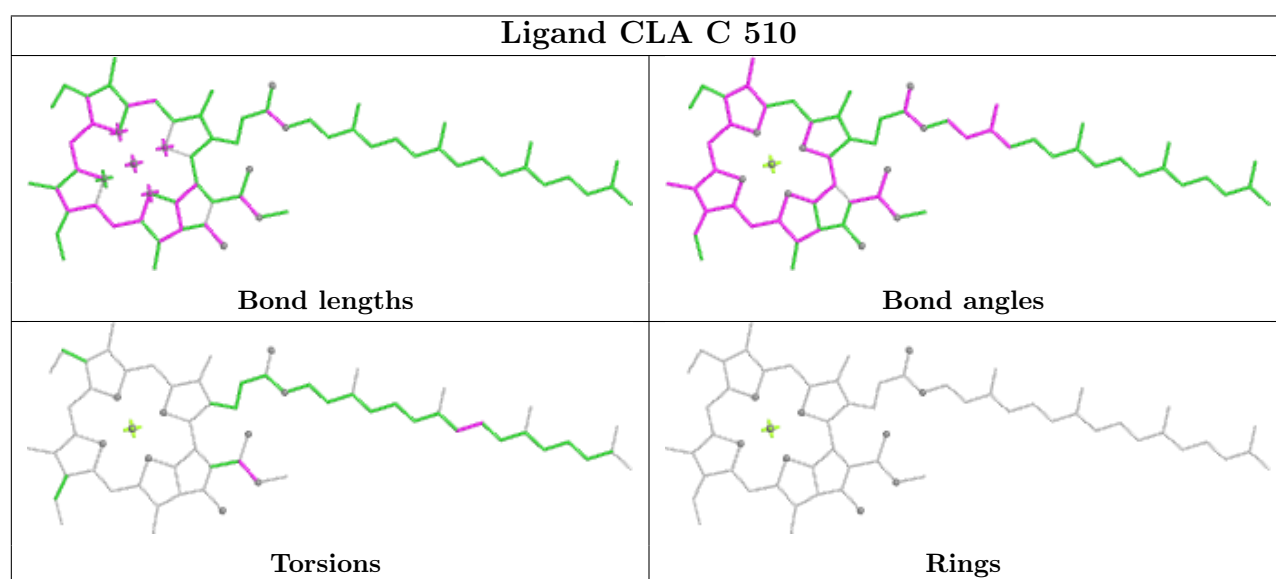
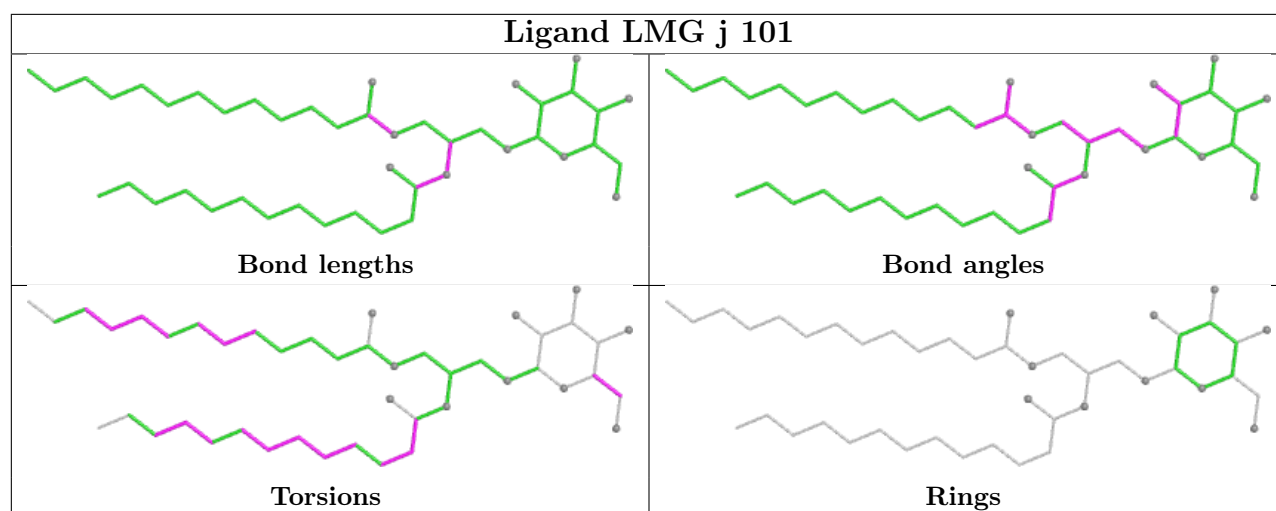
| Ligand LMG a 410                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

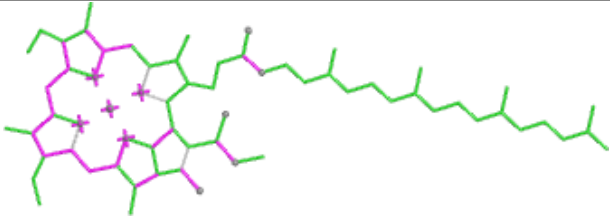
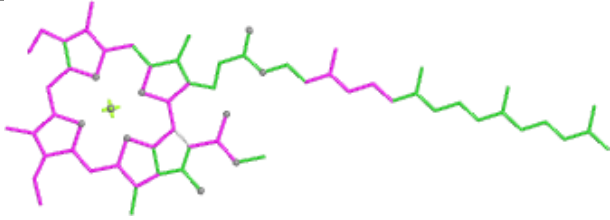
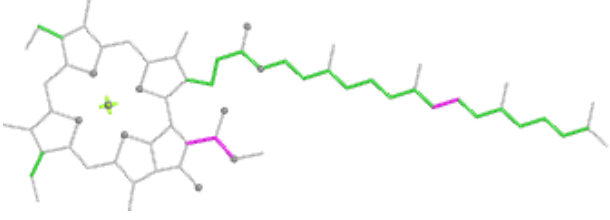
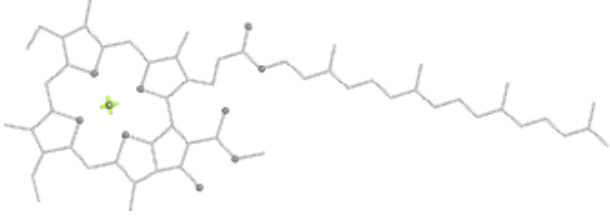
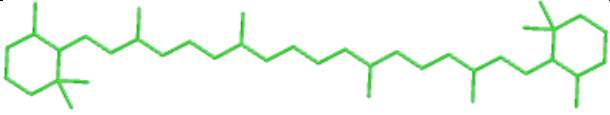
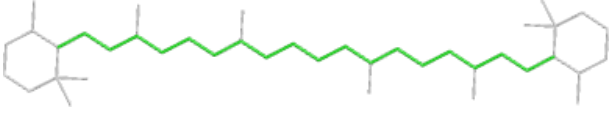
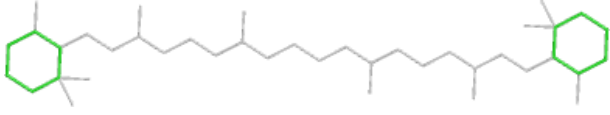
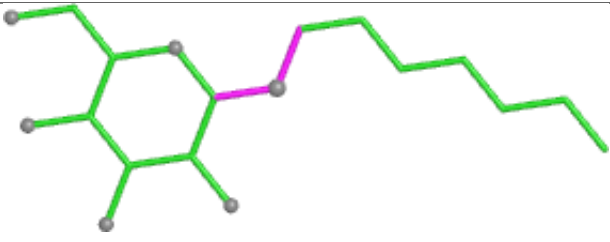
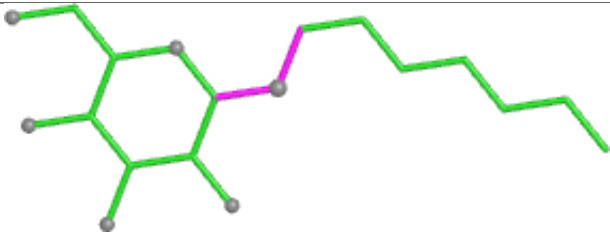
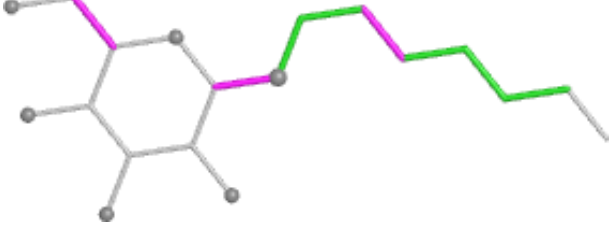
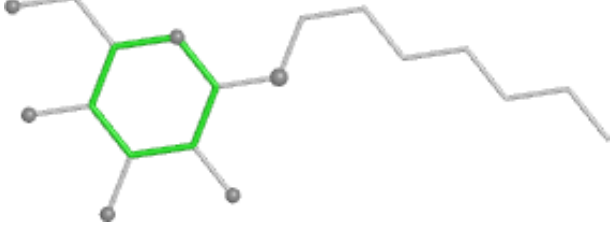
| Ligand BCR t 101                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|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

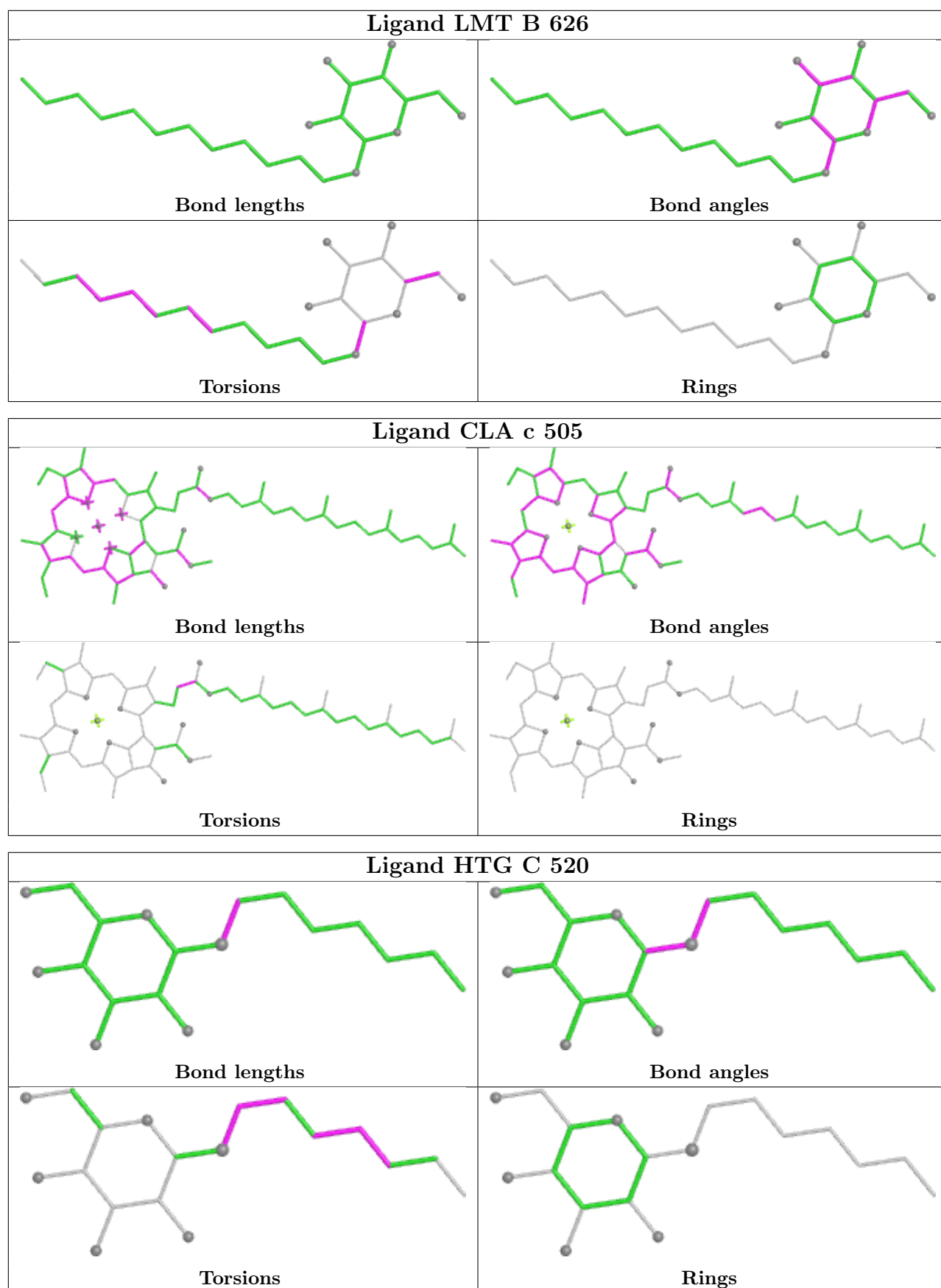
| Ligand RRX x 101                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|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

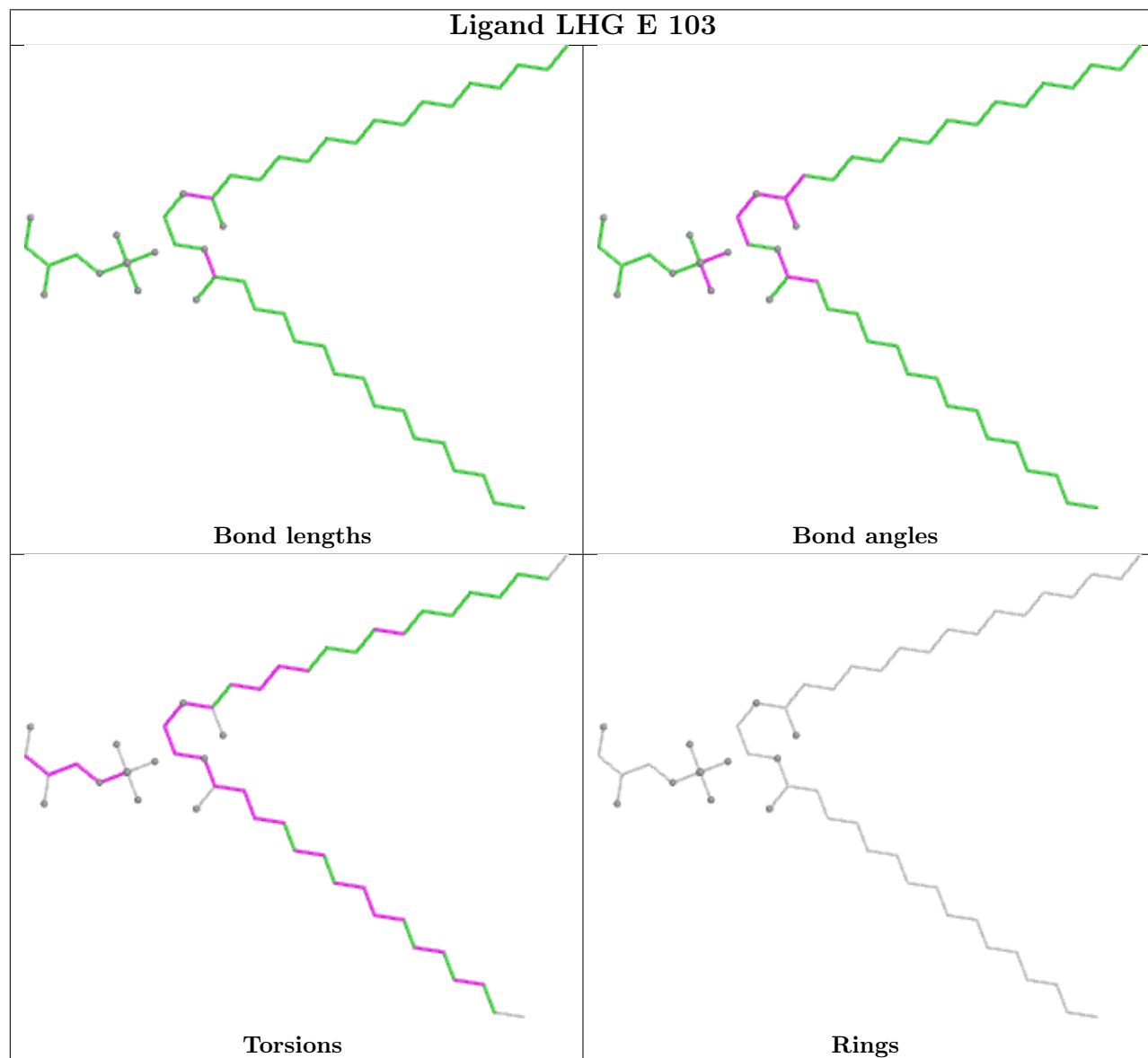
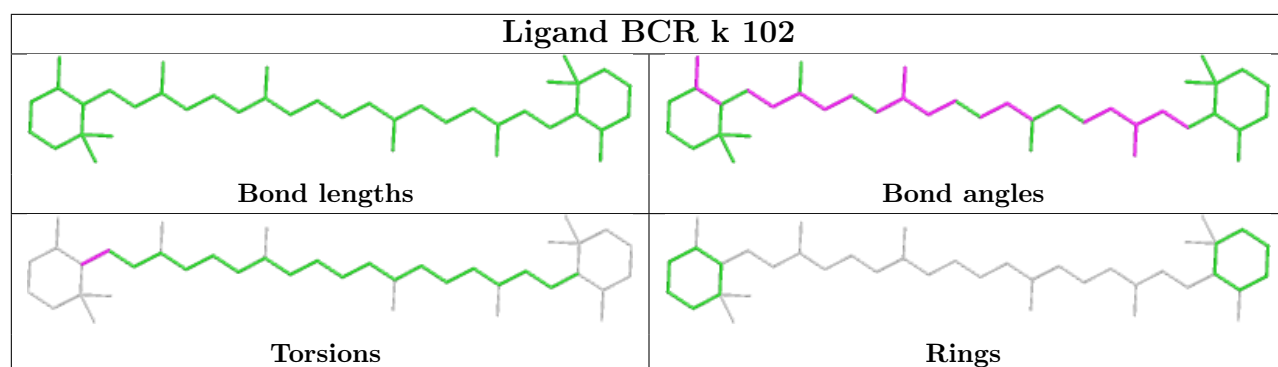
| Ligand BCR D 405                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

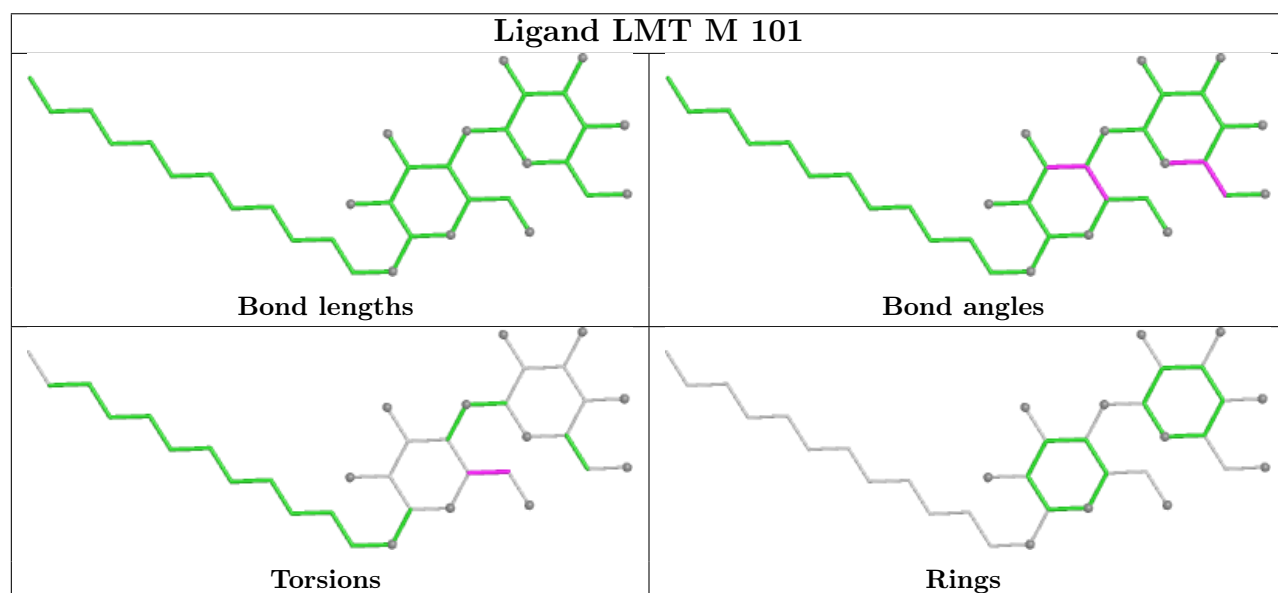
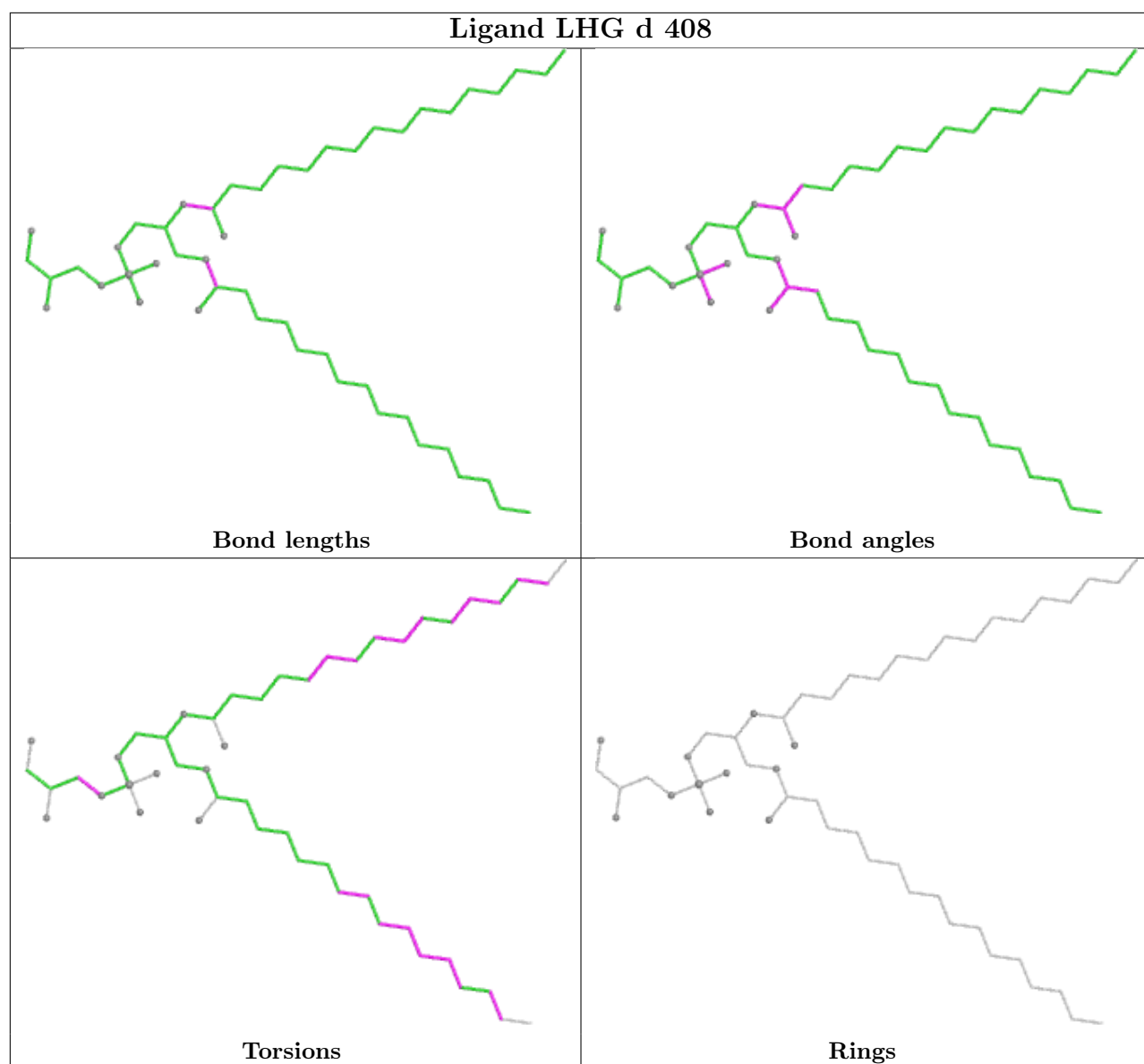


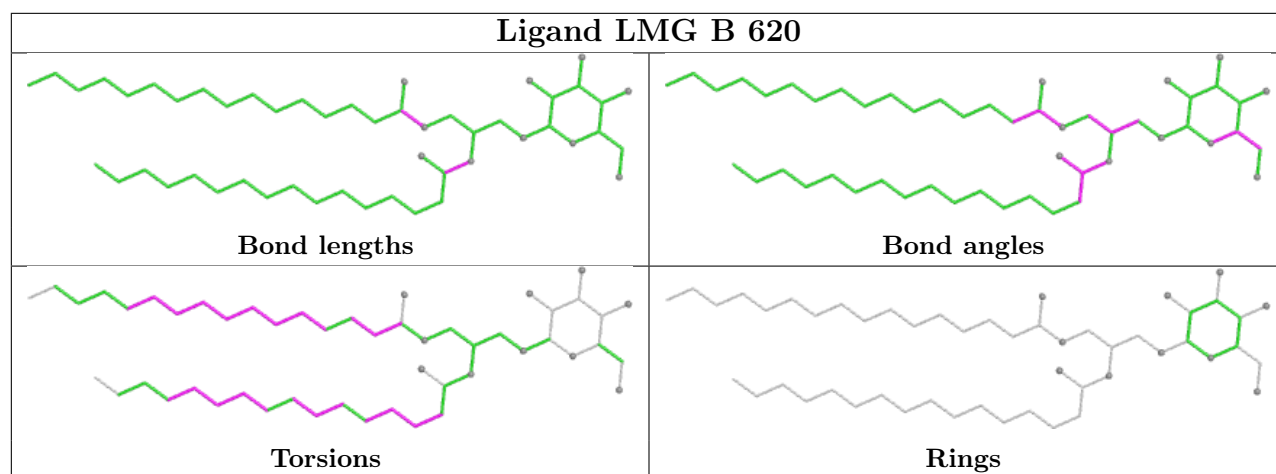
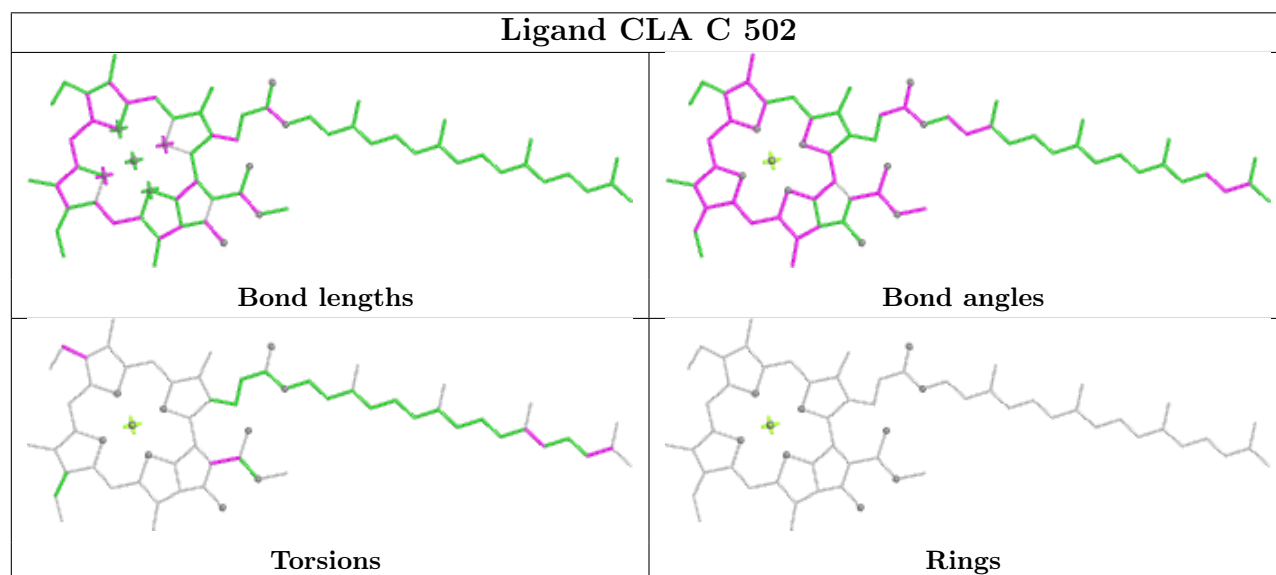
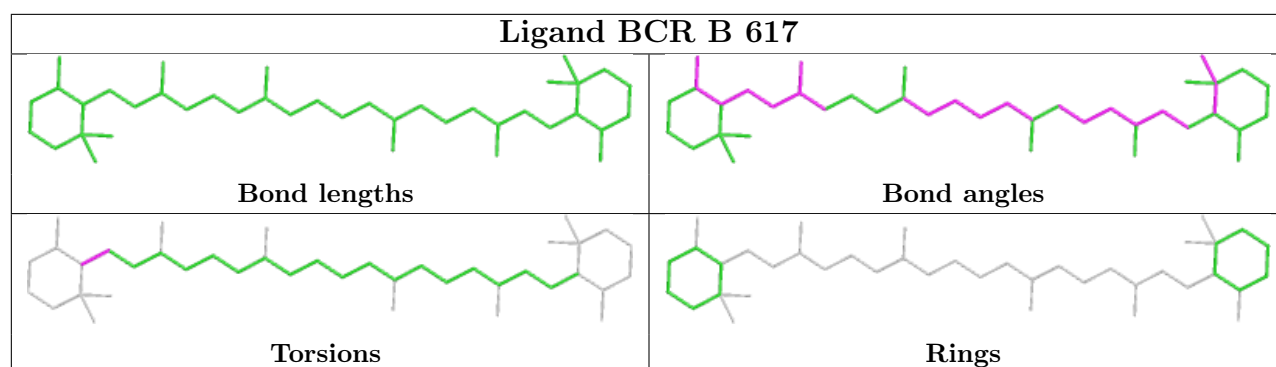


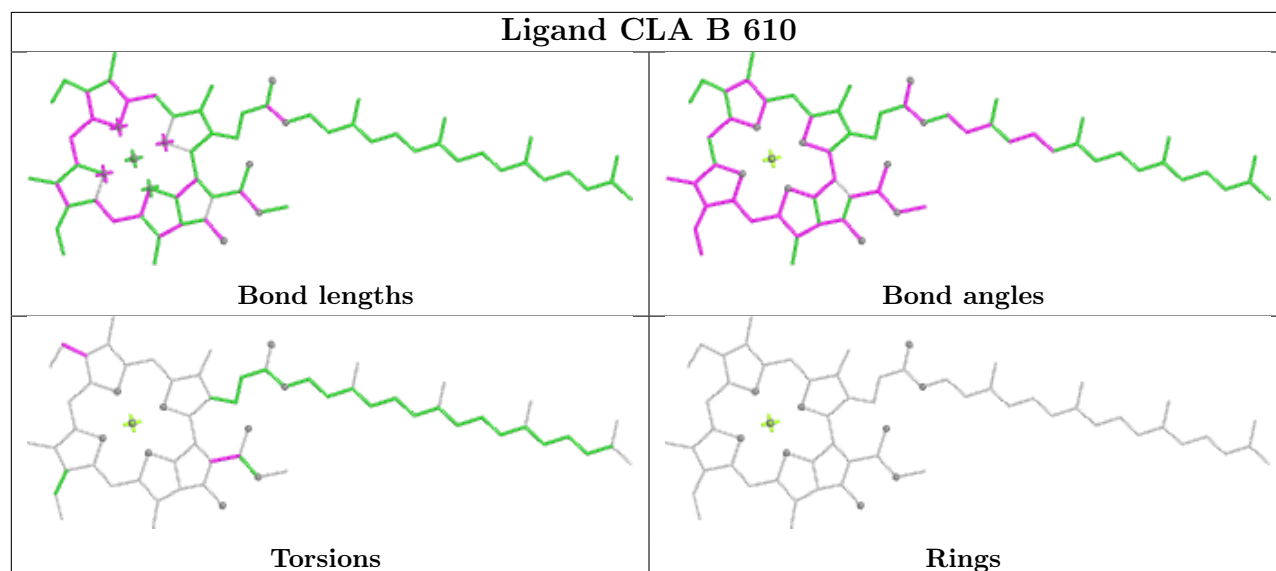
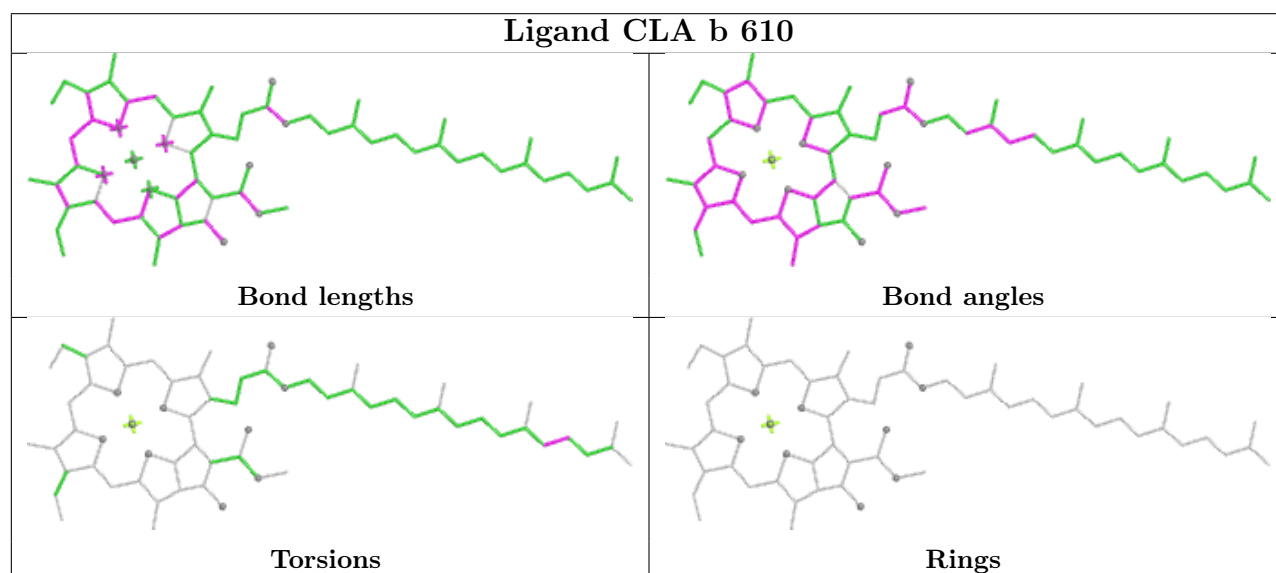
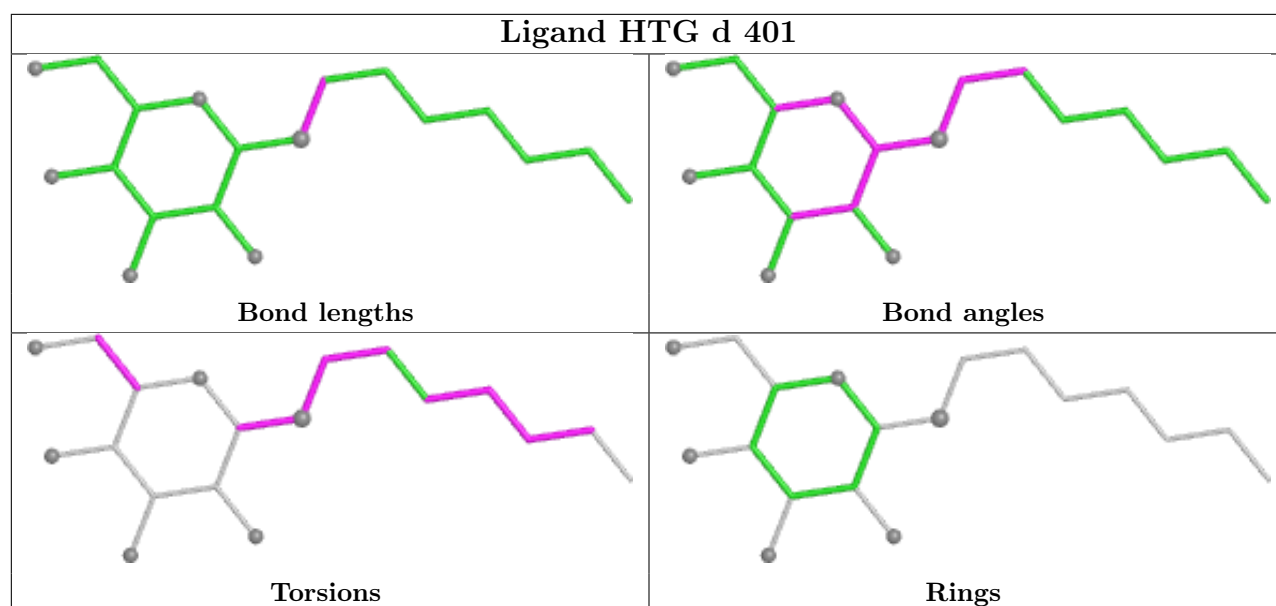
| Ligand CLA C 503                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR C 515                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand HTG C 522                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

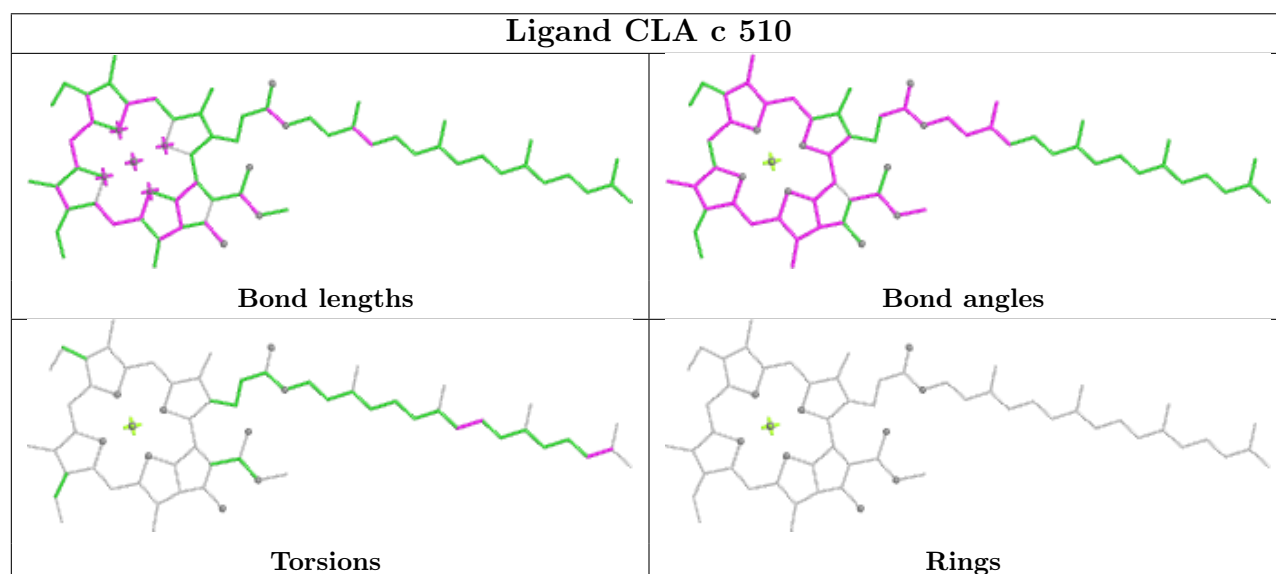
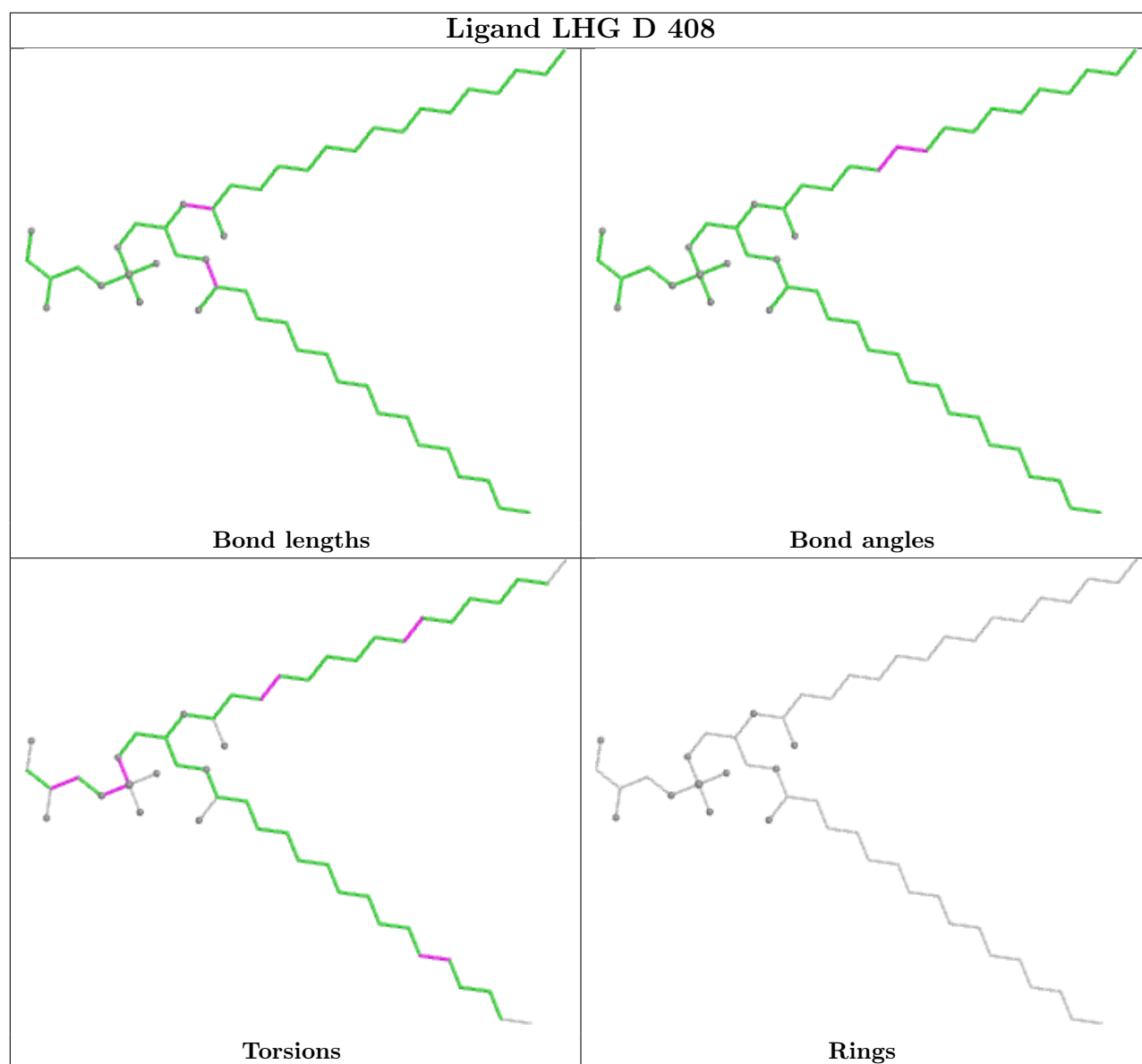






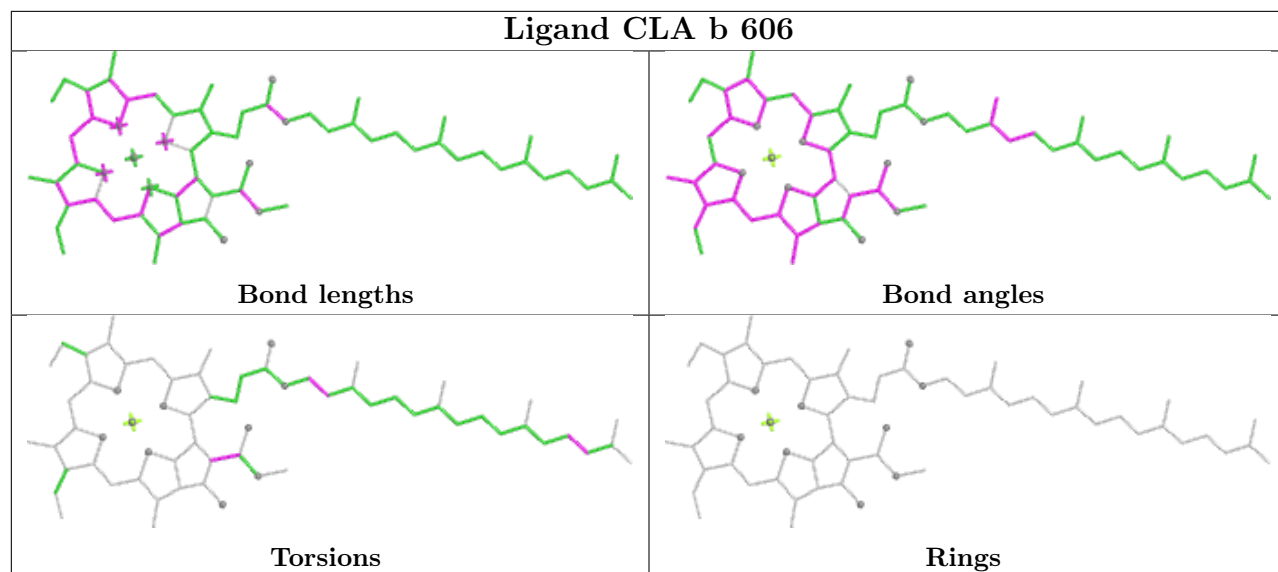




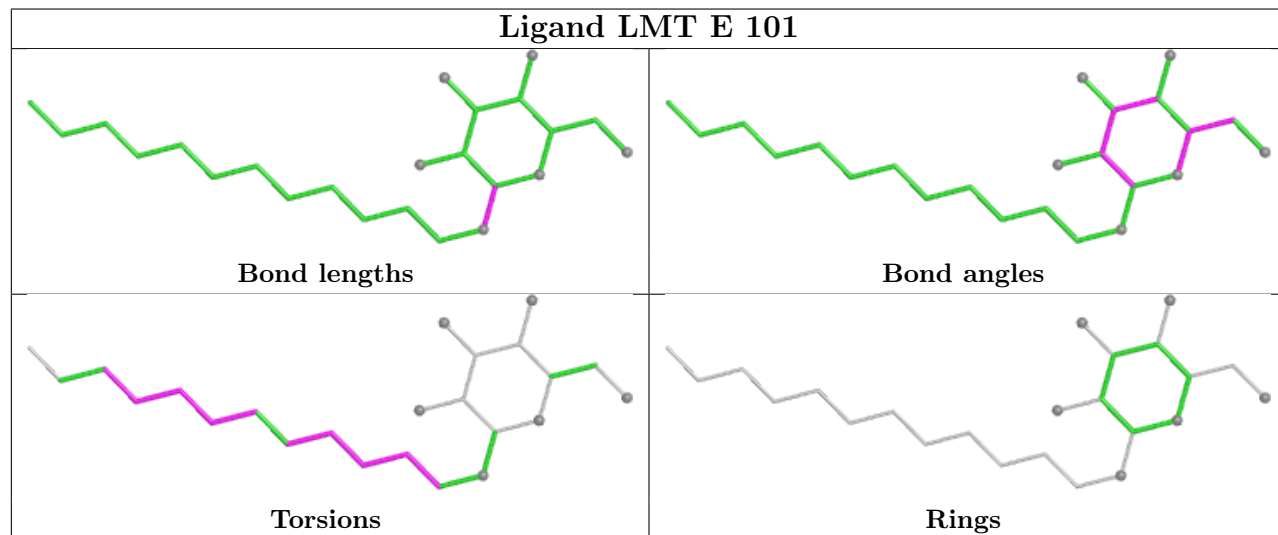




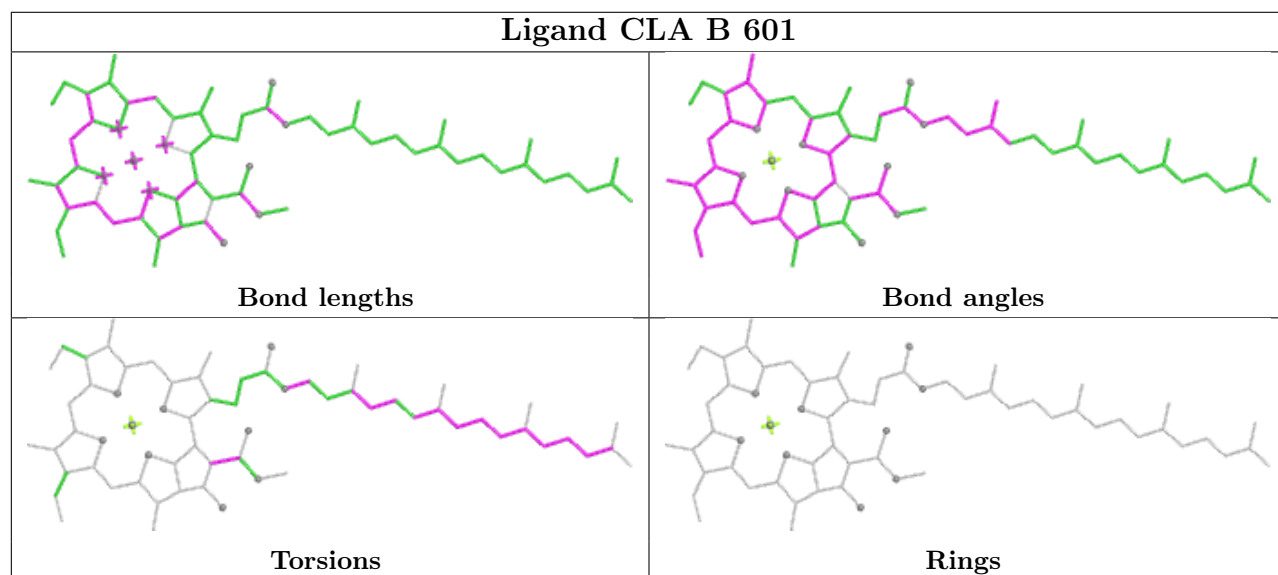
## Ligand CLA b 606

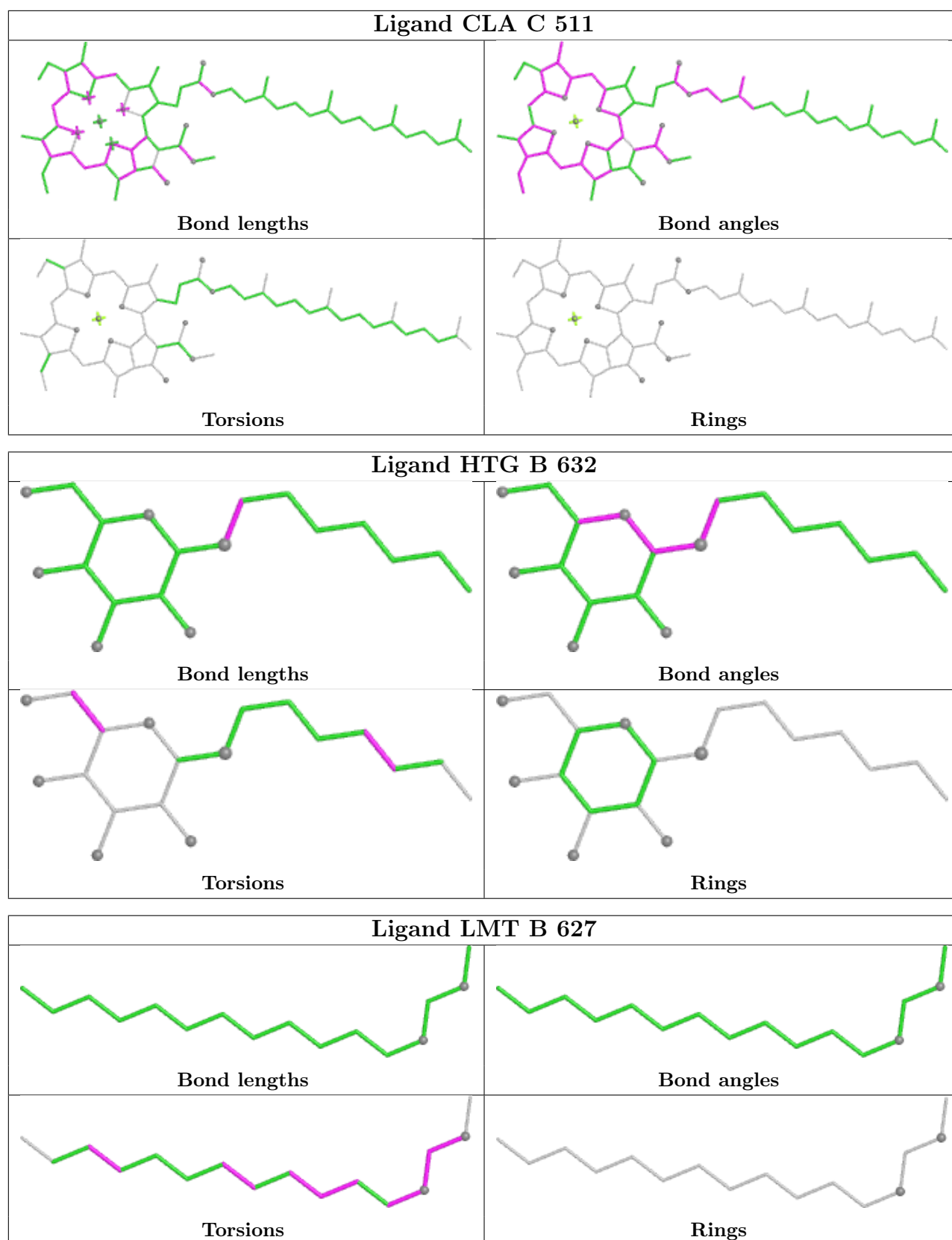


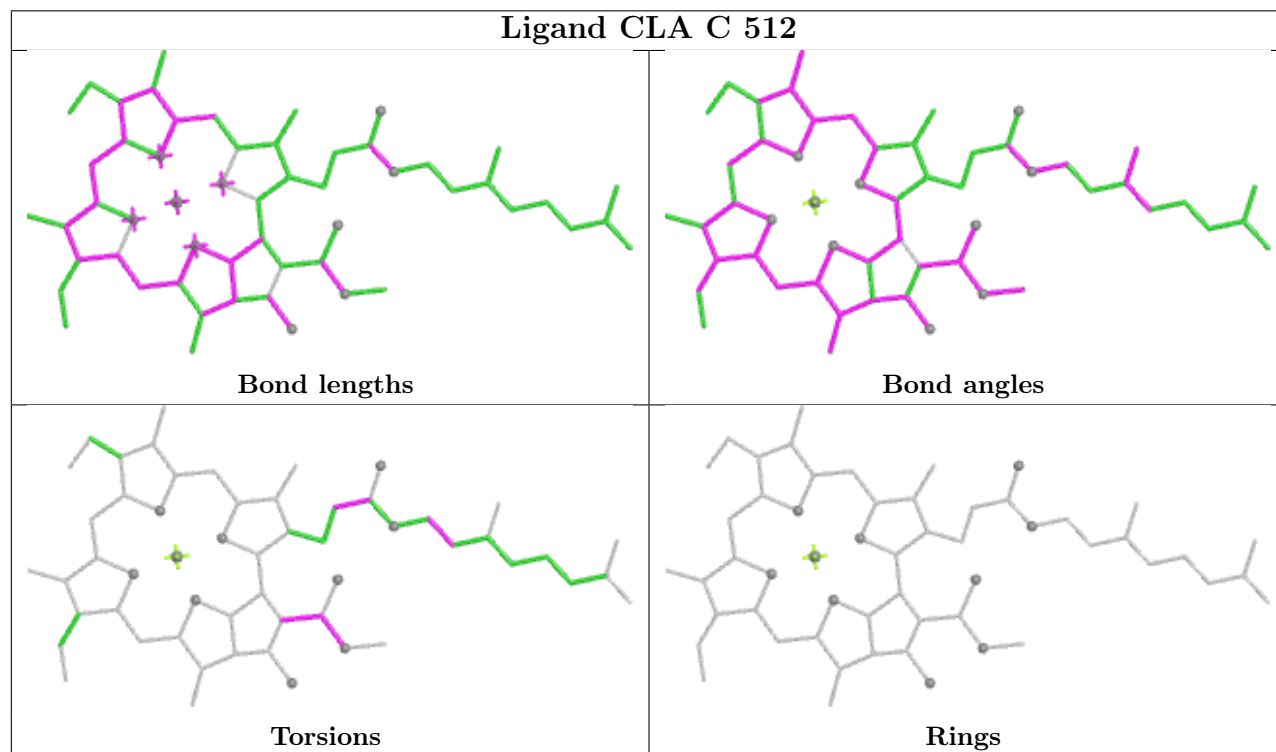
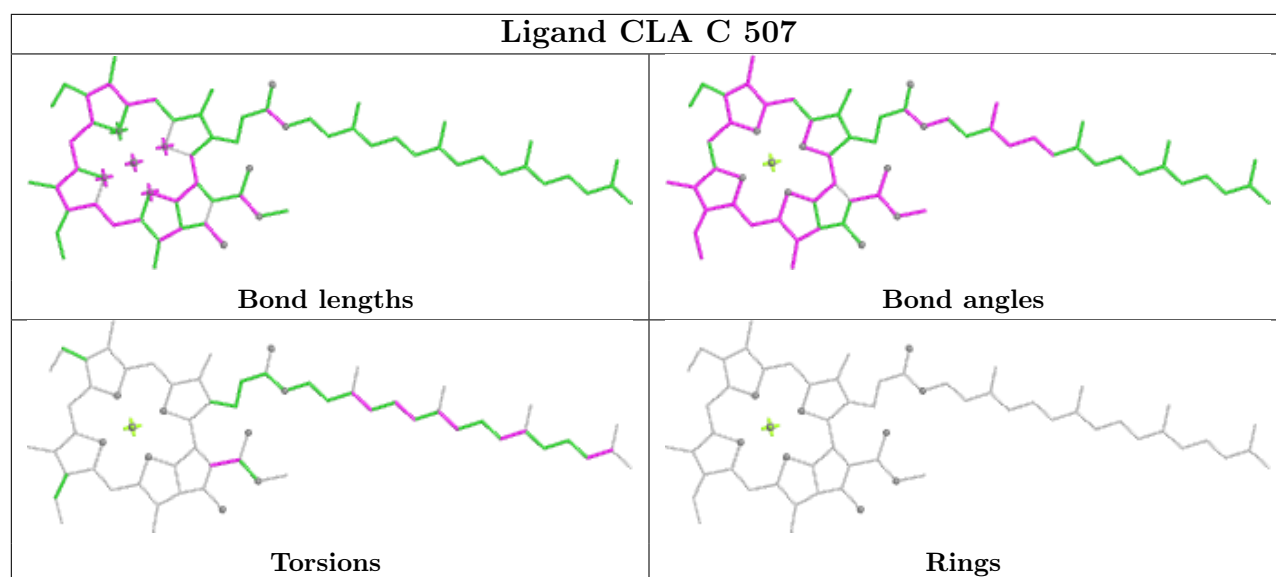
## Ligand LMT E 101

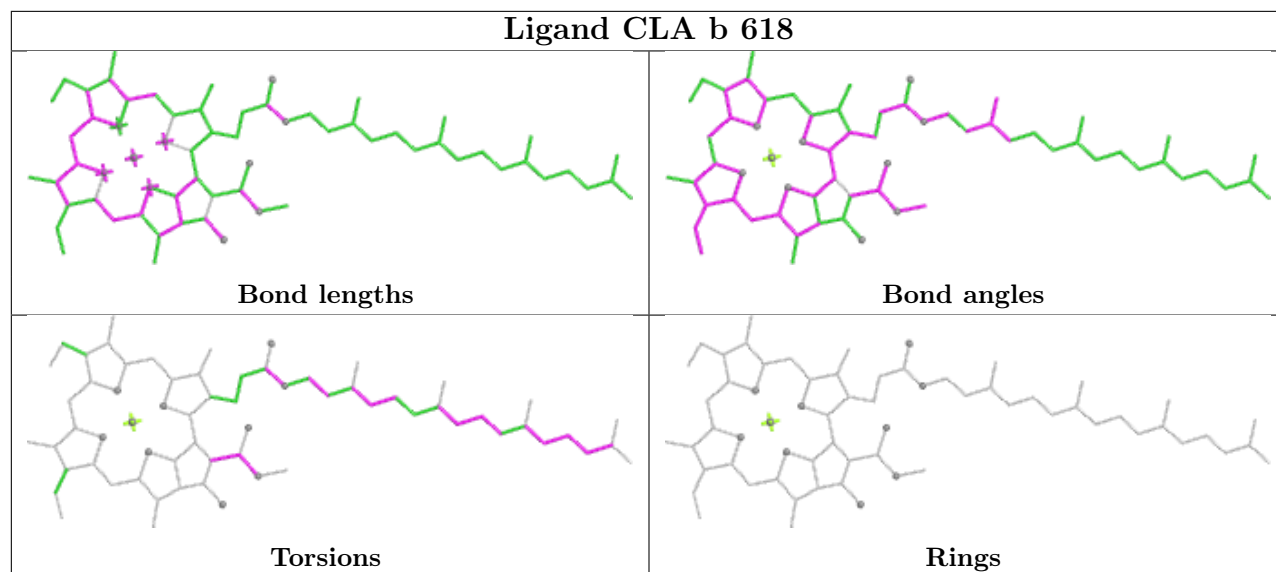
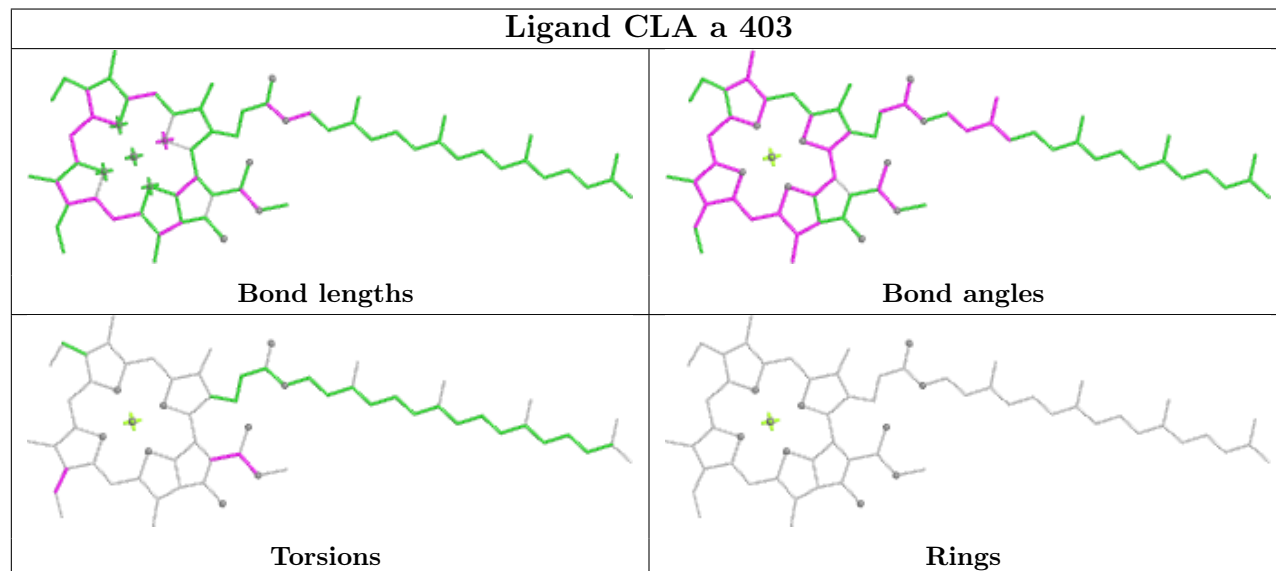


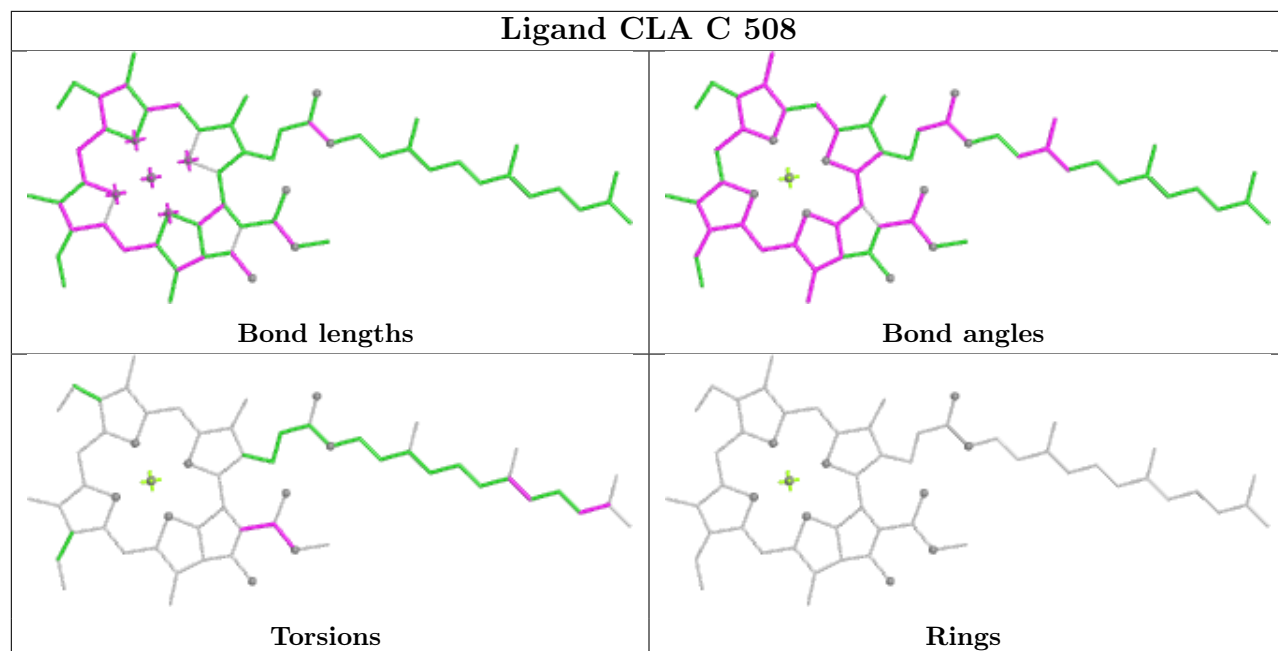
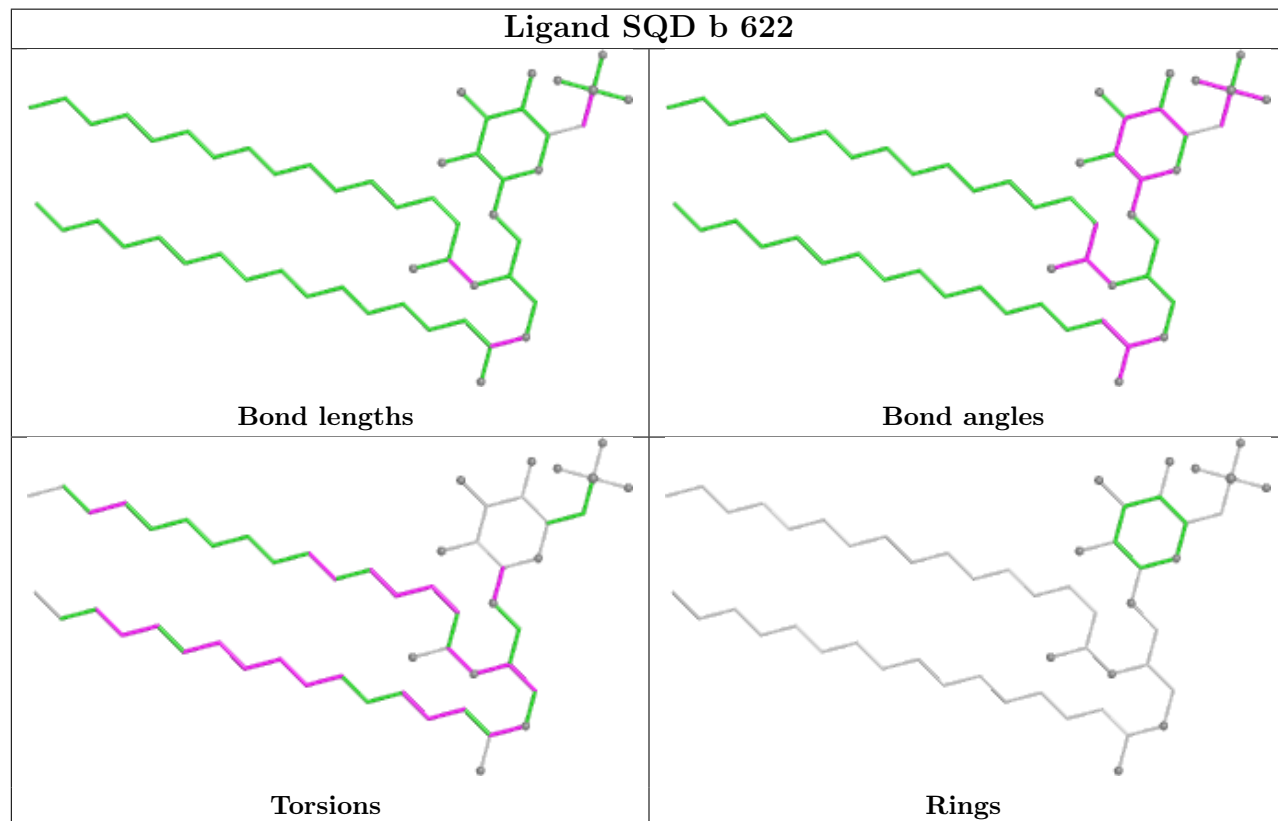
## Ligand CLA B 601

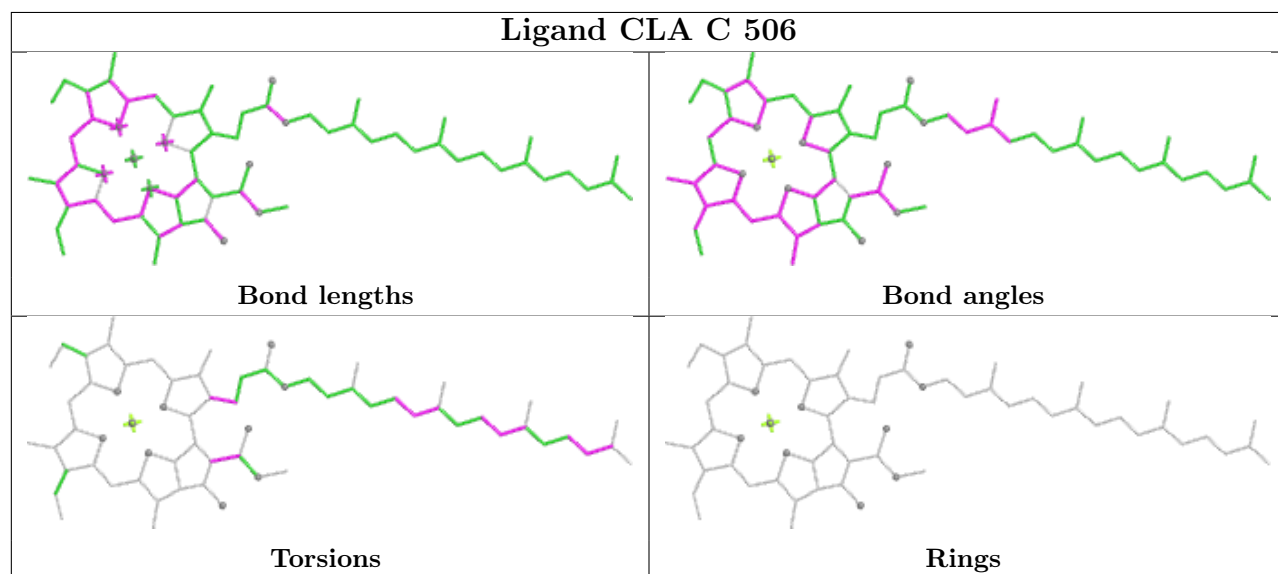
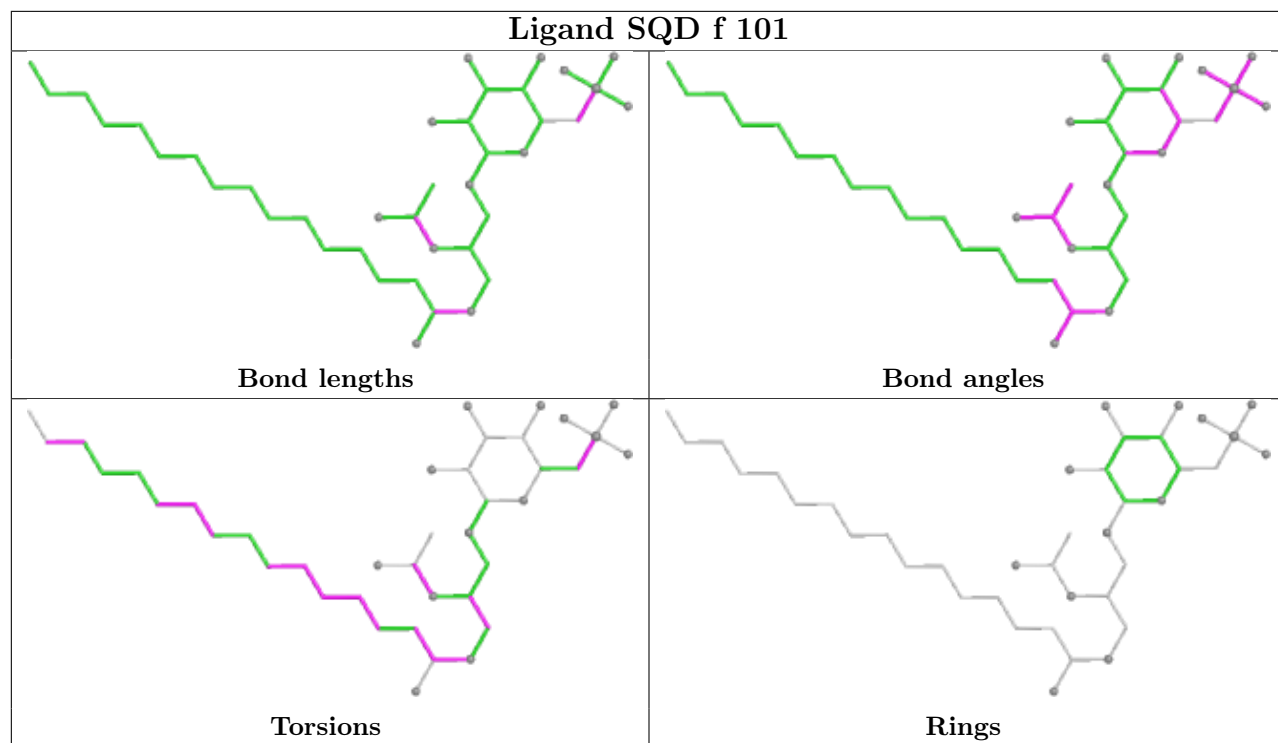




