



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:03 AM UTC

PDB ID : 4YUU / pdb\_00004yuu  
Title : Crystal structure of oxygen-evolving photosystem II from a red alga  
Authors : Ago, H.; Shen, J.-R.  
Deposited on : 2015-03-19  
Resolution : 2.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

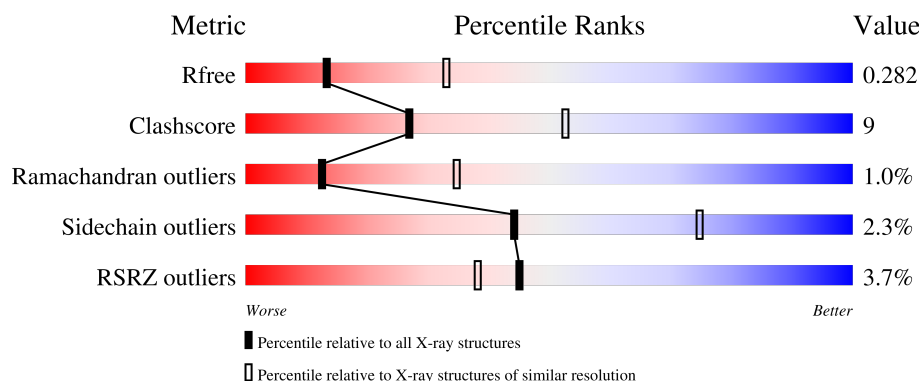
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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                      | 5248 (2.80-2.76)                                      |
| Clashscore            | 190562                      | 5693 (2.80-2.76)                                      |
| Ramachandran outliers | 187476                      | 5590 (2.80-2.76)                                      |
| Sidechain outliers    | 187428                      | 5592 (2.80-2.76)                                      |
| RSRZ outliers         | 180081                      | 5251 (2.80-2.76)                                      |

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   | A1    | 344    | <div> <div>%</div> <div>80%19%.</div> </div>    |
| 1   | A2    | 344    | <div> <div>2%</div> <div>81%15%..</div> </div>  |
| 1   | a1    | 344    | <div> <div>%</div> <div>78%18%..</div> </div>   |
| 1   | a2    | 344    | <div> <div>80%16%..</div> </div>                |
| 2   | B1    | 509    | <div> <div>%</div> <div>79%14%. 5%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | B2    | 509    |                  |
| 2   | b1    | 509    |                  |
| 2   | b2    | 509    |                  |
| 3   | C1    | 460    |                  |
| 3   | C2    | 460    |                  |
| 3   | c1    | 460    |                  |
| 3   | c2    | 460    |                  |
| 4   | D1    | 351    |                  |
| 4   | D2    | 351    |                  |
| 4   | d1    | 351    |                  |
| 4   | d2    | 351    |                  |
| 5   | E1    | 84     |                  |
| 5   | E2    | 84     |                  |
| 5   | e1    | 84     |                  |
| 5   | e2    | 84     |                  |
| 6   | F1    | 43     |                  |
| 6   | F2    | 43     |                  |
| 6   | f1    | 43     |                  |
| 6   | f2    | 43     |                  |
| 7   | H1    | 67     |                  |
| 7   | H2    | 67     |                  |
| 7   | h1    | 67     |                  |
| 7   | h2    | 67     |                  |
| 8   | I1    | 38     |                  |
| 8   | I2    | 38     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8   | i1    | 38     |                  |
| 8   | i2    | 38     |                  |
| 9   | J1    | 39     |                  |
| 9   | J2    | 39     |                  |
| 9   | j1    | 39     |                  |
| 9   | j2    | 39     |                  |
| 10  | K1    | 41     |                  |
| 10  | K2    | 41     |                  |
| 10  | k1    | 41     |                  |
| 10  | k2    | 41     |                  |
| 11  | L1    | 38     |                  |
| 11  | L2    | 38     |                  |
| 11  | l1    | 38     |                  |
| 11  | l2    | 38     |                  |
| 12  | M1    | 108    |                  |
| 12  | M2    | 108    |                  |
| 12  | m1    | 108    |                  |
| 12  | m2    | 108    |                  |
| 13  | O1    | 329    |                  |
| 13  | O2    | 329    |                  |
| 13  | o1    | 329    |                  |
| 13  | o2    | 329    |                  |
| 14  | T1    | 32     |                  |
| 14  | T2    | 32     |                  |
| 14  | t1    | 32     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 14  | t2    | 32     |                  |
| 15  | U1    | 155    |                  |
| 15  | U2    | 155    |                  |
| 15  | u1    | 155    |                  |
| 15  | u2    | 155    |                  |
| 16  | V1    | 155    |                  |
| 16  | V2    | 155    |                  |
| 16  | v1    | 155    |                  |
| 16  | v2    | 155    |                  |
| 17  | Y1    | 35     |                  |
| 17  | Y2    | 35     |                  |
| 17  | y1    | 35     |                  |
| 17  | y2    | 35     |                  |
| 18  | X1    | 40     |                  |
| 18  | X2    | 40     |                  |
| 18  | x1    | 40     |                  |
| 18  | x2    | 40     |                  |
| 19  | S1    | 46     |                  |
| 19  | S2    | 46     |                  |
| 19  | s1    | 46     |                  |
| 19  | s2    | 46     |                  |
| 20  | W1    | 25     |                  |
| 20  | W2    | 25     |                  |
| 20  | w1    | 25     |                  |
| 20  | w2    | 25     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 21  | Q2    | 218    |                  |
| 21  | q1    | 218    |                  |
| 22  | Z2    | 62     |                  |
| 22  | z2    | 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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | A1    | 403 | X         | -        | -       | -                |
| 25  | CLA  | A1    | 404 | X         | -        | -       | -                |
| 25  | CLA  | A1    | 405 | X         | -        | -       | -                |
| 25  | CLA  | A1    | 406 | X         | -        | -       | -                |
| 25  | CLA  | A2    | 402 | X         | -        | -       | -                |
| 25  | CLA  | A2    | 403 | X         | -        | -       | -                |
| 25  | CLA  | A2    | 404 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 604 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 605 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 606 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 607 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 608 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 609 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 610 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 612 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 613 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 614 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 615 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 616 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 617 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 618 | X         | -        | -       | -                |
| 25  | CLA  | B1    | 619 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 604 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 605 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 606 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 607 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 608 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 609 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 610 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 611 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | B2    | 612 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 613 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 614 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 615 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 616 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 617 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 618 | X         | -        | -       | -                |
| 25  | CLA  | B2    | 619 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 502 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 503 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 504 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 505 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 506 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 507 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 508 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 509 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 510 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 511 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 512 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 513 | X         | -        | -       | -                |
| 25  | CLA  | C1    | 514 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 503 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 504 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 505 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 506 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 507 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 508 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 509 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 510 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 511 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 513 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 516 | X         | -        | -       | -                |
| 25  | CLA  | C2    | 518 | X         | -        | -       | -                |
| 25  | CLA  | D1    | 402 | X         | -        | -       | -                |
| 25  | CLA  | D1    | 403 | X         | -        | -       | -                |
| 25  | CLA  | D2    | 401 | X         | -        | -       | -                |
| 25  | CLA  | D2    | 404 | X         | -        | -       | -                |
| 25  | CLA  | D2    | 406 | X         | -        | -       | -                |
| 25  | CLA  | K2    | 101 | X         | -        | -       | -                |
| 25  | CLA  | a1    | 403 | X         | -        | -       | -                |
| 25  | CLA  | a1    | 404 | X         | -        | -       | -                |
| 25  | CLA  | a1    | 405 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | a2    | 404 | X         | -        | -       | -                |
| 25  | CLA  | a2    | 405 | X         | -        | -       | -                |
| 25  | CLA  | a2    | 413 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 604 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 605 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 606 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 607 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 608 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 609 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 610 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 611 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 612 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 613 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 614 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 615 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 616 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 617 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 619 | X         | -        | -       | -                |
| 25  | CLA  | b1    | 620 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 604 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 606 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 608 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 609 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 610 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 611 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 612 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 613 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 614 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 615 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 616 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 617 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 618 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 619 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 620 | X         | -        | -       | -                |
| 25  | CLA  | b2    | 624 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 503 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 504 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 505 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 506 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 507 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 508 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 509 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CLA  | c1    | 510 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 511 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 512 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 513 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 515 | X         | -        | -       | -                |
| 25  | CLA  | c1    | 516 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 502 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 503 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 504 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 505 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 506 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 507 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 508 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 509 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 510 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 511 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 512 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 513 | X         | -        | -       | -                |
| 25  | CLA  | c2    | 515 | X         | -        | -       | -                |
| 25  | CLA  | d1    | 401 | X         | -        | -       | -                |
| 25  | CLA  | d1    | 404 | X         | -        | -       | -                |
| 25  | CLA  | d2    | 402 | X         | -        | -       | -                |
| 25  | CLA  | d2    | 404 | X         | -        | -       | -                |
| 25  | CLA  | d2    | 405 | X         | -        | -       | -                |

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 92765 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   | A1    | 344      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2609  | 1708 | 425 | 462 | 14 |         |         |       |
| 1   | a1    | 334      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2564  | 1676 | 421 | 454 | 13 |         |         |       |
| 1   | A2    | 332      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2475  | 1607 | 411 | 444 | 13 |         |         |       |
| 1   | a2    | 334      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2513  | 1638 | 410 | 452 | 13 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B1    | 483      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3703  | 2426 | 624 | 641 | 12 |         |         |       |
| 2   | b1    | 503      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3881  | 2549 | 646 | 674 | 12 |         |         |       |
| 2   | B2    | 503      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3770  | 2460 | 645 | 654 | 11 |         |         |       |
| 2   | b2    | 481      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3681  | 2418 | 620 | 631 | 12 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C1    | 449      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3392  | 2215 | 573 | 594 | 10 |         |         |       |
| 3   | c1    | 449      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 3439  | 2241 | 577 | 611 | 10 |         |         |       |
| 3   | C2    | 444      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3145  | 2028 | 545 | 564 | 8  |         |         |       |
| 3   | c2    | 448      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3386  | 2201 | 578 | 597 | 10 |         |         |       |



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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D1    | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2615  | 1736 | 422 | 447 | 10 |         |         |       |
| 4   | d1    | 339      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2678  | 1775 | 433 | 460 | 10 |         |         |       |
| 4   | D2    | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2585  | 1713 | 422 | 440 | 10 |         |         |       |
| 4   | d2    | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2643  | 1756 | 425 | 452 | 10 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 5   | E1    | 61       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 405   | 264 | 68 | 73 |         |         |       |
| 5   | e1    | 57       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 427   | 280 | 71 | 76 |         |         |       |
| 5   | E2    | 63       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 430   | 279 | 72 | 79 |         |         |       |
| 5   | e2    | 60       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 421   | 279 | 71 | 71 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | F1    | 28       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 213   | 144 | 36 | 32 | 1 |         |         |       |
| 6   | f1    | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 227   | 158 | 36 | 32 | 1 |         |         |       |
| 6   | F2    | 31       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 229   | 153 | 41 | 34 | 1 |         |         |       |
| 6   | f2    | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 225   | 157 | 34 | 33 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | H1    | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 433   | 289 | 69 | 73 | 2 |         |         |       |
| 7   | h1    | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 470   | 317 | 71 | 80 | 2 |         |         |       |
| 7   | H2    | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 443   | 294 | 72 | 75 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | h2    | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 450   | 302 | 69 | 77 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | I1    | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 274   | 184 | 42 | 45 | 3 |         |         |       |
| 8   | i1    | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 280   | 188 | 44 | 45 | 3 |         |         |       |
| 8   | I2    | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 265   | 177 | 41 | 45 | 2 |         |         |       |
| 8   | i2    | 33       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 261   | 174 | 40 | 44 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 9   | J1    | 32       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 220   | 148 | 33 | 39 |         |         |       |
| 9   | j1    | 32       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 224   | 152 | 33 | 39 |         |         |       |
| 9   | J2    | 35       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 231   | 154 | 36 | 41 |         |         |       |
| 9   | j2    | 33       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 228   | 153 | 34 | 41 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | K1    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 279   | 195 | 39 | 44 | 1 |         |         |       |
| 10  | k1    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 280   | 198 | 39 | 42 | 1 |         |         |       |
| 10  | K2    | 37       | Total | C   | N  | O  |   | 0       | 0       | 0     |
|     |       |          | 250   | 171 | 39 | 40 |   |         |         |       |
| 10  | k2    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 269   | 185 | 40 | 43 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 11  | L1    | 37       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 292   | 197 | 46 | 49 |         |         |       |
| 11  | l1    | 37       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 299   | 203 | 47 | 49 |         |         |       |
| 11  | L2    | 37       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 299   | 202 | 46 | 51 |         |         |       |
| 11  | l2    | 37       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 299   | 202 | 46 | 51 |         |         |       |

- Molecule 12 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN M.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | M1    | 40       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 285   | 189 | 44 | 50 | 2 |         |         |       |
| 12  | m1    | 40       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 285   | 189 | 44 | 50 | 2 |         |         |       |
| 12  | M2    | 40       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 284   | 188 | 46 | 48 | 2 |         |         |       |
| 12  | m2    | 40       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 287   | 189 | 46 | 50 | 2 |         |         |       |

- Molecule 13 is a protein called PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | O1    | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1074 | 276 | 316 | 8 |         |         |       |
| 13  | o1    | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1070 | 282 | 332 | 8 |         |         |       |
| 13  | O2    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1376  | 870  | 237 | 262 | 7 |         |         |       |
| 13  | o2    | 245      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1768  | 1123 | 296 | 341 | 8 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14  | T1    | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 241   | 168 | 36 | 36 | 1 |         |         |       |
| 14  | t1    | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 246   | 173 | 36 | 36 | 1 |         |         |       |
| 14  | T2    | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 240   | 170 | 33 | 36 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14  | t2    | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 235   | 167 | 32 | 35 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | U1    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 691   | 445 | 116 | 129 | 1 |         |         |       |
| 15  | u1    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 703   | 449 | 119 | 134 | 1 |         |         |       |
| 15  | U2    | 90       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 577   | 355 | 103 | 118 | 1 |         |         |       |
| 15  | u2    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 708   | 455 | 120 | 132 | 1 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| U1    | -51     | MET      | -      | initiating methionine | UNP Q9ZQS5 |
| u1    | -51     | MET      | -      | initiating methionine | UNP Q9ZQS5 |
| U2    | -51     | MET      | -      | initiating methionine | UNP Q9ZQS5 |
| u2    | -51     | MET      | -      | initiating methionine | UNP Q9ZQS5 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | V1    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 579 | 159 | 175 | 4 |         |         |       |
| 16  | v1    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 921   | 577 | 163 | 177 | 4 |         |         |       |
| 16  | V2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 845   | 521 | 152 | 168 | 4 |         |         |       |
| 16  | v2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 963   | 608 | 168 | 183 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17  | Y1    | 27       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 170   | 111 | 29 | 30 |         |         |       |
| 17  | y1    | 27       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 195   | 133 | 30 | 32 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17  | Y2    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 159   | 104 | 27 | 28 |         |         |       |
| 17  | y2    | 27       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 188   | 126 | 30 | 32 |         |         |       |

- Molecule 18 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN X.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18  | X1    | 29       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 197   | 135 | 30 | 32 |         |         |       |
| 18  | x1    | 36       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 255   | 174 | 38 | 42 |         |         |       |
| 18  | X2    | 31       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 215   | 149 | 33 | 32 |         |         |       |
| 18  | x2    | 32       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 218   | 147 | 35 | 36 |         |         |       |

- Molecule 19 is a protein called PEPTIDE CHAIN UNASSIGNED.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 19  | S1    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 164   | 113 | 26 | 25 |         |         |       |
| 19  | s1    | 40       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 263   | 182 | 41 | 40 |         |         |       |
| 19  | S2    | 30       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 191   | 130 | 31 | 30 |         |         |       |
| 19  | s2    | 46       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 281   | 188 | 47 | 46 |         |         |       |

- Molecule 20 is a protein called PEPTIDE CHAIN UNASSIGNED.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 20  | W1    | 21       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 134   | 91  | 21 | 22 |         |         |       |
| 20  | w1    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 152   | 101 | 25 | 26 |         |         |       |
| 20  | W2    | 21       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 129   | 86  | 21 | 22 |         |         |       |
| 20  | w2    | 20       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 127   | 86  | 20 | 21 |         |         |       |

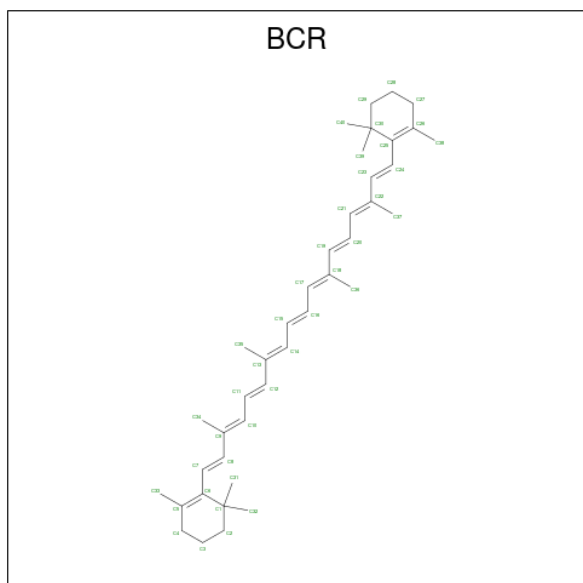
- Molecule 21 is a protein called Extrinsic protein in photosystem II.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | q1    | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 645   | 399 | 115 | 127 | 4 |         |         |       |
| 21  | Q2    | 111      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 417 | 123 | 133 | 3 |         |         |       |

- Molecule 22 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 22  | Z2    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 351   | 224 | 61 | 65 | 1 |         |         |       |
| 22  | z2    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 381   | 250 | 63 | 67 | 1 |         |         |       |

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 23  | A1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 23  | B1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 23  | B1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 23  | B1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 23  | C1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 23  | C1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 23  | D1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | H1    | 1        | Total C<br>22 22 | 0       | 0       |
| 23  | J1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | K1    | 1        | Total C<br>31 31 | 0       | 0       |
| 23  | a1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | b1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | b1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | b1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | c1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | c1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | d1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | h1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | k1    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | A2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | B2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | B2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | B2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | C2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | F2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | H2    | 1        | Total C<br>24 24 | 0       | 0       |
| 23  | K2    | 1        | Total C<br>40 40 | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 23  | K2    | 1        | Total C<br>29 29 | 0       | 0       |
| 23  | a2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | b2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | b2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | b2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | c2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | d2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | h2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | j2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | k2    | 1        | Total C<br>40 40 | 0       | 0       |
| 23  | z2    | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 24  | A1    | 1        | Total Cl<br>1 1 | 0       | 0       |
| 24  | a1    | 1        | Total Cl<br>1 1 | 0       | 0       |
| 24  | A2    | 1        | Total Cl<br>1 1 | 0       | 0       |
| 24  | a2    | 1        | Total Cl<br>1 1 | 0       | 0       |

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).





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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 25  | B1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | B1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | B1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | B1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | B1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |         |
| 25  | B1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |         |
| 25  | C1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 25  | D1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | D1    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 25  | a1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | a1    | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | a1    | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 25  | c1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | d1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | d1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | d1    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | A2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | A2    | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | A2    | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | B2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | C2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | C2    | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | C2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | C2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | C2    | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | C2    | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | C2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | C2    | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | C2    | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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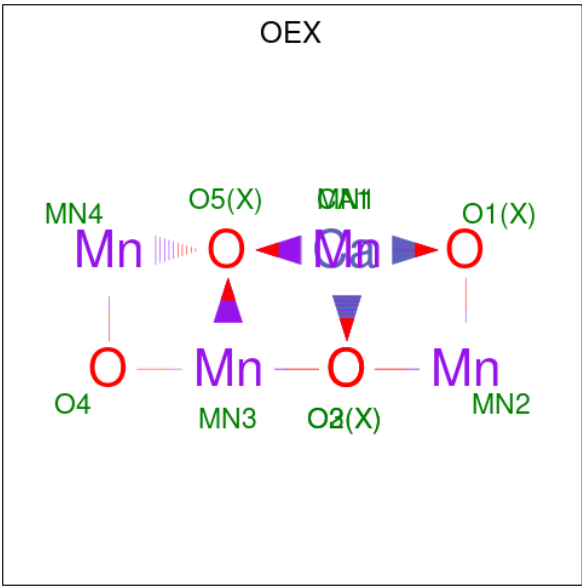
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 25  | C2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 53    | 43 | 1  | 4 | 5 |         |         |
| 25  | C2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 25  | C2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 25  | D2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | D2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |         |
| 25  | D2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | K2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 25  | a2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | a2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | a2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 25  | b2    | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |

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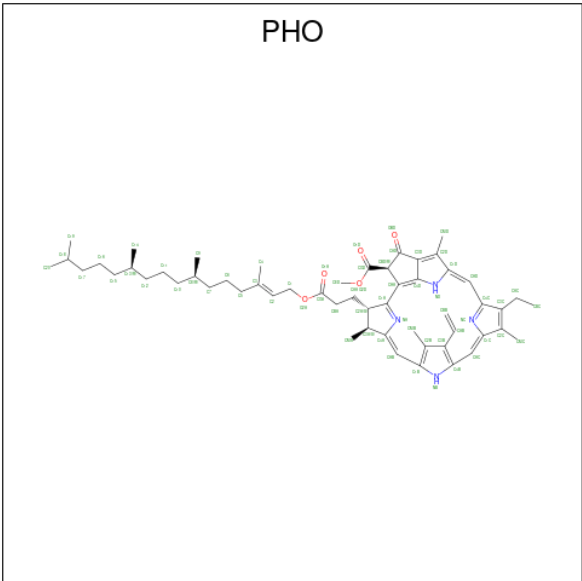
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 25  | b2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b2    | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | b2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | c2    | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | d2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | d2    | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 25  | d2    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26  | A1    | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |
| 26  | a1    | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |
| 26  | A2    | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |
| 26  | a2    | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$ ).





| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 27  | A1    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 27  | D1    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 63    | 54 | 4 | 5 |         |         |
| 27  | a1    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 27  | d1    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 27  | A2    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 27  | D2    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 27  | a2    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 27  | d2    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |

- Molecule 28 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

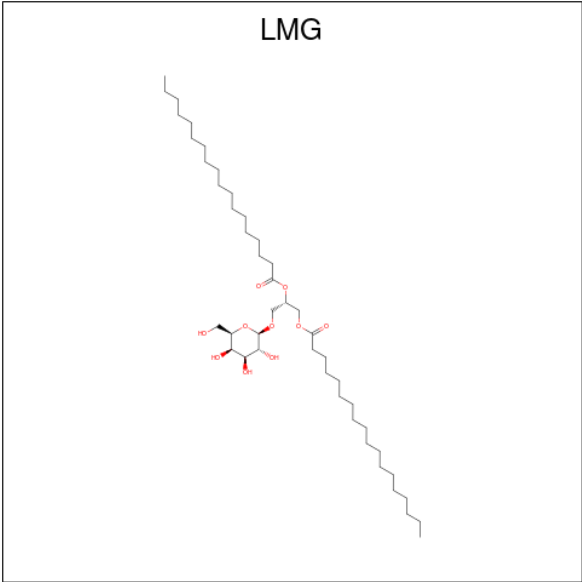
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 28  | A1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 28  | B1    | 3        | Total | C  | 0       | 0       |
|     |       |          | 41    | 41 |         |         |
| 28  | D1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 28  | a1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 28  | b1    | 7        | Total | C  | 0       | 0       |
|     |       |          | 92    | 92 |         |         |
| 28  | d1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 28  | j1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 28  | l1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 28  | m1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 28  | t1    | 2        | Total | C  | 0       | 0       |
|     |       |          | 27    | 27 |         |         |
| 28  | x1    | 1        | Total | C  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 28  | A2    | 2        | Total | C  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 28  | B2    | 4        | Total C<br>58 58 | 0       | 0       |
| 28  | C2    | 2        | Total C<br>24 24 | 0       | 0       |
| 28  | F2    | 1        | Total C<br>16 16 | 0       | 0       |
| 28  | H2    | 1        | Total C<br>5 5   | 0       | 0       |
| 28  | I2    | 2        | Total C<br>31 31 | 0       | 0       |
| 28  | J2    | 1        | Total C<br>10 10 | 0       | 0       |
| 28  | K2    | 1        | Total C<br>5 5   | 0       | 0       |
| 28  | M2    | 1        | Total C<br>11 11 | 0       | 0       |
| 28  | X2    | 1        | Total C<br>7 7   | 0       | 0       |
| 28  | W2    | 1        | Total C<br>9 9   | 0       | 0       |
| 28  | a2    | 4        | Total C<br>55 55 | 0       | 0       |
| 28  | b2    | 1        | Total C<br>12 12 | 0       | 0       |
| 28  | c2    | 1        | Total C<br>15 15 | 0       | 0       |
| 28  | d2    | 2        | Total C<br>25 25 | 0       | 0       |
| 28  | i2    | 1        | Total C<br>14 14 | 0       | 0       |
| 28  | k2    | 4        | Total C<br>30 30 | 0       | 0       |
| 28  | m2    | 2        | Total C<br>36 36 | 0       | 0       |

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 29  | A1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 43    | 33 | 10 |         |         |
| 29  | A1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 41    | 31 | 10 |         |         |
| 29  | B1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 31    | 21 | 10 |         |         |
| 29  | B1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 29  | C1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 29  | D1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 25 | 10 |         |         |
| 29  | M1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 31    | 27 | 4  |         |         |
| 29  | a1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 29  | b1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 38    | 28 | 10 |         |         |
| 29  | b1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 39    | 29 | 10 |         |         |
| 29  | b1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 40    | 30 | 10 |         |         |
| 29  | c1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 55    | 45 | 10 |         |         |
| 29  | d1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 23 | 10 |         |         |
| 29  | d1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 30 | 5  |         |         |

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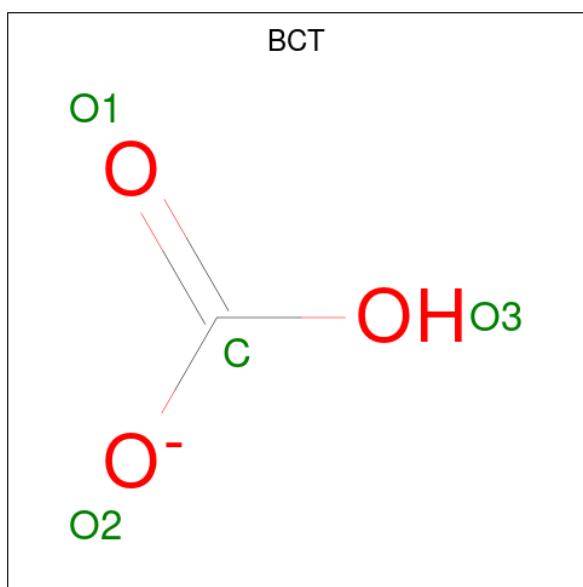
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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 29  | A2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 29    | 19 | 10 |         |         |
| 29  | B2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 40    | 30 | 10 |         |         |
| 29  | B2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 37    | 27 | 10 |         |         |
| 29  | C2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 14 | 10 |         |         |
| 29  | F2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 25 | 10 |         |         |
| 29  | I2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 34    | 24 | 10 |         |         |
| 29  | a2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 44    | 34 | 10 |         |         |
| 29  | b2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 39    | 29 | 10 |         |         |
| 29  | c2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 26    | 16 | 10 |         |         |
| 29  | d2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 27    | 17 | 10 |         |         |
| 29  | j2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 50    | 40 | 10 |         |         |

- Molecule 30 is FE (III) ION (CCD ID: FE) (formula: Fe).

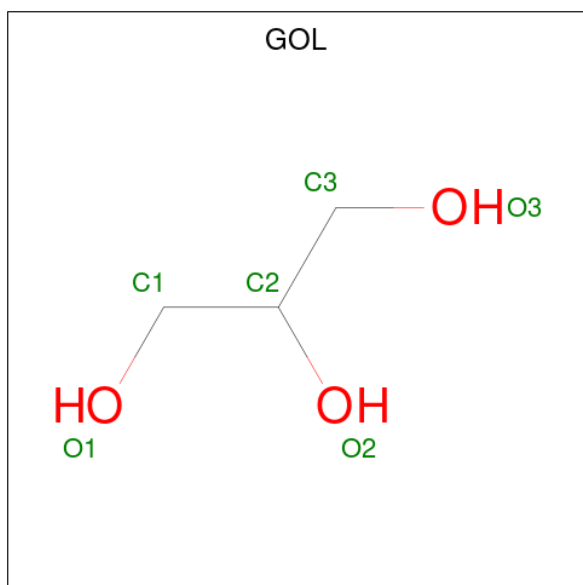
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 30  | A1    | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 30  | a1    | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 30  | A2    | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 30  | a2    | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO<sub>3</sub>).



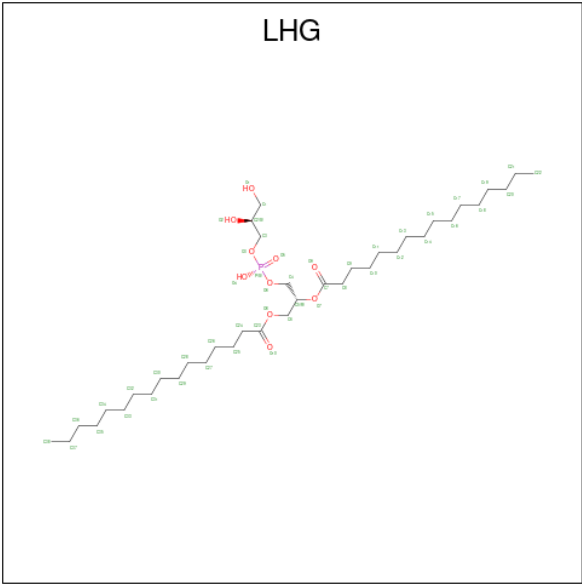
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 31  | A1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 31  | a1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 31  | A2    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 31  | a2    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |

- Molecule 32 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 32  | B1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 32  | C1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 32  | a1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 32  | b1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 32  | c1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 32  | i1    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 32  | C2    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 32  | a2    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 32  | c2    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



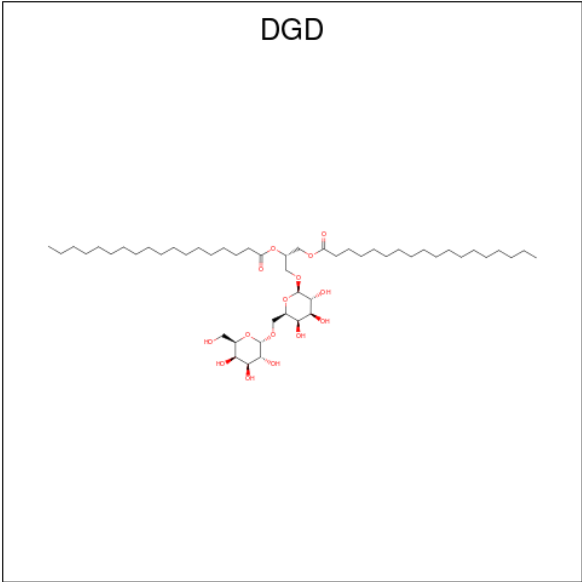
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 33  | B1    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | D1    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 33  | D1    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | L1    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 41    | 30 | 10 | 1 |         |         |
| 33  | a1    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |         |
| 33  | b1    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | d1    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 32    | 21 | 10 | 1 |         |         |
| 33  | d1    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | l1    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | A2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 33    | 22 | 10 | 1 |         |         |
| 33  | B2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |         |
| 33  | D2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | D2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | L2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | a2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 30    | 19 | 10 | 1 |         |         |
| 33  | b2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |         |
| 33  | d2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | d2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 33  | l2    | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 44    | 33 | 10 | 1 |         |         |

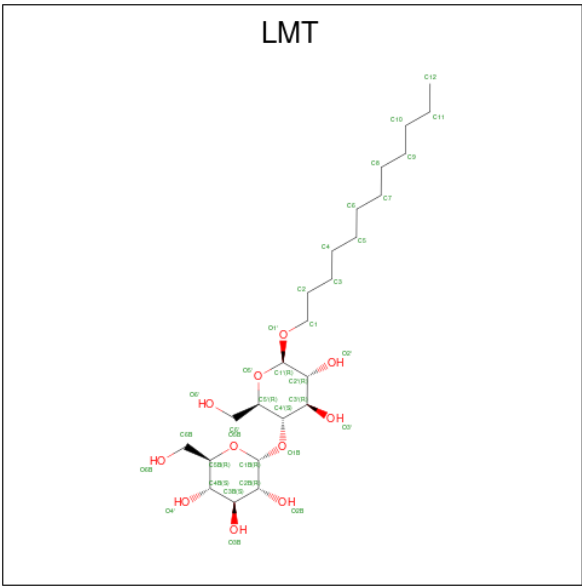
- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 34  | C1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 52    | 37 | 15 |         |         |
| 34  | C1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 34  | C1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 64    | 49 | 15 |         |         |
| 34  | H1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 34  | c1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 36 | 15 |         |         |
| 34  | c1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 34  | c1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 34  | h1    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 34  | C2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 18 | 15 |         |         |
| 34  | H2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 34  | c2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 34  | c2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 52    | 37 | 15 |         |         |
| 34  | c2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 34  | h2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |



- Molecule 35 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



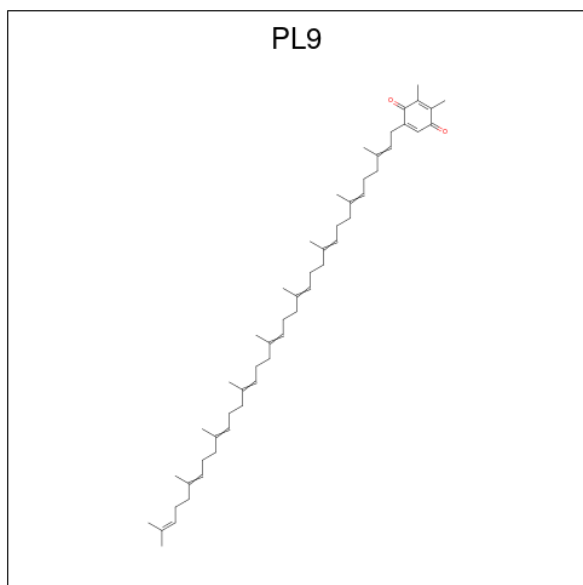
| Mol | Chain | Residues | Atoms                 | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 35  | C1    | 1        | Total C O<br>35 24 11 | 0       | 0       |
| 35  | L1    | 1        | Total C<br>12 12      | 0       | 0       |
| 35  | M1    | 1        | Total C<br>11 11      | 0       | 0       |
| 35  | M1    | 1        | Total C O<br>24 18 6  | 0       | 0       |
| 35  | T1    | 1        | Total C<br>12 12      | 0       | 0       |
| 35  | c1    | 1        | Total C O<br>33 22 11 | 0       | 0       |
| 35  | l1    | 1        | Total C O<br>24 18 6  | 0       | 0       |
| 35  | m1    | 1        | Total C O<br>35 24 11 | 0       | 0       |
| 35  | a2    | 1        | Total C O<br>35 24 11 | 0       | 0       |
| 35  | b2    | 1        | Total C O<br>35 24 11 | 0       | 0       |
| 35  | b2    | 1        | Total C O<br>35 24 11 | 0       | 0       |
| 35  | i2    | 1        | Total C<br>7 7        | 0       | 0       |
| 35  | m2    | 1        | Total C O<br>30 19 11 | 0       | 0       |

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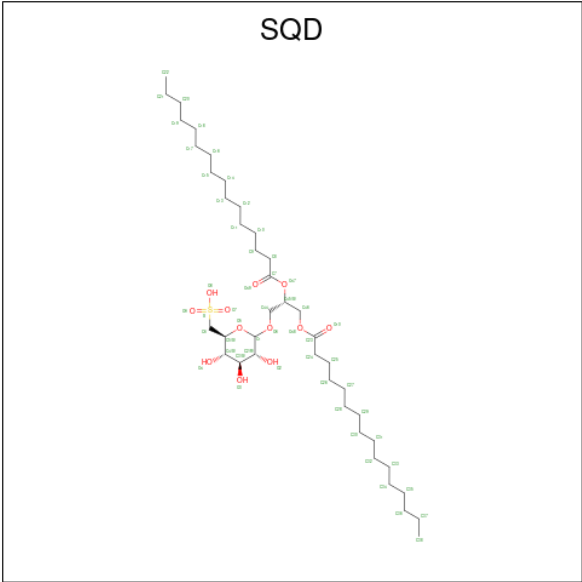
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 35  | m2    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 29    | 18 | 11 |         |         |

- Molecule 36 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>).