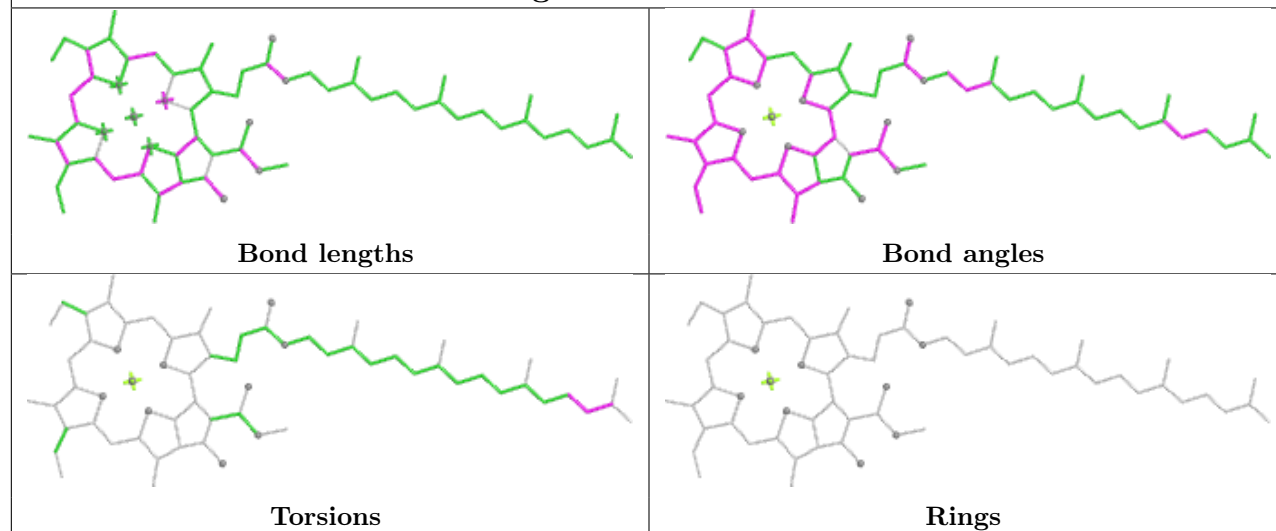


**Ligand CLA b 618****Ligand CLA a 403**

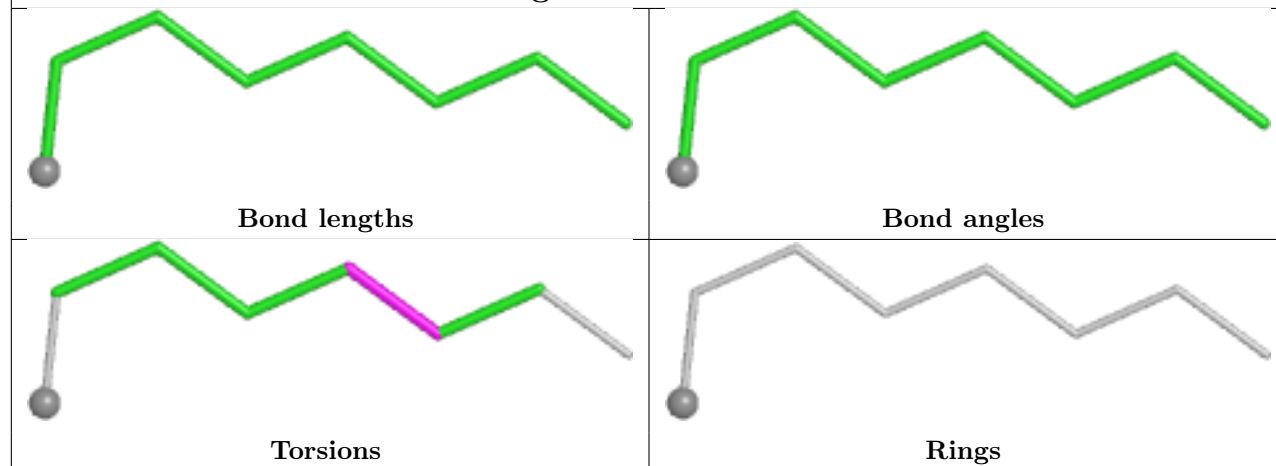
**Ligand CLA C 508****Ligand SQD b 622**



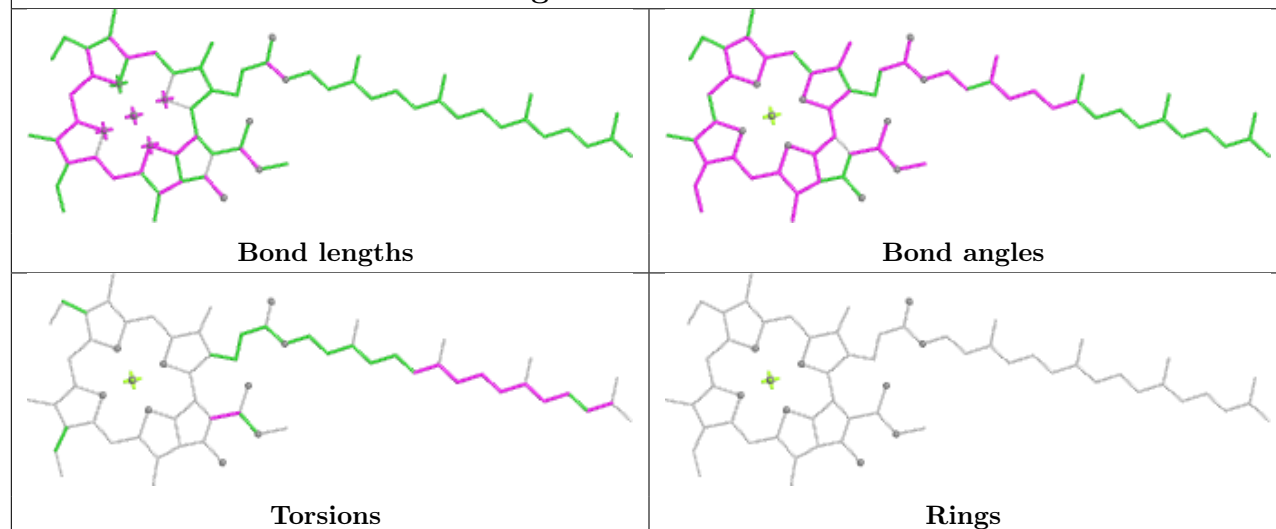
## Ligand CLA B 612

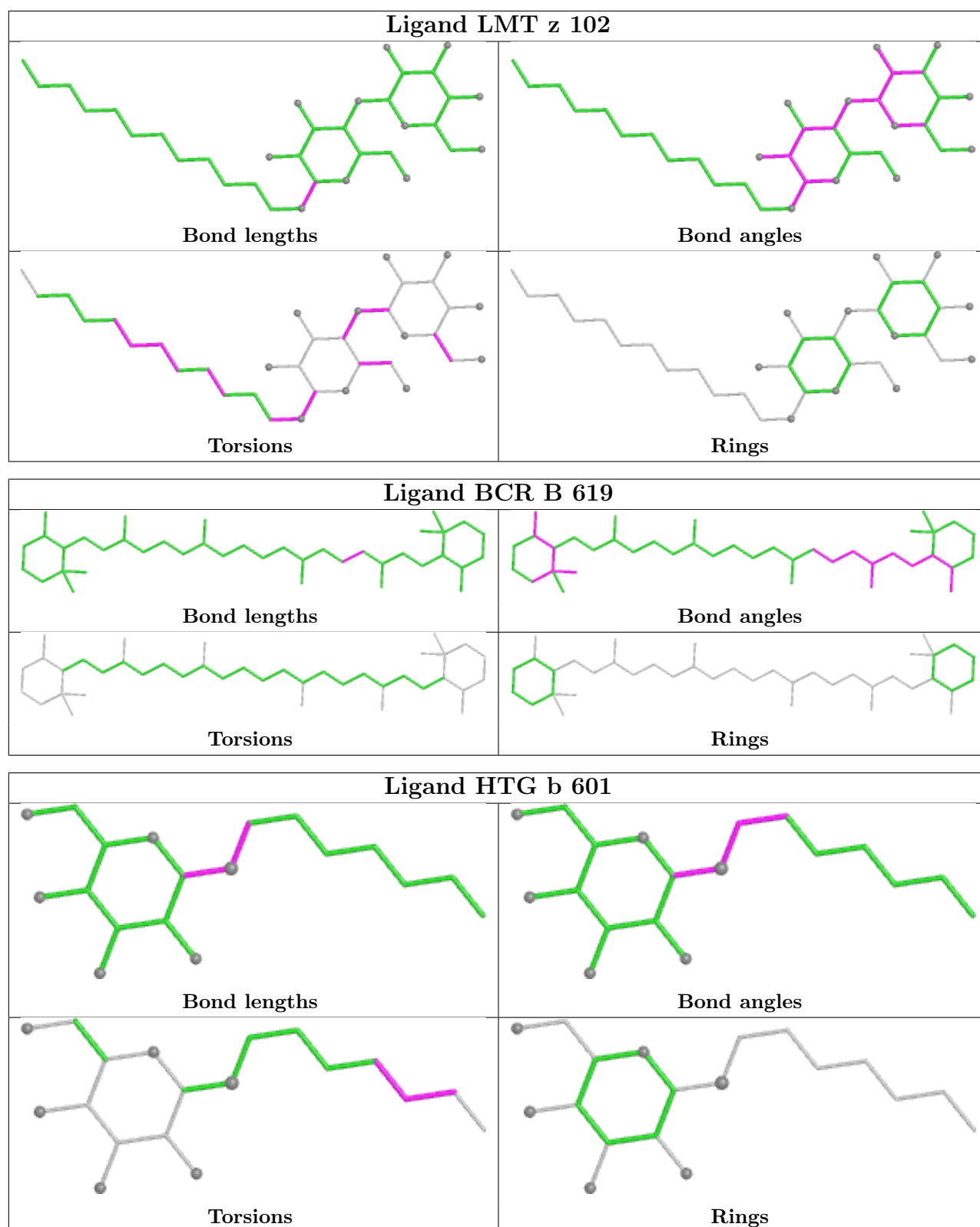


## Ligand HTG u 201

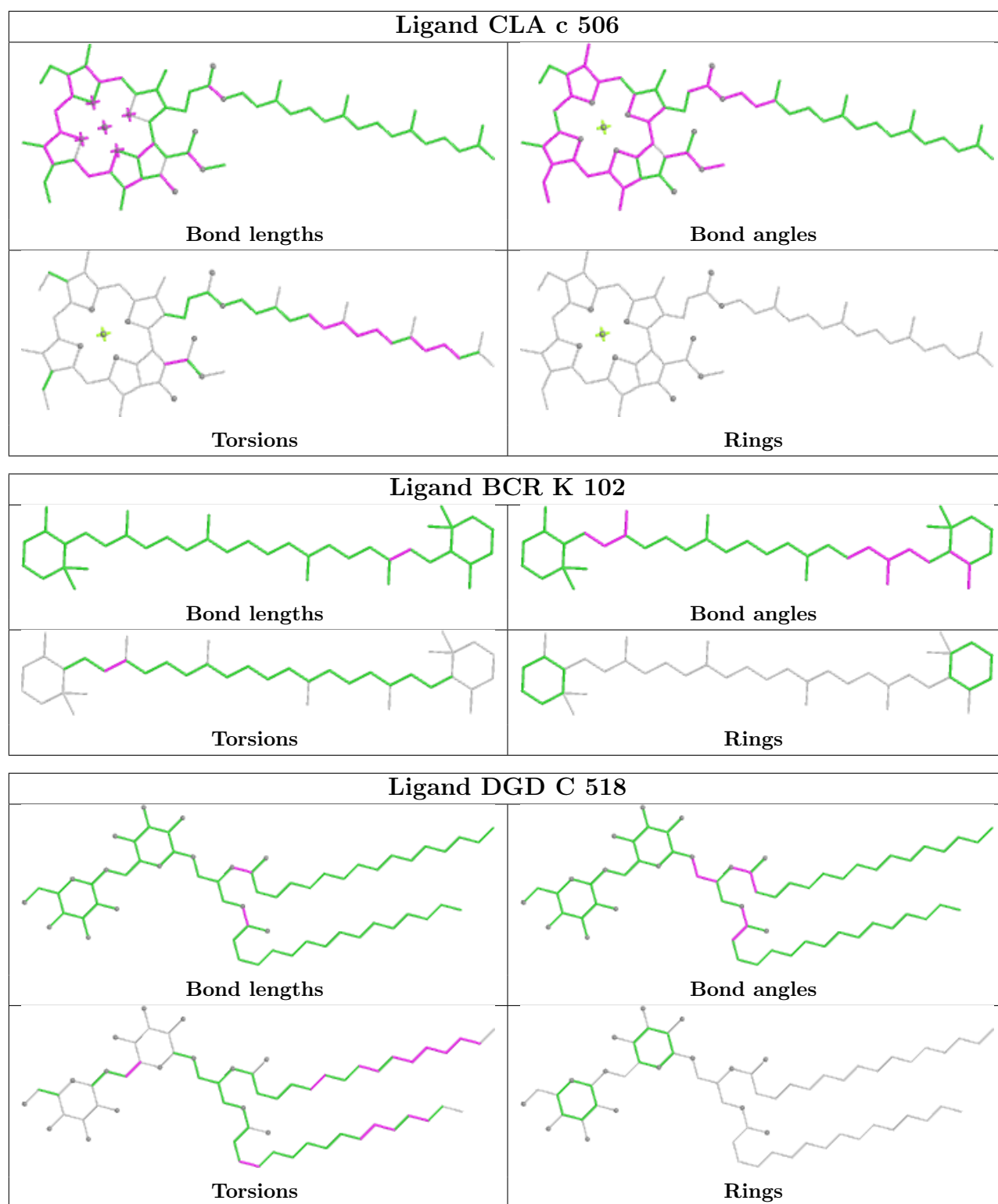


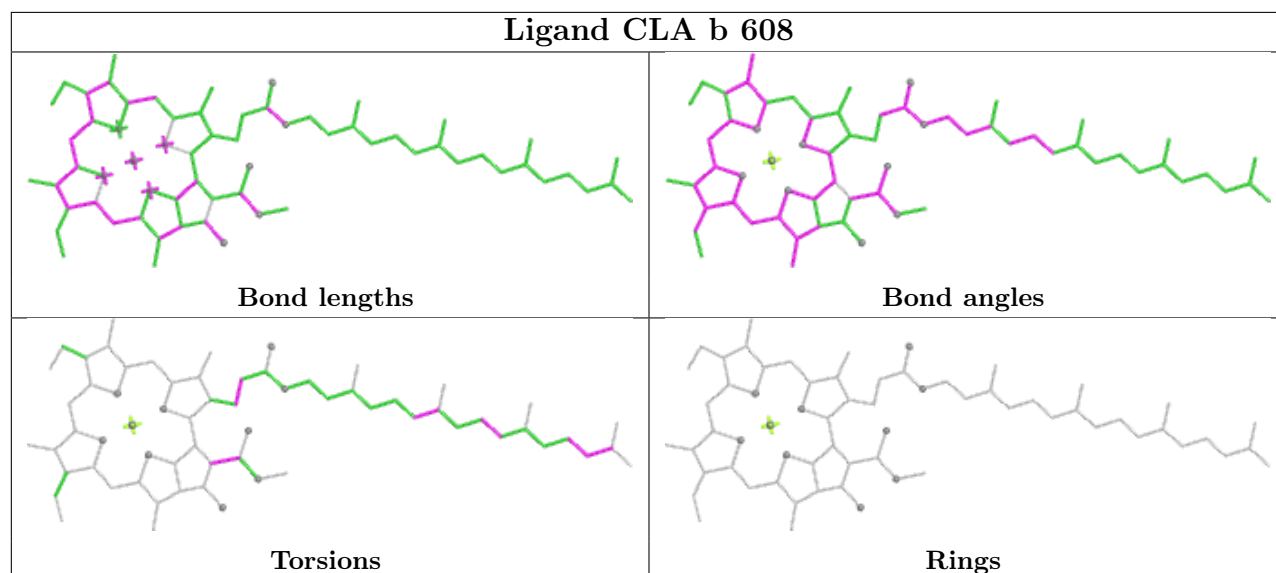
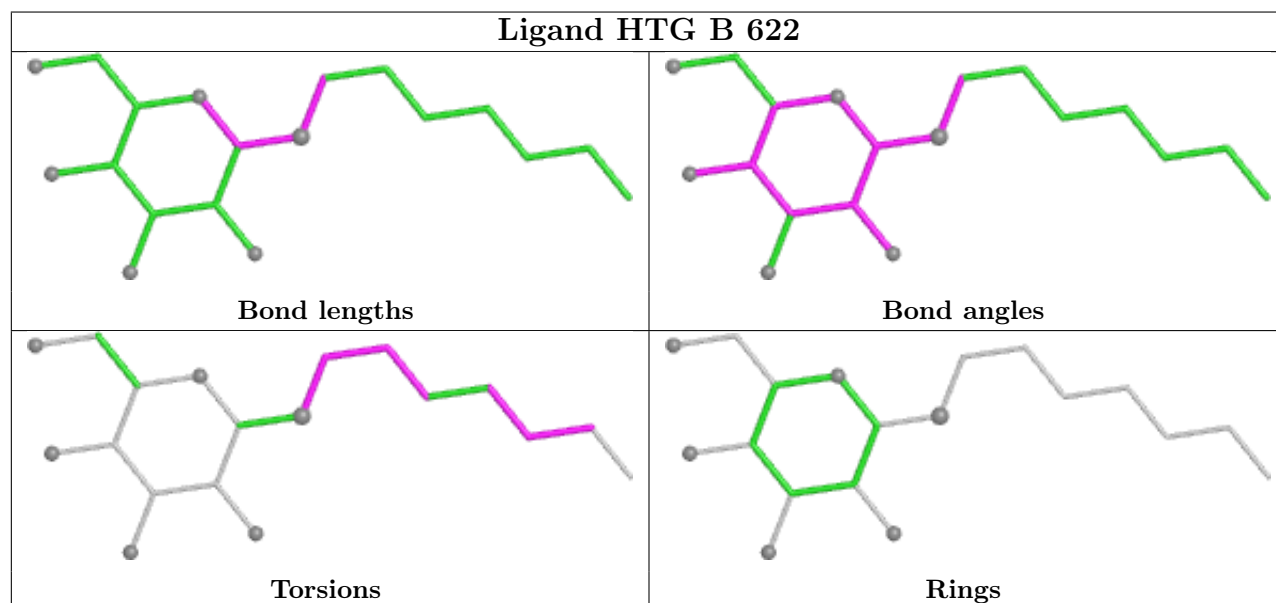
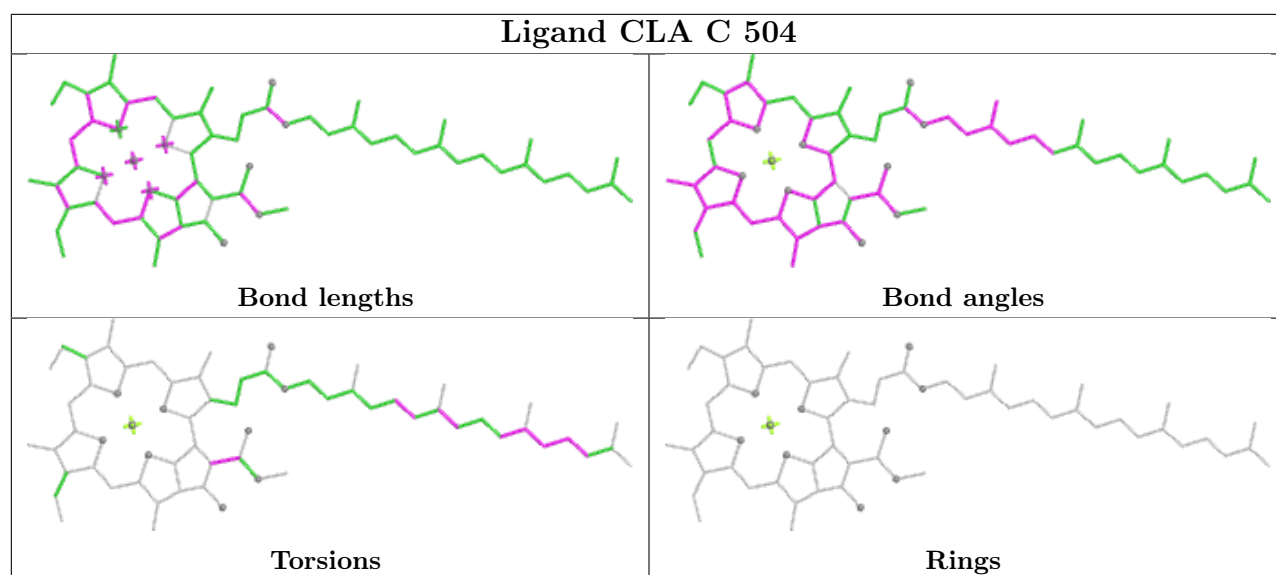
## Ligand CLA D 404



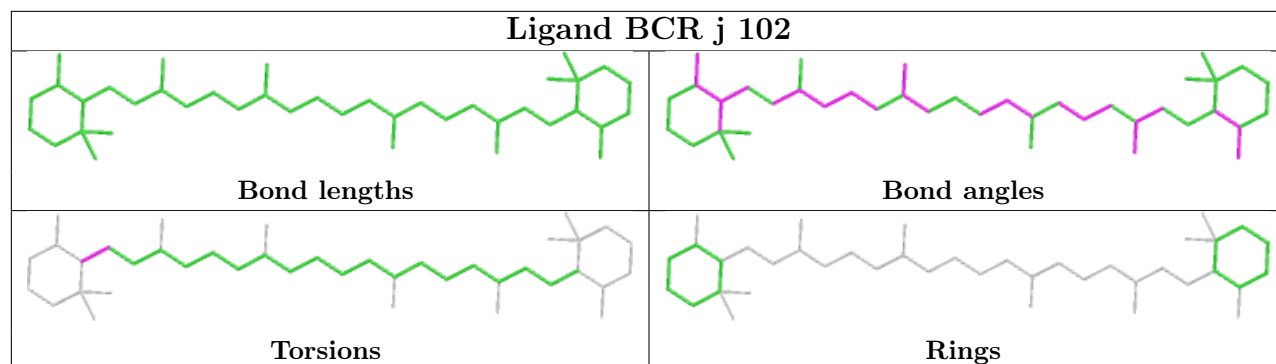




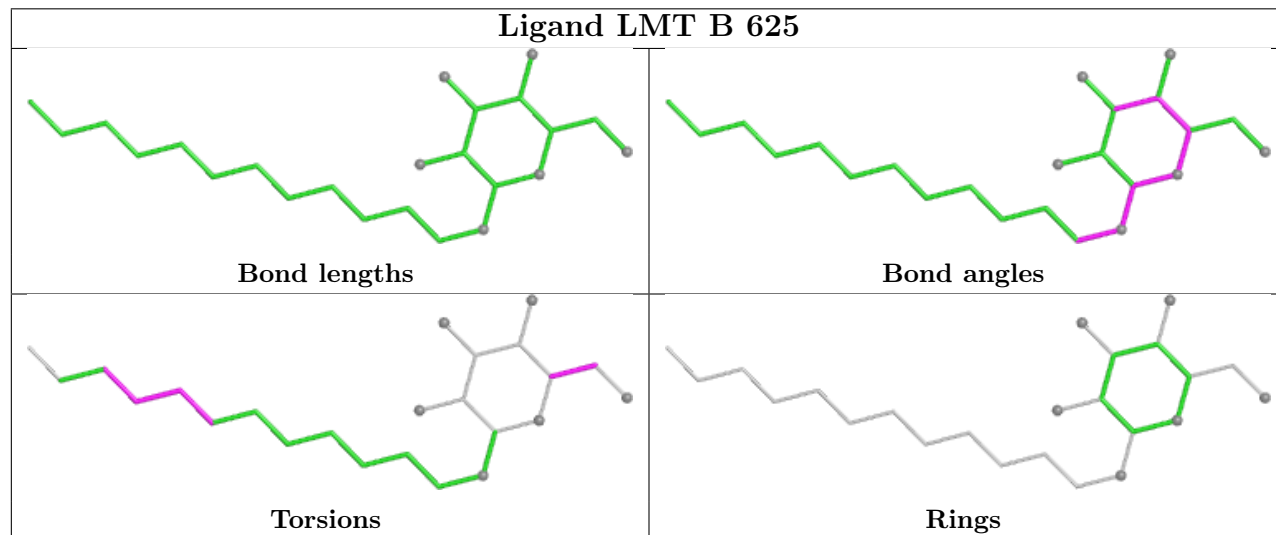




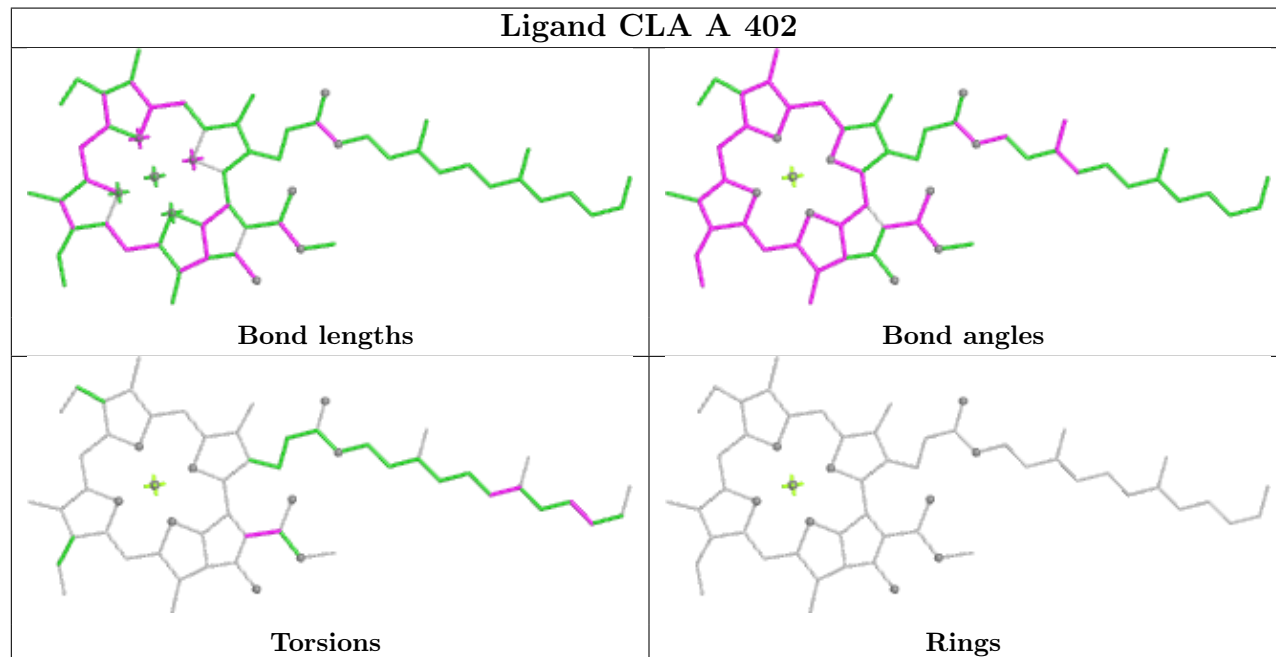
## Ligand BCR j 102

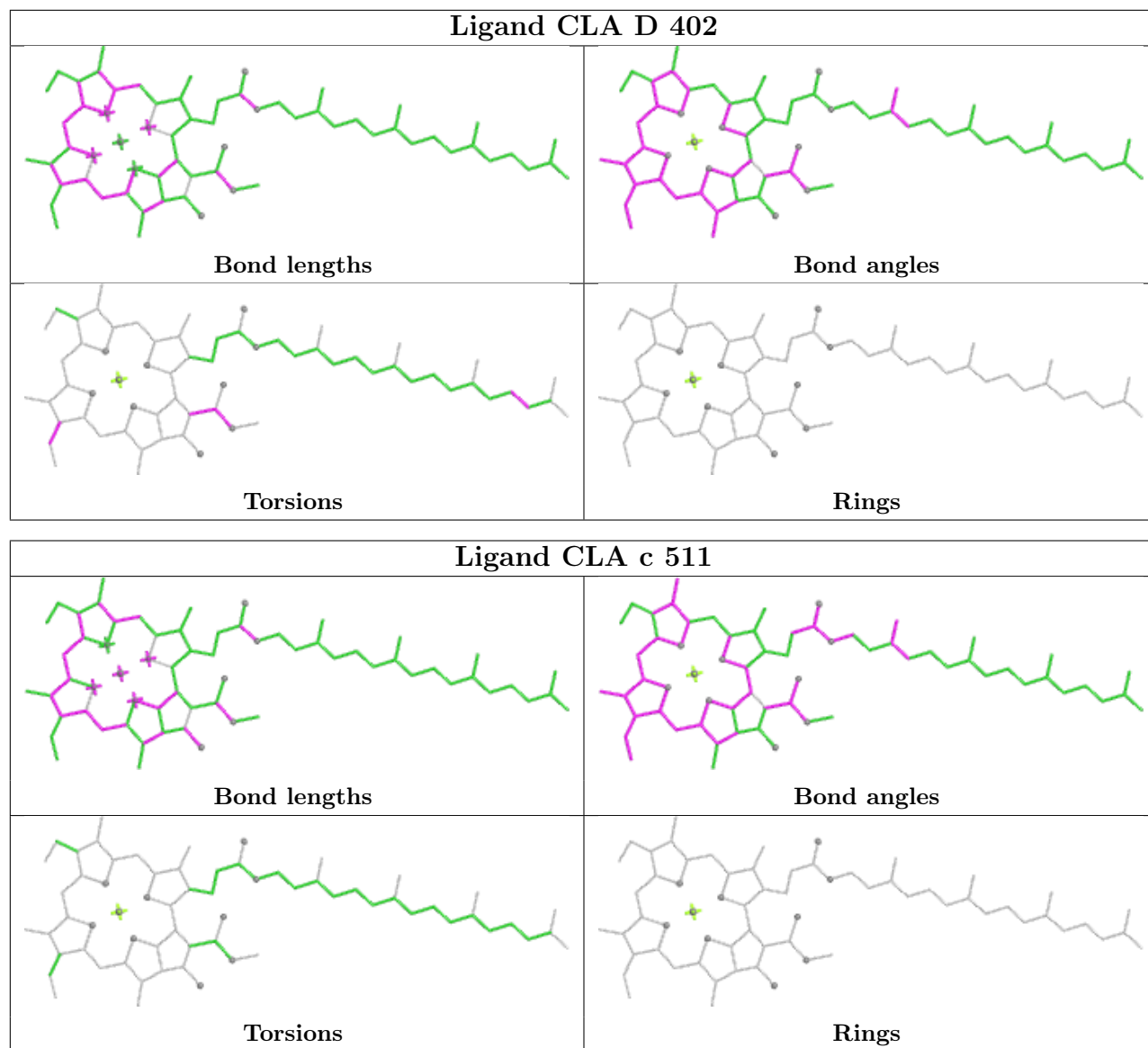


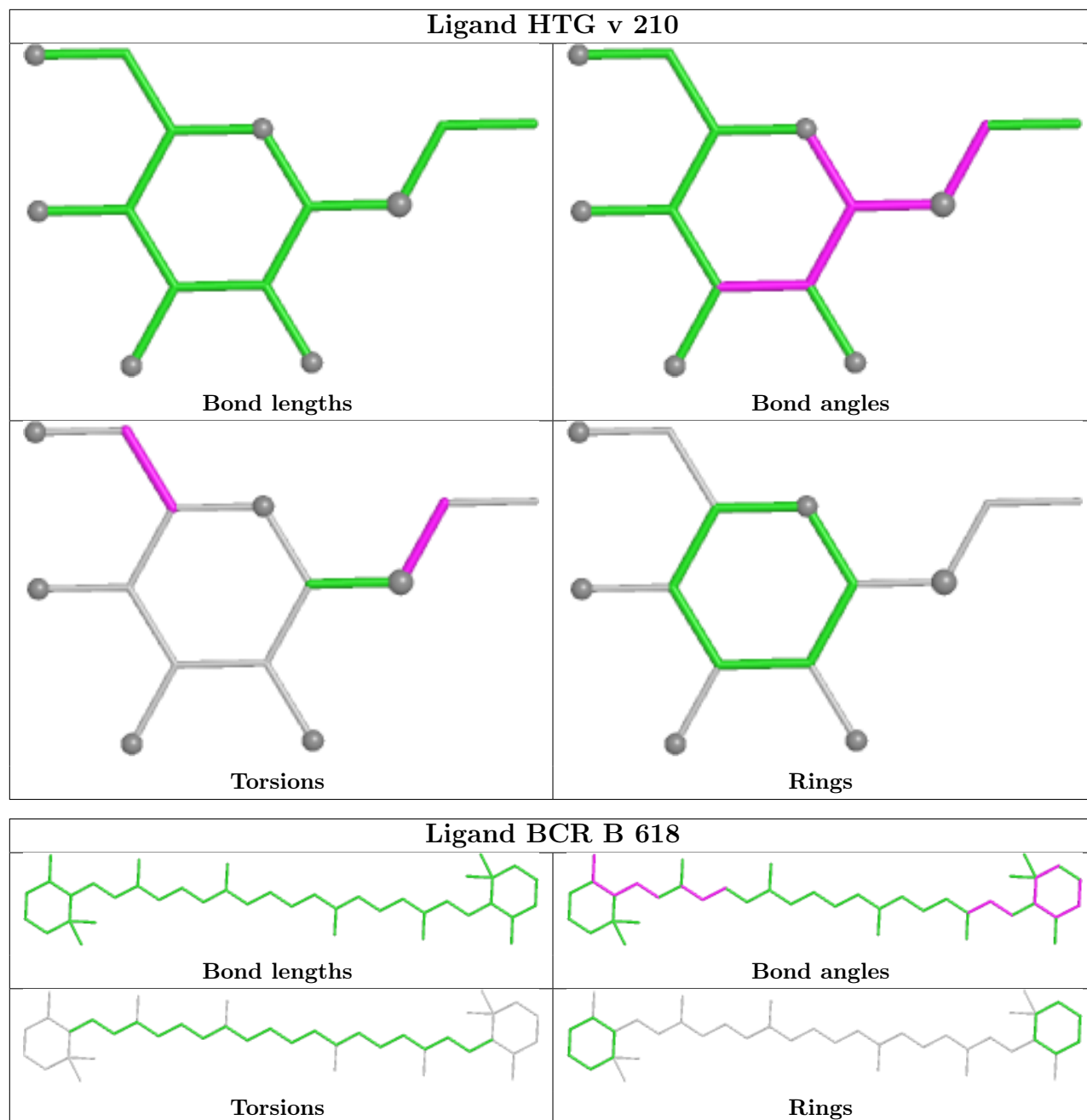
## Ligand LMT B 625



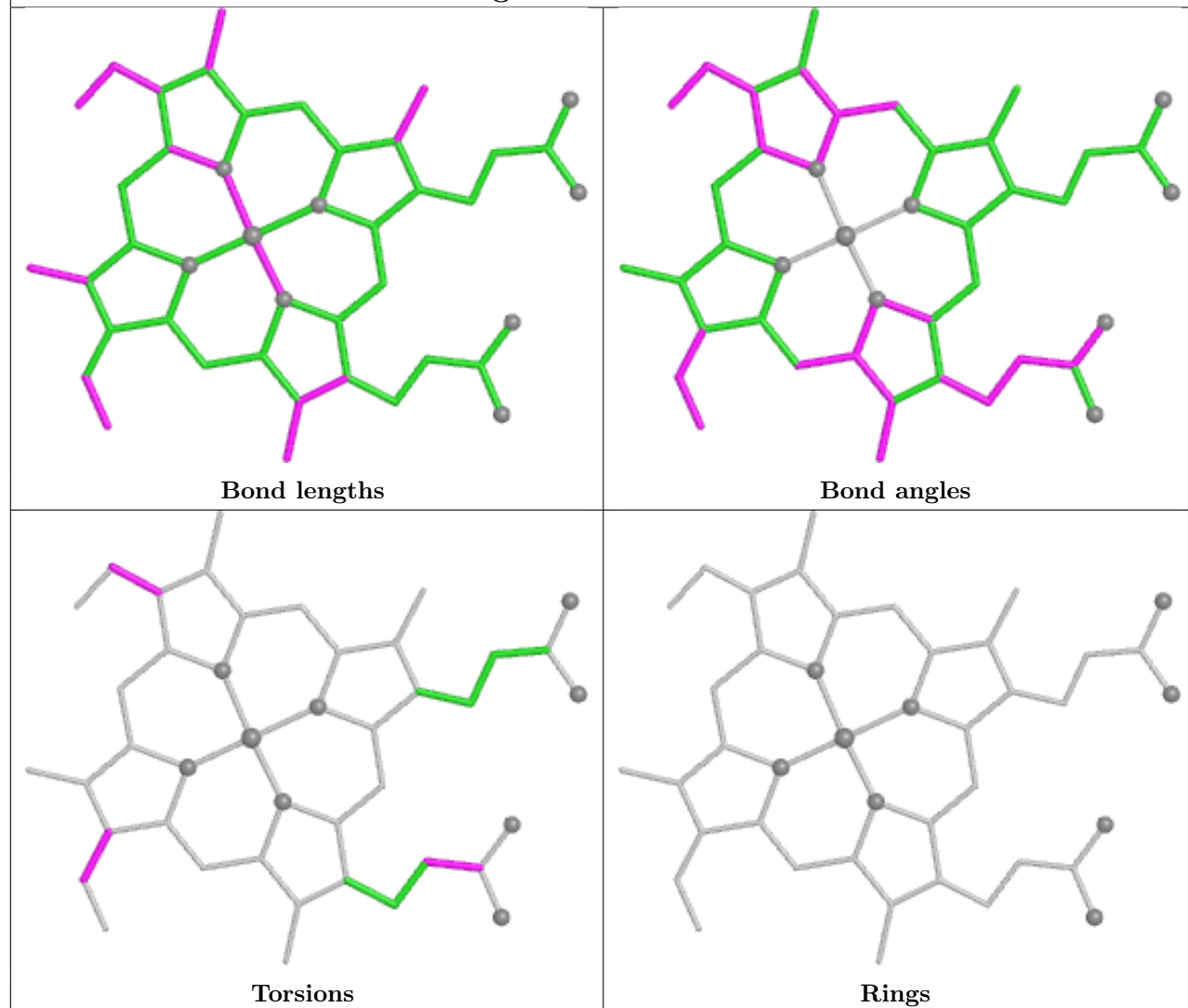
## Ligand CLA A 402



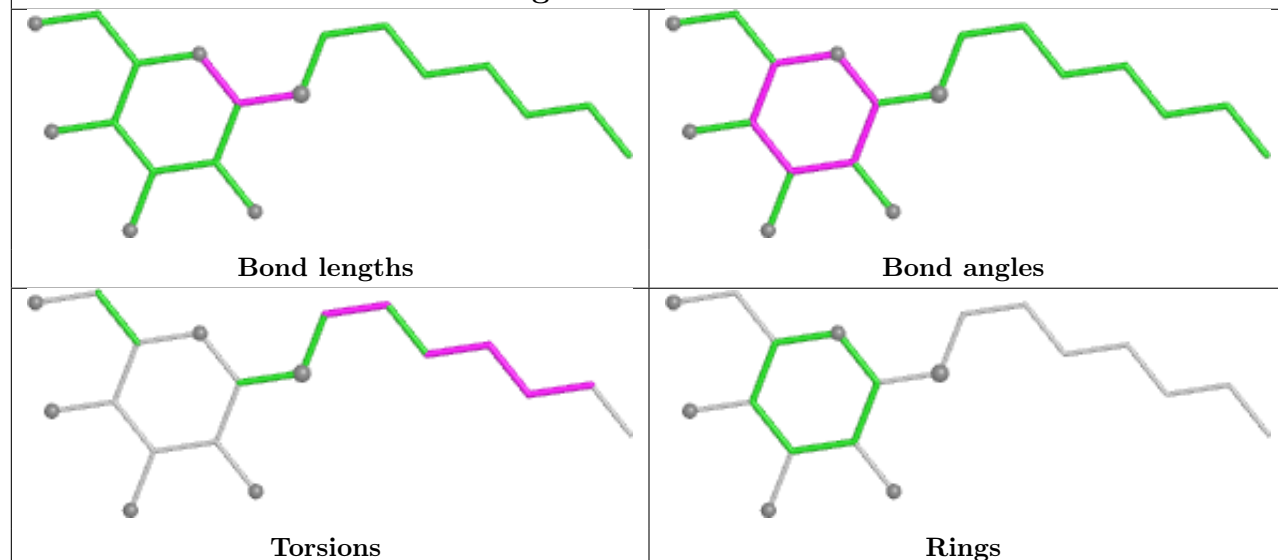


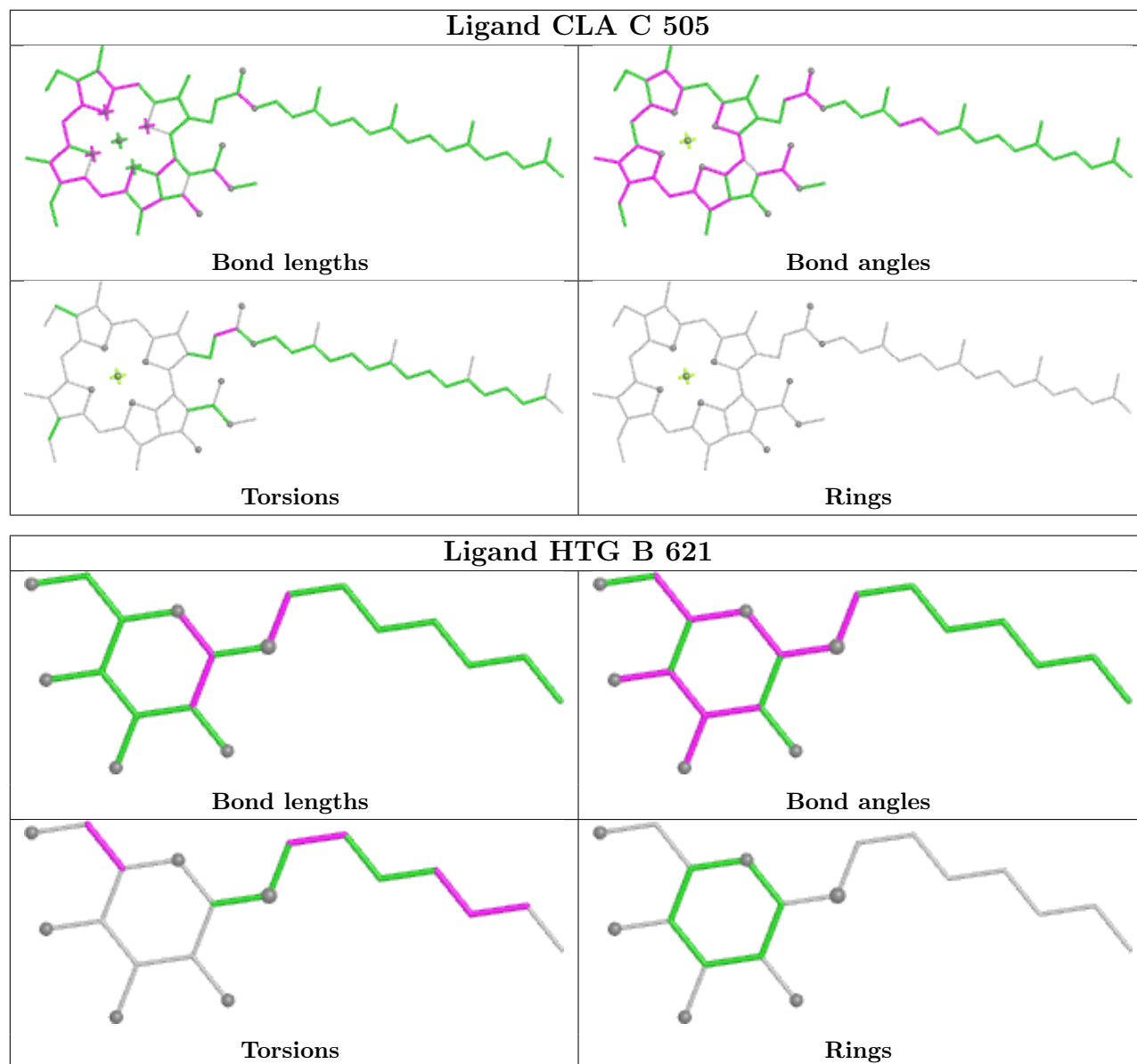


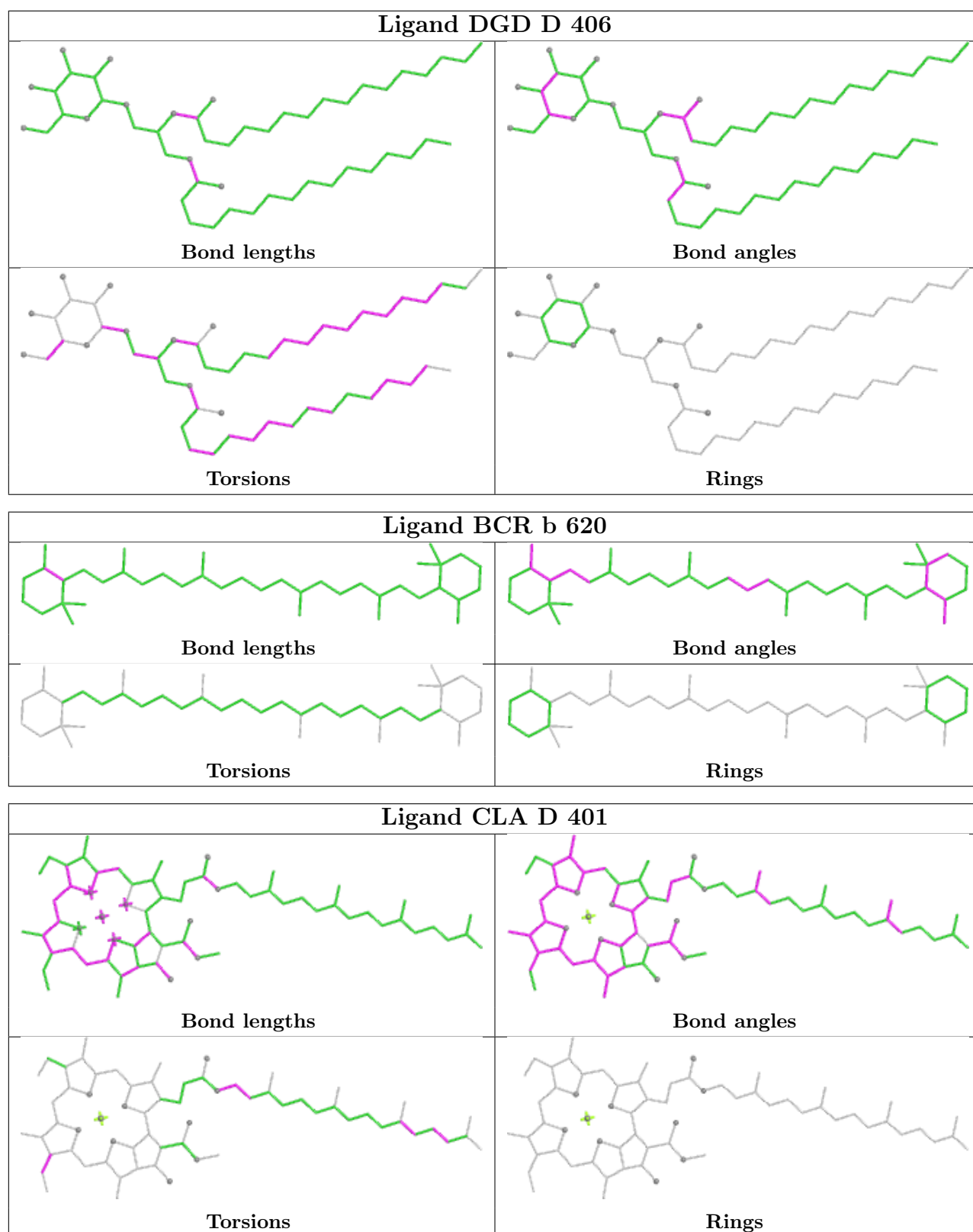
## Ligand HEC V 201



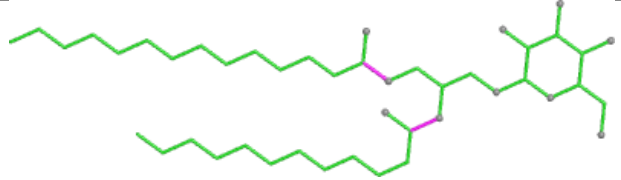
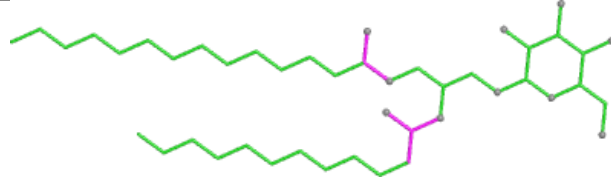
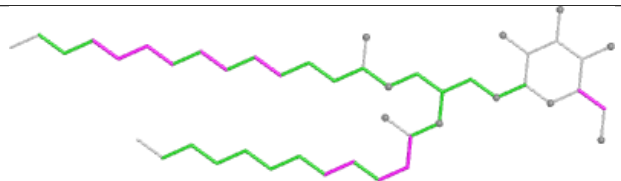
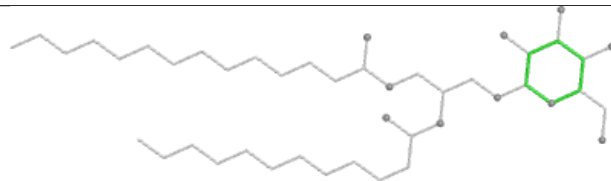
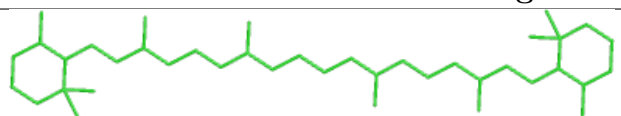
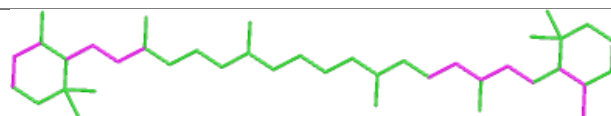
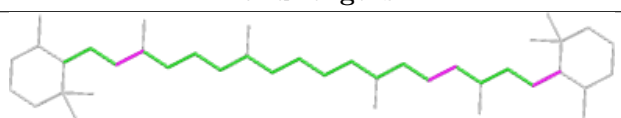
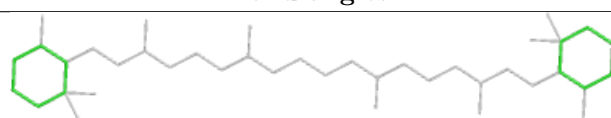
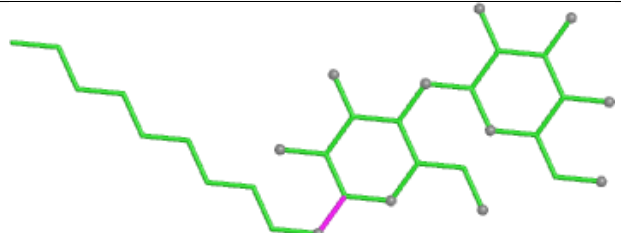
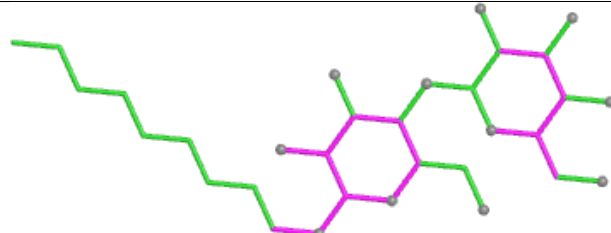
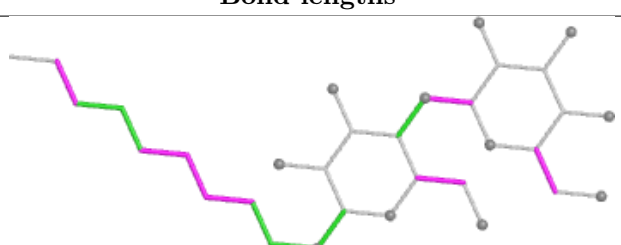
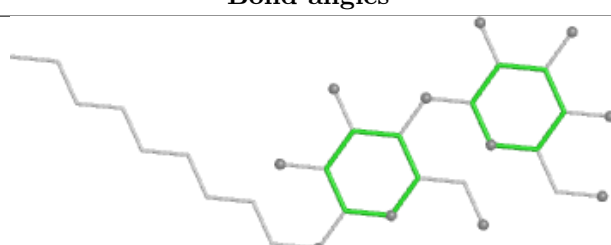
## Ligand HTG b 625

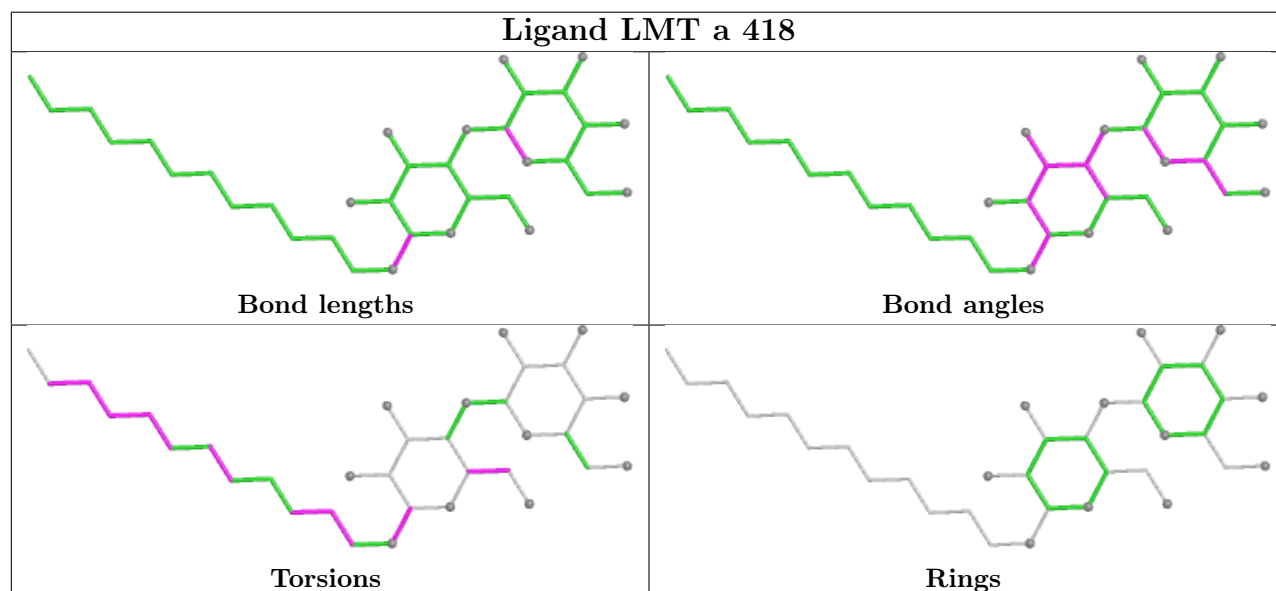
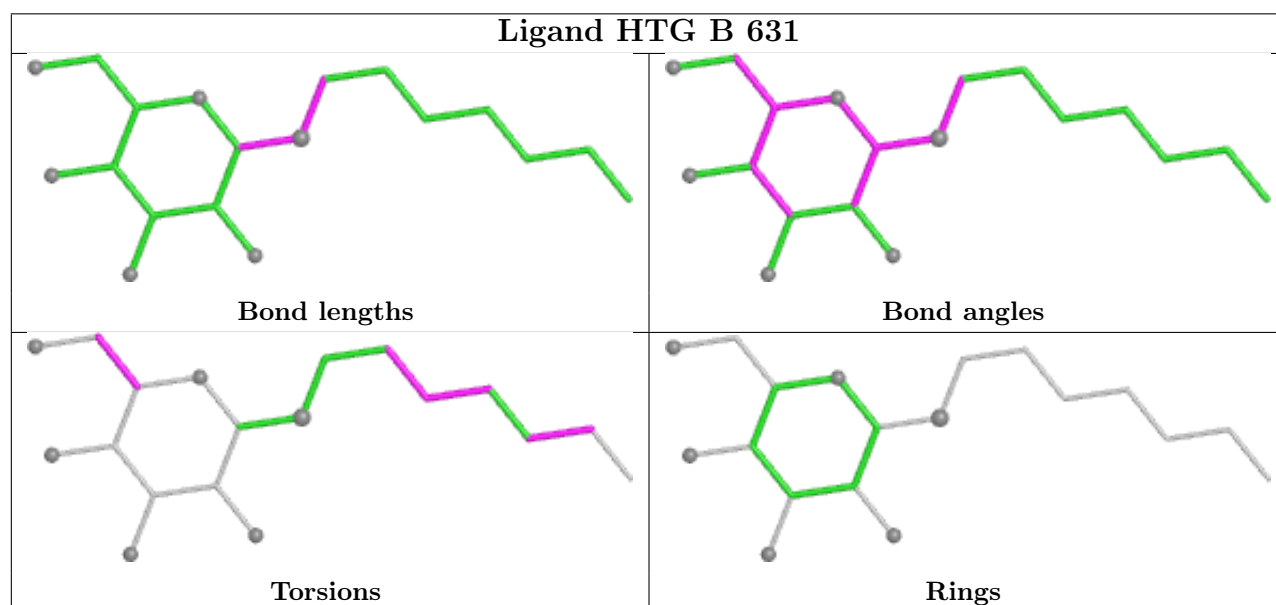
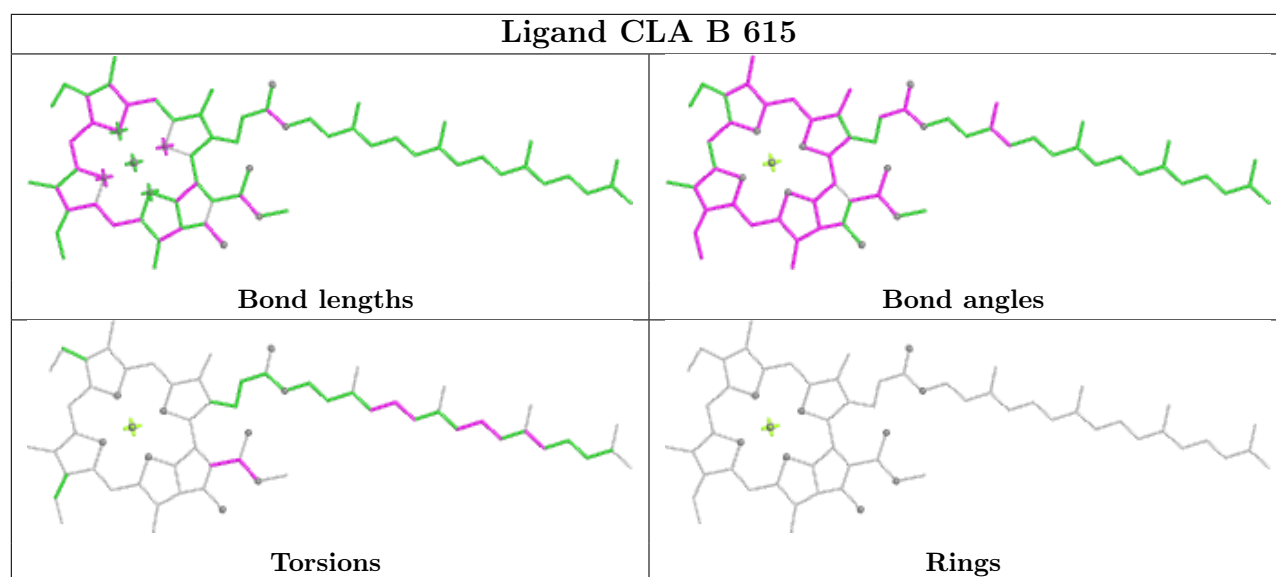


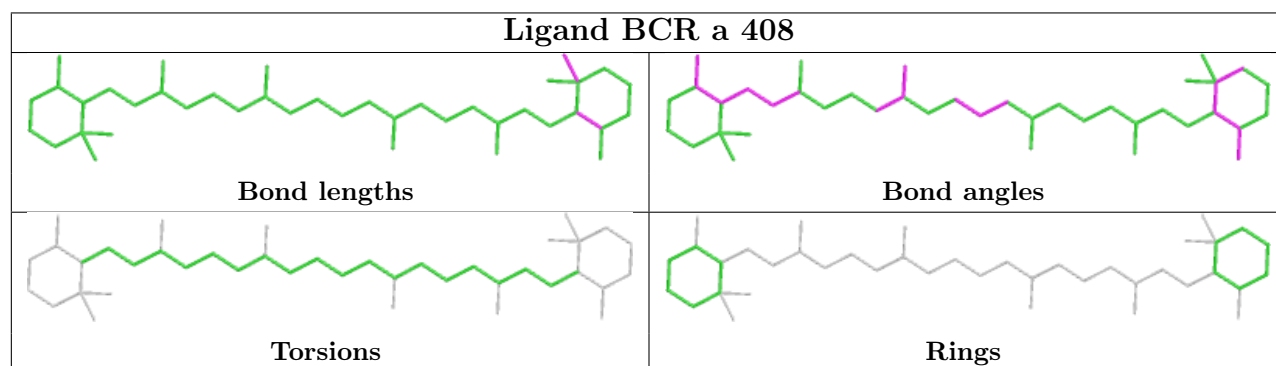
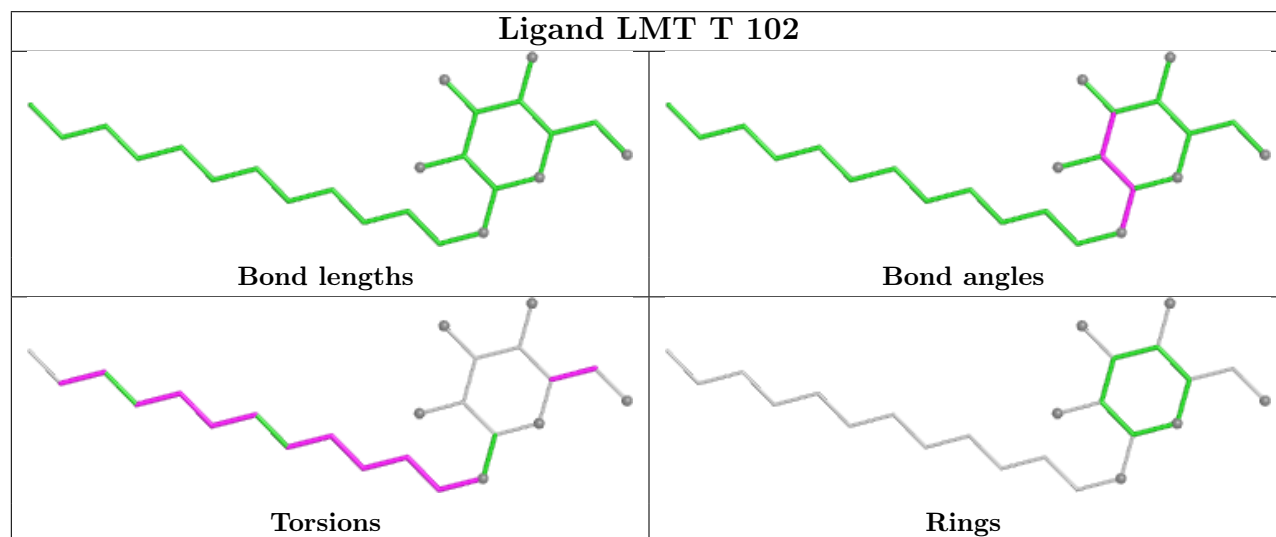
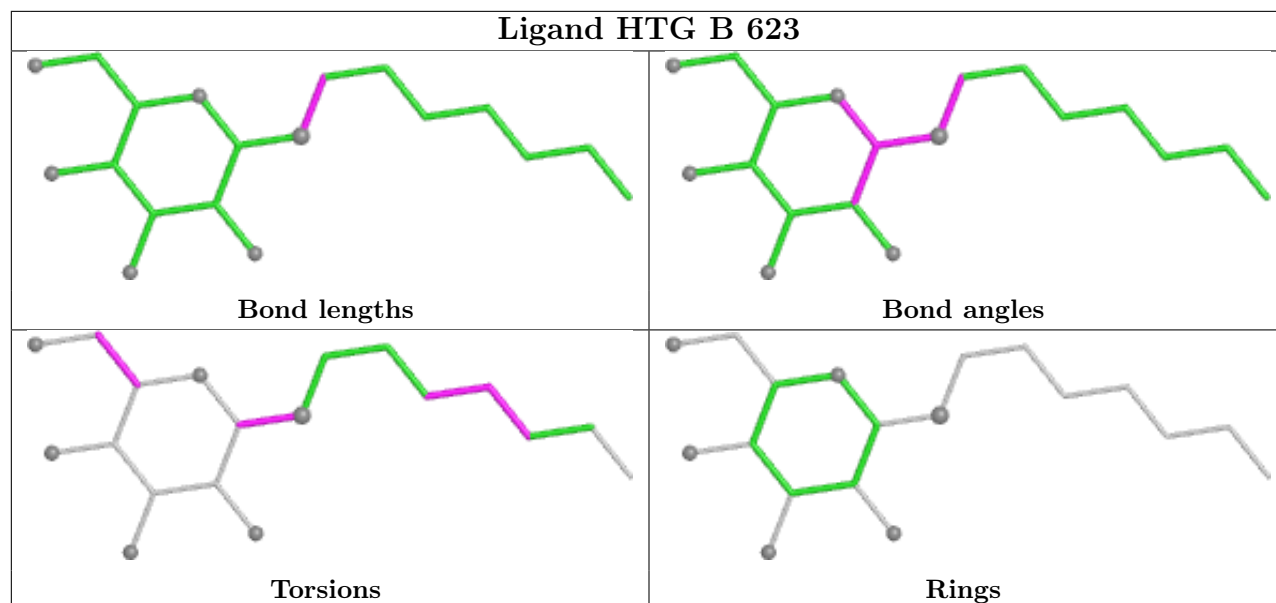


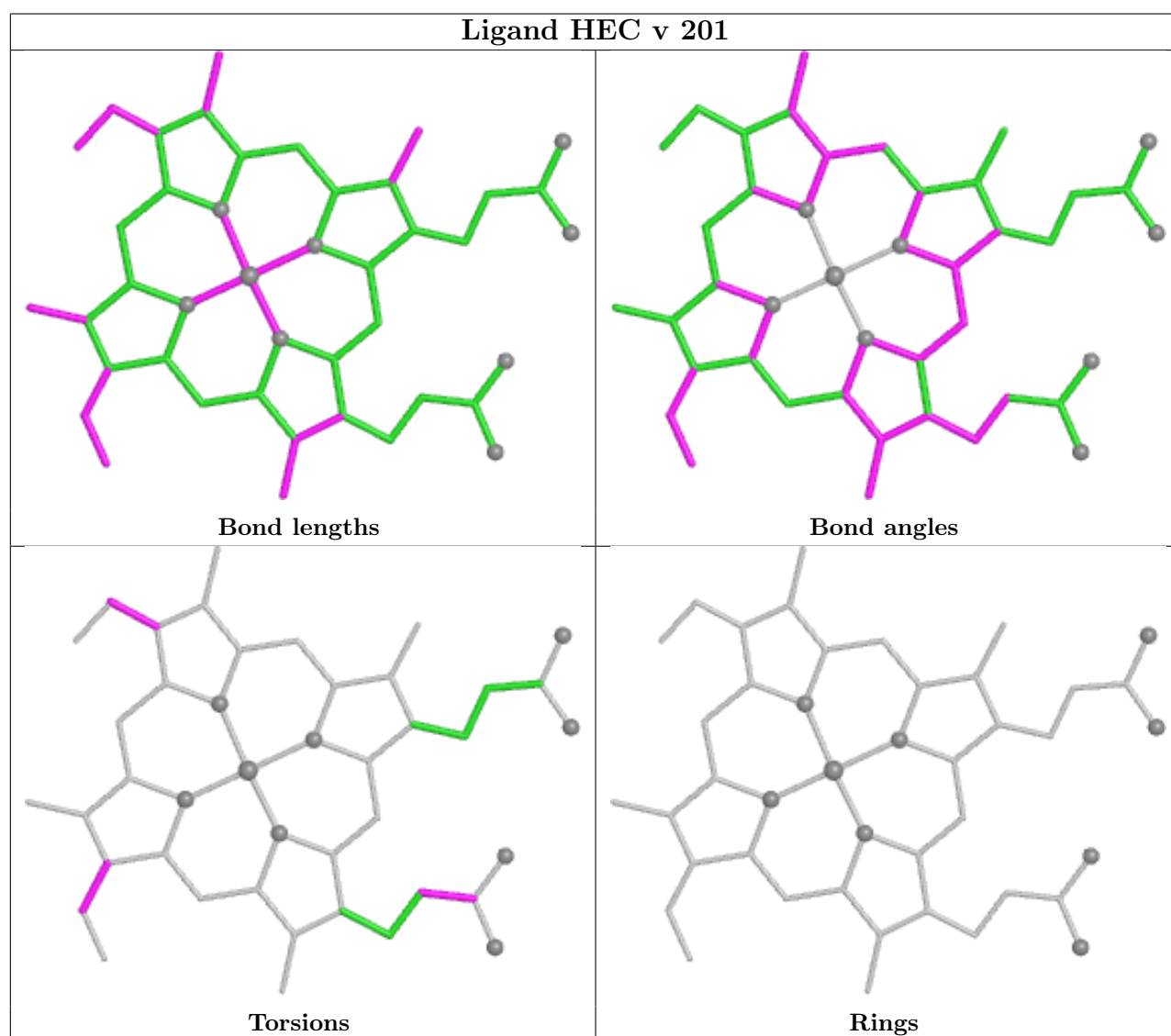
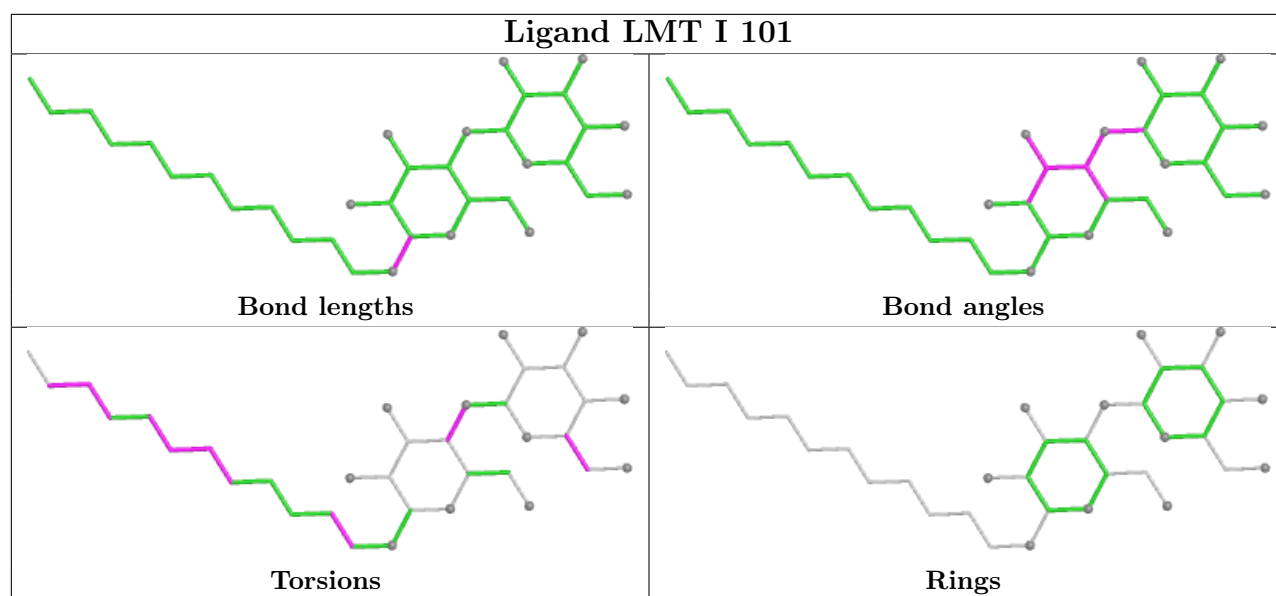


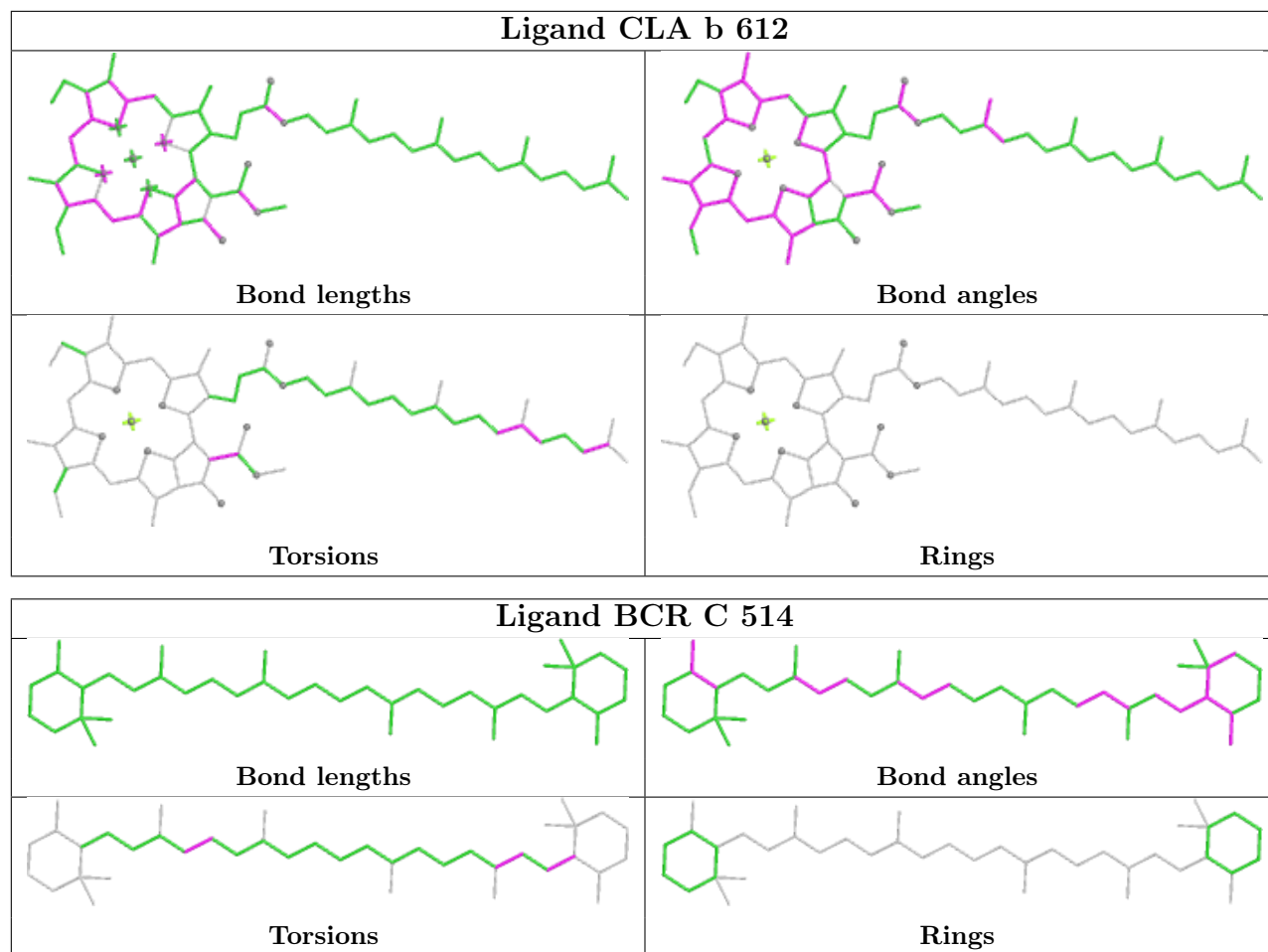


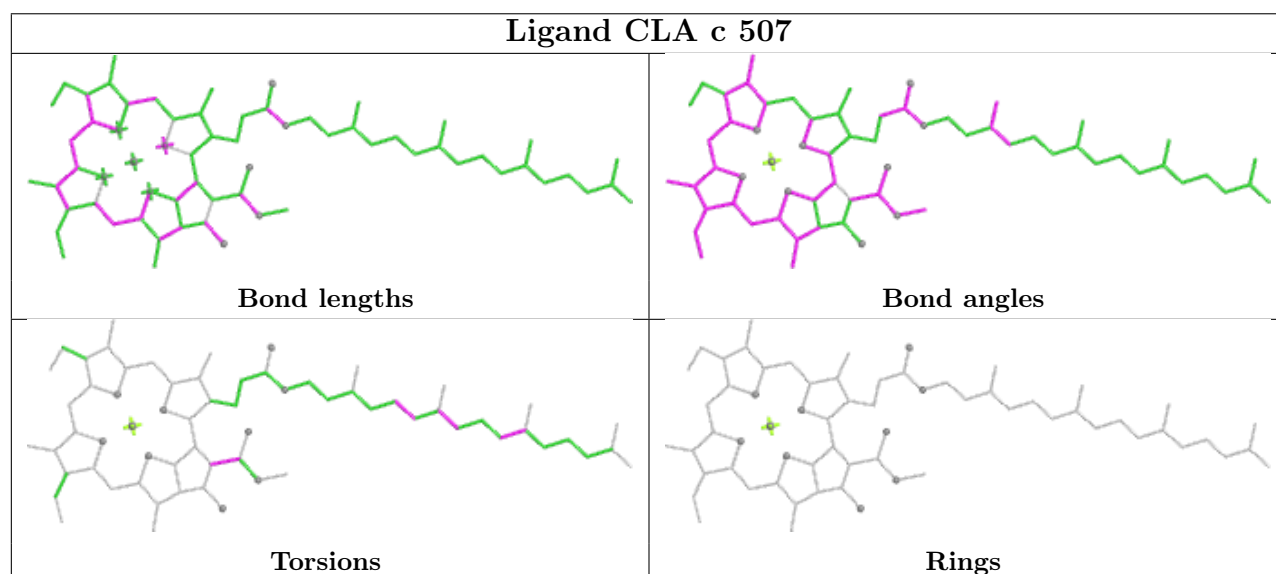
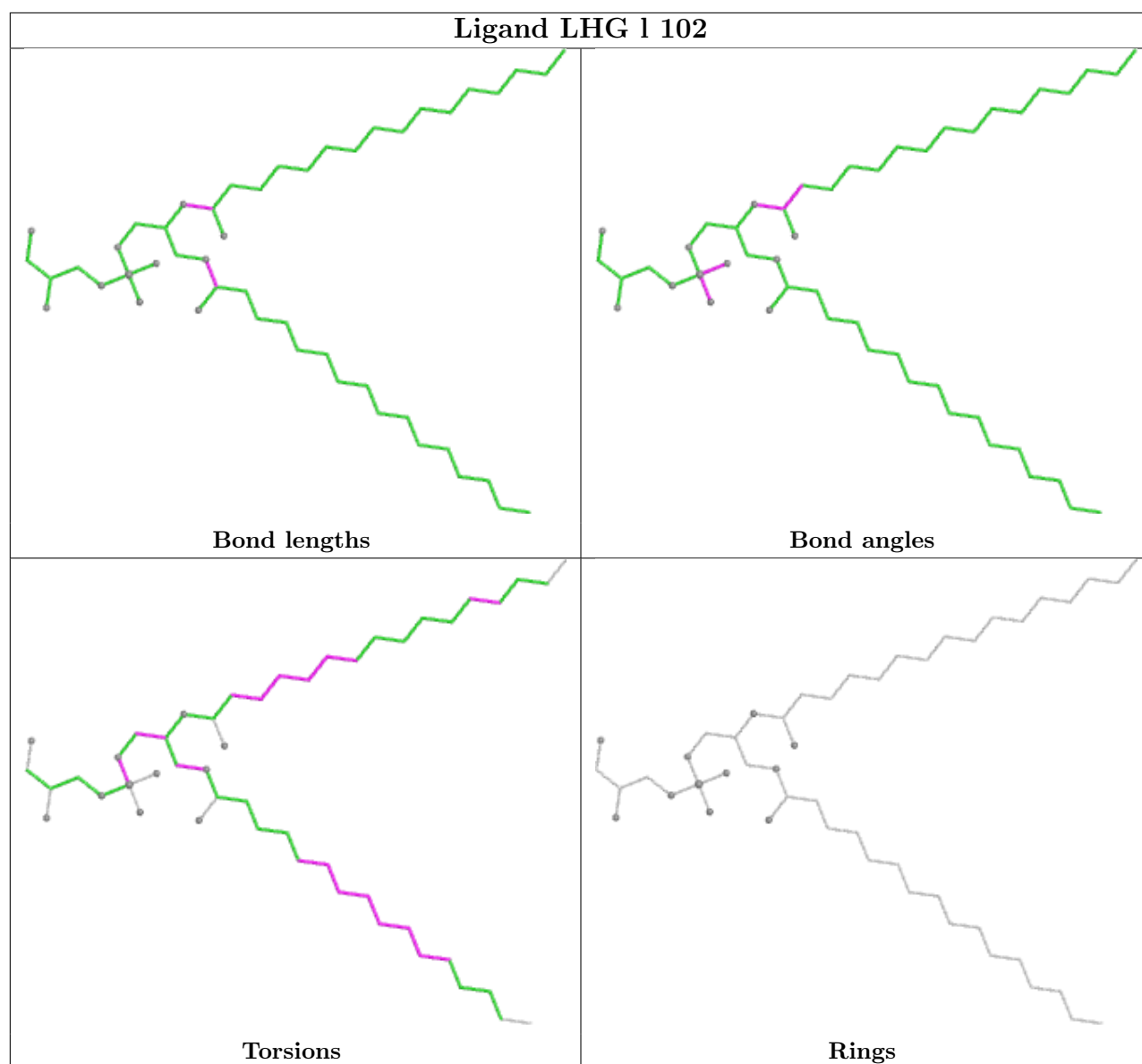
| Ligand LMG J 101                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR k 101                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMT b 627                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