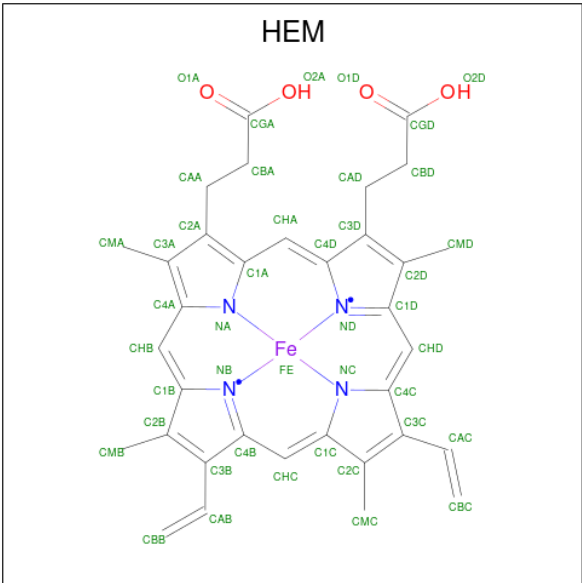
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 36  | D1    | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 36  | d1    | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 36  | D2    | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 36  | d2    | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |

- Molecule 37 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 |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 37  | D1    | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 35    | 22 | 12 | 1 |         |         |
| 37  | B2    | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 45    | 32 | 12 | 1 |         |         |
| 37  | D2    | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 25    | 12 | 12 | 1 |         |         |
| 37  | b2    | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 45    | 32 | 12 | 1 |         |         |

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms       |         |         |        | ZeroOcc | AltConf |   |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 38  | E1    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 38  | V1    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 38  | f1    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 38  | v1    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 38  | E2    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 38  | V2    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 38  | e2    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 38  | v2    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |

- Molecule 39 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 39  | O1    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 39  | o2    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

- Molecule 40 is water.

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 40  | A1    | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 40  | B1    | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 40  | a1    | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 40  | c1    | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 40  | A2    | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 40  | a2    | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 40  | b2    | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 40  | c2    | 1        | Total<br>1 | O<br>1 | 0       | 0       |

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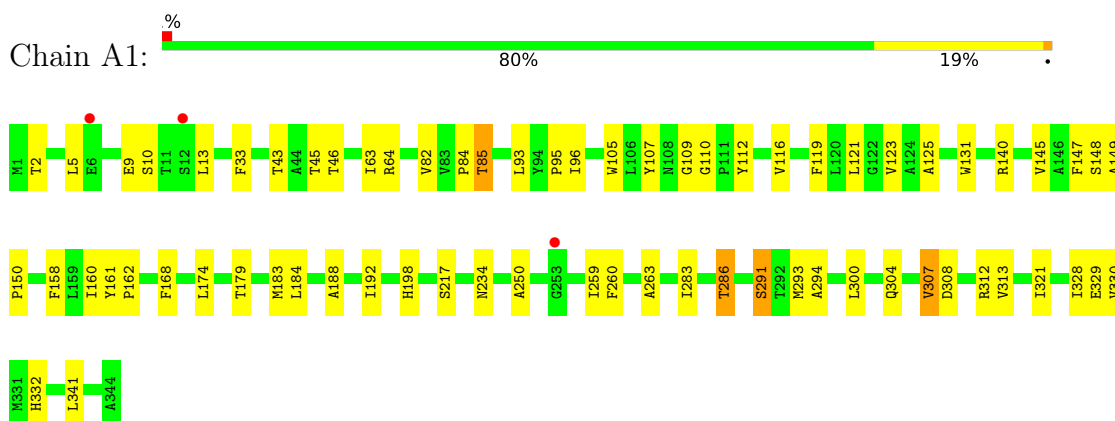
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 40  | d2    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

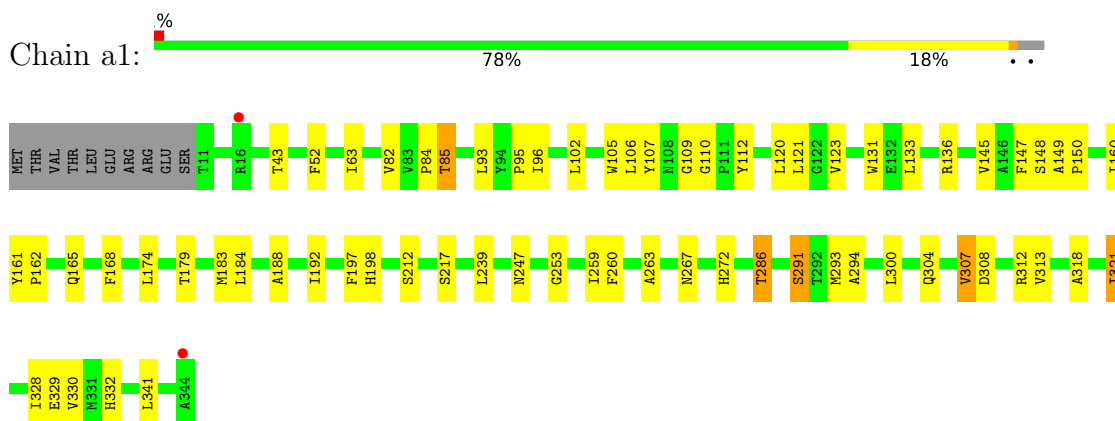
### 3 Residue-property plots

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

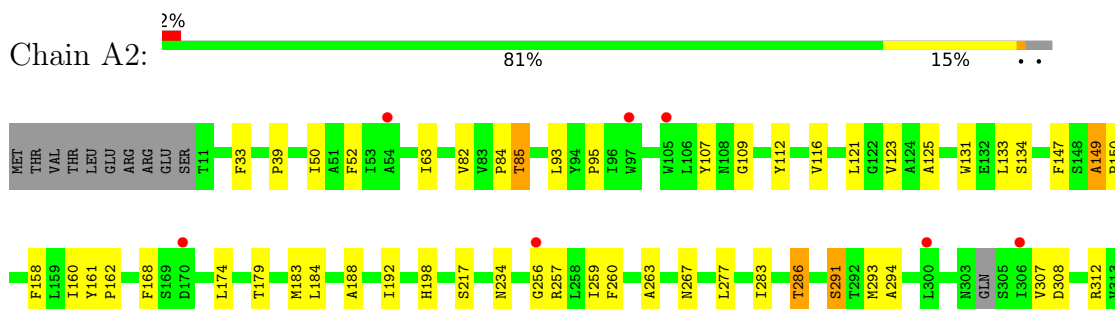
- Molecule 1: Photosystem II protein D1

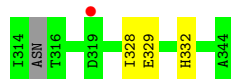


- Molecule 1: Photosystem II protein D1



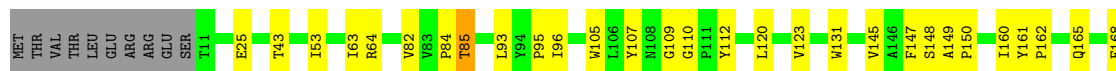
- Molecule 1: Photosystem II protein D1





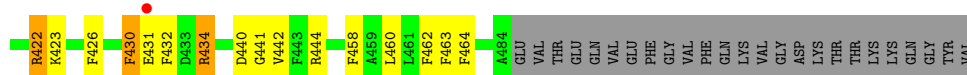
- Molecule 1: Photosystem II protein D1

Chain a2: 80% 16% ..



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B1: % 79% 14% 5%



- Molecule 2: Photosystem II CP47 reaction center protein

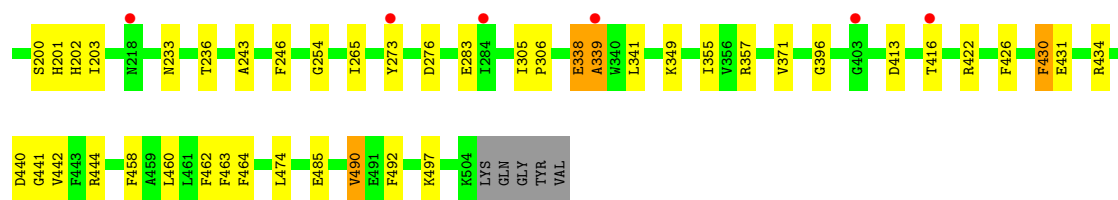
Chain b1: 83% 14% ..



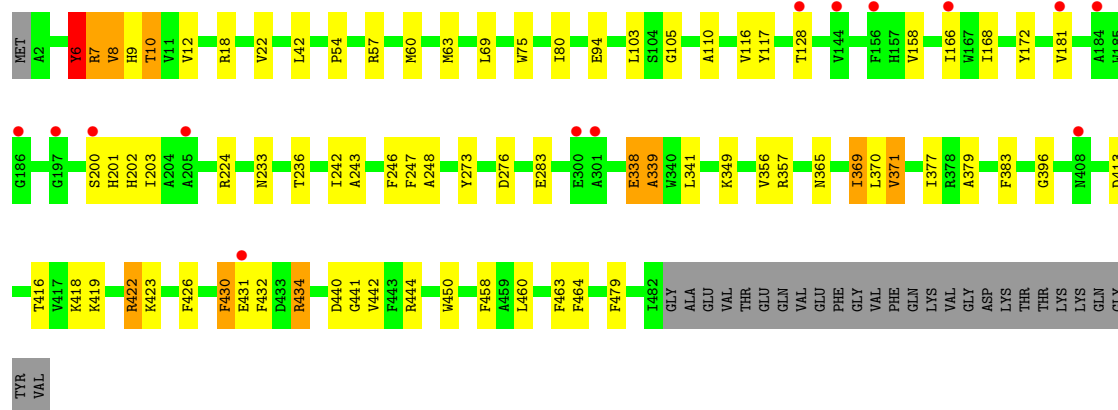
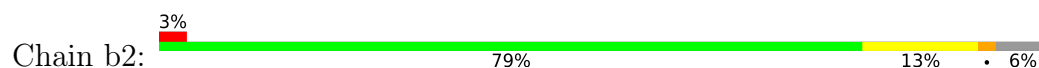
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B2: 2% 84% 13% ..

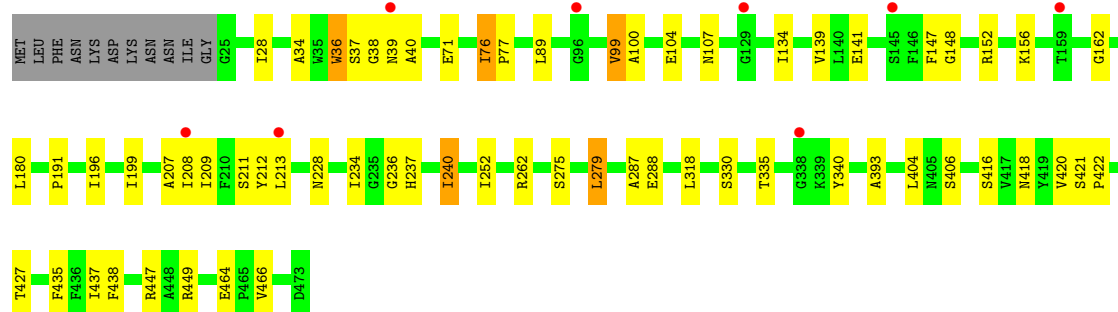
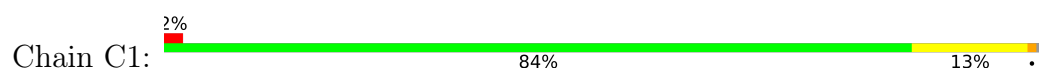




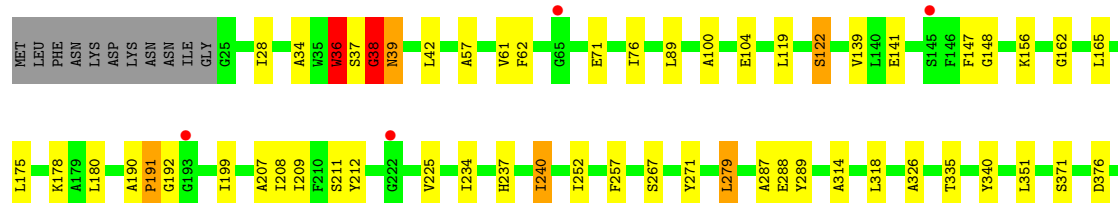
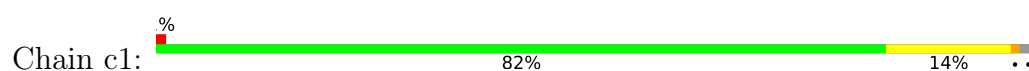
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein



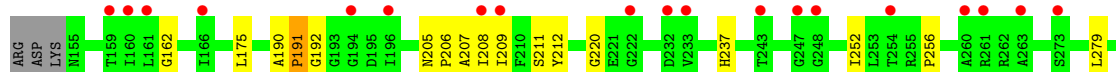
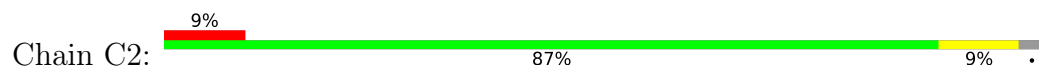
• Molecule 3: Photosystem II CP43 reaction center protein



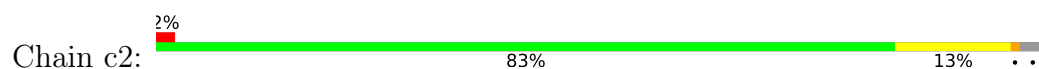




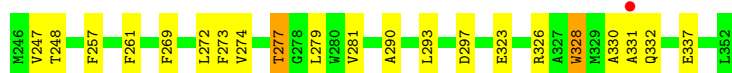
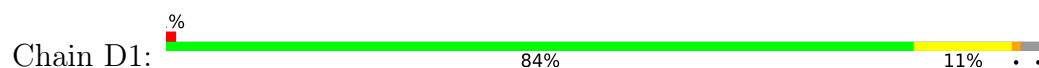
• Molecule 3: Photosystem II CP43 reaction center protein



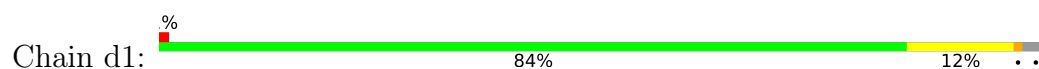
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II D2 protein

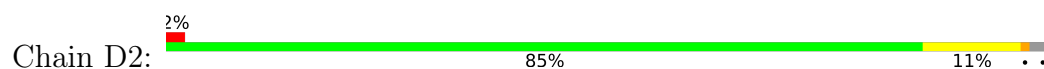


• Molecule 4: Photosystem II D2 protein

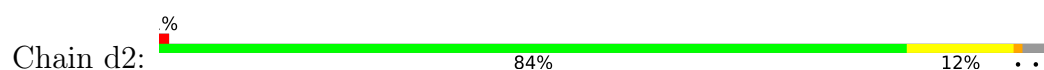




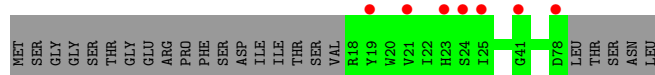
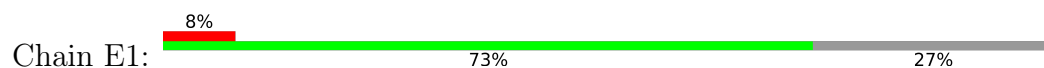
• Molecule 4: Photosystem II D2 protein



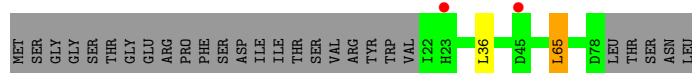
• Molecule 4: Photosystem II D2 protein



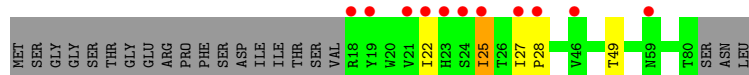
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

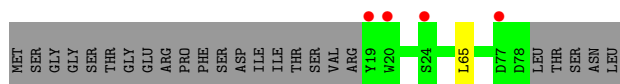


• Molecule 5: Cytochrome b559 subunit alpha

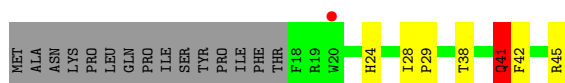


• Molecule 5: Cytochrome b559 subunit alpha





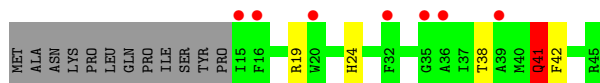
- Molecule 6: Cytochrome b559 subunit beta



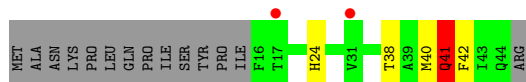
- Molecule 6: Cytochrome b559 subunit beta



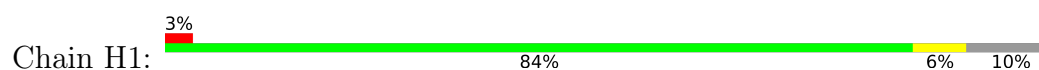
- Molecule 6: Cytochrome b559 subunit beta



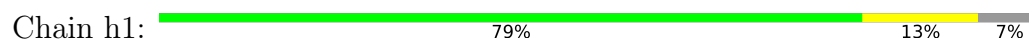
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H

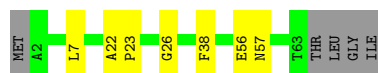


- Molecule 7: Photosystem II reaction center protein H



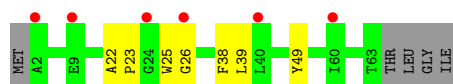
- Molecule 7: Photosystem II reaction center protein H

Chain H2:  82% 10% 7%



- Molecule 7: Photosystem II reaction center protein H

Chain h2:  9% 82% 10% 7%



- Molecule 8: Photosystem II reaction center protein I

Chain I1:  74% 16% 11%



- Molecule 8: Photosystem II reaction center protein I

Chain i1:  68% 21% 11%



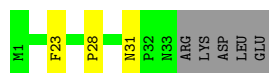
- Molecule 8: Photosystem II reaction center protein I

Chain I2:  3% 79% 13% 8%



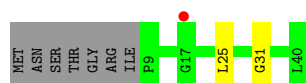
- Molecule 8: Photosystem II reaction center protein I

Chain i2:  79% 8% 13%



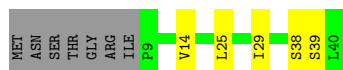
- Molecule 9: Photosystem II reaction center protein J

Chain J1:  3% 77% 5% 18%



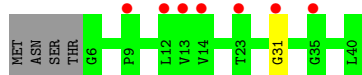
- Molecule 9: Photosystem II reaction center protein J

Chain j1:  69% 13% 18%



- Molecule 9: Photosystem II reaction center protein J

Chain J2:  18% 87% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j2:  3% 67% 15% 15%



- Molecule 10: Photosystem II reaction center protein K

Chain K1:  2% 56% 29% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain k1:  61% 24% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K2:  15% 73% 12% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain k2:  5% 61% 27% 10%



- Molecule 11: Photosystem II reaction center protein L

Chain L1:  74% 24% .



- Molecule 11: Photosystem II reaction center protein L

Chain l1:  71% 26% .



- Molecule 11: Photosystem II reaction center protein L

Chain L2:  74% 24% .



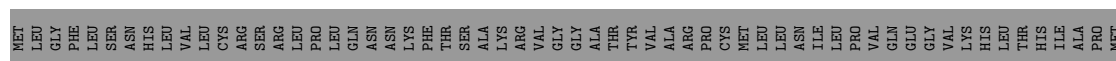
- Molecule 11: Photosystem II reaction center protein L

Chain l2:  71% 26% .



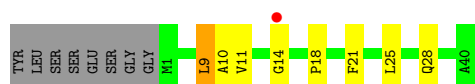
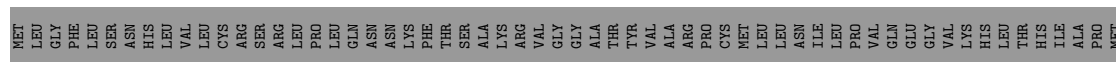
- Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain M1:  27% 10% 63%



- Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain m1:  30% 6% 63%

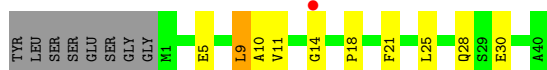


- Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

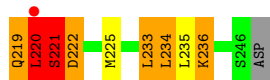
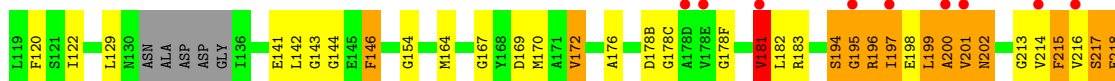
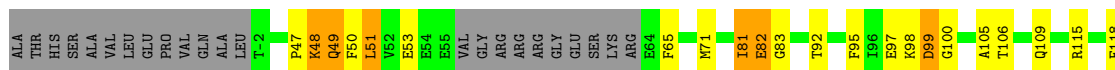
Chain M2:  30% 6% 63%



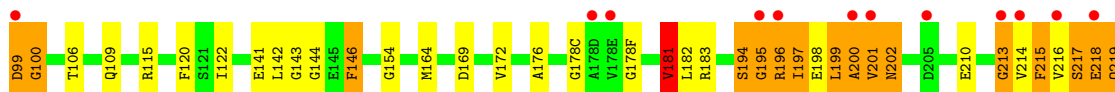
Chain m2:  %

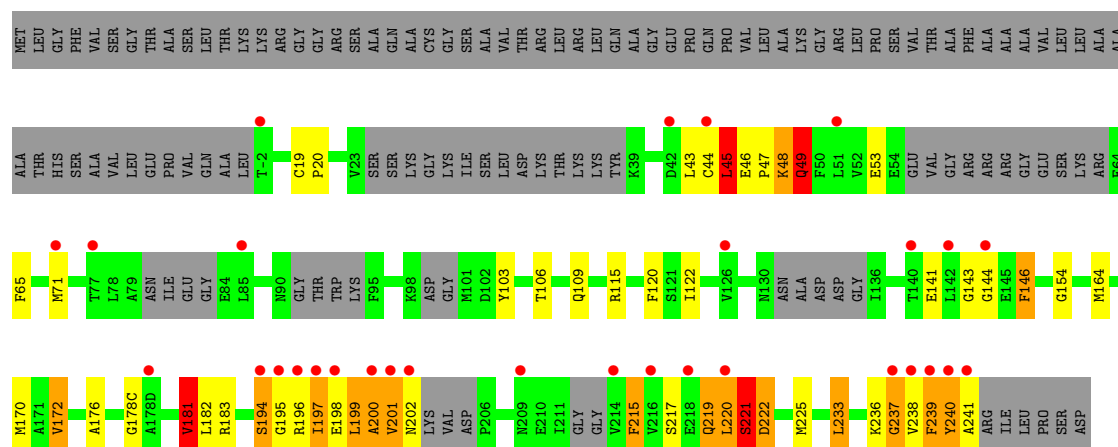


Chain O1: 

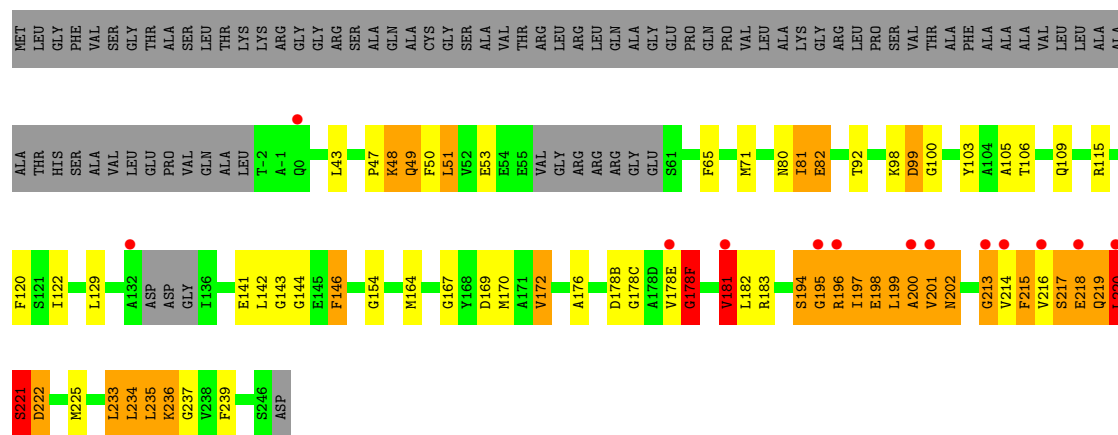


Chain 01:  5% 54% 9% 8% 28%

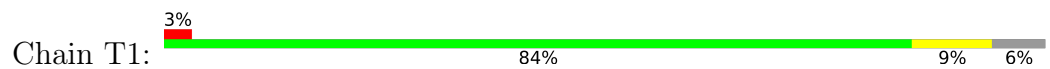




• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO



• Molecule 14: Photosystem II reaction center protein T



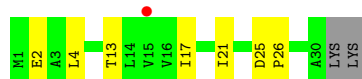
• Molecule 14: Photosystem II reaction center protein T



• Molecule 14: Photosystem II reaction center protein T



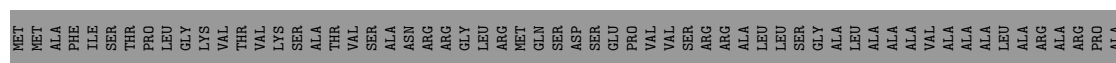




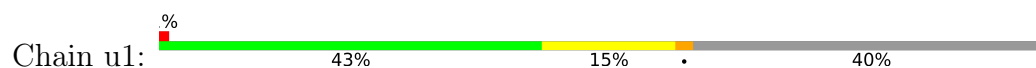
- Molecule 14: Photosystem II reaction center protein T



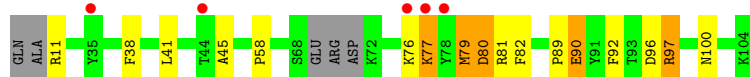
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



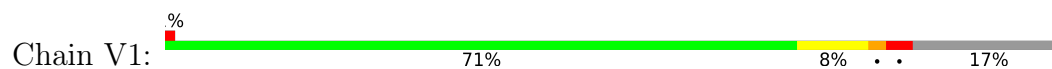
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



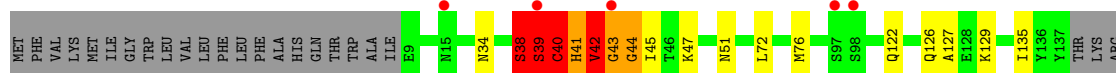
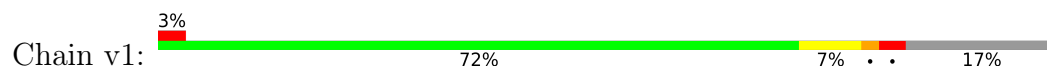
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



- Molecule 16: Cytochrome c-550

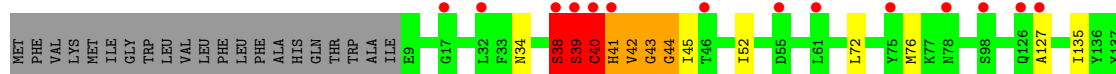
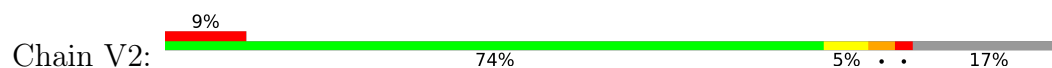


- Molecule 16: Cytochrome c-550



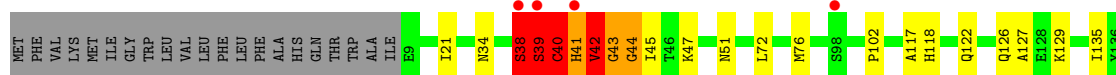
SER  
MET

- Molecule 16: Cytochrome c-550



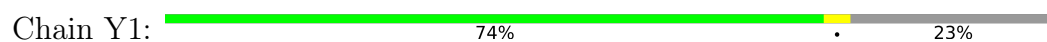
THR  
LYS  
ARG  
SER  
MET

- Molecule 16: Cytochrome c-550



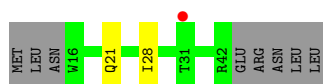
Y137  
THR  
LYS  
ARG  
SER  
MET

- Molecule 17: Photosystem II reaction center protein Ycf12

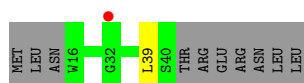


- Molecule 17: Photosystem II reaction center protein Ycf12





- Molecule 17: Photosystem II reaction center protein Ycf12



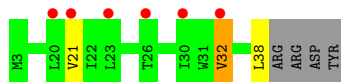
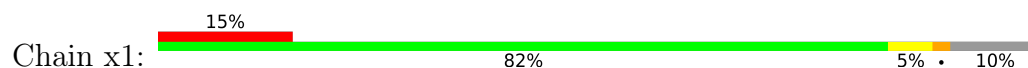
- Molecule 17: Photosystem II reaction center protein Ycf12



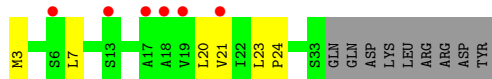
- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



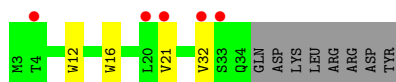
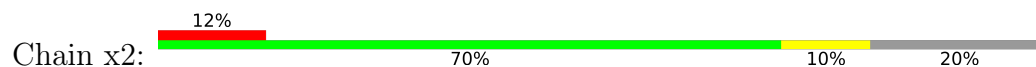
- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

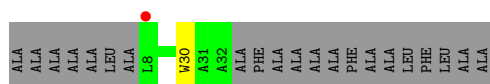


- Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

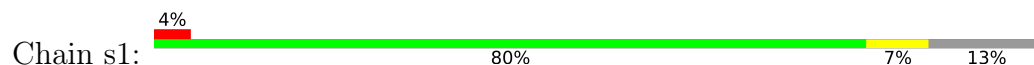


- Molecule 19: PEPTIDE CHAIN UNASSIGNED





- Molecule 19: PEPTIDE CHAIN UNASSIGNED



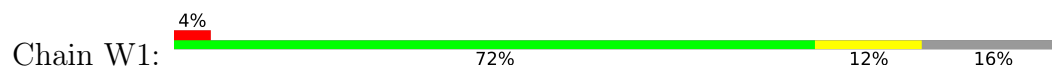
- Molecule 19: PEPTIDE CHAIN UNASSIGNED



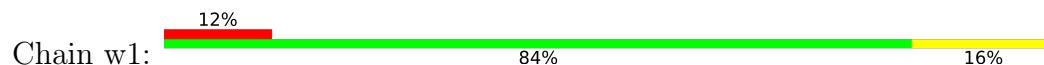
- Molecule 19: PEPTIDE CHAIN UNASSIGNED



- Molecule 20: PEPTIDE CHAIN UNASSIGNED



- Molecule 20: PEPTIDE CHAIN UNASSIGNED

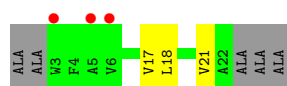


- Molecule 20: PEPTIDE CHAIN UNASSIGNED

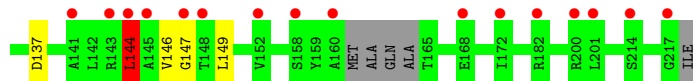
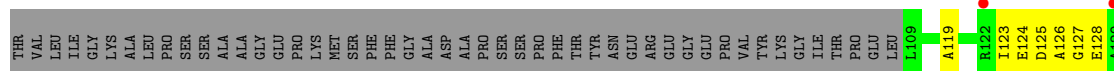
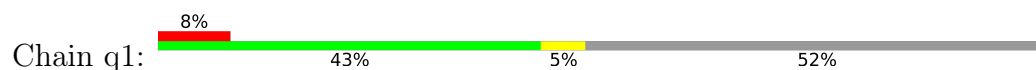


- Molecule 20: PEPTIDE CHAIN UNASSIGNED

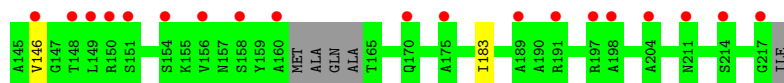
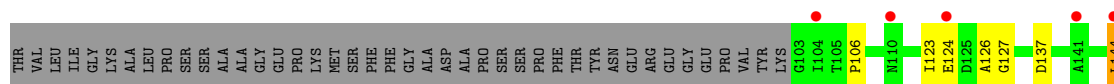




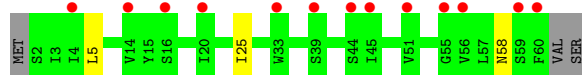
- Molecule 21: Extrinsic protein in photosystem II



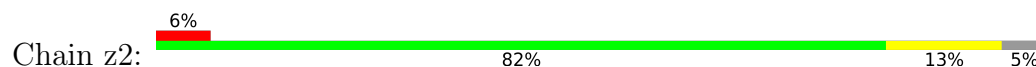
- Molecule 21: Extrinsic protein in photosystem II



- Molecule 22: Photosystem II reaction center protein Z



- Molecule 22: 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, $\alpha$ , $\beta$ , $\gamma$                | 210.44Å 240.31Å 300.06Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 10.00 – 2.77<br>10.00 – 2.77                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (10.00-2.77)<br>97.5 (10.00-2.77)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.48 (at 2.76Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.9_1692                                             | Depositor        |
| R, $R_{free}$                                                           | 0.249 , 0.278<br>0.255 , 0.282                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 19164 reflections (4.99%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 68.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.616                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 78.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 92765                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 68.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: GOL, CL, OEX, LMG, UNL, FE, BCT, CLA, SQD, DGD, BCR, PL9, PHO, LMT, HEM, CA, LHG

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   | A1    | 0.38         | 0/2685        | 0.77        | 1/3673 (0.0%) |
| 1   | A2    | 0.40         | 1/2548 (0.0%) | 0.77        | 0/3481        |
| 1   | a1    | 0.37         | 0/2642        | 0.76        | 0/3612        |
| 1   | a2    | 0.37         | 0/2586        | 0.76        | 0/3538        |
| 2   | B1    | 0.41         | 2/3830 (0.1%) | 0.83        | 6/5227 (0.1%) |
| 2   | B2    | 0.41         | 2/3897 (0.1%) | 0.83        | 6/5323 (0.1%) |
| 2   | b1    | 0.46         | 3/4015 (0.1%) | 0.83        | 9/5473 (0.2%) |
| 2   | b2    | 0.41         | 2/3808 (0.1%) | 0.83        | 6/5197 (0.1%) |
| 3   | C1    | 0.35         | 0/3501        | 0.77        | 2/4782 (0.0%) |
| 3   | C2    | 0.34         | 0/3242        | 0.79        | 2/4441 (0.0%) |
| 3   | c1    | 0.38         | 2/3555 (0.1%) | 0.77        | 4/4850 (0.1%) |
| 3   | c2    | 0.34         | 0/3495        | 0.77        | 2/4773 (0.0%) |
| 4   | D1    | 0.44         | 1/2704 (0.0%) | 0.77        | 2/3688 (0.1%) |
| 4   | D2    | 0.44         | 1/2675 (0.0%) | 0.78        | 4/3655 (0.1%) |
| 4   | d1    | 0.44         | 1/2772 (0.0%) | 0.78        | 2/3783 (0.1%) |
| 4   | d2    | 0.44         | 1/2736 (0.0%) | 0.77        | 2/3734 (0.1%) |
| 5   | E1    | 0.33         | 0/418         | 0.74        | 0/577         |
| 5   | E2    | 0.34         | 0/443         | 0.73        | 0/614         |
| 5   | e1    | 0.32         | 0/440         | 0.69        | 0/603         |
| 5   | e2    | 0.32         | 0/434         | 0.72        | 0/598         |
| 6   | F1    | 0.67         | 0/220         | 0.95        | 3/299 (1.0%)  |
| 6   | F2    | 0.61         | 0/236         | 0.95        | 3/320 (0.9%)  |
| 6   | f1    | 0.64         | 0/235         | 0.92        | 3/319 (0.9%)  |
| 6   | f2    | 0.63         | 0/234         | 0.92        | 3/318 (0.9%)  |
| 7   | H1    | 0.29         | 0/443         | 0.70        | 0/606         |
| 7   | H2    | 0.30         | 0/453         | 0.72        | 0/619         |
| 7   | h1    | 0.29         | 0/481         | 0.71        | 0/657         |
| 7   | h2    | 0.28         | 0/461         | 0.70        | 0/631         |
| 8   | I1    | 0.30         | 0/283         | 0.68        | 0/381         |
| 8   | I2    | 0.30         | 0/273         | 0.71        | 0/371         |
| 8   | i1    | 0.29         | 0/289         | 0.69        | 0/389         |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 8   | i2    | 0.30         | 0/270          | 0.71        | 0/364          |
| 9   | J1    | 0.27         | 0/225          | 0.70        | 0/307          |
| 9   | J2    | 0.26         | 0/236          | 0.72        | 0/324          |
| 9   | j1    | 0.26         | 0/229          | 0.70        | 0/313          |
| 9   | j2    | 0.27         | 0/233          | 0.82        | 2/319 (0.6%)   |
| 10  | K1    | 0.50         | 0/289          | 0.84        | 0/399          |
| 10  | K2    | 0.54         | 0/258          | 0.87        | 0/359          |
| 10  | k1    | 0.50         | 0/290          | 0.85        | 0/401          |
| 10  | k2    | 0.53         | 0/278          | 0.85        | 0/385          |
| 11  | L1    | 0.66         | 0/301          | 0.88        | 0/410          |
| 11  | L2    | 0.64         | 0/308          | 0.87        | 0/419          |
| 11  | l1    | 0.65         | 0/308          | 0.88        | 0/418          |
| 11  | l2    | 0.65         | 0/308          | 0.87        | 0/418          |
| 12  | M1    | 0.49         | 0/288          | 0.93        | 0/391          |
| 12  | M2    | 0.48         | 0/287          | 0.93        | 0/390          |
| 12  | m1    | 0.48         | 0/288          | 0.92        | 0/391          |
| 12  | m2    | 0.46         | 0/290          | 0.93        | 0/394          |
| 13  | O1    | 0.98         | 15/1700 (0.9%) | 1.46        | 35/2315 (1.5%) |
| 13  | O2    | 0.89         | 9/1387 (0.6%)  | 1.35        | 27/1881 (1.4%) |
| 13  | o1    | 0.94         | 13/1716 (0.8%) | 1.41        | 38/2330 (1.6%) |
| 13  | o2    | 0.95         | 14/1794 (0.8%) | 1.46        | 40/2434 (1.6%) |
| 14  | T1    | 0.28         | 0/248          | 0.78        | 0/337          |
| 14  | T2    | 0.28         | 0/247          | 0.77        | 0/337          |
| 14  | t1    | 0.29         | 0/253          | 0.77        | 0/344          |
| 14  | t2    | 0.29         | 0/242          | 0.77        | 0/330          |
| 15  | U1    | 0.63         | 1/709 (0.1%)   | 1.03        | 7/970 (0.7%)   |
| 15  | U2    | 0.67         | 2/588 (0.3%)   | 1.25        | 10/809 (1.2%)  |
| 15  | u1    | 0.63         | 1/721 (0.1%)   | 1.02        | 5/981 (0.5%)   |
| 15  | u2    | 0.62         | 2/726 (0.3%)   | 1.00        | 5/988 (0.5%)   |
| 16  | V1    | 0.66         | 3/937 (0.3%)   | 0.98        | 8/1281 (0.6%)  |
| 16  | V2    | 0.68         | 3/858 (0.3%)   | 0.98        | 8/1177 (0.7%)  |
| 16  | v1    | 0.64         | 2/941 (0.2%)   | 0.98        | 8/1284 (0.6%)  |
| 16  | v2    | 0.63         | 2/983 (0.2%)   | 0.96        | 8/1337 (0.6%)  |
| 17  | Y1    | 0.61         | 0/171          | 1.00        | 0/236          |
| 17  | Y2    | 0.62         | 0/159          | 1.05        | 0/219          |
| 17  | y1    | 0.58         | 0/198          | 0.93        | 0/274          |
| 17  | y2    | 0.59         | 0/191          | 0.98        | 0/264          |
| 18  | X1    | 0.37         | 0/202          | 0.80        | 1/278 (0.4%)   |
| 18  | X2    | 0.35         | 0/222          | 0.82        | 1/307 (0.3%)   |
| 18  | x1    | 0.41         | 0/262          | 0.80        | 1/363 (0.3%)   |
| 18  | x2    | 0.44         | 0/225          | 0.88        | 1/312 (0.3%)   |
| 19  | S1    | 0.32         | 0/167          | 0.65        | 0/231          |
| 19  | S2    | 0.32         | 0/194          | 0.66        | 0/268          |



| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 19  | s1    | 0.32         | 0/269           | 0.63        | 0/371             |
| 19  | s2    | 0.33         | 0/285           | 0.68        | 0/395             |
| 20  | W1    | 0.34         | 0/134           | 0.77        | 0/186             |
| 20  | W2    | 0.35         | 0/129           | 0.81        | 0/179             |
| 20  | w1    | 0.34         | 0/152           | 0.77        | 0/211             |
| 20  | w2    | 0.32         | 0/127           | 0.79        | 0/176             |
| 21  | Q2    | 0.55         | 1/682 (0.1%)    | 0.85        | 0/937             |
| 21  | q1    | 0.55         | 1/650 (0.2%)    | 0.84        | 0/893             |
| 22  | Z2    | 0.33         | 0/353           | 0.81        | 0/487             |
| 22  | z2    | 0.34         | 0/387           | 0.77        | 0/532             |
| All | All   | 0.50         | 85/79929 (0.1%) | 0.88        | 265/109188 (0.2%) |

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  | O1    | 0                   | 2                   |
| 13  | O2    | 0                   | 4                   |
| 13  | o1    | 0                   | 3                   |
| 13  | o2    | 0                   | 3                   |
| 16  | V1    | 0                   | 3                   |
| 16  | V2    | 0                   | 3                   |
| 16  | v1    | 0                   | 3                   |
| 16  | v2    | 0                   | 3                   |
| All | All   | 0                   | 24                  |

The worst 5 of 85 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 16  | V2    | 42  | VAL  | CA-C  | -11.01 | 1.38        | 1.52     |
| 13  | O1    | 220 | LEU  | N-CA  | 10.34  | 1.57        | 1.45     |
| 13  | o2    | 220 | LEU  | N-CA  | 10.33  | 1.57        | 1.45     |
| 13  | o1    | 220 | LEU  | N-CA  | 10.19  | 1.57        | 1.45     |
| 13  | O1    | 221 | SER  | N-CA  | 9.74   | 1.58        | 1.46     |

The worst 5 of 265 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13  | O1    | 219 | GLN  | N-CA-C | 12.94 | 128.74      | 109.07   |
| 13  | o2    | 219 | GLN  | N-CA-C | 12.93 | 128.73      | 109.07   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 13  | o1    | 219 | GLN  | N-CA-C | 12.60  | 128.22      | 109.07   |
| 13  | O1    | 215 | PHE  | CA-C-N | -12.49 | 102.53      | 122.64   |
| 13  | O1    | 215 | PHE  | C-N-CA | -12.49 | 102.53      | 122.64   |

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 13  | O1    | 194 | SER  | Peptide |
| 13  | O1    | 220 | LEU  | Peptide |
| 16  | V1    | 38  | SER  | Peptide |
| 16  | V1    | 41  | HIS  | Peptide |
| 16  | V1    | 44  | GLY  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A1    | 2609  | 0        | 2500     | 51      | 0            |
| 1   | A2    | 2475  | 0        | 2296     | 41      | 0            |
| 1   | a1    | 2564  | 0        | 2462     | 54      | 0            |
| 1   | a2    | 2513  | 0        | 2376     | 46      | 0            |
| 2   | B1    | 3703  | 0        | 3485     | 59      | 0            |
| 2   | B2    | 3770  | 0        | 3462     | 47      | 0            |
| 2   | b1    | 3881  | 0        | 3672     | 64      | 0            |
| 2   | b2    | 3681  | 0        | 3452     | 59      | 0            |
| 3   | C1    | 3392  | 0        | 3206     | 54      | 0            |
| 3   | C2    | 3145  | 0        | 2751     | 34      | 0            |
| 3   | c1    | 3439  | 0        | 3293     | 57      | 0            |
| 3   | c2    | 3386  | 0        | 3189     | 50      | 0            |
| 4   | D1    | 2615  | 0        | 2465     | 42      | 0            |
| 4   | D2    | 2585  | 0        | 2371     | 41      | 0            |
| 4   | d1    | 2678  | 0        | 2544     | 39      | 0            |
| 4   | d2    | 2643  | 0        | 2489     | 40      | 0            |
| 5   | E1    | 405   | 0        | 304      | 0       | 0            |
| 5   | E2    | 430   | 0        | 345      | 3       | 0            |
| 5   | e1    | 427   | 0        | 374      | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | e2    | 421   | 0        | 354      | 0       | 0            |
| 6   | F1    | 213   | 0        | 198      | 5       | 0            |
| 6   | F2    | 229   | 0        | 204      | 5       | 0            |
| 6   | f1    | 227   | 0        | 221      | 4       | 0            |
| 6   | f2    | 225   | 0        | 205      | 4       | 0            |
| 7   | H1    | 433   | 0        | 407      | 3       | 0            |
| 7   | H2    | 443   | 0        | 414      | 4       | 0            |
| 7   | h1    | 470   | 0        | 474      | 4       | 0            |
| 7   | h2    | 450   | 0        | 432      | 5       | 0            |
| 8   | I1    | 274   | 0        | 262      | 4       | 0            |
| 8   | I2    | 265   | 0        | 236      | 4       | 0            |
| 8   | i1    | 280   | 0        | 276      | 6       | 0            |
| 8   | i2    | 261   | 0        | 238      | 1       | 0            |
| 9   | J1    | 220   | 0        | 209      | 2       | 0            |
| 9   | J2    | 231   | 0        | 208      | 1       | 0            |
| 9   | j1    | 224   | 0        | 223      | 4       | 0            |
| 9   | j2    | 228   | 0        | 220      | 6       | 0            |
| 10  | K1    | 279   | 0        | 268      | 15      | 0            |
| 10  | K2    | 250   | 0        | 218      | 6       | 0            |
| 10  | k1    | 280   | 0        | 280      | 12      | 0            |
| 10  | k2    | 269   | 0        | 252      | 10      | 0            |
| 11  | L1    | 292   | 0        | 284      | 8       | 0            |
| 11  | L2    | 299   | 0        | 297      | 11      | 0            |
| 11  | l1    | 299   | 0        | 304      | 9       | 0            |
| 11  | l2    | 299   | 0        | 294      | 12      | 0            |
| 12  | M1    | 285   | 0        | 295      | 10      | 0            |
| 12  | M2    | 284   | 0        | 296      | 9       | 0            |
| 12  | m1    | 285   | 0        | 295      | 7       | 0            |
| 12  | m2    | 287   | 0        | 298      | 9       | 0            |
| 13  | O1    | 1674  | 0        | 1534     | 65      | 0            |
| 13  | O2    | 1376  | 0        | 1198     | 57      | 0            |
| 13  | o1    | 1692  | 0        | 1547     | 60      | 0            |
| 13  | o2    | 1768  | 0        | 1663     | 71      | 0            |
| 14  | T1    | 241   | 0        | 248      | 3       | 0            |
| 14  | T2    | 240   | 0        | 253      | 6       | 0            |
| 14  | t1    | 246   | 0        | 264      | 5       | 0            |
| 14  | t2    | 235   | 0        | 248      | 4       | 0            |
| 15  | U1    | 691   | 0        | 628      | 14      | 0            |
| 15  | U2    | 577   | 0        | 435      | 10      | 0            |
| 15  | u1    | 703   | 0        | 645      | 15      | 0            |
| 15  | u2    | 708   | 0        | 671      | 19      | 0            |
| 16  | V1    | 917   | 0        | 847      | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | V2    | 845   | 0        | 719      | 15      | 0            |
| 16  | v1    | 921   | 0        | 842      | 17      | 0            |
| 16  | v2    | 963   | 0        | 937      | 22      | 0            |
| 17  | Y1    | 170   | 0        | 141      | 1       | 0            |
| 17  | Y2    | 159   | 0        | 148      | 1       | 0            |
| 17  | y1    | 195   | 0        | 194      | 2       | 0            |
| 17  | y2    | 188   | 0        | 174      | 7       | 0            |
| 18  | X1    | 197   | 0        | 192      | 1       | 0            |
| 18  | X2    | 215   | 0        | 197      | 3       | 0            |
| 18  | x1    | 255   | 0        | 245      | 2       | 0            |
| 18  | x2    | 218   | 0        | 191      | 1       | 0            |
| 19  | S1    | 164   | 0        | 161      | 1       | 0            |
| 19  | S2    | 191   | 0        | 184      | 1       | 0            |
| 19  | s1    | 263   | 0        | 260      | 3       | 0            |
| 19  | s2    | 281   | 0        | 276      | 1       | 0            |
| 20  | W1    | 134   | 0        | 149      | 2       | 0            |
| 20  | W2    | 129   | 0        | 136      | 3       | 0            |
| 20  | w1    | 152   | 0        | 165      | 5       | 0            |
| 20  | w2    | 127   | 0        | 137      | 2       | 0            |
| 21  | Q2    | 676   | 0        | 484      | 4       | 0            |
| 21  | q1    | 645   | 0        | 462      | 7       | 0            |
| 22  | Z2    | 351   | 0        | 280      | 2       | 0            |
| 22  | z2    | 381   | 0        | 335      | 6       | 0            |
| 23  | A1    | 40    | 0        | 56       | 4       | 0            |
| 23  | A2    | 40    | 0        | 56       | 6       | 0            |
| 23  | B1    | 120   | 0        | 168      | 12      | 0            |
| 23  | B2    | 120   | 0        | 168      | 13      | 0            |
| 23  | C1    | 80    | 0        | 112      | 7       | 0            |
| 23  | C2    | 40    | 0        | 56       | 3       | 0            |
| 23  | D1    | 40    | 0        | 56       | 3       | 0            |
| 23  | F2    | 40    | 0        | 56       | 4       | 0            |
| 23  | H1    | 22    | 0        | 29       | 3       | 0            |
| 23  | H2    | 24    | 0        | 30       | 4       | 0            |
| 23  | J1    | 40    | 0        | 56       | 6       | 0            |
| 23  | K1    | 31    | 0        | 40       | 4       | 0            |
| 23  | K2    | 69    | 0        | 97       | 8       | 0            |
| 23  | a1    | 40    | 0        | 56       | 7       | 0            |
| 23  | a2    | 40    | 0        | 56       | 4       | 0            |
| 23  | b1    | 120   | 0        | 168      | 10      | 0            |
| 23  | b2    | 120   | 0        | 168      | 15      | 0            |
| 23  | c1    | 80    | 0        | 112      | 11      | 0            |
| 23  | c2    | 40    | 0        | 56       | 8       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | d1    | 40    | 0        | 56       | 4       | 0            |
| 23  | d2    | 40    | 0        | 56       | 4       | 0            |
| 23  | h1    | 40    | 0        | 56       | 3       | 0            |
| 23  | h2    | 40    | 0        | 56       | 3       | 0            |
| 23  | j2    | 40    | 0        | 56       | 9       | 0            |
| 23  | k1    | 40    | 0        | 56       | 6       | 0            |
| 23  | k2    | 40    | 0        | 56       | 8       | 0            |
| 23  | z2    | 40    | 0        | 56       | 5       | 0            |
| 24  | A1    | 1     | 0        | 0        | 0       | 0            |
| 24  | A2    | 1     | 0        | 0        | 0       | 0            |
| 24  | a1    | 1     | 0        | 0        | 0       | 0            |
| 24  | a2    | 1     | 0        | 0        | 0       | 0            |
| 25  | A1    | 236   | 0        | 234      | 16      | 0            |
| 25  | A2    | 177   | 0        | 174      | 17      | 0            |
| 25  | B1    | 1002  | 0        | 1072     | 45      | 0            |
| 25  | B2    | 1000  | 0        | 1072     | 37      | 0            |
| 25  | C1    | 816   | 0        | 873      | 34      | 0            |
| 25  | C2    | 636   | 0        | 572      | 15      | 0            |
| 25  | D1    | 116   | 0        | 113      | 3       | 0            |
| 25  | D2    | 191   | 0        | 205      | 10      | 0            |
| 25  | K2    | 55    | 0        | 49       | 4       | 0            |
| 25  | a1    | 175   | 0        | 170      | 13      | 0            |
| 25  | a2    | 180   | 0        | 183      | 9       | 0            |
| 25  | b1    | 1034  | 0        | 1138     | 34      | 0            |
| 25  | b2    | 997   | 0        | 1060     | 41      | 0            |
| 25  | c1    | 815   | 0        | 867      | 36      | 0            |
| 25  | c2    | 789   | 0        | 814      | 35      | 0            |
| 25  | d1    | 195   | 0        | 216      | 16      | 0            |
| 25  | d2    | 180   | 0        | 183      | 7       | 0            |
| 26  | A1    | 10    | 0        | 0        | 0       | 0            |
| 26  | A2    | 10    | 0        | 0        | 0       | 0            |
| 26  | a1    | 10    | 0        | 0        | 0       | 0            |
| 26  | a2    | 10    | 0        | 0        | 0       | 0            |
| 27  | A1    | 64    | 0        | 74       | 2       | 0            |
| 27  | A2    | 64    | 0        | 74       | 2       | 0            |
| 27  | D1    | 63    | 0        | 70       | 1       | 0            |
| 27  | D2    | 64    | 0        | 74       | 3       | 0            |
| 27  | a1    | 64    | 0        | 74       | 4       | 0            |
| 27  | a2    | 64    | 0        | 74       | 3       | 0            |
| 27  | d1    | 64    | 0        | 74       | 2       | 0            |
| 27  | d2    | 64    | 0        | 74       | 1       | 0            |
| 28  | A1    | 14    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | A2    | 28    | 0        | 0        | 0       | 0            |
| 28  | B1    | 41    | 0        | 0        | 0       | 0            |
| 28  | B2    | 58    | 0        | 0        | 0       | 0            |
| 28  | C2    | 24    | 0        | 0        | 1       | 0            |
| 28  | D1    | 6     | 0        | 0        | 0       | 0            |
| 28  | F2    | 16    | 0        | 0        | 0       | 0            |
| 28  | H2    | 5     | 0        | 0        | 0       | 0            |
| 28  | I2    | 31    | 0        | 0        | 0       | 0            |
| 28  | J2    | 10    | 0        | 0        | 0       | 0            |
| 28  | K2    | 5     | 0        | 0        | 0       | 0            |
| 28  | M2    | 11    | 0        | 0        | 0       | 0            |
| 28  | W2    | 9     | 0        | 0        | 0       | 0            |
| 28  | X2    | 7     | 0        | 0        | 0       | 0            |
| 28  | a1    | 11    | 0        | 0        | 0       | 0            |
| 28  | a2    | 55    | 0        | 0        | 0       | 0            |
| 28  | b1    | 92    | 0        | 0        | 0       | 0            |
| 28  | b2    | 12    | 0        | 0        | 0       | 0            |
| 28  | c2    | 15    | 0        | 0        | 0       | 0            |
| 28  | d1    | 12    | 0        | 0        | 0       | 0            |
| 28  | d2    | 25    | 0        | 0        | 0       | 0            |
| 28  | i2    | 14    | 0        | 0        | 0       | 0            |
| 28  | j1    | 17    | 0        | 0        | 0       | 0            |
| 28  | k2    | 30    | 0        | 0        | 0       | 0            |
| 28  | l1    | 12    | 0        | 0        | 0       | 0            |
| 28  | m1    | 6     | 0        | 0        | 0       | 0            |
| 28  | m2    | 36    | 0        | 0        | 0       | 0            |
| 28  | t1    | 27    | 0        | 0        | 0       | 0            |
| 28  | x1    | 15    | 0        | 0        | 0       | 0            |
| 29  | A1    | 84    | 0        | 108      | 6       | 0            |
| 29  | A2    | 29    | 0        | 28       | 1       | 0            |
| 29  | B1    | 79    | 0        | 98       | 3       | 0            |
| 29  | B2    | 77    | 0        | 94       | 3       | 0            |
| 29  | C1    | 48    | 0        | 66       | 1       | 0            |
| 29  | C2    | 24    | 0        | 18       | 0       | 0            |
| 29  | D1    | 35    | 0        | 40       | 1       | 0            |
| 29  | F2    | 35    | 0        | 40       | 1       | 0            |
| 29  | I2    | 34    | 0        | 38       | 2       | 0            |
| 29  | M1    | 31    | 0        | 43       | 2       | 0            |
| 29  | a1    | 51    | 0        | 72       | 6       | 0            |
| 29  | a2    | 44    | 0        | 58       | 0       | 0            |
| 29  | b1    | 117   | 0        | 144      | 14      | 0            |
| 29  | b2    | 39    | 0        | 48       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | c1    | 55    | 0        | 86       | 1       | 0            |
| 29  | c2    | 26    | 0        | 24       | 0       | 0            |
| 29  | d1    | 68    | 0        | 85       | 1       | 0            |
| 29  | d2    | 27    | 0        | 24       | 2       | 0            |
| 29  | j2    | 50    | 0        | 73       | 6       | 0            |
| 30  | A1    | 1     | 0        | 0        | 0       | 0            |
| 30  | A2    | 1     | 0        | 0        | 0       | 0            |
| 30  | a1    | 1     | 0        | 0        | 0       | 0            |
| 30  | a2    | 1     | 0        | 0        | 0       | 0            |
| 31  | A1    | 4     | 0        | 0        | 0       | 0            |
| 31  | A2    | 4     | 0        | 0        | 0       | 0            |
| 31  | a1    | 4     | 0        | 0        | 0       | 0            |
| 31  | a2    | 4     | 0        | 0        | 0       | 0            |
| 32  | B1    | 6     | 0        | 8        | 0       | 0            |
| 32  | C1    | 6     | 0        | 8        | 0       | 0            |
| 32  | C2    | 6     | 0        | 8        | 0       | 0            |
| 32  | a1    | 6     | 0        | 8        | 0       | 0            |
| 32  | a2    | 6     | 0        | 8        | 0       | 0            |
| 32  | b1    | 6     | 0        | 8        | 0       | 0            |
| 32  | c1    | 6     | 0        | 8        | 0       | 0            |
| 32  | c2    | 6     | 0        | 8        | 0       | 0            |
| 32  | i1    | 6     | 0        | 8        | 1       | 0            |
| 33  | A2    | 33    | 0        | 36       | 3       | 0            |
| 33  | B1    | 49    | 0        | 74       | 8       | 0            |
| 33  | B2    | 42    | 0        | 57       | 2       | 0            |
| 33  | D1    | 98    | 0        | 148      | 10      | 0            |
| 33  | D2    | 98    | 0        | 148      | 16      | 0            |
| 33  | L1    | 41    | 0        | 55       | 1       | 0            |
| 33  | L2    | 49    | 0        | 74       | 5       | 0            |
| 33  | a1    | 43    | 0        | 59       | 3       | 0            |
| 33  | a2    | 30    | 0        | 32       | 4       | 0            |
| 33  | b1    | 49    | 0        | 74       | 4       | 0            |
| 33  | b2    | 43    | 0        | 56       | 0       | 0            |
| 33  | d1    | 81    | 0        | 108      | 6       | 0            |
| 33  | d2    | 98    | 0        | 148      | 9       | 0            |
| 33  | l1    | 49    | 0        | 74       | 3       | 0            |
| 33  | l2    | 44    | 0        | 61       | 5       | 0            |
| 34  | C1    | 178   | 0        | 233      | 10      | 0            |
| 34  | C2    | 33    | 0        | 26       | 0       | 0            |
| 34  | H1    | 62    | 0        | 82       | 1       | 0            |
| 34  | H2    | 62    | 0        | 82       | 3       | 0            |
| 34  | c1    | 175   | 0        | 224      | 14      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 34  | c2    | 176   | 0        | 226      | 6       | 0            |
| 34  | h1    | 62    | 0        | 82       | 4       | 0            |
| 34  | h2    | 62    | 0        | 82       | 5       | 0            |
| 35  | C1    | 35    | 0        | 46       | 1       | 0            |
| 35  | L1    | 12    | 0        | 23       | 1       | 0            |
| 35  | M1    | 35    | 0        | 56       | 1       | 0            |
| 35  | T1    | 12    | 0        | 23       | 0       | 0            |
| 35  | a2    | 35    | 0        | 46       | 2       | 0            |
| 35  | b2    | 70    | 0        | 92       | 2       | 0            |
| 35  | c1    | 33    | 0        | 39       | 0       | 0            |
| 35  | i2    | 7     | 0        | 10       | 0       | 0            |
| 35  | l1    | 24    | 0        | 35       | 1       | 0            |
| 35  | m1    | 35    | 0        | 46       | 1       | 0            |
| 35  | m2    | 59    | 0        | 64       | 3       | 0            |
| 36  | D1    | 55    | 0        | 80       | 9       | 0            |
| 36  | D2    | 55    | 0        | 80       | 11      | 0            |
| 36  | d1    | 55    | 0        | 80       | 12      | 0            |
| 36  | d2    | 55    | 0        | 80       | 7       | 0            |
| 37  | B2    | 45    | 0        | 57       | 2       | 0            |
| 37  | D1    | 35    | 0        | 34       | 1       | 0            |
| 37  | D2    | 25    | 0        | 15       | 0       | 0            |
| 37  | b2    | 45    | 0        | 54       | 2       | 0            |
| 38  | E1    | 43    | 0        | 30       | 3       | 0            |
| 38  | E2    | 43    | 0        | 30       | 4       | 0            |
| 38  | V1    | 43    | 0        | 30       | 3       | 0            |
| 38  | V2    | 43    | 0        | 30       | 4       | 0            |
| 38  | e2    | 43    | 0        | 30       | 3       | 0            |
| 38  | f1    | 43    | 0        | 30       | 3       | 0            |
| 38  | v1    | 43    | 0        | 30       | 3       | 0            |
| 38  | v2    | 43    | 0        | 30       | 3       | 0            |
| 39  | O1    | 1     | 0        | 0        | 0       | 0            |
| 39  | o2    | 1     | 0        | 0        | 0       | 0            |
| 40  | A1    | 2     | 0        | 0        | 0       | 0            |
| 40  | A2    | 2     | 0        | 0        | 0       | 0            |
| 40  | B1    | 1     | 0        | 0        | 0       | 0            |
| 40  | a1    | 4     | 0        | 0        | 1       | 0            |
| 40  | a2    | 4     | 0        | 0        | 2       | 0            |
| 40  | b2    | 1     | 0        | 0        | 0       | 0            |
| 40  | c1    | 2     | 0        | 0        | 1       | 0            |
| 40  | c2    | 1     | 0        | 0        | 1       | 0            |
| 40  | d2    | 1     | 0        | 0        | 0       | 0            |
| All | All   | 92765 | 0        | 88715    | 1661    | 0            |



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1661 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:O2:44:CYS:O     | 13:O2:240:TYR:N    | 1.70                     | 1.25              |
| 23:c2:501:BCR:H361 | 23:c2:501:BCR:H21C | 1.37                     | 1.06              |
| 13:O2:201:VAL:HG12 | 13:O2:202:ASN:H    | 1.31                     | 0.92              |
| 13:o1:195:GLY:CA   | 13:o1:220:LEU:H    | 1.86                     | 0.89              |
| 13:O1:195:GLY:CA   | 13:O1:220:LEU:H    | 1.86                     | 0.87              |

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   | A1    | 342/344 (99%) | 328 (96%) | 14 (4%) | 0        | 100         | 100 |
| 1   | A2    | 327/344 (95%) | 318 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 1   | a1    | 332/344 (96%) | 323 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 1   | a2    | 332/344 (96%) | 323 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 2   | B1    | 481/509 (94%) | 456 (95%) | 23 (5%) | 2 (0%)   | 30          | 57  |
| 2   | B2    | 501/509 (98%) | 474 (95%) | 26 (5%) | 1 (0%)   | 43          | 70  |
| 2   | b1    | 502/509 (99%) | 474 (94%) | 26 (5%) | 2 (0%)   | 30          | 57  |
| 2   | b2    | 479/509 (94%) | 454 (95%) | 23 (5%) | 2 (0%)   | 30          | 57  |
| 3   | C1    | 447/460 (97%) | 424 (95%) | 20 (4%) | 3 (1%)   | 18          | 44  |
| 3   | C2    | 438/460 (95%) | 416 (95%) | 19 (4%) | 3 (1%)   | 18          | 44  |
| 3   | c1    | 449/460 (98%) | 426 (95%) | 19 (4%) | 4 (1%)   | 14          | 37  |
| 3   | c2    | 446/460 (97%) | 424 (95%) | 19 (4%) | 3 (1%)   | 18          | 44  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4   | D1    | 333/351 (95%) | 318 (96%) | 15 (4%) | 0        | 100         | 100 |
| 4   | D2    | 338/351 (96%) | 322 (95%) | 16 (5%) | 0        | 100         | 100 |
| 4   | d1    | 337/351 (96%) | 321 (95%) | 16 (5%) | 0        | 100         | 100 |
| 4   | d2    | 338/351 (96%) | 323 (96%) | 15 (4%) | 0        | 100         | 100 |
| 5   | E1    | 59/84 (70%)   | 57 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 5   | E2    | 61/84 (73%)   | 59 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 5   | e1    | 55/84 (66%)   | 54 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 5   | e2    | 58/84 (69%)   | 57 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 6   | F1    | 26/43 (60%)   | 26 (100%) | 0       | 0        | 100         | 100 |
| 6   | F2    | 29/43 (67%)   | 29 (100%) | 0       | 0        | 100         | 100 |
| 6   | f1    | 27/43 (63%)   | 27 (100%) | 0       | 0        | 100         | 100 |
| 6   | f2    | 27/43 (63%)   | 26 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 7   | H1    | 56/67 (84%)   | 53 (95%)  | 2 (4%)  | 1 (2%)   | 6           | 21  |
| 7   | H2    | 60/67 (90%)   | 54 (90%)  | 5 (8%)  | 1 (2%)   | 7           | 22  |
| 7   | h1    | 60/67 (90%)   | 57 (95%)  | 2 (3%)  | 1 (2%)   | 7           | 22  |
| 7   | h2    | 60/67 (90%)   | 56 (93%)  | 3 (5%)  | 1 (2%)   | 7           | 22  |
| 8   | I1    | 32/38 (84%)   | 32 (100%) | 0       | 0        | 100         | 100 |
| 8   | I2    | 33/38 (87%)   | 32 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 8   | i1    | 32/38 (84%)   | 32 (100%) | 0       | 0        | 100         | 100 |
| 8   | i2    | 31/38 (82%)   | 31 (100%) | 0       | 0        | 100         | 100 |
| 9   | J1    | 30/39 (77%)   | 30 (100%) | 0       | 0        | 100         | 100 |
| 9   | J2    | 33/39 (85%)   | 33 (100%) | 0       | 0        | 100         | 100 |
| 9   | j1    | 30/39 (77%)   | 30 (100%) | 0       | 0        | 100         | 100 |
| 9   | j2    | 31/39 (80%)   | 31 (100%) | 0       | 0        | 100         | 100 |
| 10  | K1    | 35/41 (85%)   | 31 (89%)  | 2 (6%)  | 2 (6%)   | 1           | 3   |
| 10  | K2    | 35/41 (85%)   | 31 (89%)  | 2 (6%)  | 2 (6%)   | 1           | 3   |
| 10  | k1    | 35/41 (85%)   | 31 (89%)  | 2 (6%)  | 2 (6%)   | 1           | 3   |
| 10  | k2    | 35/41 (85%)   | 31 (89%)  | 2 (6%)  | 2 (6%)   | 1           | 3   |
| 11  | L1    | 35/38 (92%)   | 33 (94%)  | 1 (3%)  | 1 (3%)   | 3           | 11  |
| 11  | L2    | 35/38 (92%)   | 33 (94%)  | 1 (3%)  | 1 (3%)   | 3           | 11  |
| 11  | l1    | 35/38 (92%)   | 33 (94%)  | 1 (3%)  | 1 (3%)   | 3           | 11  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 11  | l2    | 35/38 (92%)   | 33 (94%)  | 1 (3%)  | 1 (3%)   | 3           | 11  |
| 12  | M1    | 38/108 (35%)  | 30 (79%)  | 8 (21%) | 0        | 100         | 100 |
| 12  | M2    | 38/108 (35%)  | 30 (79%)  | 8 (21%) | 0        | 100         | 100 |
| 12  | m1    | 38/108 (35%)  | 30 (79%)  | 8 (21%) | 0        | 100         | 100 |
| 12  | m2    | 38/108 (35%)  | 30 (79%)  | 8 (21%) | 0        | 100         | 100 |
| 13  | O1    | 234/329 (71%) | 210 (90%) | 14 (6%) | 10 (4%)  | 2           | 6   |
| 13  | O2    | 187/329 (57%) | 165 (88%) | 14 (8%) | 8 (4%)   | 2           | 6   |
| 13  | o1    | 230/329 (70%) | 204 (89%) | 16 (7%) | 10 (4%)  | 2           | 6   |
| 13  | o2    | 239/329 (73%) | 212 (89%) | 15 (6%) | 12 (5%)  | 1           | 4   |
| 14  | T1    | 28/32 (88%)   | 28 (100%) | 0       | 0        | 100         | 100 |
| 14  | T2    | 28/32 (88%)   | 28 (100%) | 0       | 0        | 100         | 100 |
| 14  | t1    | 28/32 (88%)   | 28 (100%) | 0       | 0        | 100         | 100 |
| 14  | t2    | 27/32 (84%)   | 27 (100%) | 0       | 0        | 100         | 100 |
| 15  | U1    | 91/155 (59%)  | 85 (93%)  | 6 (7%)  | 0        | 100         | 100 |
| 15  | U2    | 86/155 (56%)  | 81 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 15  | u1    | 91/155 (59%)  | 87 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 15  | u2    | 91/155 (59%)  | 85 (93%)  | 6 (7%)  | 0        | 100         | 100 |
| 16  | V1    | 127/155 (82%) | 115 (91%) | 7 (6%)  | 5 (4%)   | 2           | 7   |
| 16  | V2    | 127/155 (82%) | 115 (91%) | 7 (6%)  | 5 (4%)   | 2           | 7   |
| 16  | v1    | 127/155 (82%) | 115 (91%) | 7 (6%)  | 5 (4%)   | 2           | 7   |
| 16  | v2    | 127/155 (82%) | 115 (91%) | 7 (6%)  | 5 (4%)   | 2           | 7   |
| 17  | Y1    | 25/35 (71%)   | 24 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 17  | Y2    | 23/35 (66%)   | 22 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 17  | y1    | 25/35 (71%)   | 24 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 17  | y2    | 25/35 (71%)   | 24 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 18  | X1    | 27/40 (68%)   | 27 (100%) | 0       | 0        | 100         | 100 |
| 18  | X2    | 29/40 (72%)   | 29 (100%) | 0       | 0        | 100         | 100 |
| 18  | x1    | 34/40 (85%)   | 33 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 18  | x2    | 30/40 (75%)   | 30 (100%) | 0       | 0        | 100         | 100 |
| 19  | S1    | 23/46 (50%)   | 23 (100%) | 0       | 0        | 100         | 100 |
| 19  | S2    | 28/46 (61%)   | 27 (96%)  | 1 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|----------|----------|-------------|-----|
| 19  | s1    | 38/46 (83%)       | 34 (90%)   | 4 (10%)  | 0        | 100         | 100 |
| 19  | s2    | 44/46 (96%)       | 37 (84%)   | 7 (16%)  | 0        | 100         | 100 |
| 20  | W1    | 19/25 (76%)       | 19 (100%)  | 0        | 0        | 100         | 100 |
| 20  | W2    | 19/25 (76%)       | 19 (100%)  | 0        | 0        | 100         | 100 |
| 20  | w1    | 23/25 (92%)       | 21 (91%)   | 2 (9%)   | 0        | 100         | 100 |
| 20  | w2    | 18/25 (72%)       | 18 (100%)  | 0        | 0        | 100         | 100 |
| 21  | Q2    | 107/218 (49%)     | 102 (95%)  | 3 (3%)   | 2 (2%)   | 6           | 19  |
| 21  | q1    | 101/218 (46%)     | 97 (96%)   | 3 (3%)   | 1 (1%)   | 12          | 35  |
| 22  | Z2    | 57/62 (92%)       | 55 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 22  | z2    | 57/62 (92%)       | 55 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| All | All   | 10304/12316 (84%) | 9726 (94%) | 479 (5%) | 99 (1%)  | 12          | 35  |