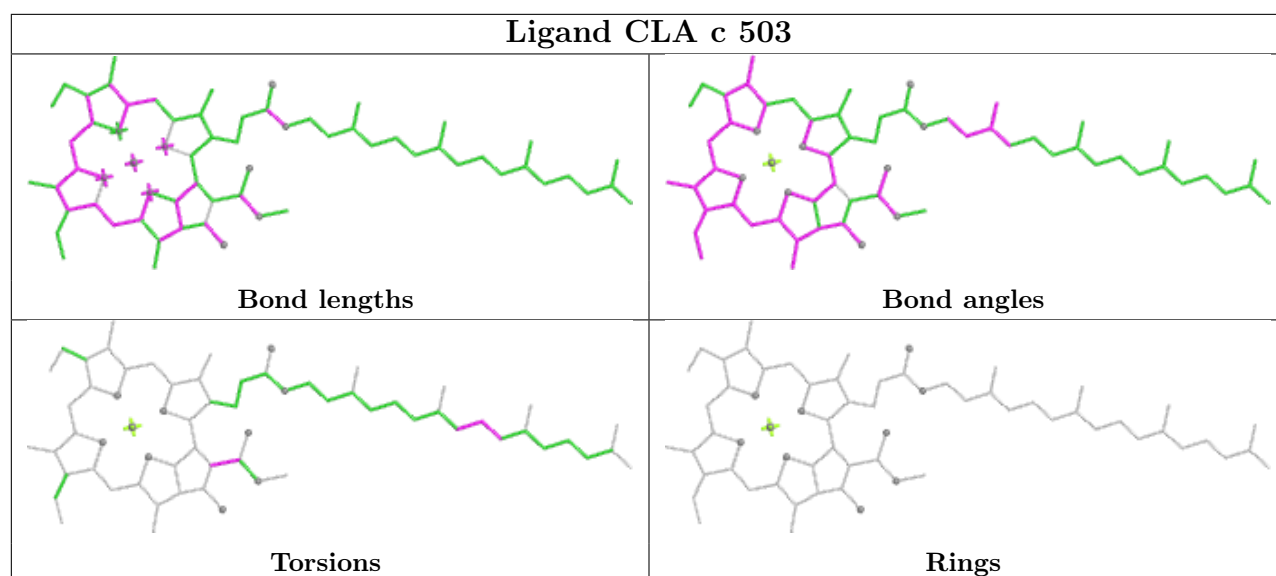
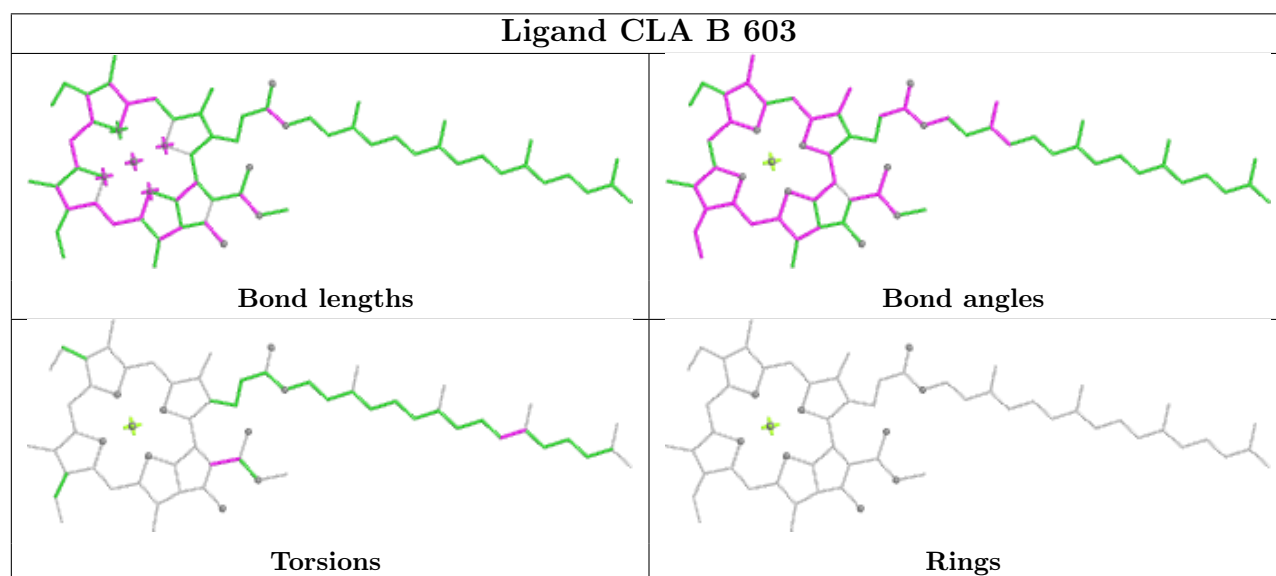
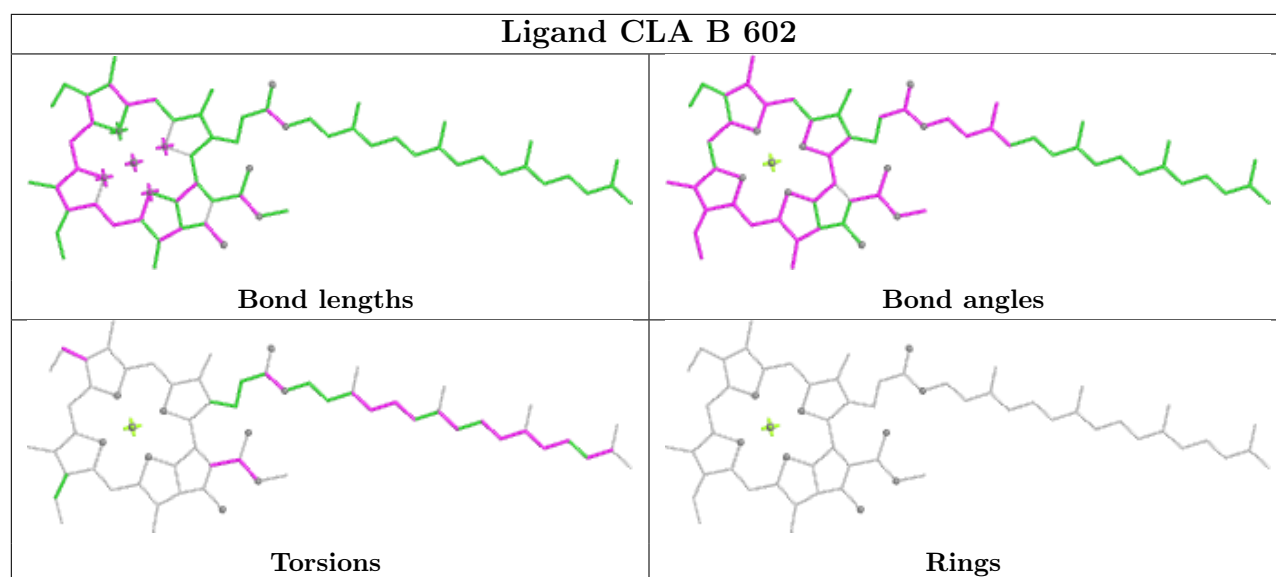


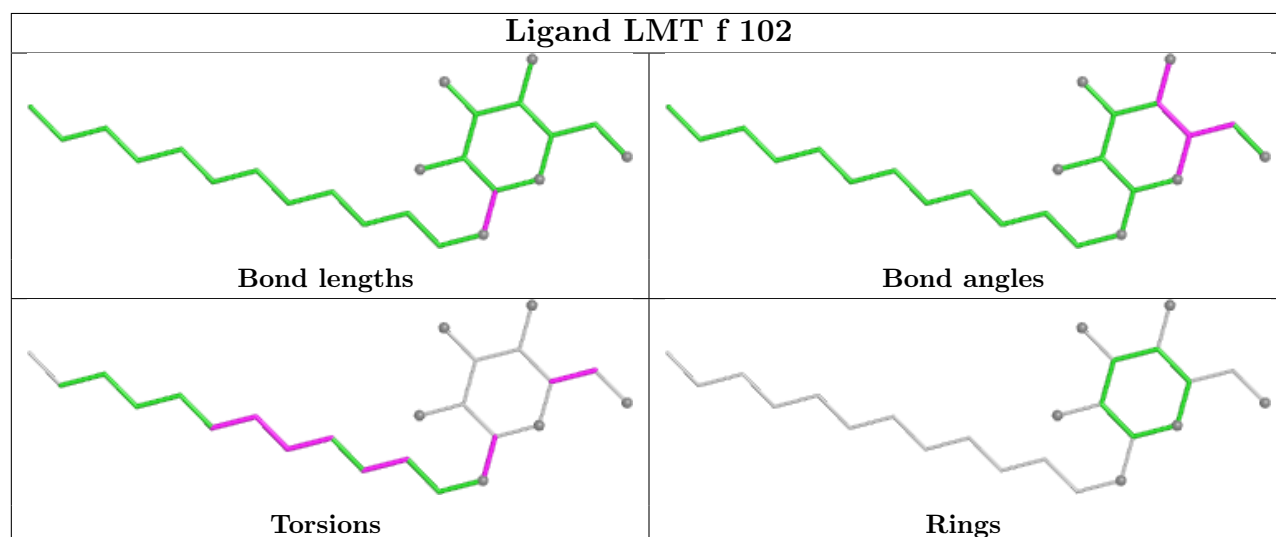
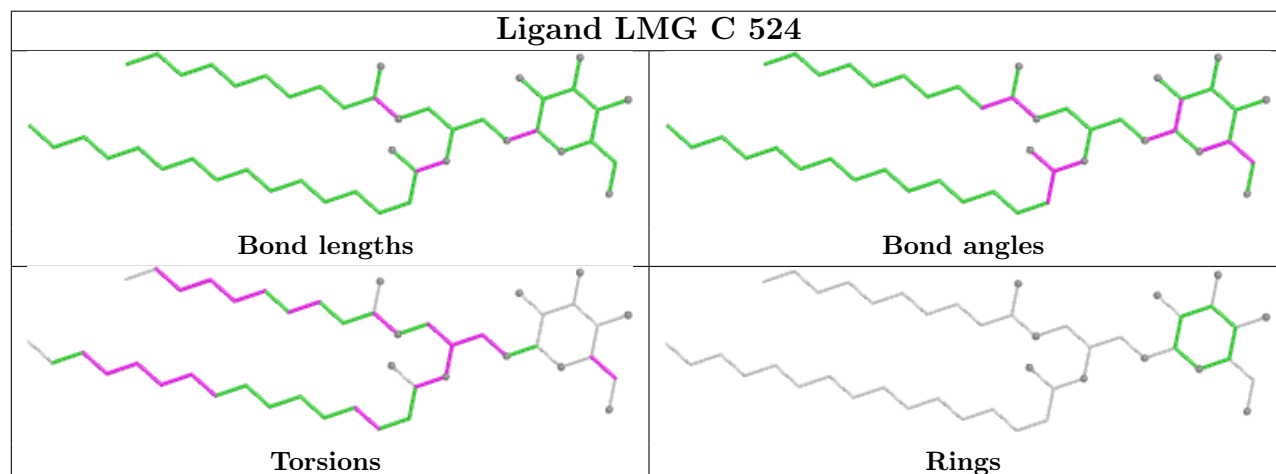
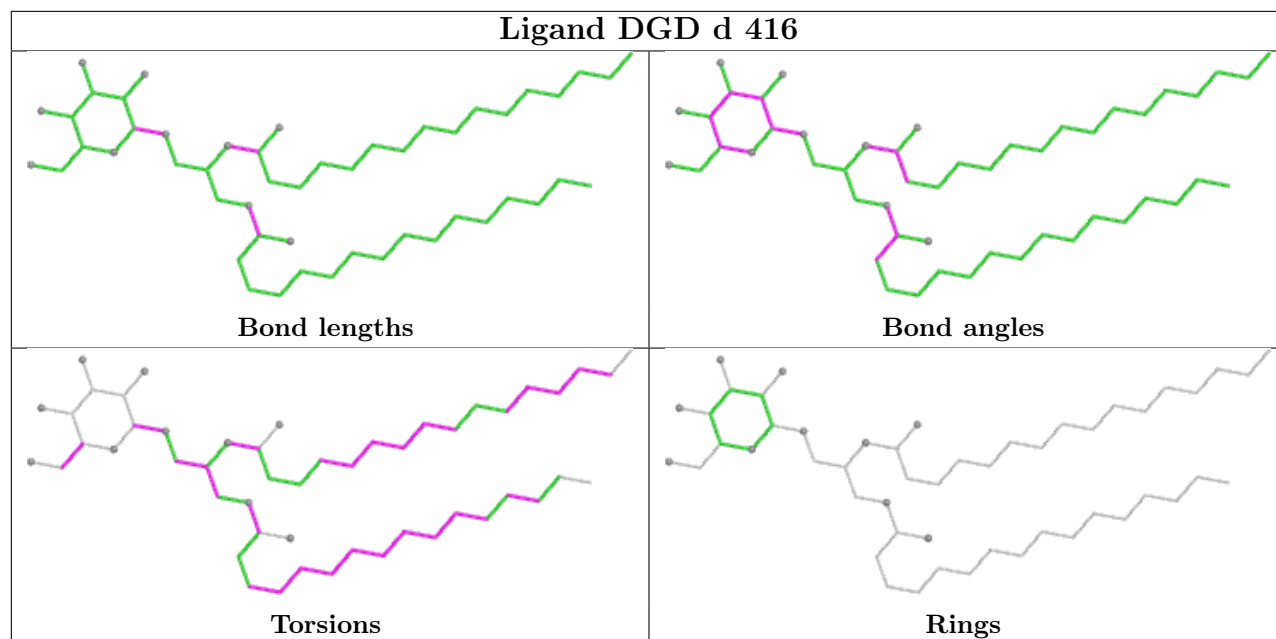




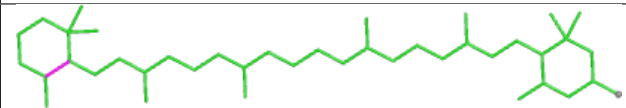
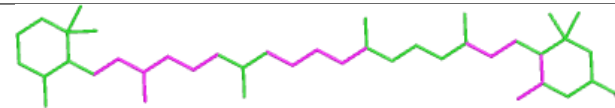
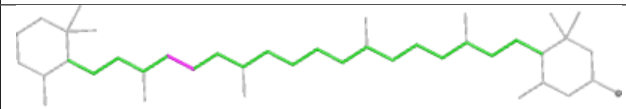
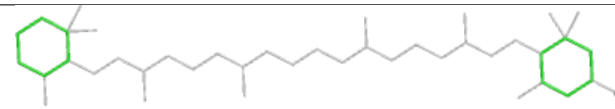


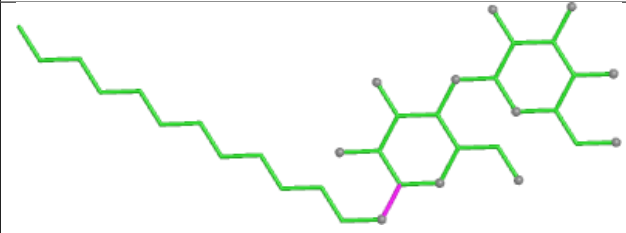
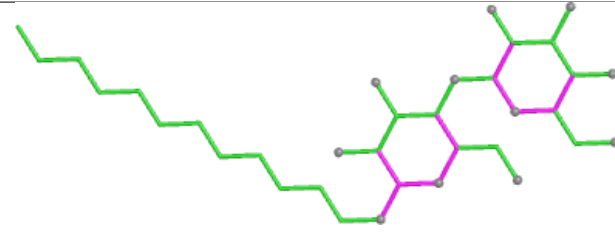
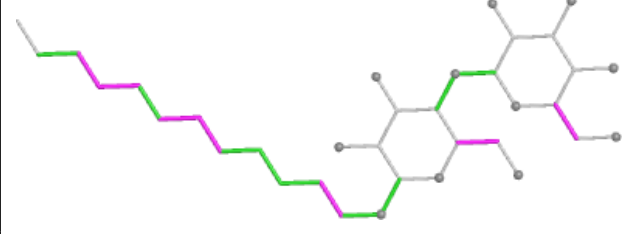
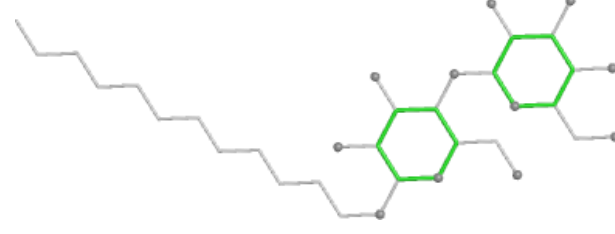


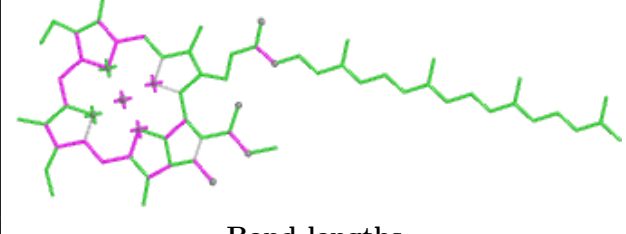
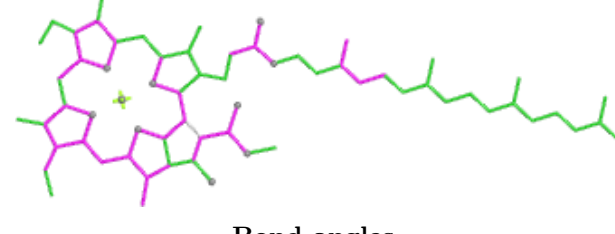
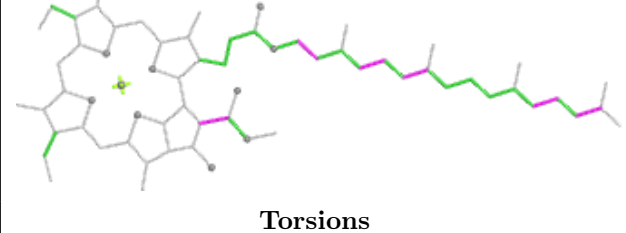
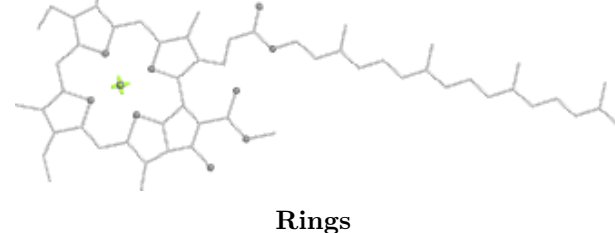


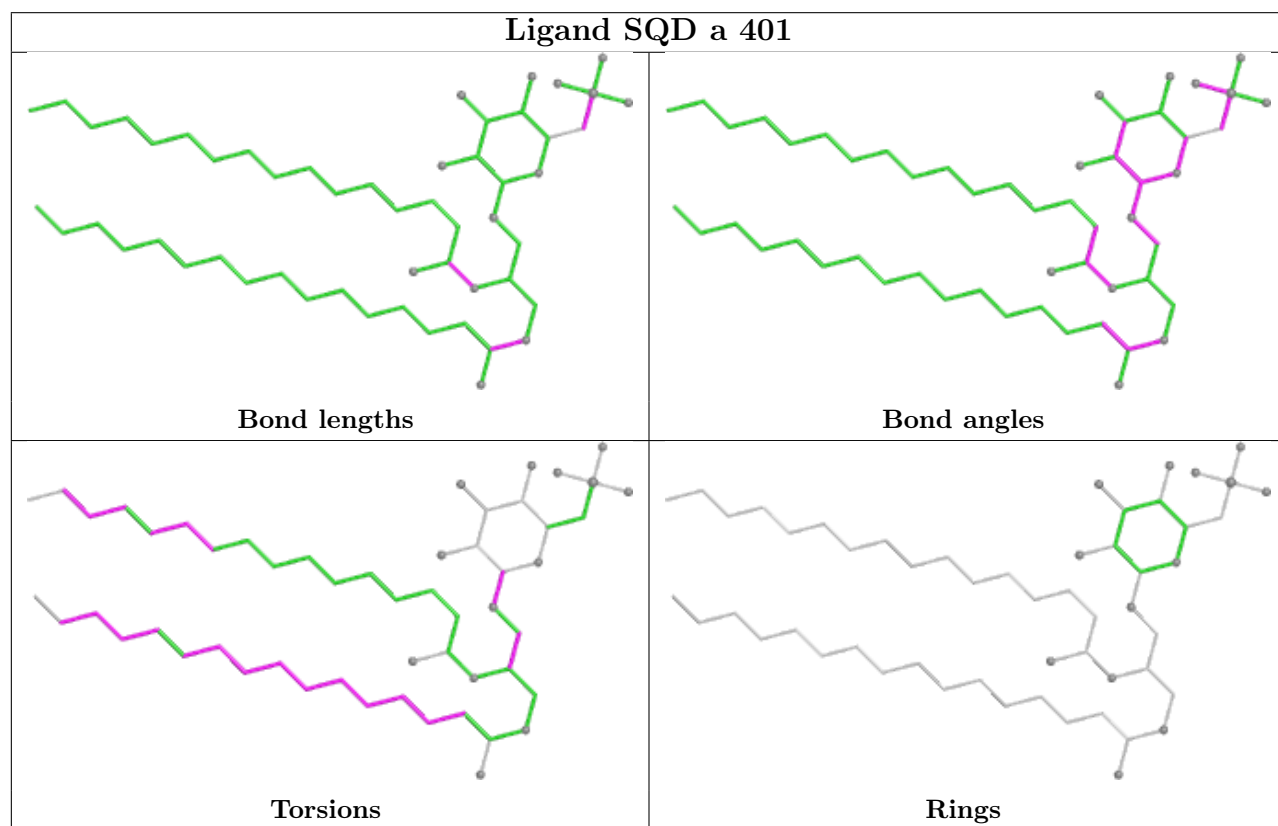
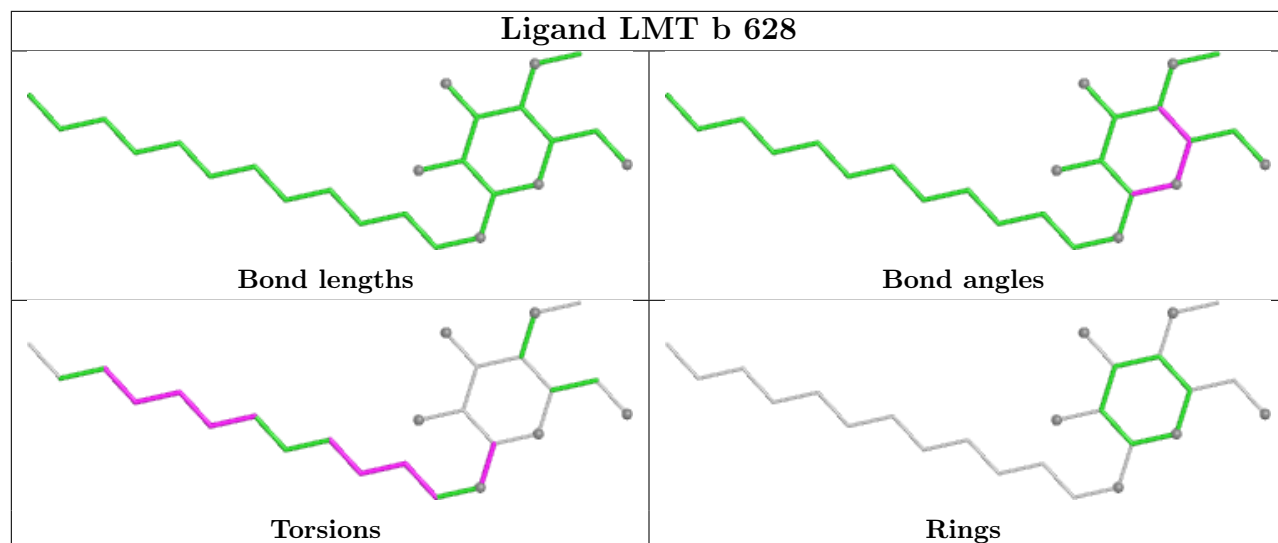


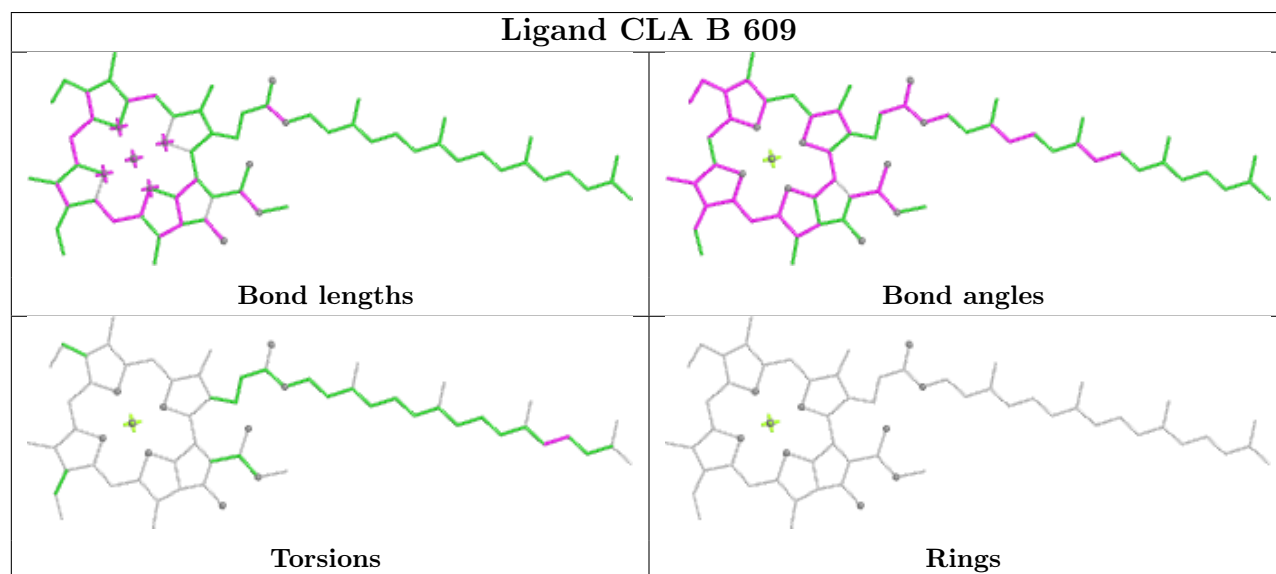
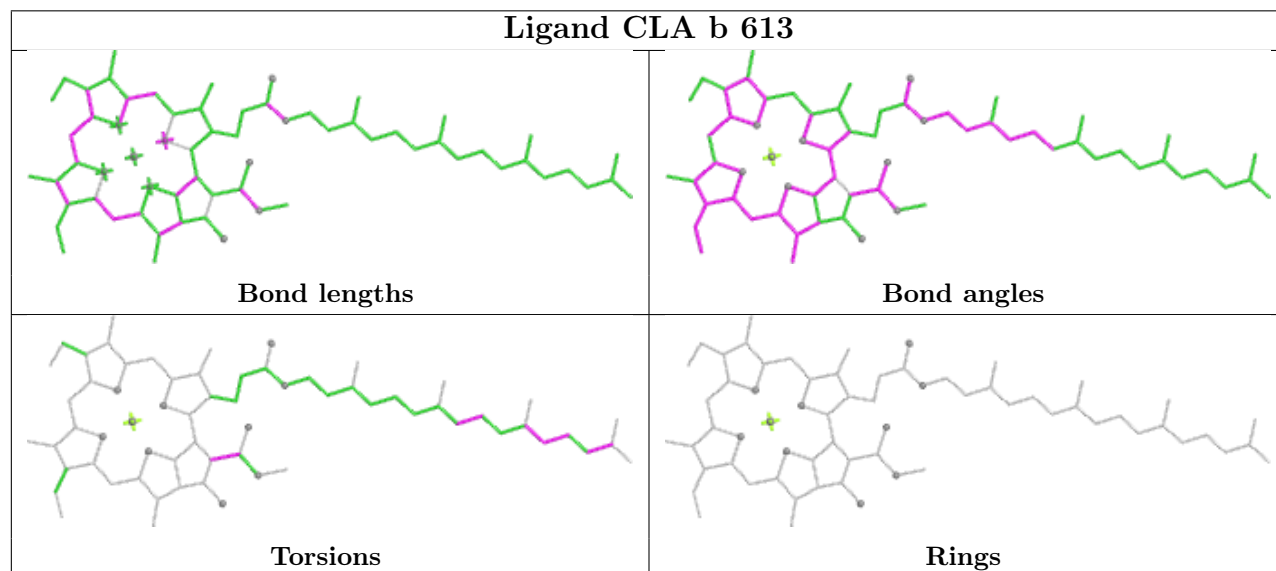
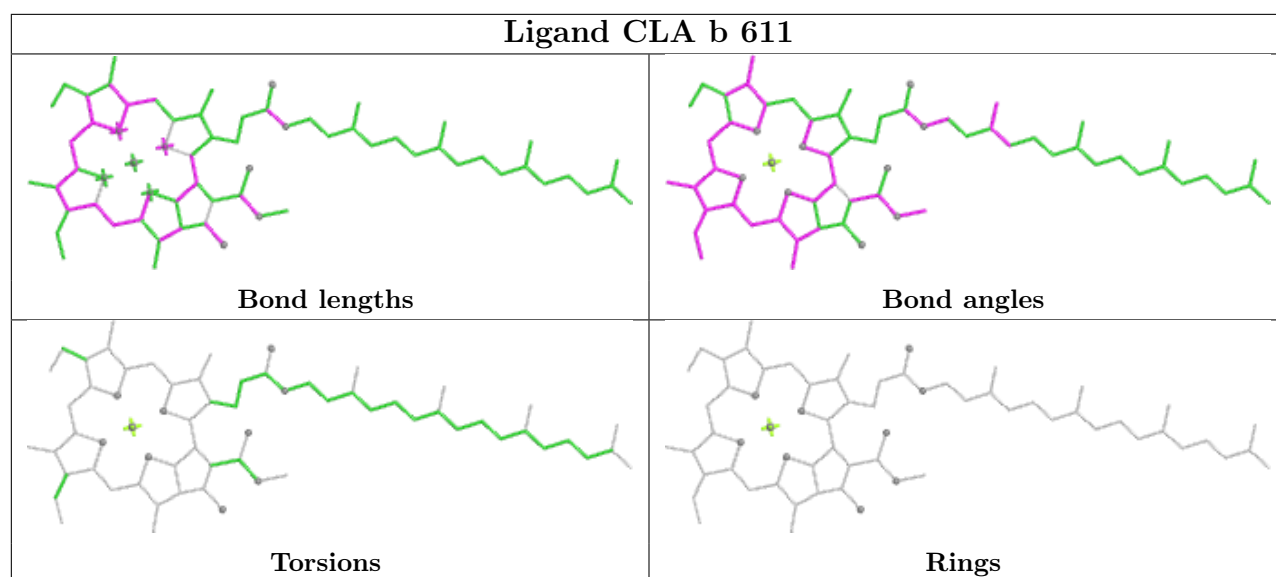


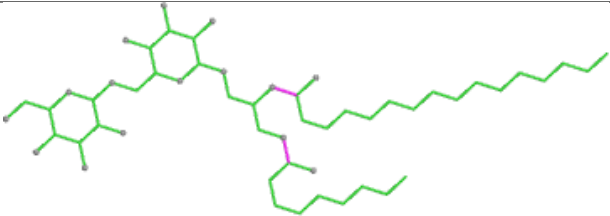
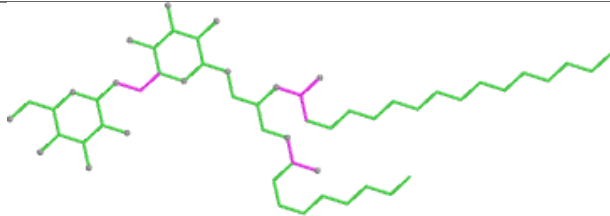
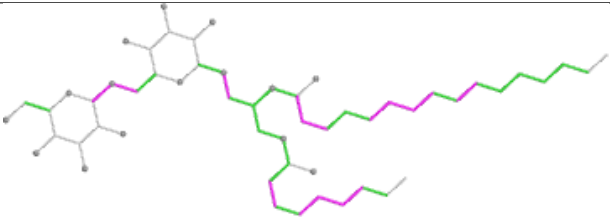
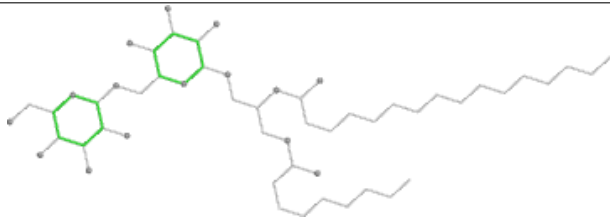
| Ligand RRX H 101                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|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

| Ligand LMT c 523                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

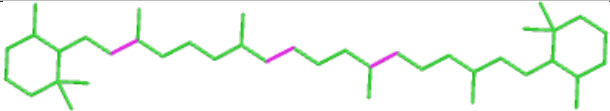
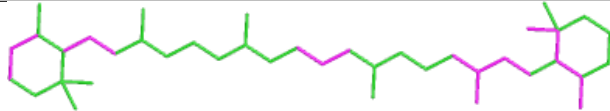
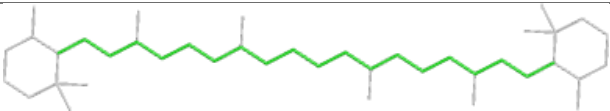
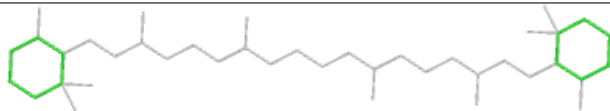
| Ligand CLA B 605                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



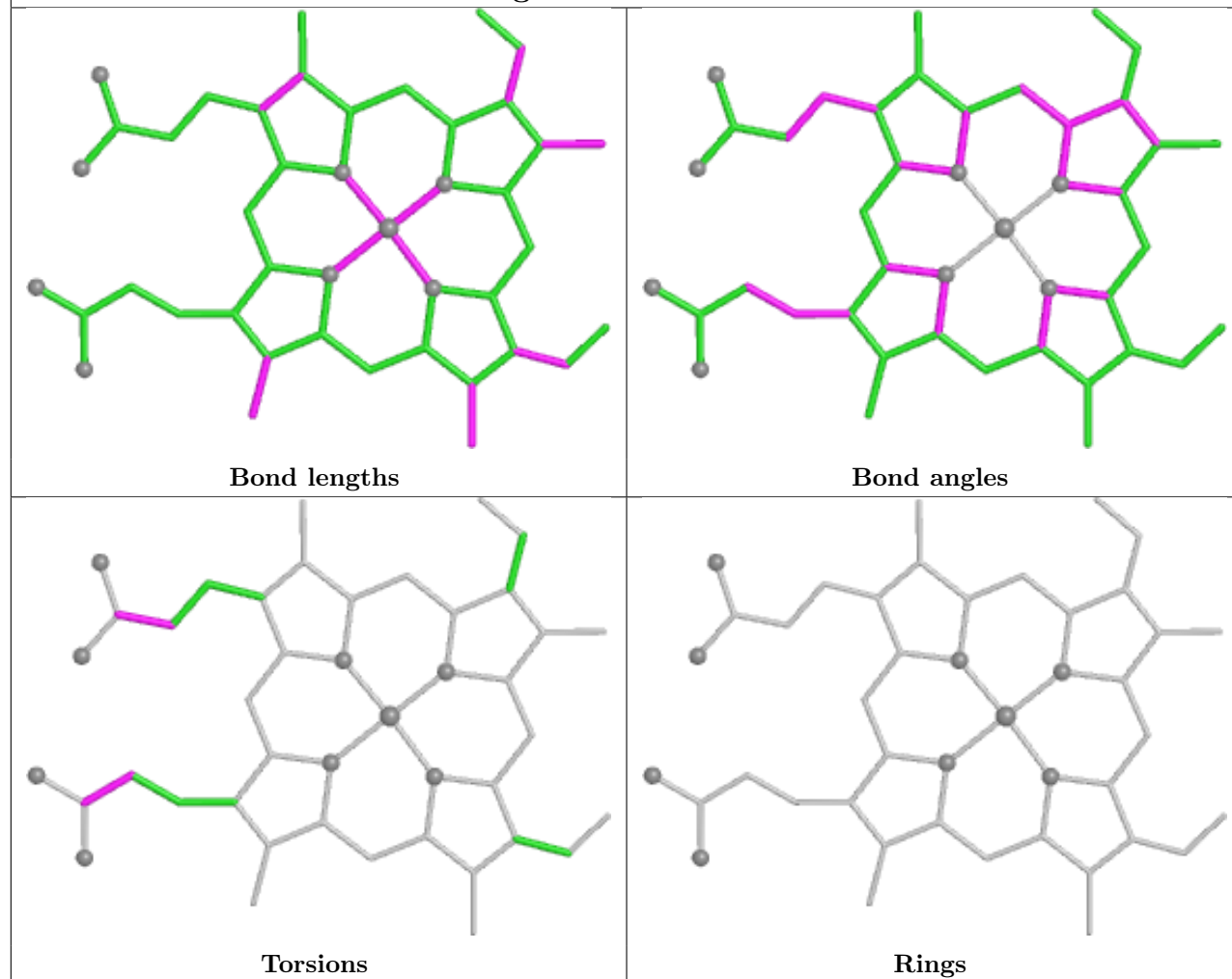


| Ligand DGD C 517                                                                  |                                                                                    |  |  |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|--|--|
|  |  |  |  |
| Bond lengths                                                                      | Bond angles                                                                        |  |  |
|  |  |  |  |
| Torsions                                                                          | Rings                                                                              |  |  |

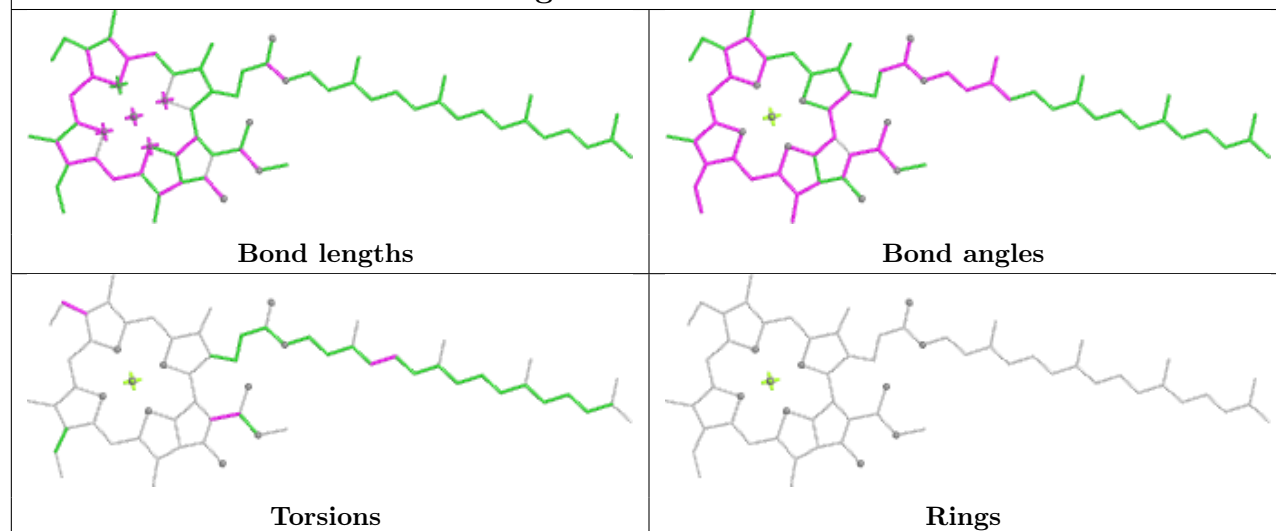
  

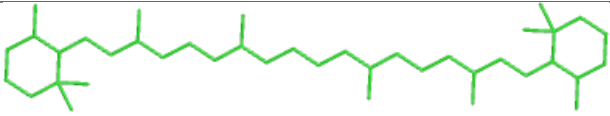
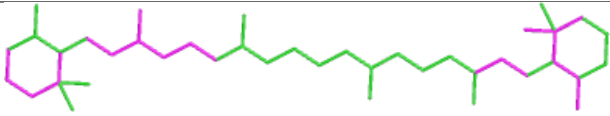
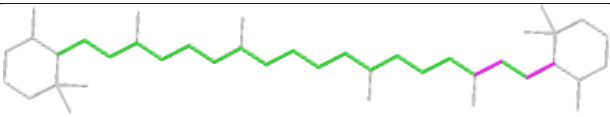
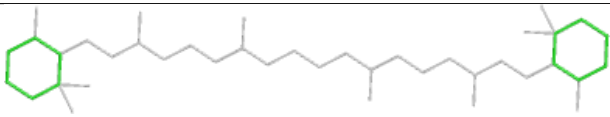
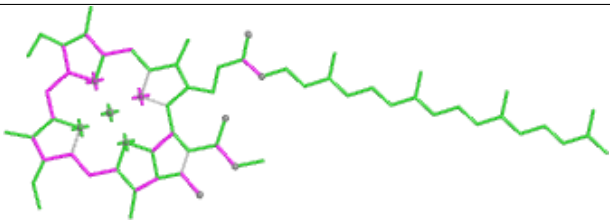
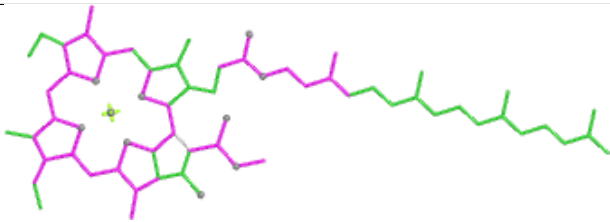
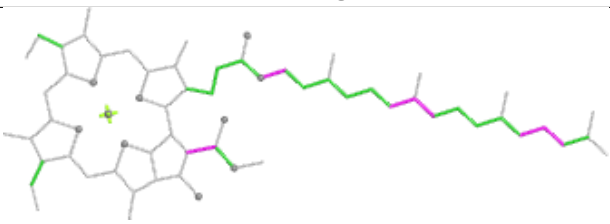
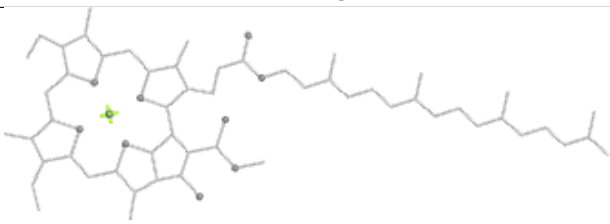
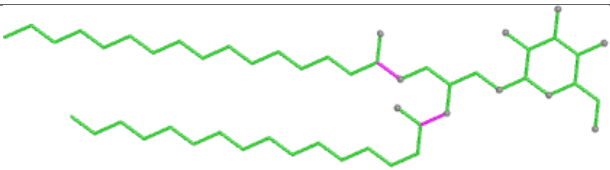
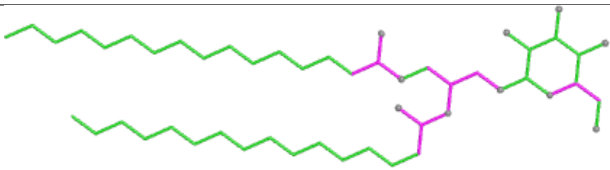
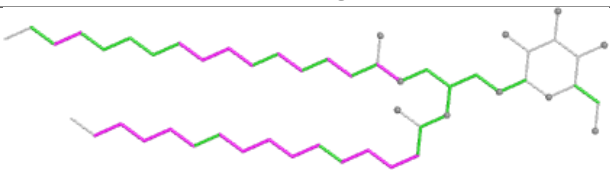
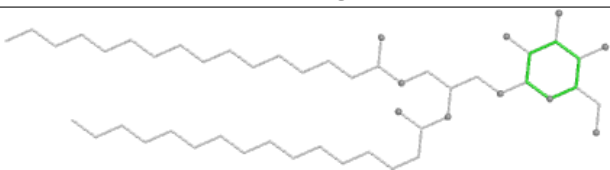
| Ligand BCR A 405                                                                   |                                                                                     |  |  |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|--|--|
|   |   |  |  |
| Bond lengths                                                                       | Bond angles                                                                         |  |  |
|  |  |  |  |
| Torsions                                                                           | Rings                                                                               |  |  |

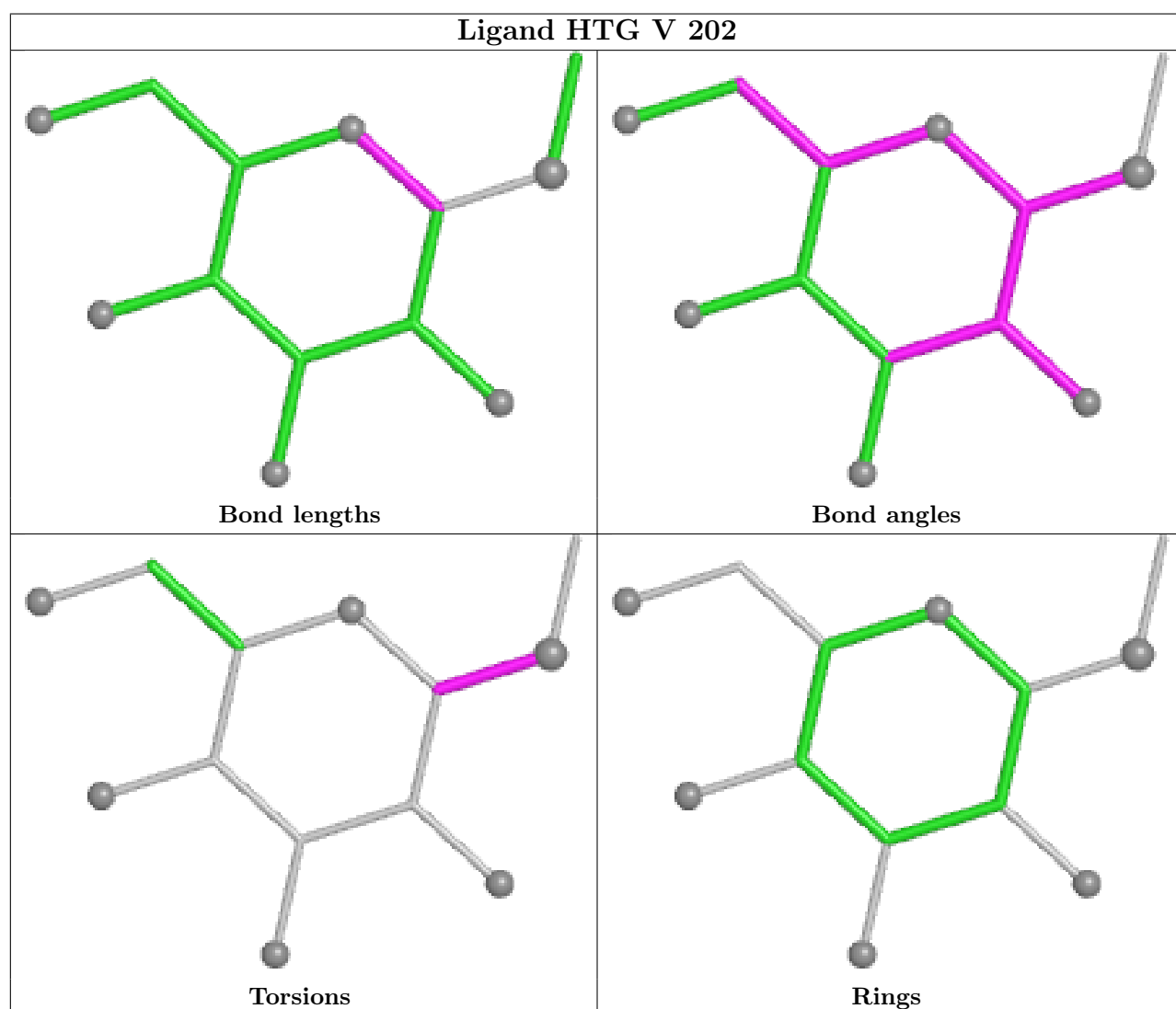
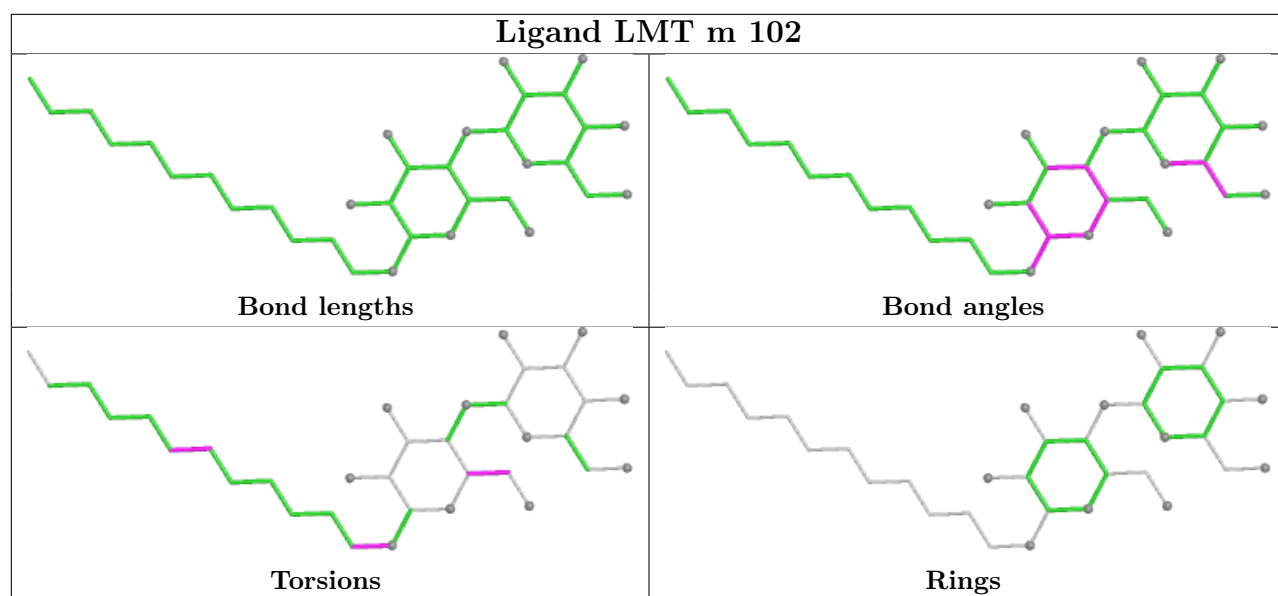
## Ligand HEM e 102

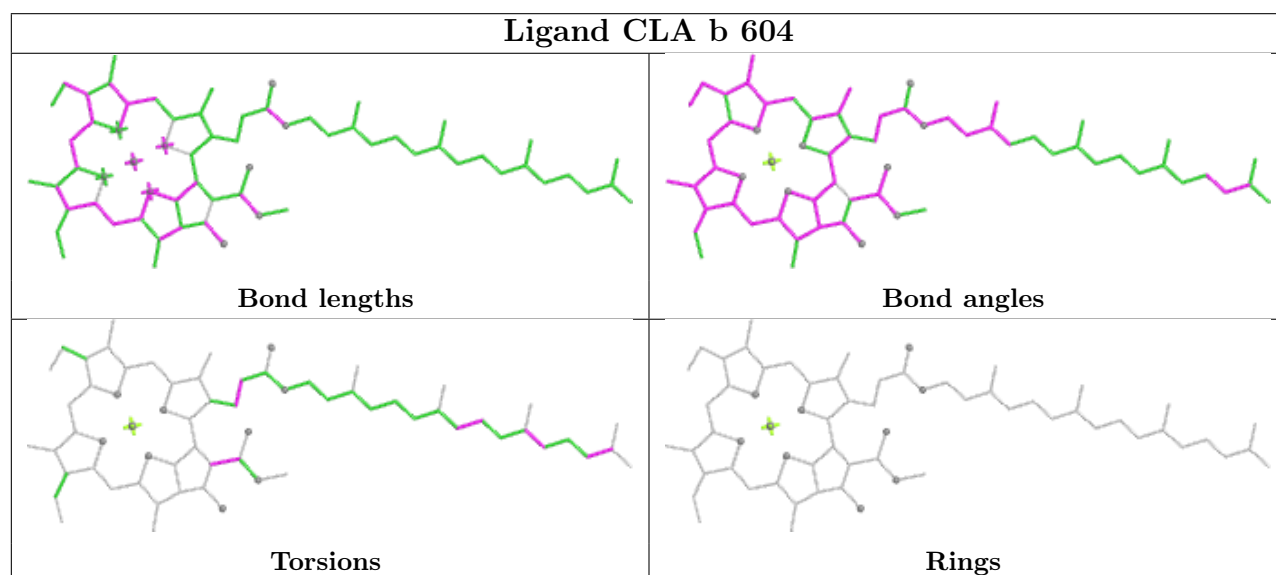
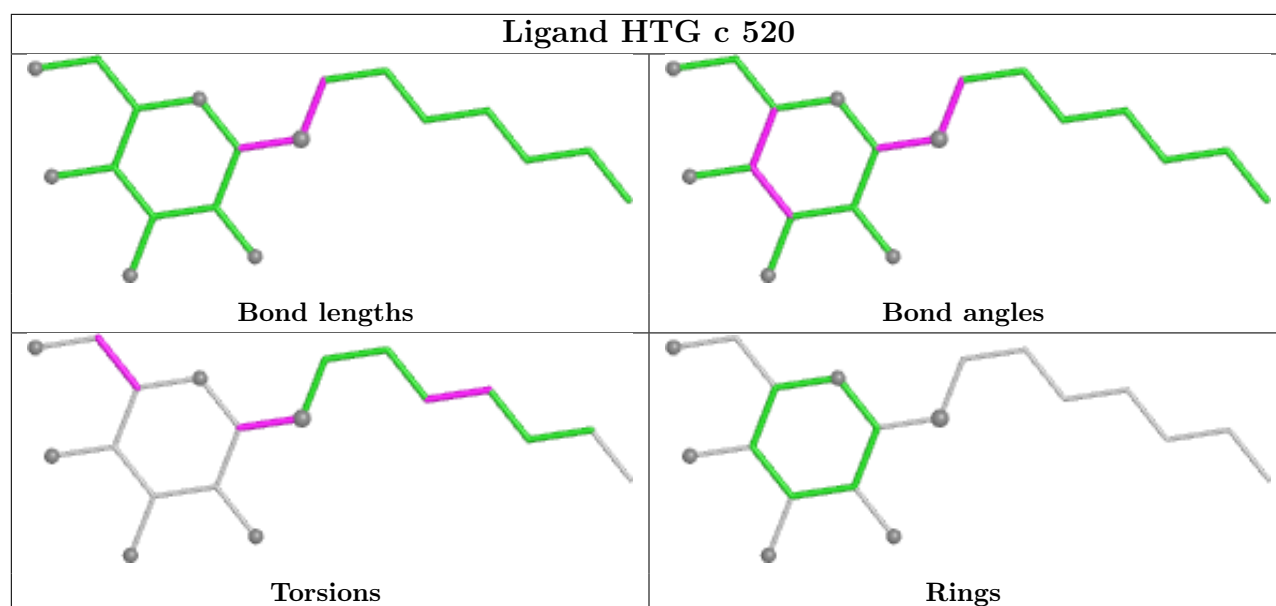


## Ligand CLA b 609

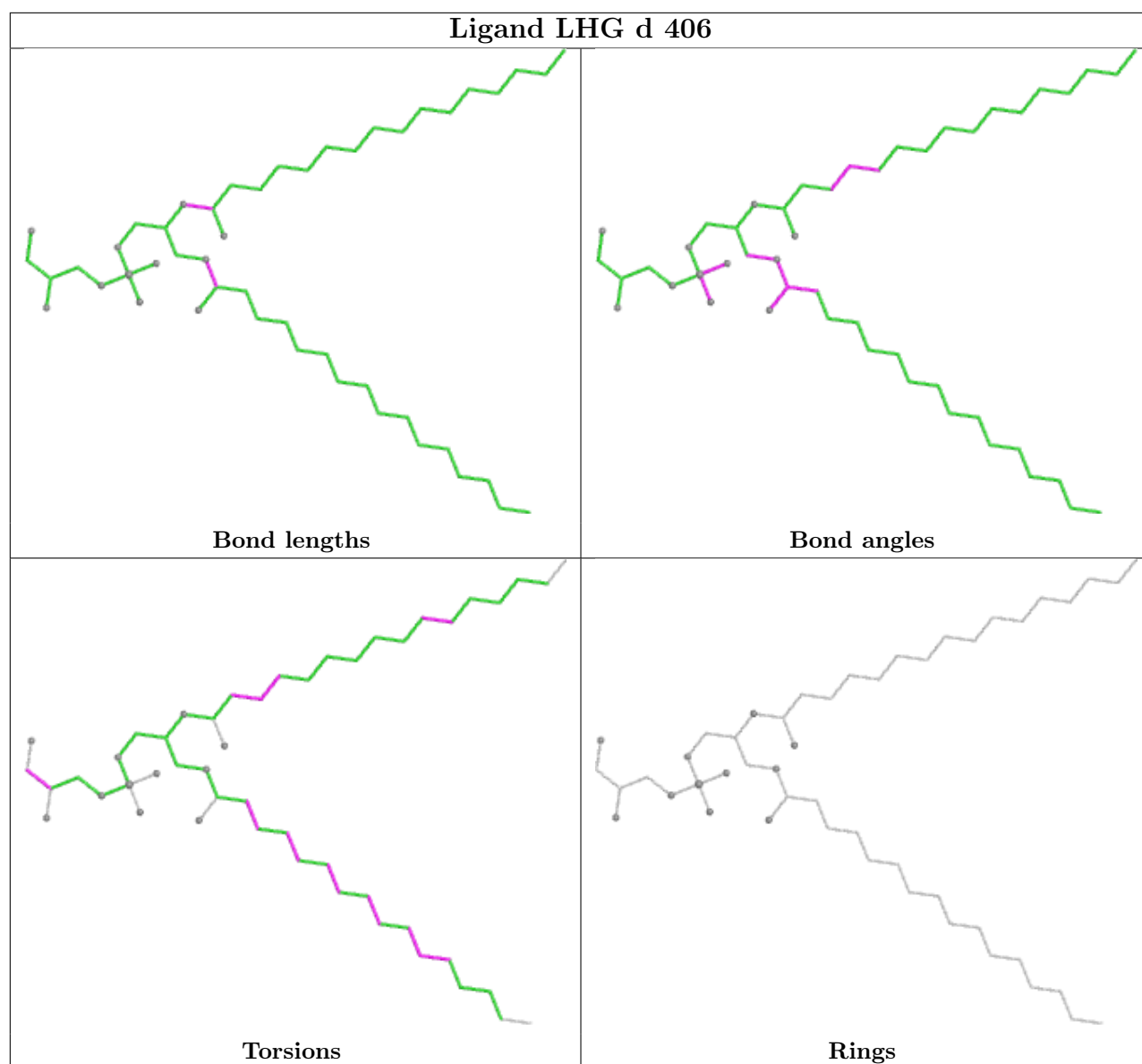


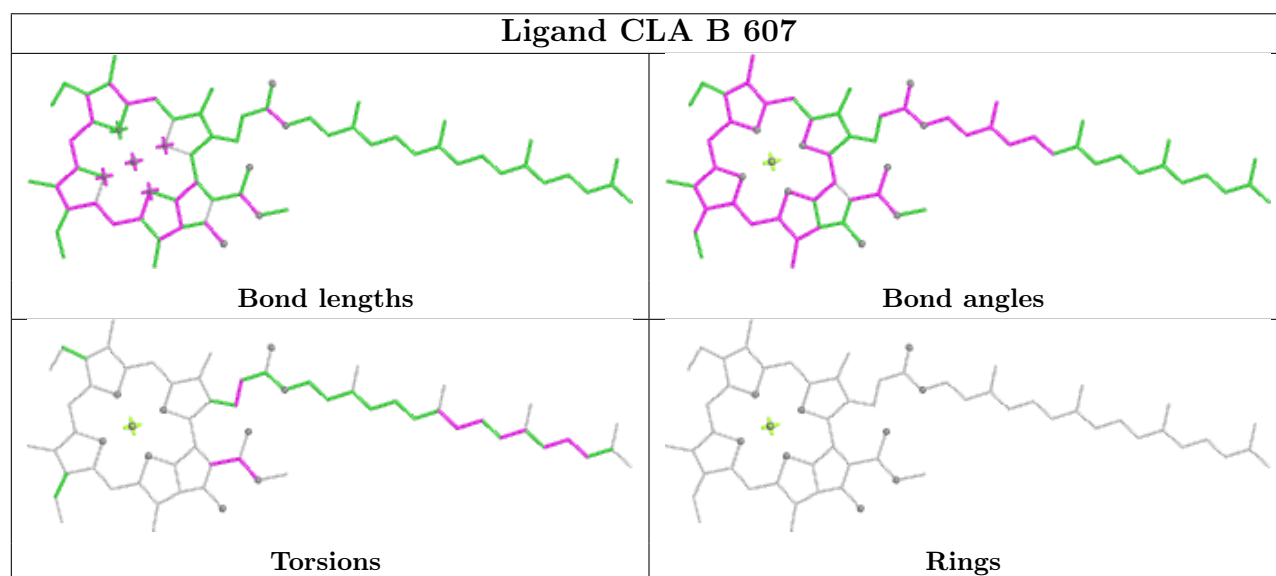
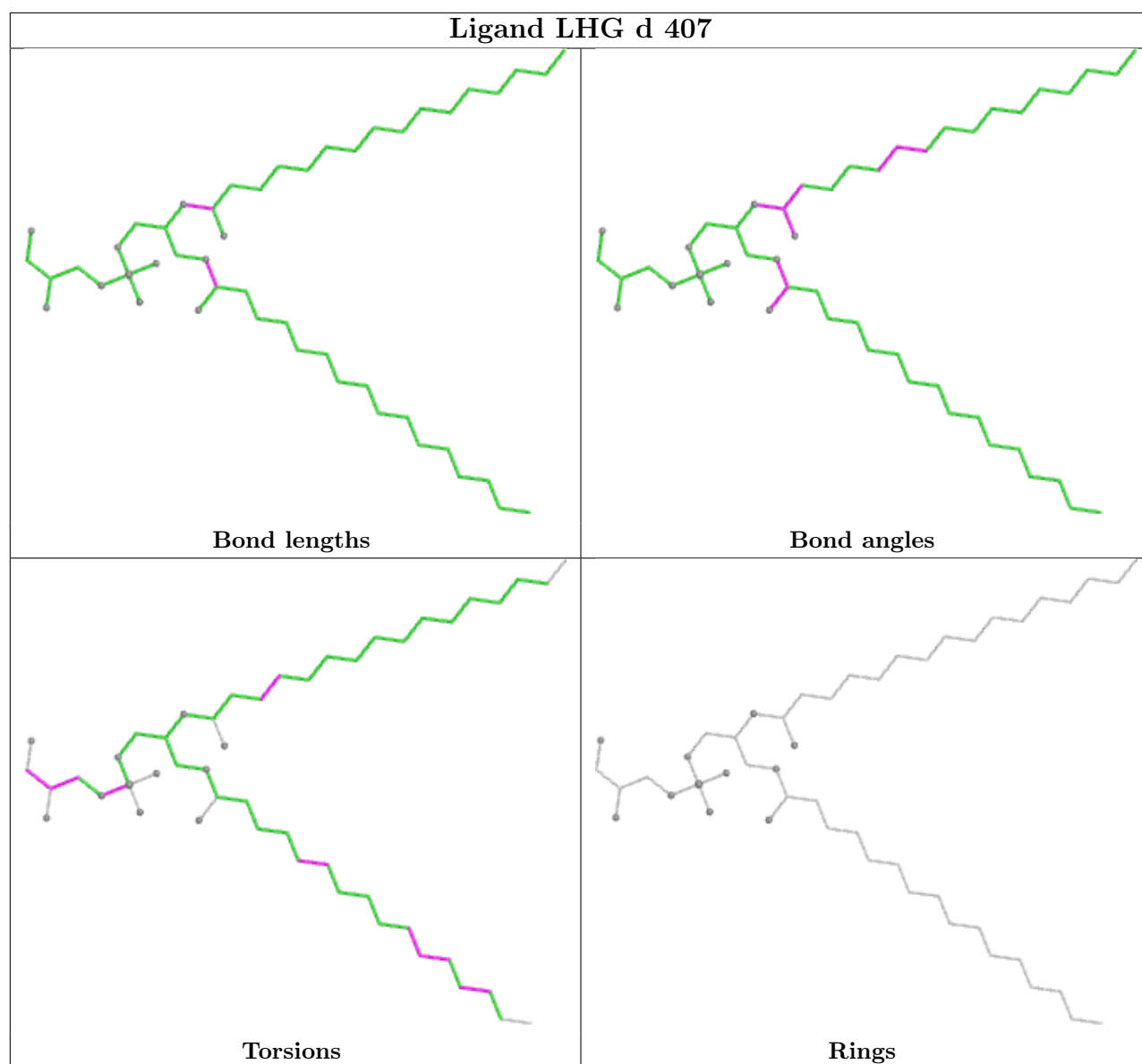
| Ligand BCR d 405                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand CLA C 509                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand LMG C 519                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

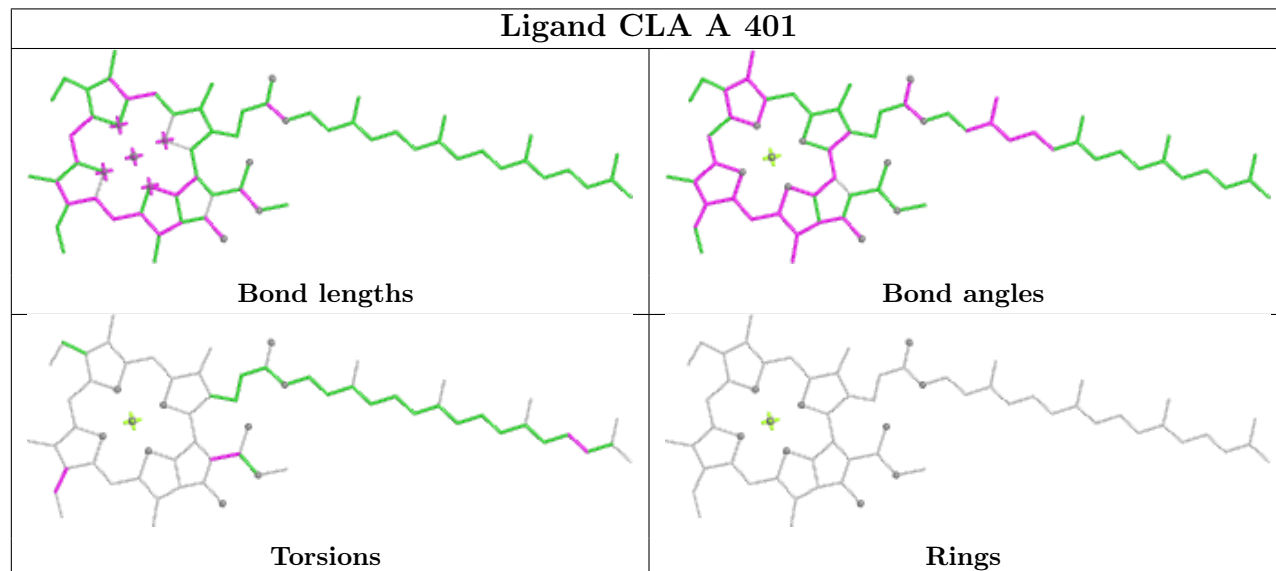
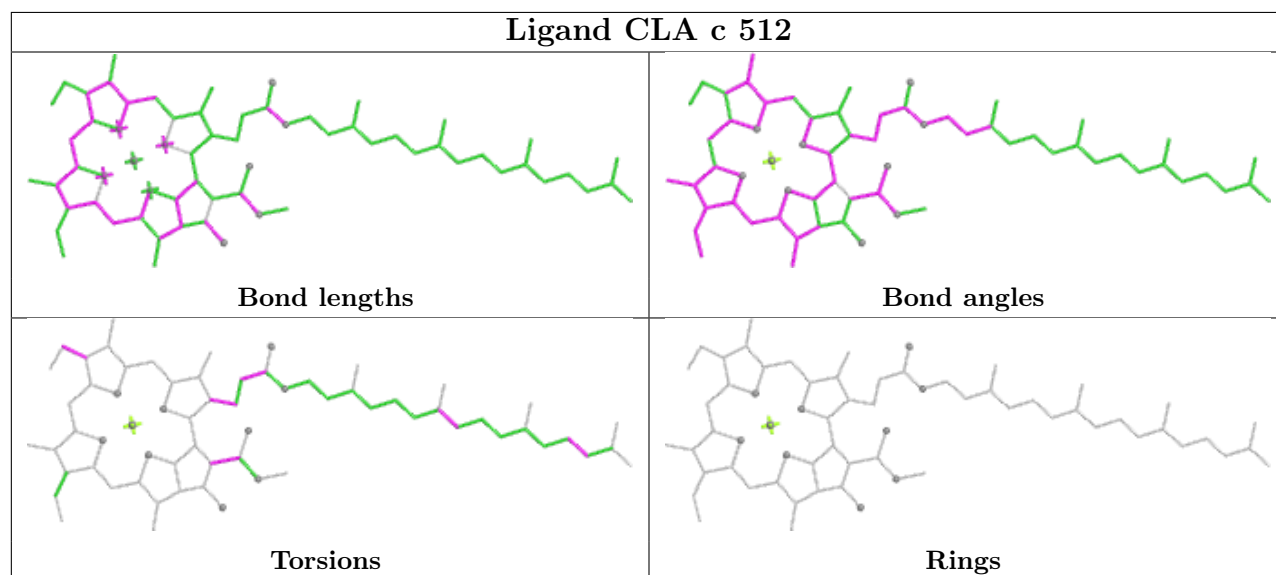
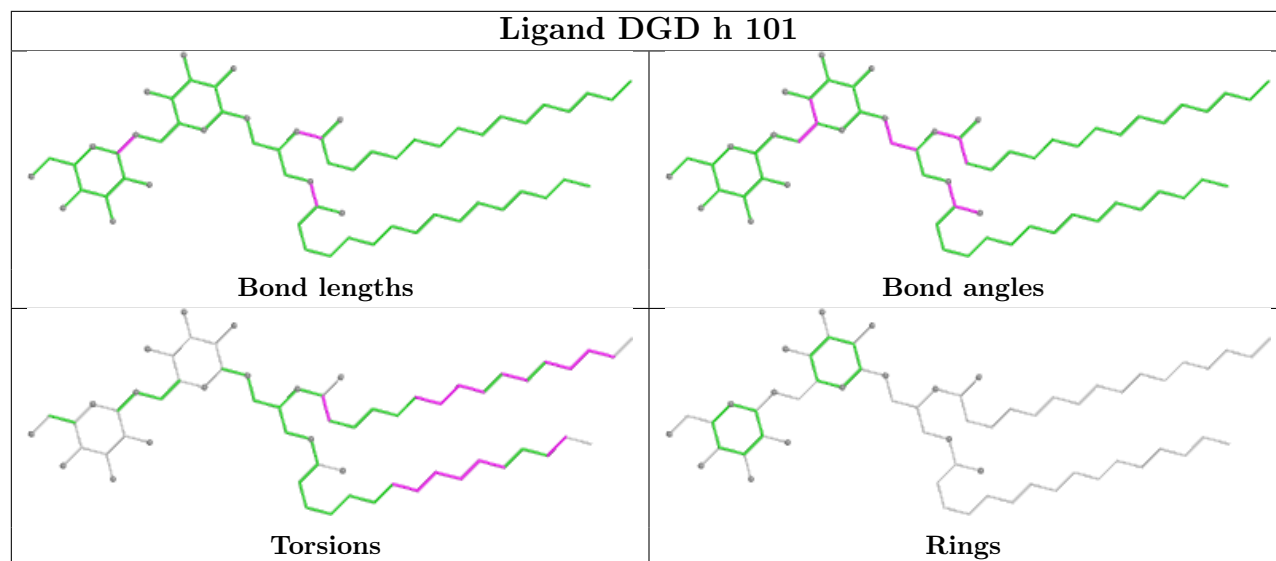