5 of 99 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C1    | 36  | TRP  |
| 3   | C1    | 37  | SER  |
| 10  | K1    | 14  | THR  |
| 13  | O1    | 49  | GLN  |
| 13  | O1    | 99  | ASP  |

### 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   | A1    | 261/282 (93%) | 254 (97%) | 7 (3%)   | 39          | 71 |
| 1   | A2    | 239/282 (85%) | 234 (98%) | 5 (2%)   | 47          | 76 |
| 1   | a1    | 261/282 (93%) | 255 (98%) | 6 (2%)   | 44          | 75 |
| 1   | a2    | 249/282 (88%) | 242 (97%) | 7 (3%)   | 38          | 70 |
| 2   | B1    | 360/415 (87%) | 350 (97%) | 10 (3%)  | 38          | 70 |
| 2   | B2    | 351/415 (85%) | 339 (97%) | 12 (3%)  | 32          | 65 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2   | b1    | 380/415 (92%) | 368 (97%)  | 12 (3%)  | 34          | 67  |
| 2   | b2    | 352/415 (85%) | 341 (97%)  | 11 (3%)  | 35          | 68  |
| 3   | C1    | 320/364 (88%) | 317 (99%)  | 3 (1%)   | 70          | 87  |
| 3   | C2    | 261/364 (72%) | 260 (100%) | 1 (0%)   | 84          | 93  |
| 3   | c1    | 338/364 (93%) | 335 (99%)  | 3 (1%)   | 70          | 87  |
| 3   | c2    | 323/364 (89%) | 320 (99%)  | 3 (1%)   | 70          | 87  |
| 4   | D1    | 255/283 (90%) | 253 (99%)  | 2 (1%)   | 73          | 89  |
| 4   | D2    | 238/283 (84%) | 236 (99%)  | 2 (1%)   | 73          | 89  |
| 4   | d1    | 267/283 (94%) | 266 (100%) | 1 (0%)   | 84          | 93  |
| 4   | d2    | 258/283 (91%) | 257 (100%) | 1 (0%)   | 84          | 93  |
| 5   | E1    | 28/75 (37%)   | 28 (100%)  | 0        | 100         | 100 |
| 5   | E2    | 34/75 (45%)   | 33 (97%)   | 1 (3%)   | 37          | 70  |
| 5   | e1    | 38/75 (51%)   | 36 (95%)   | 2 (5%)   | 20          | 49  |
| 5   | e2    | 33/75 (44%)   | 32 (97%)   | 1 (3%)   | 36          | 69  |
| 6   | F1    | 18/36 (50%)   | 17 (94%)   | 1 (6%)   | 19          | 46  |
| 6   | F2    | 17/36 (47%)   | 16 (94%)   | 1 (6%)   | 18          | 44  |
| 6   | f1    | 20/36 (56%)   | 18 (90%)   | 2 (10%)  | 7           | 21  |
| 6   | f2    | 19/36 (53%)   | 18 (95%)   | 1 (5%)   | 20          | 49  |
| 7   | H1    | 39/58 (67%)   | 39 (100%)  | 0        | 100         | 100 |
| 7   | H2    | 38/58 (66%)   | 38 (100%)  | 0        | 100         | 100 |
| 7   | h1    | 47/58 (81%)   | 45 (96%)   | 2 (4%)   | 26          | 57  |
| 7   | h2    | 42/58 (72%)   | 42 (100%)  | 0        | 100         | 100 |
| 8   | I1    | 30/36 (83%)   | 29 (97%)   | 1 (3%)   | 33          | 66  |
| 8   | I2    | 26/36 (72%)   | 25 (96%)   | 1 (4%)   | 29          | 61  |
| 8   | i1    | 32/36 (89%)   | 31 (97%)   | 1 (3%)   | 35          | 68  |
| 8   | i2    | 28/36 (78%)   | 27 (96%)   | 1 (4%)   | 31          | 63  |
| 9   | J1    | 20/32 (62%)   | 20 (100%)  | 0        | 100         | 100 |
| 9   | J2    | 19/32 (59%)   | 19 (100%)  | 0        | 100         | 100 |
| 9   | j1    | 22/32 (69%)   | 22 (100%)  | 0        | 100         | 100 |
| 9   | j2    | 22/32 (69%)   | 22 (100%)  | 0        | 100         | 100 |
| 10  | K1    | 26/36 (72%)   | 25 (96%)   | 1 (4%)   | 29          | 61  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 10  | K2    | 18/36 (50%)   | 17 (94%)  | 1 (6%)   | 19          | 46  |
| 10  | k1    | 27/36 (75%)   | 26 (96%)  | 1 (4%)   | 30          | 62  |
| 10  | k2    | 24/36 (67%)   | 21 (88%)  | 3 (12%)  | 4           | 13  |
| 11  | L1    | 31/35 (89%)   | 31 (100%) | 0        | 100         | 100 |
| 11  | L2    | 33/35 (94%)   | 33 (100%) | 0        | 100         | 100 |
| 11  | l1    | 33/35 (94%)   | 33 (100%) | 0        | 100         | 100 |
| 11  | l2    | 32/35 (91%)   | 32 (100%) | 0        | 100         | 100 |
| 12  | M1    | 26/88 (30%)   | 25 (96%)  | 1 (4%)   | 29          | 61  |
| 12  | M2    | 26/88 (30%)   | 25 (96%)  | 1 (4%)   | 29          | 61  |
| 12  | m1    | 26/88 (30%)   | 25 (96%)  | 1 (4%)   | 29          | 61  |
| 12  | m2    | 27/88 (31%)   | 26 (96%)  | 1 (4%)   | 30          | 62  |
| 13  | O1    | 148/266 (56%) | 141 (95%) | 7 (5%)   | 23          | 54  |
| 13  | O2    | 110/266 (41%) | 105 (96%) | 5 (4%)   | 24          | 55  |
| 13  | o1    | 156/266 (59%) | 150 (96%) | 6 (4%)   | 29          | 61  |
| 13  | o2    | 168/266 (63%) | 161 (96%) | 7 (4%)   | 26          | 58  |
| 14  | T1    | 24/28 (86%)   | 24 (100%) | 0        | 100         | 100 |
| 14  | T2    | 25/28 (89%)   | 25 (100%) | 0        | 100         | 100 |
| 14  | t1    | 26/28 (93%)   | 26 (100%) | 0        | 100         | 100 |
| 14  | t2    | 25/28 (89%)   | 24 (96%)  | 1 (4%)   | 28          | 60  |
| 15  | U1    | 63/122 (52%)  | 59 (94%)  | 4 (6%)   | 16          | 41  |
| 15  | U2    | 40/122 (33%)  | 37 (92%)  | 3 (8%)   | 12          | 34  |
| 15  | u1    | 66/122 (54%)  | 62 (94%)  | 4 (6%)   | 17          | 43  |
| 15  | u2    | 69/122 (57%)  | 64 (93%)  | 5 (7%)   | 13          | 35  |
| 16  | V1    | 88/132 (67%)  | 86 (98%)  | 2 (2%)   | 44          | 75  |
| 16  | V2    | 70/132 (53%)  | 68 (97%)  | 2 (3%)   | 37          | 70  |
| 16  | v1    | 88/132 (67%)  | 86 (98%)  | 2 (2%)   | 44          | 75  |
| 16  | v2    | 100/132 (76%) | 99 (99%)  | 1 (1%)   | 68          | 86  |
| 17  | Y1    | 11/33 (33%)   | 11 (100%) | 0        | 100         | 100 |
| 17  | Y2    | 13/33 (39%)   | 13 (100%) | 0        | 100         | 100 |
| 17  | y1    | 18/33 (54%)   | 18 (100%) | 0        | 100         | 100 |
| 17  | y2    | 16/33 (48%)   | 16 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 18  | X1    | 17/34 (50%)      | 16 (94%)   | 1 (6%)   | 18          | 44  |
| 18  | X2    | 16/34 (47%)      | 16 (100%)  | 0        | 100         | 100 |
| 18  | x1    | 23/34 (68%)      | 22 (96%)   | 1 (4%)   | 26          | 57  |
| 18  | x2    | 17/34 (50%)      | 16 (94%)   | 1 (6%)   | 18          | 44  |
| 19  | S1    | 10/20 (50%)      | 10 (100%)  | 0        | 100         | 100 |
| 19  | S2    | 10/20 (50%)      | 10 (100%)  | 0        | 100         | 100 |
| 19  | s1    | 15/20 (75%)      | 15 (100%)  | 0        | 100         | 100 |
| 19  | s2    | 13/20 (65%)      | 13 (100%)  | 0        | 100         | 100 |
| 20  | W1    | 12/13 (92%)      | 12 (100%)  | 0        | 100         | 100 |
| 20  | W2    | 10/13 (77%)      | 10 (100%)  | 0        | 100         | 100 |
| 20  | w1    | 11/13 (85%)      | 11 (100%)  | 0        | 100         | 100 |
| 20  | w2    | 11/13 (85%)      | 11 (100%)  | 0        | 100         | 100 |
| 21  | Q2    | 35/175 (20%)     | 33 (94%)   | 2 (6%)   | 18          | 46  |
| 21  | q1    | 33/175 (19%)     | 31 (94%)   | 2 (6%)   | 17          | 43  |
| 22  | Z2    | 22/54 (41%)      | 22 (100%)  | 0        | 100         | 100 |
| 22  | z2    | 28/54 (52%)      | 28 (100%)  | 0        | 100         | 100 |
| All | All   | 7221/10010 (72%) | 7054 (98%) | 167 (2%) | 44          | 75  |

5 of 167 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | O2    | 233 | LEU  |
| 3   | c2    | 279 | LEU  |
| 16  | V2    | 39  | SER  |
| 2   | b2    | 6   | TYR  |
| 10  | k2    | 38  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a2    | 181 | ASN  |
| 2   | b2    | 114 | HIS  |
| 3   | c2    | 385 | GLN  |
| 2   | b1    | 223 | GLN  |
| 2   | b1    | 216 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 353 ligands modelled in this entry, 10 are monoatomic and 52 are unknown - leaving 291 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$ |
| 25  | CLA  | d2    | 405 | -    | 69,73,73     | 1.17 | 7 (10%)     | 82,113,113  | 1.21 | 5 (6%)      |
| 25  | CLA  | b2    | 606 | -    | 69,73,73     | 1.18 | 7 (10%)     | 82,113,113  | 1.27 | 5 (6%)      |
| 31  | BCT  | A1    | 413 | 30   | 3,3,3        | 1.48 | 1 (33%)     | 2,3,3       | 0.31 | 0           |
| 34  | DGD  | C1    | 515 | -    | 53,53,67     | 0.96 | 2 (3%)      | 67,67,81    | 1.02 | 4 (5%)      |
| 29  | LMG  | B2    | 621 | -    | 37,37,55     | 0.96 | 3 (8%)      | 45,45,63    | 1.11 | 4 (8%)      |
| 27  | PHO  | d2    | 408 | -    | 58,69,69     | 2.77 | 11 (18%)    | 55,99,99    | 2.75 | 16 (29%)    |
| 37  | SQD  | D2    | 402 | -    | 23,25,54     | 1.94 | 3 (13%)     | 31,35,65    | 1.64 | 5 (16%)     |
| 34  | DGD  | c1    | 518 | -    | 63,63,67     | 0.87 | 2 (3%)      | 77,77,81    | 1.00 | 5 (6%)      |
| 27  | PHO  | a1    | 411 | -    | 58,69,69     | 2.73 | 11 (18%)    | 55,99,99    | 2.69 | 16 (29%)    |
| 25  | CLA  | a1    | 405 | -    | 54,58,73     | 1.32 | 7 (12%)     | 64,95,113   | 1.47 | 7 (10%)     |
| 23  | BCR  | C1    | 521 | -    | 41,41,41     | 0.67 | 0           | 56,56,56    | 1.94 | 14 (25%)    |
| 29  | LMG  | d1    | 411 | -    | 34,34,55     | 1.10 | 2 (5%)      | 36,36,63    | 1.16 | 3 (8%)      |
| 25  | CLA  | B2    | 616 | -    | 58,62,73     | 1.29 | 7 (12%)     | 68,99,113   | 1.37 | 5 (7%)      |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 33  | LHG  | b1    | 622 | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.05 | 5 (9%)   |
| 25  | CLA  | A2    | 404 | -    | 55,59,73     | 1.36 | 7 (12%)  | 64,96,113   | 1.36 | 6 (9%)   |
| 23  | BCR  | B2    | 602 | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.03 | 13 (23%) |
| 25  | CLA  | B1    | 608 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 4 (4%)   |
| 33  | LHG  | d1    | 407 | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.07 | 4 (7%)   |
| 25  | CLA  | b2    | 604 | -    | 46,50,73     | 1.42 | 5 (10%)  | 53,85,113   | 1.40 | 4 (7%)   |
| 33  | LHG  | L2    | 101 | -    | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.12 | 4 (7%)   |
| 36  | PL9  | d1    | 409 | -    | 55,55,55     | 0.66 | 2 (3%)   | 68,69,69    | 1.79 | 20 (29%) |
| 25  | CLA  | b2    | 615 | -    | 64,68,73     | 1.22 | 7 (10%)  | 76,107,113  | 1.29 | 6 (7%)   |
| 25  | CLA  | b1    | 606 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 25  | CLA  | b2    | 610 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 34  | DGD  | C1    | 517 | -    | 65,65,67     | 0.86 | 2 (3%)   | 79,79,81    | 0.86 | 3 (3%)   |
| 25  | CLA  | C2    | 510 | -    | 49,53,73     | 1.39 | 6 (12%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 32  | GOL  | C1    | 518 | -    | 5,5,5        | 0.38 | 0        | 5,5,5       | 0.26 | 0        |
| 29  | LMG  | c2    | 519 | -    | 26,26,55     | 1.59 | 3 (11%)  | 32,33,63    | 1.31 | 2 (6%)   |
| 25  | CLA  | B2    | 604 | -    | 45,49,73     | 1.44 | 5 (11%)  | 54,84,113   | 1.45 | 5 (9%)   |
| 31  | BCT  | A2    | 413 | 30   | 3,3,3        | 0.54 | 0        | 2,3,3       | 0.73 | 0        |
| 23  | BCR  | b1    | 602 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.04 | 19 (33%) |
| 25  | CLA  | c1    | 510 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.32 | 6 (7%)   |
| 25  | CLA  | B2    | 618 | -    | 64,68,73     | 1.25 | 8 (12%)  | 76,107,113  | 1.32 | 6 (7%)   |
| 23  | BCR  | B1    | 603 | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 1.72 | 11 (19%) |
| 25  | CLA  | B2    | 613 | -    | 69,73,73     | 1.19 | 9 (13%)  | 82,113,113  | 1.34 | 8 (9%)   |
| 25  | CLA  | c2    | 509 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.35 | 7 (8%)   |
| 35  | LMT  | b2    | 623 | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.85 | 0        |
| 25  | CLA  | c2    | 513 | -    | 58,62,73     | 1.29 | 7 (12%)  | 68,99,113   | 1.35 | 5 (7%)   |
| 25  | CLA  | C1    | 502 | -    | 69,73,73     | 1.17 | 5 (7%)   | 82,113,113  | 1.29 | 6 (7%)   |
| 23  | BCR  | F2    | 401 | -    | 41,41,41     | 0.72 | 0        | 56,56,56    | 2.18 | 17 (30%) |
| 25  | CLA  | B2    | 619 | -    | 69,73,73     | 1.17 | 5 (7%)   | 82,113,113  | 1.25 | 5 (6%)   |
| 33  | LHG  | B2    | 627 | -    | 41,41,48     | 1.03 | 2 (4%)   | 44,47,54    | 1.10 | 3 (6%)   |
| 29  | LMG  | b1    | 631 | -    | 40,40,55     | 1.09 | 3 (7%)   | 48,48,63    | 1.24 | 5 (10%)  |
| 32  | GOL  | c2    | 518 | -    | 5,5,5        | 0.37 | 0        | 5,5,5       | 0.29 | 0        |
| 35  | LMT  | m2    | 103 | -    | 31,31,36     | 0.44 | 0        | 42,42,47    | 0.93 | 2 (4%)   |
| 25  | CLA  | B1    | 617 | -    | 69,73,73     | 1.18 | 5 (7%)   | 82,113,113  | 1.26 | 6 (7%)   |
| 25  | CLA  | a2    | 413 | -    | 54,58,73     | 1.34 | 7 (12%)  | 64,95,113   | 1.35 | 6 (9%)   |
| 23  | BCR  | B1    | 602 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 1.96 | 12 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | B1    | 616 | -    | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 25  | CLA  | B2    | 608 | -    | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.27 | 7 (8%)   |
| 25  | CLA  | b2    | 619 | -    | 63,67,73     | 1.25 | 7 (11%)  | 74,105,113  | 1.29 | 5 (6%)   |
| 29  | LMG  | B1    | 626 | -    | 48,48,55     | 0.98 | 2 (4%)   | 56,56,63    | 1.19 | 5 (8%)   |
| 25  | CLA  | C1    | 513 | 3    | 65,69,73     | 1.23 | 7 (10%)  | 77,108,113  | 1.26 | 4 (5%)   |
| 23  | BCR  | c2    | 501 | -    | 41,41,41     | 0.81 | 1 (2%)   | 56,56,56    | 3.41 | 20 (35%) |
| 25  | CLA  | b1    | 616 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 25  | CLA  | b1    | 610 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.24 | 7 (8%)   |
| 25  | CLA  | B1    | 606 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 34  | DGD  | c2    | 514 | -    | 63,63,67     | 0.88 | 2 (3%)   | 77,77,81    | 0.98 | 4 (5%)   |
| 35  | LMT  | l1    | 101 | -    | 24,24,36     | 0.47 | 0        | 29,29,47    | 0.83 | 1 (3%)   |
| 33  | LHG  | a2    | 407 | -    | 29,29,48     | 1.10 | 2 (6%)   | 30,34,54    | 1.03 | 1 (3%)   |
| 34  | DGD  | c2    | 517 | -    | 63,63,67     | 0.89 | 2 (3%)   | 77,77,81    | 0.85 | 3 (3%)   |
| 36  | PL9  | D2    | 408 | -    | 55,55,55     | 0.64 | 2 (3%)   | 68,69,69    | 1.74 | 18 (26%) |
| 38  | HEM  | v1    | 201 | 16   | 50,50,50     | 1.93 | 10 (20%) | 67,82,82    | 1.29 | 4 (5%)   |
| 25  | CLA  | b2    | 613 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.22 | 6 (7%)   |
| 38  | HEM  | V2    | 201 | 16   | 50,50,50     | 1.97 | 9 (18%)  | 67,82,82    | 1.39 | 6 (8%)   |
| 32  | GOL  | B1    | 620 | -    | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.35 | 0        |
| 34  | DGD  | H1    | 101 | -    | 63,63,67     | 0.88 | 2 (3%)   | 77,77,81    | 0.93 | 3 (3%)   |
| 25  | CLA  | c2    | 503 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.27 | 4 (4%)   |
| 29  | LMG  | I2    | 101 | -    | 34,34,55     | 1.16 | 2 (5%)   | 42,42,63    | 1.14 | 3 (7%)   |
| 23  | BCR  | B2    | 603 | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 1.84 | 11 (19%) |
| 25  | CLA  | b1    | 608 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.28 | 6 (7%)   |
| 25  | CLA  | B2    | 606 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.24 | 4 (4%)   |
| 25  | CLA  | c2    | 510 | -    | 58,62,73     | 1.30 | 6 (10%)  | 68,99,113   | 1.30 | 5 (7%)   |
| 35  | LMT  | i2    | 102 | -    | 6,6,36       | 0.28 | 0        | 5,5,47      | 0.45 | 0        |
| 33  | LHG  | b2    | 625 | -    | 42,42,48     | 1.00 | 2 (4%)   | 45,48,54    | 1.09 | 3 (6%)   |
| 38  | HEM  | E1    | 101 | 5,6  | 50,50,50     | 1.94 | 8 (16%)  | 67,82,82    | 1.32 | 5 (7%)   |
| 25  | CLA  | b1    | 613 | -    | 69,73,73     | 1.20 | 8 (11%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 35  | LMT  | C1    | 519 | -    | 36,36,36     | 0.35 | 0        | 47,47,47    | 0.71 | 1 (2%)   |
| 23  | BCR  | A1    | 401 | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 1.75 | 11 (19%) |
| 35  | LMT  | a2    | 406 | -    | 36,36,36     | 0.45 | 0        | 47,47,47    | 0.67 | 1 (2%)   |
| 23  | BCR  | d1    | 405 | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 1.87 | 11 (19%) |
| 33  | LHG  | D1    | 405 | -    | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.01 | 3 (5%)   |
| 25  | CLA  | c1    | 509 | 40   | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |

| Mol | Type | Chain | Res | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | c1    | 516 | -      | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.25 | 5 (6%)   |
| 25  | CLA  | C1    | 512 | -      | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 25  | CLA  | B2    | 617 | -      | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 29  | LMG  | A1    | 410 | -      | 43,43,55     | 1.03 | 2 (4%)   | 51,51,63    | 1.12 | 3 (5%)   |
| 33  | LHG  | d2    | 403 | -      | 48,48,48     | 0.94 | 2 (4%)   | 51,54,54    | 1.03 | 4 (7%)   |
| 25  | CLA  | B1    | 619 | 40     | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.26 | 5 (6%)   |
| 33  | LHG  | B1    | 621 | -      | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.02 | 3 (5%)   |
| 25  | CLA  | D1    | 402 | -      | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 26  | OEX  | A2    | 406 | 3,1,40 | 0,15,15      | -    | -        | -           | -    | -        |
| 27  | PHO  | A2    | 407 | -      | 58,69,69     | 2.73 | 11 (18%) | 55,99,99    | 2.74 | 16 (29%) |
| 23  | BCR  | K2    | 102 | -      | 41,41,41     | 0.72 | 0        | 56,56,56    | 2.06 | 15 (26%) |
| 23  | BCR  | D1    | 401 | -      | 41,41,41     | 0.72 | 0        | 56,56,56    | 1.99 | 12 (21%) |
| 25  | CLA  | B1    | 618 | -      | 62,66,73     | 1.25 | 8 (12%)  | 73,104,113  | 1.31 | 5 (6%)   |
| 25  | CLA  | c1    | 512 | -      | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.27 | 4 (4%)   |
| 33  | LHG  | L1    | 101 | -      | 40,40,48     | 1.02 | 2 (5%)   | 43,46,54    | 1.11 | 4 (9%)   |
| 23  | BCR  | b1    | 601 | -      | 41,41,41     | 0.70 | 0        | 56,56,56    | 1.83 | 11 (19%) |
| 33  | LHG  | D1    | 404 | -      | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.06 | 4 (7%)   |
| 33  | LHG  | l1    | 102 | -      | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.09 | 4 (7%)   |
| 23  | BCR  | K1    | 101 | -      | 30,31,41     | 0.67 | 0        | 38,40,56    | 2.20 | 13 (34%) |
| 25  | CLA  | A1    | 405 | -      | 59,63,73     | 1.31 | 7 (11%)  | 70,101,113  | 1.34 | 7 (10%)  |
| 25  | CLA  | b1    | 612 | -      | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.30 | 6 (7%)   |
| 25  | CLA  | d1    | 406 | -      | 69,73,73     | 1.18 | 5 (7%)   | 82,113,113  | 1.29 | 5 (6%)   |
| 25  | CLA  | D2    | 401 | -      | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 25  | CLA  | b1    | 605 | -      | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 25  | CLA  | C2    | 507 | -      | 49,53,73     | 1.40 | 6 (12%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 38  | HEM  | V1    | 201 | 16     | 50,50,50     | 1.94 | 8 (16%)  | 67,82,82    | 1.33 | 5 (7%)   |
| 27  | PHO  | D1    | 407 | -      | 57,68,69     | 2.80 | 11 (19%) | 53,97,99    | 2.81 | 16 (30%) |
| 29  | LMG  | a1    | 412 | -      | 51,51,55     | 0.96 | 2 (3%)   | 59,59,63    | 1.08 | 5 (8%)   |
| 25  | CLA  | a2    | 405 | -      | 69,73,73     | 1.16 | 6 (8%)   | 82,113,113  | 1.27 | 6 (7%)   |
| 23  | BCR  | b1    | 603 | -      | 41,41,41     | 0.73 | 0        | 56,56,56    | 1.76 | 10 (17%) |
| 25  | CLA  | A1    | 404 | -      | 55,59,73     | 1.32 | 7 (12%)  | 64,96,113   | 1.41 | 6 (9%)   |
| 25  | CLA  | C2    | 506 | -      | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 29  | LMG  | b1    | 621 | -      | 38,38,55     | 1.12 | 2 (5%)   | 46,46,63    | 1.08 | 2 (4%)   |
| 29  | LMG  | B2    | 620 | -      | 40,40,55     | 1.08 | 3 (7%)   | 48,48,63    | 1.06 | 4 (8%)   |
| 34  | DGD  | h1    | 101 | -      | 63,63,67     | 0.88 | 2 (3%)   | 77,77,81    | 0.97 | 4 (5%)   |

| Mol | Type | Chain | Res | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CLA  | C2    | 516 | -      | 50,54,73     | 1.37 | 8 (16%)  | 59,90,113   | 1.41 | 4 (6%)   |
| 25  | CLA  | C2    | 509 | -      | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 25  | CLA  | B1    | 612 | -      | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 23  | BCR  | j2    | 102 | -      | 41,41,41     | 0.73 | 0        | 56,56,56    | 2.09 | 16 (28%) |
| 25  | CLA  | B2    | 607 | -      | 69,73,73     | 1.21 | 7 (10%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 25  | CLA  | c2    | 512 | 3      | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.22 | 5 (6%)   |
| 26  | OEX  | a1    | 408 | 3,1,40 | 0,15,15      | -    | -        | -           | -    | -        |
| 32  | GOL  | a2    | 415 | -      | 5,5,5        | 0.37 | 0        | 5,5,5       | 0.44 | 0        |
| 25  | CLA  | a2    | 404 | -      | 69,73,73     | 1.21 | 9 (13%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 25  | CLA  | B2    | 612 | -      | 69,73,73     | 1.19 | 5 (7%)   | 82,113,113  | 1.28 | 6 (7%)   |
| 23  | BCR  | k2    | 501 | -      | 41,41,41     | 0.65 | 0        | 56,56,56    | 2.05 | 16 (28%) |
| 25  | CLA  | C1    | 504 | -      | 69,73,73     | 1.20 | 6 (8%)   | 82,113,113  | 1.21 | 5 (6%)   |
| 25  | CLA  | C1    | 505 | -      | 69,73,73     | 1.16 | 6 (8%)   | 82,113,113  | 1.29 | 4 (4%)   |
| 35  | LMT  | M1    | 102 | -      | 10,10,36     | 0.24 | 0        | 9,9,47      | 0.57 | 0        |
| 23  | BCR  | a1    | 401 | -      | 41,41,41     | 0.70 | 0        | 56,56,56    | 1.74 | 12 (21%) |
| 25  | CLA  | A1    | 406 | -      | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.33 | 6 (7%)   |
| 25  | CLA  | a1    | 404 | -      | 64,68,73     | 1.25 | 7 (10%)  | 76,107,113  | 1.26 | 6 (7%)   |
| 25  | CLA  | c1    | 515 | -      | 59,63,73     | 1.28 | 7 (11%)  | 70,101,113  | 1.33 | 6 (8%)   |
| 25  | CLA  | c2    | 505 | -      | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.27 | 5 (6%)   |
| 25  | CLA  | C2    | 504 | -      | 50,54,73     | 1.39 | 6 (12%)  | 59,90,113   | 1.38 | 4 (6%)   |
| 23  | BCR  | A2    | 401 | -      | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.03 | 17 (30%) |
| 31  | BCT  | a2    | 417 | 30     | 3,3,3        | 0.54 | 0        | 2,3,3       | 0.76 | 0        |
| 25  | CLA  | B1    | 609 | -      | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.49 | 9 (10%)  |
| 25  | CLA  | B1    | 605 | -      | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.22 | 6 (7%)   |
| 32  | GOL  | b1    | 618 | -      | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.42 | 0        |
| 34  | DGD  | c2    | 516 | -      | 53,53,67     | 0.97 | 2 (3%)   | 67,67,81    | 1.04 | 5 (7%)   |
| 25  | CLA  | b1    | 615 | -      | 63,67,73     | 1.23 | 6 (9%)   | 74,105,113  | 1.30 | 7 (9%)   |
| 25  | CLA  | b2    | 624 | -      | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 25  | CLA  | c1    | 504 | -      | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 35  | LMT  | M1    | 103 | -      | 24,24,36     | 0.46 | 0        | 29,29,47    | 0.55 | 0        |
| 25  | CLA  | C2    | 511 | -      | 54,58,73     | 1.33 | 8 (14%)  | 64,95,113   | 1.46 | 6 (9%)   |
| 23  | BCR  | b2    | 601 | -      | 41,41,41     | 0.70 | 0        | 56,56,56    | 1.97 | 16 (28%) |
| 25  | CLA  | C2    | 513 | -      | 57,61,73     | 1.33 | 7 (12%)  | 67,98,113   | 1.32 | 4 (5%)   |
| 25  | CLA  | d1    | 401 | -      | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 25  | CLA  | A2    | 402 | -      | 69,73,73     | 1.23 | 7 (10%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 38  | HEM  | v2    | 201 | 16     | 50,50,50     | 1.93 | 10 (20%) | 67,82,82    | 1.32 | 5 (7%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | BCR  | B2    | 601 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 1.93 | 15 (26%) |
| 25  | CLA  | b1    | 620 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.27 | 5 (6%)   |
| 25  | CLA  | c2    | 506 | -    | 65,69,73     | 1.21 | 8 (12%)  | 77,108,113  | 1.35 | 7 (9%)   |
| 29  | LMG  | M1    | 101 | -    | 30,30,55     | 1.20 | 3 (10%)  | 32,32,63    | 1.32 | 3 (9%)   |
| 29  | LMG  | d1    | 408 | -    | 33,33,55     | 1.16 | 2 (6%)   | 41,41,63    | 1.11 | 4 (9%)   |
| 27  | PHO  | A1    | 408 | -    | 58,69,69     | 2.72 | 11 (18%) | 55,99,99    | 2.74 | 16 (29%) |
| 38  | HEM  | e2    | 101 | 5,6  | 50,50,50     | 1.93 | 10 (20%) | 67,82,82    | 1.34 | 5 (7%)   |
| 25  | CLA  | C2    | 518 | -    | 45,49,73     | 1.43 | 6 (13%)  | 54,84,113   | 1.50 | 6 (11%)  |
| 25  | CLA  | b2    | 612 | -    | 69,73,73     | 1.21 | 9 (13%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 23  | BCR  | a2    | 402 | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 1.65 | 13 (23%) |
| 25  | CLA  | b2    | 617 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.25 | 5 (6%)   |
| 35  | LMT  | c1    | 517 | -    | 34,34,36     | 0.44 | 0        | 45,45,47    | 0.69 | 1 (2%)   |
| 32  | GOL  | C2    | 514 | -    | 5,5,5        | 0.37 | 0        | 5,5,5       | 0.34 | 0        |
| 25  | CLA  | C2    | 503 | -    | 69,73,73     | 1.17 | 5 (7%)   | 82,113,113  | 1.30 | 4 (4%)   |
| 25  | CLA  | c2    | 504 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.26 | 5 (6%)   |
| 33  | LHG  | D2    | 403 | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.04 | 4 (7%)   |
| 29  | LMG  | C1    | 520 | -    | 48,48,55     | 0.98 | 2 (4%)   | 56,56,63    | 1.01 | 4 (7%)   |
| 23  | BCR  | K2    | 104 | -    | 29,29,41     | 0.59 | 0        | 41,41,56    | 1.72 | 11 (26%) |
| 37  | SQD  | b2    | 605 | -    | 43,45,54     | 1.23 | 3 (6%)   | 53,56,65    | 1.13 | 4 (7%)   |
| 25  | CLA  | B1    | 614 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.25 | 7 (8%)   |
| 25  | CLA  | C1    | 503 | -    | 64,68,73     | 1.23 | 6 (9%)   | 76,107,113  | 1.27 | 4 (5%)   |
| 25  | CLA  | c1    | 505 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.24 | 5 (6%)   |
| 23  | BCR  | d2    | 401 | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.11 | 16 (28%) |
| 25  | CLA  | C2    | 508 | -    | 54,58,73     | 1.33 | 6 (11%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 25  | CLA  | c1    | 513 | 3    | 64,68,73     | 1.23 | 6 (9%)   | 76,107,113  | 1.29 | 5 (6%)   |
| 25  | CLA  | K2    | 101 | -    | 59,63,73     | 1.28 | 7 (11%)  | 70,101,113  | 1.34 | 6 (8%)   |
| 23  | BCR  | J1    | 101 | -    | 41,41,41     | 0.74 | 0        | 56,56,56    | 2.11 | 14 (25%) |
| 25  | CLA  | a1    | 403 | -    | 69,73,73     | 1.23 | 7 (10%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 25  | CLA  | b2    | 609 | -    | 65,69,73     | 1.21 | 8 (12%)  | 77,108,113  | 1.32 | 6 (7%)   |
| 25  | CLA  | c2    | 511 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.25 | 4 (4%)   |
| 25  | CLA  | B2    | 614 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 23  | BCR  | h2    | 101 | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 1.80 | 14 (25%) |
| 25  | CLA  | A2    | 403 | -    | 65,69,73     | 1.23 | 6 (9%)   | 77,108,113  | 1.26 | 6 (7%)   |
| 25  | CLA  | c1    | 508 | -    | 54,58,73     | 1.35 | 7 (12%)  | 64,95,113   | 1.39 | 7 (10%)  |
| 25  | CLA  | b2    | 620 | 40   | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.29 | 5 (6%)   |