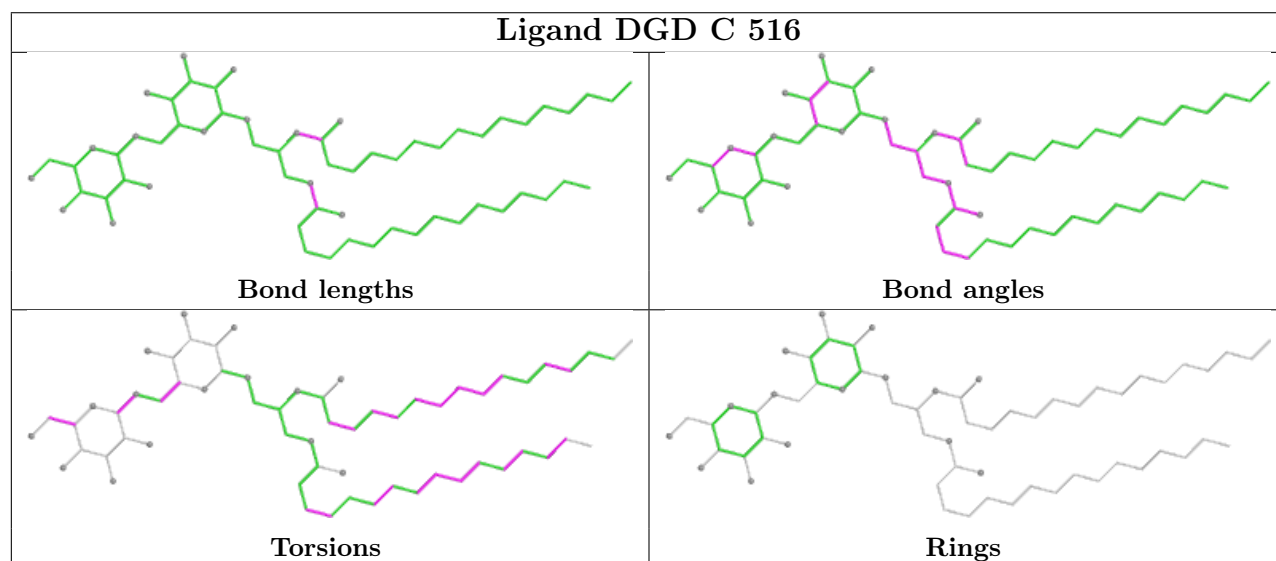
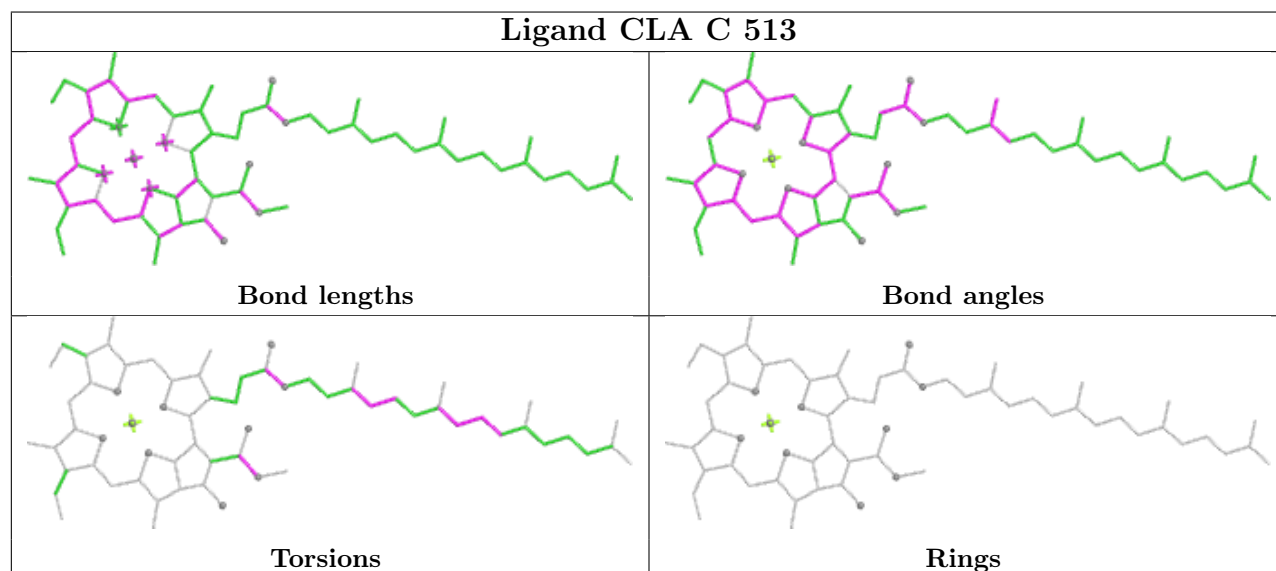
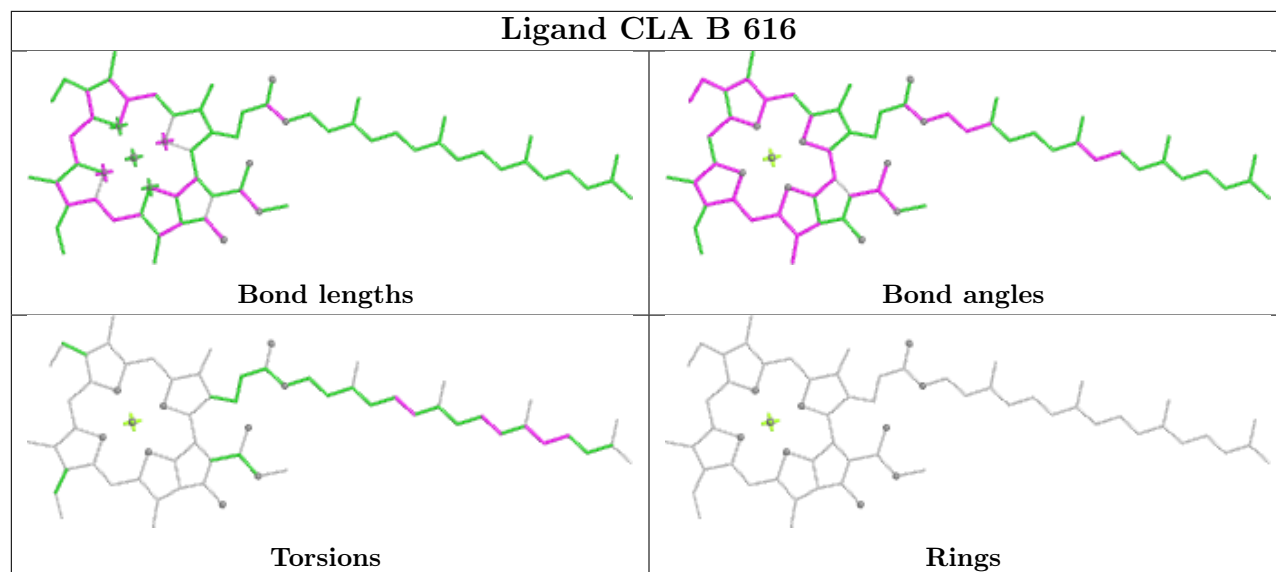


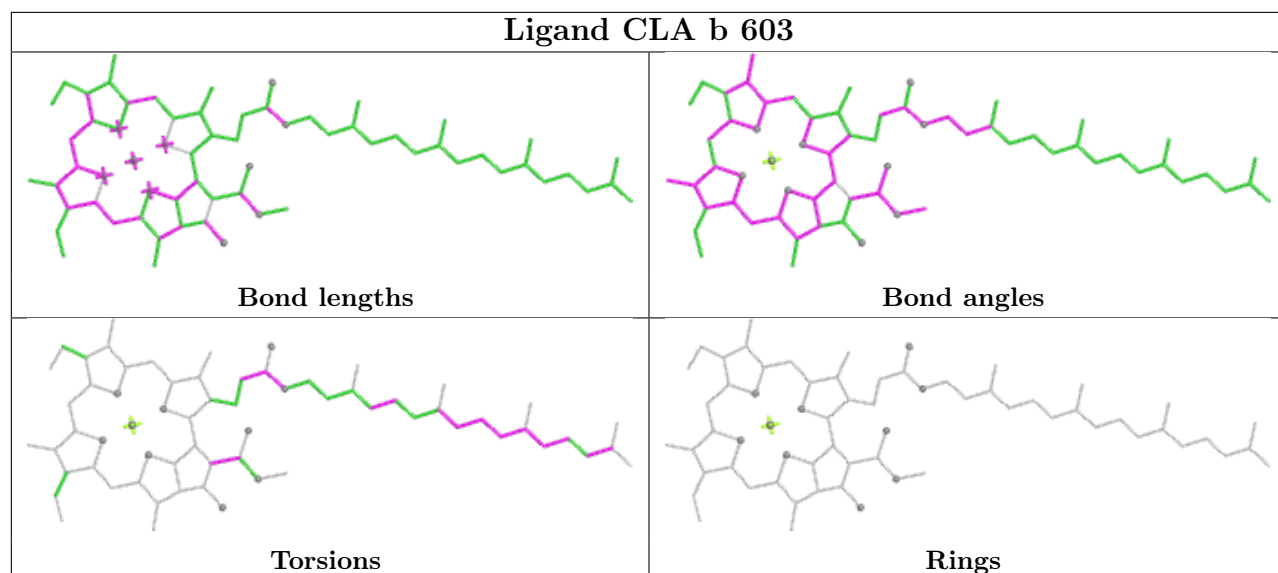
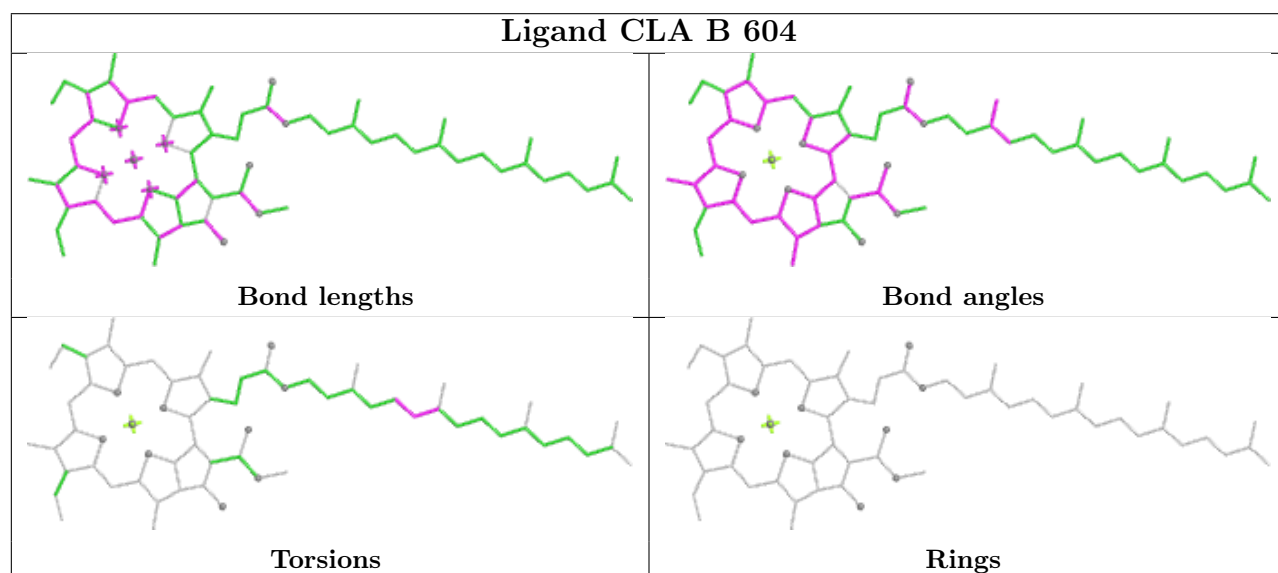
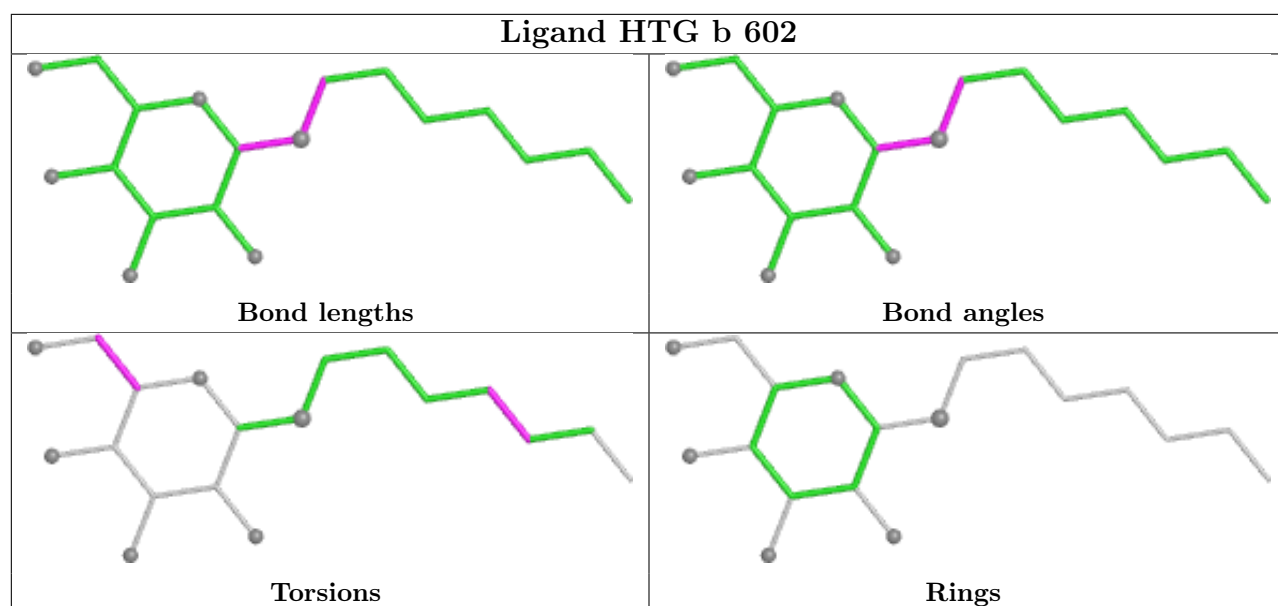


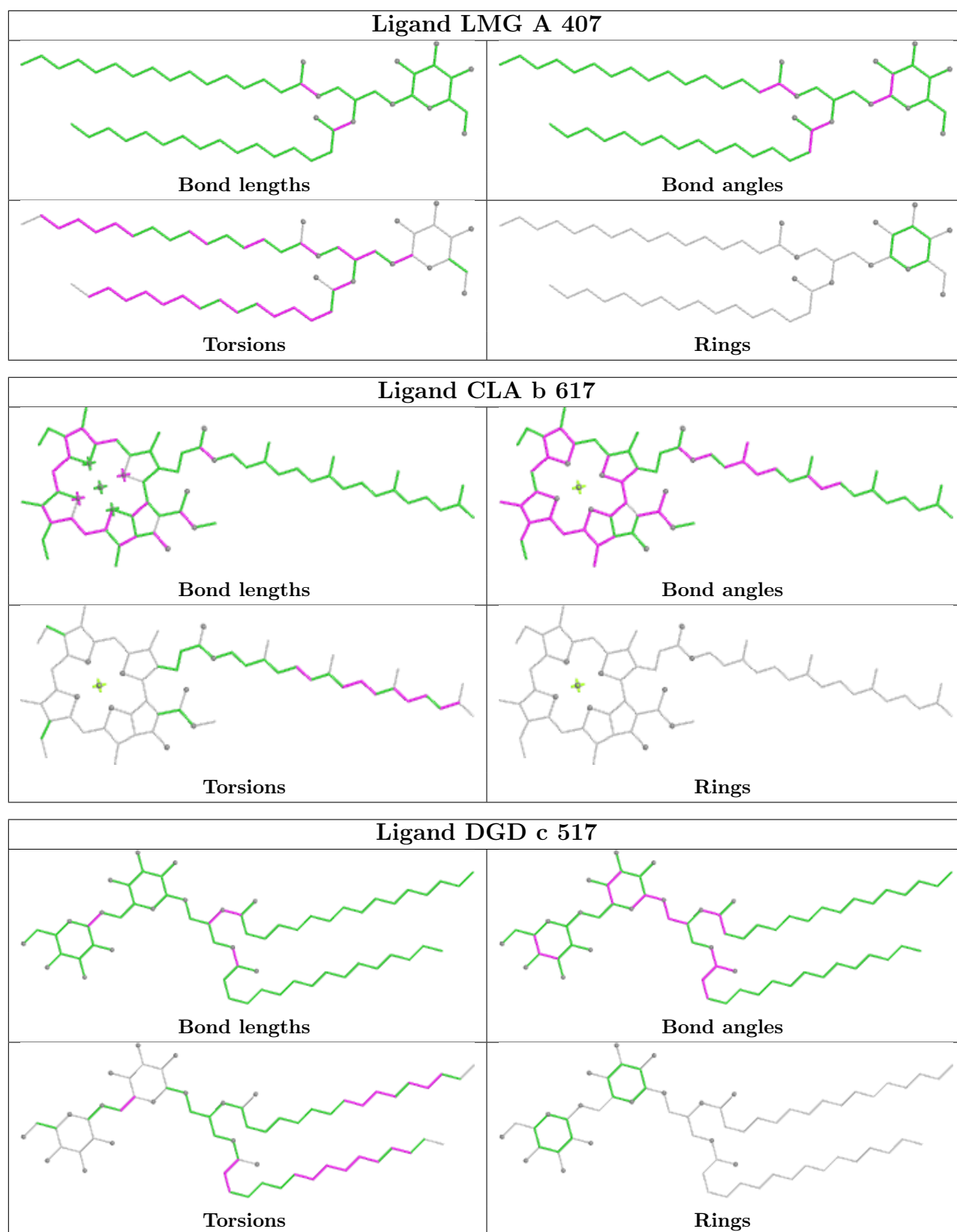


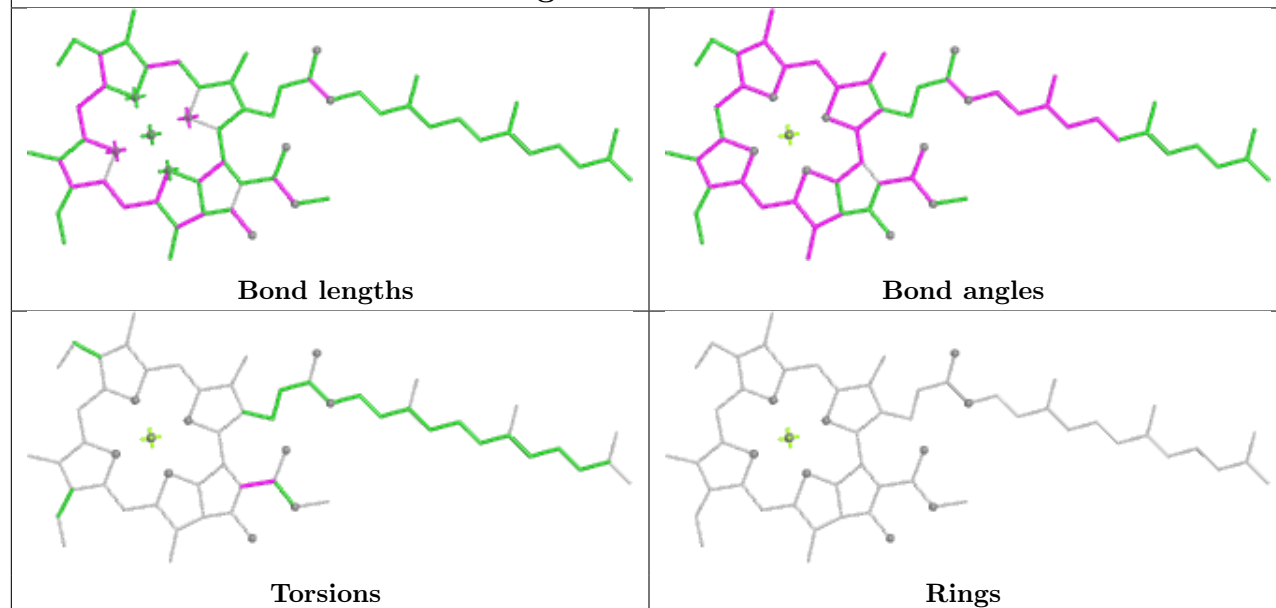
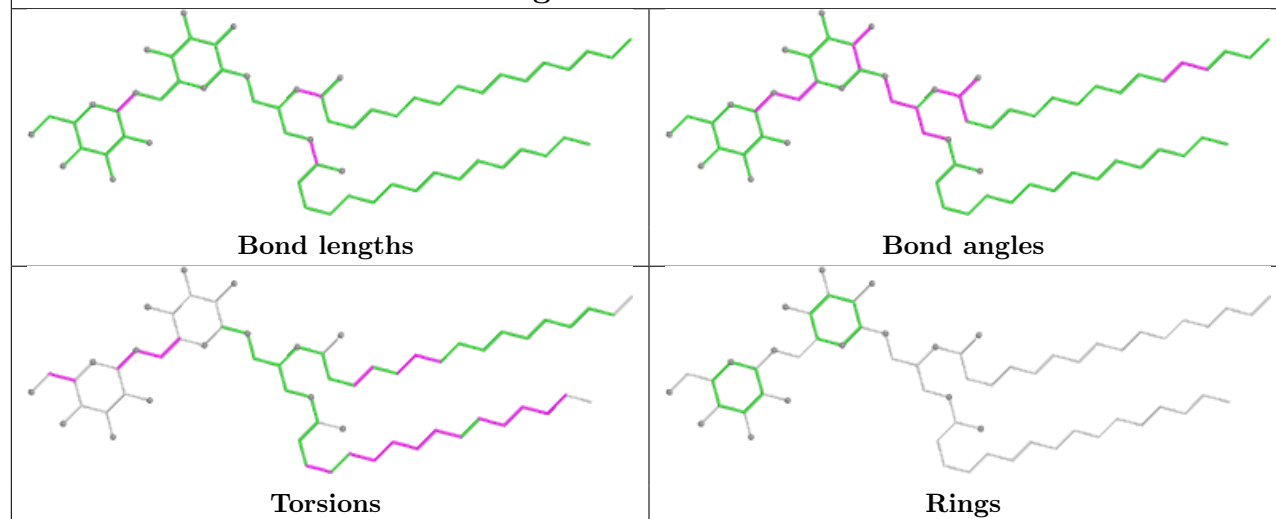


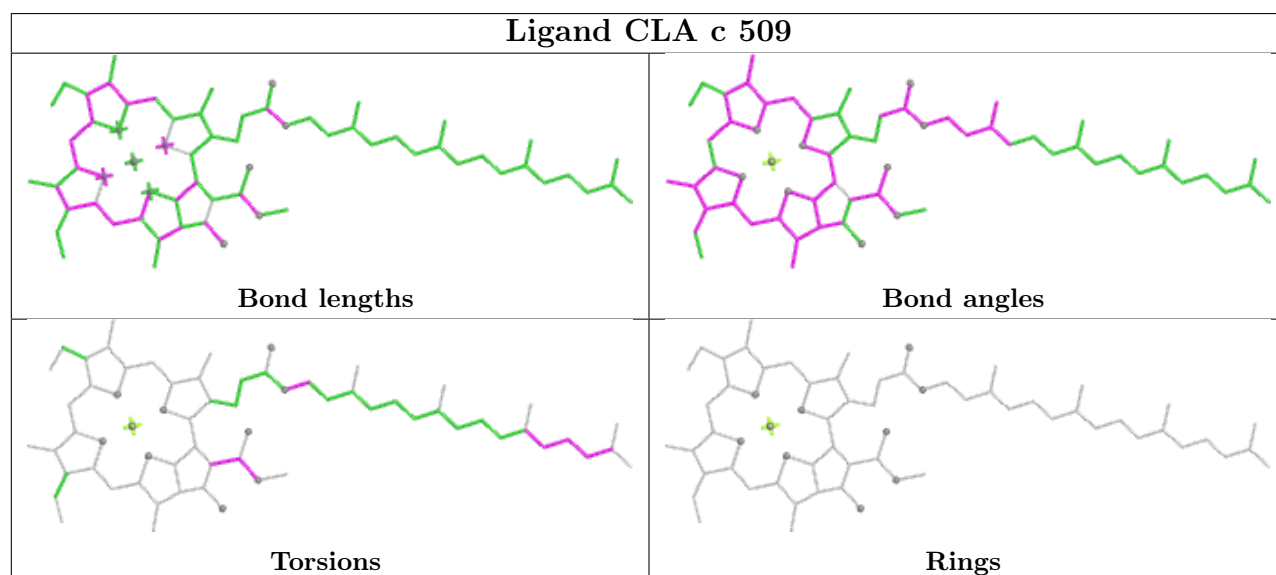
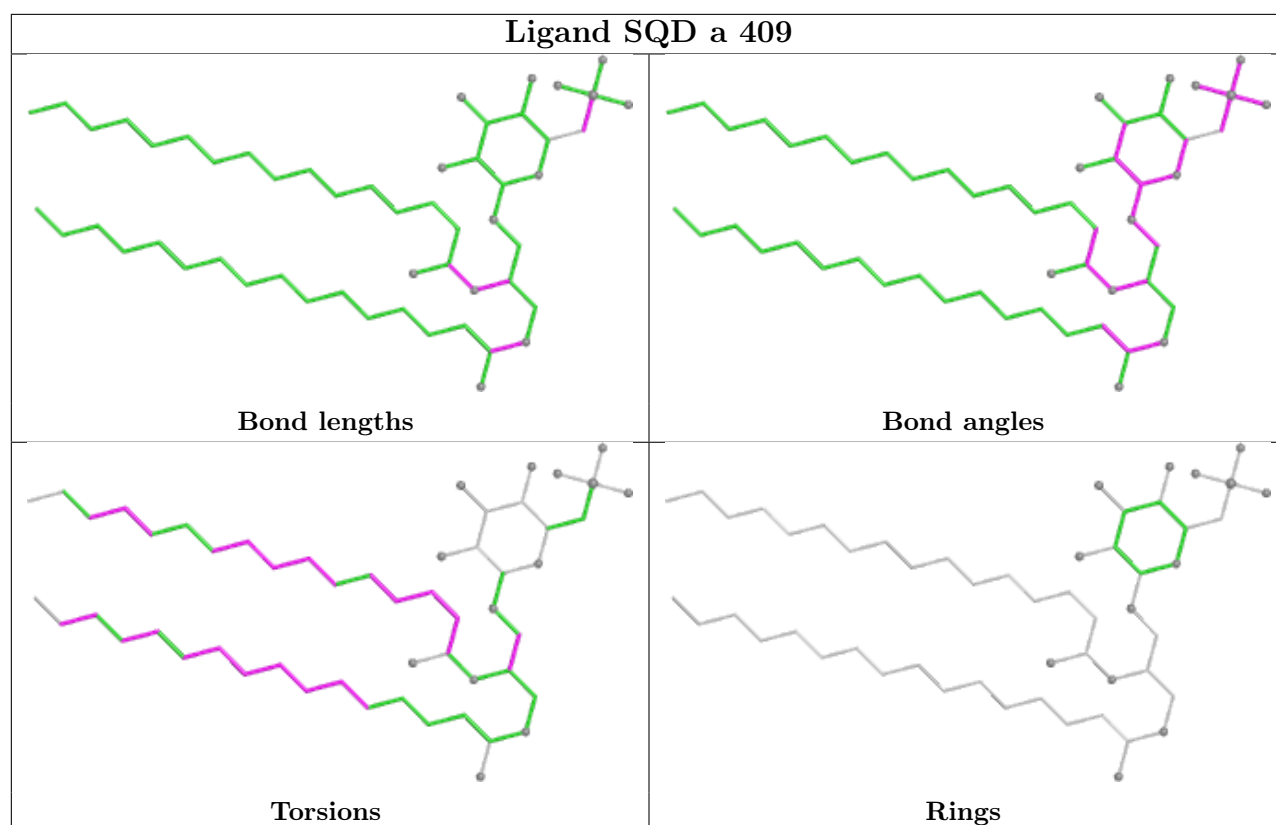




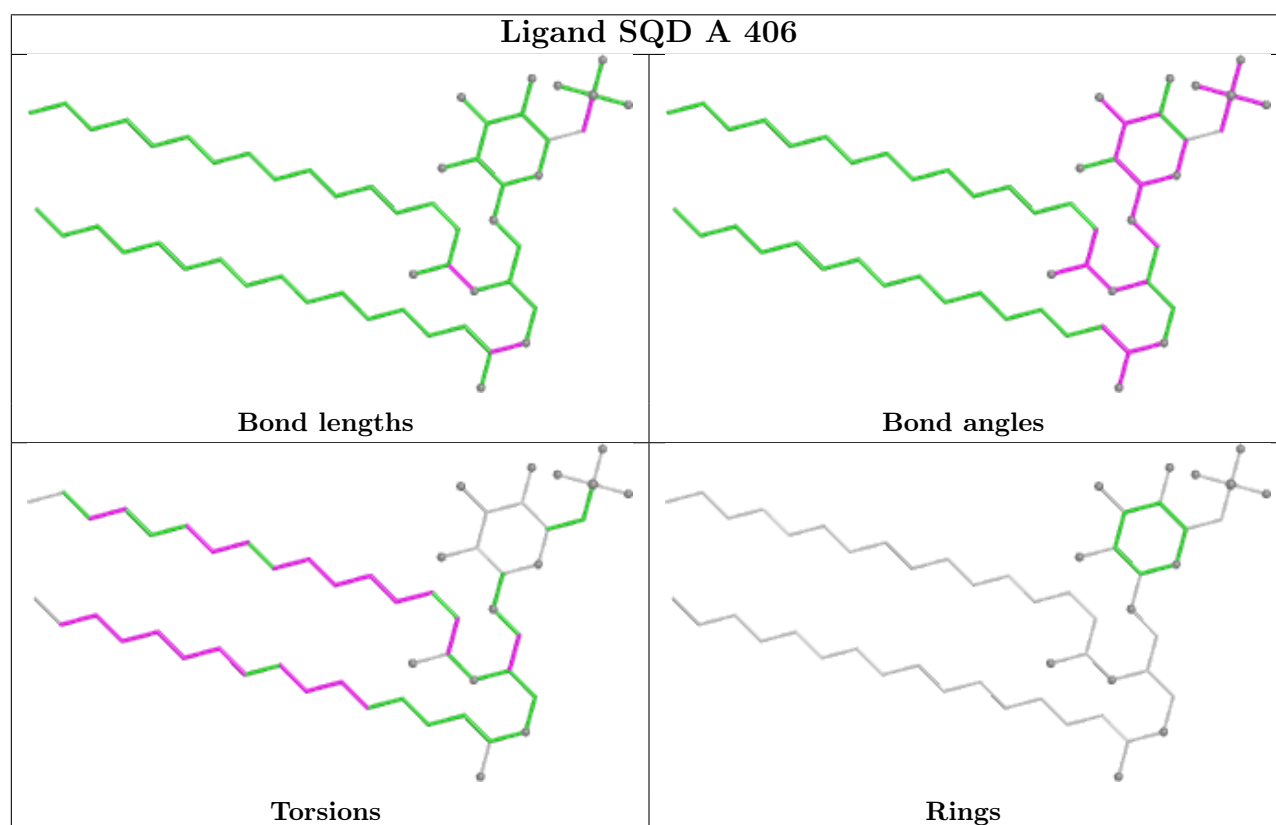
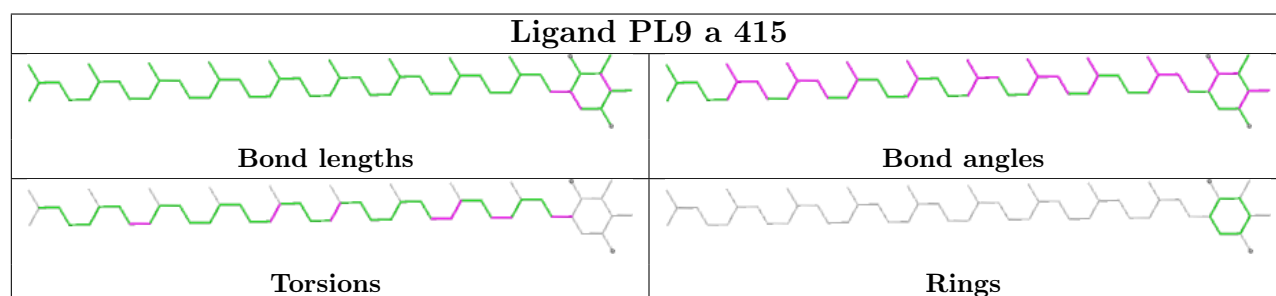
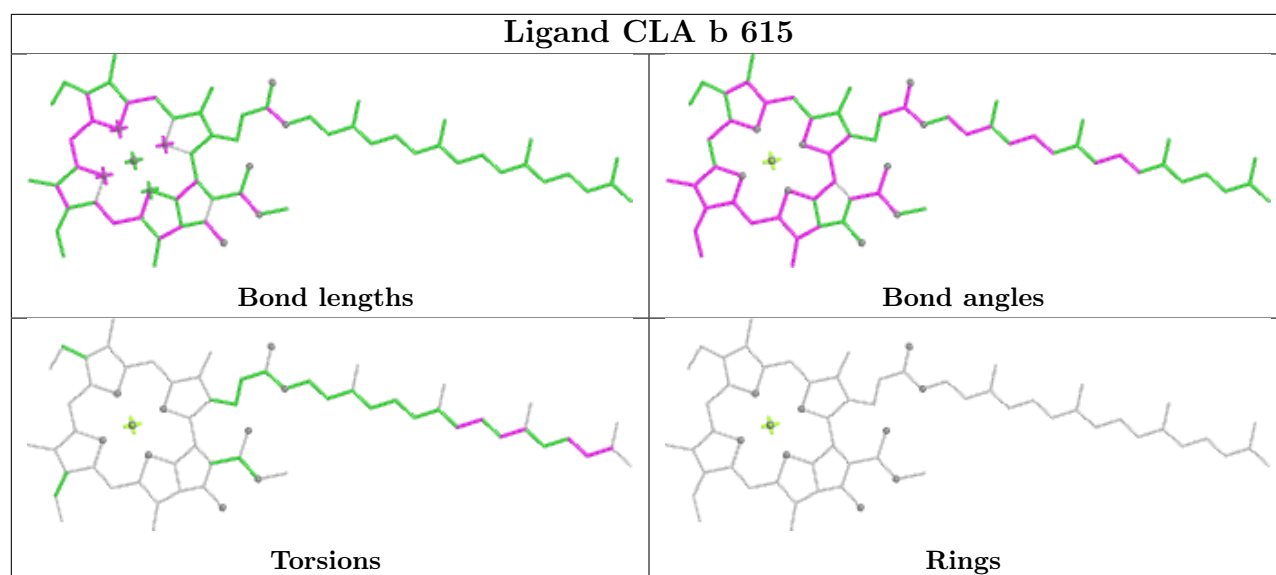


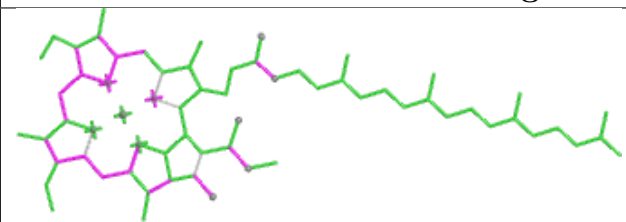
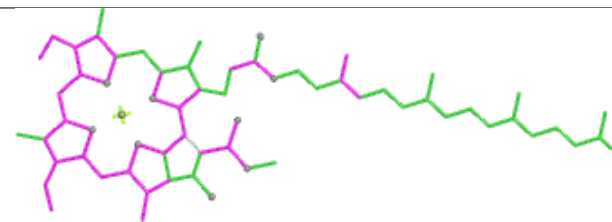
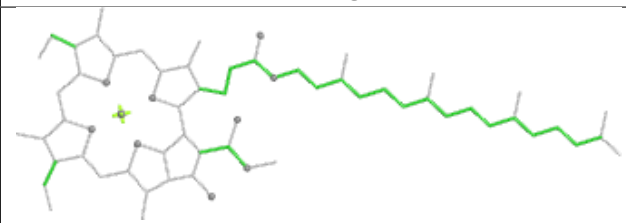
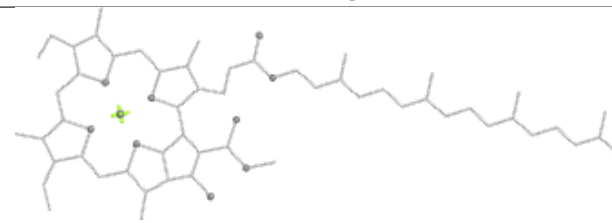


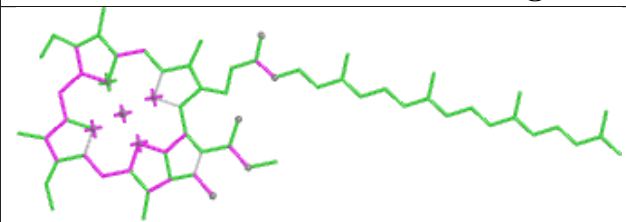
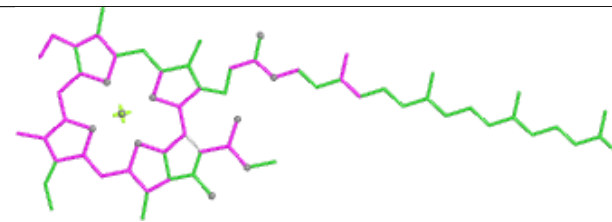
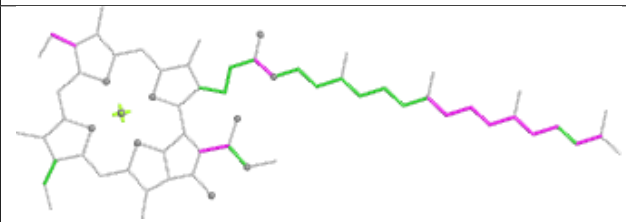
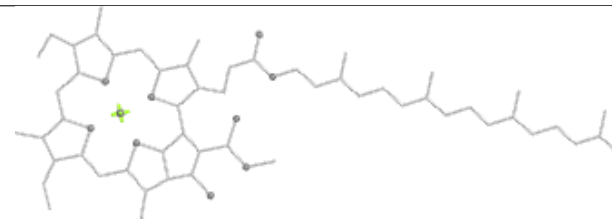
**Ligand CLA c 508****Ligand DGD c 515**

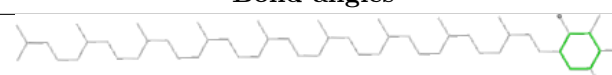


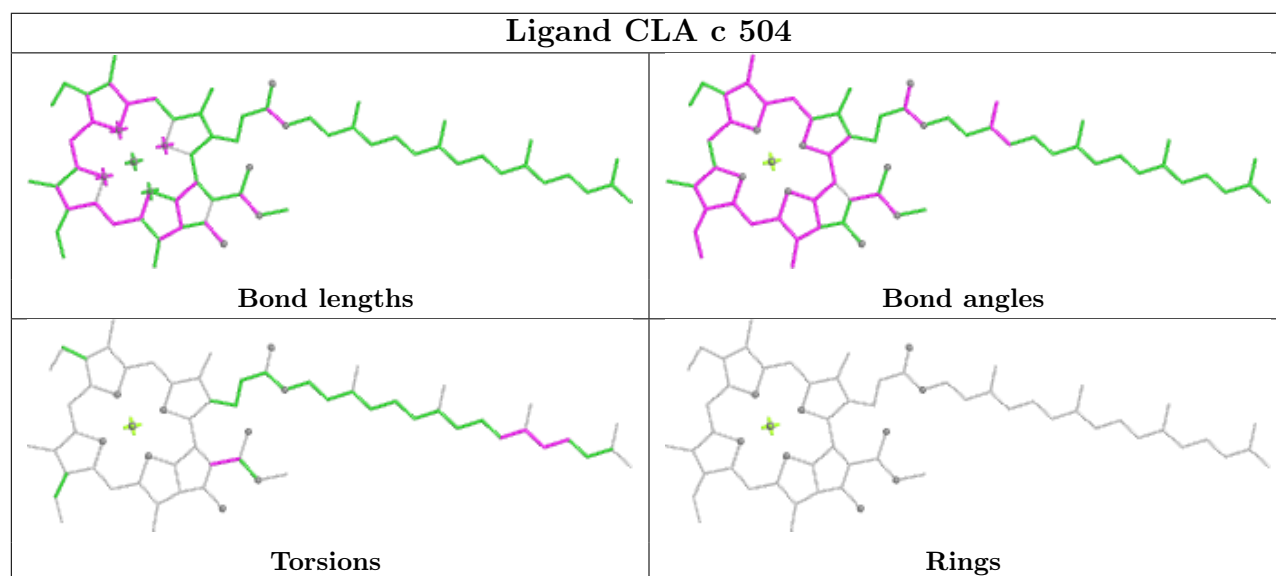
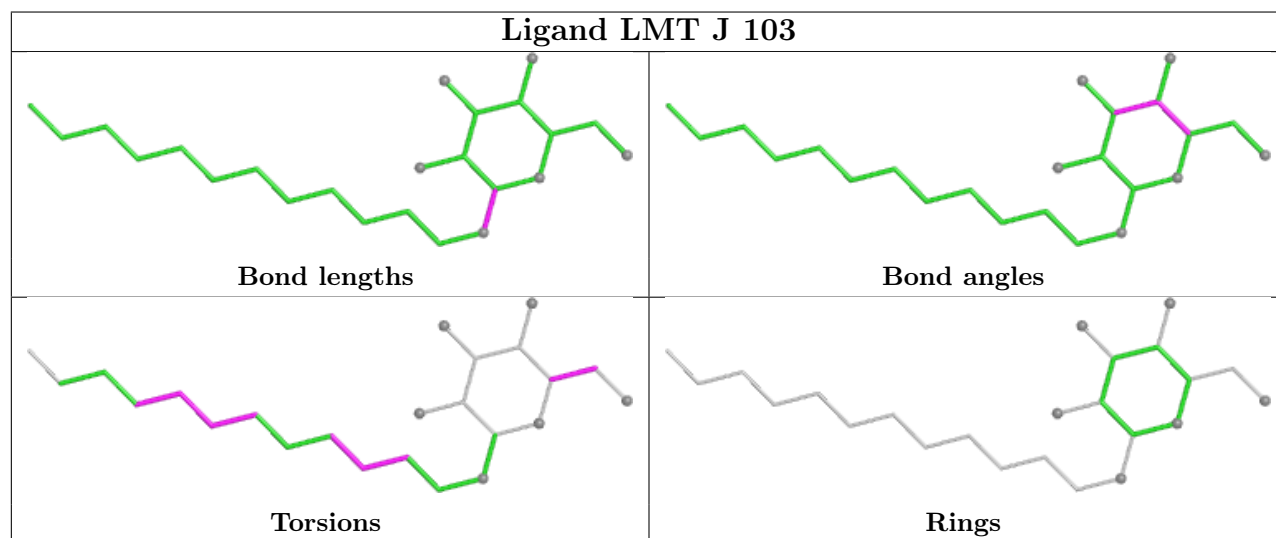
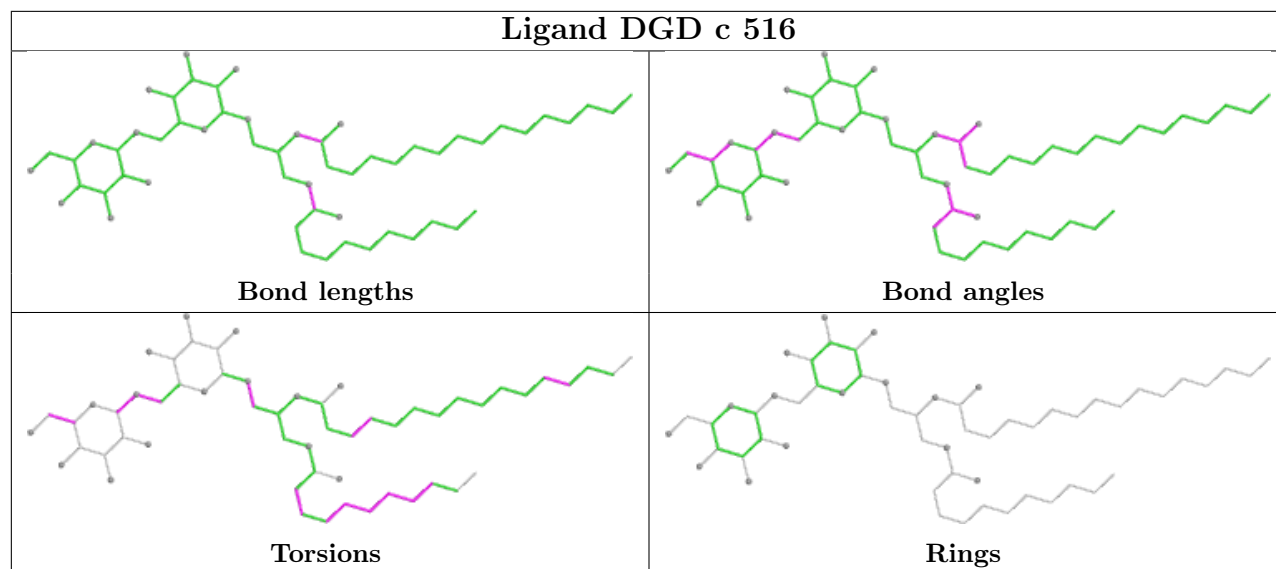


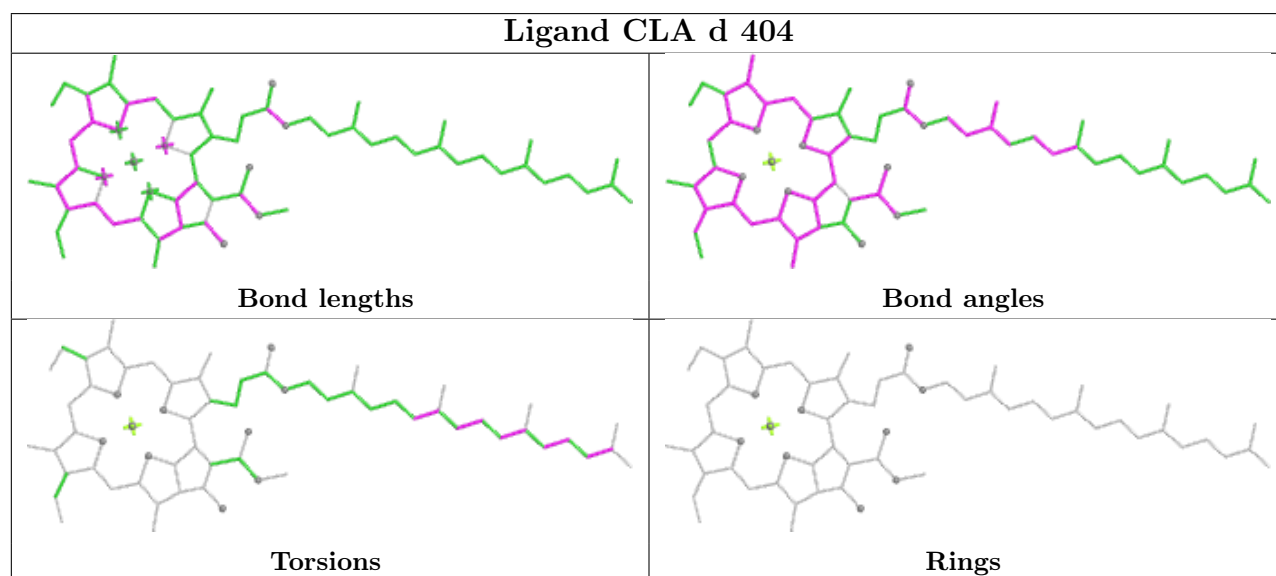
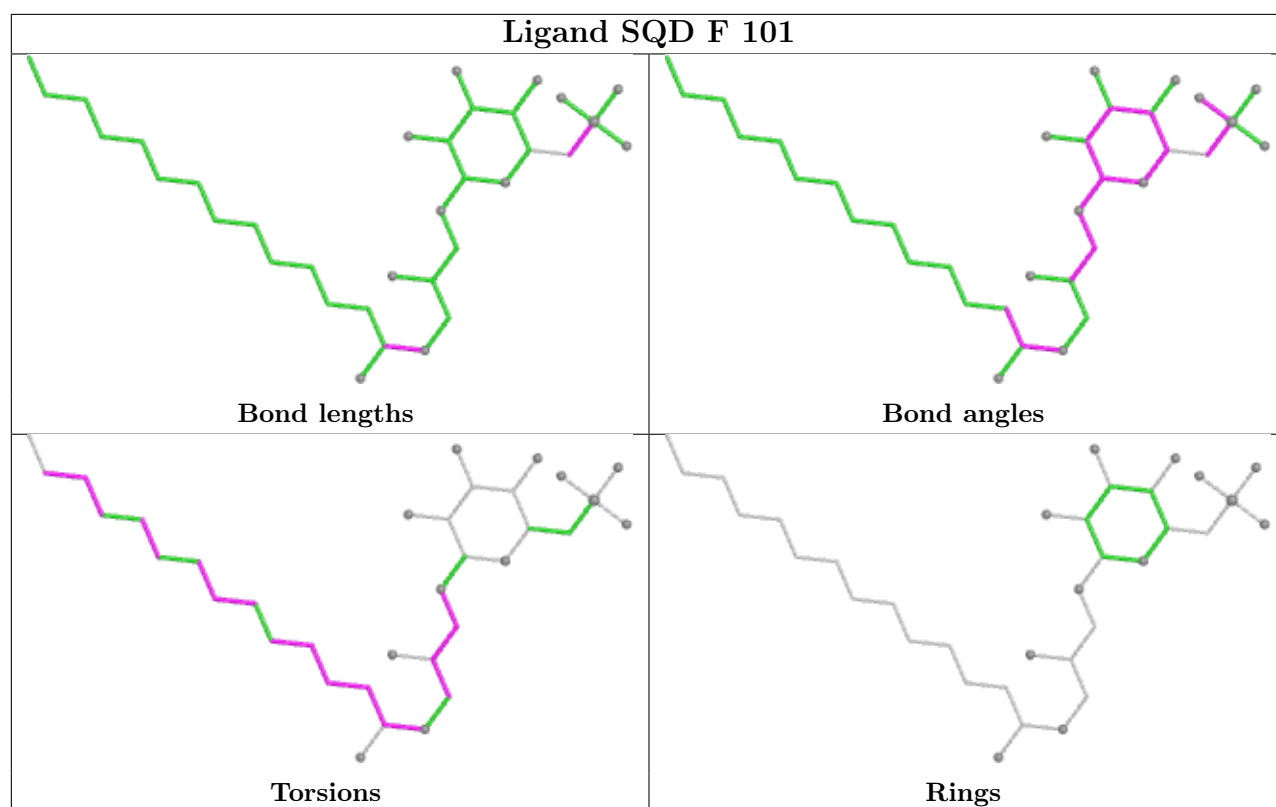


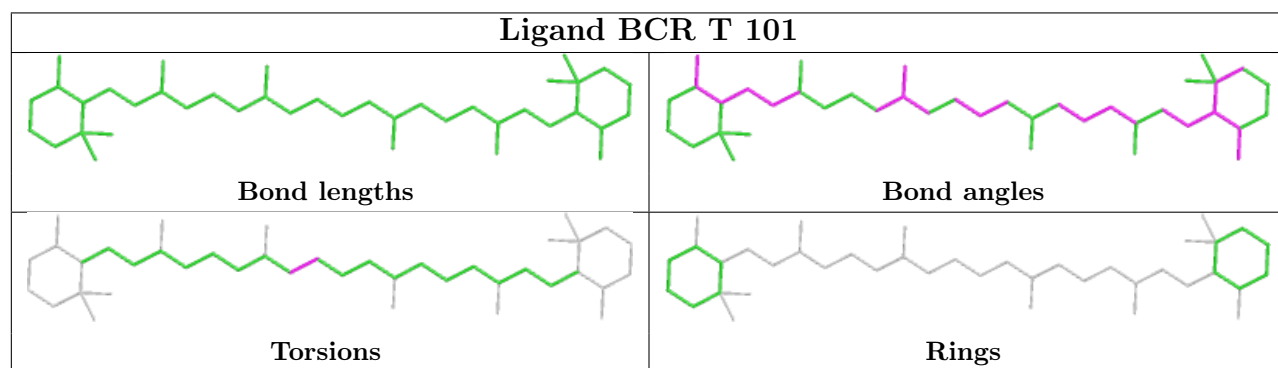
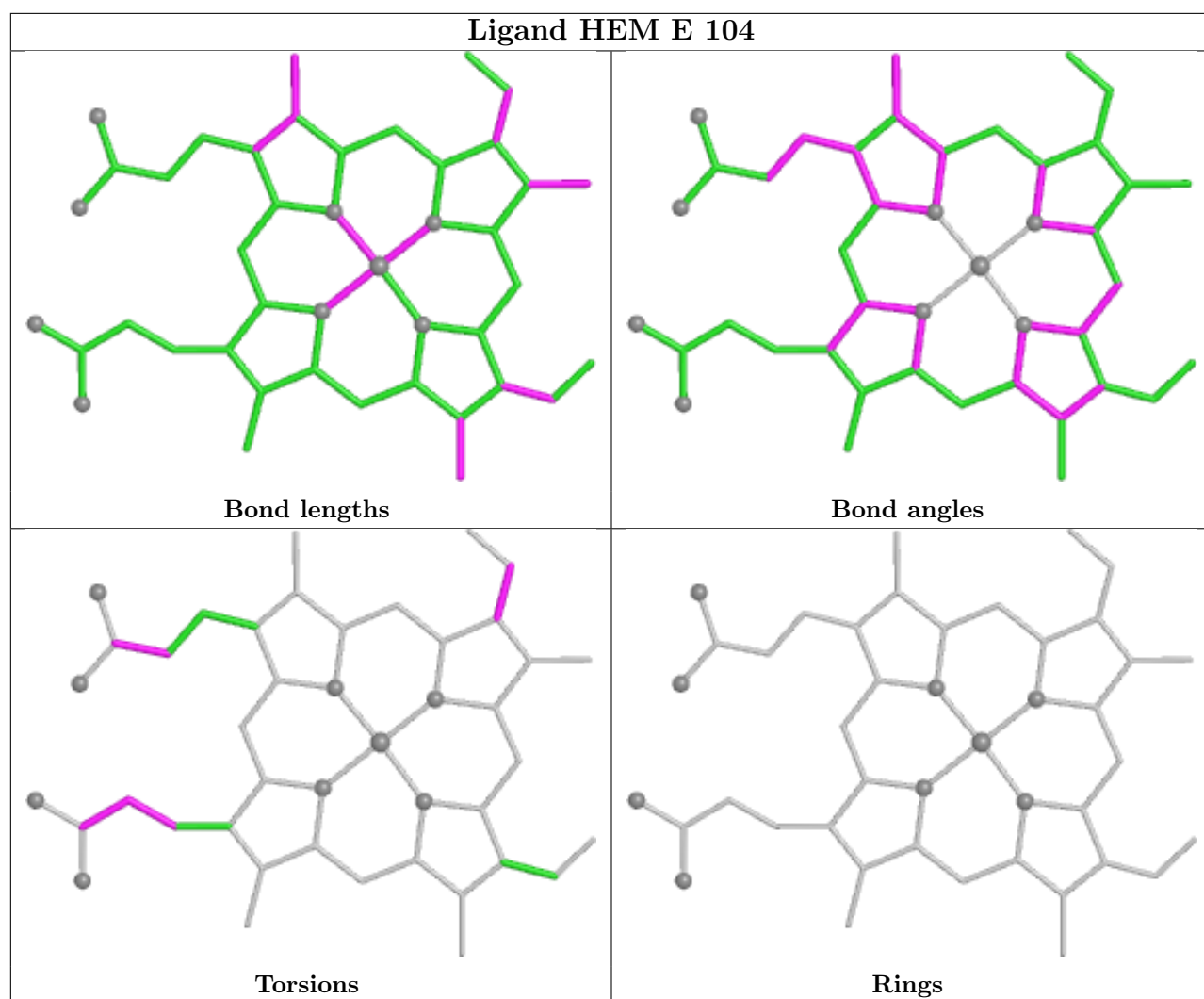
| Ligand CLA B 613                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

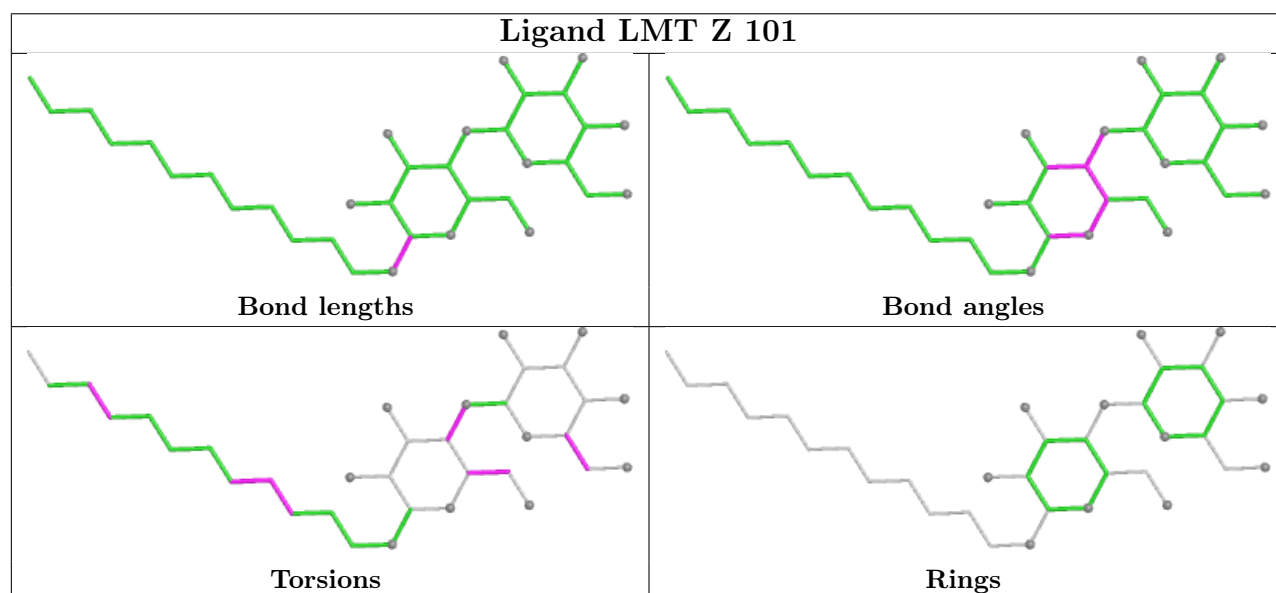
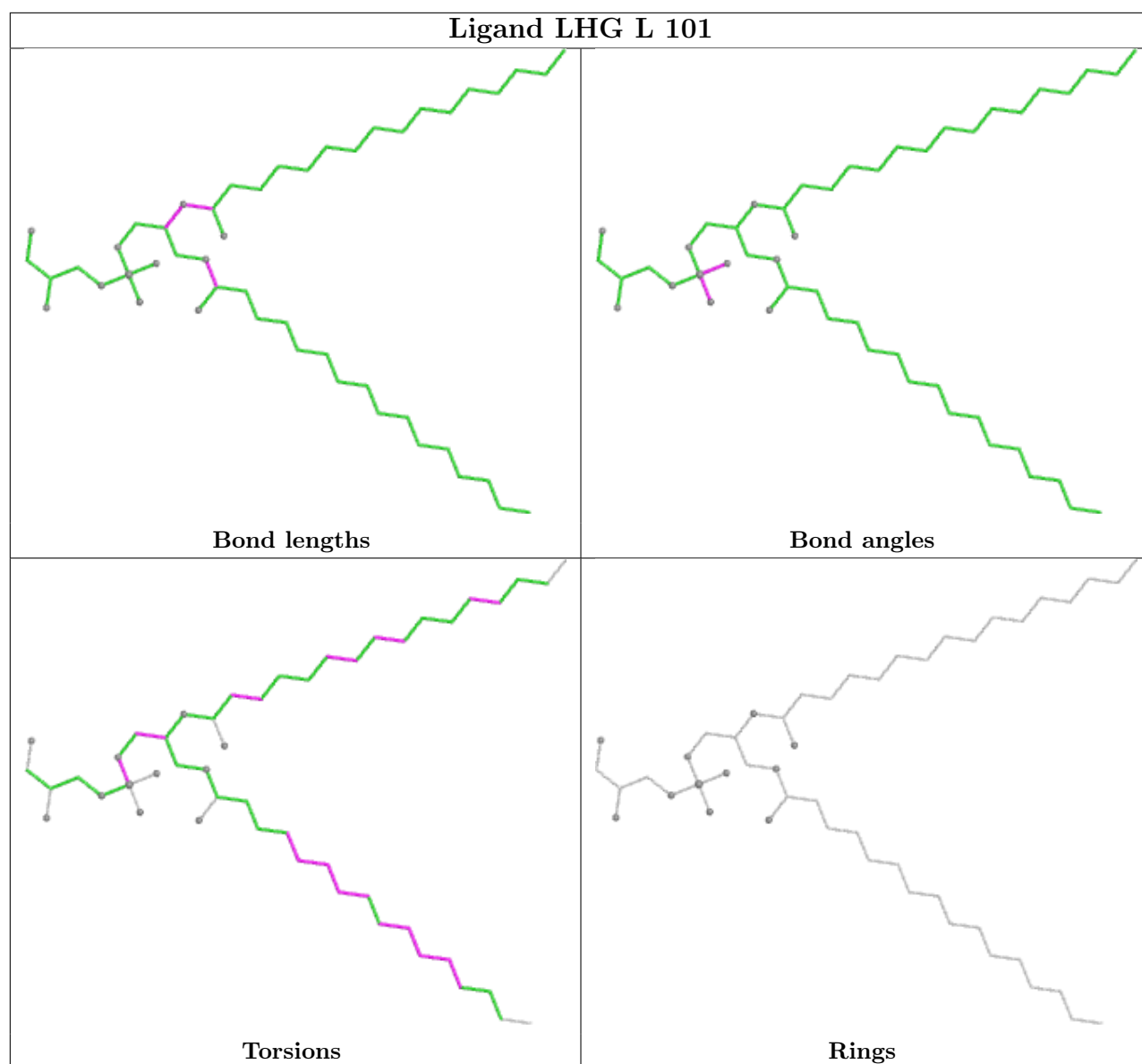
| Ligand CLA c 513                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

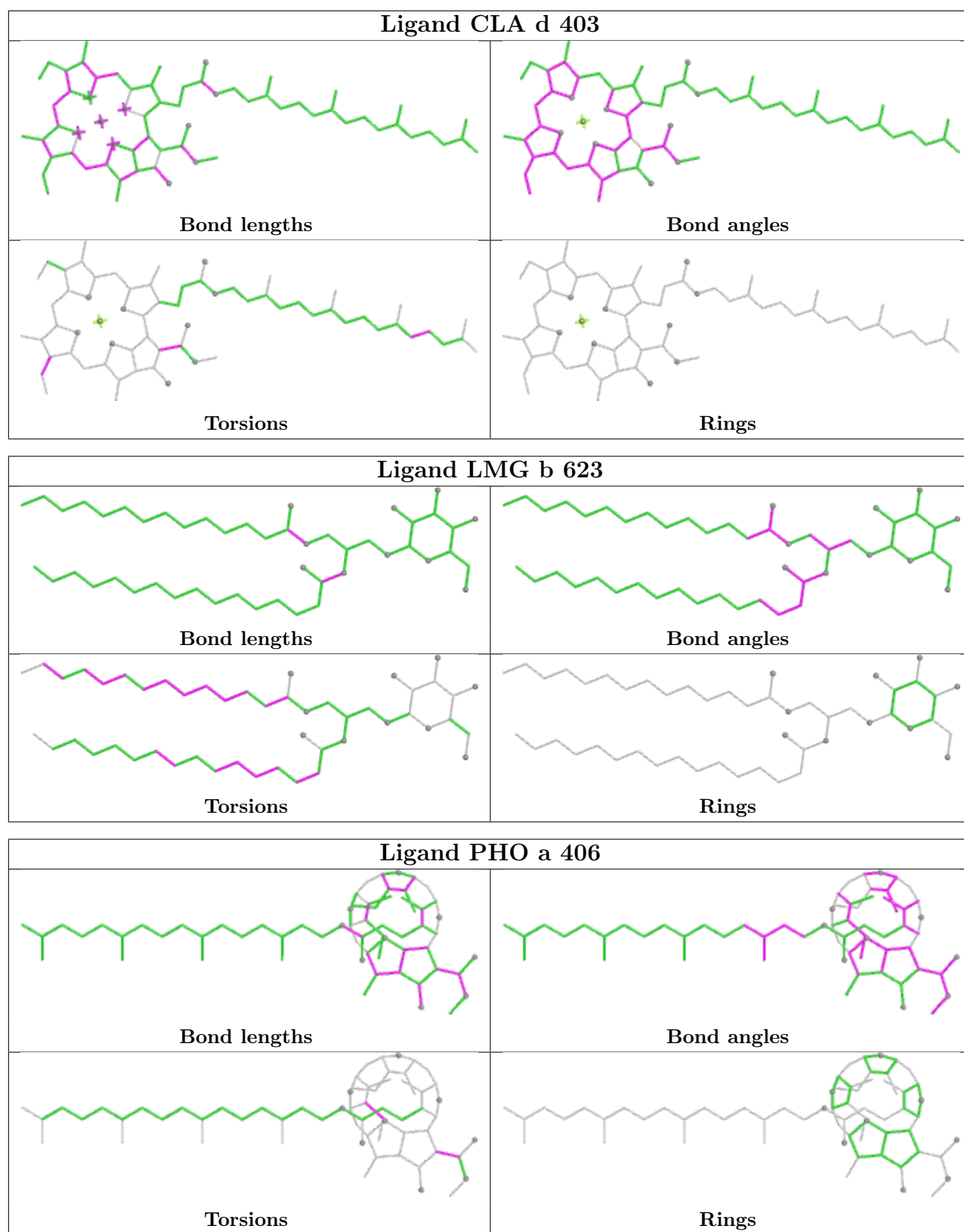
| Ligand PL9 D 412                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |











## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|----------------|--------|---------------|-----------------------|---------|
| 1   | A     | 334/344 (97%)  | -0.66  | 2 (0%) 85 88  | 15, 23, 46, 68        | 3 (0%)  |
| 1   | a     | 334/344 (97%)  | -0.64  | 0 100 100     | 14, 23, 48, 78        | 4 (1%)  |
| 2   | B     | 505/505 (100%) | -0.49  | 10 (1%) 65 68 | 15, 28, 54, 85        | 11 (2%) |
| 2   | b     | 495/505 (98%)  | -0.42  | 13 (2%) 57 61 | 16, 27, 53, 95        | 4 (0%)  |
| 3   | C     | 451/455 (99%)  | -0.31  | 1 (0%) 91 93  | 21, 33, 49, 83        | 1 (0%)  |
| 3   | c     | 455/455 (100%) | -0.34  | 0 100 100     | 22, 33, 46, 79        | 1 (0%)  |
| 4   | D     | 342/342 (100%) | -0.66  | 1 (0%) 90 92  | 17, 24, 44, 90        | 1 (0%)  |
| 4   | d     | 342/342 (100%) | -0.72  | 1 (0%) 90 92  | 18, 25, 42, 86        | 0       |
| 5   | E     | 78/83 (93%)    | 0.44   | 6 (7%) 19 20  | 28, 47, 75, 87        | 1 (1%)  |
| 5   | e     | 78/83 (93%)    | 0.20   | 2 (2%) 57 61  | 29, 43, 63, 81        | 2 (2%)  |
| 6   | F     | 33/44 (75%)    | -0.05  | 2 (6%) 27 29  | 28, 36, 63, 66        | 0       |
| 6   | f     | 32/44 (72%)    | -0.11  | 1 (3%) 51 55  | 28, 34, 72, 90        | 0       |
| 7   | H     | 64/65 (98%)    | 0.07   | 2 (3%) 51 55  | 26, 36, 50, 78        | 1 (1%)  |
| 7   | h     | 62/65 (95%)    | -0.06  | 0 100 100     | 25, 36, 48, 58        | 1 (1%)  |
| 8   | I     | 34/38 (89%)    | -0.05  | 0 100 100     | 29, 36, 60, 78        | 0       |
| 8   | i     | 35/38 (92%)    | -0.14  | 0 100 100     | 29, 34, 47, 85        | 1 (2%)  |
| 9   | J     | 36/40 (90%)    | -0.01  | 1 (2%) 55 58  | 26, 41, 74, 90        | 0       |
| 9   | j     | 40/40 (100%)   | 0.09   | 2 (5%) 34 37  | 27, 39, 56, 65        | 0       |
| 10  | K     | 37/37 (100%)   | -0.22  | 0 100 100     | 33, 40, 52, 59        | 0       |
| 10  | k     | 37/37 (100%)   | -0.06  | 0 100 100     | 32, 40, 56, 64        | 0       |
| 11  | L     | 37/37 (100%)   | -0.65  | 0 100 100     | 12, 22, 65, 81        | 1 (2%)  |
| 11  | l     | 37/37 (100%)   | -0.67  | 0 100 100     | 12, 22, 76, 91        | 1 (2%)  |
| 12  | M     | 33/36 (91%)    | -0.67  | 1 (3%) 52 56  | 15, 25, 39, 57        | 1 (3%)  |
| 12  | m     | 34/36 (94%)    | -0.64  | 0 100 100     | 16, 26, 53, 74        | 1 (2%)  |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 13  | O     | 243/244 (99%)   | -0.26  | 2 (0%) 82 86  | 17, 32, 56, 85        | 6 (2%)  |
| 13  | o     | 243/244 (99%)   | -0.21  | 2 (0%) 82 86  | 17, 35, 67, 89        | 2 (0%)  |
| 14  | T     | 28/32 (87%)     | -0.70  | 0 100 100     | 19, 23, 37, 54        | 1 (3%)  |
| 14  | t     | 29/32 (90%)     | -0.52  | 0 100 100     | 20, 23, 49, 74        | 0       |
| 15  | U     | 97/104 (93%)    | -0.38  | 0 100 100     | 22, 29, 49, 67        | 0       |
| 15  | u     | 97/104 (93%)    | -0.39  | 0 100 100     | 24, 29, 44, 75        | 0       |
| 16  | V     | 137/137 (100%)  | -0.55  | 0 100 100     | 17, 28, 43, 60        | 3 (2%)  |
| 16  | v     | 137/137 (100%)  | -0.18  | 0 100 100     | 25, 36, 53, 74        | 0       |
| 17  | Y     | 29/30 (96%)     | 0.52   | 2 (6%) 23 25  | 41, 51, 72, 79        | 0       |
| 17  | y     | 29/30 (96%)     | 0.30   | 0 100 100     | 41, 50, 66, 70        | 0       |
| 18  | X     | 38/40 (95%)     | 0.38   | 1 (2%) 57 61  | 32, 42, 68, 72        | 0       |
| 18  | x     | 35/40 (87%)     | 0.18   | 1 (2%) 53 57  | 33, 40, 63, 67        | 0       |
| 19  | Z     | 62/62 (100%)    | 0.61   | 4 (6%) 25 27  | 38, 48, 86, 98        | 0       |
| 19  | z     | 61/62 (98%)     | 0.88   | 6 (9%) 13 13  | 45, 54, 86, 96        | 0       |
| All | All   | 5230/5350 (97%) | -0.36  | 63 (1%) 76 80 | 12, 30, 57, 98        | 47 (0%) |

The worst 5 of 63 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | b     | 496 | TYR  | 5.1  |
| 7   | H     | 65  | LEU  | 4.9  |
| 2   | b     | 495 | PHE  | 4.3  |
| 2   | b     | 499 | VAL  | 4.3  |
| 2   | b     | 502 | VAL  | 3.9  |