| Mol | Type | Chain | Res | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 29  | LMG  | A2    | 412 | -      | 29,29,55     | 1.08 | 2 (6%)   | 37,37,63    | 1.11 | 2 (5%)   |
| 23  | BCR  | H2    | 103 | -      | 24,24,41     | 0.69 | 0        | 31,31,56    | 1.63 | 7 (22%)  |
| 25  | CLA  | B1    | 613 | -      | 69,73,73     | 1.20 | 8 (11%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 35  | LMT  | L1    | 102 | -      | 11,11,36     | 0.24 | 0        | 10,10,47    | 0.57 | 0        |
| 23  | BCR  | h1    | 102 | -      | 41,41,41     | 0.67 | 0        | 56,56,56    | 1.90 | 16 (28%) |
| 25  | CLA  | b1    | 617 | -      | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 23  | BCR  | B1    | 601 | -      | 41,41,41     | 0.69 | 0        | 56,56,56    | 1.91 | 14 (25%) |
| 25  | CLA  | B1    | 611 | -      | 66,70,73     | 1.22 | 6 (9%)   | 78,109,113  | 1.26 | 6 (7%)   |
| 27  | PHO  | d1    | 403 | -      | 58,69,69     | 2.78 | 11 (18%) | 55,99,99    | 2.79 | 15 (27%) |
| 29  | LMG  | F2    | 402 | -      | 35,35,55     | 1.14 | 2 (5%)   | 43,43,63    | 1.04 | 3 (6%)   |
| 25  | CLA  | c1    | 507 | -      | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 29  | LMG  | d2    | 407 | -      | 27,27,55     | 1.38 | 2 (7%)   | 35,35,63    | 1.32 | 3 (8%)   |
| 25  | CLA  | D1    | 403 | -      | 55,59,73     | 1.33 | 6 (10%)  | 64,96,113   | 1.34 | 4 (6%)   |
| 34  | DGD  | h2    | 102 | -      | 63,63,67     | 0.88 | 2 (3%)   | 77,77,81    | 0.91 | 2 (2%)   |
| 32  | GOL  | a1    | 406 | -      | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.31 | 0        |
| 37  | SQD  | D1    | 409 | -      | 33,35,54     | 1.46 | 3 (9%)   | 43,46,65    | 1.41 | 5 (11%)  |
| 25  | CLA  | C1    | 511 | -      | 69,73,73     | 1.20 | 6 (8%)   | 82,113,113  | 1.25 | 4 (4%)   |
| 27  | PHO  | a2    | 416 | -      | 58,69,69     | 2.72 | 11 (18%) | 55,99,99    | 2.73 | 17 (30%) |
| 38  | HEM  | f1    | 101 | 6      | 50,50,50     | 1.94 | 8 (16%)  | 67,82,82    | 1.32 | 5 (7%)   |
| 35  | LMT  | m2    | 104 | -      | 30,30,36     | 0.48 | 0        | 41,41,47    | 0.83 | 1 (2%)   |
| 33  | LHG  | a1    | 407 | -      | 42,42,48     | 1.01 | 2 (4%)   | 45,48,54    | 1.11 | 3 (6%)   |
| 23  | BCR  | z2    | 101 | -      | 41,41,41     | 0.68 | 0        | 56,56,56    | 1.77 | 10 (17%) |
| 25  | CLA  | b2    | 618 | -      | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 25  | CLA  | D2    | 404 | -      | 65,69,73     | 1.22 | 6 (9%)   | 77,108,113  | 1.29 | 7 (9%)   |
| 29  | LMG  | C2    | 515 | -      | 24,24,55     | 1.19 | 3 (12%)  | 32,32,63    | 0.99 | 2 (6%)   |
| 25  | CLA  | C1    | 507 | -      | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.23 | 6 (7%)   |
| 29  | LMG  | b2    | 622 | -      | 39,39,55     | 1.08 | 2 (5%)   | 47,47,63    | 1.02 | 3 (6%)   |
| 25  | CLA  | b1    | 614 | -      | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 26  | OEX  | a2    | 408 | 3,1,40 | 0,15,15      | -    | -        | -           | -    | -        |
| 25  | CLA  | c1    | 511 | -      | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.27 | 6 (7%)   |
| 25  | CLA  | c1    | 506 | 40     | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.28 | 7 (8%)   |
| 25  | CLA  | C2    | 505 | -      | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.26 | 6 (7%)   |
| 32  | GOL  | i1    | 101 | -      | 5,5,5        | 0.42 | 0        | 5,5,5       | 0.24 | 0        |
| 25  | CLA  | b2    | 616 | -      | 64,68,73     | 1.25 | 7 (10%)  | 76,107,113  | 1.32 | 6 (7%)   |
| 38  | HEM  | E2    | 101 | 5      | 50,50,50     | 1.89 | 9 (18%)  | 67,82,82    | 1.32 | 5 (7%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 29  | LMG  | b1    | 624 | -    | 39,39,55     | 1.09 | 2 (5%)   | 47,47,63    | 1.33 | 5 (10%)  |
| 23  | BCR  | b2    | 602 | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.13 | 16 (28%) |
| 25  | CLA  | B1    | 610 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.23 | 7 (8%)   |
| 25  | CLA  | C1    | 508 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 25  | CLA  | D2    | 406 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.27 | 5 (6%)   |
| 23  | BCR  | H1    | 102 | -    | 22,22,41     | 0.68 | 0        | 29,29,56    | 1.70 | 7 (24%)  |
| 29  | LMG  | c1    | 519 | -    | 55,55,55     | 0.91 | 2 (3%)   | 63,63,63    | 0.96 | 2 (3%)   |
| 33  | LHG  | D2    | 405 | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.03 | 5 (9%)   |
| 37  | SQD  | B2    | 623 | -    | 43,45,54     | 1.24 | 4 (9%)   | 53,56,65    | 1.20 | 6 (11%)  |
| 25  | CLA  | B2    | 611 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.26 | 6 (7%)   |
| 34  | DGD  | C1    | 516 | -    | 63,63,67     | 0.85 | 2 (3%)   | 77,77,81    | 1.00 | 4 (5%)   |
| 25  | CLA  | A1    | 403 | -    | 69,73,73     | 1.22 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 35  | LMT  | b2    | 621 | -    | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.70 | 0        |
| 29  | LMG  | A1    | 412 | -    | 41,41,55     | 1.06 | 2 (4%)   | 49,49,63    | 1.03 | 3 (6%)   |
| 34  | DGD  | c1    | 520 | -    | 63,63,67     | 0.88 | 2 (3%)   | 77,77,81    | 0.86 | 2 (2%)   |
| 35  | LMT  | m1    | 101 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.69 | 1 (2%)   |
| 25  | CLA  | B2    | 605 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.25 | 6 (7%)   |
| 25  | CLA  | C1    | 506 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 25  | CLA  | C1    | 514 | -    | 49,53,73     | 1.40 | 7 (14%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 29  | LMG  | B1    | 622 | -    | 31,31,55     | 1.20 | 2 (6%)   | 39,39,63    | 1.21 | 4 (10%)  |
| 27  | PHO  | D2    | 407 | -    | 58,69,69     | 2.78 | 11 (18%) | 55,99,99    | 2.78 | 16 (29%) |
| 33  | LHG  | A2    | 405 | -    | 32,32,48     | 1.14 | 2 (6%)   | 35,38,54    | 1.04 | 3 (8%)   |
| 33  | LHG  | d2    | 406 | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.01 | 5 (9%)   |
| 34  | DGD  | c1    | 514 | -    | 52,52,67     | 0.97 | 2 (3%)   | 66,66,81    | 1.04 | 4 (6%)   |
| 25  | CLA  | c2    | 502 | -    | 69,73,73     | 1.19 | 5 (7%)   | 82,113,113  | 1.25 | 6 (7%)   |
| 23  | BCR  | C1    | 501 | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 1.82 | 14 (25%) |
| 25  | CLA  | d1    | 404 | 40   | 69,73,73     | 1.21 | 6 (8%)   | 82,113,113  | 1.29 | 5 (6%)   |
| 25  | CLA  | B2    | 609 | -    | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.32 | 6 (7%)   |
| 25  | CLA  | b2    | 611 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 25  | CLA  | c2    | 508 | 40   | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.23 | 5 (6%)   |
| 29  | LMG  | D1    | 406 | -    | 35,35,55     | 1.11 | 2 (5%)   | 43,43,63    | 1.08 | 3 (6%)   |
| 29  | LMG  | j2    | 101 | -    | 50,50,55     | 0.94 | 2 (4%)   | 58,58,63    | 1.03 | 2 (3%)   |
| 25  | CLA  | b1    | 607 | -    | 69,73,73     | 1.22 | 7 (10%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 25  | CLA  | b2    | 608 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.20 | 5 (6%)   |
| 25  | CLA  | c2    | 507 | -    | 58,62,73     | 1.30 | 7 (12%)  | 68,99,113   | 1.34 | 6 (8%)   |

| Mol | Type | Chain | Res | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 33  | LHG  | l2    | 101 | -      | 43,43,48     | 1.00 | 2 (4%)   | 46,49,54    | 1.08 | 5 (10%)  |
| 25  | CLA  | C1    | 510 | -      | 69,73,73     | 1.20 | 8 (11%)  | 82,113,113  | 1.21 | 4 (4%)   |
| 25  | CLA  | d2    | 402 | -      | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.32 | 7 (8%)   |
| 23  | BCR  | c1    | 502 | -      | 41,41,41     | 0.76 | 0        | 56,56,56    | 2.09 | 14 (25%) |
| 23  | BCR  | c1    | 501 | -      | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.11 | 16 (28%) |
| 35  | LMT  | T1    | 101 | -      | 11,11,36     | 0.24 | 0        | 10,10,47    | 0.58 | 0        |
| 25  | CLA  | b1    | 609 | -      | 69,73,73     | 1.19 | 9 (13%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 25  | CLA  | C1    | 509 | -      | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.36 | 9 (10%)  |
| 25  | CLA  | B2    | 610 | -      | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.23 | 7 (8%)   |
| 25  | CLA  | c2    | 515 | -      | 50,54,73     | 1.36 | 6 (12%)  | 59,90,113   | 1.41 | 4 (6%)   |
| 25  | CLA  | b1    | 611 | -      | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.21 | 6 (7%)   |
| 23  | BCR  | b2    | 603 | -      | 41,41,41     | 0.70 | 0        | 56,56,56    | 1.90 | 10 (17%) |
| 32  | GOL  | c1    | 521 | -      | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.34 | 0        |
| 34  | DGD  | H2    | 101 | -      | 63,63,67     | 0.89 | 2 (3%)   | 77,77,81    | 0.91 | 3 (3%)   |
| 36  | PL9  | d2    | 409 | -      | 55,55,55     | 0.66 | 2 (3%)   | 68,69,69    | 1.72 | 17 (25%) |
| 25  | CLA  | b2    | 614 | -      | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 23  | BCR  | k1    | 101 | -      | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.03 | 15 (26%) |
| 25  | CLA  | B1    | 604 | -      | 46,50,73     | 1.44 | 6 (13%)  | 53,85,113   | 1.41 | 4 (7%)   |
| 25  | CLA  | c1    | 503 | -      | 69,73,73     | 1.16 | 6 (8%)   | 82,113,113  | 1.30 | 5 (6%)   |
| 25  | CLA  | B1    | 615 | -      | 69,73,73     | 1.19 | 5 (7%)   | 82,113,113  | 1.23 | 5 (6%)   |
| 25  | CLA  | b1    | 604 | -      | 69,73,73     | 1.20 | 6 (8%)   | 82,113,113  | 1.19 | 5 (6%)   |
| 34  | DGD  | C2    | 512 | -      | 34,34,67     | 1.18 | 2 (5%)   | 46,47,81    | 1.09 | 2 (4%)   |
| 25  | CLA  | d2    | 404 | -      | 54,58,73     | 1.33 | 6 (11%)  | 64,95,113   | 1.39 | 5 (7%)   |
| 29  | LMG  | a2    | 412 | -      | 44,44,55     | 1.01 | 2 (4%)   | 52,52,63    | 1.12 | 5 (9%)   |
| 33  | LHG  | d1    | 402 | -      | 31,31,48     | 1.16 | 2 (6%)   | 34,37,54    | 1.35 | 4 (11%)  |
| 25  | CLA  | B1    | 607 | -      | 64,68,73     | 1.25 | 8 (12%)  | 76,107,113  | 1.27 | 5 (6%)   |
| 23  | BCR  | C2    | 502 | -      | 41,41,41     | 0.69 | 0        | 56,56,56    | 1.88 | 11 (19%) |
| 26  | OEX  | A1    | 407 | 3,1,40 | 0,15,15      | -    | -        | -           | -    | -        |
| 25  | CLA  | B2    | 615 | -      | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.23 | 6 (7%)   |
| 31  | BCT  | a1    | 413 | 30     | 3,3,3        | 0.54 | 0        | 2,3,3       | 0.70 | 0        |
| 36  | PL9  | D1    | 408 | -      | 55,55,55     | 0.66 | 2 (3%)   | 68,69,69    | 1.75 | 17 (25%) |
| 25  | CLA  | b1    | 619 | -      | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | d2    | 405 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | b2    | 606 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 34  | DGD  | C1    | 515 | -    | -         | 10/41/81/95   | 0/2/2/2 |
| 29  | LMG  | B2    | 621 | -    | -         | 8/31/51/70    | 0/1/1/1 |
| 27  | PHO  | d2    | 408 | -    | -         | 0/37/103/103  | 0/5/6/6 |
| 37  | SQD  | D2    | 402 | -    | -         | 2/18/38/69    | 0/1/1/1 |
| 34  | DGD  | c1    | 518 | -    | -         | 11/51/91/95   | 0/2/2/2 |
| 27  | PHO  | a1    | 411 | -    | -         | 5/37/103/103  | 0/5/6/6 |
| 25  | CLA  | a1    | 405 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 23  | BCR  | C1    | 521 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 29  | LMG  | d1    | 411 | -    | -         | 2/36/36/70    | -       |
| 25  | CLA  | B2    | 616 | -    | 1/1/12/20 | 7/26/102/115  | -       |
| 33  | LHG  | b1    | 622 | -    | -         | 13/53/53/53   | -       |
| 25  | CLA  | A2    | 404 | -    | 1/1/12/20 | 7/23/99/115   | -       |
| 23  | BCR  | B2    | 602 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B1    | 608 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 33  | LHG  | d1    | 407 | -    | -         | 13/53/53/53   | -       |
| 25  | CLA  | b2    | 604 | -    | 1/1/10/20 | 4/12/88/115   | -       |
| 33  | LHG  | L2    | 101 | -    | -         | 14/53/53/53   | -       |
| 36  | PL9  | d1    | 409 | -    | -         | 9/53/73/73    | 0/1/1/1 |
| 25  | CLA  | b2    | 615 | -    | 1/1/14/20 | 7/33/109/115  | -       |
| 25  | CLA  | b1    | 606 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | b2    | 610 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 34  | DGD  | C1    | 517 | -    | -         | 6/53/93/95    | 0/2/2/2 |
| 25  | CLA  | C2    | 510 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 32  | GOL  | C1    | 518 | -    | -         | 2/4/4/4       | -       |
| 29  | LMG  | c2    | 519 | -    | -         | 3/20/40/70    | 0/1/1/1 |
| 25  | CLA  | B2    | 604 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 25  | CLA  | c1    | 510 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 23  | BCR  | b1    | 602 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B2    | 618 | -    | 1/1/14/20 | 3/33/109/115  | -       |
| 25  | CLA  | c2    | 509 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | CLA  | B2    | 613 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 23  | BCR  | B1    | 603 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 35  | LMT  | b2    | 623 | -    | -         | 1/21/61/61    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | c2    | 513 | -    | 1/1/12/20 | 8/26/102/115  | -       |
| 25  | CLA  | C1    | 502 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 23  | BCR  | F2    | 401 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B2    | 619 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 33  | LHG  | B2    | 627 | -    | -         | 6/46/46/53    | -       |
| 29  | LMG  | b1    | 631 | -    | -         | 7/35/55/70    | 0/1/1/1 |
| 32  | GOL  | c2    | 518 | -    | -         | 2/4/4/4       | -       |
| 35  | LMT  | m2    | 103 | -    | -         | 5/16/56/61    | 0/2/2/2 |
| 25  | CLA  | B1    | 617 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 25  | CLA  | a2    | 413 | -    | 1/1/12/20 | 5/21/97/115   | -       |
| 25  | CLA  | B2    | 608 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 25  | CLA  | B1    | 616 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | CLA  | b2    | 619 | -    | 1/1/13/20 | 9/32/108/115  | -       |
| 23  | BCR  | B1    | 602 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 29  | LMG  | B1    | 626 | -    | -         | 12/43/63/70   | 0/1/1/1 |
| 25  | CLA  | C1    | 513 | 3    | 1/1/14/20 | 14/35/111/115 | -       |
| 23  | BCR  | c2    | 501 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 25  | CLA  | b1    | 616 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 25  | CLA  | b1    | 610 | -    | 1/1/15/20 | 2/39/115/115  | -       |
| 25  | CLA  | B1    | 606 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 34  | DGD  | c2    | 514 | -    | -         | 15/51/91/95   | 0/2/2/2 |
| 35  | LMT  | l1    | 101 | -    | -         | 3/15/35/61    | 0/1/1/2 |
| 33  | LHG  | a2    | 407 | -    | -         | 9/33/33/53    | -       |
| 34  | DGD  | c2    | 517 | -    | -         | 7/51/91/95    | 0/2/2/2 |
| 36  | PL9  | D2    | 408 | -    | -         | 7/53/73/73    | 0/1/1/1 |
| 38  | HEM  | v1    | 201 | 16   | -         | 4/14/54/54    | -       |
| 25  | CLA  | b2    | 613 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 38  | HEM  | V2    | 201 | 16   | -         | 3/14/54/54    | -       |
| 32  | GOL  | B1    | 620 | -    | -         | 2/4/4/4       | -       |
| 34  | DGD  | H1    | 101 | -    | -         | 12/51/91/95   | 0/2/2/2 |
| 25  | CLA  | c2    | 503 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 29  | LMG  | I2    | 101 | -    | -         | 3/29/49/70    | 0/1/1/1 |
| 25  | CLA  | b1    | 608 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 25  | CLA  | c2    | 510 | -    | 1/1/12/20 | 8/26/102/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | B2    | 606 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 23  | BCR  | B2    | 603 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 35  | LMT  | i2    | 102 | -    | -         | 0/4/4/61      | -       |
| 33  | LHG  | b2    | 625 | -    | -         | 4/47/47/53    | -       |
| 38  | HEM  | E1    | 101 | 5,6  | -         | 3/14/54/54    | -       |
| 25  | CLA  | b1    | 613 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 35  | LMT  | C1    | 519 | -    | -         | 1/21/61/61    | 0/2/2/2 |
| 23  | BCR  | A1    | 401 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 35  | LMT  | a2    | 406 | -    | -         | 5/21/61/61    | 0/2/2/2 |
| 23  | BCR  | d1    | 405 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 33  | LHG  | D1    | 405 | -    | -         | 12/53/53/53   | -       |
| 25  | CLA  | c1    | 509 | 40   | 1/1/15/20 | 17/39/115/115 | -       |
| 25  | CLA  | c1    | 516 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | CLA  | C1    | 512 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | B2    | 617 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 29  | LMG  | A1    | 410 | -    | -         | 4/38/58/70    | 0/1/1/1 |
| 33  | LHG  | d2    | 403 | -    | -         | 12/53/53/53   | -       |
| 25  | CLA  | B1    | 619 | 40   | 1/1/15/20 | 17/39/115/115 | -       |
| 33  | LHG  | B1    | 621 | -    | -         | 11/53/53/53   | -       |
| 25  | CLA  | D1    | 402 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 27  | PHO  | A2    | 407 | -    | -         | 7/37/103/103  | 0/5/6/6 |
| 23  | BCR  | K2    | 102 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B1    | 618 | -    | 1/1/13/20 | 4/31/107/115  | -       |
| 23  | BCR  | D1    | 401 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 25  | CLA  | c1    | 512 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 33  | LHG  | L1    | 101 | -    | -         | 14/45/45/53   | -       |
| 23  | BCR  | b1    | 601 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 33  | LHG  | D1    | 404 | -    | -         | 10/53/53/53   | -       |
| 33  | LHG  | l1    | 102 | -    | -         | 18/53/53/53   | -       |
| 25  | CLA  | A1    | 405 | -    | 1/1/13/20 | 3/27/103/115  | -       |
| 25  | CLA  | b1    | 612 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 23  | BCR  | K1    | 101 | -    | -         | 5/26/43/63    | 0/1/1/2 |
| 25  | CLA  | d1    | 406 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | D2    | 401 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 25  | CLA  | b1    | 605 | -    | 1/1/15/20 | 6/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | C2    | 507 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 38  | HEM  | V1    | 201 | 16   | -         | 4/14/54/54    | -       |
| 27  | PHO  | D1    | 407 | -    | -         | 3/35/101/103  | 0/5/6/6 |
| 29  | LMG  | a1    | 412 | -    | -         | 12/46/66/70   | 0/1/1/1 |
| 25  | CLA  | a2    | 405 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | A1    | 404 | -    | 1/1/12/20 | 7/23/99/115   | -       |
| 25  | CLA  | C2    | 506 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 23  | BCR  | b1    | 603 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 29  | LMG  | b1    | 621 | -    | -         | 6/33/53/70    | 0/1/1/1 |
| 29  | LMG  | B2    | 620 | -    | -         | 8/35/55/70    | 0/1/1/1 |
| 34  | DGD  | h1    | 101 | -    | -         | 9/51/91/95    | 0/2/2/2 |
| 25  | CLA  | C2    | 516 | -    | 1/1/11/20 | 10/17/93/115  | -       |
| 25  | CLA  | C2    | 509 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 25  | CLA  | B1    | 612 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 23  | BCR  | j2    | 102 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B2    | 607 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 25  | CLA  | c2    | 512 | 3    | 1/1/15/20 | 15/39/115/115 | -       |
| 32  | GOL  | a2    | 415 | -    | -         | 2/4/4/4       | -       |
| 25  | CLA  | a2    | 404 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 25  | CLA  | B2    | 612 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 23  | BCR  | k2    | 501 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 25  | CLA  | C1    | 504 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | CLA  | C1    | 505 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 35  | LMT  | M1    | 102 | -    | -         | 1/8/8/61      | -       |
| 25  | CLA  | c1    | 515 | -    | 1/1/13/20 | 8/27/103/115  | -       |
| 25  | CLA  | A1    | 406 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | CLA  | a1    | 404 | -    | 1/1/14/20 | 7/33/109/115  | -       |
| 23  | BCR  | a1    | 401 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 25  | CLA  | c2    | 505 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | C2    | 504 | -    | 1/1/11/20 | 6/17/93/115   | -       |
| 23  | BCR  | A2    | 401 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B1    | 609 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | B1    | 605 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 32  | GOL  | b1    | 618 | -    | -         | 4/4/4/4       | -       |
| 34  | DGD  | c2    | 516 | -    | -         | 7/41/81/95    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | b1    | 615 | -    | 1/1/13/20 | 7/32/108/115  | -       |
| 25  | CLA  | b2    | 624 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | CLA  | c1    | 504 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 35  | LMT  | M1    | 103 | -    | -         | 3/15/35/61    | 0/1/1/2 |
| 25  | CLA  | C2    | 511 | -    | 1/1/12/20 | 2/21/97/115   | -       |
| 23  | BCR  | b2    | 601 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 25  | CLA  | C2    | 513 | -    | 1/1/12/20 | 2/25/101/115  | -       |
| 25  | CLA  | d1    | 401 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 25  | CLA  | A2    | 402 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 38  | HEM  | v2    | 201 | 16   | -         | 2/14/54/54    | -       |
| 25  | CLA  | c2    | 506 | -    | 1/1/14/20 | 11/35/111/115 | -       |
| 25  | CLA  | b1    | 620 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 23  | BCR  | B2    | 601 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 29  | LMG  | M1    | 101 | -    | -         | 5/31/31/70    | -       |
| 29  | LMG  | d1    | 408 | -    | -         | 2/28/48/70    | 0/1/1/1 |
| 27  | PHO  | A1    | 408 | -    | -         | 6/37/103/103  | 0/5/6/6 |
| 38  | HEM  | e2    | 101 | 5,6  | -         | 2/14/54/54    | -       |
| 25  | CLA  | C2    | 518 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 25  | CLA  | b2    | 612 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | CLA  | b2    | 617 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 23  | BCR  | a2    | 402 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 35  | LMT  | c1    | 517 | -    | -         | 0/19/59/61    | 0/2/2/2 |
| 32  | GOL  | C2    | 514 | -    | -         | 2/4/4/4       | -       |
| 25  | CLA  | C2    | 503 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 25  | CLA  | c2    | 504 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 33  | LHG  | D2    | 403 | -    | -         | 11/53/53/53   | -       |
| 29  | LMG  | C1    | 520 | -    | -         | 8/43/63/70    | 0/1/1/1 |
| 23  | BCR  | K2    | 104 | -    | -         | 0/12/46/63    | 0/2/2/2 |
| 37  | SQD  | b2    | 605 | -    | -         | 10/40/60/69   | 0/1/1/1 |
| 25  | CLA  | B1    | 614 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | C1    | 503 | -    | 1/1/14/20 | 12/33/109/115 | -       |
| 25  | CLA  | c1    | 505 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 23  | BCR  | d2    | 401 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 25  | CLA  | C2    | 508 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 25  | CLA  | c1    | 513 | 3    | 1/1/14/20 | 5/33/109/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | K2    | 101 | -    | 1/1/13/20 | 13/27/103/115 | -       |
| 25  | CLA  | a1    | 403 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 25  | CLA  | b2    | 609 | -    | 1/1/14/20 | 12/35/111/115 | -       |
| 25  | CLA  | c2    | 511 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 23  | BCR  | J1    | 101 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B2    | 614 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | b2    | 620 | 40   | 1/1/15/20 | 22/39/115/115 | -       |
| 25  | CLA  | A2    | 403 | -    | 1/1/14/20 | 7/35/111/115  | -       |
| 25  | CLA  | c1    | 508 | -    | 1/1/12/20 | 5/21/97/115   | -       |
| 23  | BCR  | h2    | 101 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 29  | LMG  | A2    | 412 | -    | -         | 5/23/43/70    | 0/1/1/1 |
| 23  | BCR  | H2    | 103 | -    | -         | 2/17/34/63    | 0/1/1/2 |
| 25  | CLA  | B1    | 613 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 35  | LMT  | L1    | 102 | -    | -         | 1/9/9/61      | -       |
| 23  | BCR  | h1    | 102 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 25  | CLA  | b1    | 617 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 23  | BCR  | B1    | 601 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B1    | 611 | -    | -         | 9/36/112/115  | -       |
| 27  | PHO  | d1    | 403 | -    | -         | 3/37/103/103  | 0/5/6/6 |
| 29  | LMG  | F2    | 402 | -    | -         | 3/30/50/70    | 0/1/1/1 |
| 25  | CLA  | c1    | 507 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 29  | LMG  | d2    | 407 | -    | -         | 3/21/41/70    | 0/1/1/1 |
| 25  | CLA  | D1    | 403 | -    | 1/1/12/20 | 4/23/99/115   | -       |
| 34  | DGD  | h2    | 102 | -    | -         | 9/51/91/95    | 0/2/2/2 |
| 32  | GOL  | a1    | 406 | -    | -         | 1/4/4/4       | -       |
| 37  | SQD  | D1    | 409 | -    | -         | 2/29/49/69    | 0/1/1/1 |
| 25  | CLA  | C1    | 511 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 27  | PHO  | a2    | 416 | -    | -         | 5/37/103/103  | 0/5/6/6 |
| 38  | HEM  | f1    | 101 | 6    | -         | 5/14/54/54    | -       |
| 35  | LMT  | m2    | 104 | -    | -         | 4/15/55/61    | 0/2/2/2 |
| 33  | LHG  | a1    | 407 | -    | -         | 14/47/47/53   | -       |
| 25  | CLA  | b2    | 618 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 23  | BCR  | z2    | 101 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 25  | CLA  | D2    | 404 | -    | 1/1/14/20 | 11/35/111/115 | -       |
| 29  | LMG  | C2    | 515 | -    | -         | 0/18/38/70    | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | C1    | 507 | -    | 1/1/15/20 | 21/39/115/115 | -       |
| 29  | LMG  | b2    | 622 | -    | -         | 0/34/54/70    | 0/1/1/1 |
| 25  | CLA  | b1    | 614 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | c1    | 511 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | c1    | 506 | 40   | 1/1/15/20 | 13/39/115/115 | -       |
| 25  | CLA  | C2    | 505 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 32  | GOL  | i1    | 101 | -    | -         | 2/4/4/4       | -       |
| 25  | CLA  | b2    | 616 | -    | 1/1/14/20 | 6/33/109/115  | -       |
| 38  | HEM  | E2    | 101 | 5    | -         | 1/14/54/54    | -       |
| 29  | LMG  | b1    | 624 | -    | -         | 3/34/54/70    | 0/1/1/1 |
| 23  | BCR  | b2    | 602 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B1    | 610 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | C1    | 508 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | D2    | 406 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 23  | BCR  | H1    | 102 | -    | -         | 3/15/32/63    | 0/1/1/2 |
| 29  | LMG  | c1    | 519 | -    | -         | 9/50/70/70    | 0/1/1/1 |
| 33  | LHG  | D2    | 405 | -    | -         | 15/53/53/53   | -       |
| 37  | SQD  | B2    | 623 | -    | -         | 2/40/60/69    | 0/1/1/1 |
| 25  | CLA  | B2    | 611 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 34  | DGD  | C1    | 516 | -    | -         | 10/51/91/95   | 0/2/2/2 |
| 25  | CLA  | A1    | 403 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 35  | LMT  | b2    | 621 | -    | -         | 1/21/61/61    | 0/2/2/2 |
| 29  | LMG  | A1    | 412 | -    | -         | 7/36/56/70    | 0/1/1/1 |
| 34  | DGD  | c1    | 520 | -    | -         | 8/51/91/95    | 0/2/2/2 |
| 35  | LMT  | m1    | 101 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 25  | CLA  | B2    | 605 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 25  | CLA  | C1    | 506 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | CLA  | C1    | 514 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 29  | LMG  | B1    | 622 | -    | -         | 2/26/46/70    | 0/1/1/1 |
| 27  | PHO  | D2    | 407 | -    | -         | 6/37/103/103  | 0/5/6/6 |
| 33  | LHG  | A2    | 405 | -    | -         | 10/37/37/53   | -       |
| 33  | LHG  | d2    | 406 | -    | -         | 9/53/53/53    | -       |
| 34  | DGD  | c1    | 514 | -    | -         | 9/40/80/95    | 0/2/2/2 |
| 25  | CLA  | c2    | 502 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 25  | CLA  | b2    | 611 | -    | 1/1/15/20 | 7/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 25  | CLA  | d1    | 404 | 40   | 1/1/15/20 | 4/39/115/115  | -       |
| 25  | CLA  | B2    | 609 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 25  | CLA  | c2    | 508 | 40   | 1/1/15/20 | 16/39/115/115 | -       |
| 23  | BCR  | C1    | 501 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 29  | LMG  | D1    | 406 | -    | -         | 5/30/50/70    | 0/1/1/1 |
| 29  | LMG  | j2    | 101 | -    | -         | 7/45/65/70    | 0/1/1/1 |
| 25  | CLA  | b1    | 607 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | CLA  | b2    | 608 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 25  | CLA  | c2    | 507 | -    | 1/1/12/20 | 5/26/102/115  | -       |
| 33  | LHG  | l2    | 101 | -    | -         | 20/48/48/53   | -       |
| 25  | CLA  | C1    | 510 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | CLA  | d2    | 402 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 23  | BCR  | c1    | 502 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 23  | BCR  | c1    | 501 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 35  | LMT  | T1    | 101 | -    | -         | 0/9/9/61      | -       |
| 25  | CLA  | b1    | 609 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | CLA  | C1    | 509 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 25  | CLA  | B2    | 610 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 25  | CLA  | c2    | 515 | -    | 1/1/11/20 | 4/17/93/115   | -       |
| 25  | CLA  | b1    | 611 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 23  | BCR  | b2    | 603 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 32  | GOL  | c1    | 521 | -    | -         | 2/4/4/4       | -       |
| 34  | DGD  | H2    | 101 | -    | -         | 7/51/91/95    | 0/2/2/2 |
| 36  | PL9  | d2    | 409 | -    | -         | 8/53/73/73    | 0/1/1/1 |
| 25  | CLA  | b2    | 614 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 25  | CLA  | B1    | 604 | -    | 1/1/10/20 | 5/12/88/115   | -       |
| 23  | BCR  | k1    | 101 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 25  | CLA  | c1    | 503 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 25  | CLA  | B1    | 615 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | CLA  | b1    | 604 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 34  | DGD  | C2    | 512 | -    | -         | 1/20/60/95    | 0/2/2/2 |
| 25  | CLA  | d2    | 404 | -    | 1/1/12/20 | 4/21/97/115   | -       |
| 29  | LMG  | a2    | 412 | -    | -         | 6/39/59/70    | 0/1/1/1 |
| 33  | LHG  | d1    | 402 | -    | -         | 12/36/36/53   | -       |
| 25  | CLA  | B1    | 607 | -    | 1/1/14/20 | 9/33/109/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23  | BCR  | C2    | 502 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 25  | CLA  | B2    | 615 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 36  | PL9  | D1    | 408 | -    | -         | 8/53/73/73    | 0/1/1/1 |
| 25  | CLA  | b1    | 619 | -    | 1/1/15/20 | 16/39/115/115 | -       |

The worst 5 of 1254 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27  | d2    | 408 | PHO  | C1D-C2D | 10.28 | 1.50        | 1.39     |
| 27  | D1    | 407 | PHO  | C1D-C2D | 10.23 | 1.50        | 1.39     |
| 27  | D2    | 407 | PHO  | C1D-C2D | 10.14 | 1.50        | 1.39     |
| 27  | d1    | 403 | PHO  | C1D-C2D | 10.11 | 1.50        | 1.39     |
| 27  | A2    | 407 | PHO  | C1D-C2D | 10.09 | 1.50        | 1.39     |

The worst 5 of 1762 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | c2    | 501 | BCR  | C24-C23-C22 | -9.56 | 112.09      | 126.23   |
| 23  | c2    | 501 | BCR  | C36-C18-C17 | -9.33 | 107.70      | 122.82   |
| 23  | c2    | 501 | BCR  | C16-C17-C18 | 9.19  | 140.16      | 127.28   |
| 27  | a1    | 411 | PHO  | O2D-CGD-CBD | 8.48  | 120.27      | 110.95   |
| 27  | A1    | 408 | PHO  | O2D-CGD-CBD | 8.45  | 120.24      | 110.95   |

5 of 139 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25  | A1    | 403 | CLA  | ND   |
| 25  | A1    | 404 | CLA  | ND   |
| 25  | A1    | 405 | CLA  | ND   |
| 25  | A1    | 406 | CLA  | ND   |
| 25  | B1    | 604 | CLA  | ND   |

5 of 2137 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 23  | C1    | 501 | BCR  | C7-C8-C9-C10 |
| 23  | D1    | 401 | BCR  | C7-C8-C9-C10 |
| 23  | K1    | 101 | BCR  | C1-C6-C7-C8  |
| 23  | K1    | 101 | BCR  | C5-C6-C7-C8  |
| 23  | d1    | 405 | BCR  | C7-C8-C9-C10 |

There are no ring outliers.

250 monomers are involved in 721 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | d2    | 405 | CLA  | 3       | 0            |
| 25  | b2    | 606 | CLA  | 7       | 0            |
| 34  | C1    | 515 | DGD  | 2       | 0            |
| 29  | B2    | 621 | LMG  | 2       | 0            |
| 27  | d2    | 408 | PHO  | 1       | 0            |
| 34  | c1    | 518 | DGD  | 7       | 0            |
| 27  | a1    | 411 | PHO  | 4       | 0            |
| 25  | a1    | 405 | CLA  | 1       | 0            |
| 23  | C1    | 521 | BCR  | 3       | 0            |
| 25  | B2    | 616 | CLA  | 3       | 0            |
| 33  | b1    | 622 | LHG  | 4       | 0            |
| 25  | A2    | 404 | CLA  | 1       | 0            |
| 23  | B2    | 602 | BCR  | 6       | 0            |
| 25  | B1    | 608 | CLA  | 3       | 0            |
| 33  | d1    | 407 | LHG  | 4       | 0            |
| 33  | L2    | 101 | LHG  | 5       | 0            |
| 36  | d1    | 409 | PL9  | 12      | 0            |
| 25  | b2    | 615 | CLA  | 4       | 0            |
| 25  | b1    | 606 | CLA  | 5       | 0            |
| 25  | b2    | 610 | CLA  | 7       | 0            |
| 34  | C1    | 517 | DGD  | 1       | 0            |
| 25  | C2    | 510 | CLA  | 1       | 0            |
| 25  | B2    | 604 | CLA  | 1       | 0            |
| 23  | b1    | 602 | BCR  | 2       | 0            |
| 25  | c1    | 510 | CLA  | 4       | 0            |
| 25  | B2    | 618 | CLA  | 1       | 0            |
| 23  | B1    | 603 | BCR  | 3       | 0            |
| 25  | B2    | 613 | CLA  | 4       | 0            |
| 25  | c2    | 509 | CLA  | 5       | 0            |
| 35  | b2    | 623 | LMT  | 2       | 0            |
| 25  | C1    | 502 | CLA  | 2       | 0            |
| 23  | F2    | 401 | BCR  | 4       | 0            |
| 25  | B2    | 619 | CLA  | 1       | 0            |
| 33  | B2    | 627 | LHG  | 2       | 0            |
| 29  | b1    | 631 | LMG  | 2       | 0            |
| 35  | m2    | 103 | LMT  | 2       | 0            |
| 25  | B1    | 617 | CLA  | 5       | 0            |
| 23  | B1    | 602 | BCR  | 5       | 0            |
| 25  | B1    | 616 | CLA  | 5       | 0            |
| 25  | B2    | 608 | CLA  | 6       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | b2    | 619 | CLA  | 2       | 0            |
| 29  | B1    | 626 | LMG  | 2       | 0            |
| 25  | C1    | 513 | CLA  | 4       | 0            |
| 23  | c2    | 501 | BCR  | 8       | 0            |
| 25  | b1    | 616 | CLA  | 3       | 0            |
| 25  | B1    | 606 | CLA  | 5       | 0            |
| 34  | c2    | 514 | DGD  | 3       | 0            |
| 35  | l1    | 101 | LMT  | 1       | 0            |
| 33  | a2    | 407 | LHG  | 4       | 0            |
| 34  | c2    | 517 | DGD  | 2       | 0            |
| 36  | D2    | 408 | PL9  | 11      | 0            |
| 38  | v1    | 201 | HEM  | 3       | 0            |
| 25  | b2    | 613 | CLA  | 2       | 0            |
| 38  | V2    | 201 | HEM  | 4       | 0            |
| 34  | H1    | 101 | DGD  | 1       | 0            |
| 25  | c2    | 503 | CLA  | 4       | 0            |
| 29  | I2    | 101 | LMG  | 2       | 0            |
| 23  | B2    | 603 | BCR  | 3       | 0            |
| 25  | b1    | 608 | CLA  | 3       | 0            |
| 25  | B2    | 606 | CLA  | 3       | 0            |
| 25  | c2    | 510 | CLA  | 3       | 0            |
| 38  | E1    | 101 | HEM  | 3       | 0            |
| 25  | b1    | 613 | CLA  | 4       | 0            |
| 35  | C1    | 519 | LMT  | 1       | 0            |
| 23  | A1    | 401 | BCR  | 4       | 0            |
| 35  | a2    | 406 | LMT  | 2       | 0            |
| 23  | d1    | 405 | BCR  | 4       | 0            |
| 33  | D1    | 405 | LHG  | 6       | 0            |
| 25  | c1    | 509 | CLA  | 4       | 0            |
| 25  | c1    | 516 | CLA  | 1       | 0            |
| 25  | C1    | 512 | CLA  | 3       | 0            |
| 25  | B2    | 617 | CLA  | 3       | 0            |
| 29  | A1    | 410 | LMG  | 3       | 0            |
| 33  | d2    | 403 | LHG  | 4       | 0            |
| 25  | B1    | 619 | CLA  | 4       | 0            |
| 33  | B1    | 621 | LHG  | 8       | 0            |
| 25  | D1    | 402 | CLA  | 3       | 0            |
| 27  | A2    | 407 | PHO  | 2       | 0            |
| 23  | K2    | 102 | BCR  | 5       | 0            |
| 23  | D1    | 401 | BCR  | 3       | 0            |
| 25  | c1    | 512 | CLA  | 5       | 0            |
| 33  | L1    | 101 | LHG  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | b1    | 601 | BCR  | 4       | 0            |
| 33  | D1    | 404 | LHG  | 4       | 0            |
| 33  | l1    | 102 | LHG  | 3       | 0            |
| 23  | K1    | 101 | BCR  | 4       | 0            |
| 25  | A1    | 405 | CLA  | 6       | 0            |
| 25  | b1    | 612 | CLA  | 3       | 0            |
| 25  | d1    | 406 | CLA  | 2       | 0            |
| 25  | D2    | 401 | CLA  | 3       | 0            |
| 25  | b1    | 605 | CLA  | 1       | 0            |
| 25  | C2    | 507 | CLA  | 2       | 0            |
| 38  | V1    | 201 | HEM  | 3       | 0            |
| 27  | D1    | 407 | PHO  | 1       | 0            |
| 29  | a1    | 412 | LMG  | 6       | 0            |
| 25  | a2    | 405 | CLA  | 2       | 0            |
| 23  | b1    | 603 | BCR  | 4       | 0            |
| 25  | A1    | 404 | CLA  | 1       | 0            |
| 29  | b1    | 621 | LMG  | 3       | 0            |
| 29  | B2    | 620 | LMG  | 1       | 0            |
| 34  | h1    | 101 | DGD  | 4       | 0            |
| 25  | C2    | 516 | CLA  | 1       | 0            |
| 25  | C2    | 509 | CLA  | 3       | 0            |
| 25  | B1    | 612 | CLA  | 3       | 0            |
| 23  | j2    | 102 | BCR  | 9       | 0            |
| 25  | B2    | 607 | CLA  | 2       | 0            |
| 25  | c2    | 512 | CLA  | 4       | 0            |
| 25  | a2    | 404 | CLA  | 7       | 0            |
| 25  | B2    | 612 | CLA  | 2       | 0            |
| 23  | k2    | 501 | BCR  | 8       | 0            |
| 25  | C1    | 504 | CLA  | 5       | 0            |
| 25  | C1    | 505 | CLA  | 2       | 0            |
| 35  | M1    | 102 | LMT  | 1       | 0            |
| 23  | a1    | 401 | BCR  | 7       | 0            |
| 25  | A1    | 406 | CLA  | 5       | 0            |
| 25  | a1    | 404 | CLA  | 7       | 0            |
| 25  | c1    | 515 | CLA  | 1       | 0            |
| 25  | c2    | 505 | CLA  | 3       | 0            |
| 23  | A2    | 401 | BCR  | 6       | 0            |
| 25  | B1    | 609 | CLA  | 2       | 0            |
| 25  | B1    | 605 | CLA  | 2       | 0            |
| 34  | c2    | 516 | DGD  | 1       | 0            |
| 25  | b2    | 624 | CLA  | 3       | 0            |
| 25  | c1    | 504 | CLA  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | C2    | 511 | CLA  | 1       | 0            |
| 23  | b2    | 601 | BCR  | 4       | 0            |
| 25  | C2    | 513 | CLA  | 2       | 0            |
| 25  | d1    | 401 | CLA  | 7       | 0            |
| 25  | A2    | 402 | CLA  | 6       | 0            |
| 38  | v2    | 201 | HEM  | 3       | 0            |
| 23  | B2    | 601 | BCR  | 5       | 0            |
| 25  | b1    | 620 | CLA  | 1       | 0            |
| 25  | c2    | 506 | CLA  | 4       | 0            |
| 29  | M1    | 101 | LMG  | 2       | 0            |
| 29  | d1    | 408 | LMG  | 1       | 0            |
| 27  | A1    | 408 | PHO  | 2       | 0            |
| 38  | e2    | 101 | HEM  | 3       | 0            |
| 25  | b2    | 612 | CLA  | 5       | 0            |
| 23  | a2    | 402 | BCR  | 4       | 0            |
| 25  | C2    | 503 | CLA  | 4       | 0            |
| 25  | c2    | 504 | CLA  | 4       | 0            |
| 33  | D2    | 403 | LHG  | 9       | 0            |
| 29  | C1    | 520 | LMG  | 1       | 0            |
| 23  | K2    | 104 | BCR  | 3       | 0            |
| 37  | b2    | 605 | SQD  | 2       | 0            |
| 25  | B1    | 614 | CLA  | 1       | 0            |
| 25  | C1    | 503 | CLA  | 2       | 0            |
| 25  | c1    | 505 | CLA  | 1       | 0            |
| 23  | d2    | 401 | BCR  | 4       | 0            |
| 25  | C2    | 508 | CLA  | 1       | 0            |
| 25  | c1    | 513 | CLA  | 3       | 0            |
| 25  | K2    | 101 | CLA  | 4       | 0            |
| 23  | J1    | 101 | BCR  | 6       | 0            |
| 25  | a1    | 403 | CLA  | 5       | 0            |
| 25  | b2    | 609 | CLA  | 5       | 0            |
| 25  | c2    | 511 | CLA  | 3       | 0            |
| 25  | B2    | 614 | CLA  | 5       | 0            |
| 23  | h2    | 101 | BCR  | 3       | 0            |
| 25  | A2    | 403 | CLA  | 10      | 0            |
| 25  | c1    | 508 | CLA  | 6       | 0            |
| 25  | b2    | 620 | CLA  | 6       | 0            |
| 29  | A2    | 412 | LMG  | 1       | 0            |
| 23  | H2    | 103 | BCR  | 4       | 0            |
| 25  | B1    | 613 | CLA  | 3       | 0            |
| 35  | L1    | 102 | LMT  | 1       | 0            |
| 23  | h1    | 102 | BCR  | 3       | 0            |

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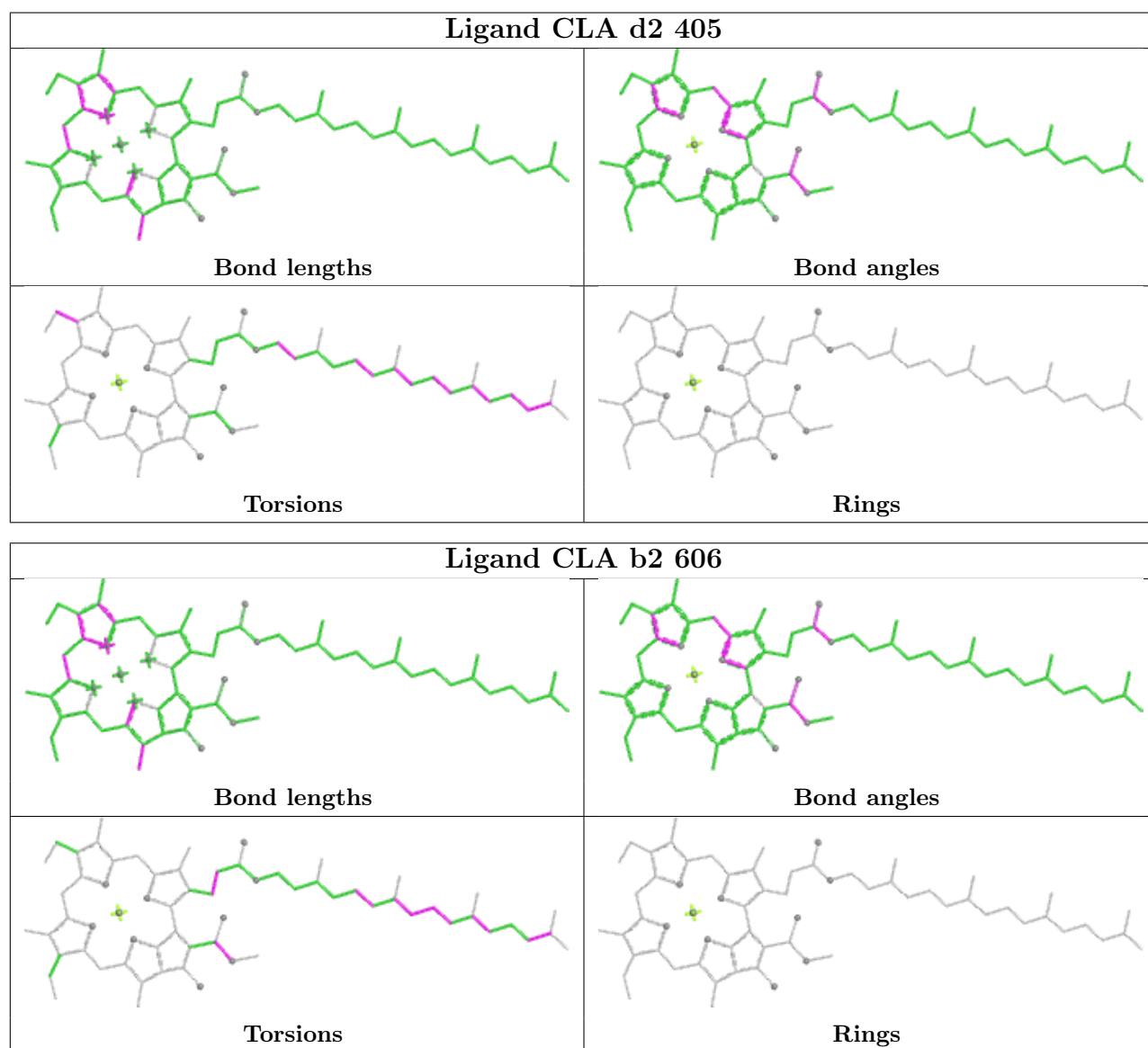
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | B1    | 601 | BCR  | 6       | 0            |
| 25  | B1    | 611 | CLA  | 6       | 0            |
| 27  | d1    | 403 | PHO  | 2       | 0            |
| 29  | F2    | 402 | LMG  | 1       | 0            |
| 25  | c1    | 507 | CLA  | 5       | 0            |
| 29  | d2    | 407 | LMG  | 2       | 0            |
| 34  | h2    | 102 | DGD  | 5       | 0            |
| 37  | D1    | 409 | SQD  | 1       | 0            |
| 25  | C1    | 511 | CLA  | 4       | 0            |
| 27  | a2    | 416 | PHO  | 3       | 0            |
| 38  | f1    | 101 | HEM  | 3       | 0            |
| 35  | m2    | 104 | LMT  | 1       | 0            |
| 33  | a1    | 407 | LHG  | 3       | 0            |
| 23  | z2    | 101 | BCR  | 5       | 0            |
| 25  | b2    | 618 | CLA  | 2       | 0            |
| 25  | D2    | 404 | CLA  | 3       | 0            |
| 25  | C1    | 507 | CLA  | 1       | 0            |
| 29  | b2    | 622 | LMG  | 3       | 0            |
| 25  | b1    | 614 | CLA  | 4       | 0            |
| 25  | c1    | 511 | CLA  | 1       | 0            |
| 25  | c1    | 506 | CLA  | 5       | 0            |
| 25  | C2    | 505 | CLA  | 4       | 0            |
| 32  | i1    | 101 | GOL  | 1       | 0            |
| 25  | b2    | 616 | CLA  | 2       | 0            |
| 38  | E2    | 101 | HEM  | 4       | 0            |
| 29  | b1    | 624 | LMG  | 9       | 0            |
| 23  | b2    | 602 | BCR  | 3       | 0            |
| 25  | B1    | 610 | CLA  | 6       | 0            |
| 25  | C1    | 508 | CLA  | 2       | 0            |
| 25  | D2    | 406 | CLA  | 4       | 0            |
| 23  | H1    | 102 | BCR  | 3       | 0            |
| 29  | c1    | 519 | LMG  | 1       | 0            |
| 33  | D2    | 405 | LHG  | 7       | 0            |
| 37  | B2    | 623 | SQD  | 2       | 0            |
| 25  | B2    | 611 | CLA  | 5       | 0            |
| 34  | C1    | 516 | DGD  | 7       | 0            |
| 25  | A1    | 403 | CLA  | 4       | 0            |
| 29  | A1    | 412 | LMG  | 3       | 0            |
| 34  | c1    | 520 | DGD  | 1       | 0            |
| 35  | m1    | 101 | LMT  | 1       | 0            |
| 25  | B2    | 605 | CLA  | 2       | 0            |
| 25  | C1    | 506 | CLA  | 4       | 0            |

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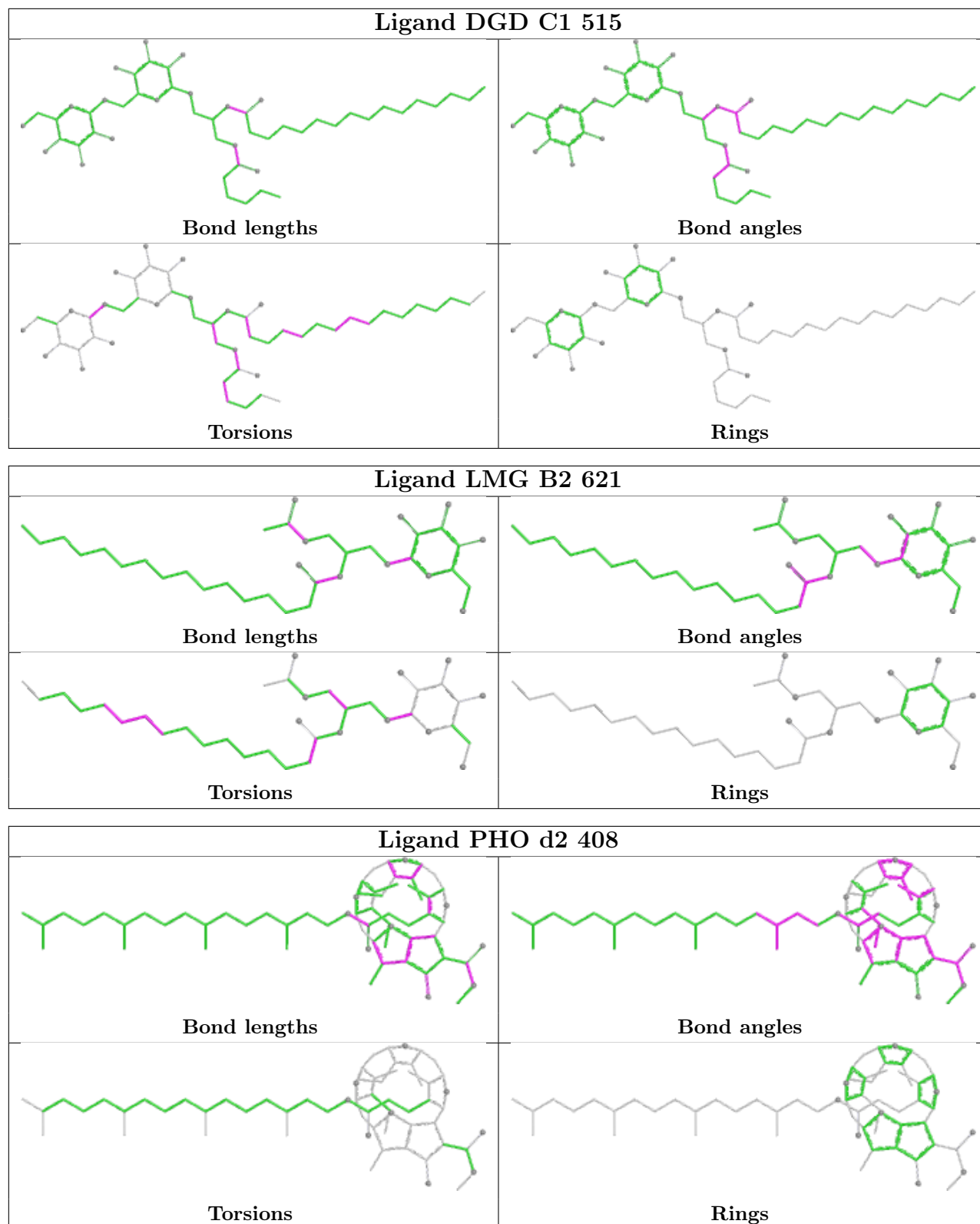
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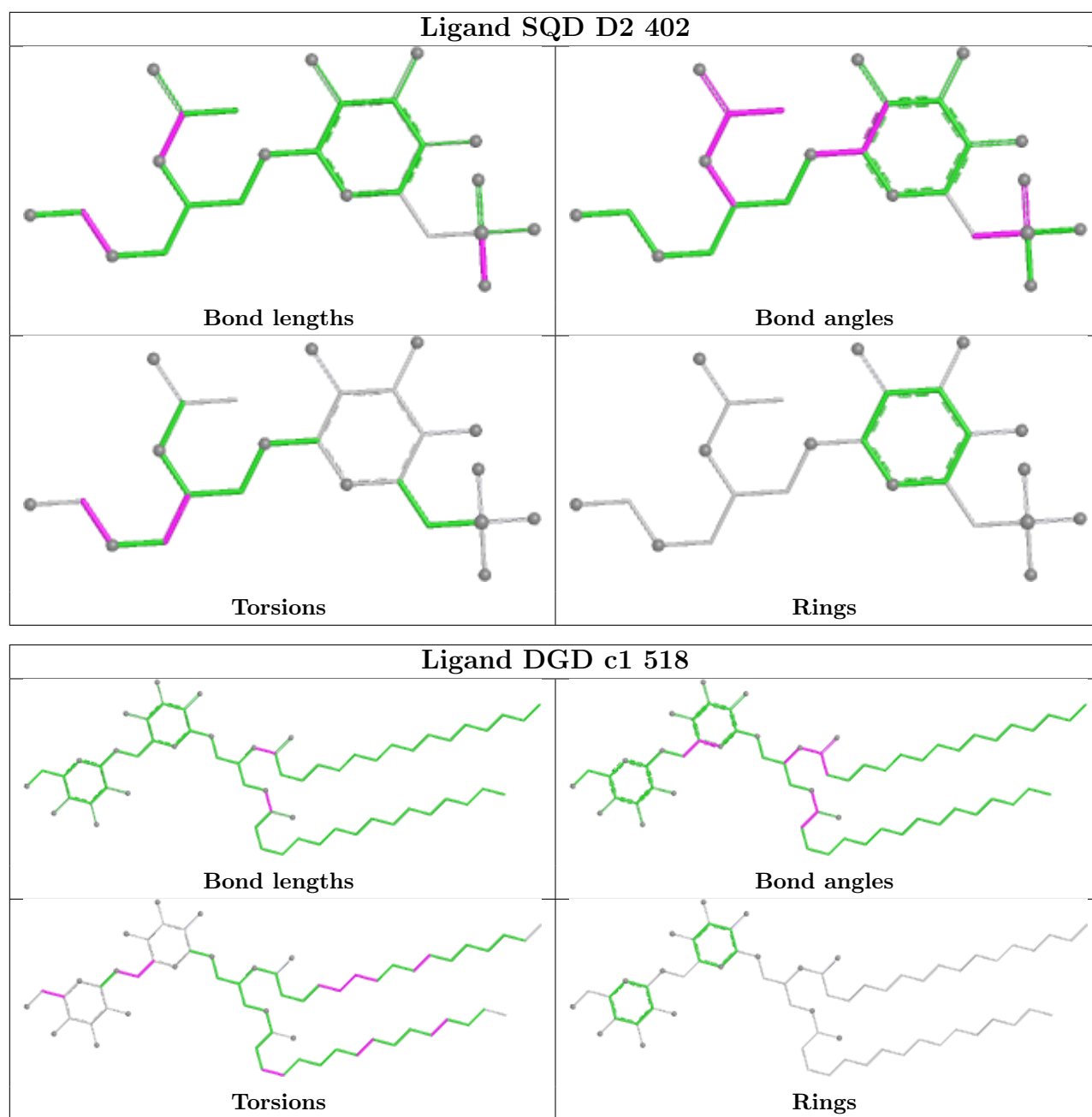
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | C1    | 514 | CLA  | 2       | 0            |
| 29  | B1    | 622 | LMG  | 1       | 0            |
| 27  | D2    | 407 | PHO  | 3       | 0            |
| 33  | A2    | 405 | LHG  | 3       | 0            |
| 33  | d2    | 406 | LHG  | 5       | 0            |
| 34  | c1    | 514 | DGD  | 6       | 0            |
| 25  | c2    | 502 | CLA  | 5       | 0            |
| 23  | C1    | 501 | BCR  | 4       | 0            |
| 25  | d1    | 404 | CLA  | 7       | 0            |
| 25  | B2    | 609 | CLA  | 2       | 0            |
| 25  | b2    | 611 | CLA  | 1       | 0            |
| 25  | c2    | 508 | CLA  | 3       | 0            |
| 29  | D1    | 406 | LMG  | 1       | 0            |
| 29  | j2    | 101 | LMG  | 6       | 0            |
| 25  | b1    | 607 | CLA  | 2       | 0            |
| 25  | b2    | 608 | CLA  | 5       | 0            |
| 25  | c2    | 507 | CLA  | 2       | 0            |
| 33  | l2    | 101 | LHG  | 5       | 0            |
| 25  | C1    | 510 | CLA  | 3       | 0            |
| 25  | d2    | 402 | CLA  | 4       | 0            |
| 23  | c1    | 502 | BCR  | 4       | 0            |
| 23  | c1    | 501 | BCR  | 7       | 0            |
| 25  | b1    | 609 | CLA  | 7       | 0            |
| 25  | C1    | 509 | CLA  | 7       | 0            |
| 25  | B2    | 610 | CLA  | 2       | 0            |
| 25  | c2    | 515 | CLA  | 3       | 0            |
| 25  | b1    | 611 | CLA  | 3       | 0            |
| 23  | b2    | 603 | BCR  | 8       | 0            |
| 34  | H2    | 101 | DGD  | 3       | 0            |
| 36  | d2    | 409 | PL9  | 7       | 0            |
| 25  | b2    | 614 | CLA  | 1       | 0            |
| 23  | k1    | 101 | BCR  | 6       | 0            |
| 25  | B1    | 604 | CLA  | 2       | 0            |
| 25  | c1    | 503 | CLA  | 4       | 0            |
| 25  | B1    | 615 | CLA  | 2       | 0            |
| 25  | b1    | 604 | CLA  | 2       | 0            |
| 33  | d1    | 402 | LHG  | 2       | 0            |
| 25  | B1    | 607 | CLA  | 2       | 0            |
| 23  | C2    | 502 | BCR  | 3       | 0            |
| 25  | B2    | 615 | CLA  | 2       | 0            |
| 36  | D1    | 408 | PL9  | 9       | 0            |
| 25  | b1    | 619 | CLA  | 1       | 0            |

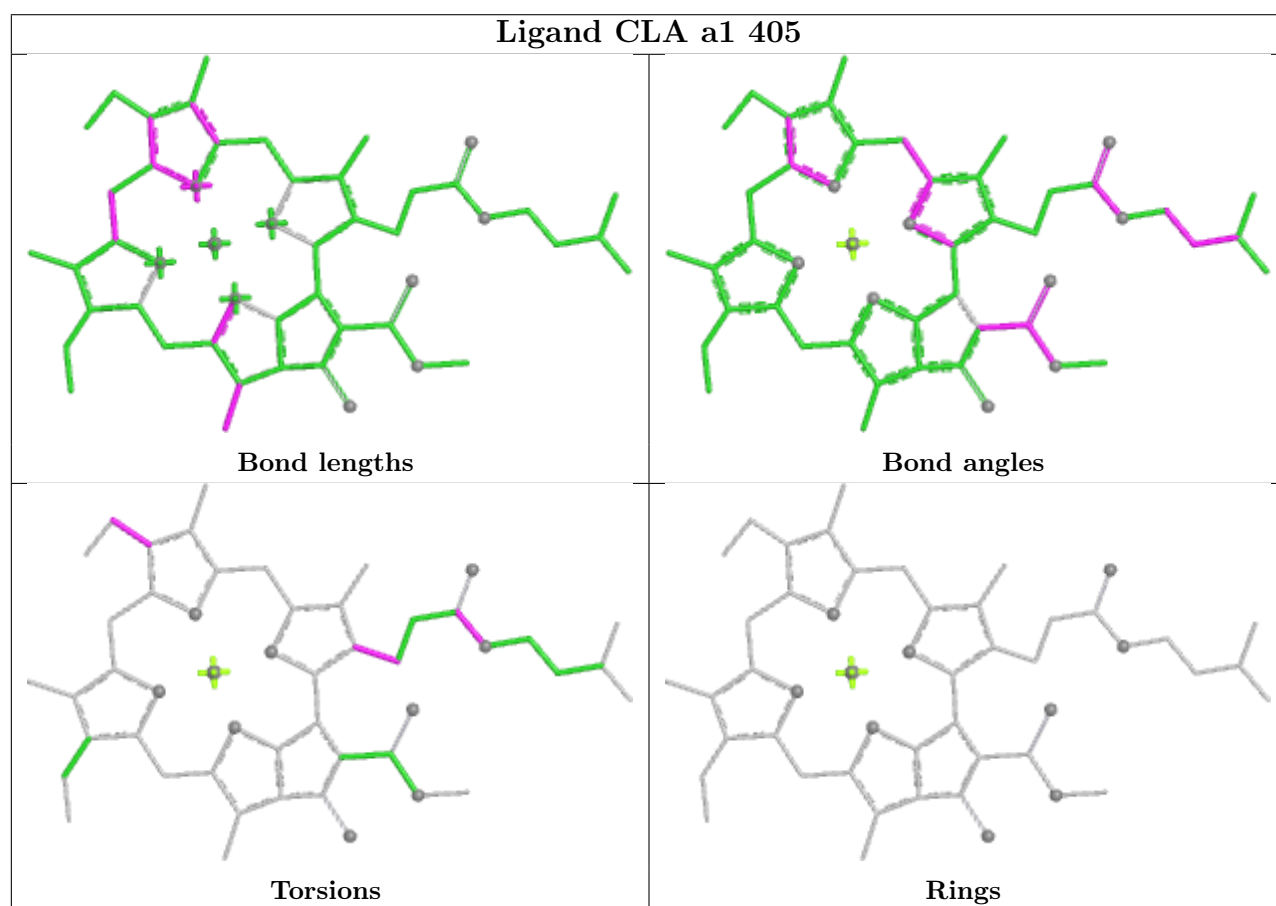
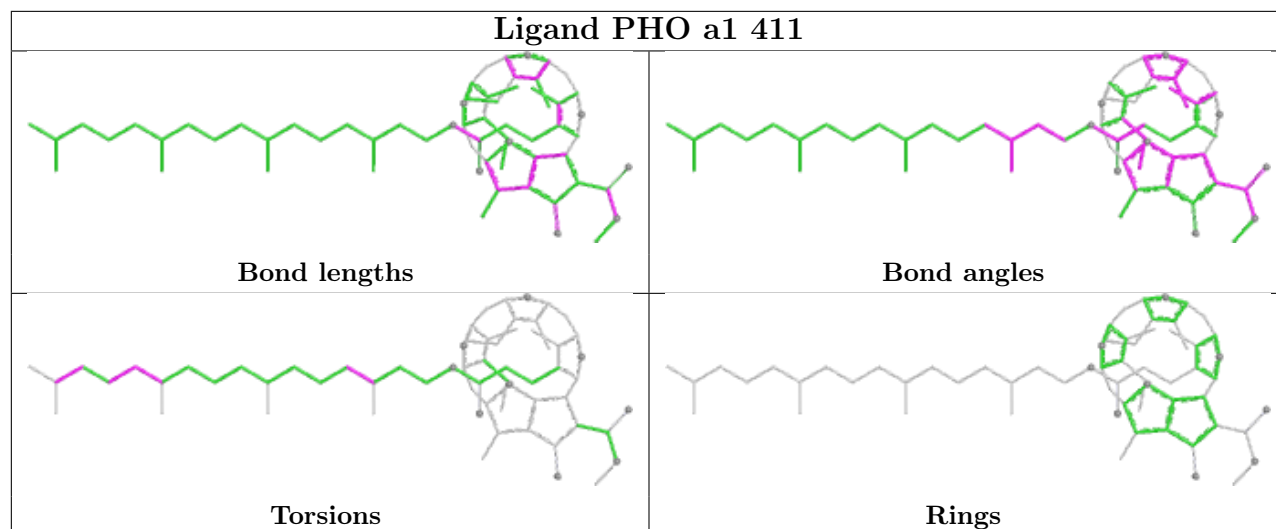
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