## 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 | 0.96 | 0.06 | 23,27,49,50                | 0     |
| 14  | FME  | T     | 1   | 10/11 | 0.97 | 0.06 | 23,29,48,51                | 0     |
| 8   | FME  | i     | 1   | 10/11 | 0.98 | 0.06 | 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 | 0.05 | 26,32,36,37                 | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 26  | UNL  | b     | 642 | 13/-  | 0.59 | 0.14 | 71,80,87,90                 | 0     |
| 35  | DGD  | D     | 406 | 51/66 | 0.62 | 0.16 | 57,74,100,108               | 0     |
| 26  | UNL  | B     | 646 | 16/-  | 0.64 | 0.14 | 85,89,93,94                 | 0     |
| 28  | DMS  | j     | 105 | 4/4   | 0.66 | 0.18 | 70,74,75,88                 | 0     |
| 26  | UNL  | B     | 629 | 10/-  | 0.66 | 0.15 | 54,69,74,74                 | 0     |
| 28  | DMS  | O     | 308 | 4/4   | 0.67 | 0.17 | 66,74,76,87                 | 0     |
| 26  | UNL  | Z     | 102 | 4/-   | 0.67 | 0.20 | 59,61,62,63                 | 0     |
| 32  | HTG  | C     | 534 | 19/19 | 0.67 | 0.14 | 68,110,128,130              | 0     |
| 26  | UNL  | b     | 643 | 9/-   | 0.67 | 0.12 | 67,67,74,74                 | 0     |
| 28  | DMS  | b     | 638 | 4/4   | 0.68 | 0.20 | 67,75,77,86                 | 0     |
| 28  | DMS  | o     | 306 | 4/4   | 0.68 | 0.19 | 55,58,65,77                 | 0     |
| 34  | LMT  | f     | 102 | 24/35 | 0.69 | 0.15 | 62,77,94,98                 | 0     |
| 28  | DMS  | U     | 904 | 4/4   | 0.69 | 0.18 | 58,66,66,83                 | 0     |
| 28  | DMS  | O     | 305 | 4/4   | 0.70 | 0.22 | 64,66,77,86                 | 0     |
| 32  | HTG  | D     | 417 | 19/19 | 0.70 | 0.15 | 67,105,119,120              | 0     |
| 28  | DMS  | B     | 636 | 4/4   | 0.71 | 0.17 | 77,86,90,96                 | 0     |
| 28  | DMS  | O     | 309 | 4/4   | 0.71 | 0.23 | 58,65,72,73                 | 0     |
| 35  | DGD  | d     | 416 | 51/66 | 0.71 | 0.14 | 56,75,96,103                | 0     |
| 28  | DMS  | H     | 103 | 4/4   | 0.72 | 0.21 | 84,101,109,112              | 0     |
| 26  | UNL  | B     | 647 | 13/-  | 0.72 | 0.13 | 71,81,90,91                 | 0     |
| 28  | DMS  | b     | 640 | 4/4   | 0.72 | 0.18 | 49,58,71,73                 | 0     |
| 26  | UNL  | A     | 413 | 4/-   | 0.72 | 0.13 | 64,64,64,66                 | 0     |
| 26  | UNL  | a     | 402 | 6/-   | 0.72 | 0.14 | 50,57,62,63                 | 0     |
| 32  | HTG  | v     | 210 | 14/19 | 0.73 | 0.16 | 60,80,92,100                | 0     |
| 26  | UNL  | T     | 103 | 13/-  | 0.73 | 0.13 | 64,68,72,72                 | 0     |
| 26  | UNL  | a     | 414 | 28/-  | 0.73 | 0.14 | 59,68,84,87                 | 0     |
| 32  | HTG  | c     | 521 | 19/19 | 0.73 | 0.14 | 57,85,102,105               | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 26  | UNL  | b     | 645 | 6/-   | 0.74 | 0.16 | 57,65,76,76                 | 0     |
| 26  | UNL  | h     | 103 | 16/-  | 0.74 | 0.14 | 61,69,73,76                 | 0     |
| 32  | HTG  | c     | 520 | 19/19 | 0.74 | 0.15 | 77,88,99,100                | 0     |
| 26  | UNL  | A     | 410 | 36/-  | 0.74 | 0.15 | 57,78,84,91                 | 0     |
| 26  | UNL  | c     | 526 | 8/-   | 0.75 | 0.17 | 54,59,64,65                 | 0     |
| 28  | DMS  | D     | 415 | 4/4   | 0.75 | 0.23 | 57,58,63,65                 | 0     |
| 34  | LMT  | I     | 101 | 35/35 | 0.75 | 0.13 | 67,82,91,92                 | 0     |
| 28  | DMS  | O     | 310 | 4/4   | 0.76 | 0.19 | 76,78,82,94                 | 0     |
| 26  | UNL  | E     | 102 | 15/-  | 0.76 | 0.17 | 55,62,76,77                 | 0     |
| 28  | DMS  | o     | 308 | 4/4   | 0.76 | 0.19 | 60,61,62,63                 | 0     |
| 34  | LMT  | b     | 627 | 32/35 | 0.77 | 0.14 | 42,67,84,87                 | 0     |
| 26  | UNL  | J     | 107 | 3/-   | 0.77 | 0.12 | 61,61,63,64                 | 0     |
| 32  | HTG  | b     | 602 | 19/19 | 0.77 | 0.13 | 51,103,117,118              | 0     |
| 28  | DMS  | b     | 641 | 4/4   | 0.77 | 0.20 | 63,65,75,80                 | 0     |
| 36  | LHG  | E     | 103 | 48/49 | 0.77 | 0.15 | 44,99,108,119               | 0     |
| 34  | LMT  | E     | 101 | 24/35 | 0.78 | 0.12 | 64,78,84,90                 | 0     |
| 26  | UNL  | I     | 105 | 10/-  | 0.78 | 0.10 | 60,66,71,72                 | 0     |
| 26  | UNL  | I     | 106 | 11/-  | 0.78 | 0.17 | 61,73,81,81                 | 0     |
| 26  | UNL  | B     | 633 | 16/-  | 0.78 | 0.16 | 53,61,69,70                 | 0     |
| 26  | UNL  | I     | 104 | 11/-  | 0.78 | 0.13 | 53,56,59,62                 | 0     |
| 32  | HTG  | u     | 201 | 8/19  | 0.78 | 0.17 | 45,52,69,89                 | 0     |
| 26  | UNL  | j     | 104 | 16/-  | 0.78 | 0.14 | 49,58,64,66                 | 0     |
| 32  | HTG  | B     | 623 | 19/19 | 0.79 | 0.12 | 53,88,93,94                 | 0     |
| 26  | UNL  | J     | 104 | 14/-  | 0.79 | 0.13 | 67,77,80,81                 | 0     |
| 26  | UNL  | I     | 103 | 13/-  | 0.79 | 0.14 | 47,53,84,87                 | 0     |
| 26  | UNL  | H     | 104 | 4/-   | 0.79 | 0.14 | 60,62,65,67                 | 0     |
| 34  | LMT  | c     | 523 | 35/35 | 0.79 | 0.12 | 67,77,83,85                 | 0     |
| 26  | UNL  | t     | 102 | 16/-  | 0.79 | 0.12 | 61,71,80,80                 | 0     |
| 26  | UNL  | c     | 524 | 30/-  | 0.79 | 0.14 | 59,74,86,87                 | 0     |
| 32  | HTG  | d     | 401 | 19/19 | 0.79 | 0.14 | 58,99,111,120               | 0     |
| 26  | UNL  | c     | 525 | 10/-  | 0.79 | 0.13 | 58,65,66,67                 | 0     |
| 26  | UNL  | U     | 901 | 14/-  | 0.80 | 0.15 | 40,49,59,59                 | 0     |
| 28  | DMS  | B     | 638 | 4/4   | 0.80 | 0.18 | 53,61,63,68                 | 0     |
| 26  | UNL  | C     | 523 | 34/-  | 0.80 | 0.12 | 59,80,92,101                | 0     |
| 26  | UNL  | b     | 644 | 7/-   | 0.80 | 0.11 | 64,65,70,70                 | 0     |
| 26  | UNL  | H     | 105 | 6/-   | 0.80 | 0.13 | 51,55,63,65                 | 0     |
| 34  | LMT  | a     | 418 | 35/35 | 0.80 | 0.13 | 45,69,78,81                 | 0     |
| 26  | UNL  | j     | 106 | 6/-   | 0.80 | 0.16 | 52,55,58,59                 | 0     |
| 23  | SQD  | f     | 101 | 40/54 | 0.80 | 0.14 | 57,86,102,107               | 0     |
| 27  | PL9  | A     | 411 | 55/55 | 0.80 | 0.15 | 43,67,89,92                 | 0     |
| 34  | LMT  | m     | 101 | 35/35 | 0.80 | 0.13 | 48,94,110,114               | 0     |
| 27  | PL9  | a     | 415 | 55/55 | 0.80 | 0.16 | 52,67,89,94                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 28  | DMS  | b     | 637 | 4/4   | 0.80 | 0.17 | 77,79,84,93                 | 0     |
| 28  | DMS  | A     | 418 | 4/4   | 0.80 | 0.21 | 68,74,80,85                 | 0     |
| 34  | LMT  | b     | 628 | 25/35 | 0.81 | 0.12 | 54,79,95,96                 | 0     |
| 28  | DMS  | u     | 204 | 4/4   | 0.81 | 0.18 | 71,78,83,86                 | 0     |
| 28  | DMS  | B     | 642 | 4/4   | 0.81 | 0.22 | 43,51,68,71                 | 0     |
| 32  | HTG  | B     | 632 | 19/19 | 0.81 | 0.12 | 51,97,108,114               | 0     |
| 34  | LMT  | z     | 102 | 35/35 | 0.81 | 0.12 | 46,85,99,101                | 0     |
| 34  | LMT  | Z     | 101 | 35/35 | 0.81 | 0.14 | 44,90,107,109               | 0     |
| 24  | LMG  | C     | 524 | 45/55 | 0.81 | 0.20 | 22,46,51,56                 | 45    |
| 26  | UNL  | b     | 630 | 11/-  | 0.81 | 0.13 | 55,60,67,68                 | 0     |
| 28  | DMS  | d     | 415 | 4/4   | 0.82 | 0.17 | 68,71,71,72                 | 0     |
| 28  | DMS  | O     | 306 | 4/4   | 0.82 | 0.18 | 66,73,73,75                 | 0     |
| 32  | HTG  | C     | 521 | 19/19 | 0.82 | 0.12 | 46,78,89,90                 | 0     |
| 28  | DMS  | V     | 205 | 4/4   | 0.82 | 0.15 | 67,76,77,79                 | 0     |
| 28  | DMS  | B     | 639 | 4/4   | 0.82 | 0.18 | 65,70,71,76                 | 0     |
| 28  | DMS  | c     | 533 | 4/4   | 0.82 | 0.16 | 73,75,77,87                 | 0     |
| 26  | UNL  | M     | 102 | 12/-  | 0.83 | 0.13 | 49,53,95,98                 | 0     |
| 26  | UNL  | B     | 630 | 14/-  | 0.83 | 0.12 | 67,74,83,84                 | 0     |
| 26  | UNL  | a     | 416 | 11/-  | 0.83 | 0.14 | 66,68,76,78                 | 0     |
| 34  | LMT  | J     | 103 | 24/35 | 0.83 | 0.12 | 53,61,81,85                 | 0     |
| 26  | UNL  | x     | 102 | 9/-   | 0.83 | 0.14 | 56,68,72,72                 | 0     |
| 26  | UNL  | L     | 102 | 14/-  | 0.84 | 0.15 | 56,60,84,84                 | 0     |
| 24  | LMG  | c     | 518 | 51/55 | 0.84 | 0.11 | 37,72,84,87                 | 0     |
| 23  | SQD  | l     | 101 | 54/54 | 0.84 | 0.13 | 47,68,101,106               | 0     |
| 28  | DMS  | b     | 636 | 4/4   | 0.84 | 0.18 | 66,71,72,79                 | 0     |
| 26  | UNL  | d     | 409 | 36/-  | 0.84 | 0.12 | 36,60,91,102                | 0     |
| 28  | DMS  | v     | 207 | 4/4   | 0.84 | 0.15 | 53,66,72,87                 | 0     |
| 23  | SQD  | b     | 622 | 54/54 | 0.84 | 0.12 | 46,63,95,100                | 0     |
| 34  | LMT  | B     | 627 | 16/35 | 0.84 | 0.12 | 52,60,78,78                 | 0     |
| 26  | UNL  | i     | 101 | 16/-  | 0.84 | 0.12 | 41,45,65,65                 | 0     |
| 26  | UNL  | i     | 103 | 11/-  | 0.84 | 0.11 | 58,61,65,66                 | 0     |
| 26  | UNL  | b     | 629 | 16/-  | 0.84 | 0.13 | 41,48,60,60                 | 0     |
| 28  | DMS  | C     | 532 | 4/4   | 0.85 | 0.17 | 33,40,41,48                 | 0     |
| 32  | HTG  | C     | 520 | 19/19 | 0.85 | 0.11 | 64,70,76,79                 | 0     |
| 28  | DMS  | O     | 311 | 4/4   | 0.85 | 0.16 | 57,65,69,72                 | 0     |
| 32  | HTG  | C     | 522 | 19/19 | 0.85 | 0.11 | 66,83,104,107               | 0     |
| 28  | DMS  | c     | 534 | 4/4   | 0.85 | 0.14 | 70,71,75,81                 | 0     |
| 23  | SQD  | F     | 101 | 35/54 | 0.85 | 0.13 | 51,76,89,90                 | 0     |
| 26  | UNL  | e     | 101 | 7/-   | 0.85 | 0.12 | 54,58,64,65                 | 0     |
| 32  | HTG  | b     | 624 | 19/19 | 0.85 | 0.12 | 49,74,80,85                 | 0     |
| 28  | DMS  | b     | 634 | 4/4   | 0.85 | 0.16 | 59,67,67,75                 | 0     |
| 28  | DMS  | A     | 417 | 4/4   | 0.85 | 0.16 | 70,72,77,81                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 26  | UNL  | J     | 105 | 12/-  | 0.85 | 0.13 | 63,67,71,71                 | 0     |
| 28  | DMS  | v     | 203 | 4/4   | 0.85 | 0.18 | 67,69,76,79                 | 0     |
| 28  | DMS  | B     | 644 | 4/4   | 0.85 | 0.16 | 52,53,61,69                 | 0     |
| 28  | DMS  | C     | 527 | 4/4   | 0.85 | 0.17 | 73,76,79,87                 | 0     |
| 26  | UNL  | z     | 101 | 6/-   | 0.86 | 0.10 | 49,55,55,57                 | 0     |
| 28  | DMS  | C     | 533 | 4/4   | 0.86 | 0.13 | 72,73,73,74                 | 0     |
| 23  | SQD  | a     | 401 | 54/54 | 0.86 | 0.11 | 39,58,82,86                 | 0     |
| 28  | DMS  | v     | 204 | 4/4   | 0.86 | 0.17 | 48,54,57,69                 | 0     |
| 28  | DMS  | U     | 902 | 4/4   | 0.86 | 0.18 | 35,44,49,58                 | 0     |
| 28  | DMS  | c     | 532 | 4/4   | 0.86 | 0.18 | 65,70,76,77                 | 0     |
| 23  | SQD  | A     | 412 | 54/54 | 0.86 | 0.11 | 41,60,78,81                 | 0     |
| 26  | UNL  | B     | 628 | 15/-  | 0.86 | 0.12 | 45,50,60,66                 | 0     |
| 34  | LMT  | B     | 625 | 24/35 | 0.86 | 0.10 | 48,67,86,89                 | 0     |
| 28  | DMS  | V     | 208 | 4/4   | 0.86 | 0.18 | 75,77,82,85                 | 0     |
| 26  | UNL  | D     | 410 | 37/-  | 0.86 | 0.11 | 42,57,93,98                 | 0     |
| 28  | DMS  | B     | 635 | 4/4   | 0.86 | 0.17 | 90,94,95,96                 | 0     |
| 32  | HTG  | B     | 622 | 19/19 | 0.87 | 0.14 | 28,46,54,54                 | 0     |
| 32  | HTG  | b     | 625 | 19/19 | 0.87 | 0.14 | 30,44,66,70                 | 0     |
| 28  | DMS  | B     | 640 | 4/4   | 0.87 | 0.23 | 45,48,49,50                 | 0     |
| 26  | UNL  | b     | 646 | 6/-   | 0.87 | 0.12 | 54,58,60,62                 | 0     |
| 28  | DMS  | u     | 203 | 4/4   | 0.87 | 0.20 | 47,55,56,65                 | 0     |
| 28  | DMS  | c     | 535 | 4/4   | 0.87 | 0.14 | 58,59,65,68                 | 0     |
| 28  | DMS  | O     | 304 | 4/4   | 0.87 | 0.15 | 63,68,72,73                 | 0     |
| 26  | UNL  | D     | 411 | 16/-  | 0.87 | 0.11 | 39,45,58,62                 | 0     |
| 34  | LMT  | m     | 102 | 35/35 | 0.87 | 0.10 | 34,53,58,59                 | 0     |
| 34  | LMT  | B     | 626 | 24/35 | 0.87 | 0.11 | 37,54,86,95                 | 0     |
| 28  | DMS  | o     | 303 | 4/4   | 0.87 | 0.15 | 66,69,75,79                 | 0     |
| 32  | HTG  | V     | 202 | 13/19 | 0.87 | 0.10 | 45,49,70,82                 | 0     |
| 28  | DMS  | v     | 208 | 4/4   | 0.87 | 0.17 | 89,92,92,95                 | 0     |
| 34  | LMT  | T     | 102 | 24/35 | 0.88 | 0.12 | 36,53,78,85                 | 0     |
| 28  | DMS  | o     | 305 | 4/4   | 0.88 | 0.14 | 73,75,77,87                 | 0     |
| 28  | DMS  | C     | 529 | 4/4   | 0.88 | 0.15 | 70,73,74,74                 | 0     |
| 28  | DMS  | C     | 531 | 4/4   | 0.88 | 0.17 | 53,54,58,74                 | 0     |
| 24  | LMG  | a     | 410 | 51/55 | 0.88 | 0.09 | 44,55,65,67                 | 0     |
| 28  | DMS  | B     | 643 | 4/4   | 0.88 | 0.13 | 51,53,62,71                 | 0     |
| 28  | DMS  | A     | 415 | 4/4   | 0.88 | 0.15 | 55,58,65,71                 | 0     |
| 28  | DMS  | D     | 416 | 4/4   | 0.88 | 0.14 | 83,87,89,91                 | 0     |
| 26  | UNL  | I     | 102 | 16/-  | 0.88 | 0.11 | 38,47,63,64                 | 0     |
| 28  | DMS  | O     | 303 | 4/4   | 0.88 | 0.14 | 63,72,77,78                 | 0     |
| 28  | DMS  | v     | 209 | 4/4   | 0.88 | 0.13 | 71,78,79,79                 | 0     |
| 28  | DMS  | o     | 304 | 4/4   | 0.88 | 0.15 | 68,79,82,83                 | 0     |
| 34  | LMT  | M     | 101 | 35/35 | 0.88 | 0.10 | 34,53,63,64                 | 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/-  | 0.89 | 0.10 | 48,54,64,65                 | 0     |
| 26  | UNL  | d     | 411    | 16/-  | 0.89 | 0.09 | 33,42,55,55                 | 0     |
| 26  | UNL  | J     | 106    | 4/-   | 0.89 | 0.12 | 57,60,61,67                 | 0     |
| 24  | LMG  | B     | 620    | 51/55 | 0.89 | 0.09 | 33,43,55,58                 | 0     |
| 28  | DMS  | v     | 205    | 4/4   | 0.89 | 0.12 | 67,70,72,73                 | 0     |
| 26  | UNL  | X     | 101    | 16/-  | 0.89 | 0.11 | 37,40,59,59                 | 0     |
| 28  | DMS  | C     | 525[A] | 4/4   | 0.89 | 0.17 | 48,49,51,57                 | 4     |
| 28  | DMS  | V     | 209    | 4/4   | 0.89 | 0.14 | 57,73,77,81                 | 0     |
| 28  | DMS  | C     | 525[B] | 4/4   | 0.89 | 0.17 | 32,33,35,35                 | 4     |
| 24  | LMG  | c     | 519    | 51/55 | 0.90 | 0.11 | 29,59,86,88                 | 0     |
| 28  | DMS  | O     | 307    | 4/4   | 0.90 | 0.15 | 69,76,77,88                 | 0     |
| 24  | LMG  | C     | 519    | 51/55 | 0.90 | 0.11 | 31,67,83,84                 | 0     |
| 28  | DMS  | B     | 645    | 4/4   | 0.90 | 0.13 | 56,59,64,71                 | 0     |
| 20  | CLA  | C     | 513    | 65/65 | 0.90 | 0.09 | 40,48,72,77                 | 0     |
| 28  | DMS  | A     | 416    | 4/4   | 0.90 | 0.12 | 59,60,69,77                 | 0     |
| 24  | LMG  | A     | 407    | 51/55 | 0.90 | 0.09 | 40,55,70,78                 | 0     |
| 28  | DMS  | U     | 903[A] | 4/4   | 0.90 | 0.16 | 32,34,40,41                 | 4     |
| 28  | DMS  | U     | 903[B] | 4/4   | 0.90 | 0.16 | 26,28,29,32                 | 4     |
| 28  | DMS  | B     | 641    | 4/4   | 0.90 | 0.12 | 68,69,75,80                 | 0     |
| 28  | DMS  | V     | 204    | 4/4   | 0.90 | 0.12 | 58,64,64,72                 | 0     |
| 20  | CLA  | C     | 506    | 65/65 | 0.90 | 0.09 | 32,45,86,87                 | 0     |
| 28  | DMS  | c     | 536    | 4/4   | 0.90 | 0.18 | 33,33,45,46                 | 0     |
| 28  | DMS  | V     | 207    | 4/4   | 0.91 | 0.14 | 62,63,63,70                 | 0     |
| 20  | CLA  | b     | 603    | 65/65 | 0.91 | 0.10 | 30,45,75,82                 | 0     |
| 24  | LMG  | b     | 623    | 49/55 | 0.91 | 0.09 | 33,42,54,61                 | 0     |
| 33  | CA   | V     | 203    | 1/1   | 0.91 | 0.10 | 63,63,63,63                 | 0     |
| 28  | DMS  | v     | 206    | 4/4   | 0.91 | 0.13 | 52,53,61,66                 | 0     |
| 28  | DMS  | u     | 202    | 4/4   | 0.91 | 0.18 | 40,46,52,54                 | 0     |
| 28  | DMS  | b     | 639    | 4/4   | 0.91 | 0.13 | 46,49,49,50                 | 0     |
| 23  | SQD  | A     | 406    | 54/54 | 0.91 | 0.10 | 34,59,71,76                 | 0     |
| 28  | DMS  | o     | 307    | 4/4   | 0.92 | 0.13 | 53,58,63,65                 | 0     |
| 22  | BCR  | C     | 514    | 40/40 | 0.92 | 0.07 | 36,45,49,50                 | 0     |
| 28  | DMS  | V     | 206    | 4/4   | 0.92 | 0.12 | 59,61,63,65                 | 0     |
| 26  | UNL  | d     | 410    | 16/-  | 0.92 | 0.10 | 33,45,63,63                 | 0     |
| 28  | DMS  | d     | 413    | 4/4   | 0.92 | 0.14 | 47,53,55,57                 | 0     |
| 28  | DMS  | d     | 414    | 4/4   | 0.92 | 0.17 | 57,62,64,68                 | 0     |
| 20  | CLA  | B     | 602    | 65/65 | 0.92 | 0.10 | 29,42,77,81                 | 0     |
| 28  | DMS  | B     | 637    | 4/4   | 0.92 | 0.14 | 53,53,54,60                 | 0     |
| 28  | DMS  | b     | 632    | 4/4   | 0.92 | 0.12 | 55,58,66,70                 | 0     |
| 32  | HTG  | b     | 601    | 19/19 | 0.92 | 0.09 | 45,61,67,80                 | 0     |
| 28  | DMS  | c     | 529    | 4/4   | 0.92 | 0.11 | 79,82,86,87                 | 0     |
| 28  | DMS  | C     | 530    | 4/4   | 0.92 | 0.17 | 44,44,46,50                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 28  | DMS  | b     | 635 | 4/4   | 0.92 | 0.12 | 58,62,69,73                 | 0     |
| 28  | DMS  | h     | 102 | 4/4   | 0.93 | 0.15 | 50,51,53,62                 | 0     |
| 33  | CA   | o     | 301 | 1/1   | 0.93 | 0.06 | 48,48,48,48                 | 0     |
| 28  | DMS  | i     | 104 | 4/4   | 0.93 | 0.11 | 63,66,67,71                 | 0     |
| 28  | DMS  | C     | 526 | 4/4   | 0.93 | 0.13 | 59,60,63,65                 | 0     |
| 32  | HTG  | B     | 631 | 19/19 | 0.93 | 0.08 | 41,57,69,73                 | 0     |
| 20  | CLA  | C     | 512 | 55/65 | 0.93 | 0.07 | 37,44,49,54                 | 0     |
| 28  | DMS  | D     | 413 | 4/4   | 0.93 | 0.11 | 50,56,60,61                 | 0     |
| 22  | BCR  | K     | 101 | 40/40 | 0.93 | 0.07 | 33,37,42,45                 | 0     |
| 22  | BCR  | k     | 102 | 40/40 | 0.93 | 0.07 | 41,46,51,51                 | 0     |
| 28  | DMS  | c     | 530 | 4/4   | 0.93 | 0.20 | 36,43,45,49                 | 0     |
| 35  | DGD  | h     | 101 | 62/66 | 0.93 | 0.08 | 25,34,41,49                 | 0     |
| 20  | CLA  | b     | 618 | 65/65 | 0.93 | 0.09 | 23,33,92,98                 | 0     |
| 22  | BCR  | D     | 405 | 40/40 | 0.94 | 0.07 | 26,30,58,60                 | 0     |
| 20  | CLA  | c     | 513 | 65/65 | 0.94 | 0.08 | 36,46,81,87                 | 0     |
| 31  | BCT  | A     | 421 | 4/4   | 0.94 | 0.07 | 31,34,40,44                 | 0     |
| 31  | BCT  | a     | 413 | 4/4   | 0.94 | 0.07 | 32,32,38,42                 | 0     |
| 32  | HTG  | B     | 621 | 19/19 | 0.94 | 0.08 | 36,41,48,52                 | 0     |
| 22  | BCR  | K     | 102 | 40/40 | 0.94 | 0.07 | 31,36,40,41                 | 0     |
| 22  | BCR  | d     | 405 | 40/40 | 0.94 | 0.07 | 24,30,56,58                 | 0     |
| 28  | DMS  | F     | 102 | 4/4   | 0.94 | 0.12 | 51,52,56,64                 | 0     |
| 23  | SQD  | a     | 409 | 54/54 | 0.94 | 0.09 | 33,56,75,78                 | 0     |
| 22  | BCR  | k     | 101 | 40/40 | 0.94 | 0.07 | 28,36,41,42                 | 0     |
| 28  | DMS  | c     | 528 | 4/4   | 0.94 | 0.13 | 58,62,63,65                 | 0     |
| 20  | CLA  | c     | 506 | 65/65 | 0.94 | 0.07 | 24,39,71,74                 | 0     |
| 28  | DMS  | b     | 633 | 4/4   | 0.94 | 0.12 | 45,48,49,53                 | 0     |
| 35  | DGD  | H     | 102 | 62/66 | 0.94 | 0.08 | 25,33,40,43                 | 0     |
| 28  | DMS  | c     | 531 | 4/4   | 0.94 | 0.11 | 73,78,85,86                 | 0     |
| 32  | HTG  | O     | 302 | 19/19 | 0.94 | 0.08 | 34,42,50,53                 | 0     |
| 36  | LHG  | D     | 407 | 49/49 | 0.94 | 0.07 | 28,37,44,52                 | 0     |
| 36  | LHG  | D     | 409 | 49/49 | 0.94 | 0.10 | 27,33,81,83                 | 0     |
| 22  | BCR  | t     | 101 | 40/40 | 0.94 | 0.06 | 22,29,41,43                 | 0     |
| 38  | RRX  | H     | 101 | 41/41 | 0.94 | 0.07 | 27,31,41,46                 | 0     |
| 38  | RRX  | x     | 101 | 41/41 | 0.94 | 0.07 | 26,32,47,58                 | 0     |
| 20  | CLA  | C     | 505 | 65/65 | 0.95 | 0.06 | 28,33,44,48                 | 0     |
| 20  | CLA  | B     | 601 | 65/65 | 0.95 | 0.08 | 23,29,82,86                 | 0     |
| 20  | CLA  | c     | 511 | 65/65 | 0.95 | 0.06 | 27,33,40,43                 | 0     |
| 20  | CLA  | c     | 512 | 65/65 | 0.95 | 0.07 | 28,41,70,72                 | 0     |
| 28  | DMS  | D     | 414 | 4/4   | 0.95 | 0.12 | 55,56,57,58                 | 0     |
| 20  | CLA  | C     | 507 | 65/65 | 0.95 | 0.07 | 28,37,52,57                 | 0     |
| 35  | DGD  | C     | 517 | 55/66 | 0.95 | 0.06 | 26,34,59,62                 | 0     |
| 24  | LMG  | j     | 101 | 45/55 | 0.95 | 0.07 | 27,32,60,64                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 20  | CLA  | C     | 508 | 60/65 | 0.95 | 0.06 | 23,31,47,51                 | 0     |
| 35  | DGD  | c     | 517 | 62/66 | 0.95 | 0.07 | 23,30,56,71                 | 0     |
| 22  | BCR  | C     | 515 | 40/40 | 0.95 | 0.06 | 31,37,43,45                 | 0     |
| 20  | CLA  | C     | 511 | 65/65 | 0.95 | 0.07 | 30,37,42,45                 | 0     |
| 20  | CLA  | B     | 610 | 65/65 | 0.95 | 0.06 | 26,31,35,38                 | 0     |
| 20  | CLA  | C     | 503 | 65/65 | 0.95 | 0.06 | 28,33,37,42                 | 0     |
| 22  | BCR  | T     | 101 | 40/40 | 0.95 | 0.06 | 24,32,43,45                 | 0     |
| 20  | CLA  | C     | 504 | 65/65 | 0.95 | 0.07 | 27,30,59,61                 | 0     |
| 20  | CLA  | b     | 608 | 65/65 | 0.95 | 0.07 | 24,31,59,63                 | 0     |
| 20  | CLA  | c     | 507 | 65/65 | 0.96 | 0.07 | 25,30,49,57                 | 0     |
| 20  | CLA  | c     | 508 | 60/65 | 0.96 | 0.06 | 24,28,52,54                 | 0     |
| 28  | DMS  | b     | 631 | 4/4   | 0.96 | 0.09 | 23,24,27,35                 | 0     |
| 33  | CA   | O     | 301 | 1/1   | 0.96 | 0.05 | 47,47,47,47                 | 0     |
| 20  | CLA  | c     | 509 | 65/65 | 0.96 | 0.07 | 25,30,53,58                 | 0     |
| 20  | CLA  | C     | 509 | 65/65 | 0.96 | 0.07 | 29,34,52,55                 | 0     |
| 28  | DMS  | v     | 202 | 4/4   | 0.96 | 0.11 | 50,51,53,55                 | 0     |
| 20  | CLA  | C     | 510 | 65/65 | 0.96 | 0.06 | 26,31,38,44                 | 0     |
| 20  | CLA  | C     | 502 | 65/65 | 0.96 | 0.06 | 24,29,41,48                 | 0     |
| 22  | BCR  | A     | 405 | 40/40 | 0.96 | 0.05 | 21,26,32,35                 | 0     |
| 22  | BCR  | B     | 618 | 40/40 | 0.96 | 0.06 | 21,28,42,45                 | 0     |
| 24  | LMG  | J     | 101 | 45/55 | 0.96 | 0.07 | 27,32,64,70                 | 0     |
| 22  | BCR  | B     | 619 | 40/40 | 0.96 | 0.06 | 22,30,42,44                 | 0     |
| 20  | CLA  | B     | 607 | 65/65 | 0.96 | 0.07 | 22,29,55,62                 | 0     |
| 20  | CLA  | B     | 603 | 65/65 | 0.96 | 0.06 | 23,28,35,39                 | 0     |
| 27  | PL9  | D     | 412 | 55/55 | 0.96 | 0.05 | 19,23,29,34                 | 0     |
| 20  | CLA  | B     | 611 | 65/65 | 0.96 | 0.06 | 21,26,34,40                 | 0     |
| 27  | PL9  | d     | 412 | 55/55 | 0.96 | 0.05 | 18,23,29,35                 | 0     |
| 20  | CLA  | b     | 604 | 65/65 | 0.96 | 0.06 | 23,27,33,35                 | 0     |
| 20  | CLA  | B     | 615 | 65/65 | 0.96 | 0.07 | 20,24,70,79                 | 0     |
| 20  | CLA  | b     | 611 | 65/65 | 0.96 | 0.06 | 24,30,34,41                 | 0     |
| 22  | BCR  | a     | 408 | 40/40 | 0.96 | 0.05 | 21,25,30,31                 | 0     |
| 22  | BCR  | b     | 619 | 40/40 | 0.96 | 0.05 | 23,26,32,35                 | 0     |
| 35  | DGD  | C     | 516 | 62/66 | 0.96 | 0.07 | 22,32,74,79                 | 0     |
| 22  | BCR  | b     | 620 | 40/40 | 0.96 | 0.05 | 22,27,43,46                 | 0     |
| 35  | DGD  | C     | 518 | 62/66 | 0.96 | 0.07 | 24,30,62,73                 | 0     |
| 22  | BCR  | c     | 514 | 40/40 | 0.96 | 0.06 | 28,36,39,39                 | 0     |
| 20  | CLA  | b     | 612 | 65/65 | 0.96 | 0.06 | 21,27,36,41                 | 0     |
| 35  | DGD  | c     | 515 | 62/66 | 0.96 | 0.07 | 23,32,71,75                 | 0     |
| 35  | DGD  | c     | 516 | 57/66 | 0.96 | 0.06 | 27,32,62,68                 | 0     |
| 22  | BCR  | j     | 102 | 40/40 | 0.96 | 0.06 | 30,35,42,45                 | 0     |
| 20  | CLA  | b     | 616 | 65/65 | 0.96 | 0.07 | 20,26,73,80                 | 0     |
| 20  | CLA  | B     | 616 | 65/65 | 0.96 | 0.06 | 25,29,48,52                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 20  | CLA  | c     | 501 | 65/65 | 0.96 | 0.06 | 26,30,41,48                 | 0     |
| 20  | CLA  | c     | 503 | 65/65 | 0.96 | 0.06 | 25,35,40,43                 | 0     |
| 20  | CLA  | c     | 504 | 65/65 | 0.96 | 0.06 | 25,29,55,60                 | 0     |
| 36  | LHG  | d     | 406 | 49/49 | 0.96 | 0.06 | 29,36,43,48                 | 0     |
| 36  | LHG  | d     | 408 | 49/49 | 0.96 | 0.09 | 24,31,83,88                 | 0     |
| 20  | CLA  | c     | 505 | 65/65 | 0.96 | 0.06 | 25,30,46,50                 | 0     |
| 20  | CLA  | C     | 501 | 65/65 | 0.96 | 0.06 | 27,33,45,52                 | 0     |
| 21  | PHO  | A     | 403 | 64/64 | 0.97 | 0.04 | 18,22,24,25                 | 0     |
| 21  | PHO  | D     | 403 | 64/64 | 0.97 | 0.04 | 18,24,29,35                 | 0     |
| 21  | PHO  | a     | 405 | 64/64 | 0.97 | 0.04 | 17,20,22,25                 | 0     |
| 21  | PHO  | a     | 406 | 64/64 | 0.97 | 0.04 | 19,24,29,32                 | 0     |
| 20  | CLA  | b     | 610 | 65/65 | 0.97 | 0.05 | 20,26,31,33                 | 0     |
| 22  | BCR  | B     | 617 | 40/40 | 0.97 | 0.05 | 22,26,32,33                 | 0     |
| 20  | CLA  | B     | 608 | 65/65 | 0.97 | 0.05 | 18,21,34,39                 | 0     |
| 20  | CLA  | B     | 609 | 65/65 | 0.97 | 0.04 | 22,25,31,33                 | 0     |
| 20  | CLA  | b     | 613 | 65/65 | 0.97 | 0.05 | 20,22,38,44                 | 0     |
| 20  | CLA  | b     | 614 | 65/65 | 0.97 | 0.05 | 21,25,31,37                 | 0     |
| 20  | CLA  | A     | 402 | 59/65 | 0.97 | 0.05 | 18,22,52,58                 | 0     |
| 20  | CLA  | b     | 617 | 65/65 | 0.97 | 0.05 | 23,30,44,50                 | 0     |
| 20  | CLA  | B     | 604 | 65/65 | 0.97 | 0.05 | 21,24,33,39                 | 0     |
| 20  | CLA  | B     | 612 | 65/65 | 0.97 | 0.05 | 19,22,36,42                 | 0     |
| 20  | CLA  | c     | 502 | 65/65 | 0.97 | 0.06 | 22,26,39,48                 | 0     |
| 20  | CLA  | D     | 401 | 65/65 | 0.97 | 0.05 | 16,20,35,41                 | 0     |
| 20  | CLA  | D     | 404 | 65/65 | 0.97 | 0.07 | 26,29,77,81                 | 0     |
| 22  | BCR  | b     | 621 | 40/40 | 0.97 | 0.05 | 27,32,42,44                 | 0     |
| 20  | CLA  | a     | 403 | 65/65 | 0.97 | 0.05 | 17,20,29,38                 | 0     |
| 20  | CLA  | a     | 407 | 47/65 | 0.97 | 0.05 | 19,22,41,48                 | 0     |
| 20  | CLA  | B     | 613 | 65/65 | 0.97 | 0.05 | 21,25,30,34                 | 0     |
| 20  | CLA  | B     | 606 | 65/65 | 0.97 | 0.05 | 19,24,35,37                 | 0     |
| 33  | CA   | b     | 626 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 36  | LHG  | D     | 408 | 49/49 | 0.97 | 0.06 | 23,30,44,49                 | 0     |
| 20  | CLA  | b     | 605 | 65/65 | 0.97 | 0.05 | 21,25,34,37                 | 0     |
| 20  | CLA  | c     | 510 | 65/65 | 0.97 | 0.05 | 23,29,39,42                 | 0     |
| 36  | LHG  | L     | 101 | 49/49 | 0.97 | 0.06 | 24,31,49,53                 | 0     |
| 20  | CLA  | b     | 606 | 65/65 | 0.97 | 0.05 | 20,24,54,59                 | 0     |
| 36  | LHG  | d     | 407 | 49/49 | 0.97 | 0.06 | 22,27,46,50                 | 0     |
| 20  | CLA  | A     | 404 | 65/65 | 0.97 | 0.07 | 20,25,88,90                 | 0     |
| 36  | LHG  | l     | 102 | 49/49 | 0.97 | 0.06 | 22,30,51,54                 | 0     |
| 37  | HEM  | E     | 104 | 43/43 | 0.97 | 0.08 | 39,44,52,56                 | 0     |
| 37  | HEM  | e     | 102 | 43/43 | 0.97 | 0.08 | 34,41,56,68                 | 0     |
| 20  | CLA  | b     | 609 | 65/65 | 0.97 | 0.05 | 19,22,33,37                 | 0     |
| 20  | CLA  | d     | 404 | 65/65 | 0.97 | 0.07 | 24,29,78,87                 | 0     |

*Continued on next page...*

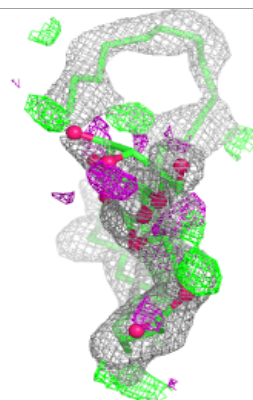
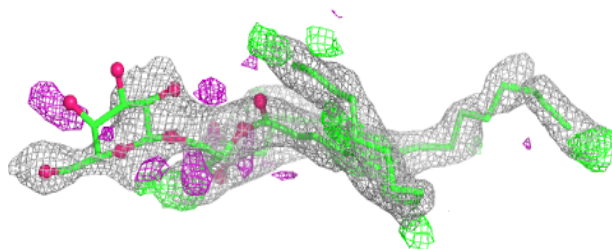
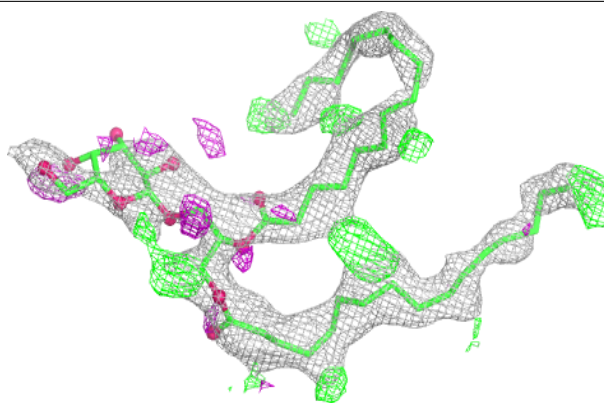
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 20  | CLA  | b     | 615 | 65/65 | 0.98 | 0.05 | 18,22,53,59                | 0     |
| 20  | CLA  | D     | 402 | 65/65 | 0.98 | 0.04 | 15,19,30,36                | 0     |
| 20  | CLA  | B     | 605 | 65/65 | 0.98 | 0.06 | 19,23,55,58                | 0     |
| 33  | CA   | c     | 522 | 1/1   | 0.98 | 0.05 | 41,41,41,41                | 0     |
| 28  | DMS  | B     | 634 | 4/4   | 0.98 | 0.07 | 23,24,25,26                | 0     |
| 20  | CLA  | d     | 402 | 65/65 | 0.98 | 0.04 | 16,20,35,41                | 0     |
| 20  | CLA  | d     | 403 | 65/65 | 0.98 | 0.04 | 17,19,27,34                | 0     |
| 20  | CLA  | B     | 614 | 65/65 | 0.98 | 0.04 | 19,22,48,53                | 0     |
| 28  | DMS  | c     | 527 | 4/4   | 0.98 | 0.06 | 33,33,34,38                | 0     |
| 20  | CLA  | a     | 404 | 60/65 | 0.98 | 0.06 | 18,22,66,75                | 0     |
| 20  | CLA  | b     | 607 | 65/65 | 0.98 | 0.05 | 20,24,33,35                | 0     |
| 28  | DMS  | C     | 528 | 4/4   | 0.98 | 0.07 | 33,37,39,41                | 0     |
| 28  | DMS  | o     | 302 | 4/4   | 0.98 | 0.08 | 20,28,31,36                | 0     |
| 20  | CLA  | A     | 401 | 65/65 | 0.98 | 0.04 | 16,19,30,36                | 0     |
| 33  | CA   | B     | 624 | 1/1   | 0.98 | 0.11 | 43,43,43,43                | 0     |
| 39  | MG   | J     | 102 | 1/1   | 0.98 | 0.05 | 33,33,33,33                | 0     |
| 40  | HEC  | v     | 201 | 43/43 | 0.98 | 0.06 | 25,29,34,37                | 0     |
| 25  | CL   | A     | 409 | 1/1   | 0.99 | 0.03 | 22,22,22,22                | 0     |
| 28  | DMS  | A     | 414 | 4/4   | 0.99 | 0.06 | 25,28,28,29                | 0     |
| 29  | FE2  | A     | 419 | 1/1   | 0.99 | 0.02 | 29,29,29,29                | 0     |
| 29  | FE2  | a     | 417 | 1/1   | 0.99 | 0.02 | 27,27,27,27                | 0     |
| 39  | MG   | j     | 103 | 1/1   | 0.99 | 0.08 | 31,31,31,31                | 0     |
| 40  | HEC  | V     | 201 | 43/43 | 0.99 | 0.04 | 21,23,27,31                | 0     |
| 25  | CL   | a     | 412 | 1/1   | 0.99 | 0.03 | 24,24,24,24                | 0     |
| 25  | CL   | A     | 408 | 1/1   | 1.00 | 0.01 | 22,22,22,22                | 0     |
| 30  | OEX  | A     | 420 | 10/10 | 1.00 | 0.03 | 21,23,24,24                | 0     |
| 30  | OEX  | a     | 419 | 10/10 | 1.00 | 0.02 | 21,24,26,26                | 0     |
| 25  | CL   | a     | 411 | 1/1   | 1.00 | 0.03 | 22,22,22,22                | 0     |

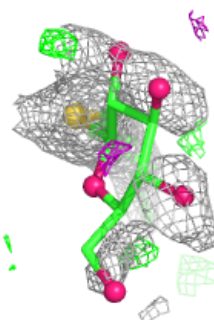
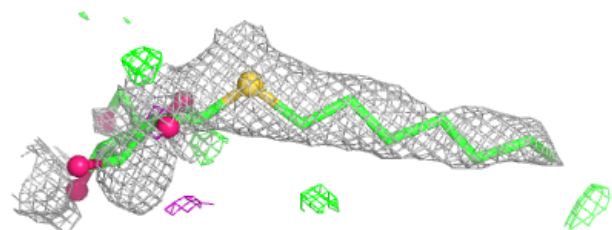
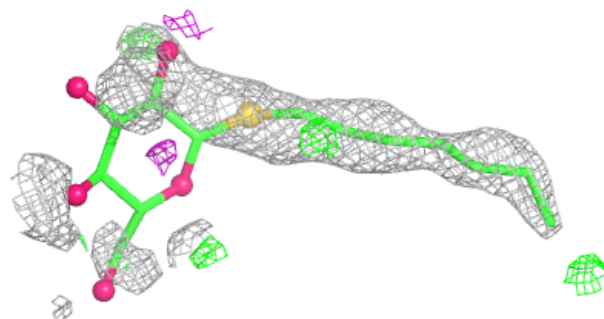
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DGD D 406:**

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

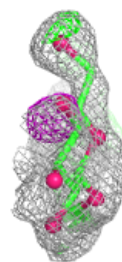
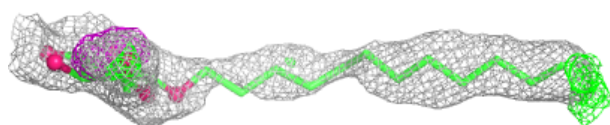
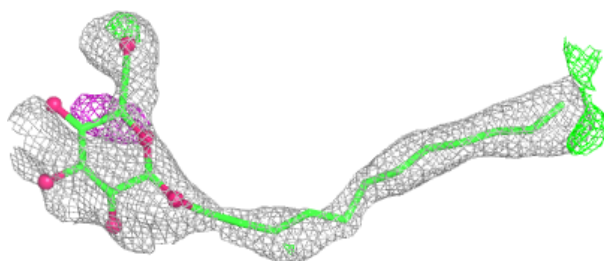
**Electron density around HTG C 534:**

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

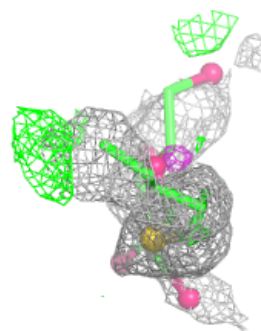
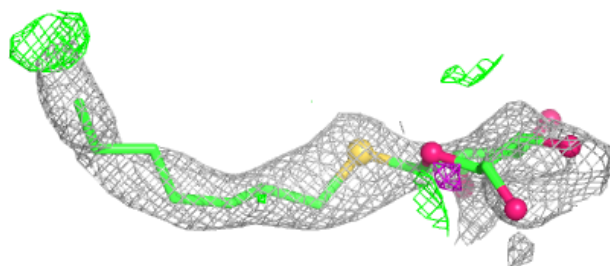
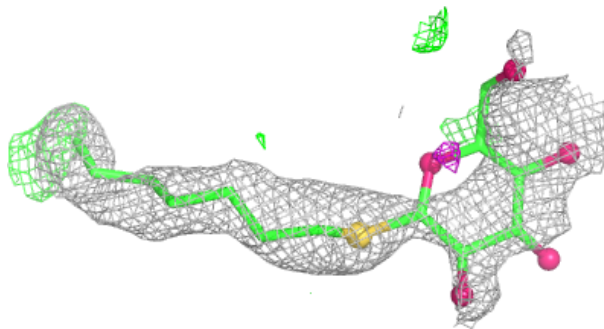


**Electron density around LMT f 102:**

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

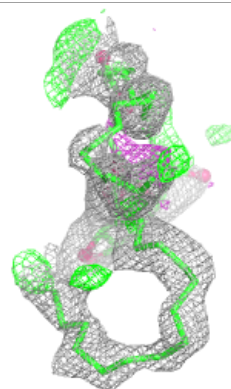
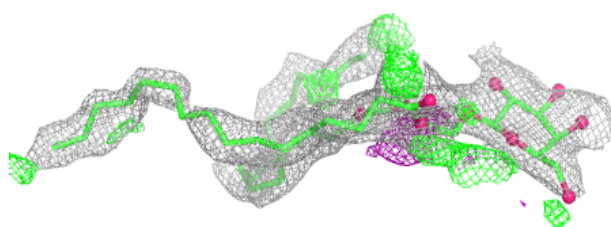
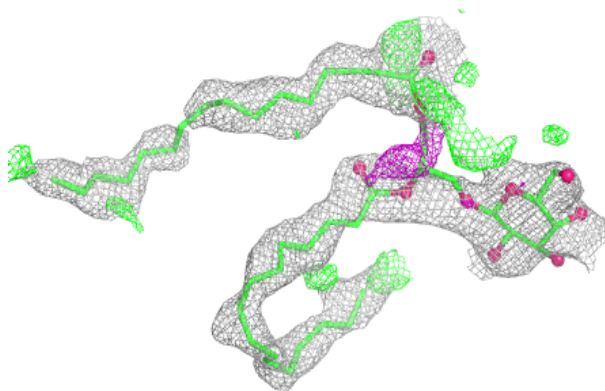
**Electron density around HTG D 417:**

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



**Electron density around DGD d 416:**

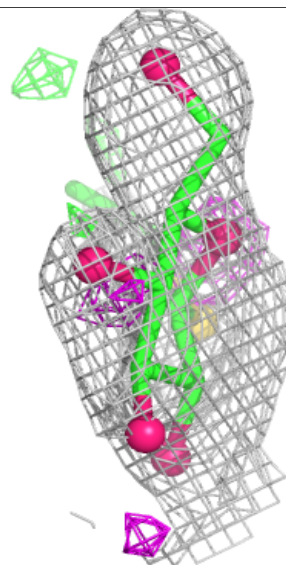
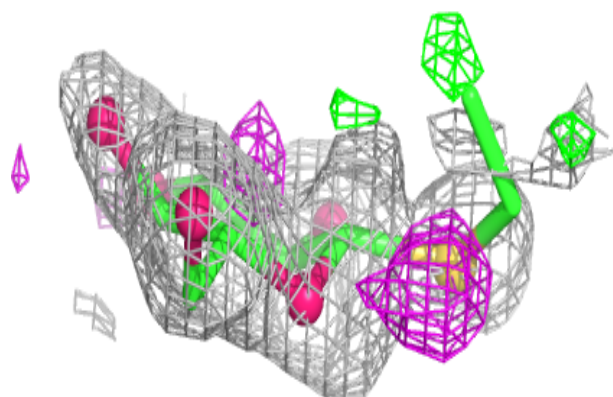
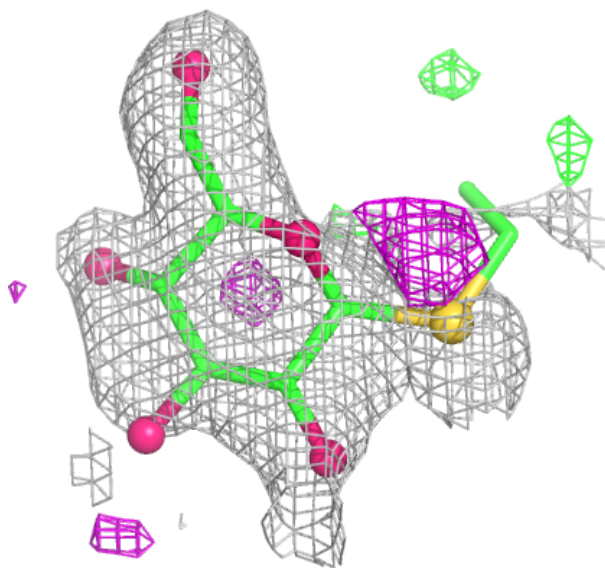
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





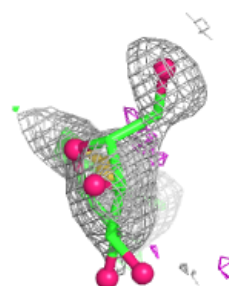
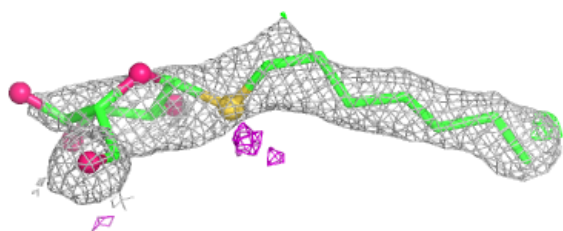
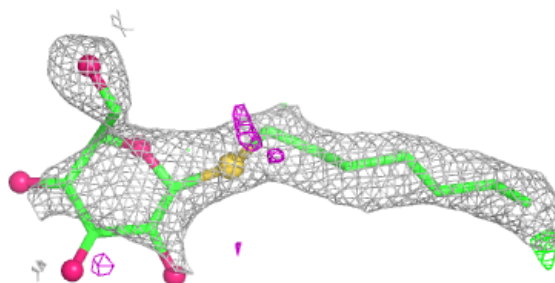
**Electron density around HTG v 210:**

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

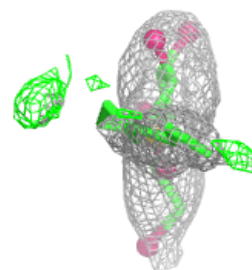
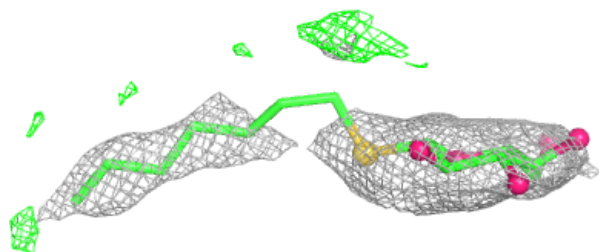
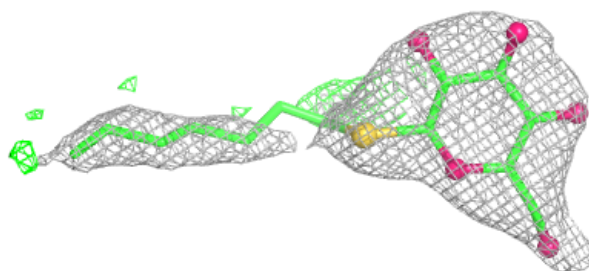


**Electron density around HTG c 521:**

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

**Electron density around HTG c 520:**

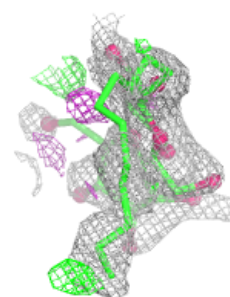
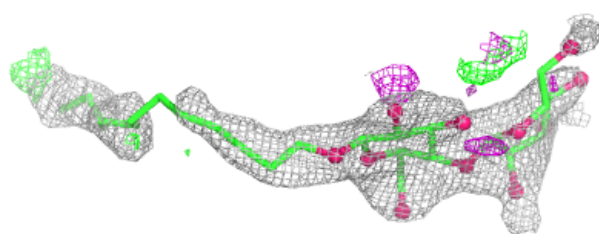
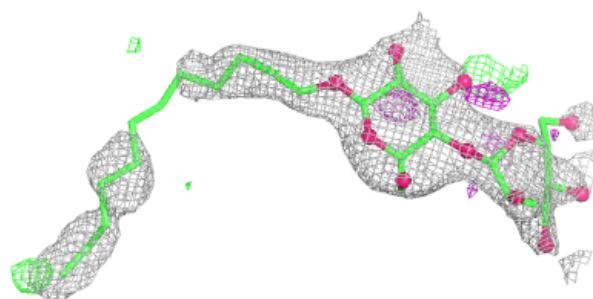
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



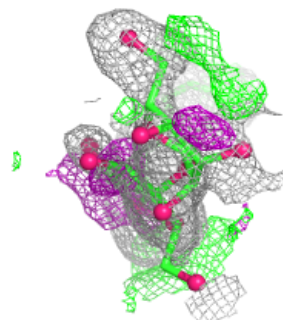
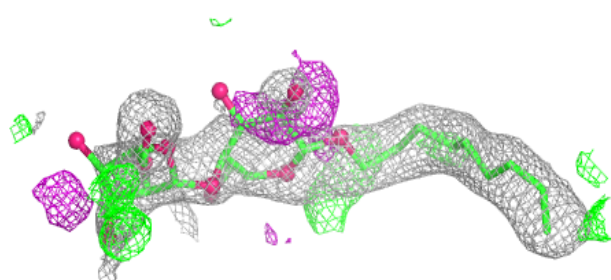
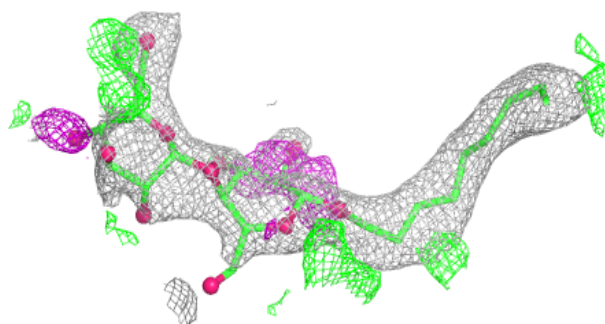


**Electron density around LMT I 101:**

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

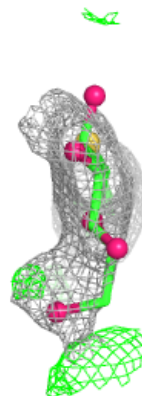
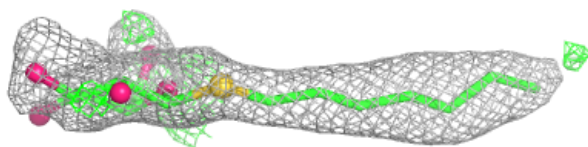
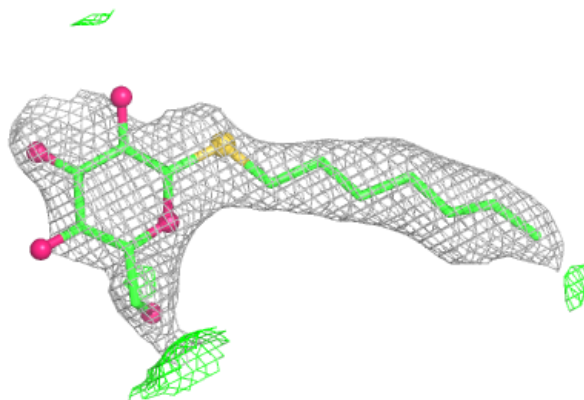
**Electron density around LMT b 627:**

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



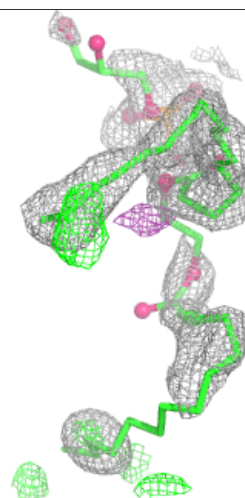
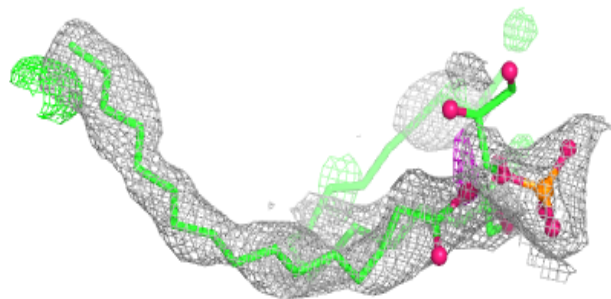
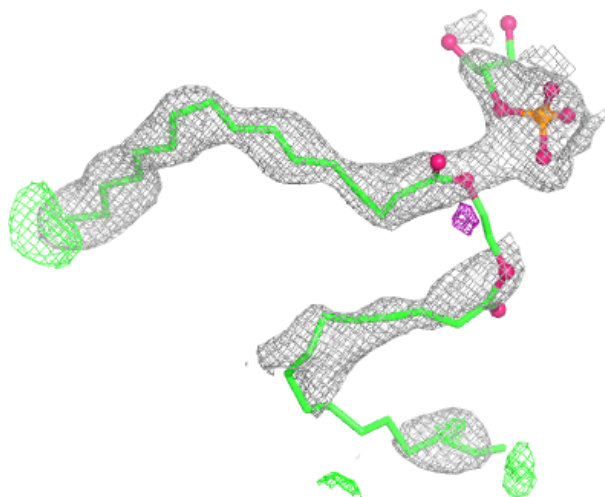
**Electron density around HTG b 602:**

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



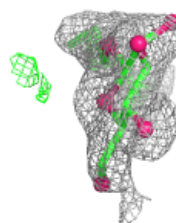
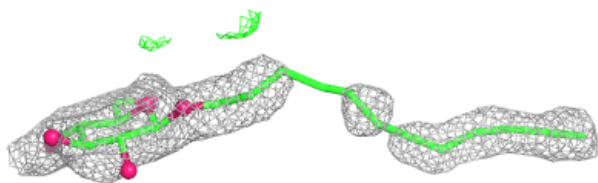
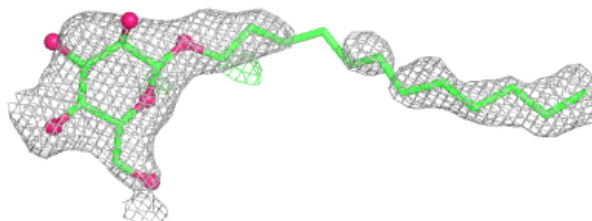
**Electron density around LHG E 103:**

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

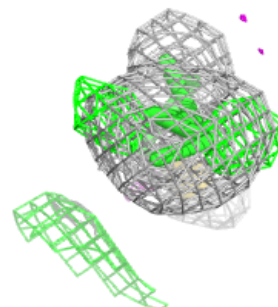
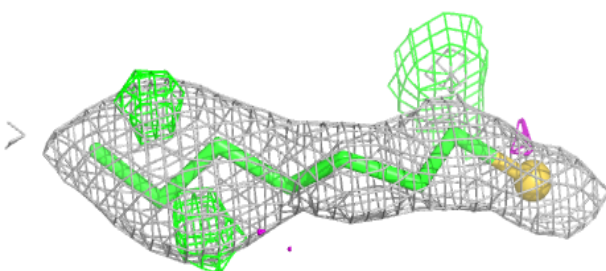
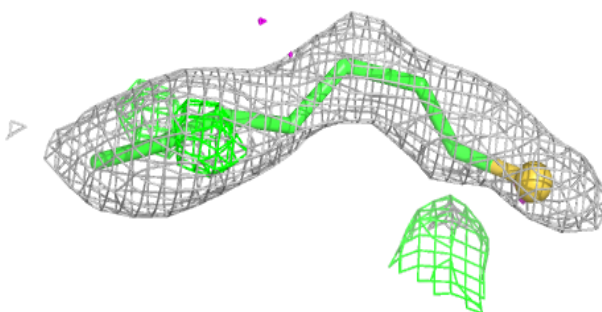


**Electron density around LMT E 101:**

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

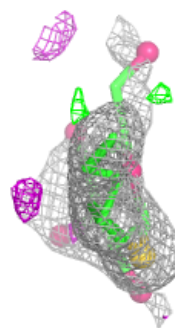
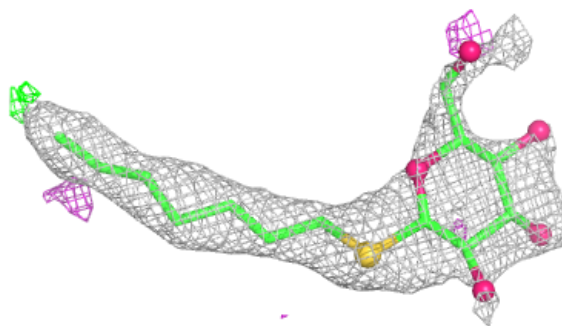
**Electron density around HTG u 201:**

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

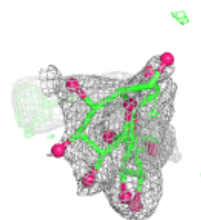
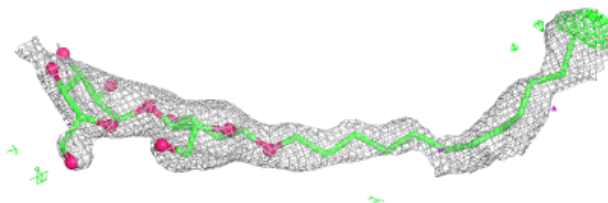
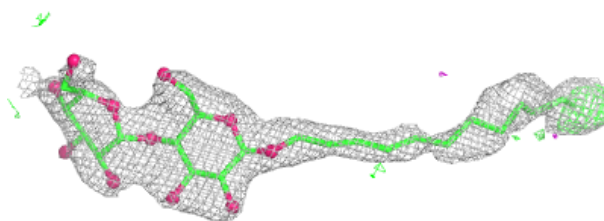


**Electron density around HTG B 623:**

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

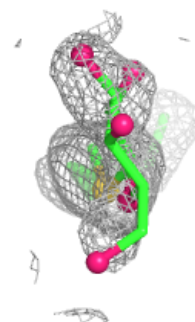
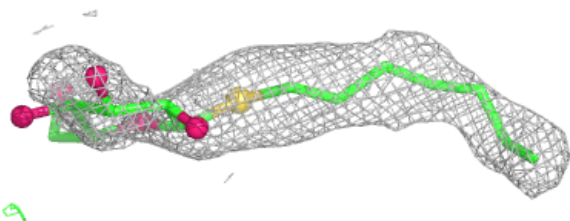
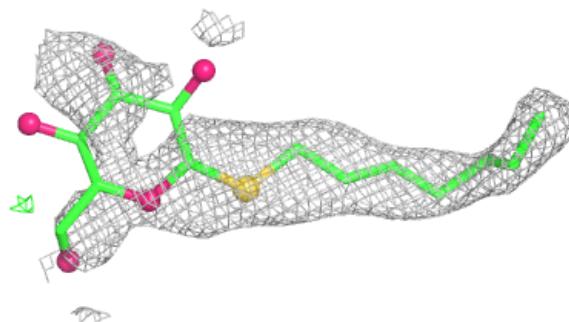
**Electron density around LMT c 523:**

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

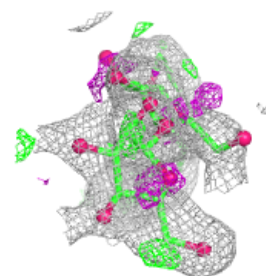
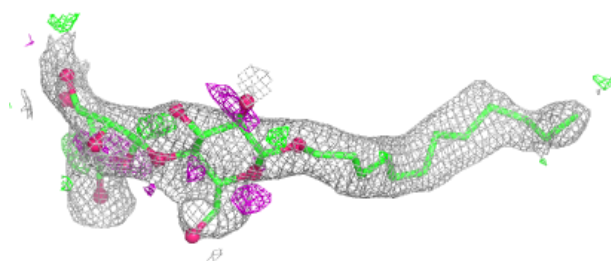
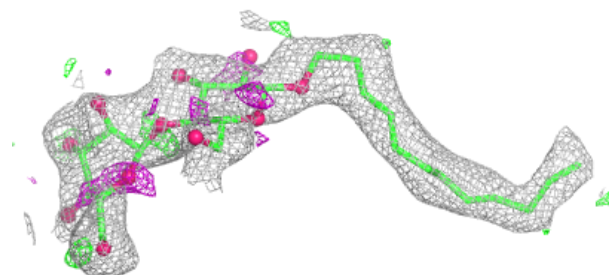


**Electron density around HTG d 401:**

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

**Electron density around LMT a 418:**

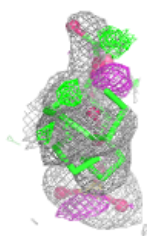
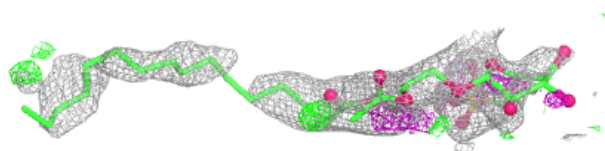
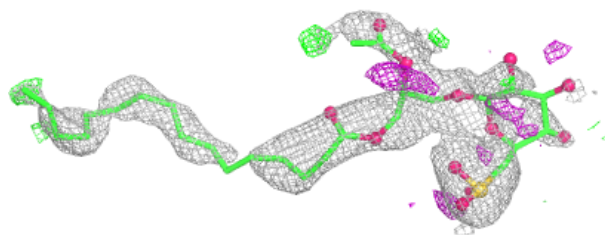
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



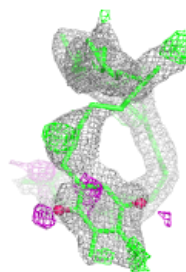
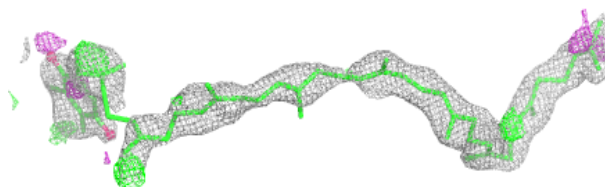
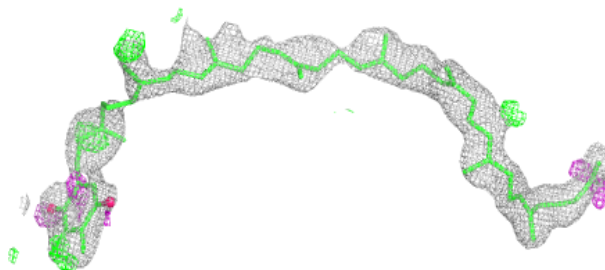


**Electron density around SQD f 101:**

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

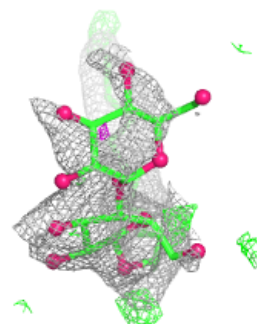
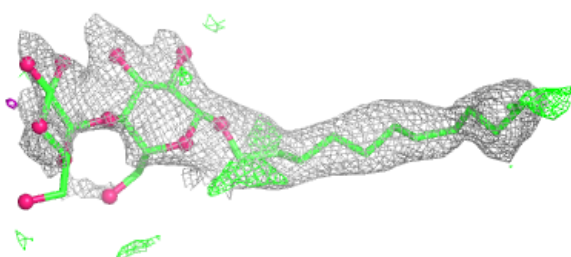
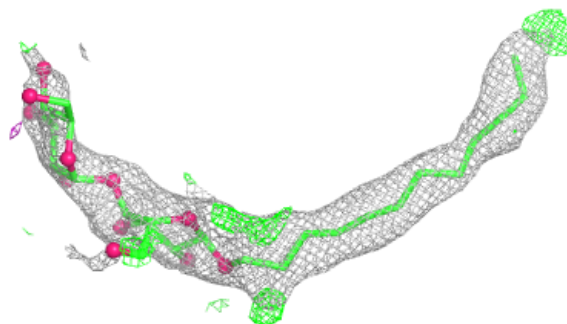
**Electron density around PL9 A 411:**

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

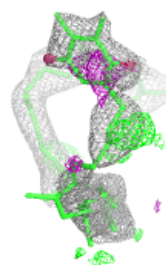
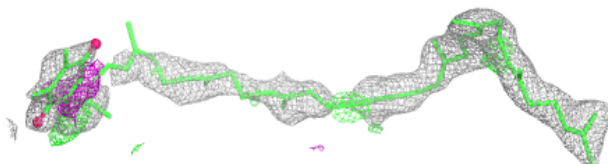
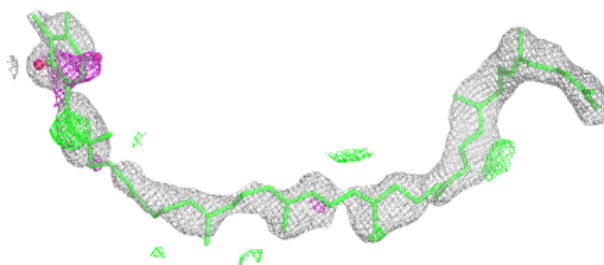


**Electron density around LMT m 101:**

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

**Electron density around PL9 a 415:**

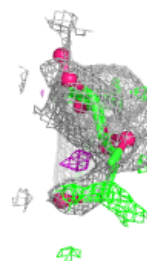
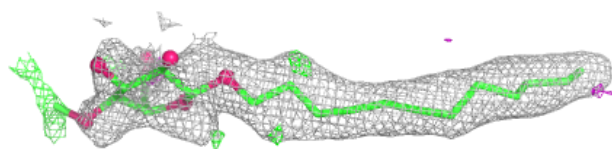
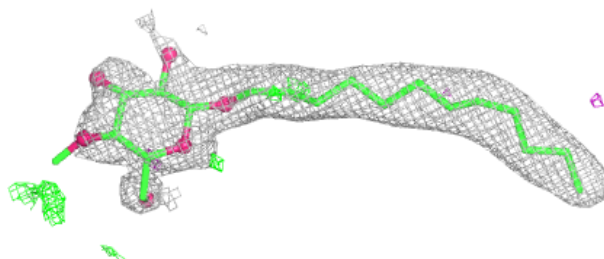
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



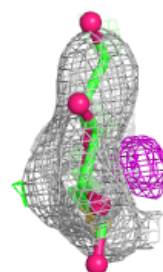
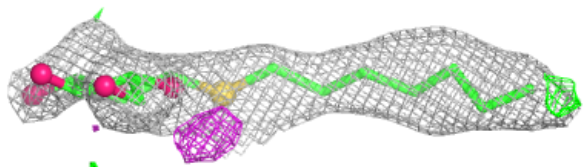
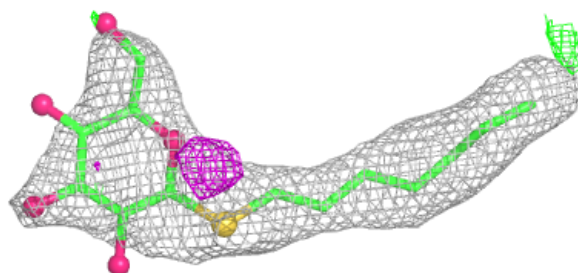


**Electron density around LMT b 628:**

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

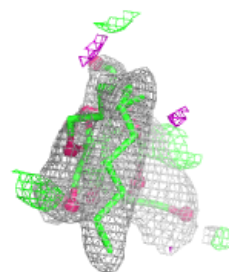
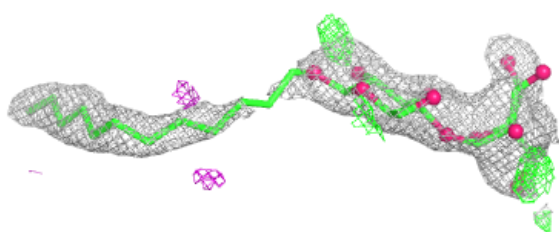
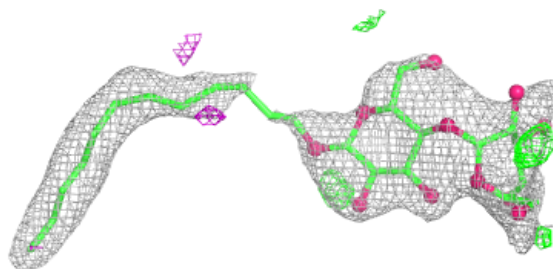
**Electron density around HTG B 632:**

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

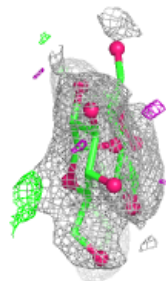
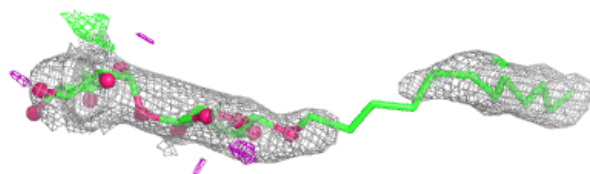
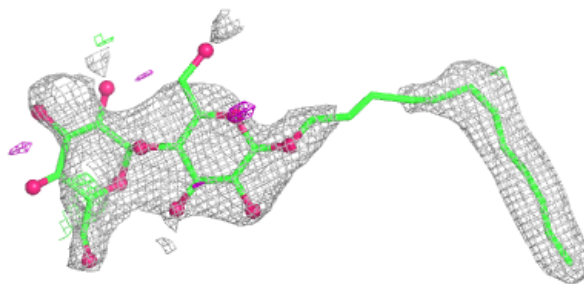


**Electron density around LMT z 102:**

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

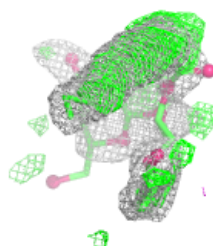
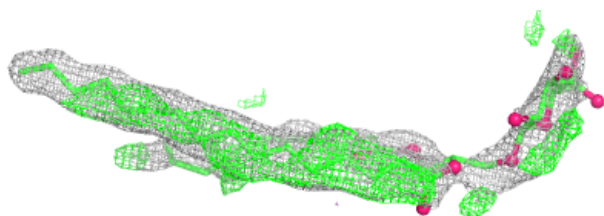
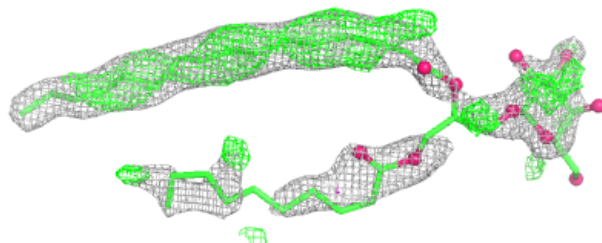
**Electron density around LMT Z 101:**

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

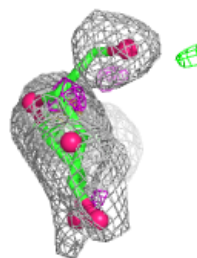
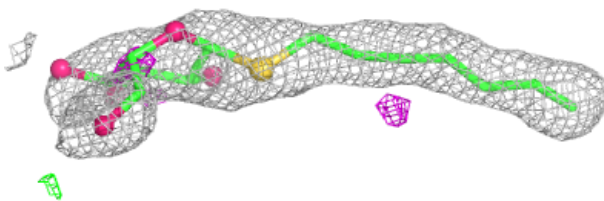
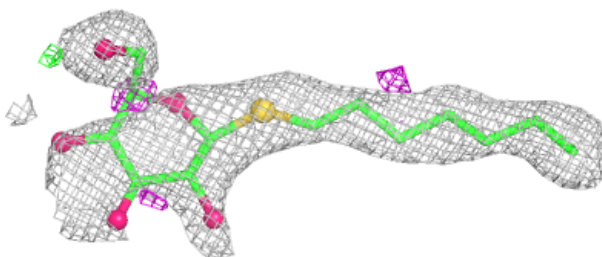


**Electron density around LMG C 524:**

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

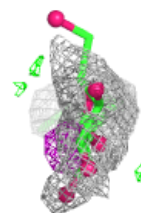
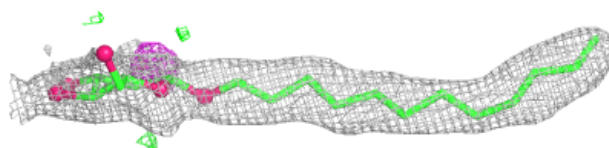
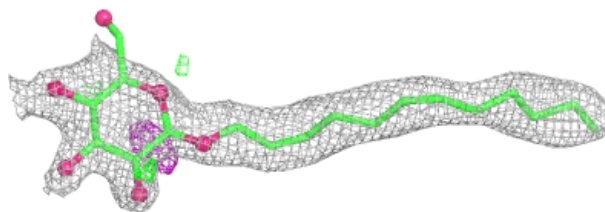
**Electron density around HTG C 521:**

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

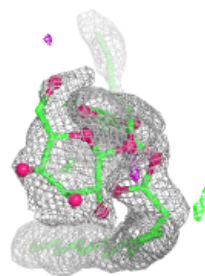
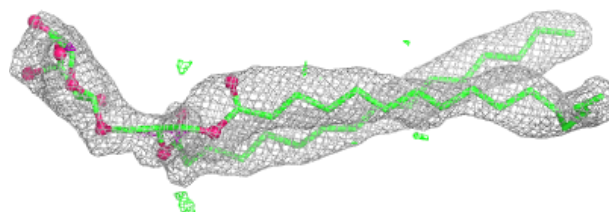
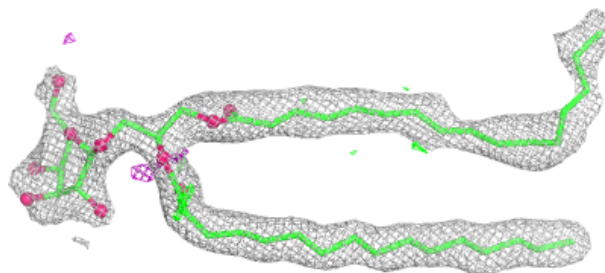


**Electron density around LMT J 103:**

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

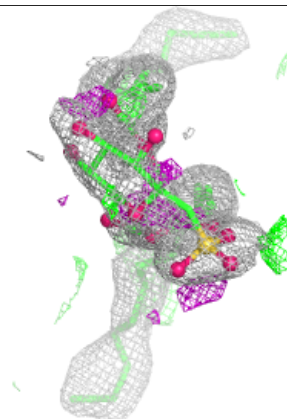
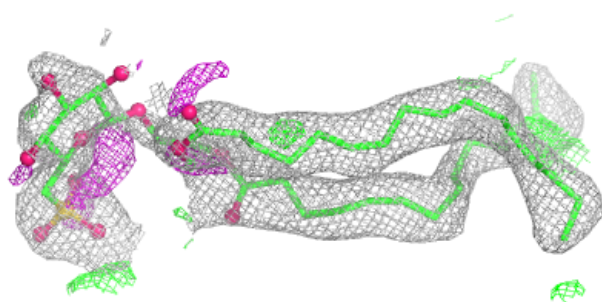
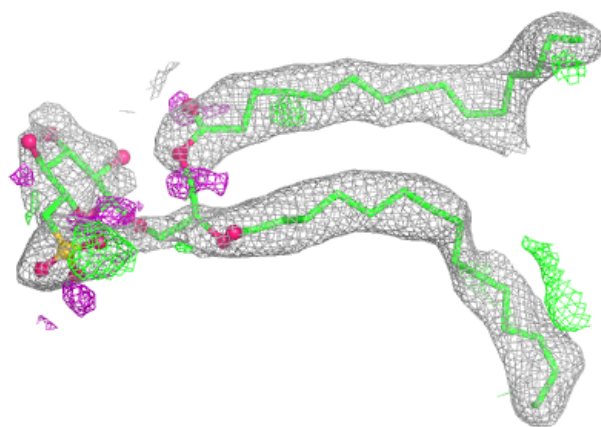
**Electron density around LMG c 518:**