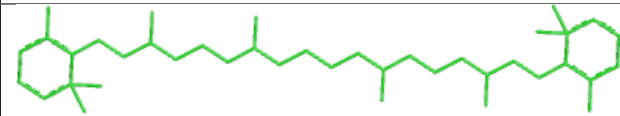
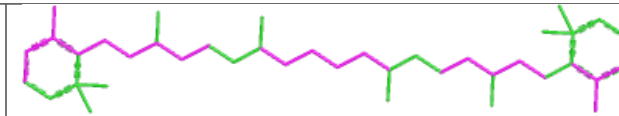
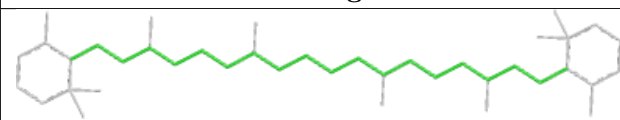
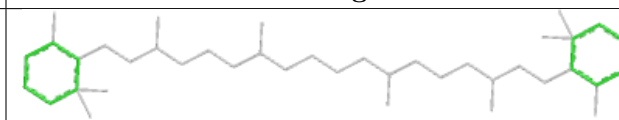


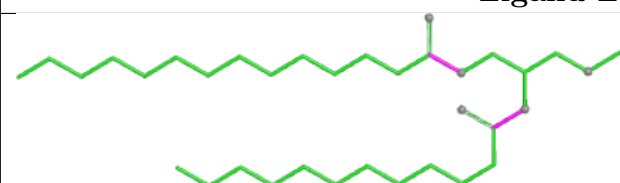
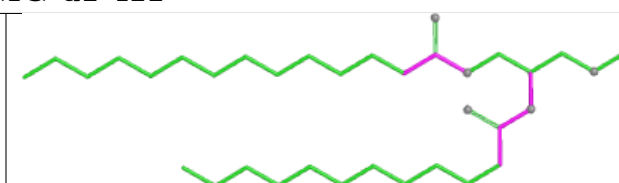
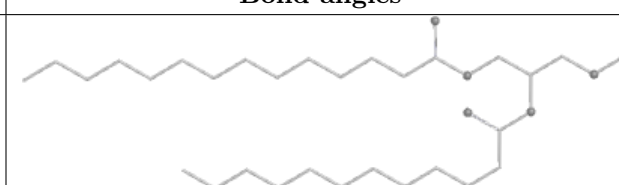


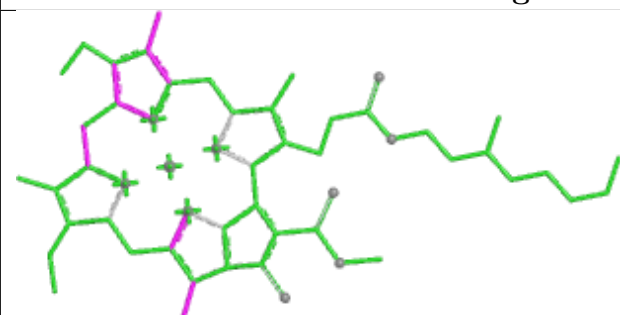
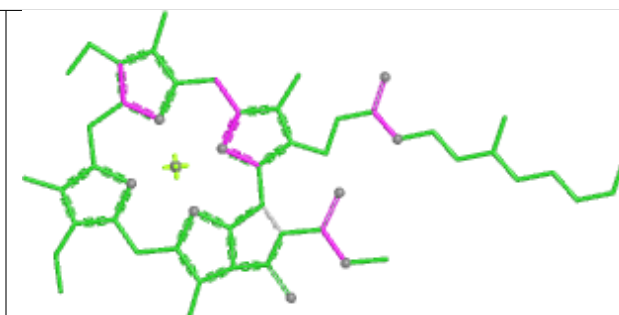
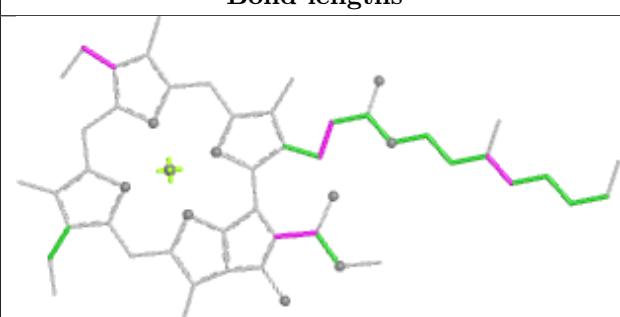
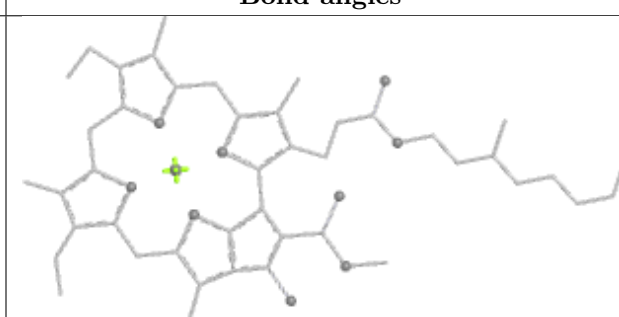


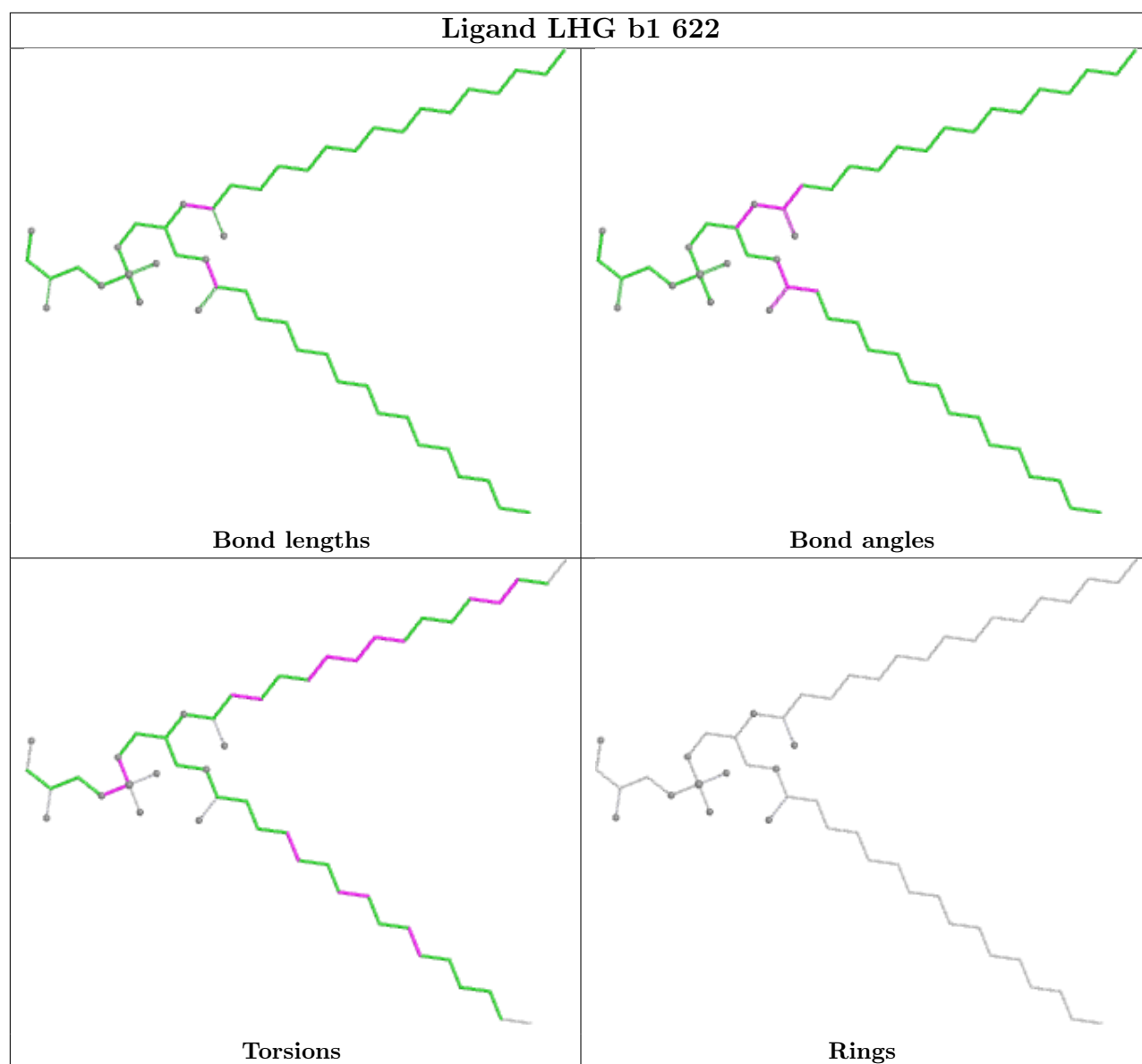




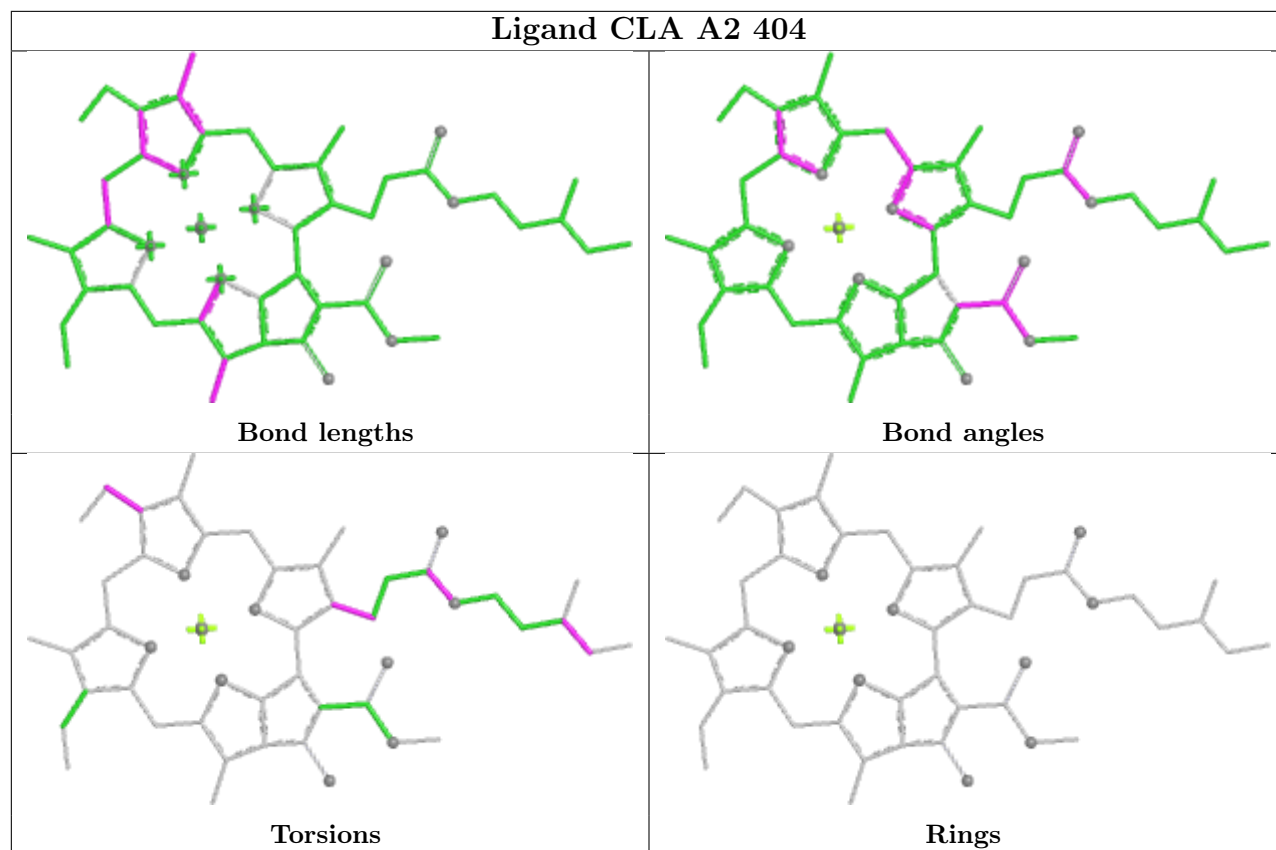
| Ligand BCR C1 521                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand LMG d1 411                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

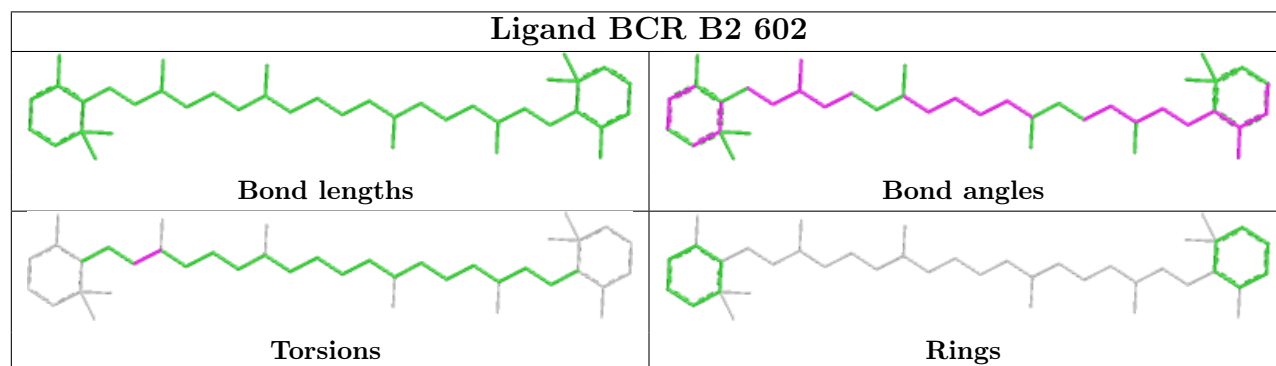
| Ligand CLA B2 616                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

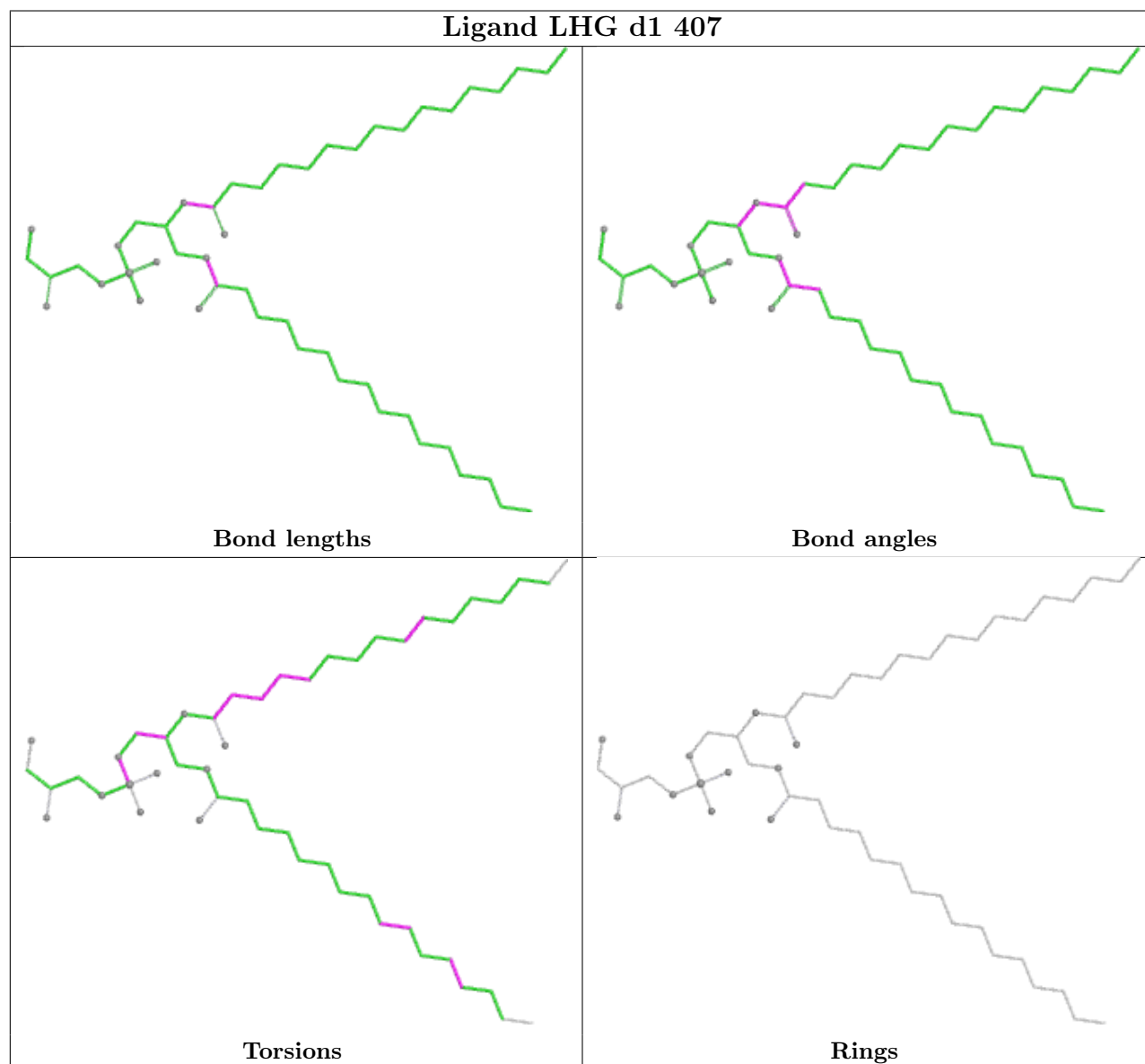
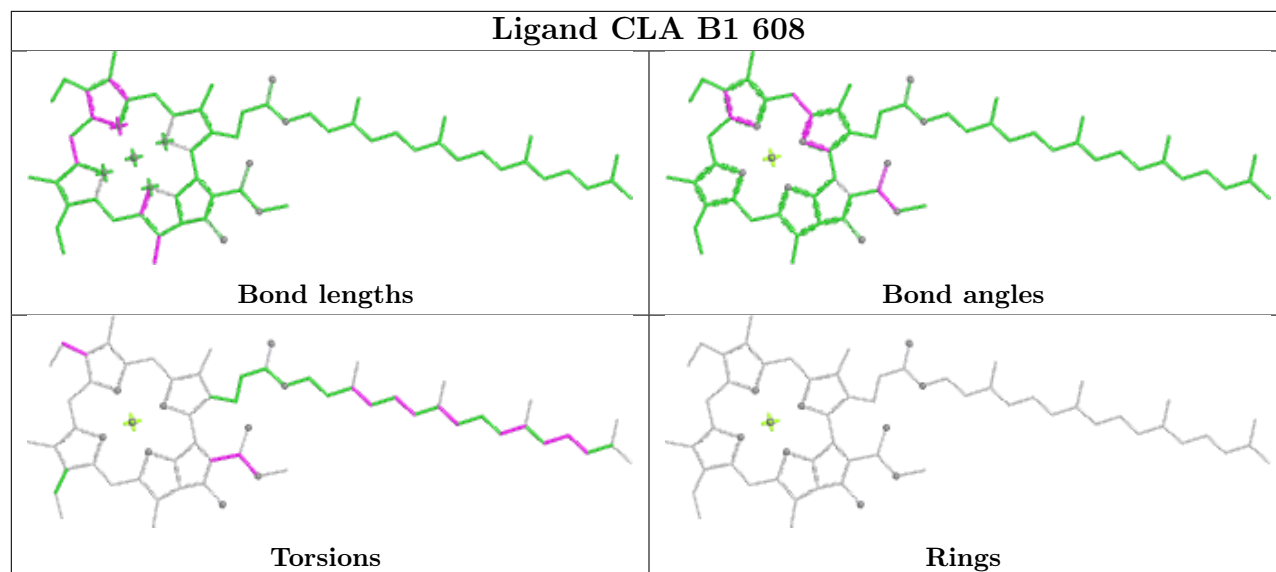


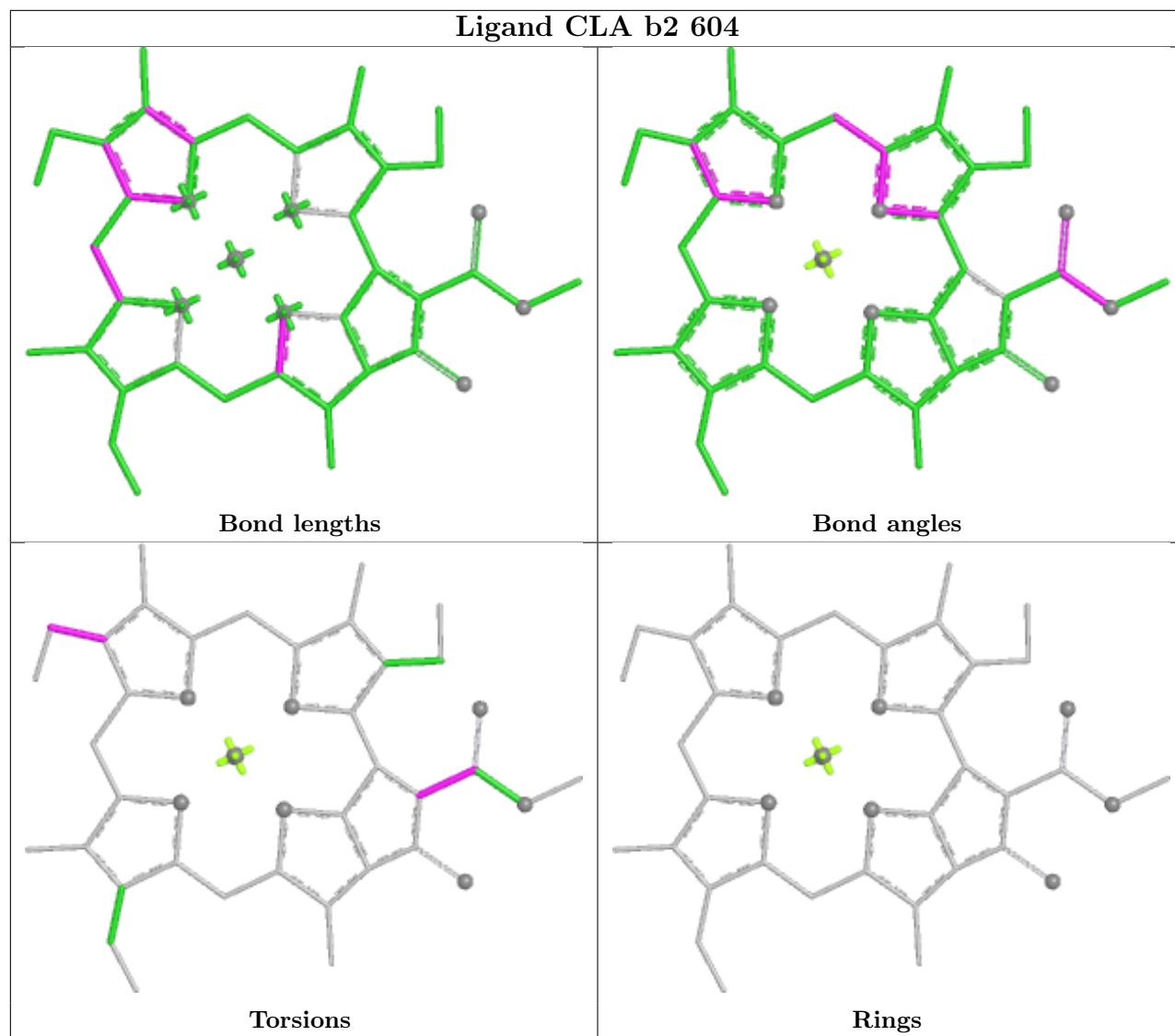
## Ligand CLA A2 404



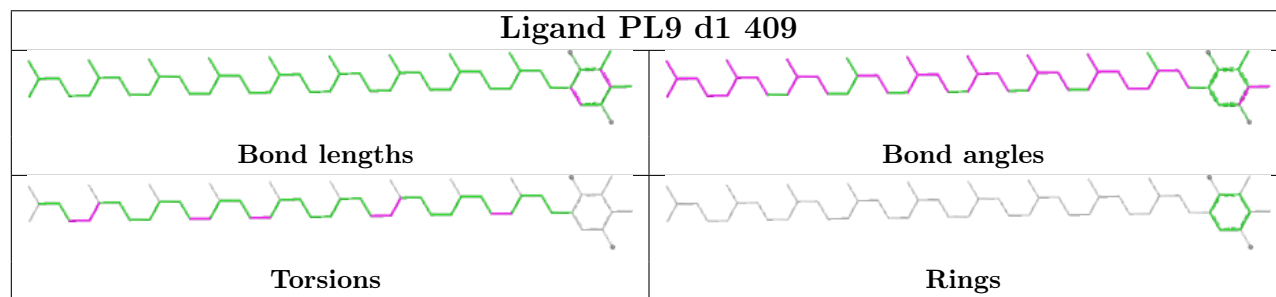
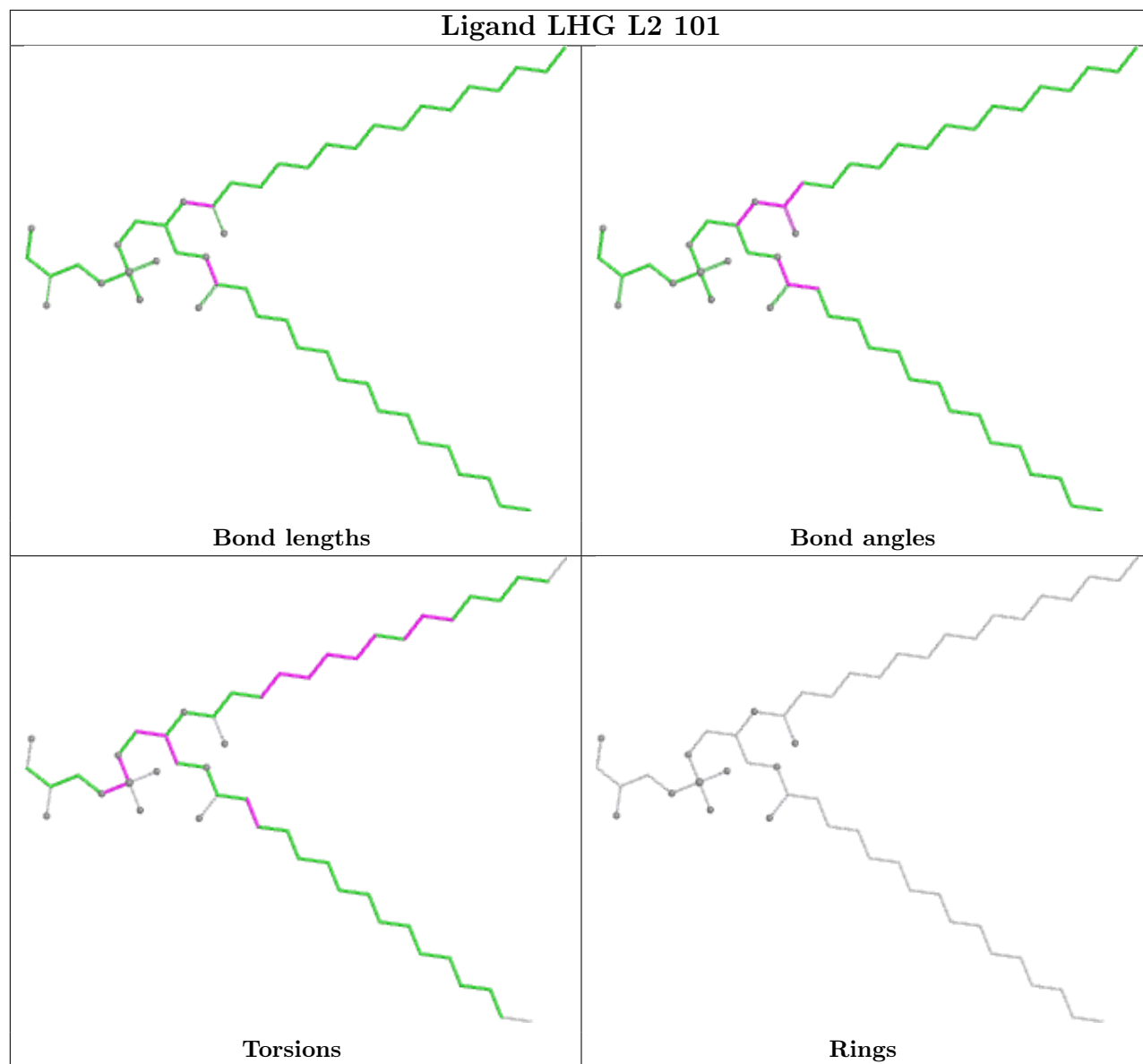
## Ligand BCR B2 602

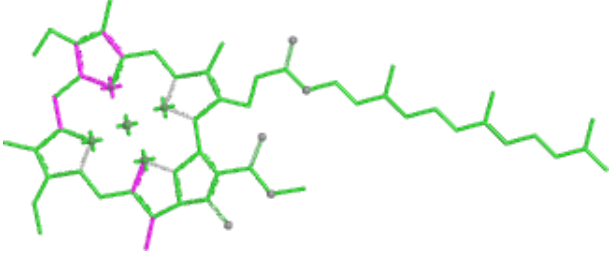
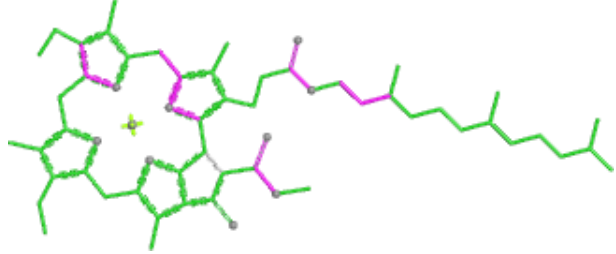
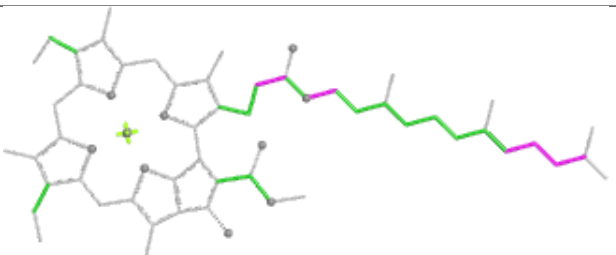
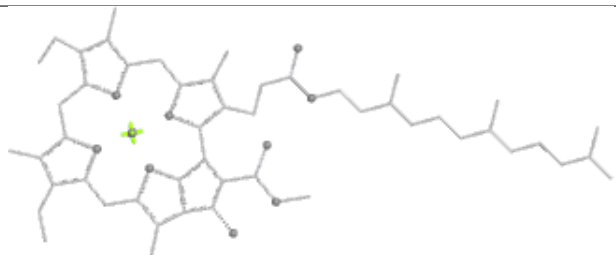
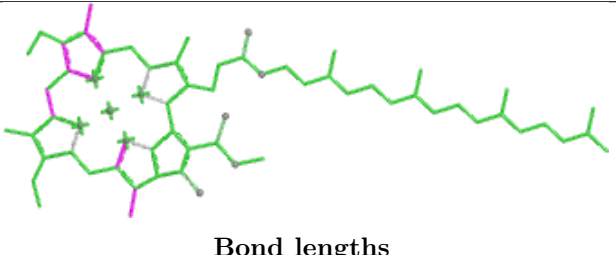
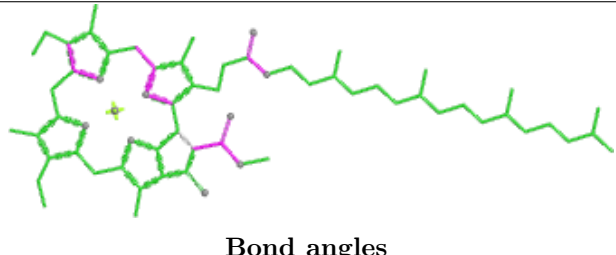
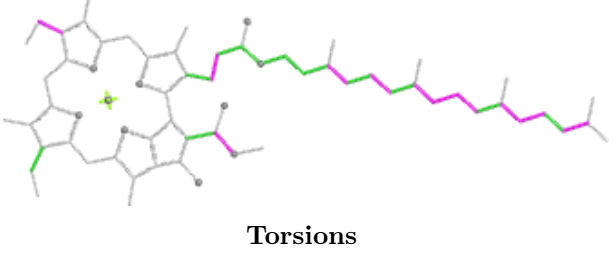
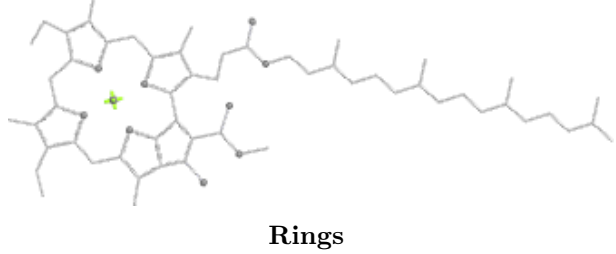


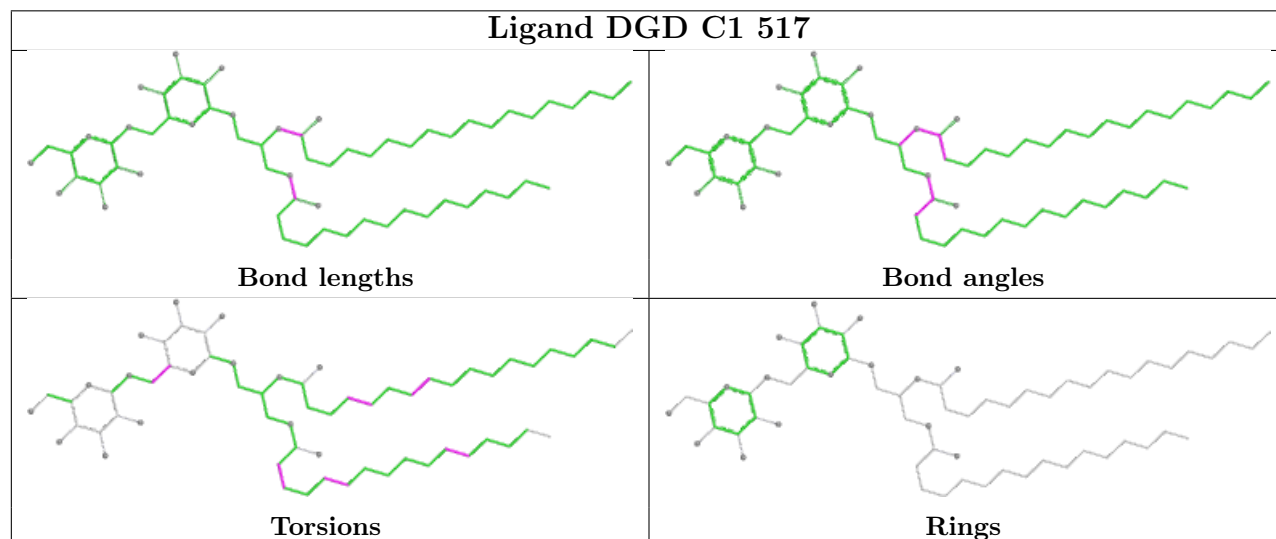
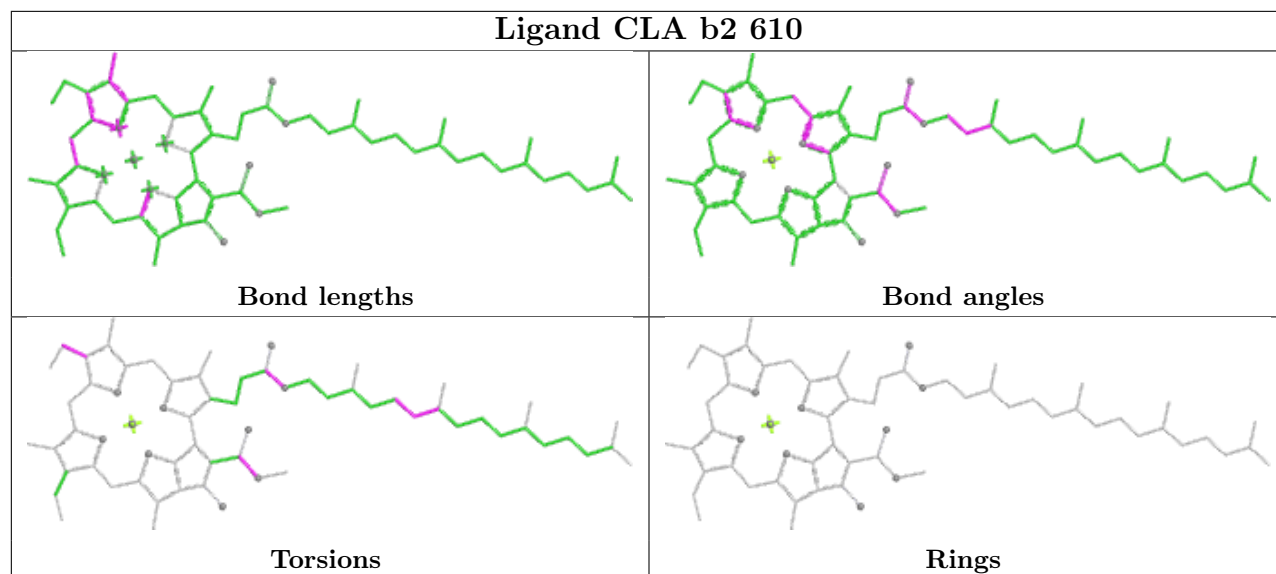