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

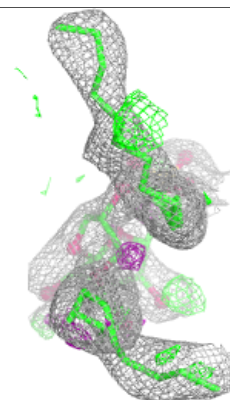
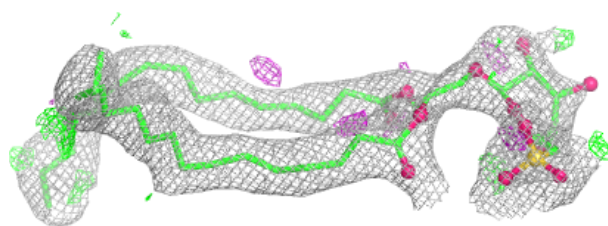
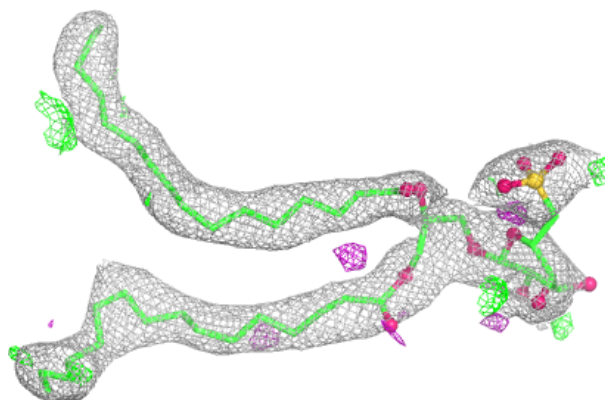


**Electron density around SQD 1 101:**

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

**Electron density around SQD b 622:**

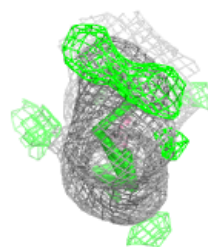
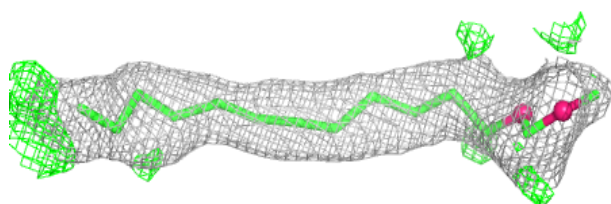
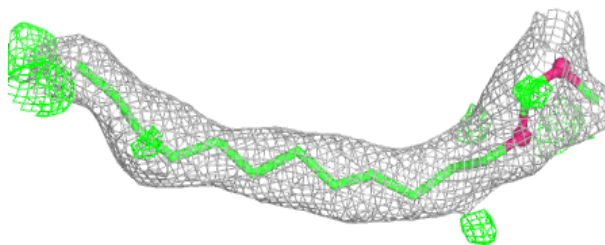
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



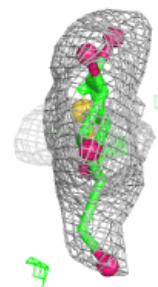
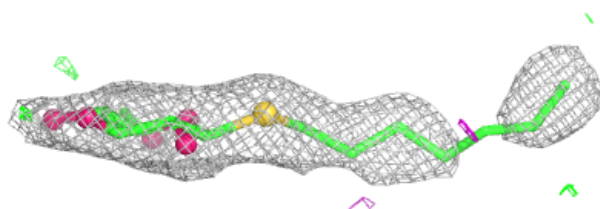
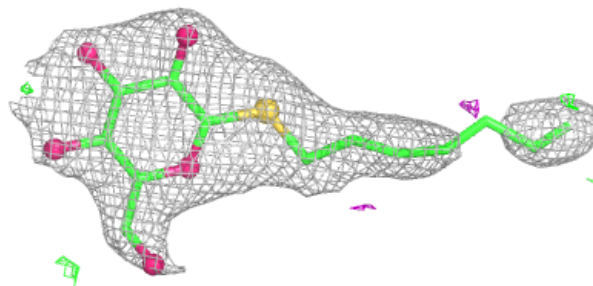


**Electron density around LMT B 627:**

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

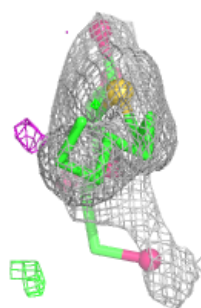
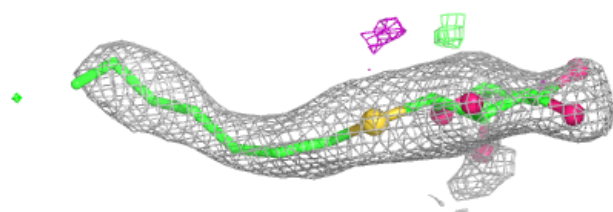
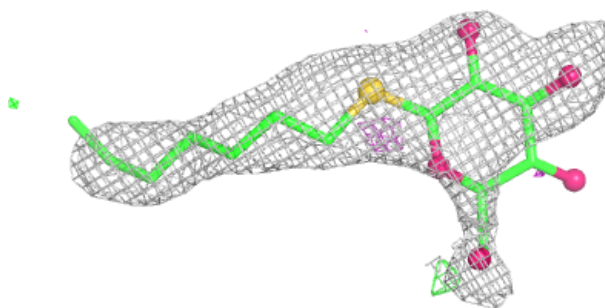
**Electron density around HTG C 520:**

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

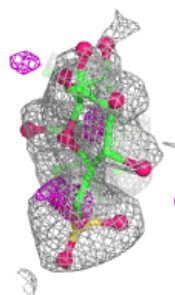
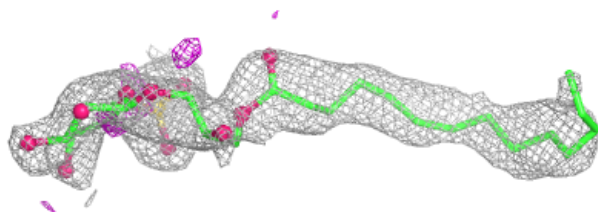
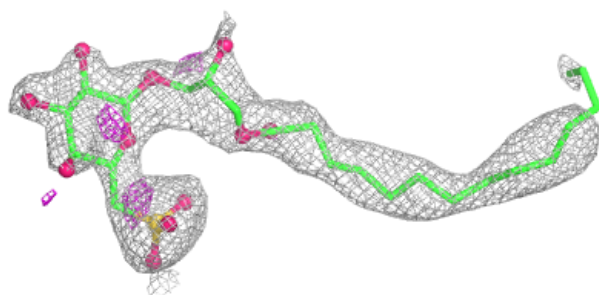


**Electron density around HTG C 522:**

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

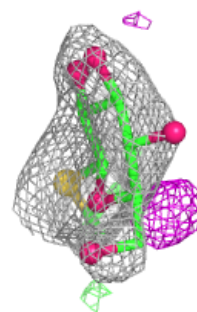
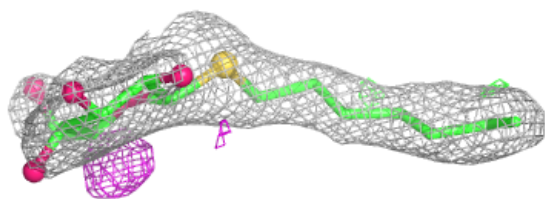
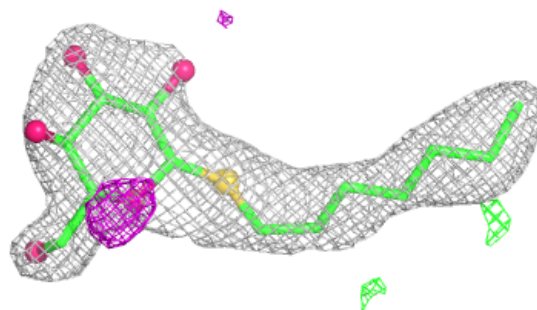
**Electron density around SQD F 101:**

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

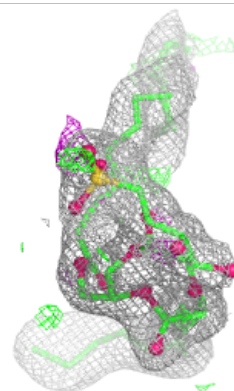
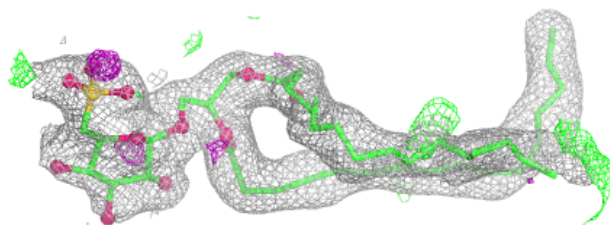
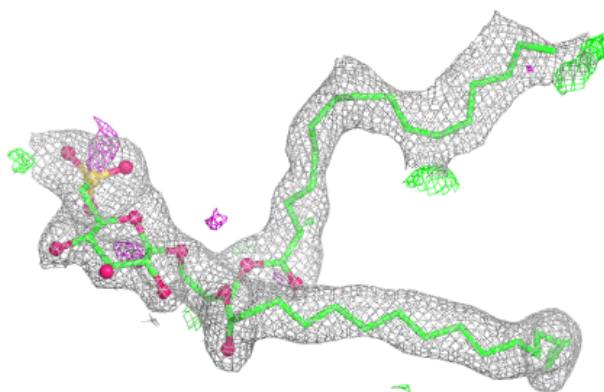


**Electron density around HTG b 624:**

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

**Electron density around SQD a 401:**

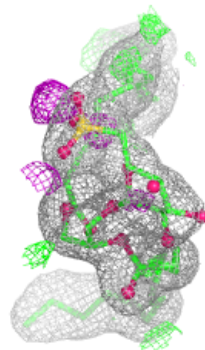
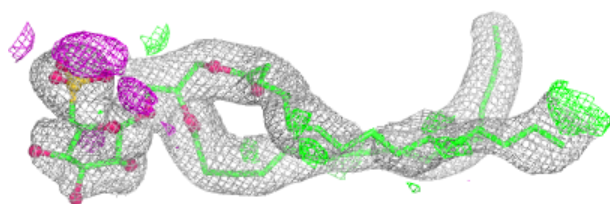
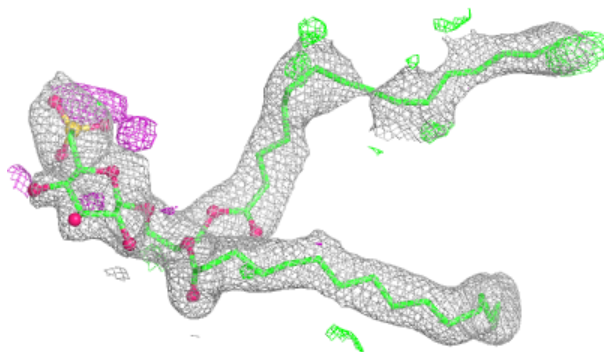
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



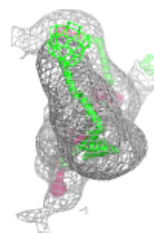
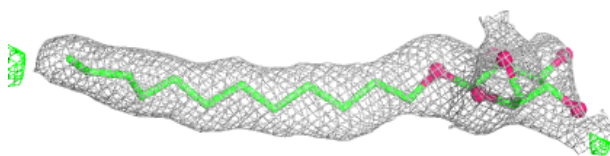
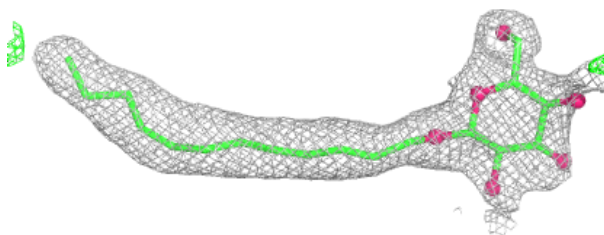


**Electron density around SQD A 412:**

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

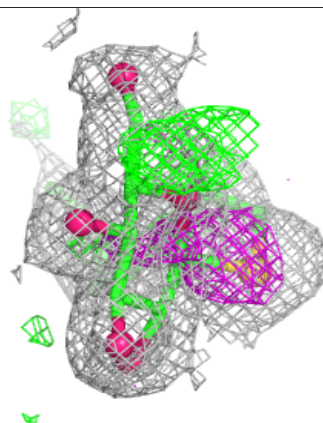
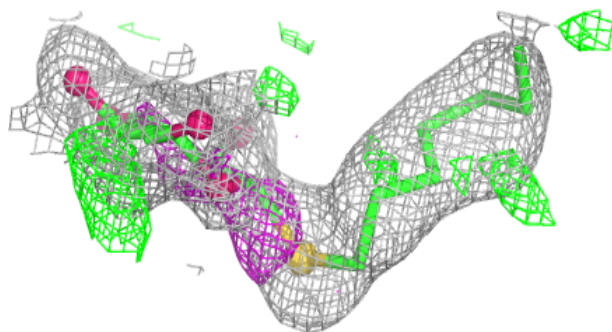
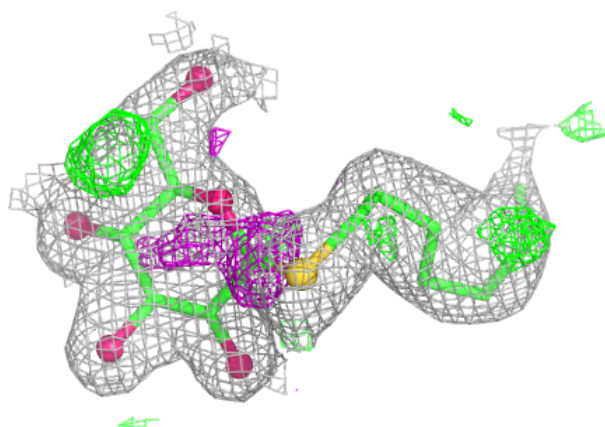
**Electron density around LMT B 625:**

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

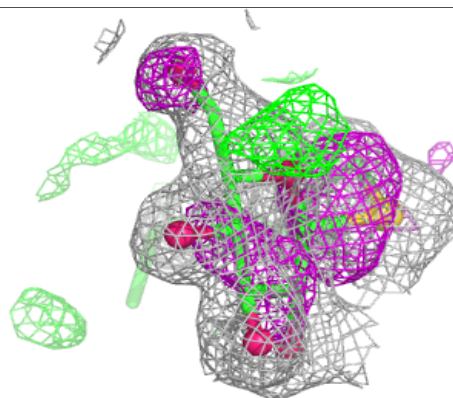
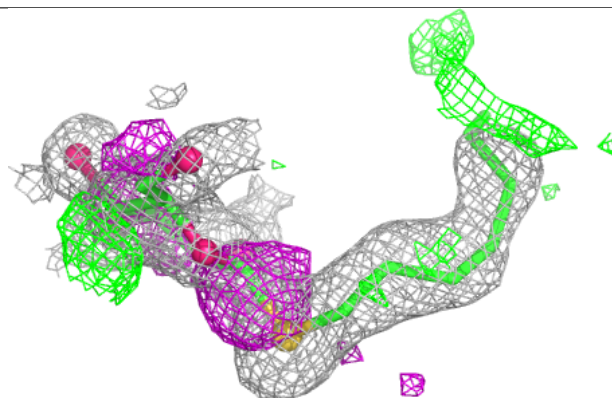
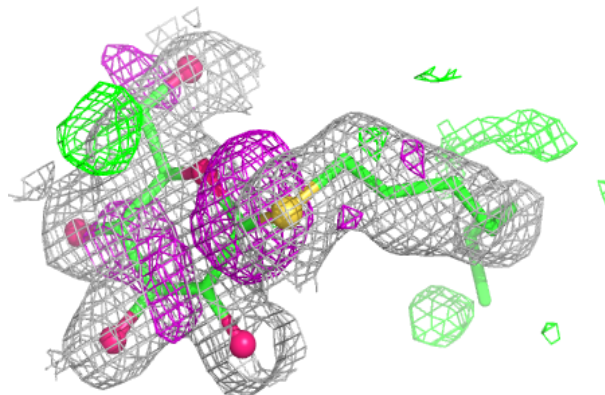


**Electron density around HTG B 622:**

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

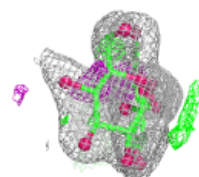
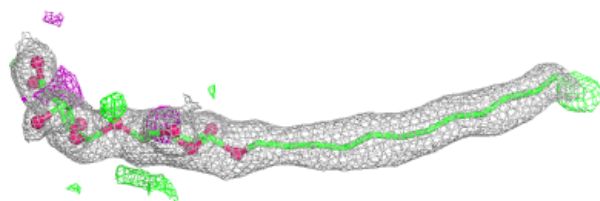
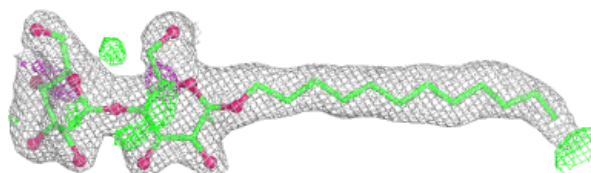
**Electron density around HTG b 625:**

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

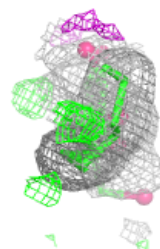
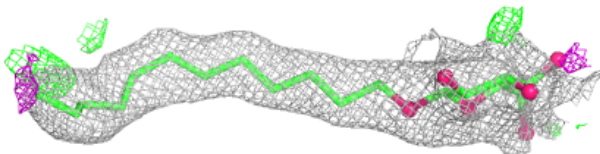
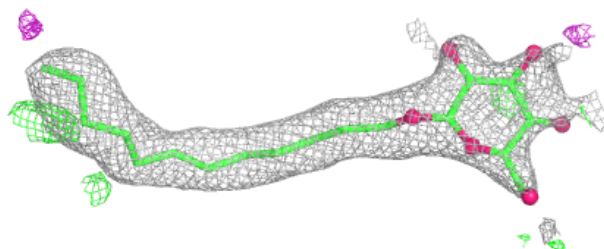


**Electron density around LMT m 102:**

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

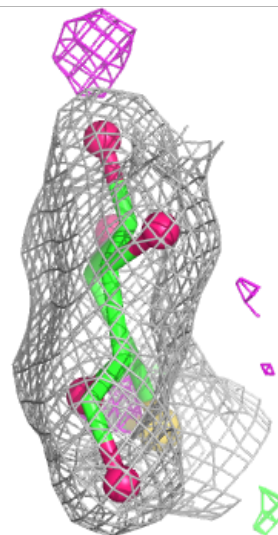
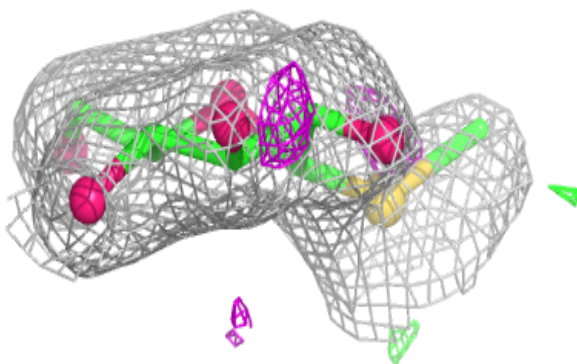
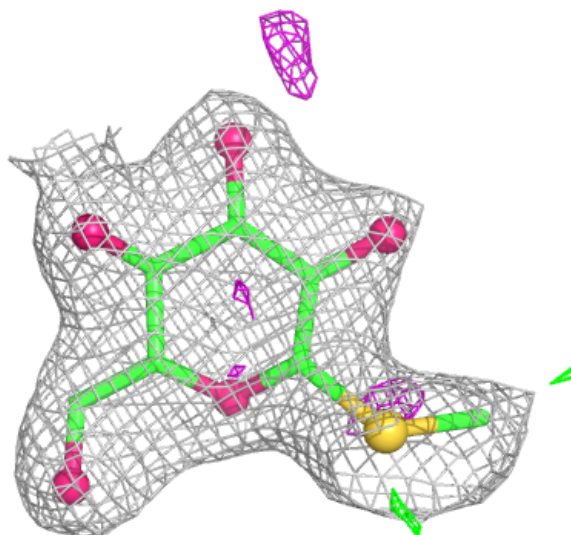
**Electron density around LMT B 626:**

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



**Electron density around HTG V 202:**

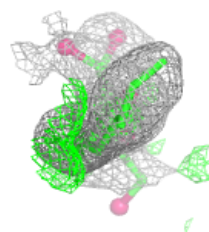
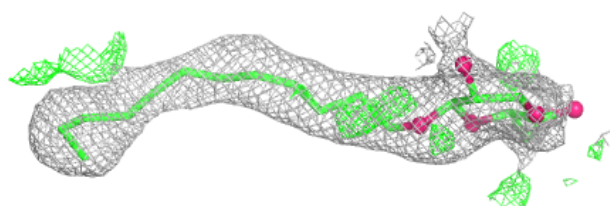
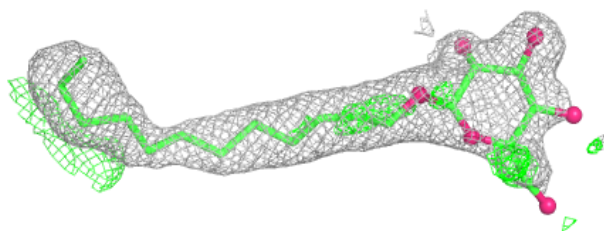
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



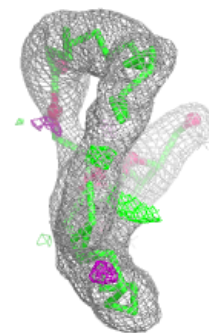
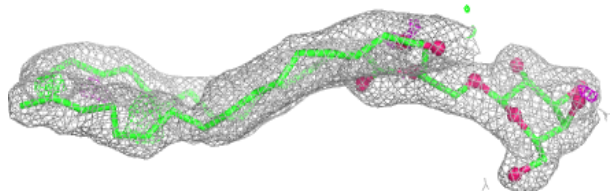
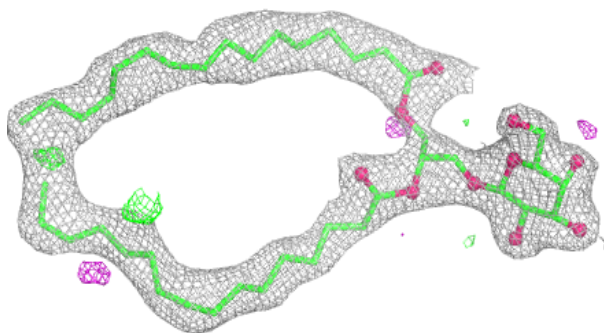


**Electron density around LMT T 102:**

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

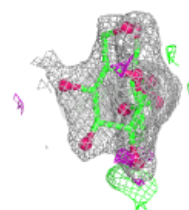
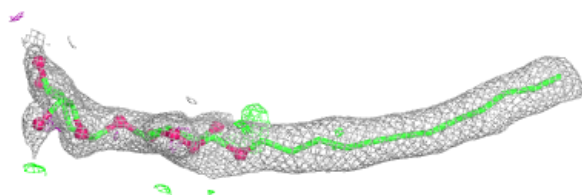
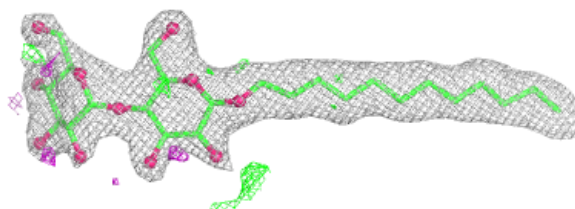
**Electron density around LMG a 410:**

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

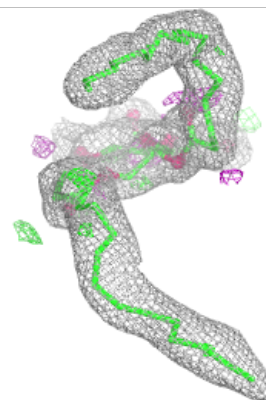
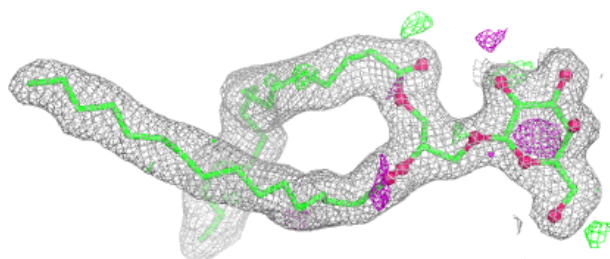
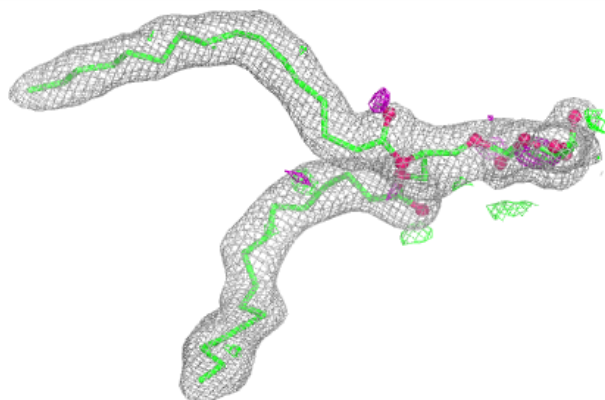


**Electron density around LMT M 101:**

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

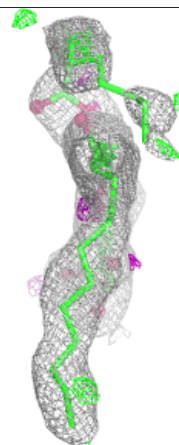
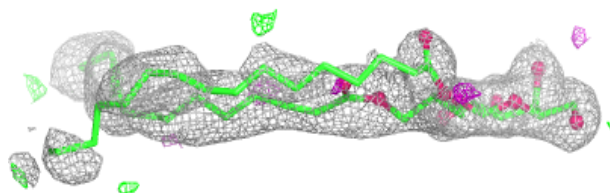
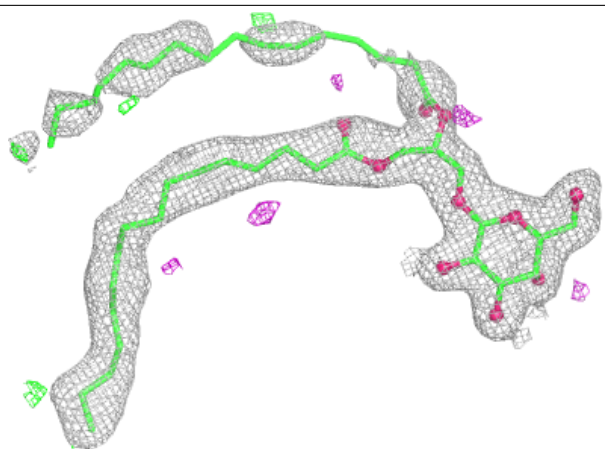
**Electron density around LMG B 620:**

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



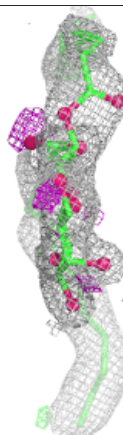
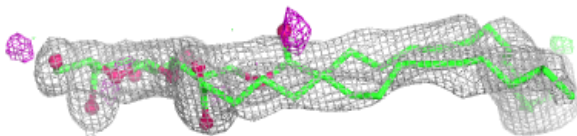
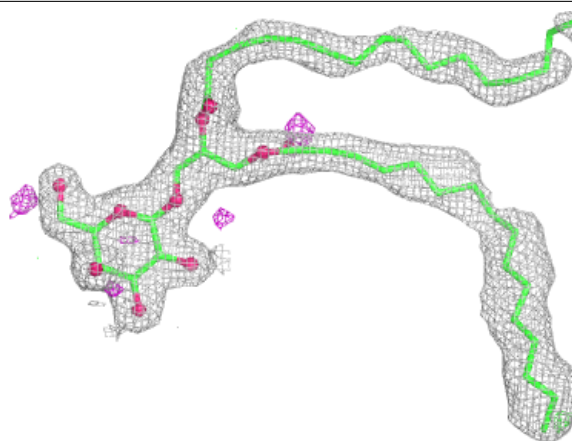
**Electron density around LMG c 519:**

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

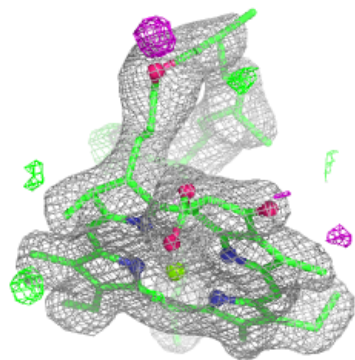
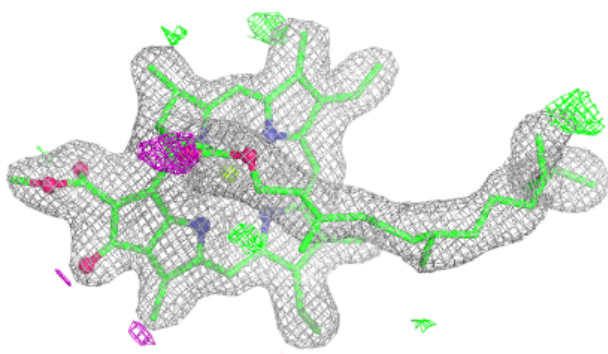
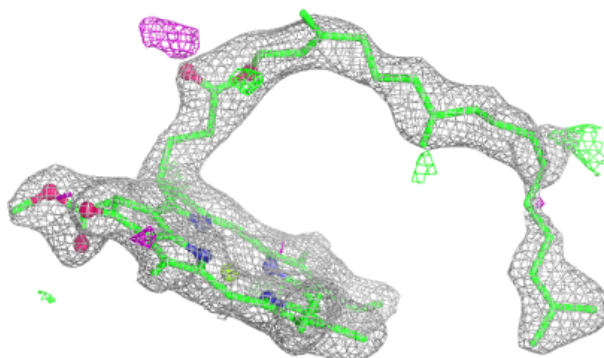


**Electron density around LMG C 519:**

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

**Electron density around CLA C 513:**

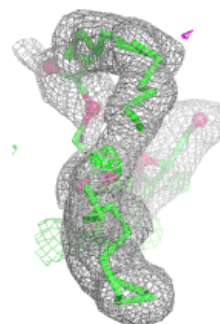
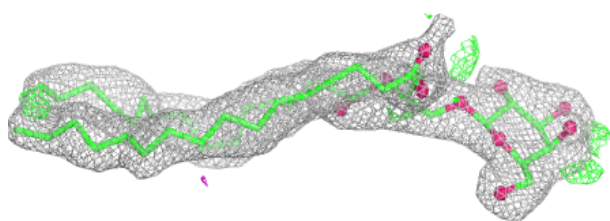
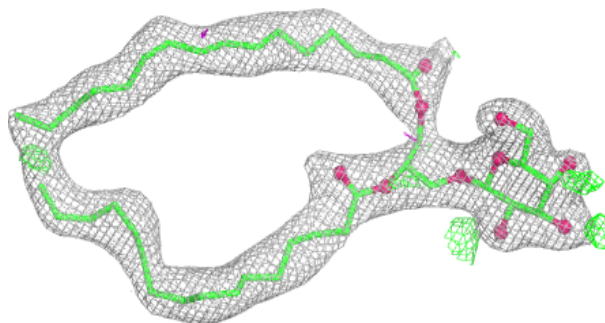
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



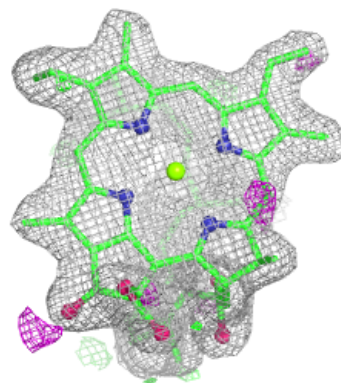
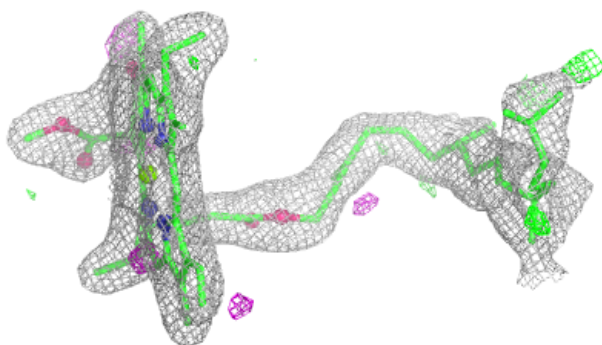
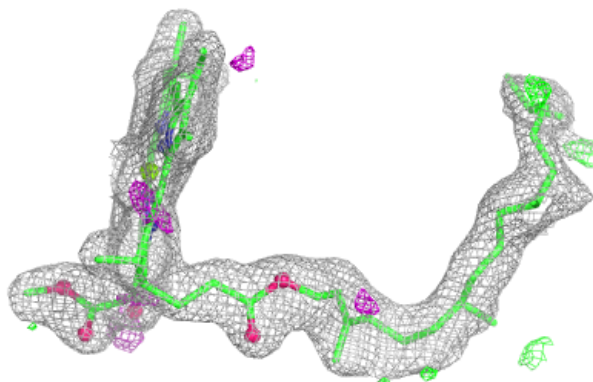


**Electron density around LMG A 407:**

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

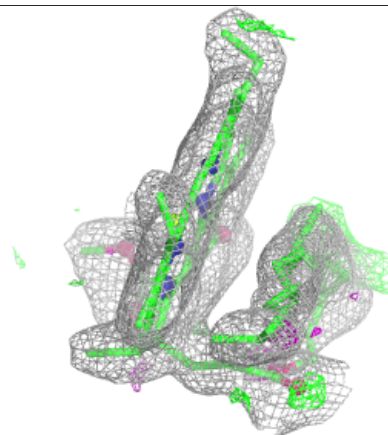
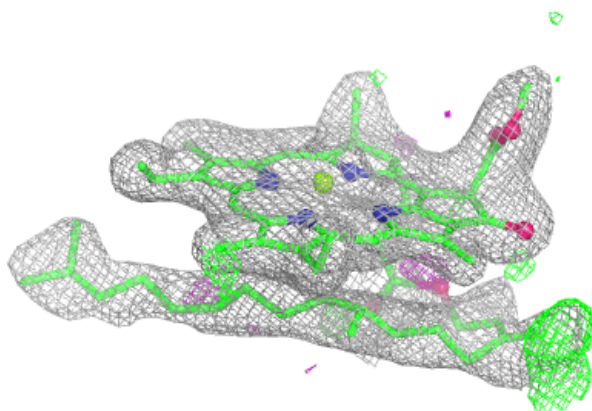
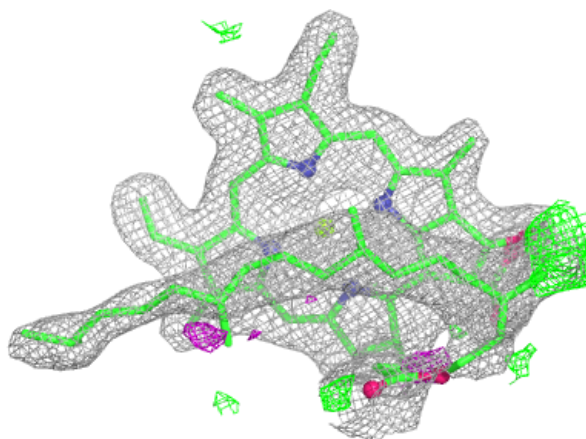
**Electron density around CLA C 506:**

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

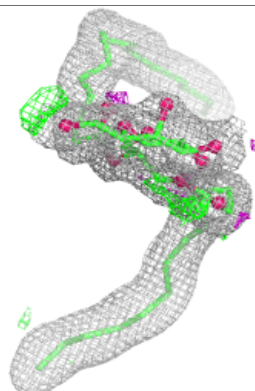
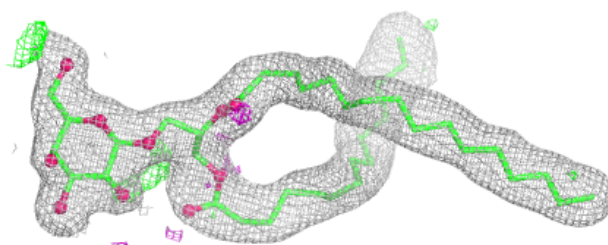
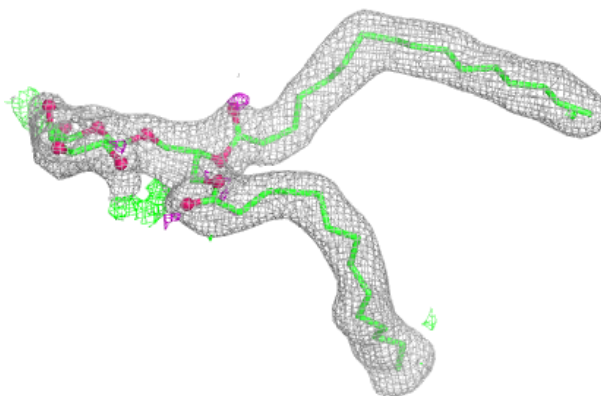


**Electron density around CLA b 603:**

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

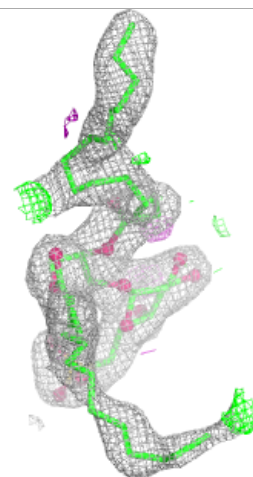
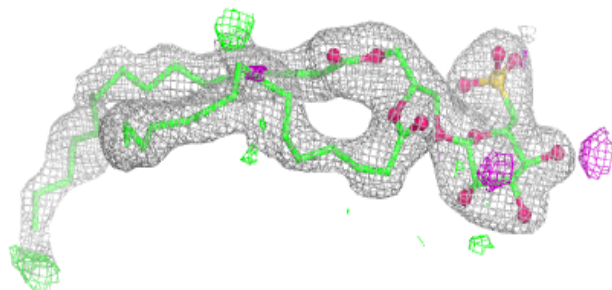
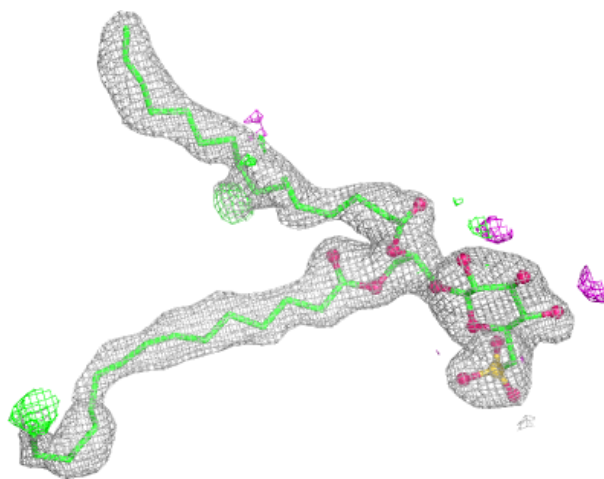
**Electron density around LMG b 623:**

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



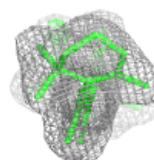
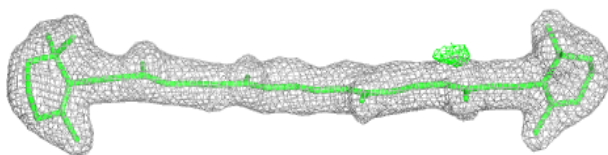
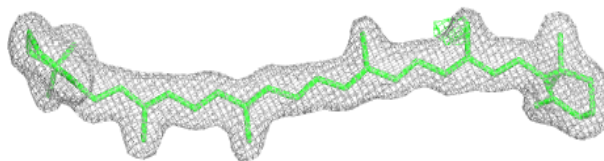
**Electron density around SQD A 406:**

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

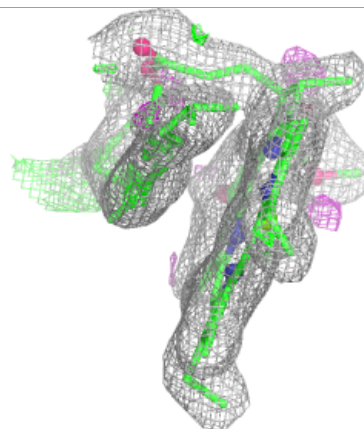
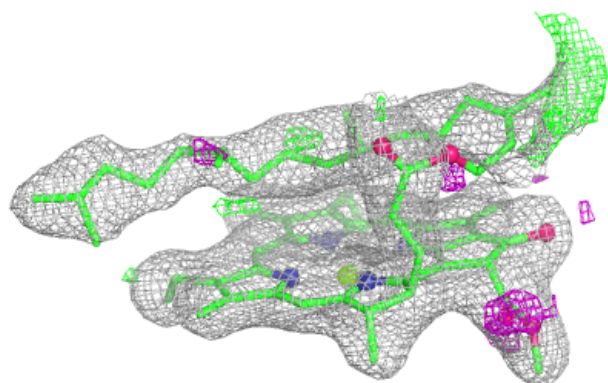
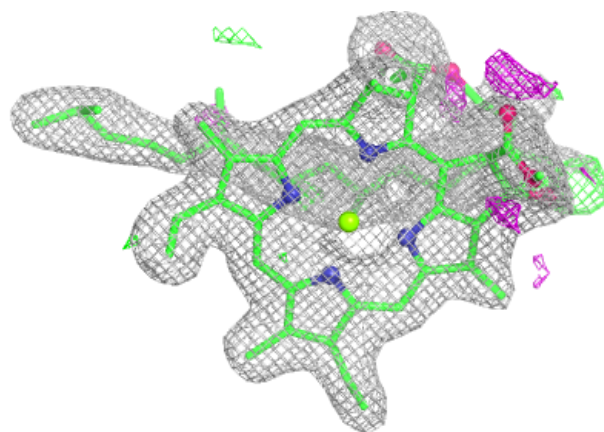


**Electron density around BCR C 514:**

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

**Electron density around CLA B 602:**

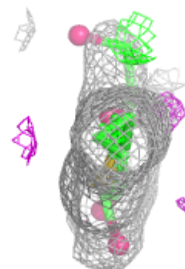
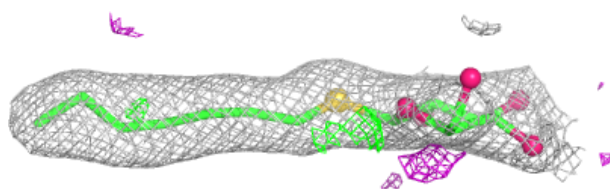
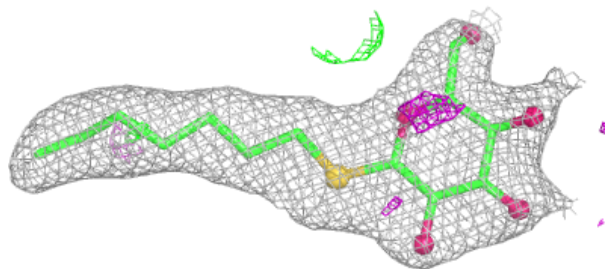
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



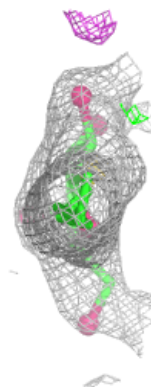
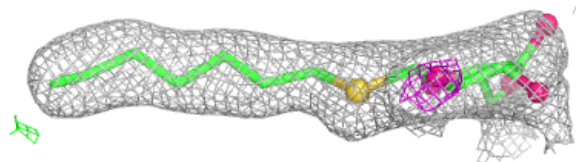
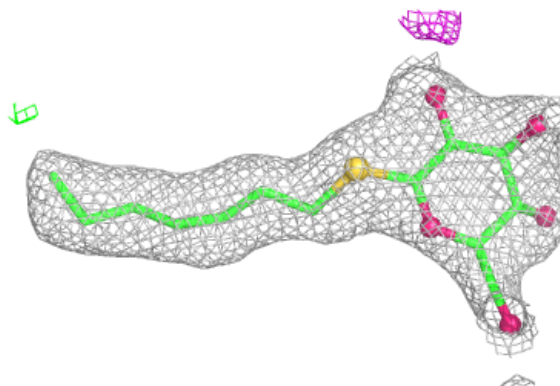


**Electron density around HTG b 601:**

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

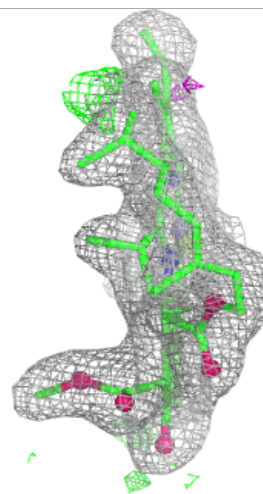
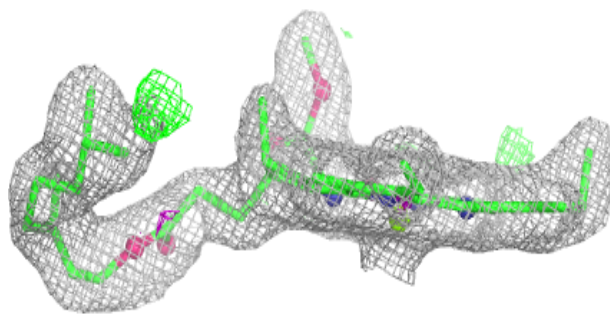
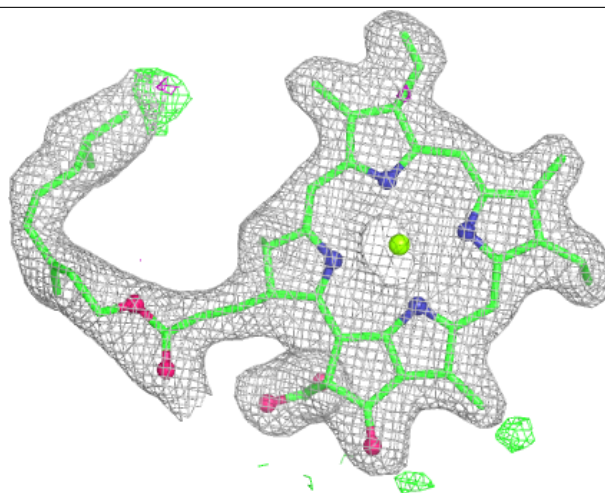
**Electron density around HTG B 631:**

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



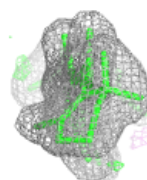
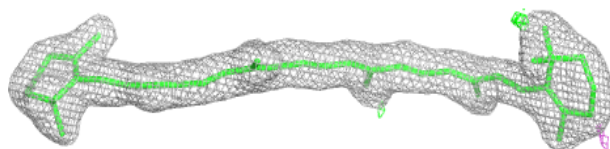
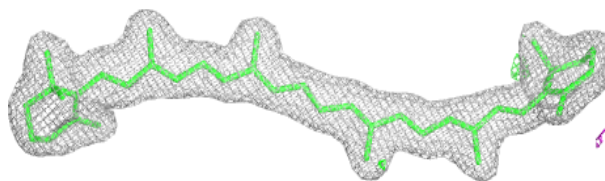
**Electron density around CLA C 512:**

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

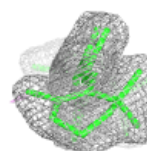
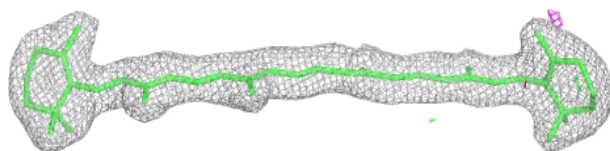
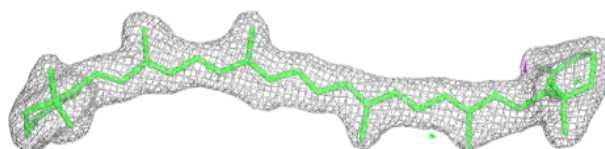


**Electron density around BCR K 101:**

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

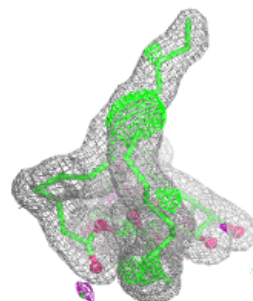
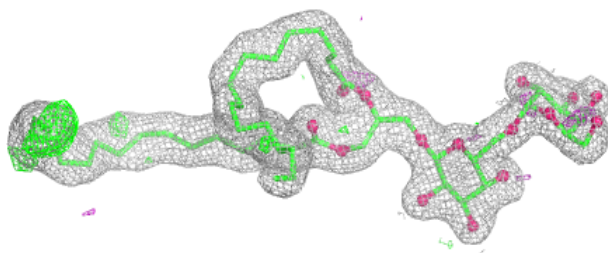
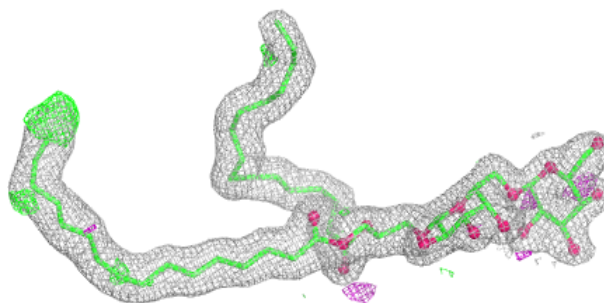
**Electron density around BCR k 102:**

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



**Electron density around DGD h 101:**

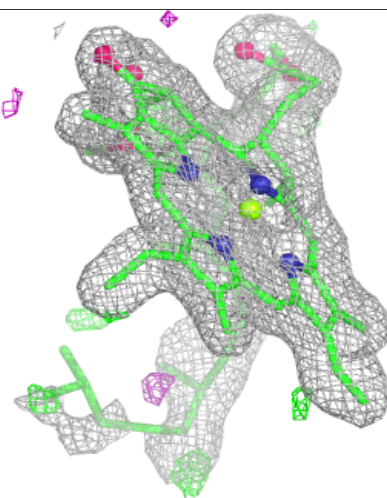
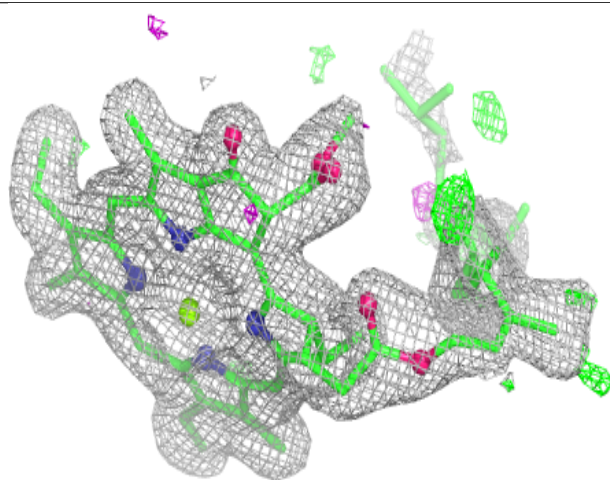
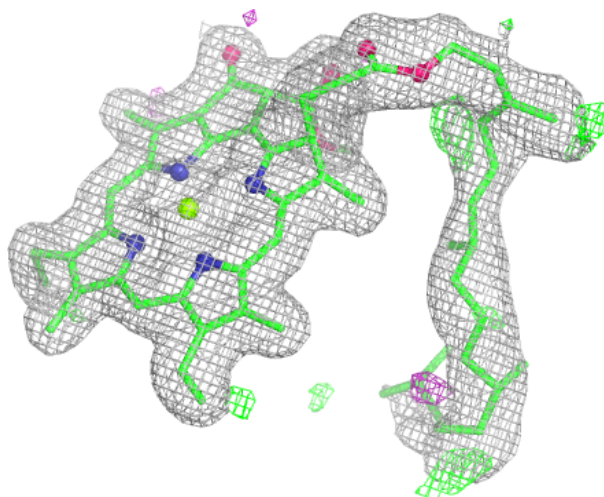
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





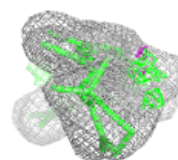
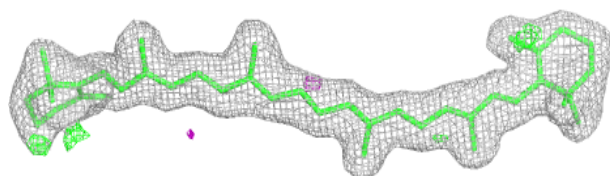
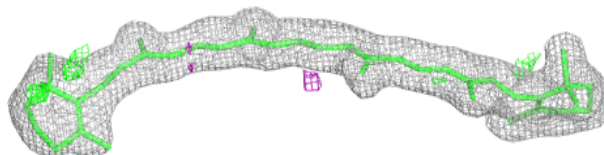
**Electron density around CLA b 618:**

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

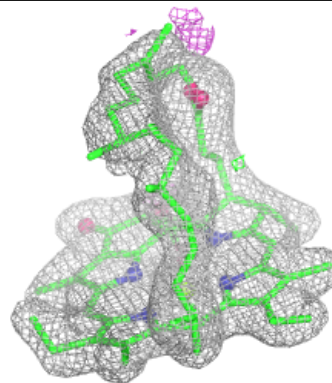
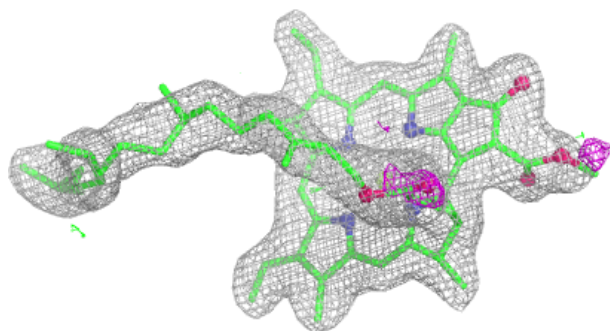
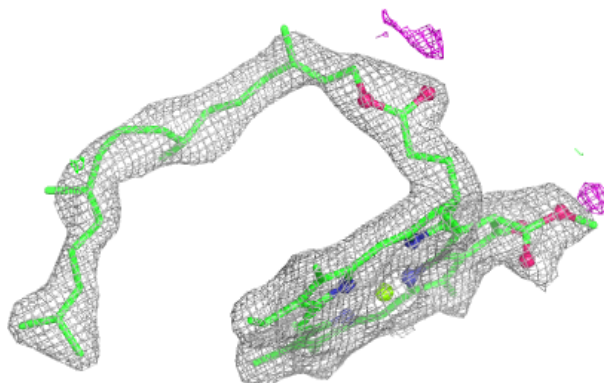


**Electron density around BCR D 405:**

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

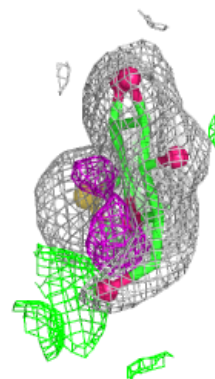
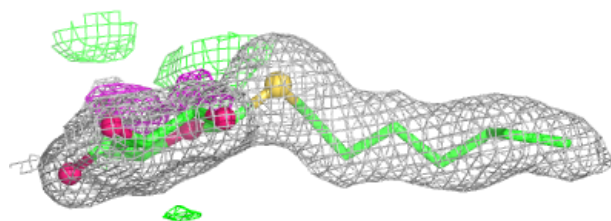
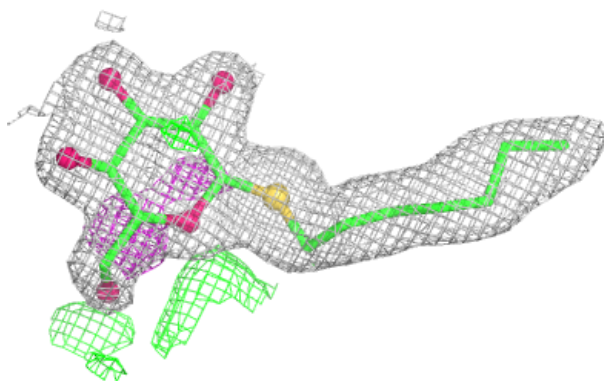
**Electron density around CLA c 513:**

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

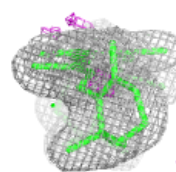
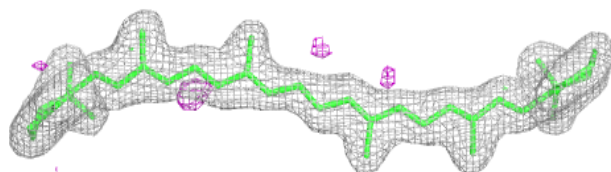
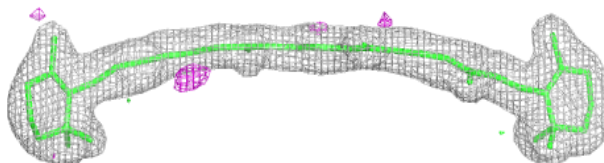


**Electron density around HTG B 621:**

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

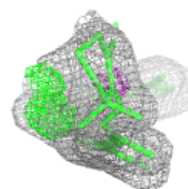
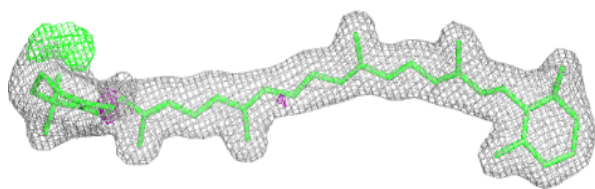
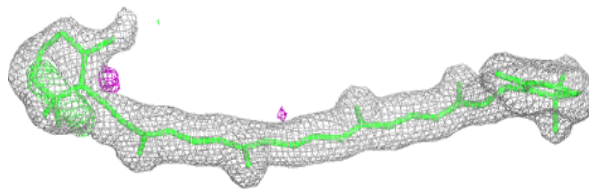
**Electron density around BCR K 102:**

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



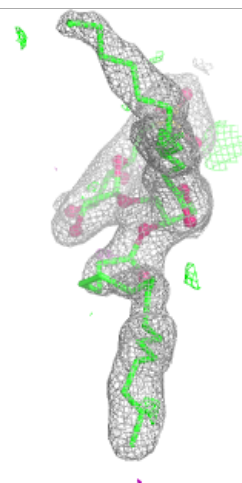
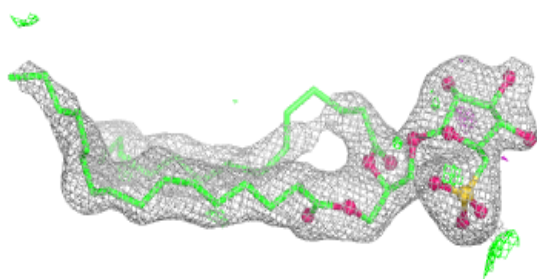
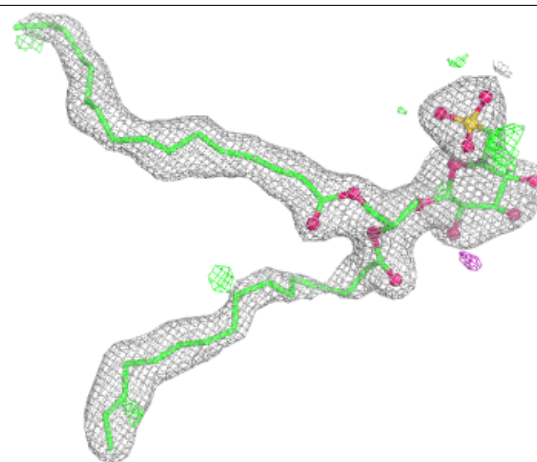
**Electron density around BCR d 405:**

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



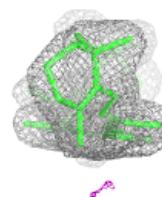
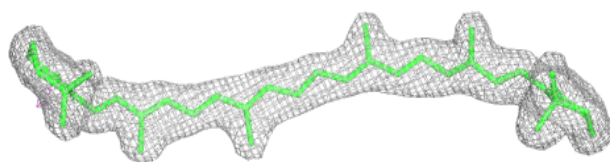
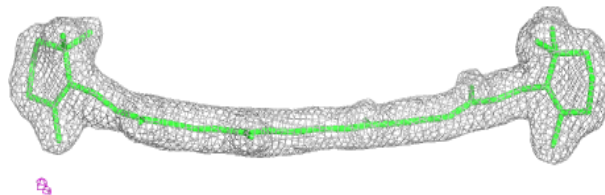
**Electron density around SQD a 409:**

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

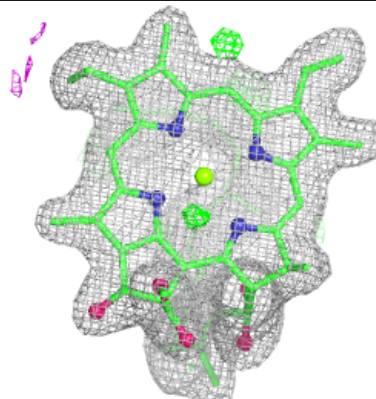
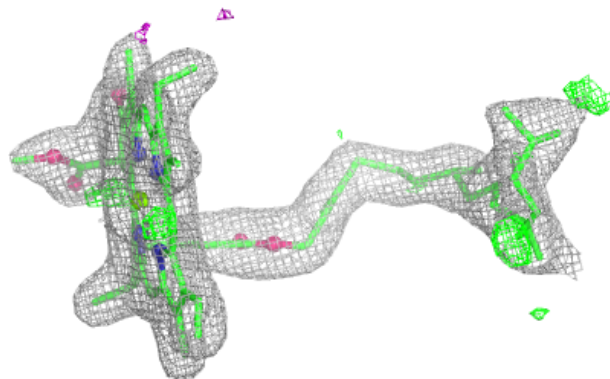
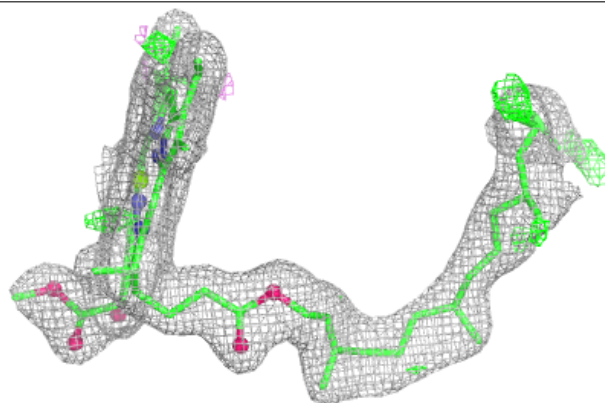


**Electron density around BCR k 101:**

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

**Electron density around CLA c 506:**

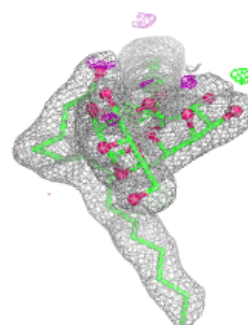
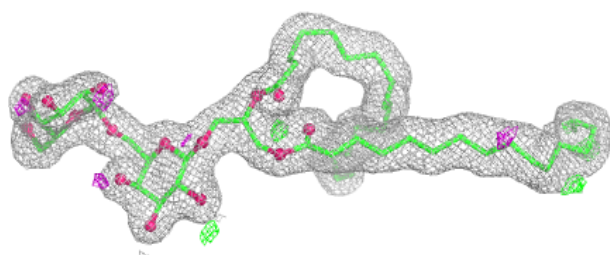
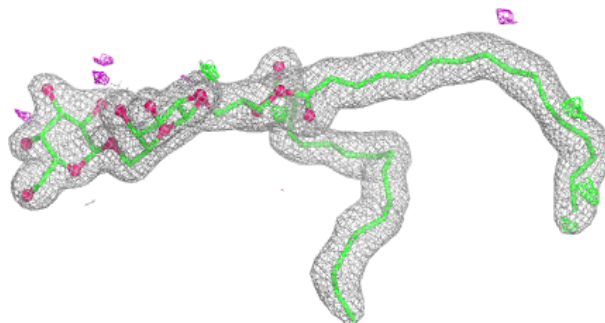
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



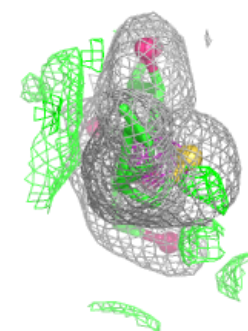
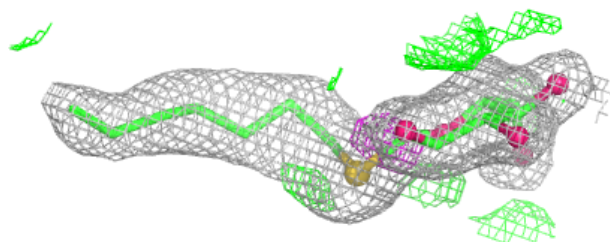
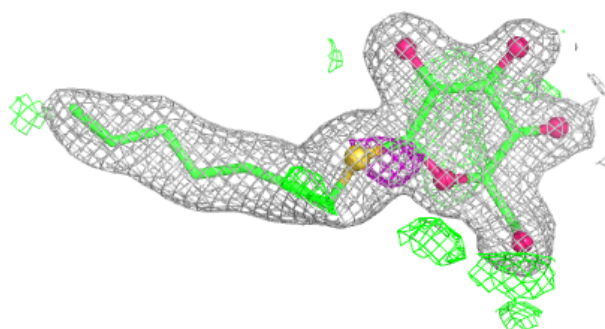


**Electron density around DGD H 102:**

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

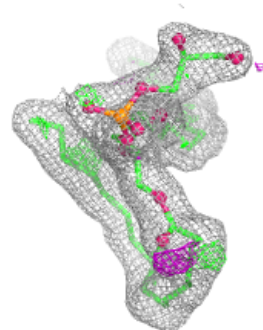
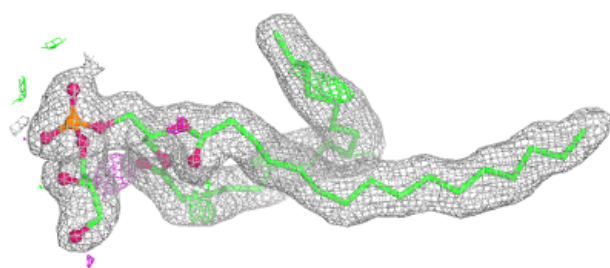
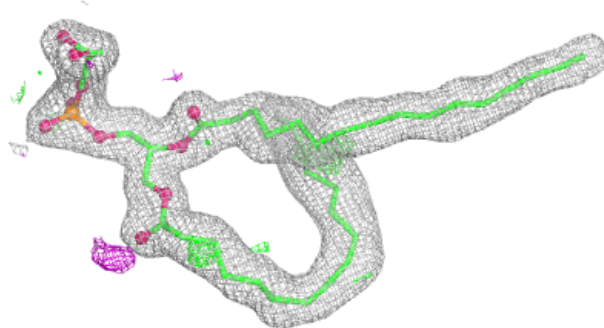
**Electron density around HTG O 302:**

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

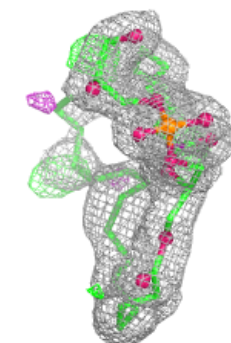
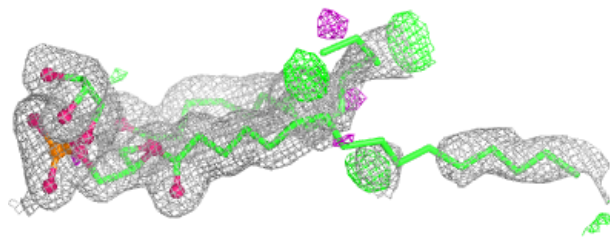
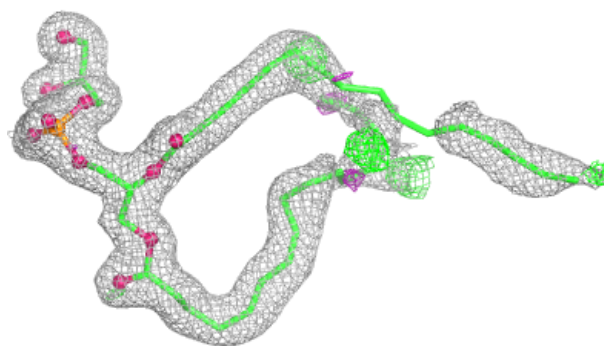


**Electron density around LHG D 407:**

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

**Electron density around LHG D 409:**

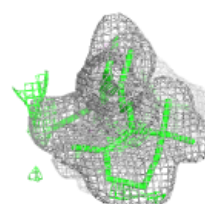
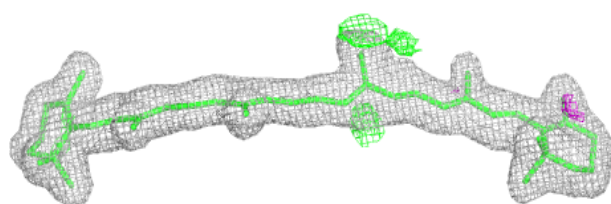
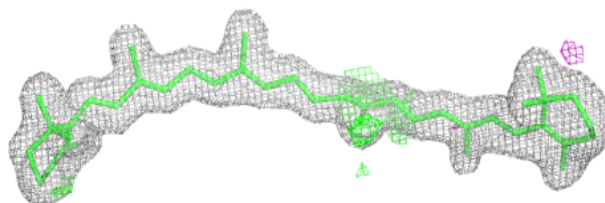
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



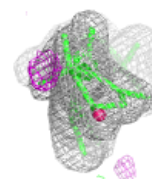
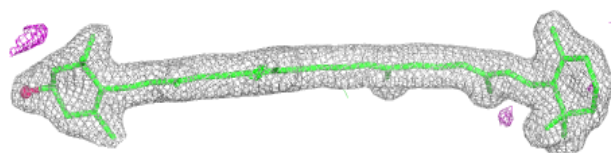
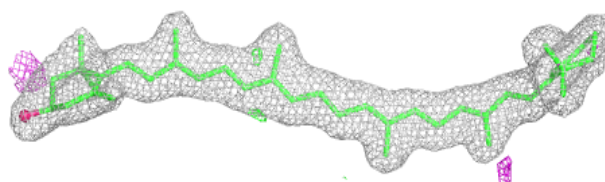


**Electron density around BCR t 101:**

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

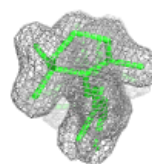
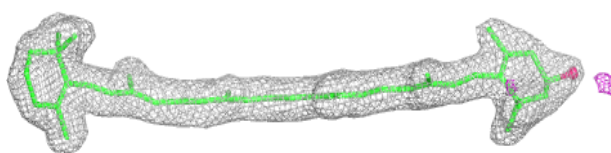
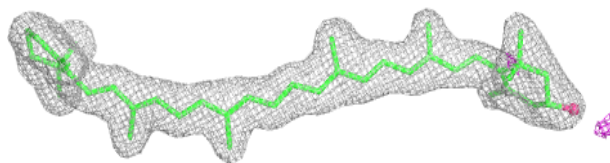
**Electron density around RRX H 101:**

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

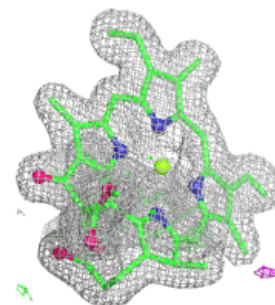
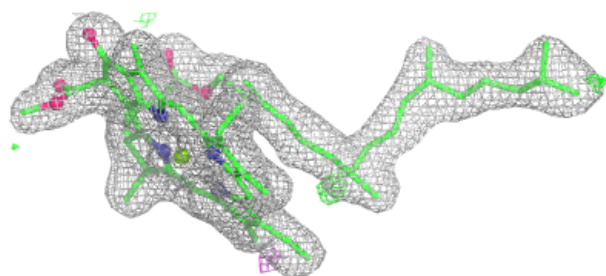
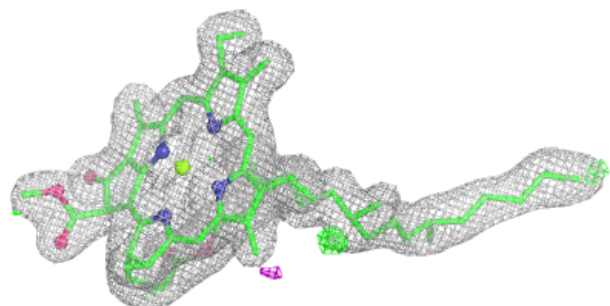


**Electron density around RRX x 101:**

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

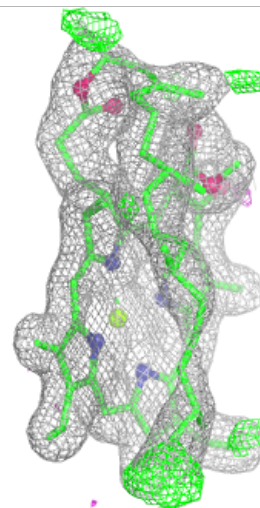
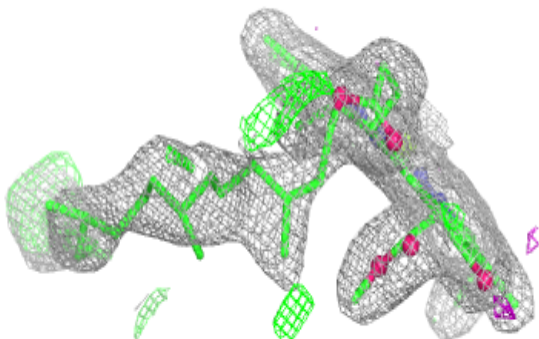
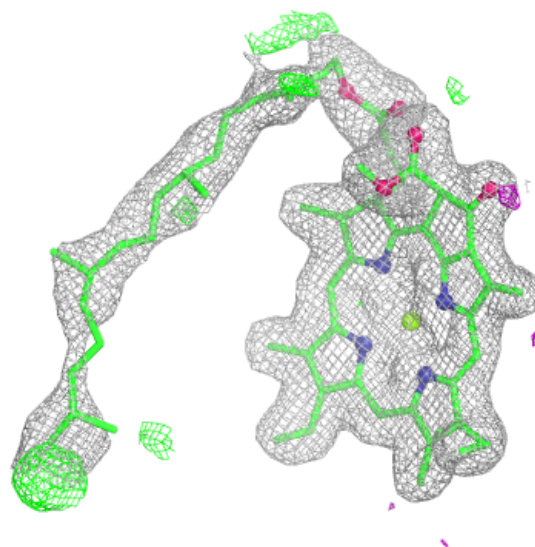
**Electron density around CLA C 505:**

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



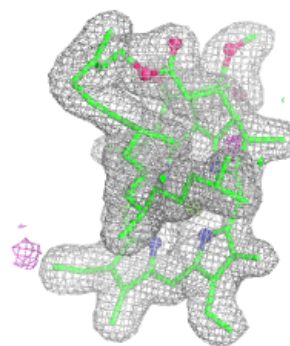
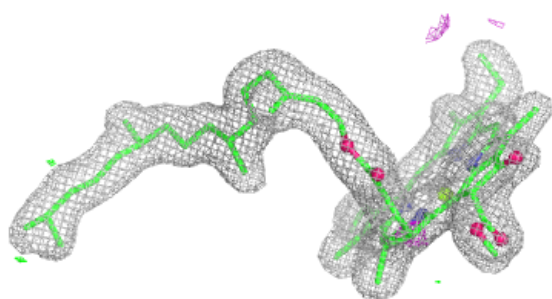
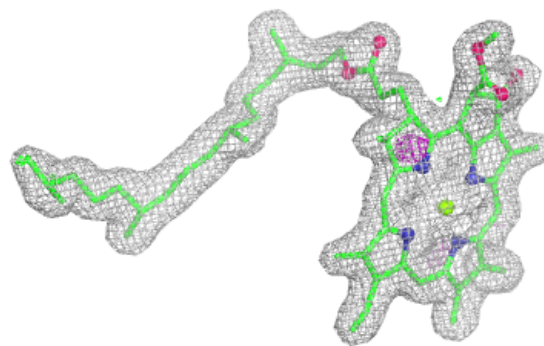
**Electron density around CLA B 601:**

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



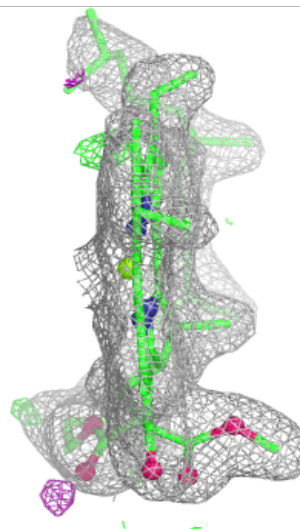
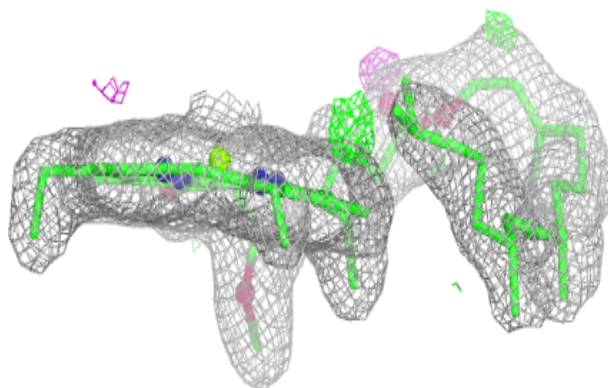
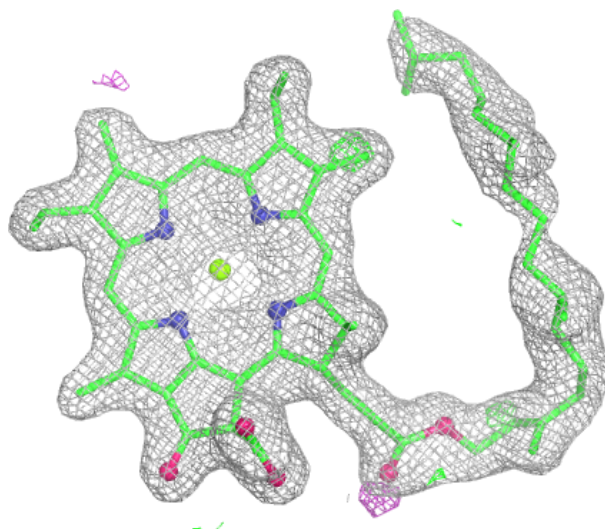
**Electron density around CLA c 511:**

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



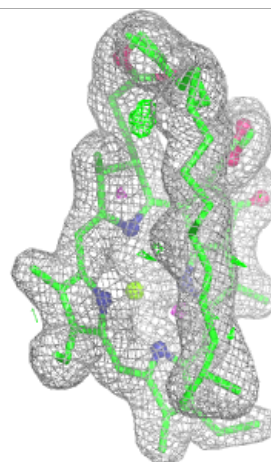
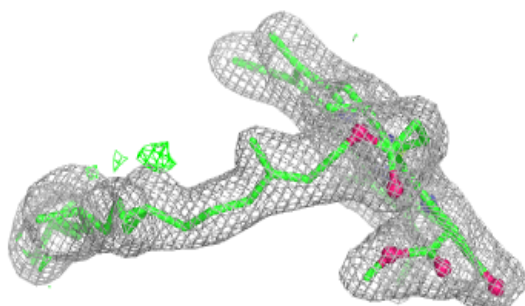
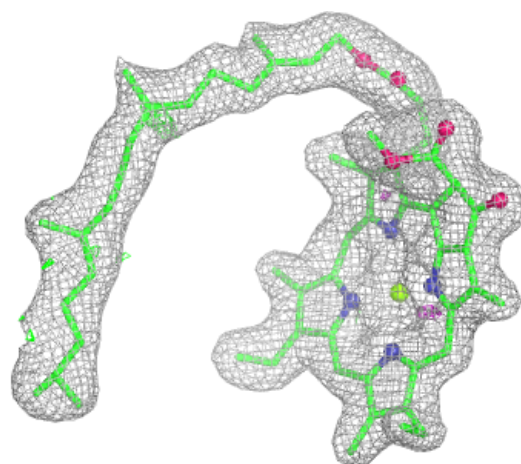
**Electron density around CLA c 512:**

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



**Electron density around CLA C 507:**

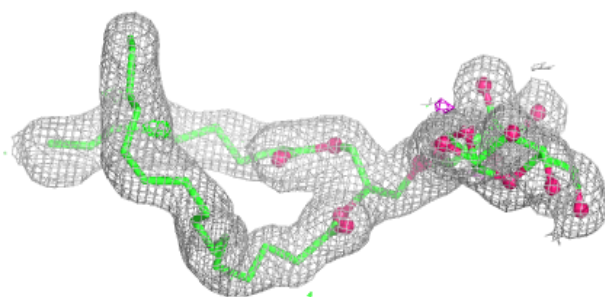
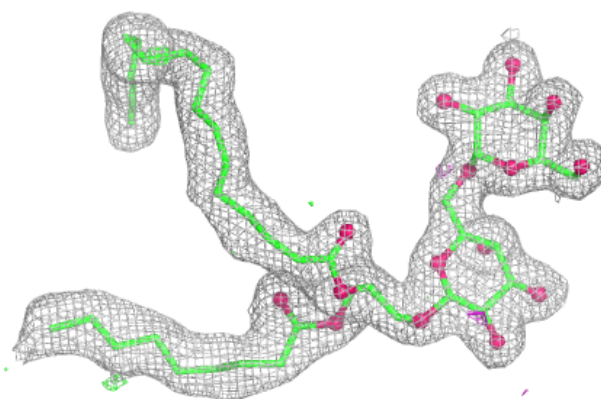
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



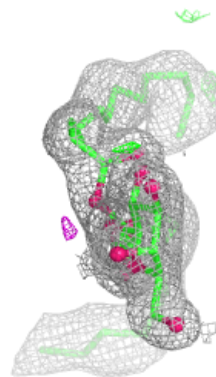
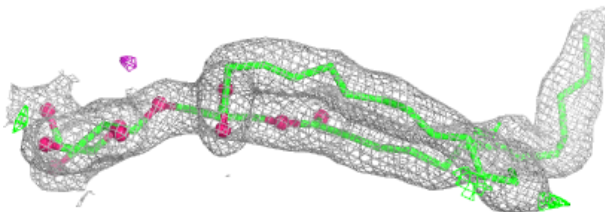
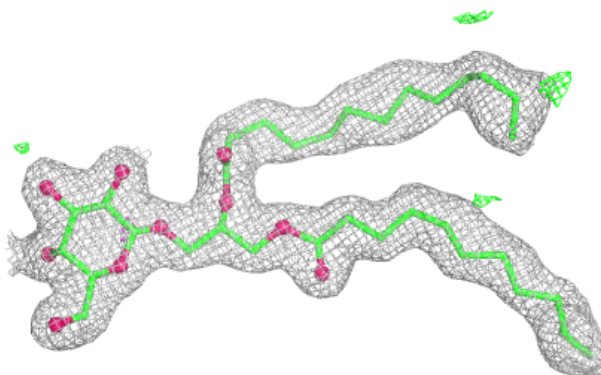


**Electron density around DGD C 517:**

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

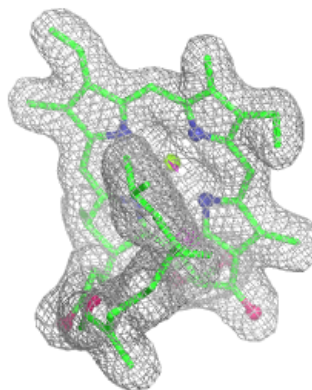
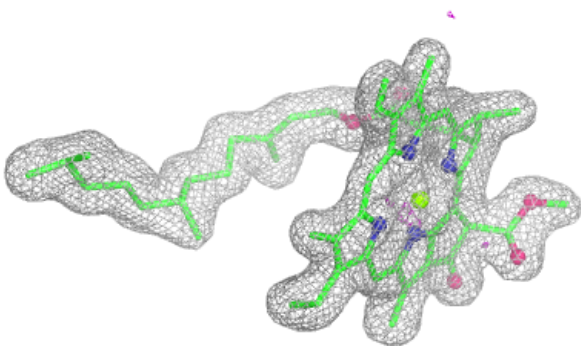
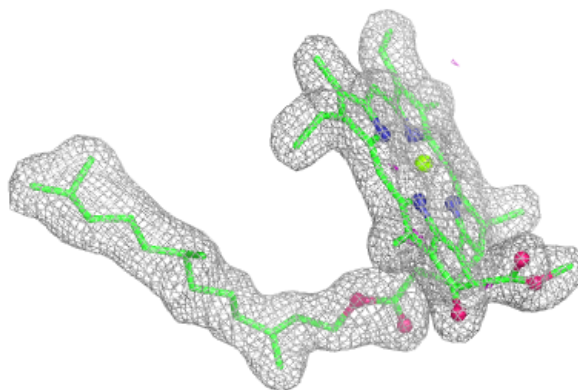
**Electron density around LMG j 101:**

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

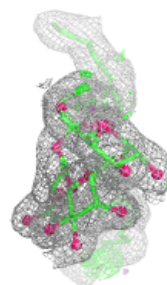
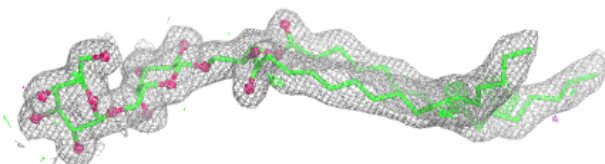
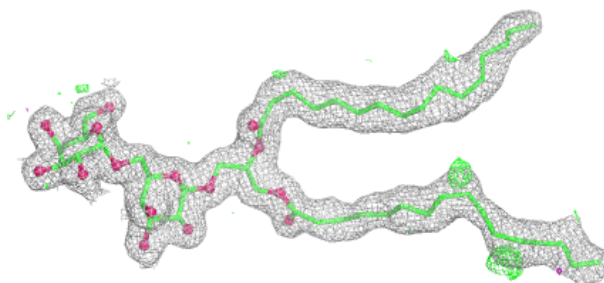


**Electron density around CLA C 508:**

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

**Electron density around DGD c 517:**

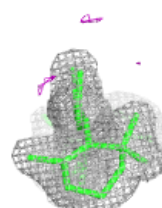
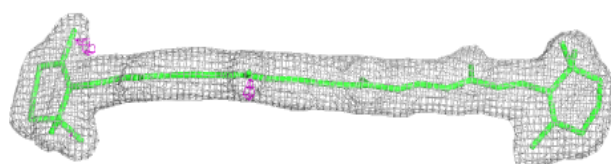
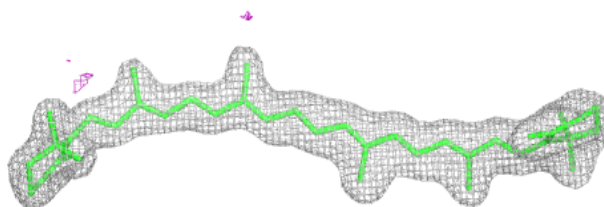
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



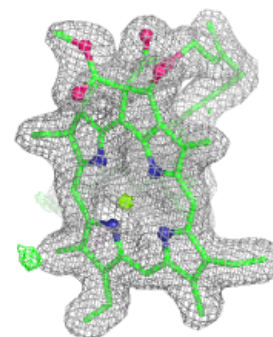
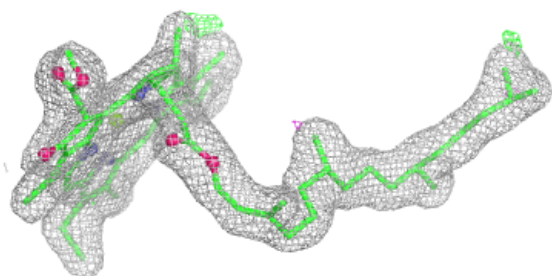
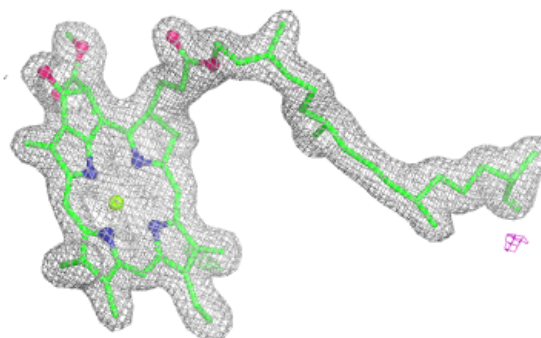


**Electron density around BCR C 515:**

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

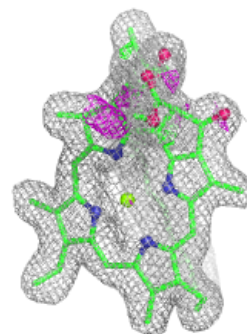
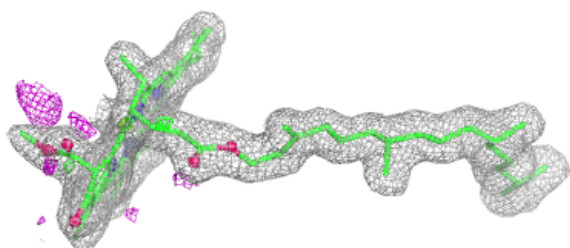
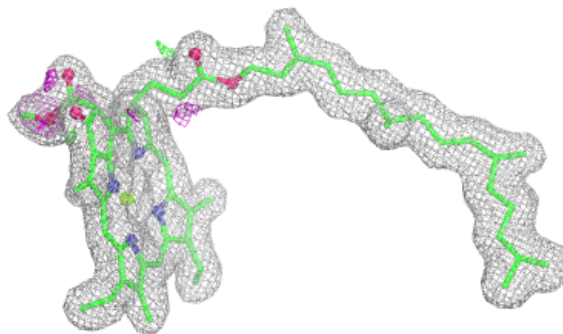
**Electron density around CLA C 511:**

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



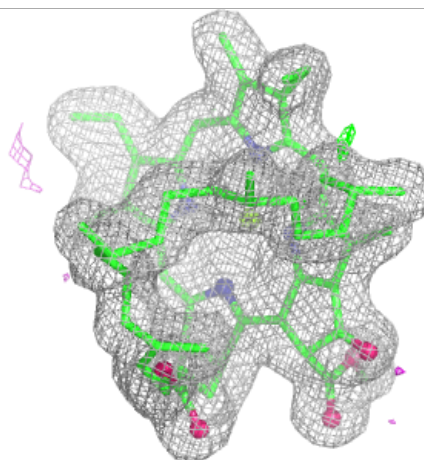
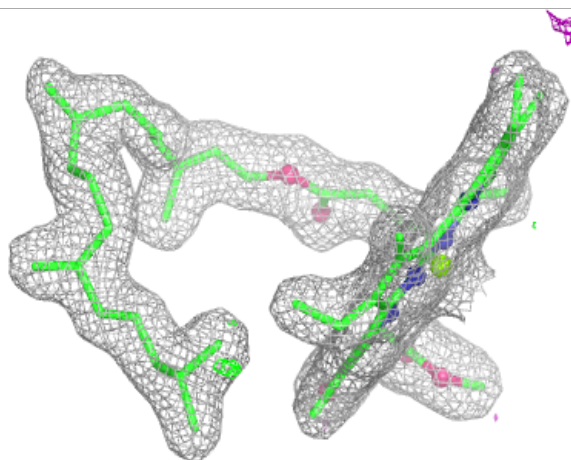
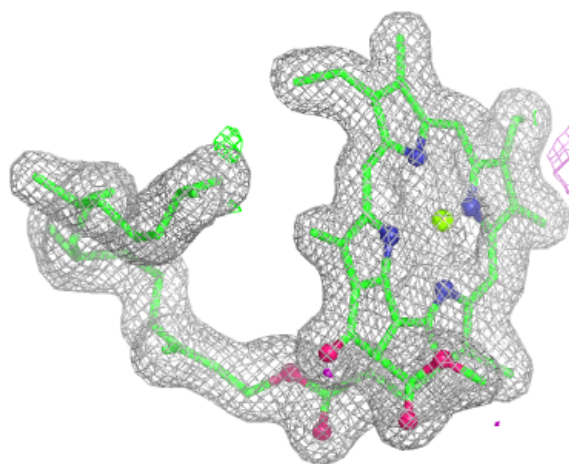
**Electron density around CLA B 610:**

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



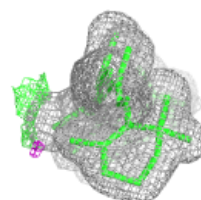
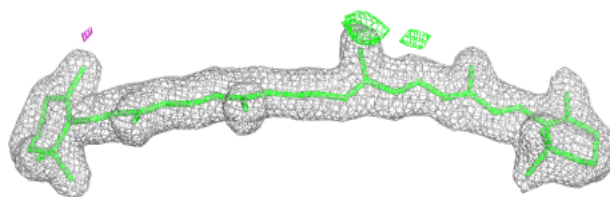
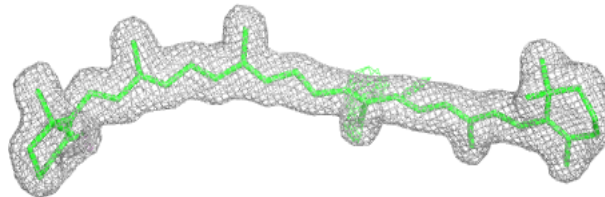
**Electron density around CLA C 503:**

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

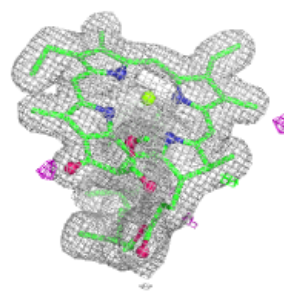
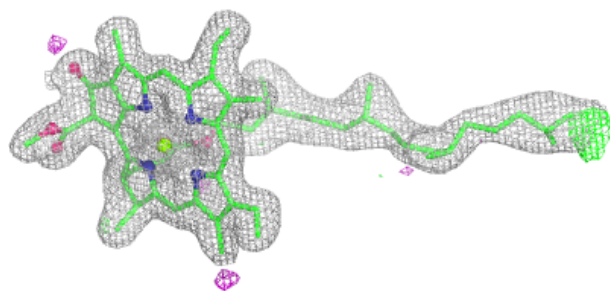
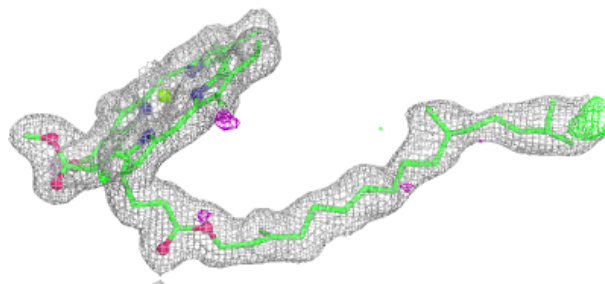


**Electron density around BCR T 101:**

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

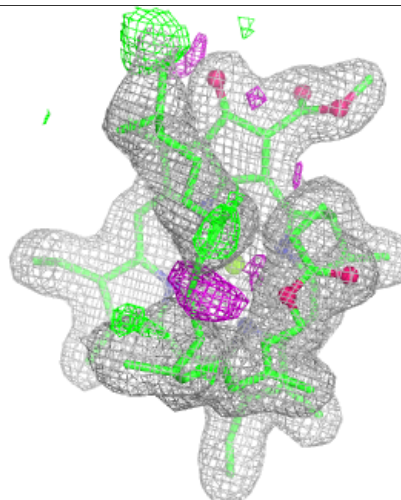
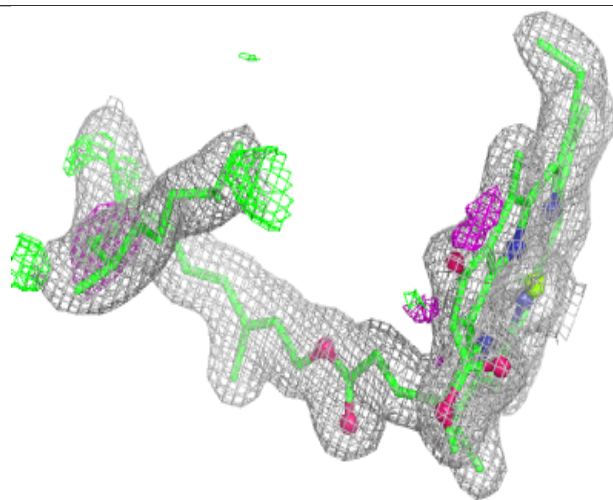
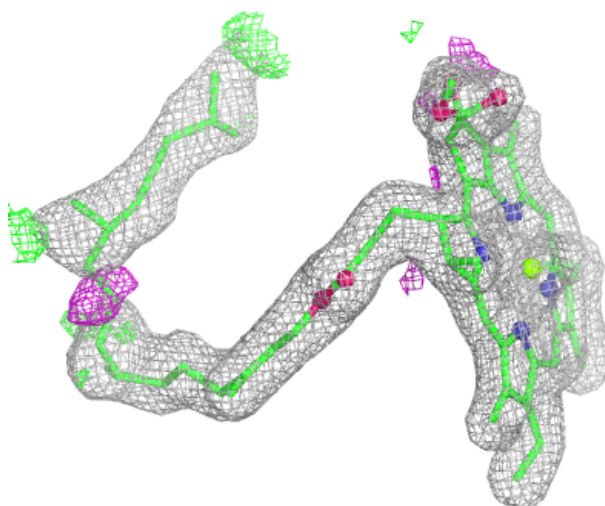
**Electron density around CLA C 504:**

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



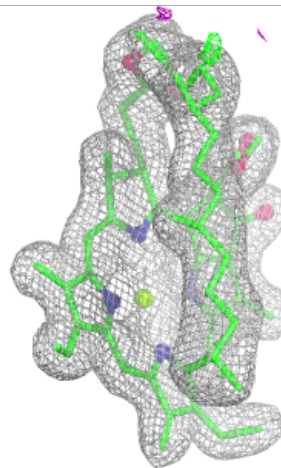
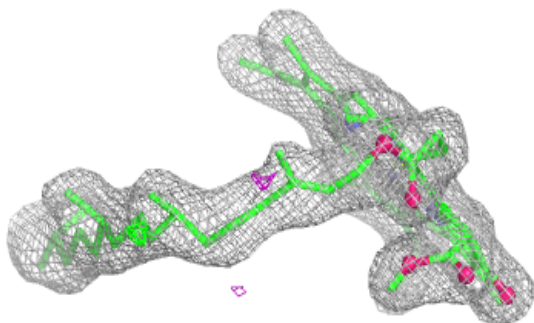
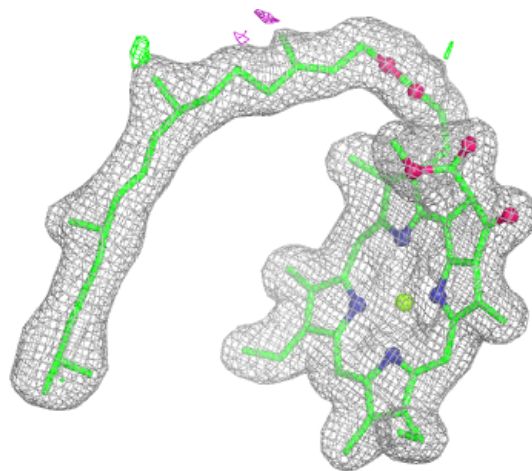
**Electron density around CLA b 608:**

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



**Electron density around CLA c 507:**

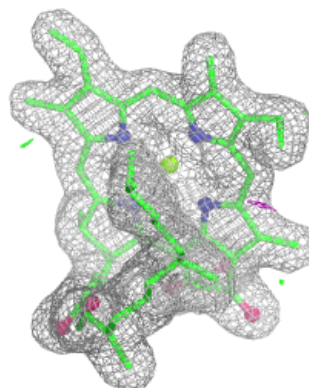
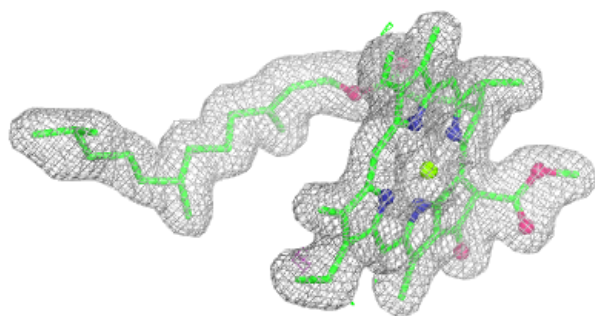
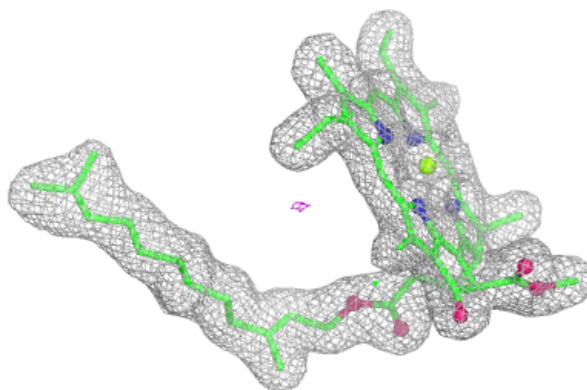
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





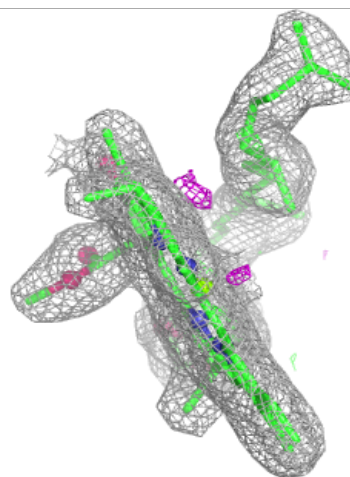
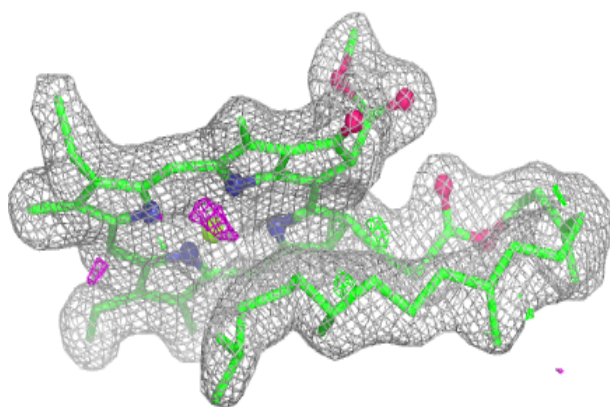
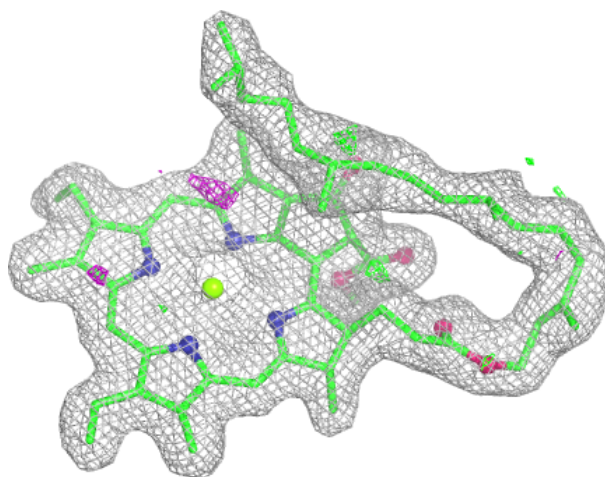
**Electron density around CLA c 508:**

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



**Electron density around CLA c 509:**

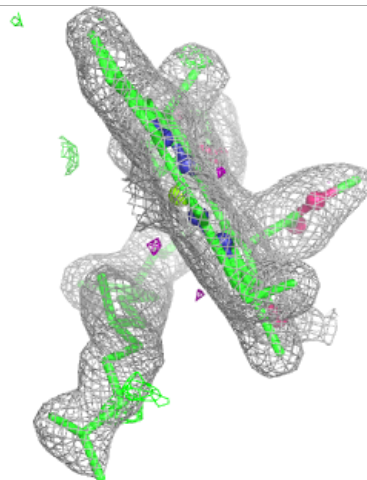
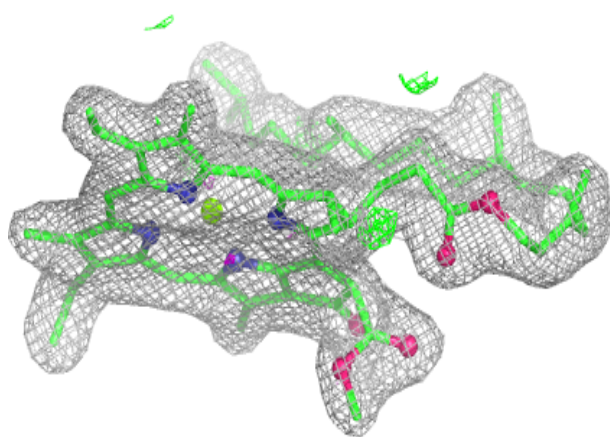
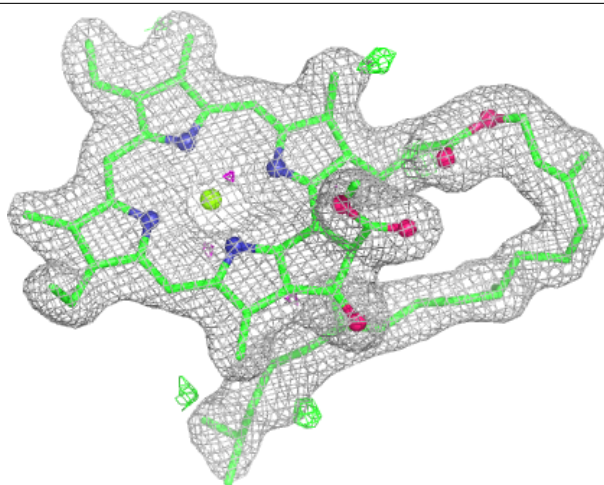
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





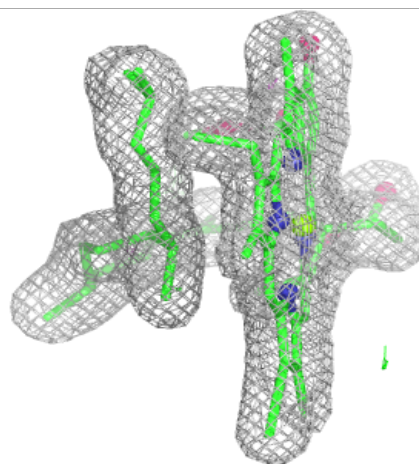
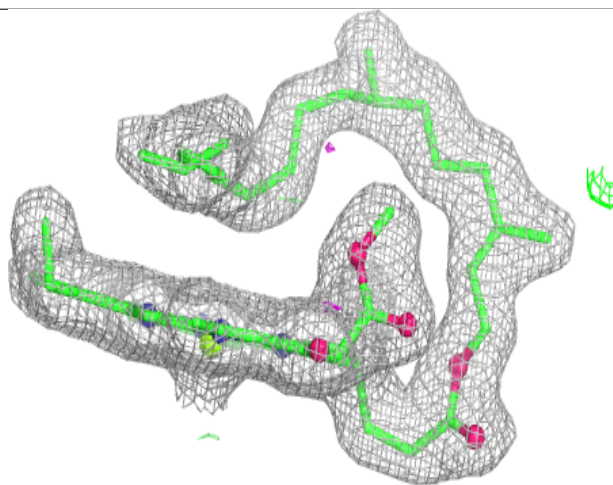
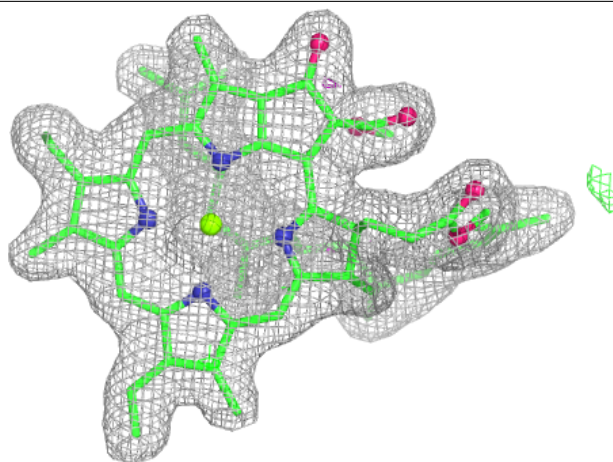
**Electron density around CLA C 509:**

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



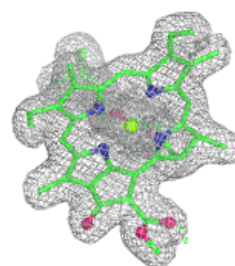
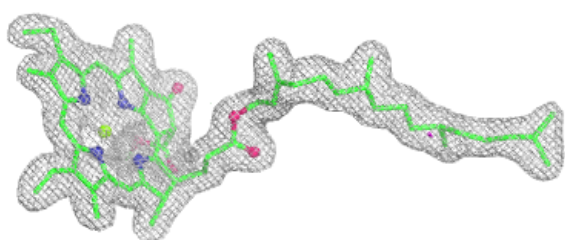
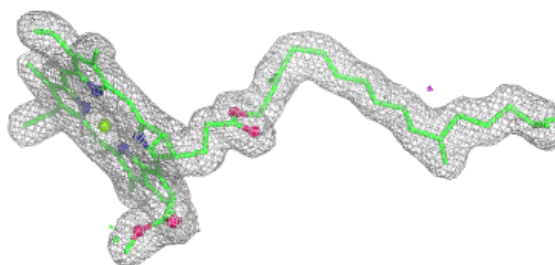
**Electron density around CLA C 510:**

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

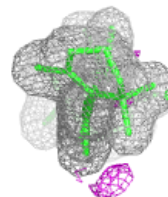
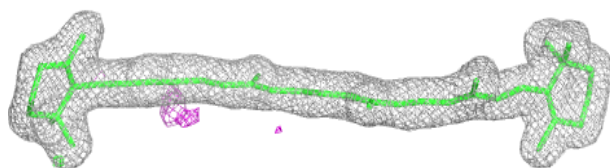
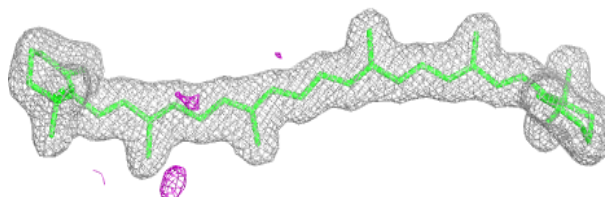


**Electron density around CLA C 502:**

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

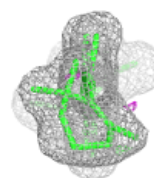
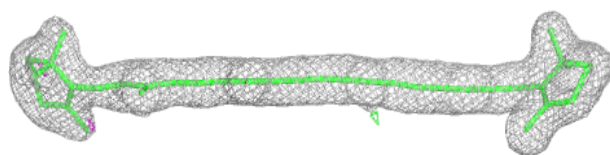
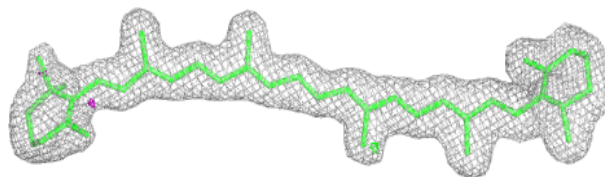
**Electron density around BCR A 405:**

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

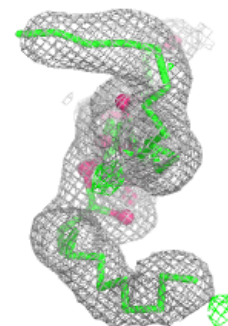
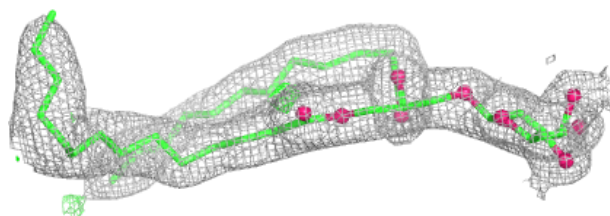
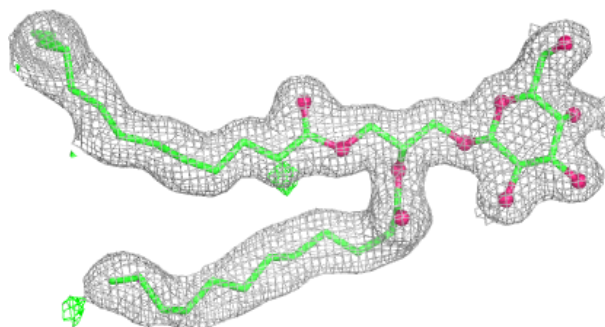


**Electron density around BCR B 618:**

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

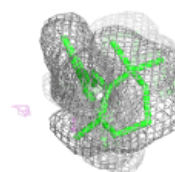
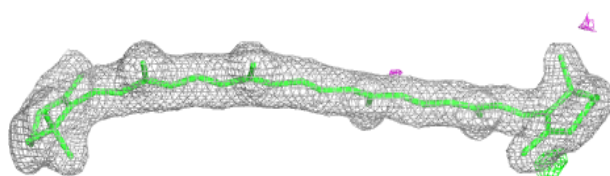
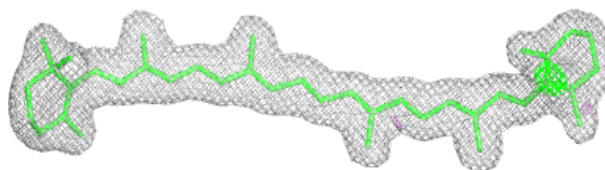
**Electron density around LMG J 101:**

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

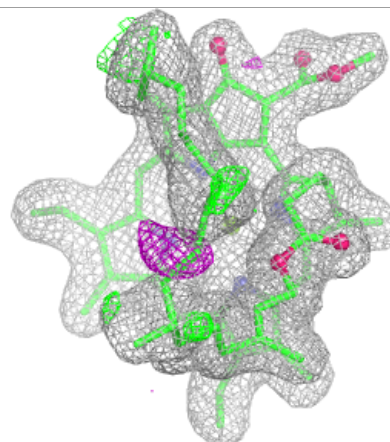
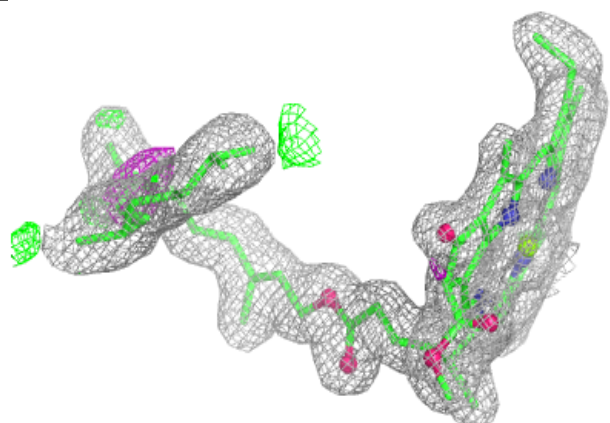
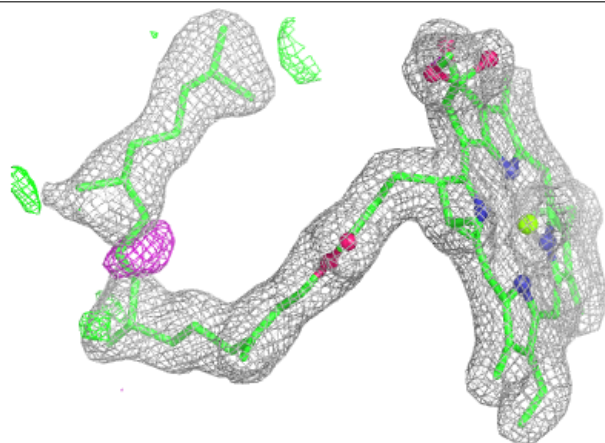


**Electron density around BCR B 619:**

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

**Electron density around CLA B 607:**

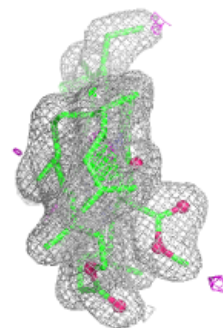
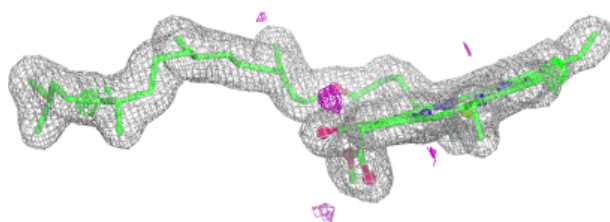
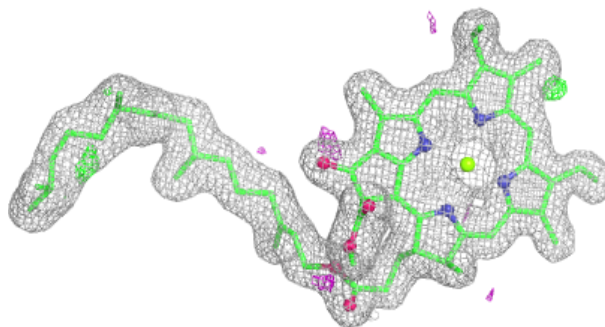
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



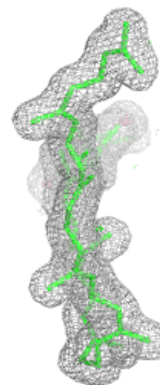
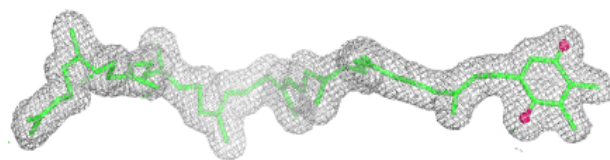
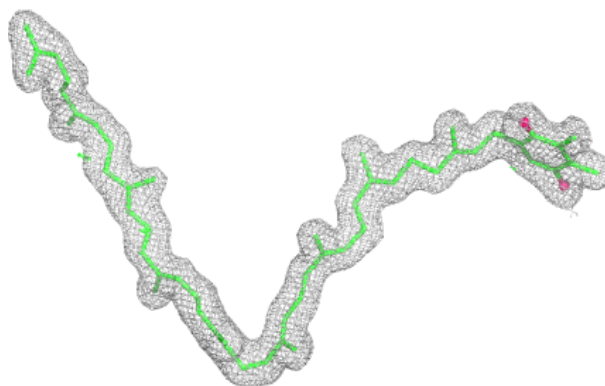


**Electron density around CLA B 603:**

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

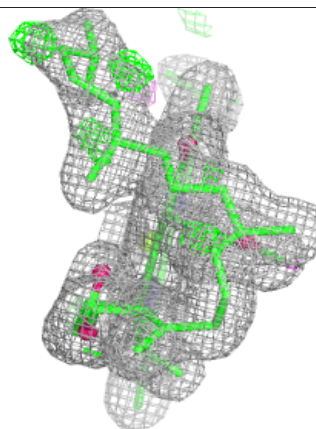
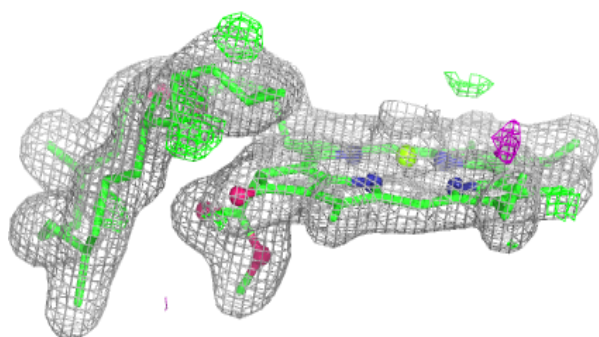
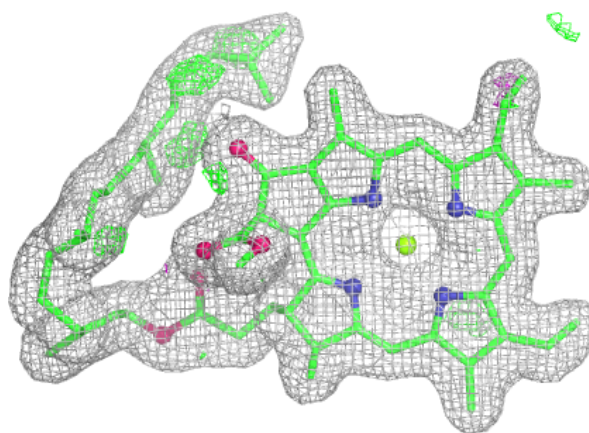
**Electron density around PL9 D 412:**

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

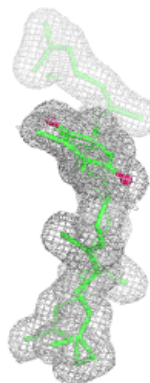
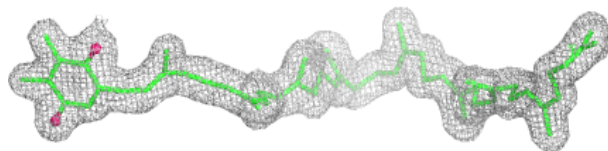
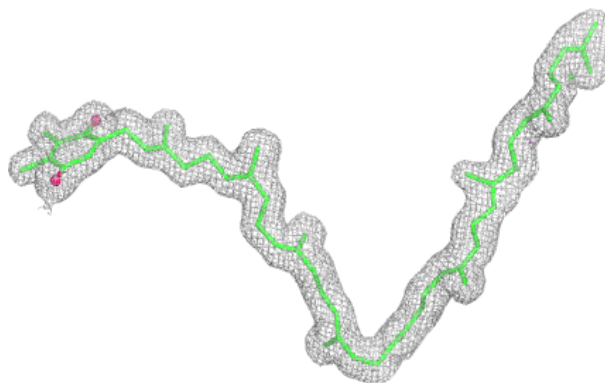


**Electron density around CLA B 611:**

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

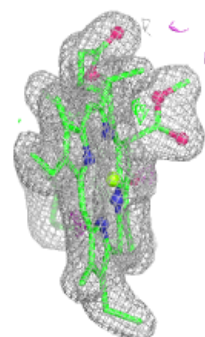
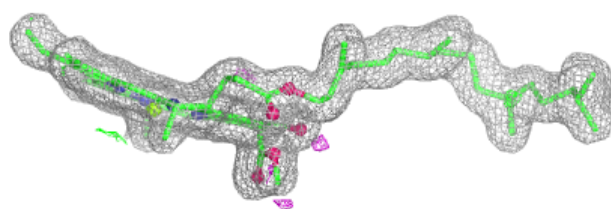
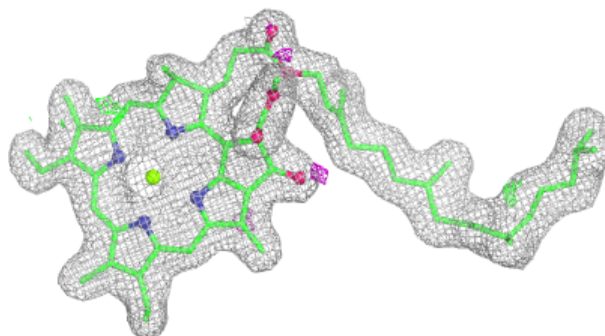
**Electron density around PL9 d 412:**

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

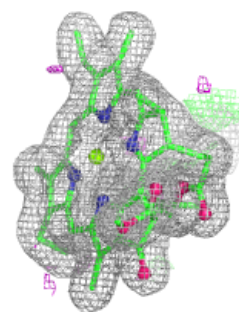
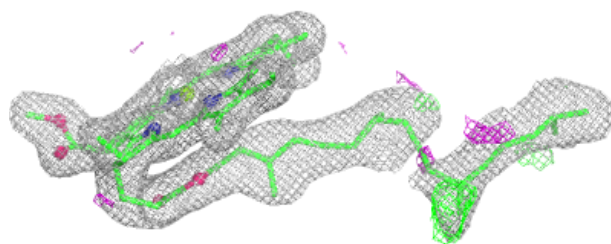
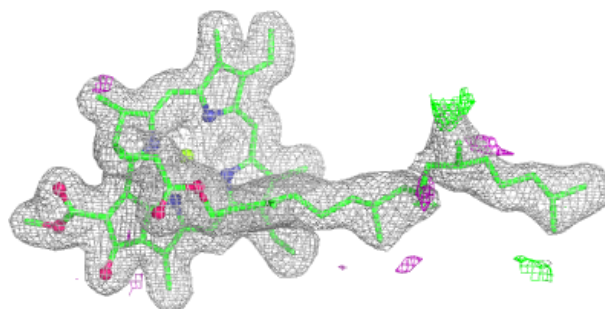


**Electron density around CLA b 604:**

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

**Electron density around CLA B 615:**

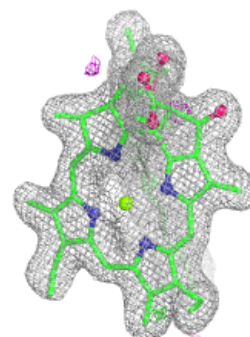
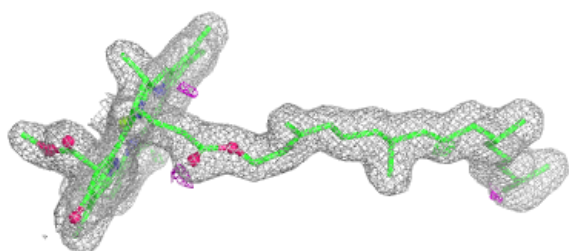
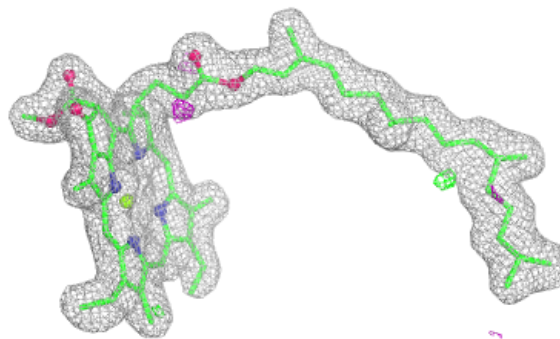
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



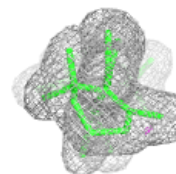
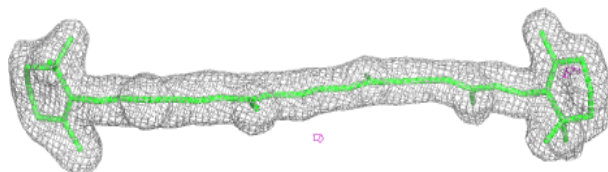
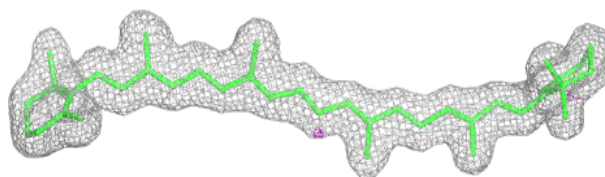


**Electron density around CLA b 611:**

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

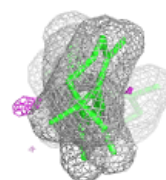
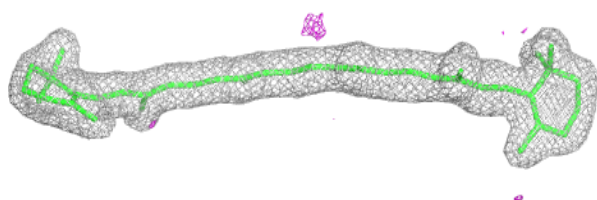
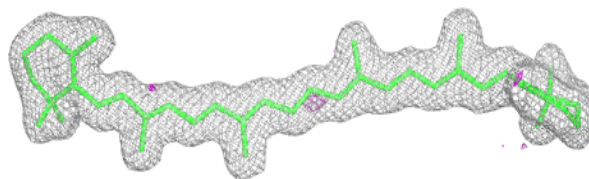
**Electron density around BCR a 408:**

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

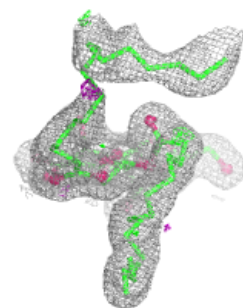
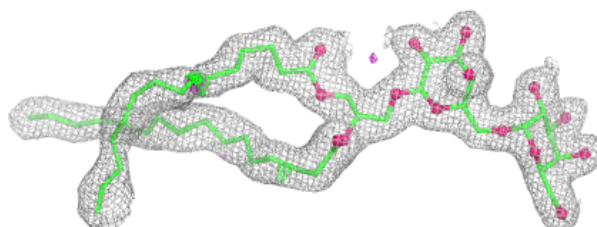
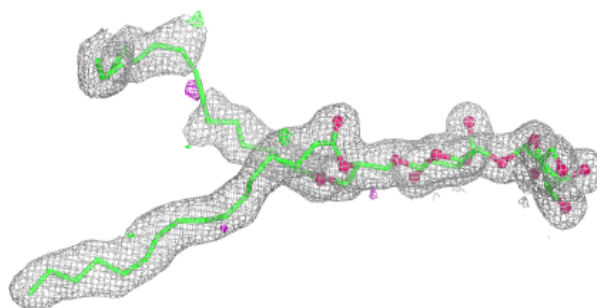


**Electron density around BCR b 619:**

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

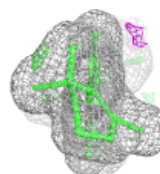
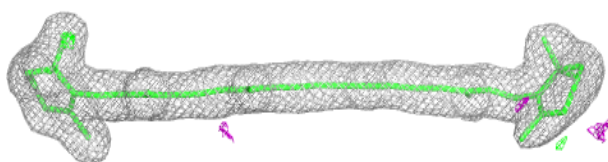
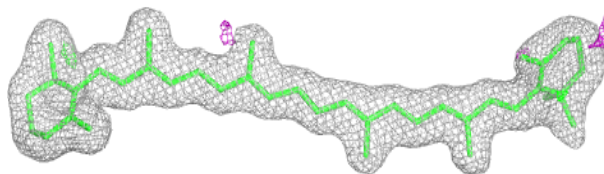
**Electron density around DGD C 516:**

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

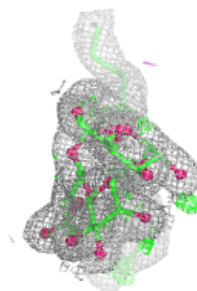
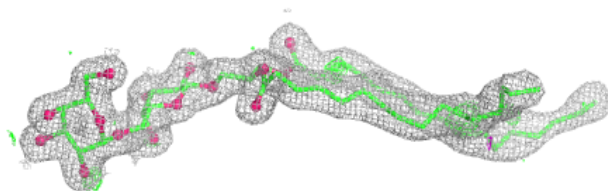
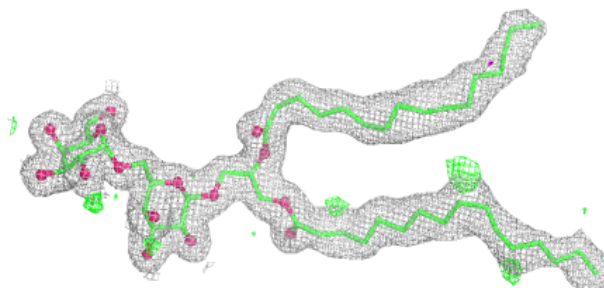


**Electron density around BCR b 620:**

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

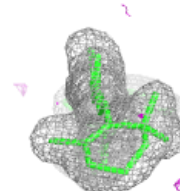
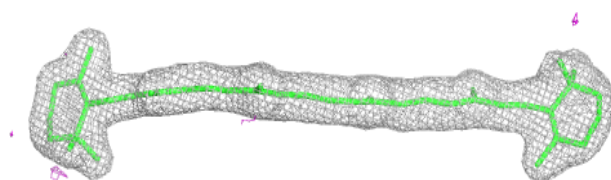
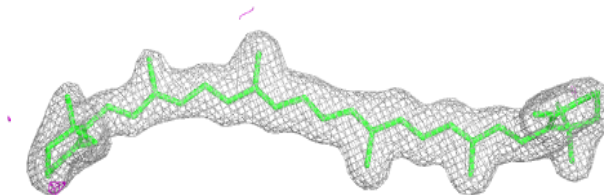
**Electron density around DGD C 518:**

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

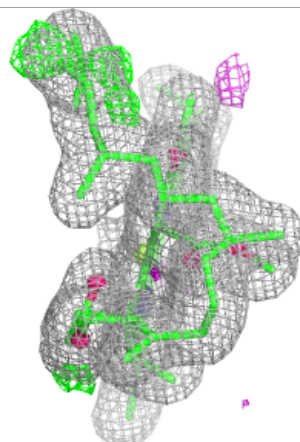
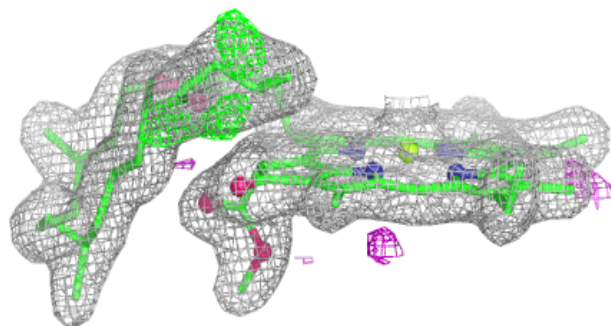
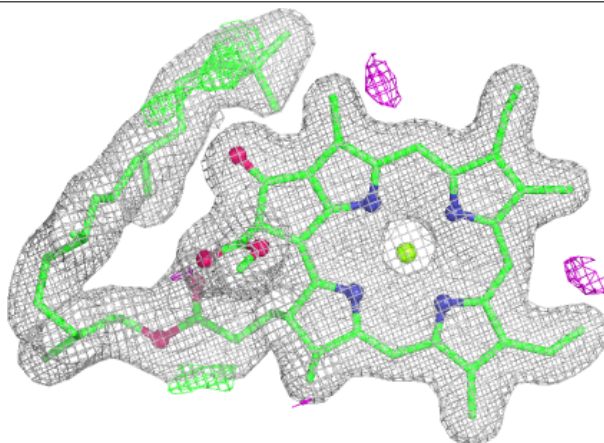


**Electron density around BCR c 514:**

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

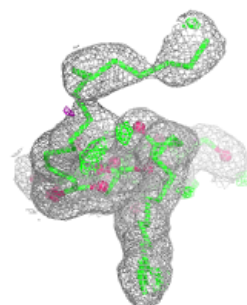
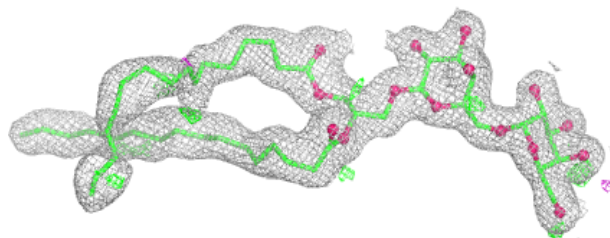
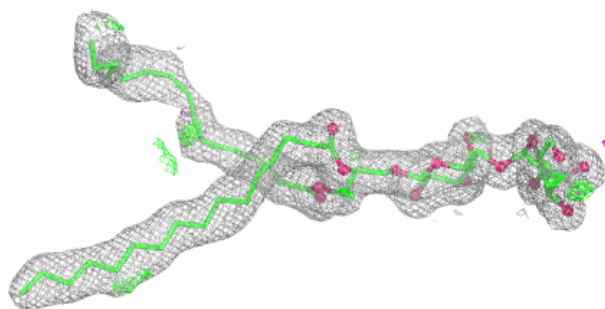
**Electron density around CLA b 612:**

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

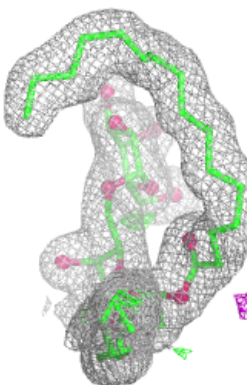
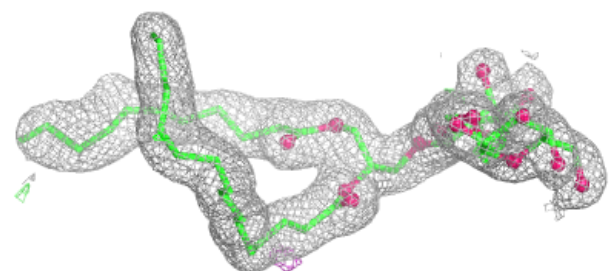
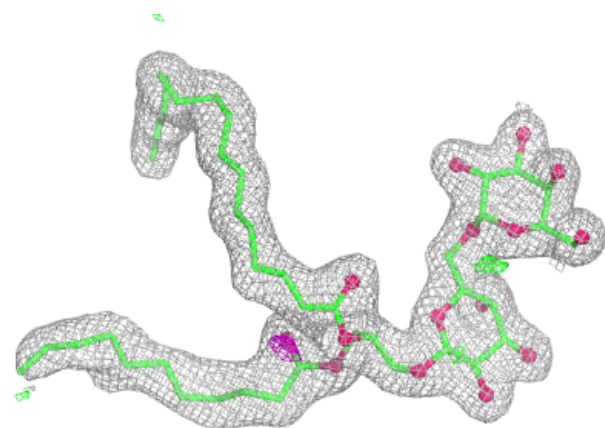


**Electron density around DGD c 515:**

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

**Electron density around DGD c 516:**

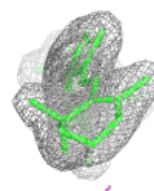
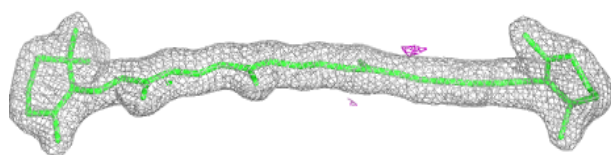
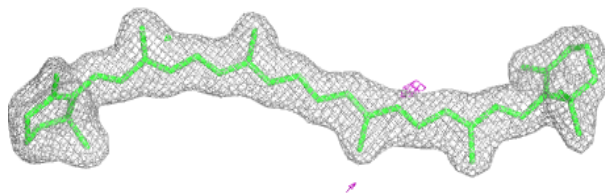
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



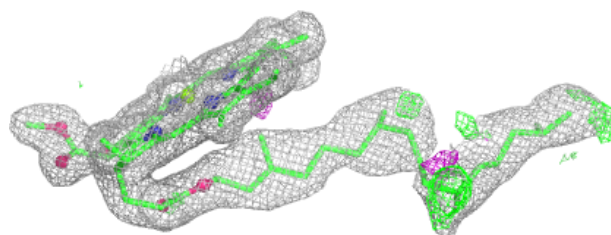
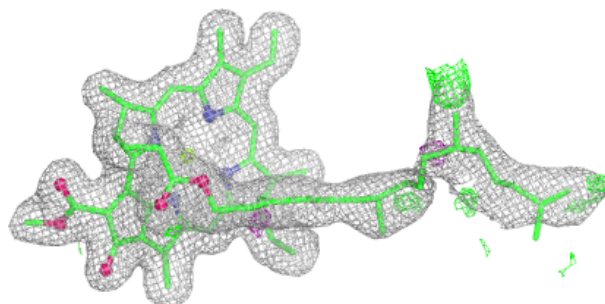


**Electron density around BCR j 102:**

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

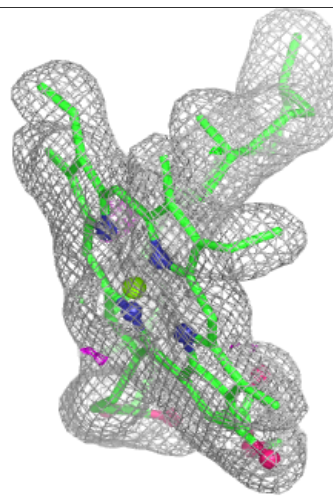
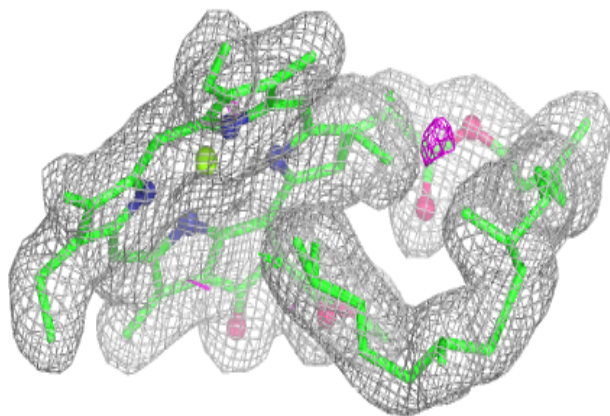
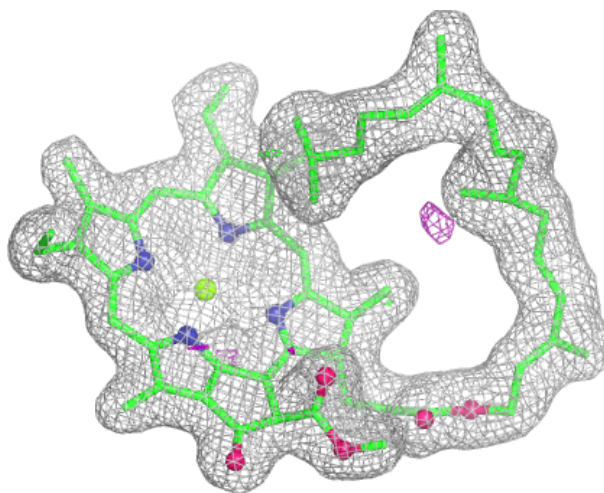
**Electron density around CLA b 616:**

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



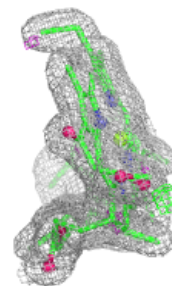
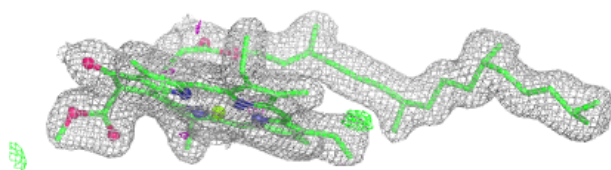
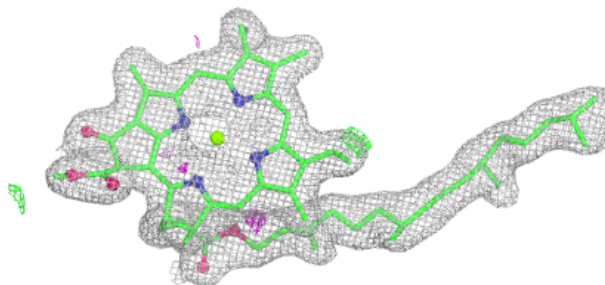
**Electron density around CLA B 616:**

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



**Electron density around CLA c 501:**

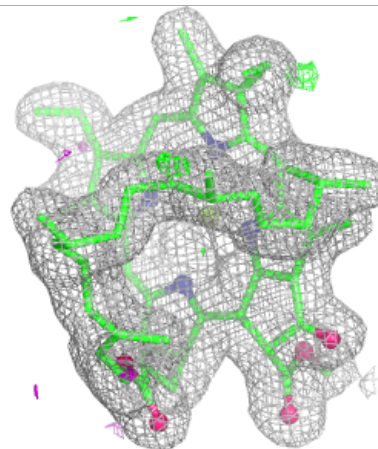
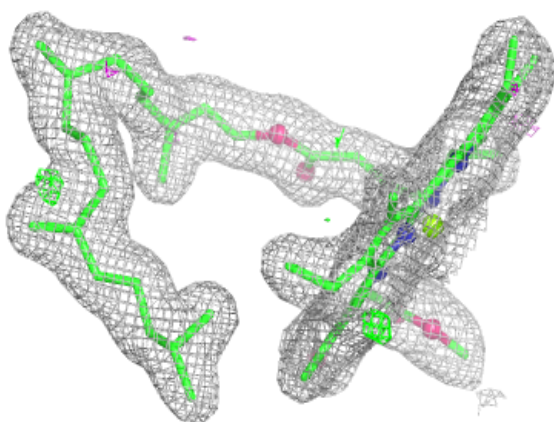
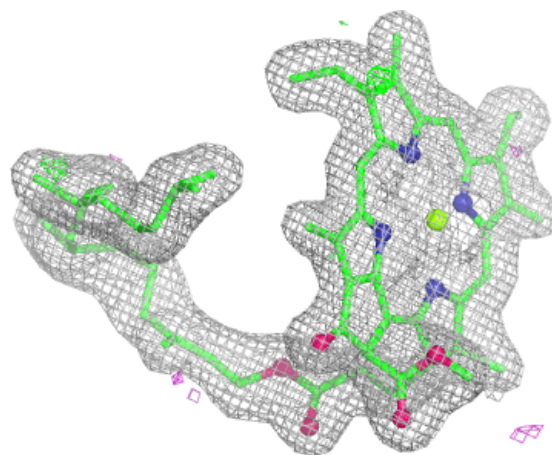
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





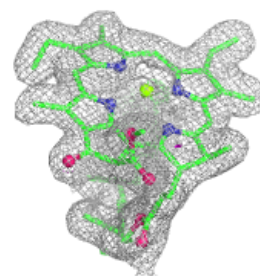
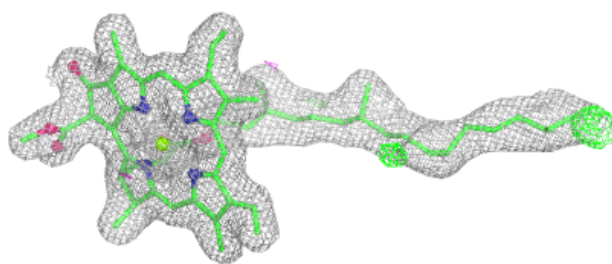
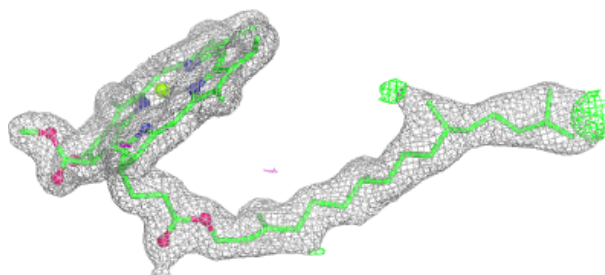
**Electron density around CLA c 503:**

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

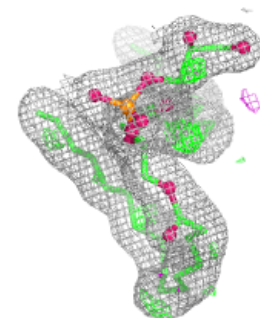
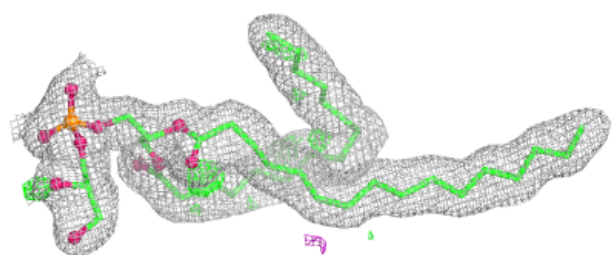
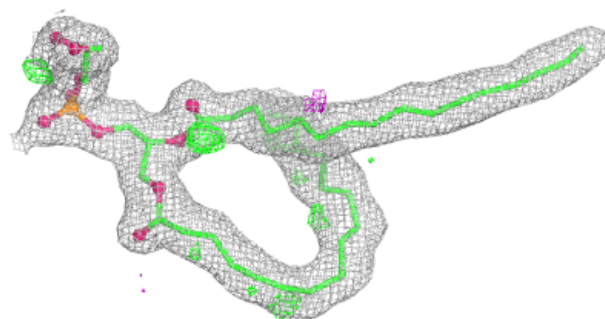


**Electron density around CLA c 504:**

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

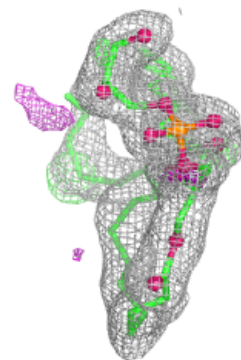
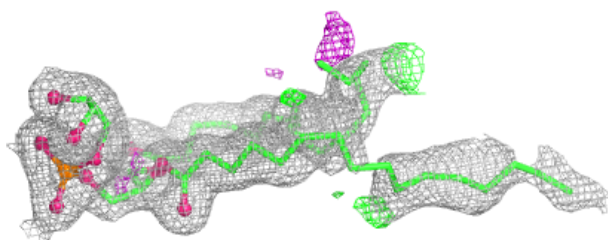
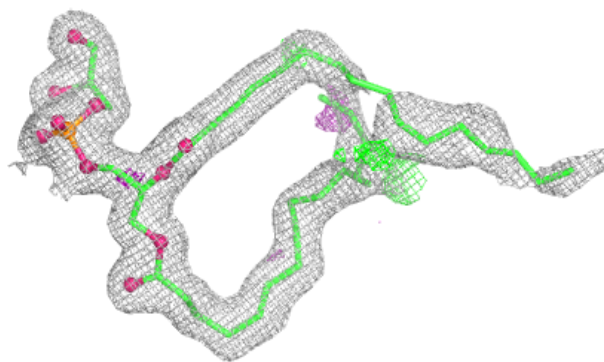
**Electron density around LHG d 406:**

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

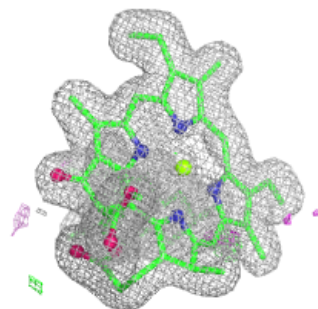
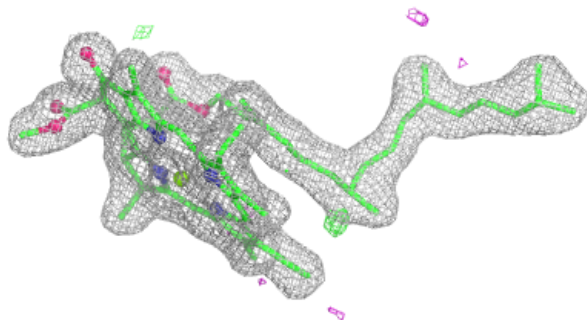
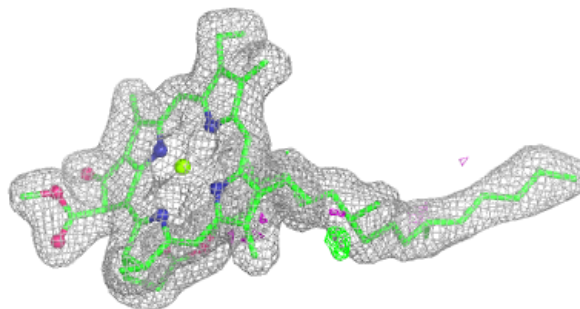


**Electron density around LHG d 408:**

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

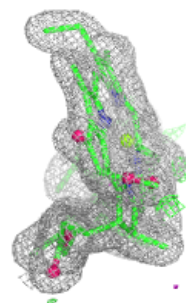
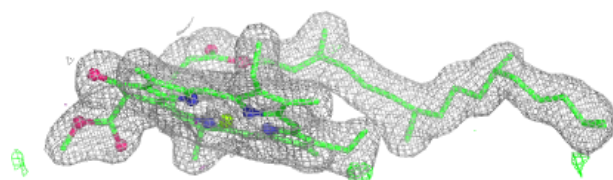
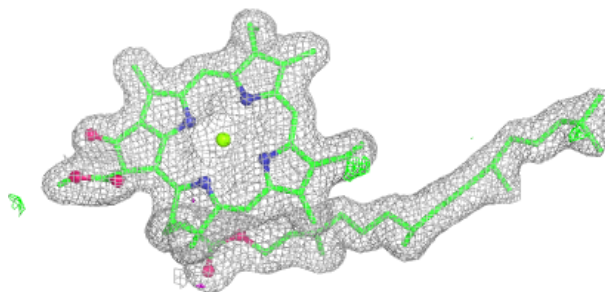
**Electron density around CLA c 505:**

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

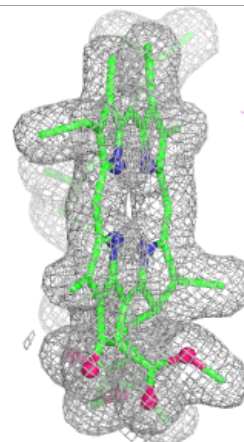
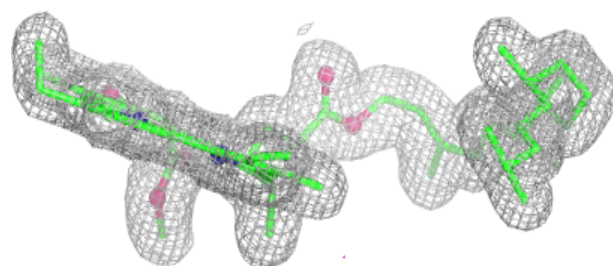
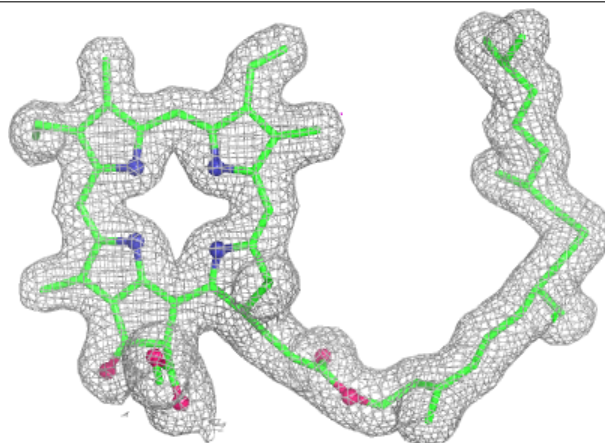


**Electron density around CLA C 501:**

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

**Electron density around PHO A 403:**

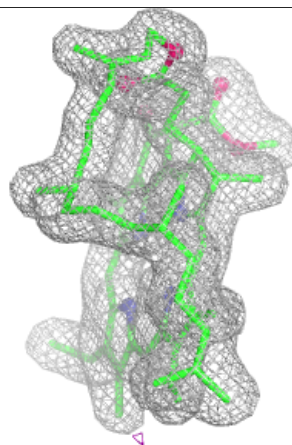
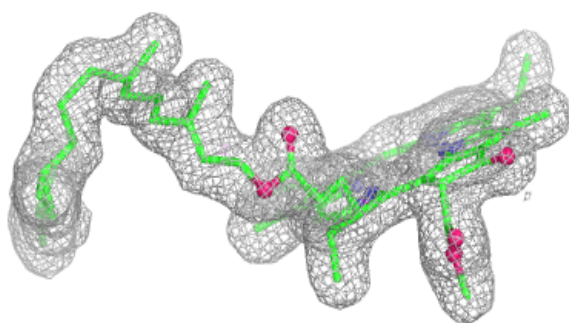
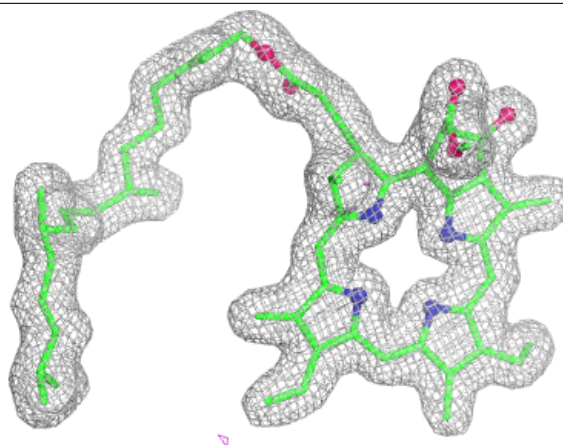
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





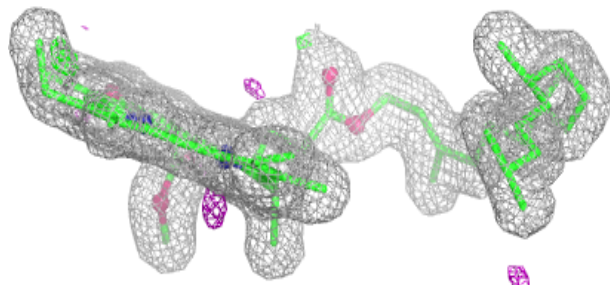
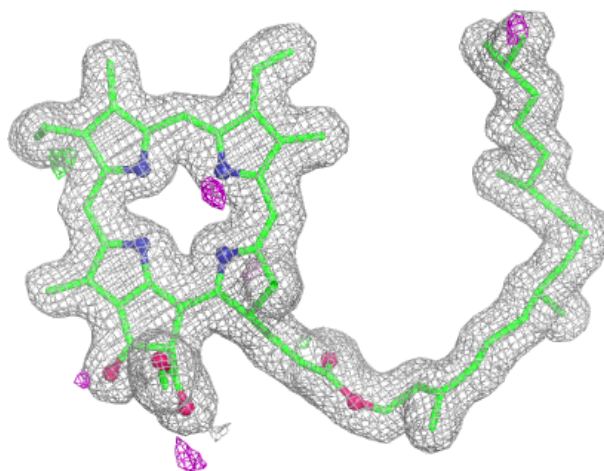
**Electron density around PHO D 403:**

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



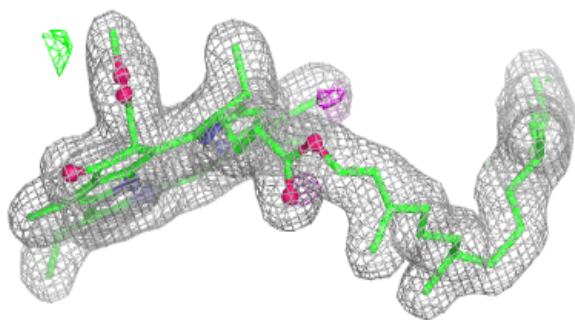
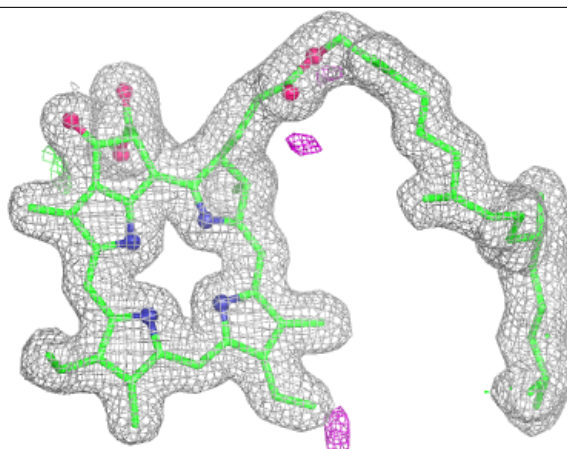
**Electron density around PHO a 405:**

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



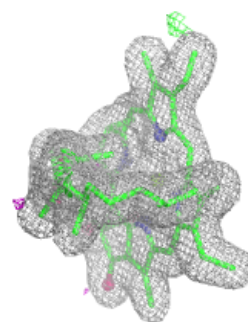
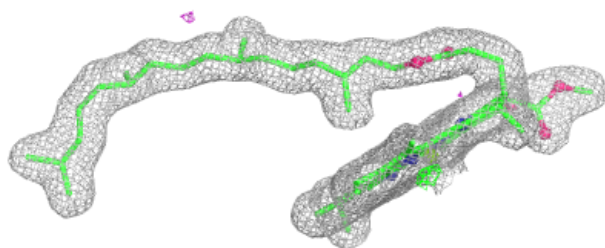
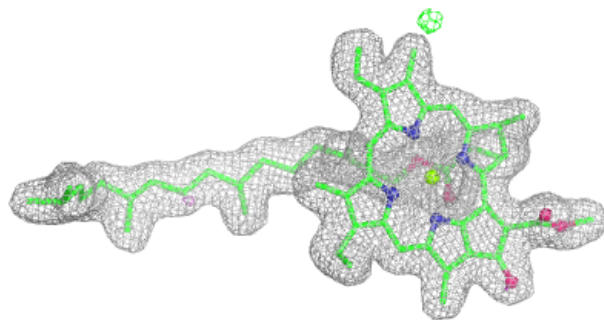
**Electron density around PHO a 406:**

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

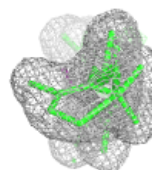
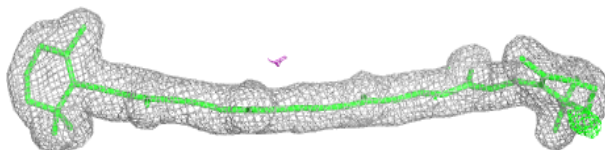
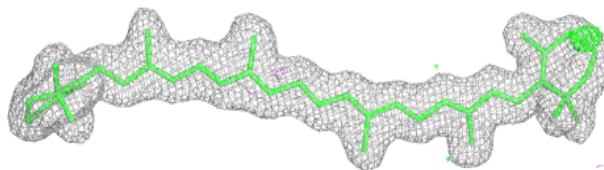


**Electron density around CLA b 610:**

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

**Electron density around BCR B 617:**

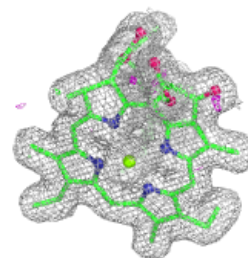
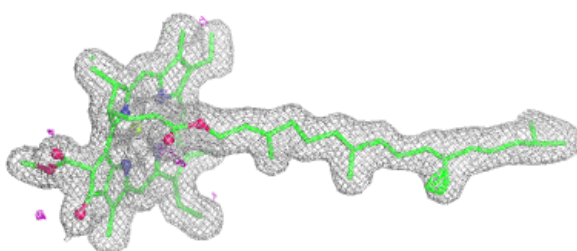
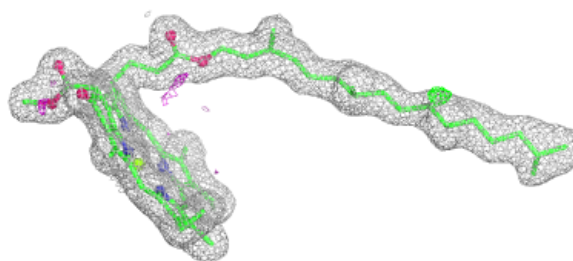
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



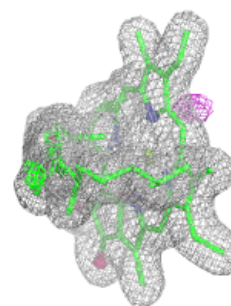
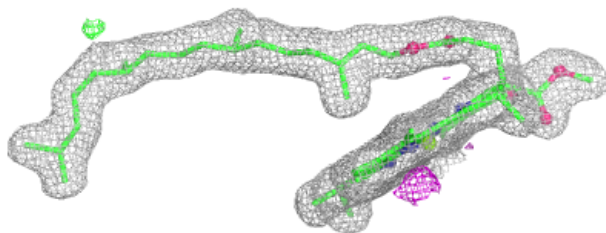
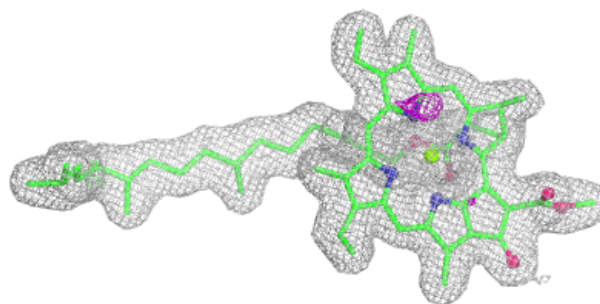


**Electron density around CLA B 608:**

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

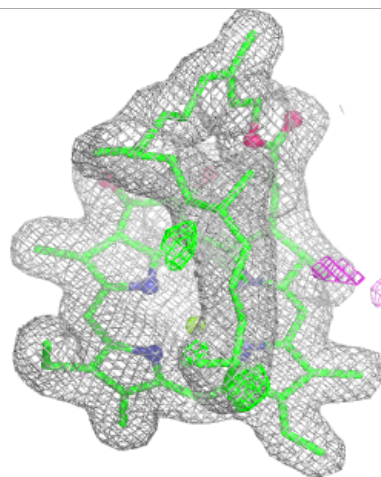
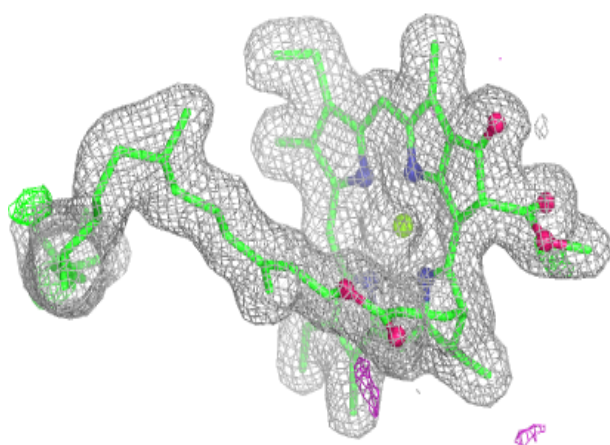
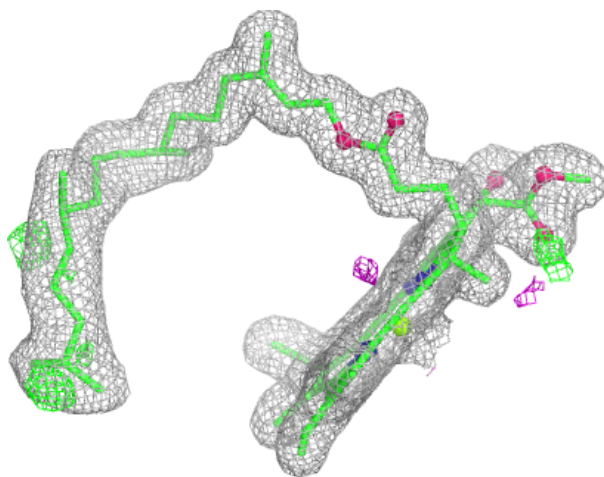
**Electron density around CLA B 609:**

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



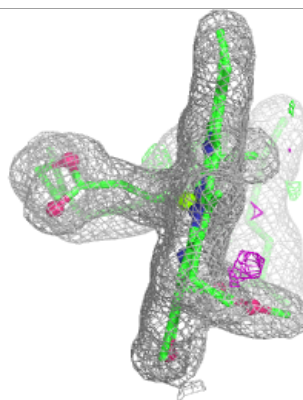
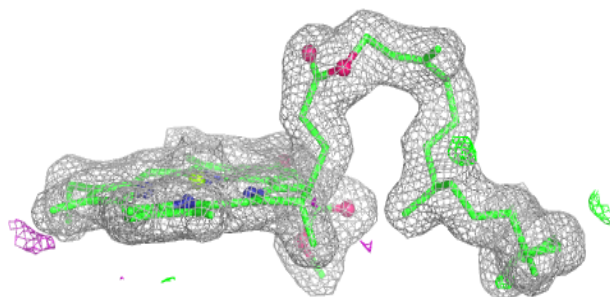
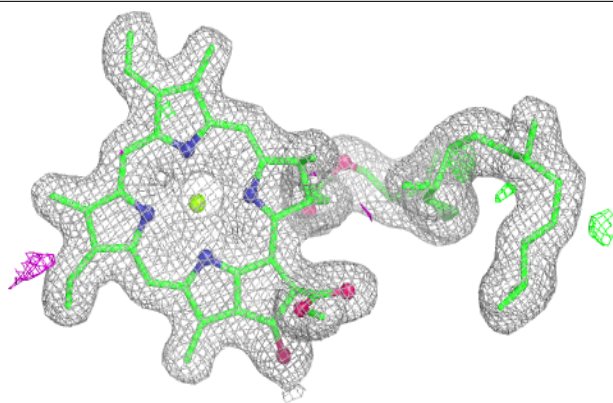
**Electron density around CLA b 613:**

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

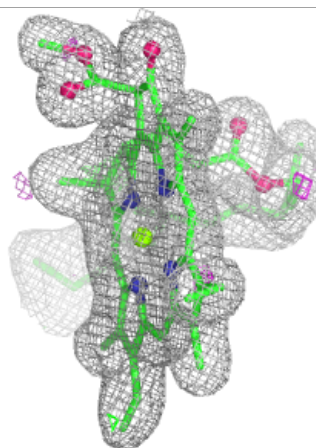
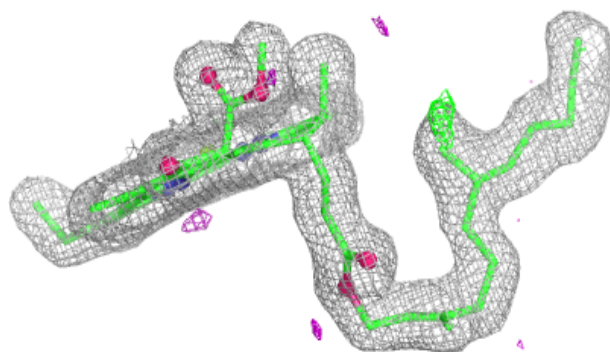
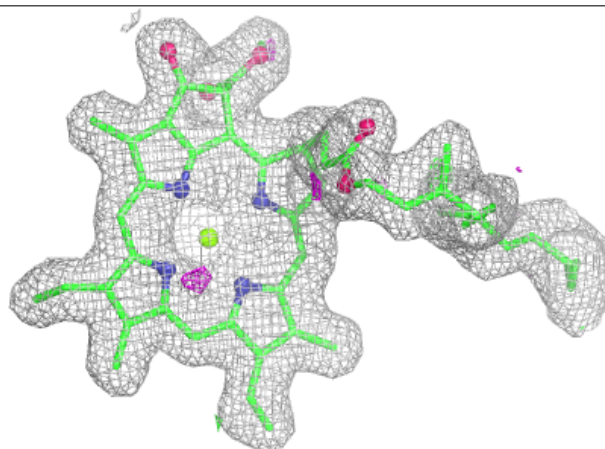


**Electron density around CLA b 614:**

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

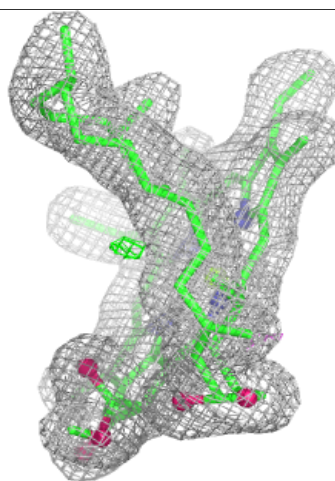
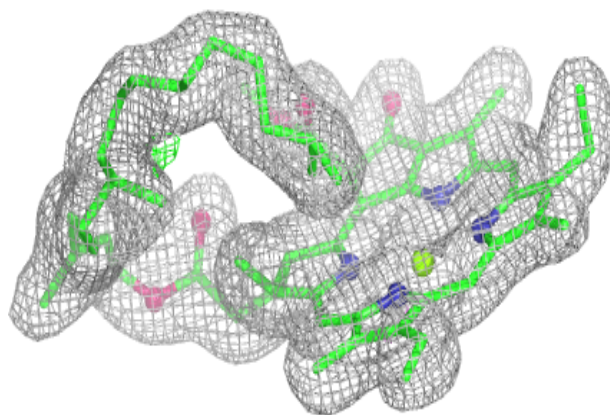
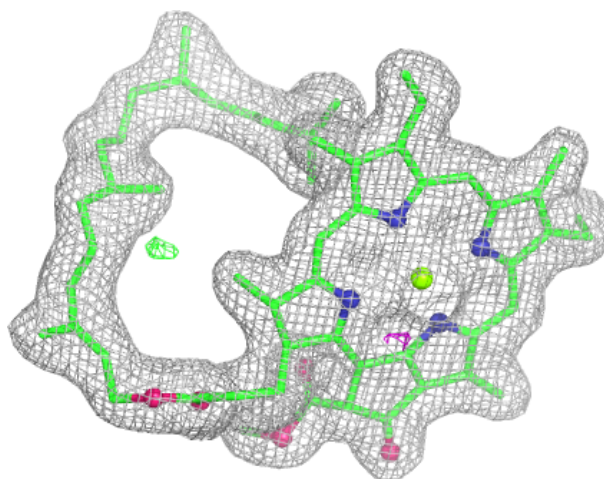
**Electron density around CLA A 402:**

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



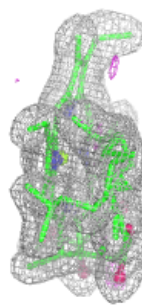
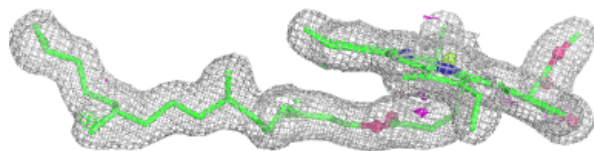
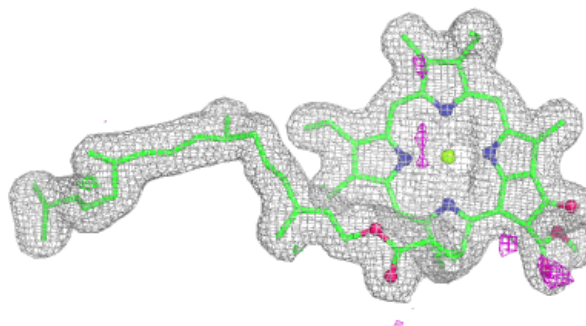
**Electron density around CLA b 617:**

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



**Electron density around CLA B 604:**

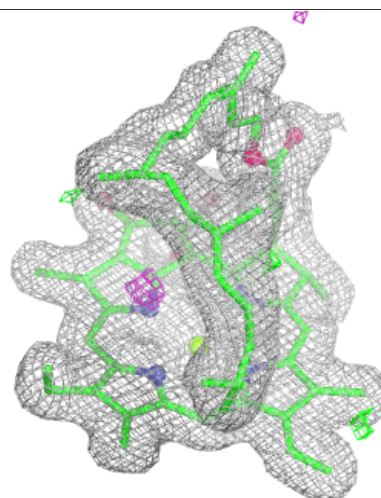
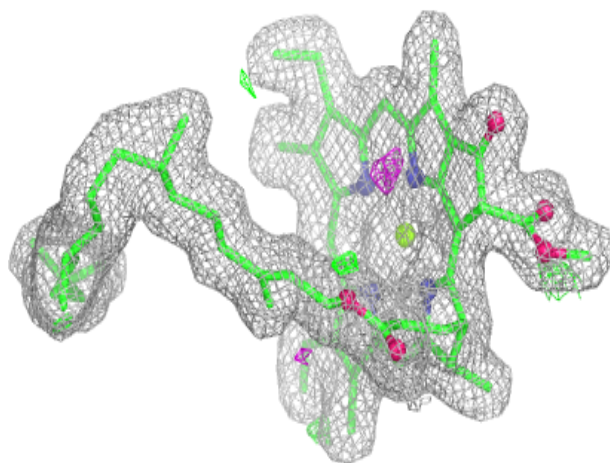
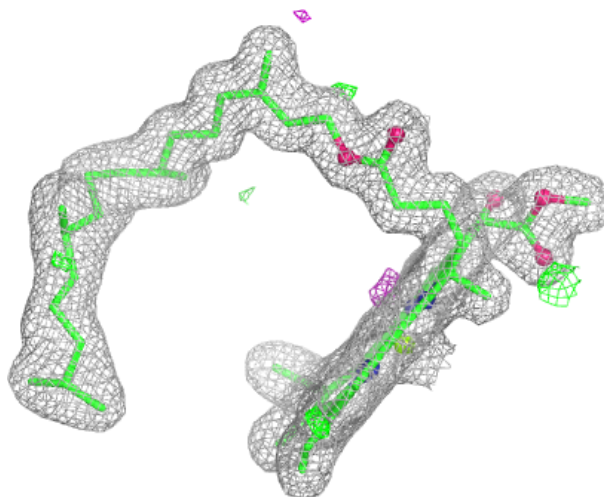
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





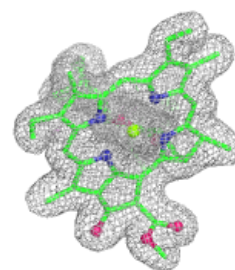
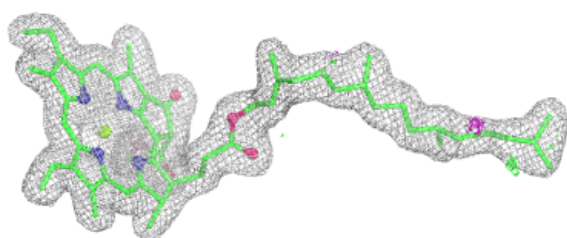
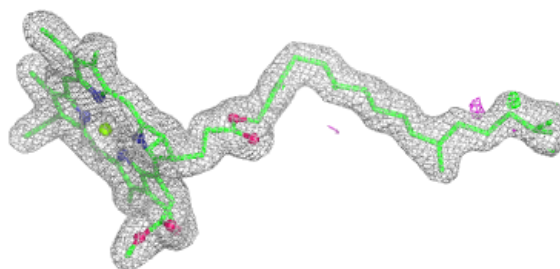
**Electron density around CLA B 612:**

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

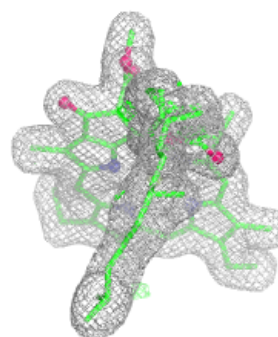
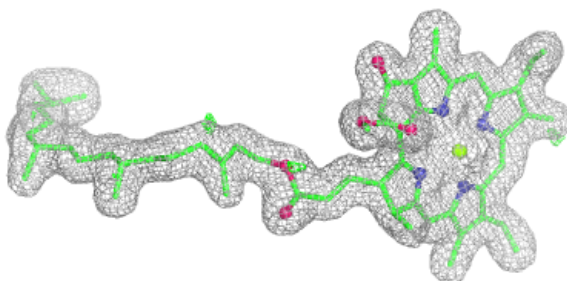
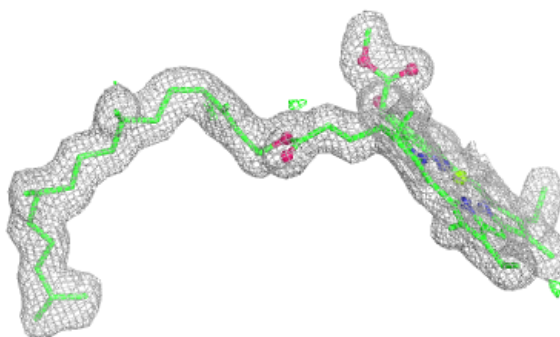


**Electron density around CLA c 502:**

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

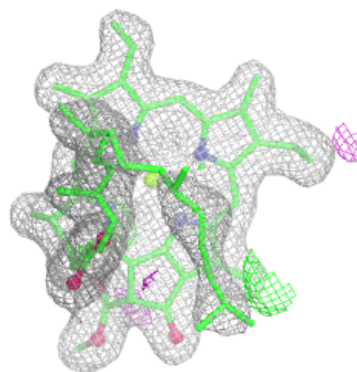
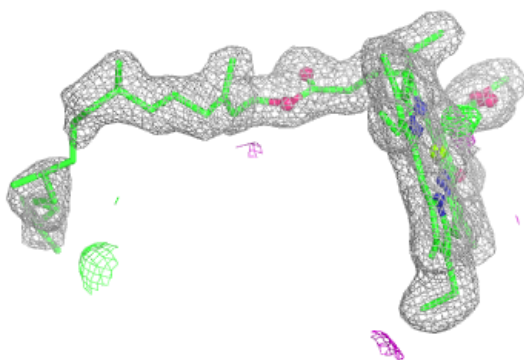
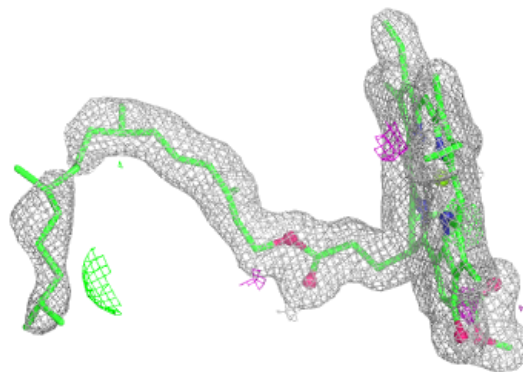
**Electron density around CLA D 401:**

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

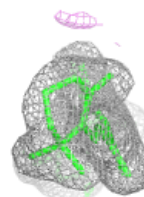
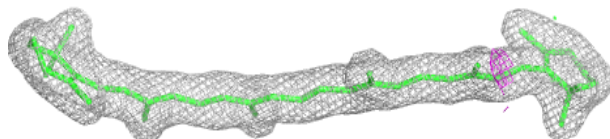
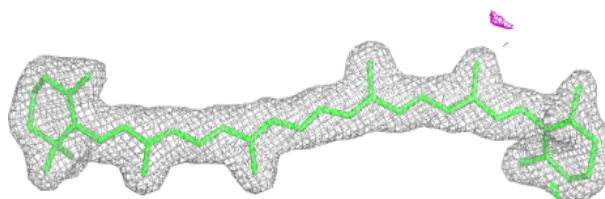


**Electron density around CLA D 404:**

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

**Electron density around BCR b 621:**

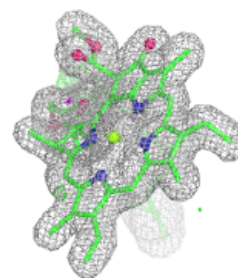
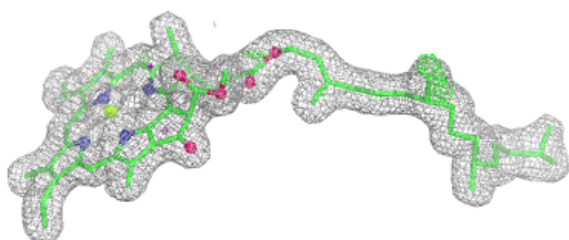
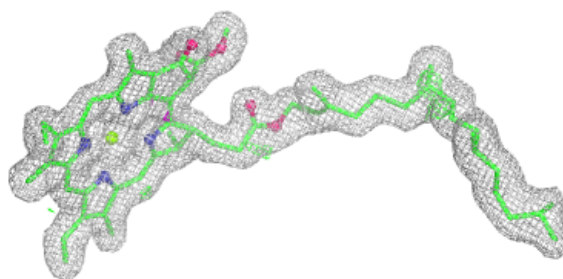
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





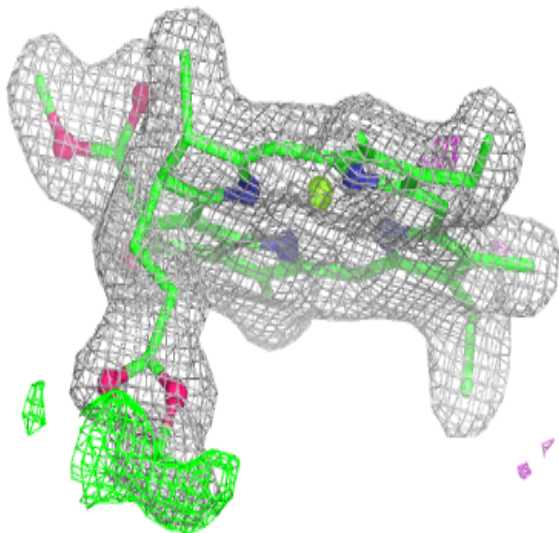
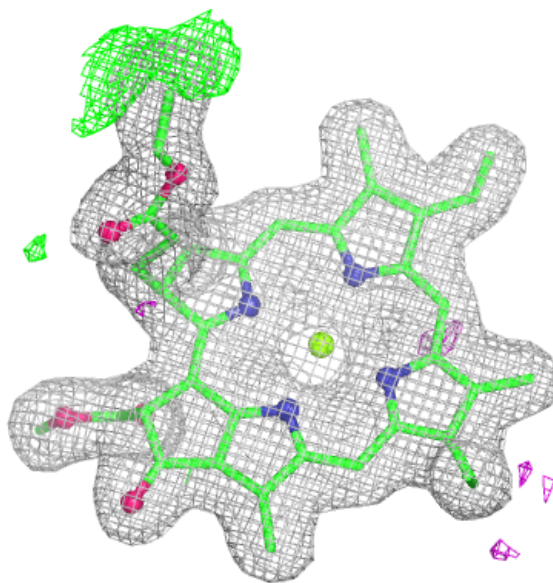
**Electron density around CLA a 403:**

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



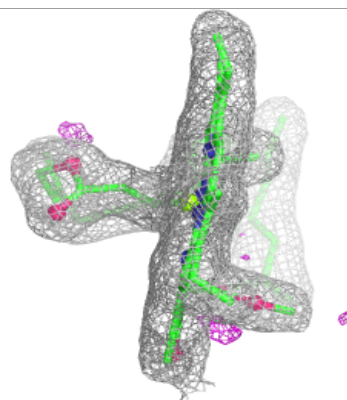
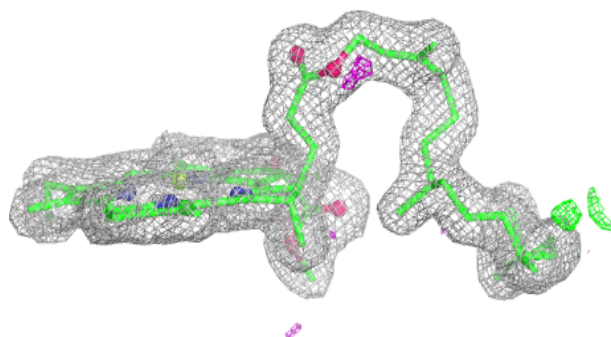
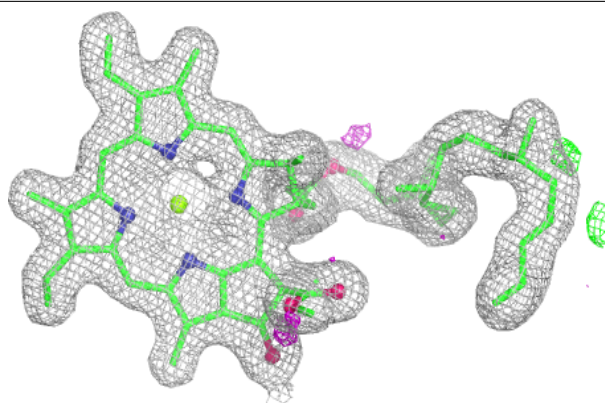
**Electron density around CLA a 407:**

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

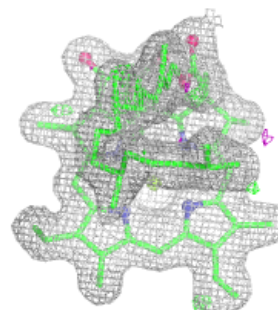
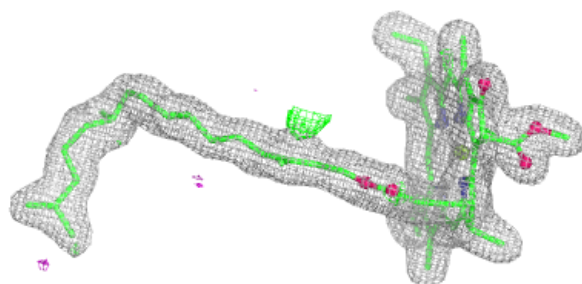
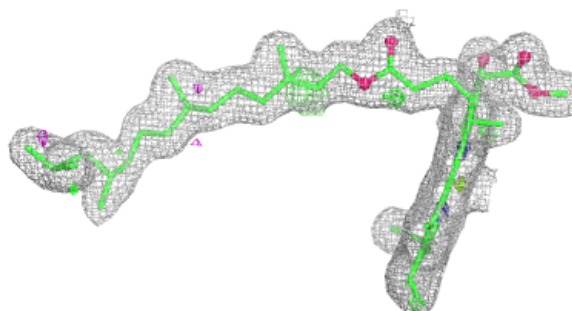


**Electron density around CLA B 613:**

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

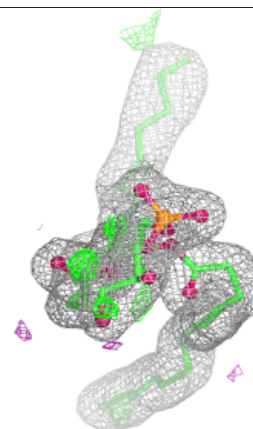
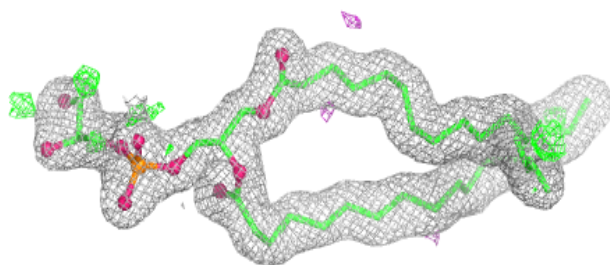
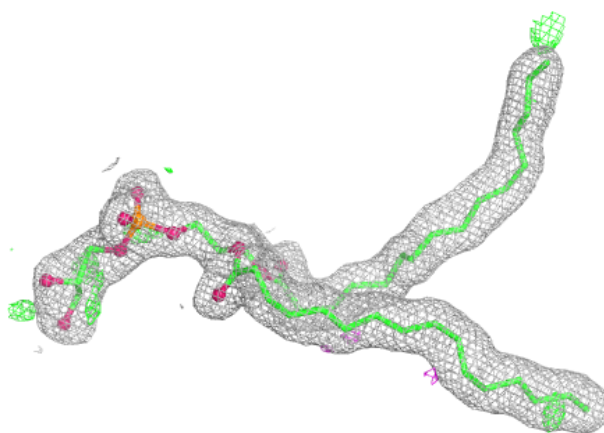
**Electron density around CLA B 606:**

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

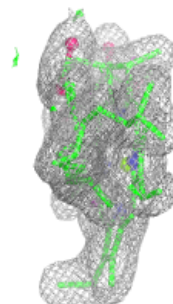
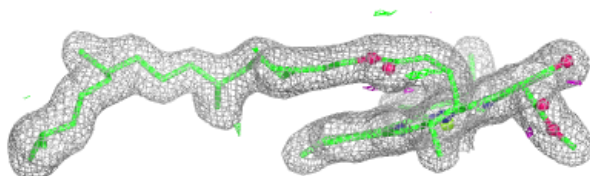
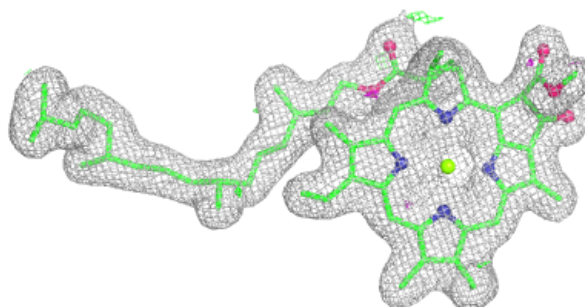


**Electron density around LHG D 408:**

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

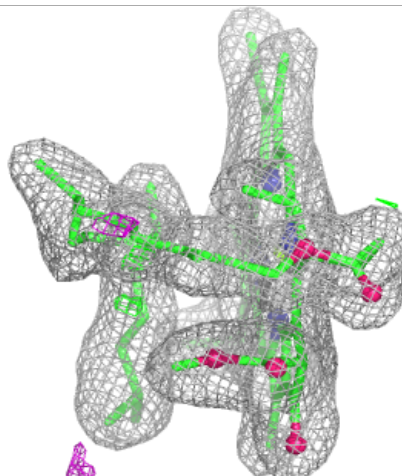
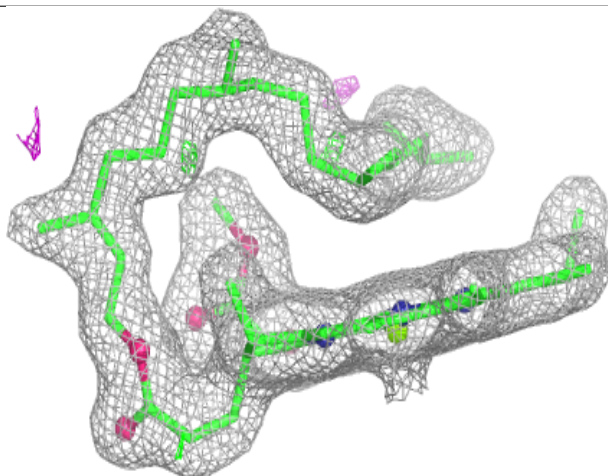
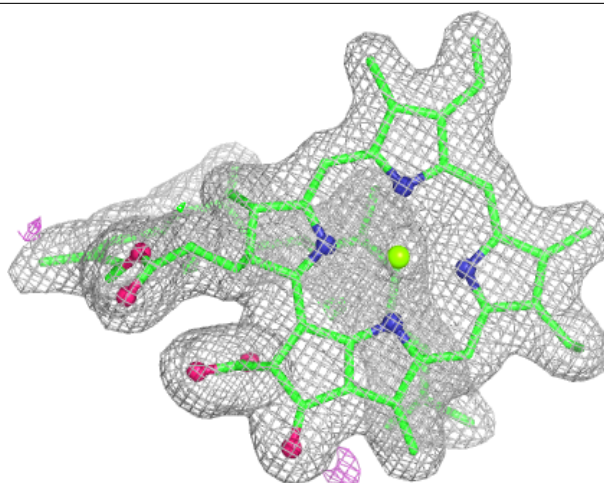
**Electron density around CLA b 605:**

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



**Electron density around CLA c 510:**

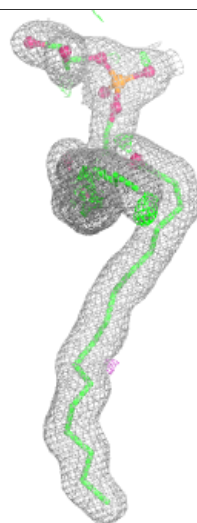
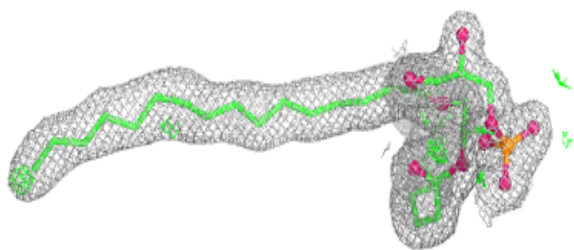
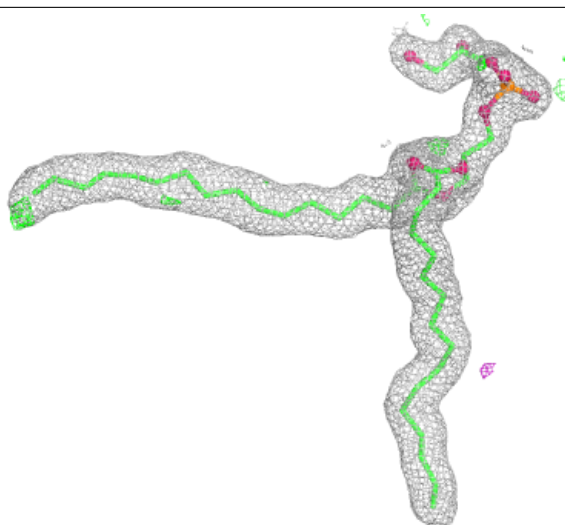
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





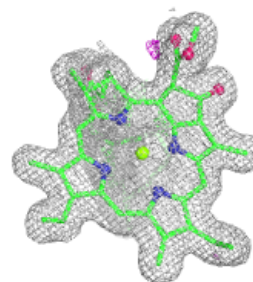
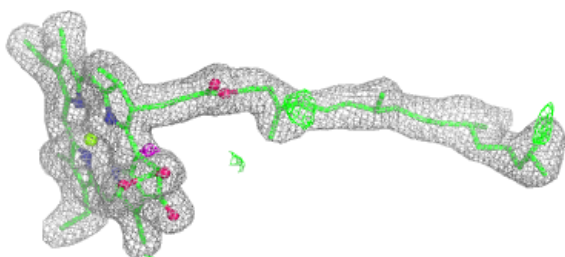
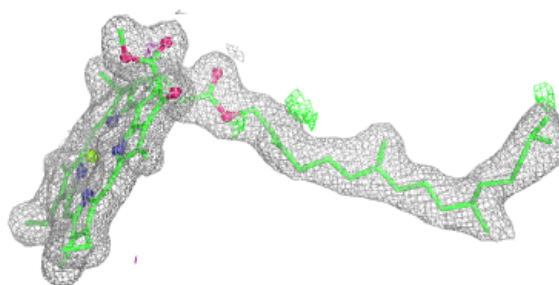
**Electron density around LHG L 101:**

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



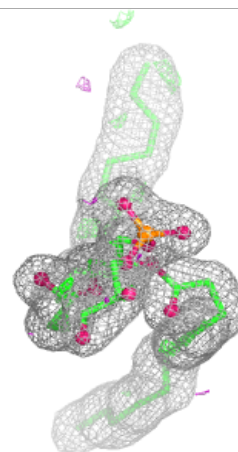
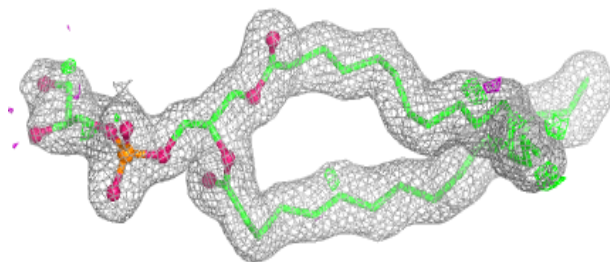
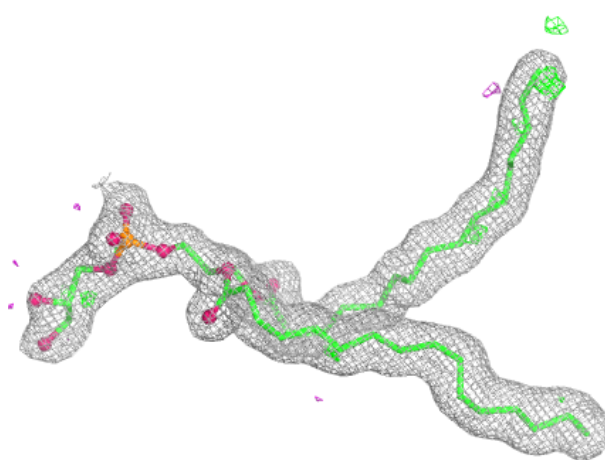
**Electron density around CLA b 606:**

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



**Electron density around LHG d 407:**

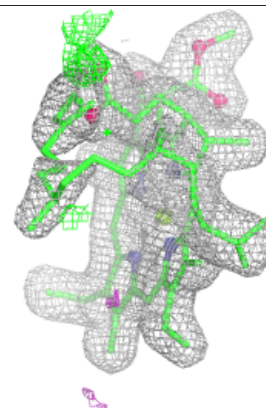
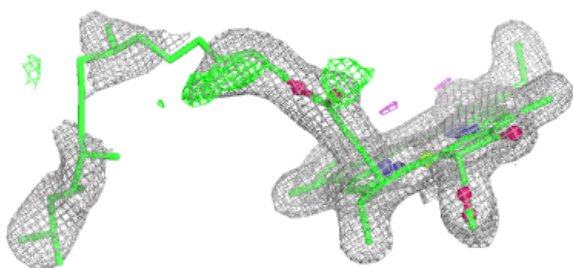
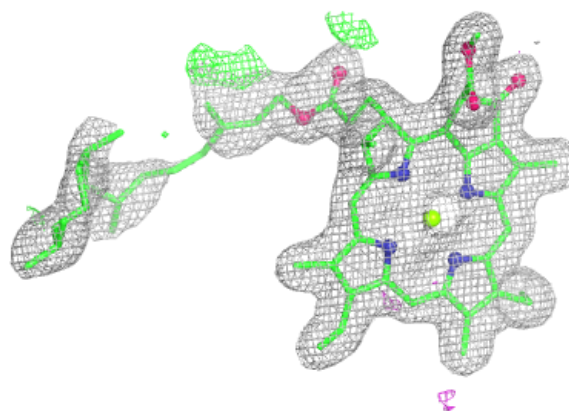
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





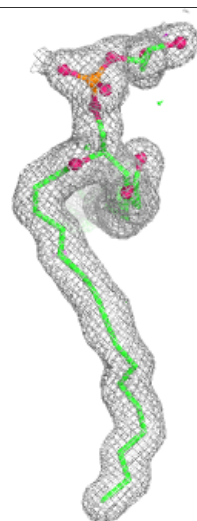
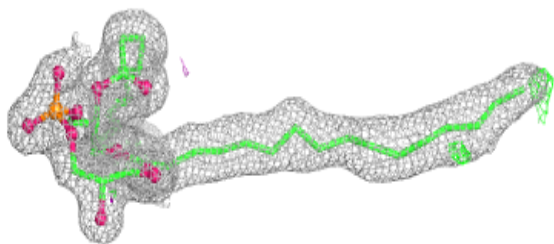
**Electron density around CLA A 404:**

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



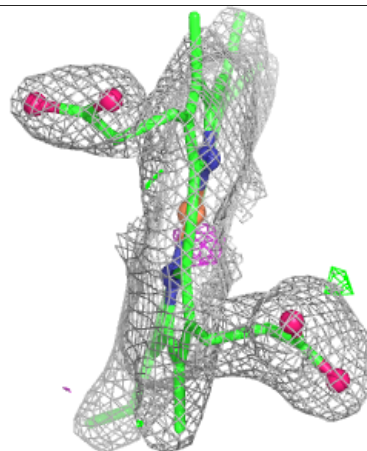
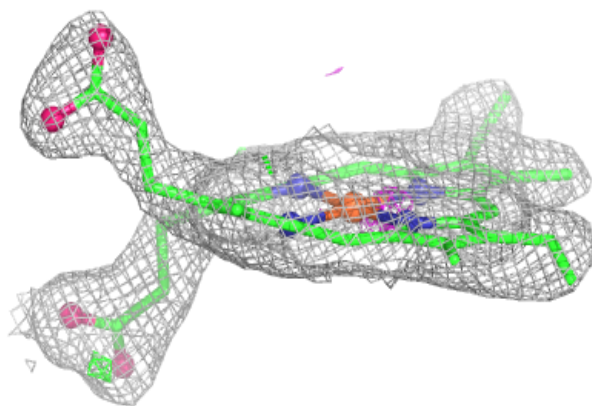
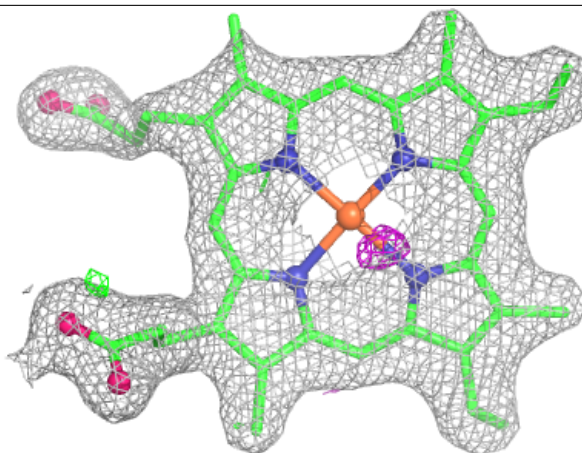
**Electron density around LHG 1 102:**

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



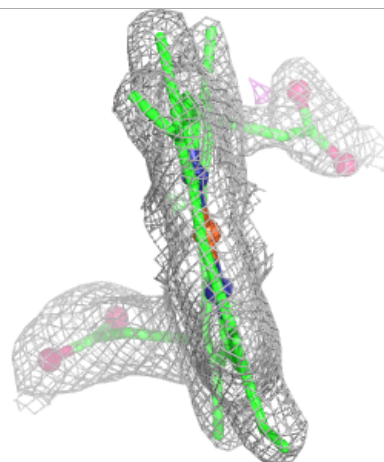
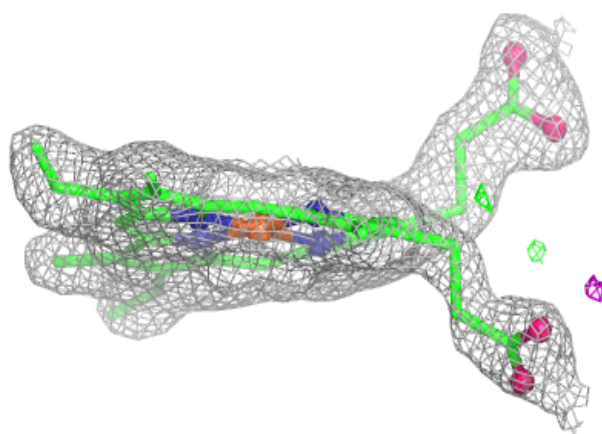
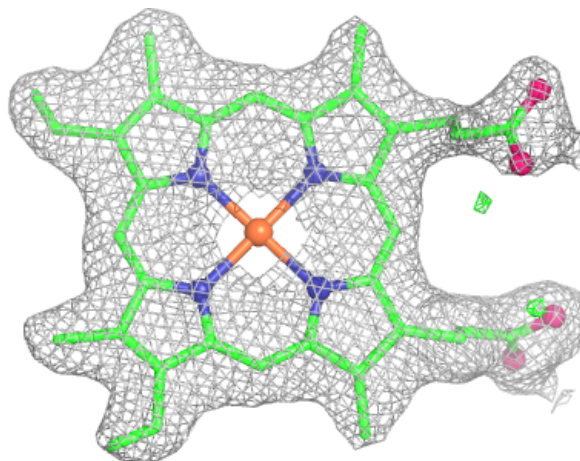
**Electron density around HEM E 104:**

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



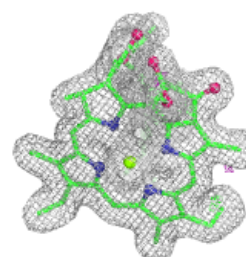
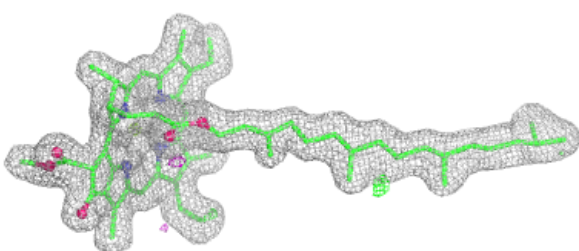
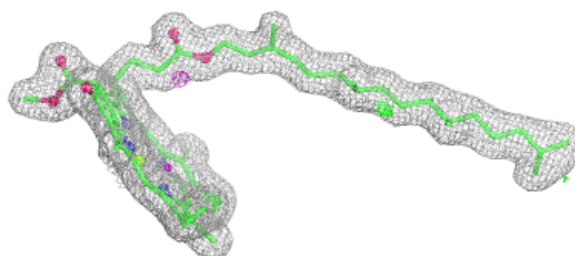
**Electron density around HEM e 102:**

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

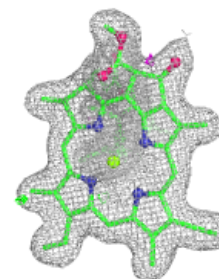
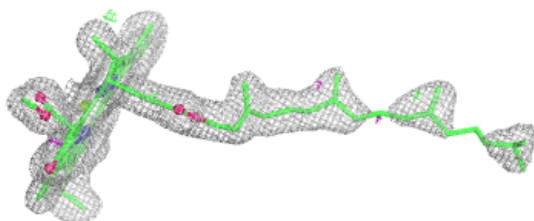
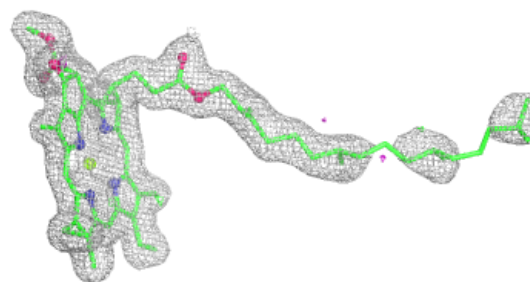


**Electron density around CLA b 609:**

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

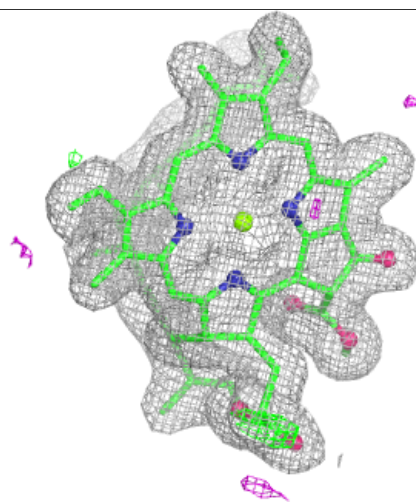
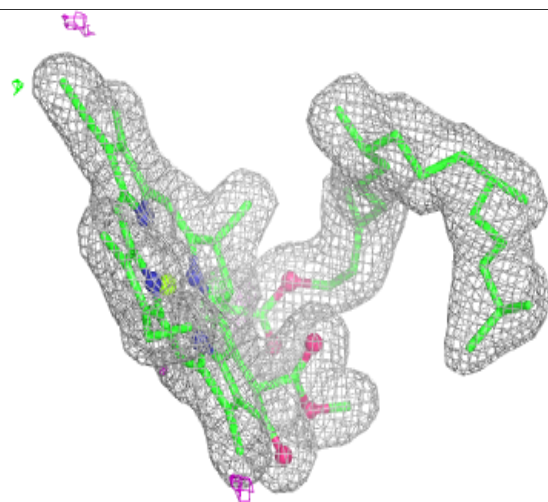
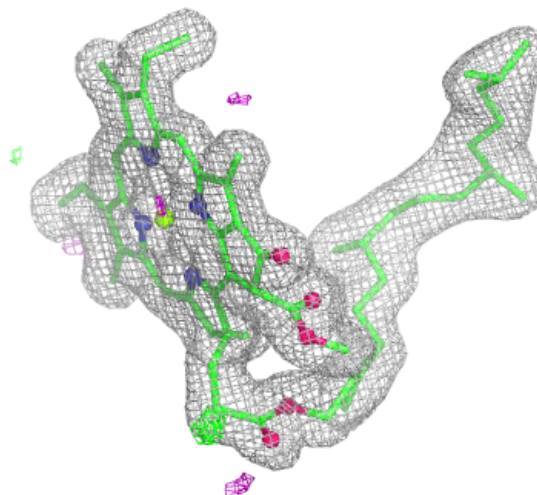
**Electron density around CLA d 404:**

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



**Electron density around CLA b 615:**

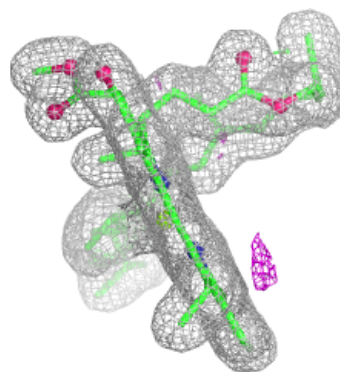
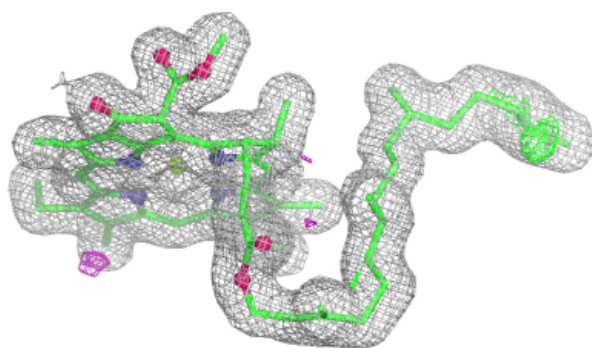
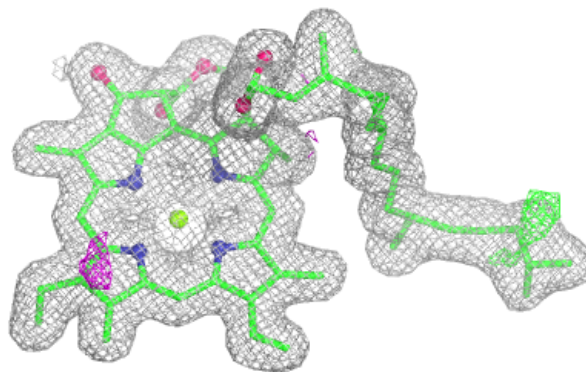
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



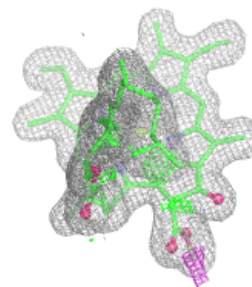
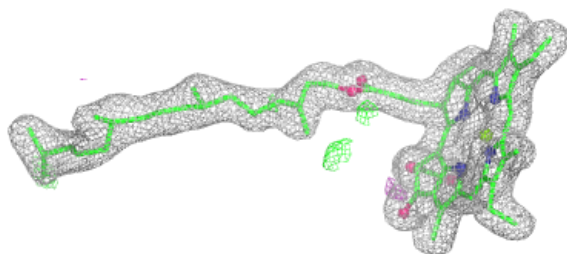
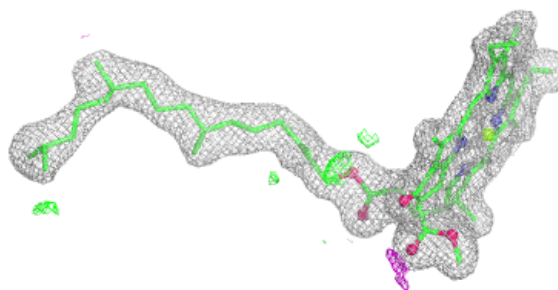


**Electron density around CLA D 402:**

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

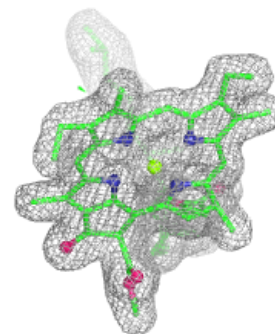
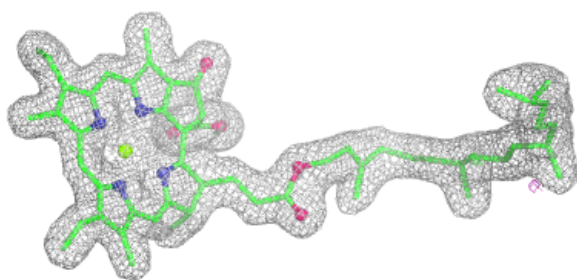
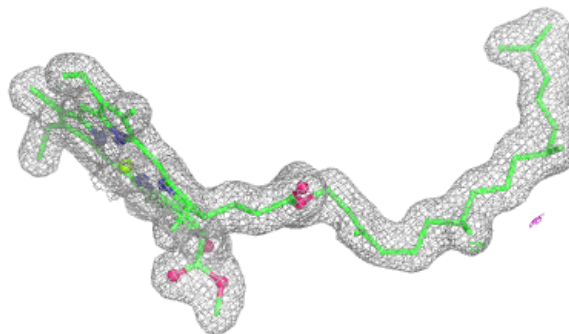
**Electron density around CLA B 605:**

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

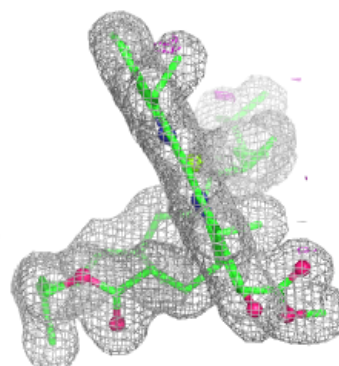
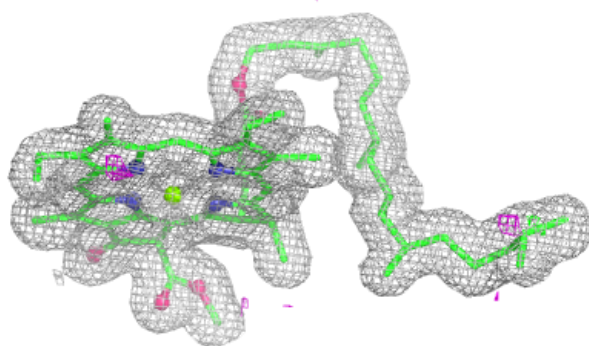
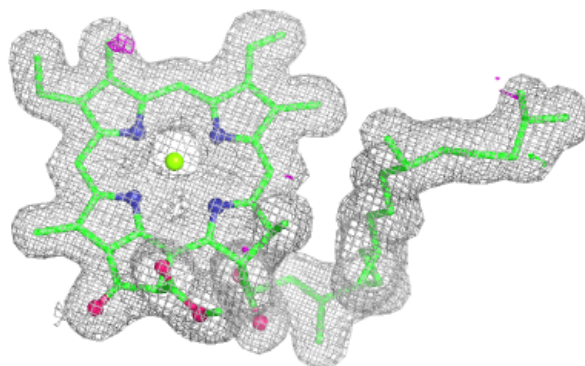


**Electron density around CLA d 402:**

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

**Electron density around CLA d 403:**

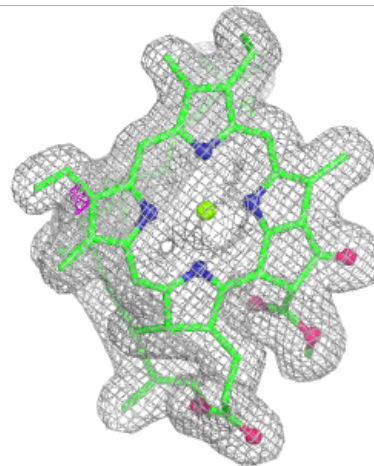
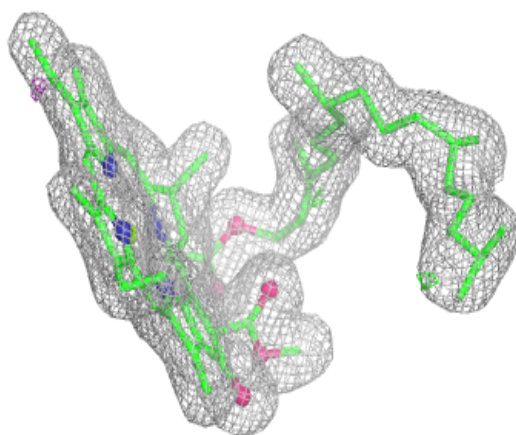
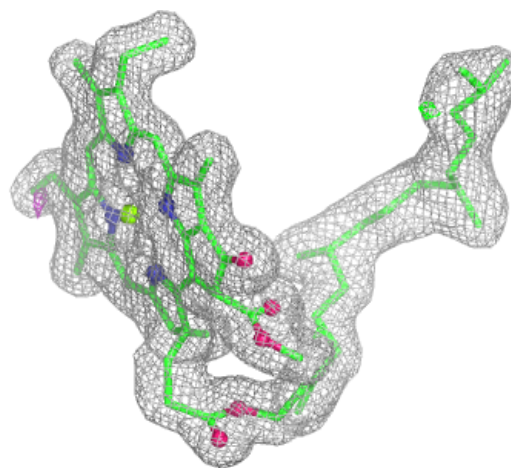
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





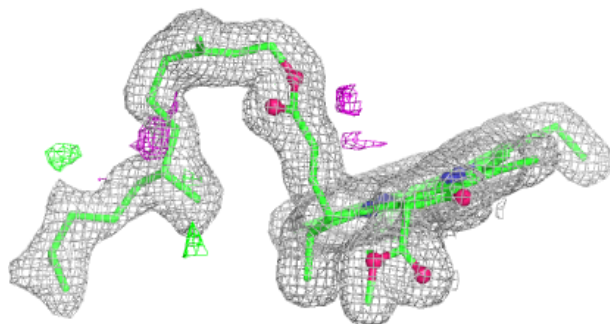
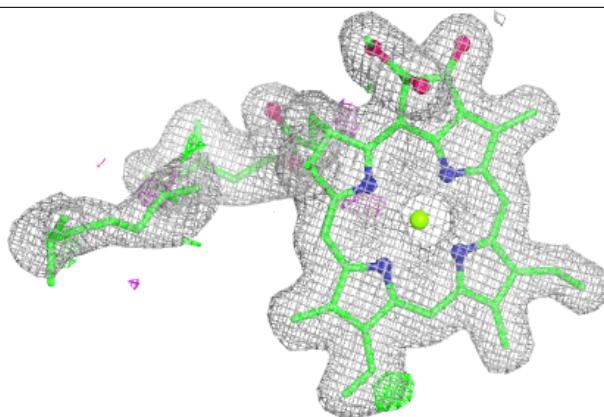
**Electron density around CLA B 614:**

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

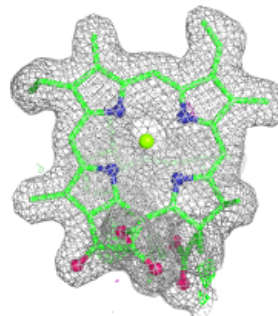
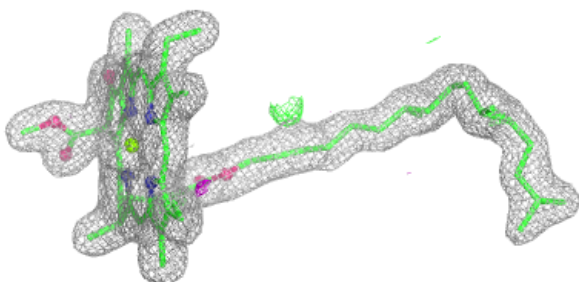
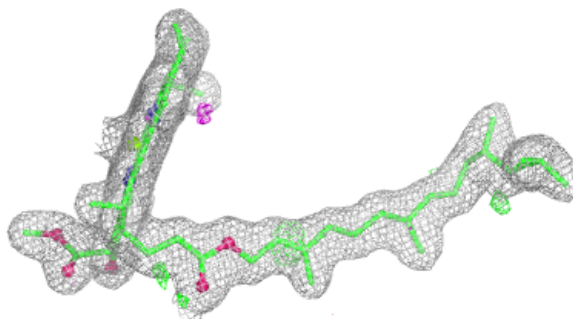


**Electron density around CLA a 404:**

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

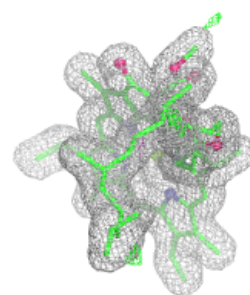
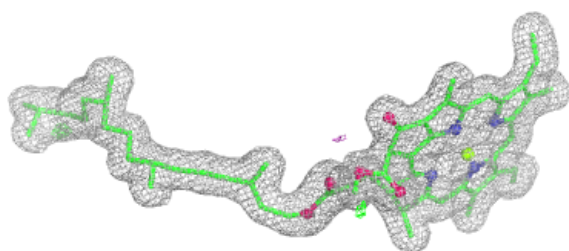
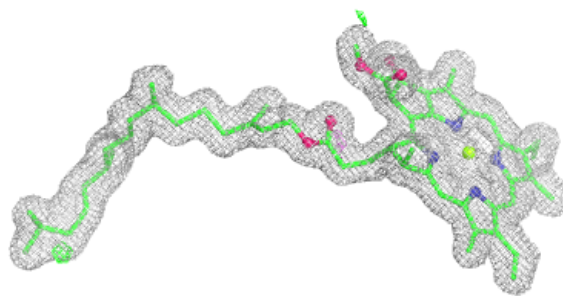
**Electron density around CLA b 607:**

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



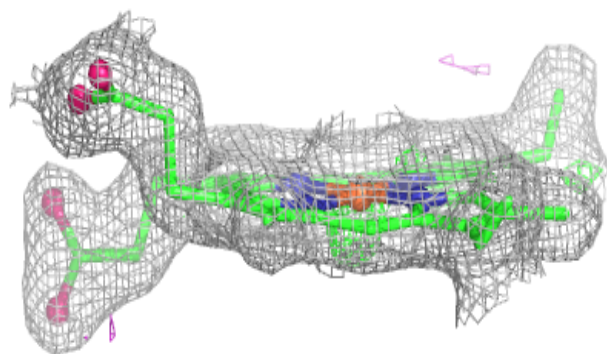
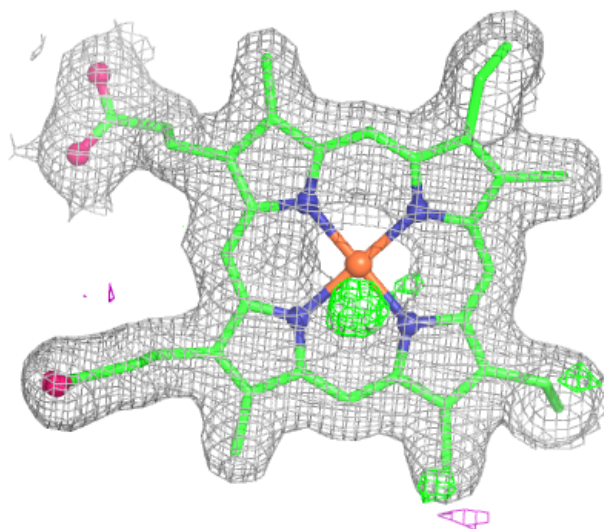
**Electron density around CLA A 401:**

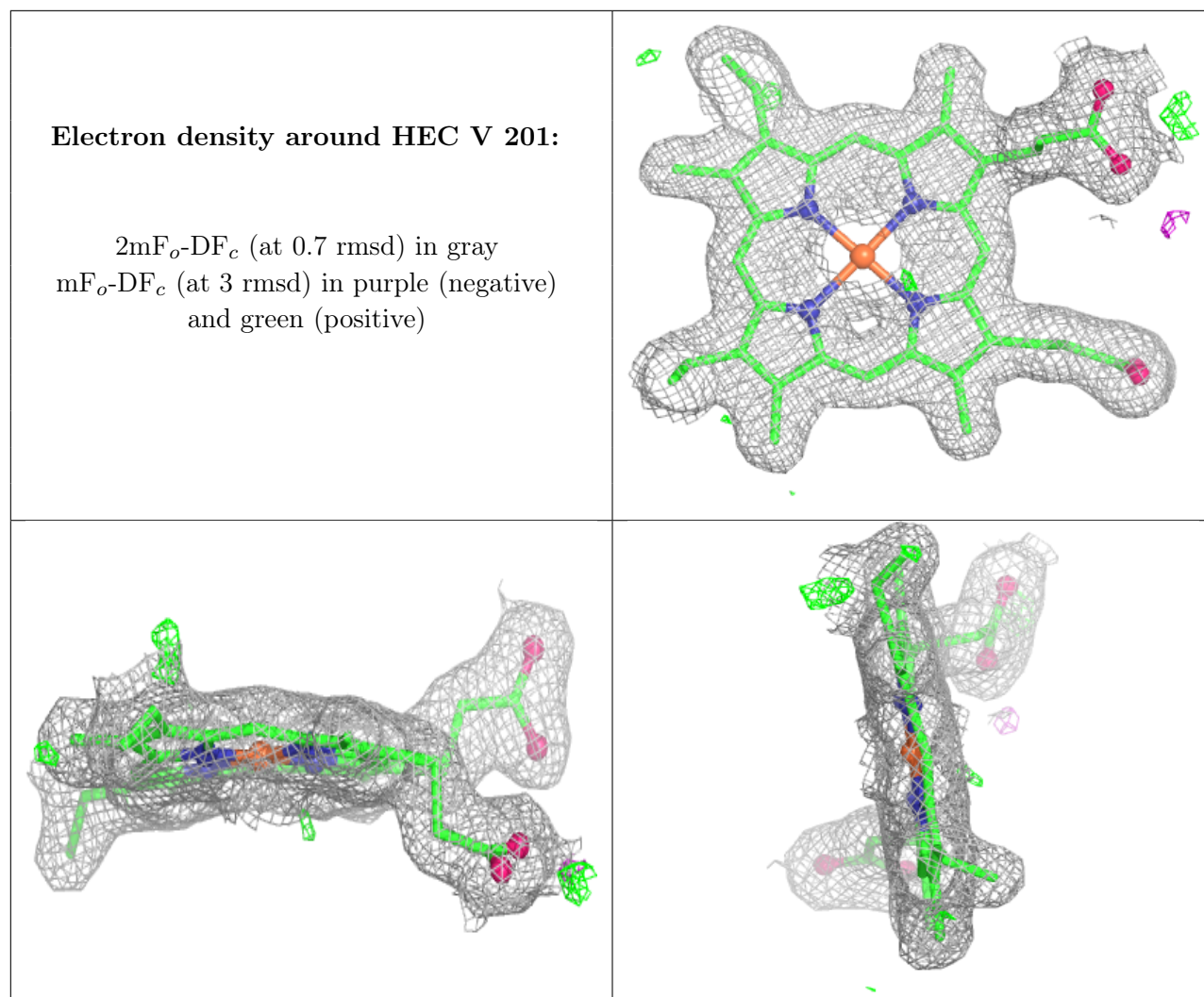
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.