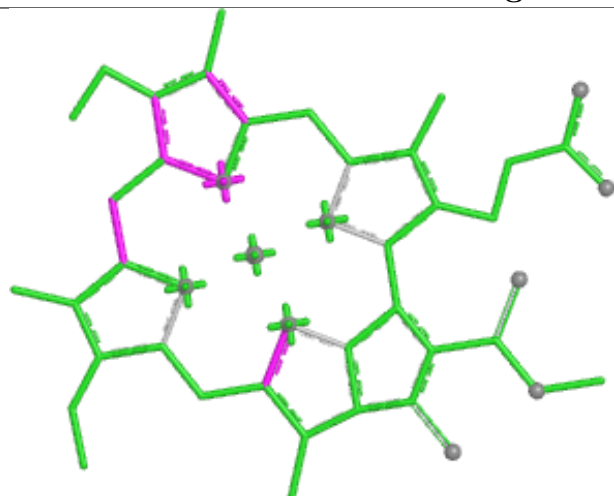




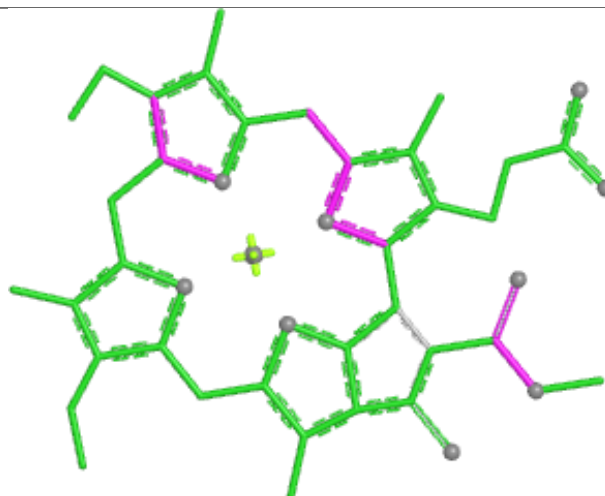
| Ligand CLA b2 615                                                                                      |                                                                                                        |
|--------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand CLA b1 606                                                                                      |                                                                                                        |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |



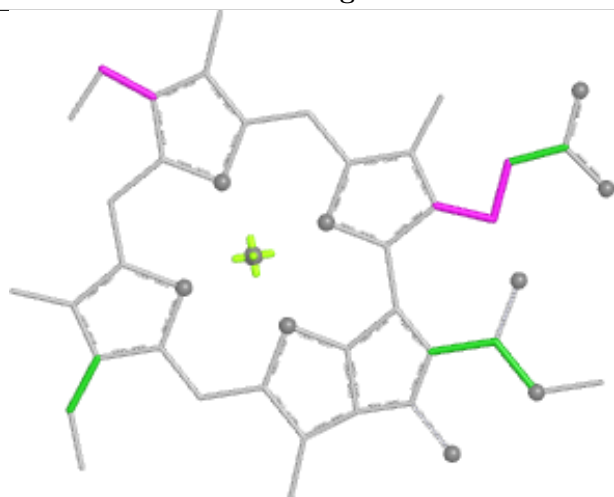
## Ligand CLA C2 510



Bond lengths



Bond angles

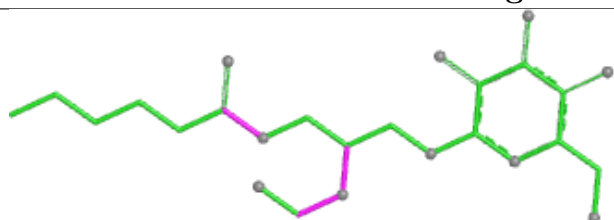


Torsions

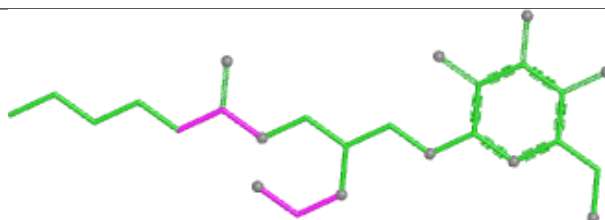


Rings

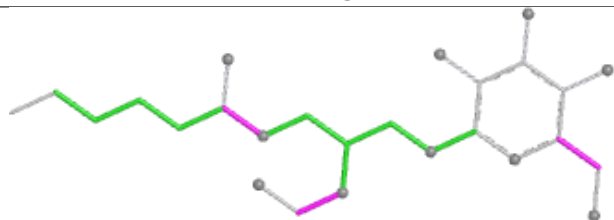
## Ligand LMG c2 519



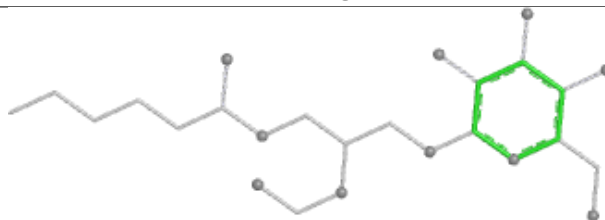
Bond lengths



Bond angles

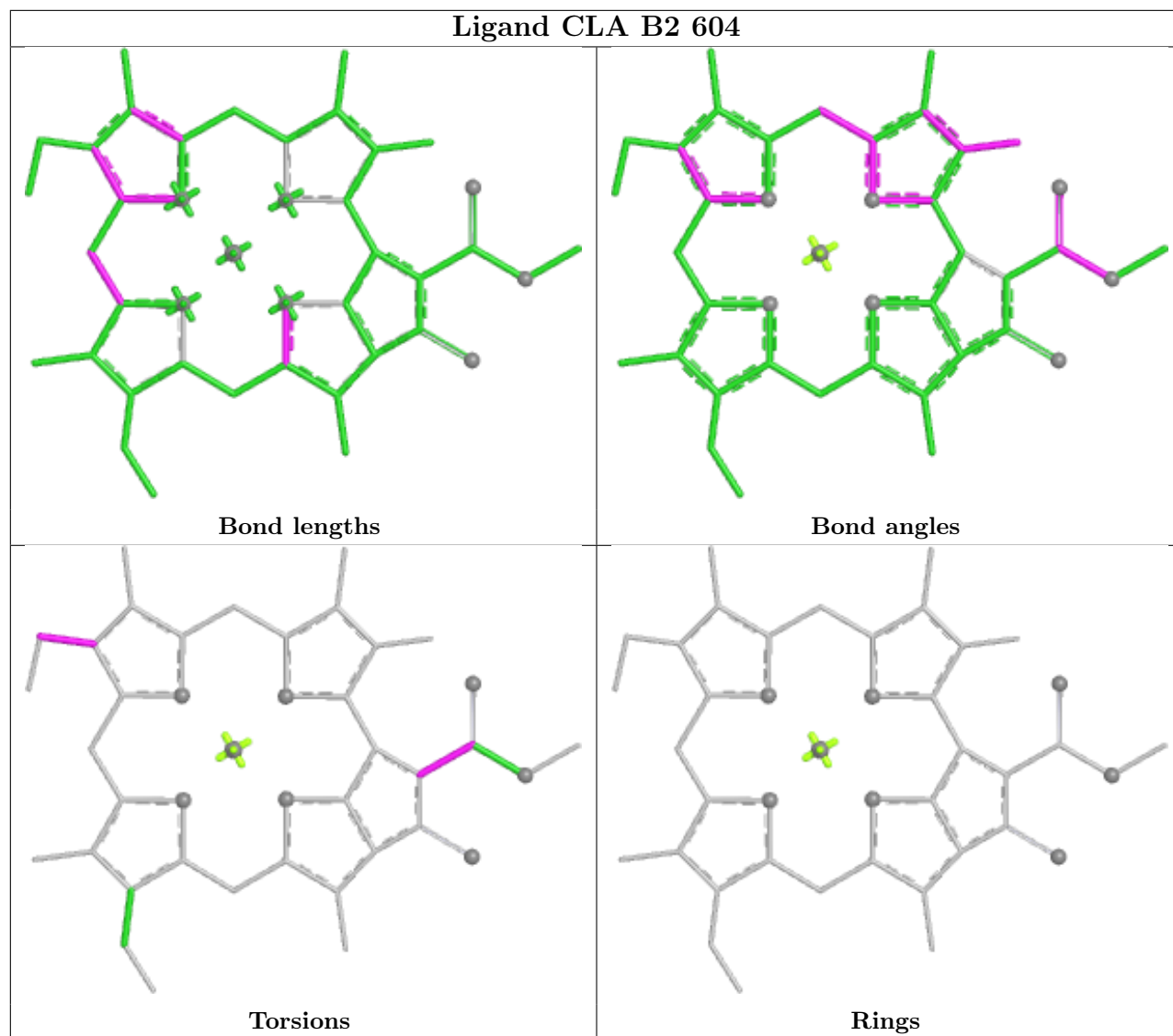


Torsions

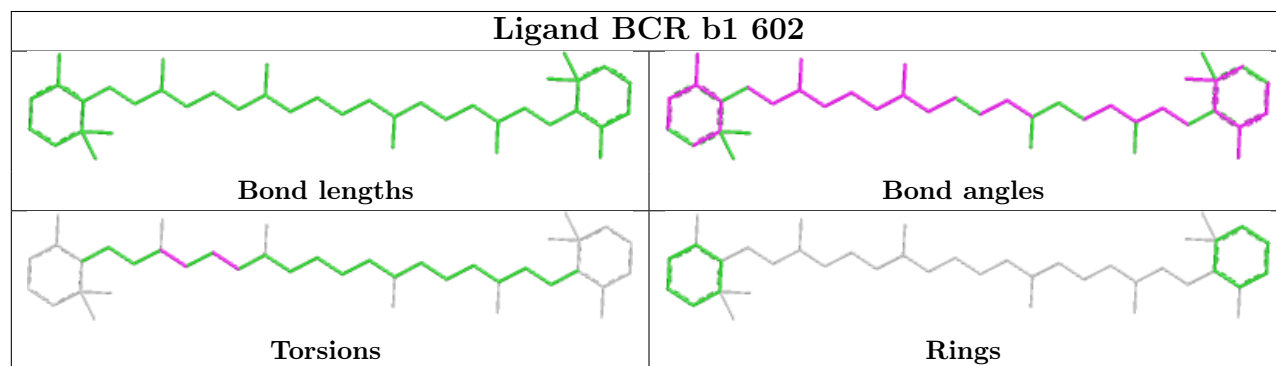


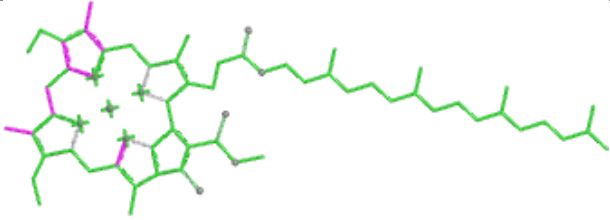
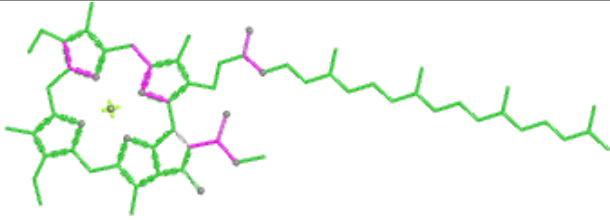
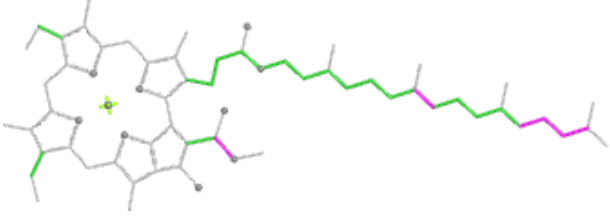
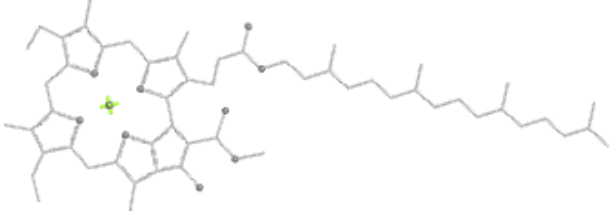
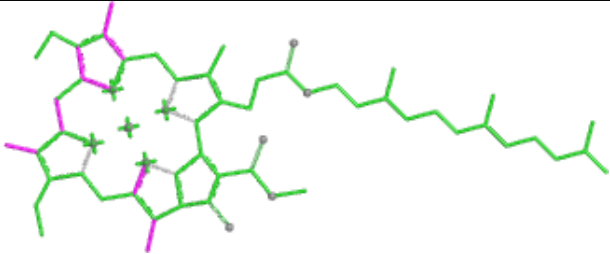
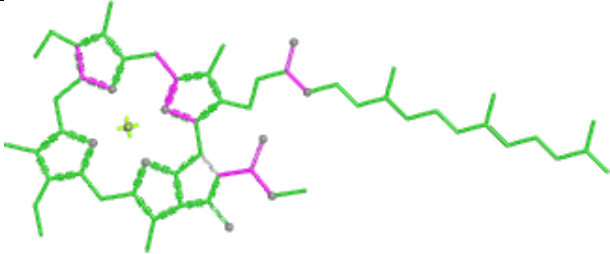
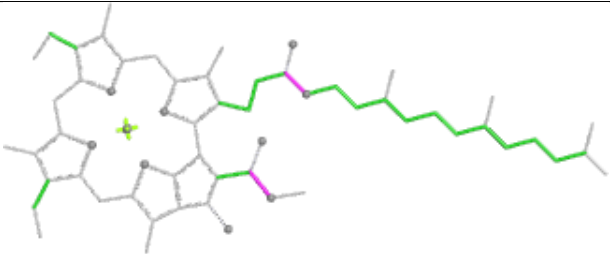
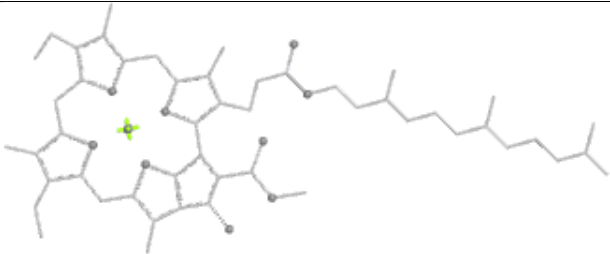
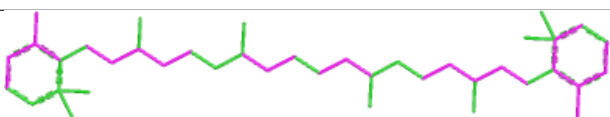
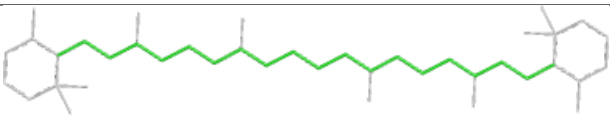
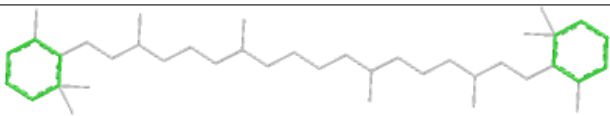
Rings

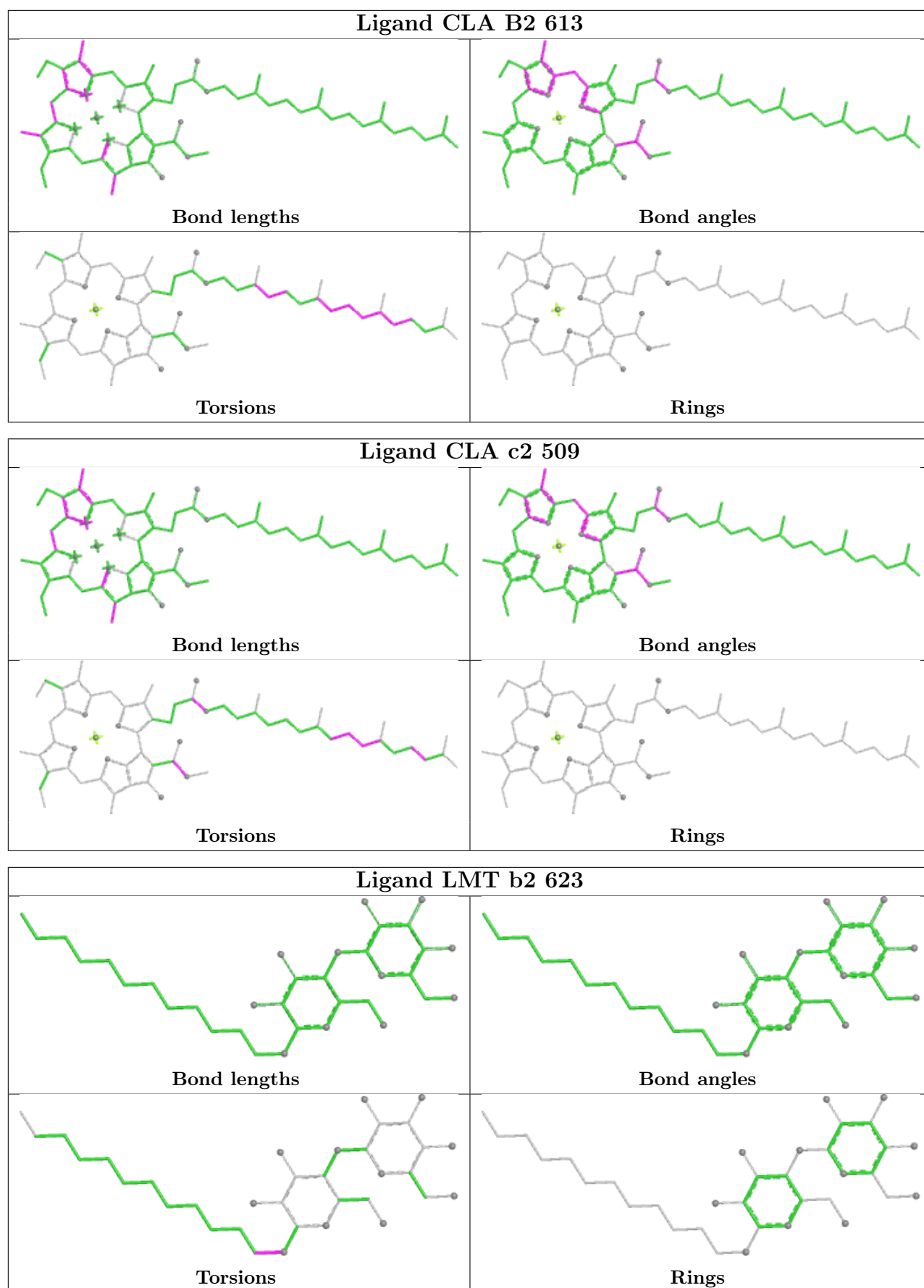
## Ligand CLA B2 604

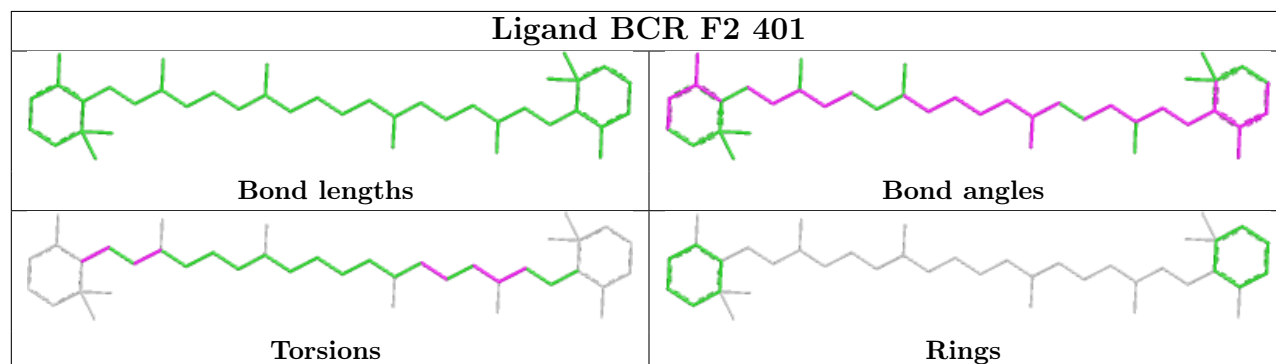
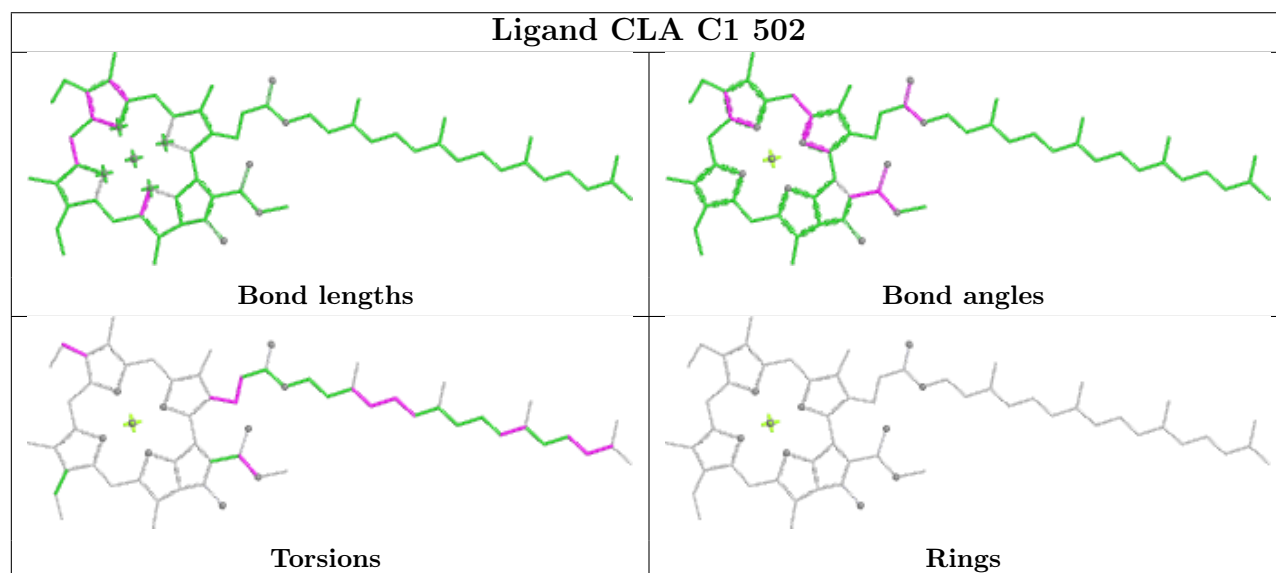
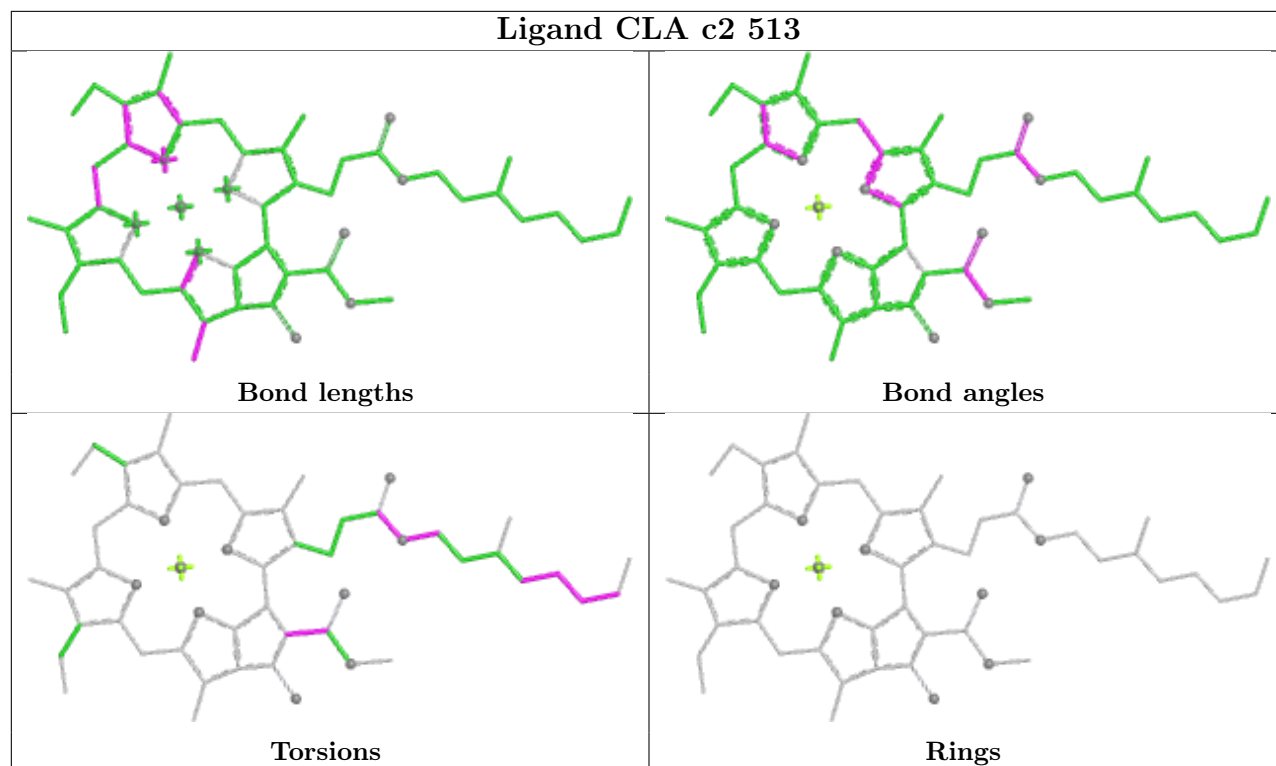


## Ligand BCR b1 602

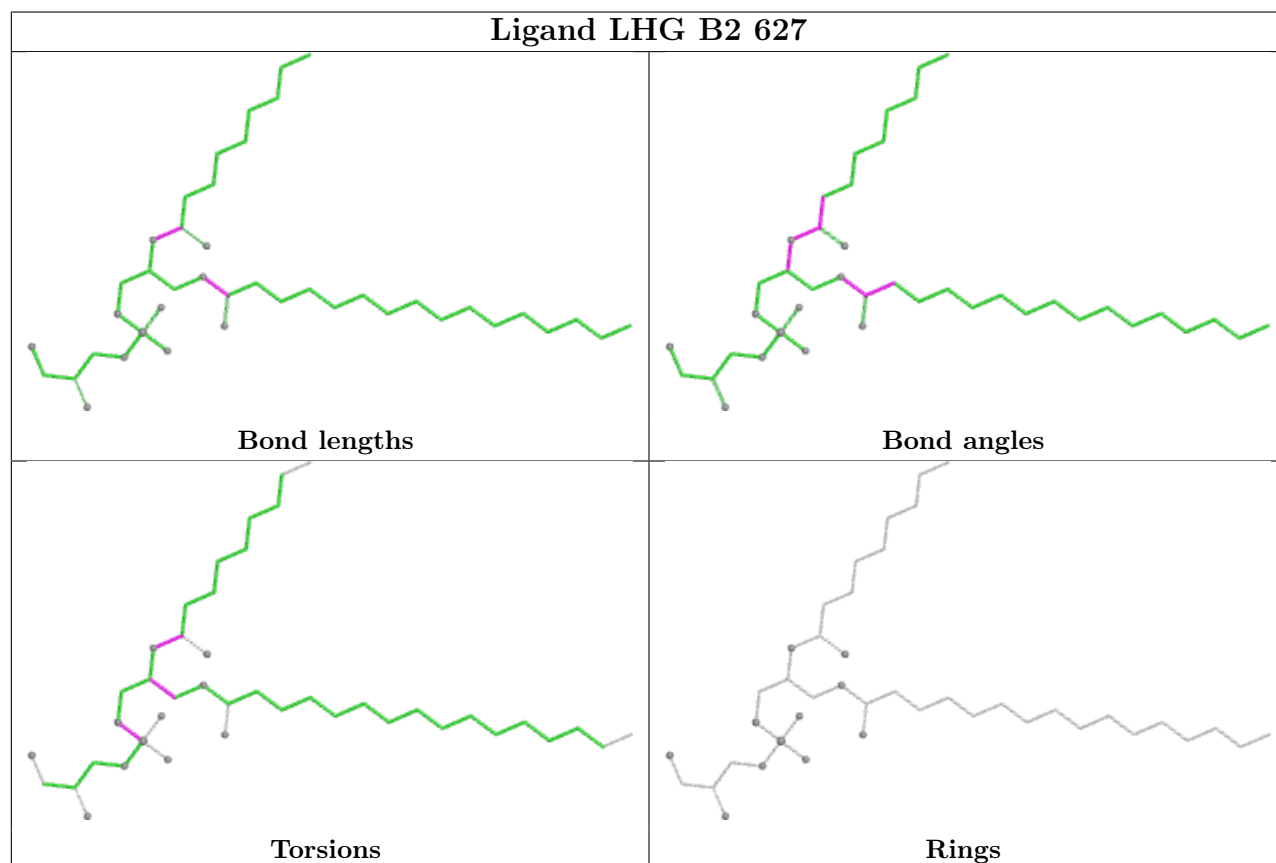
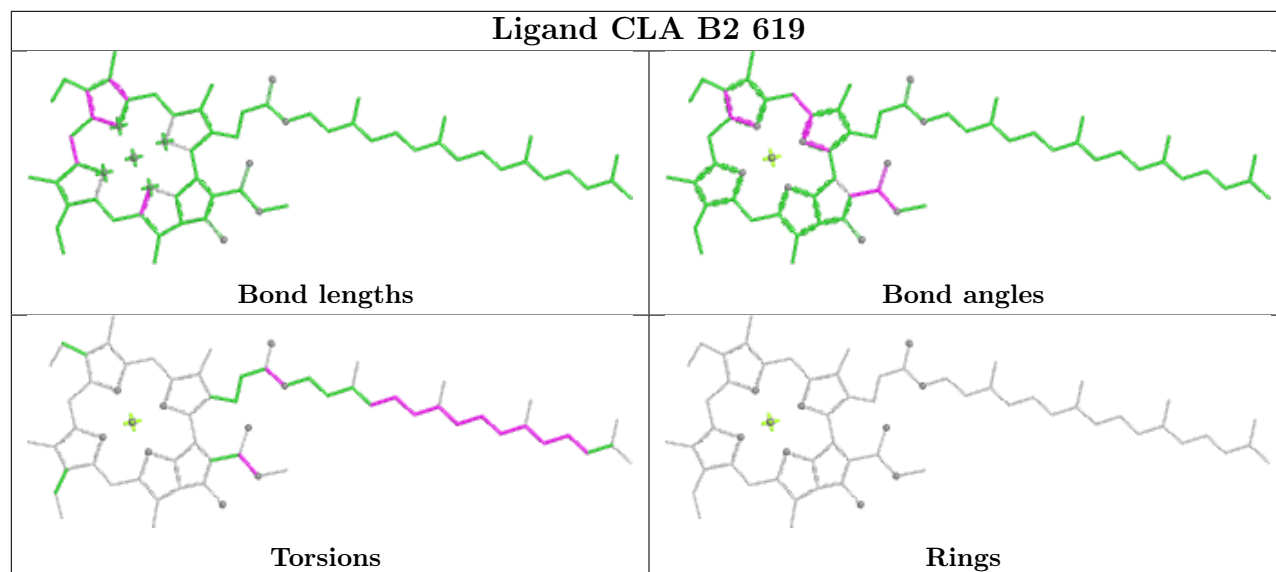


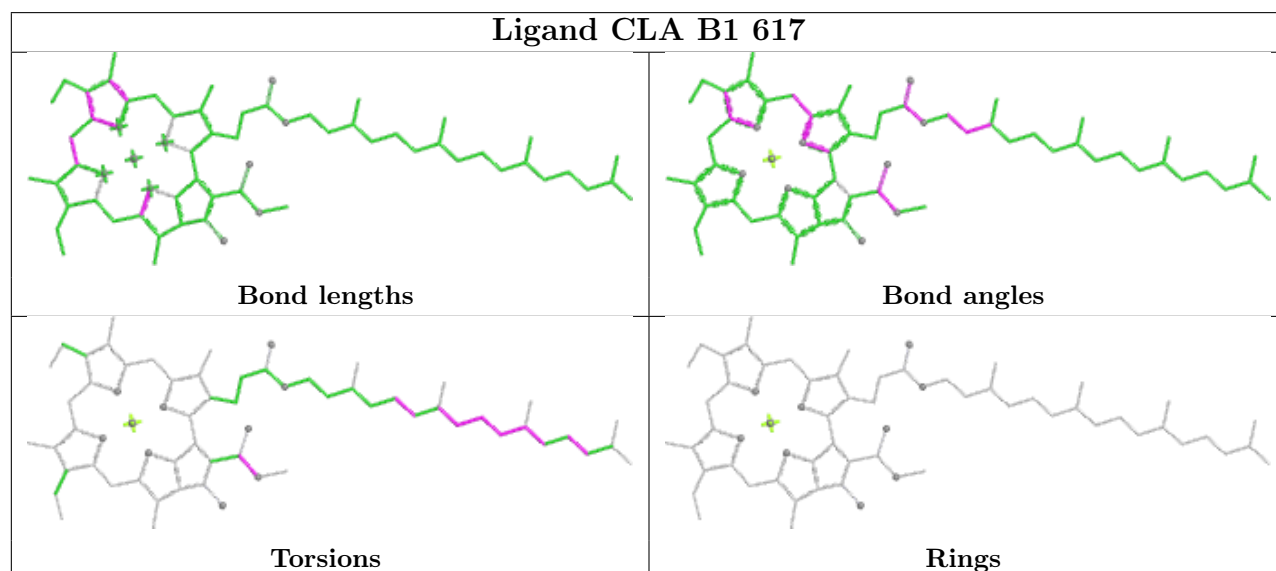
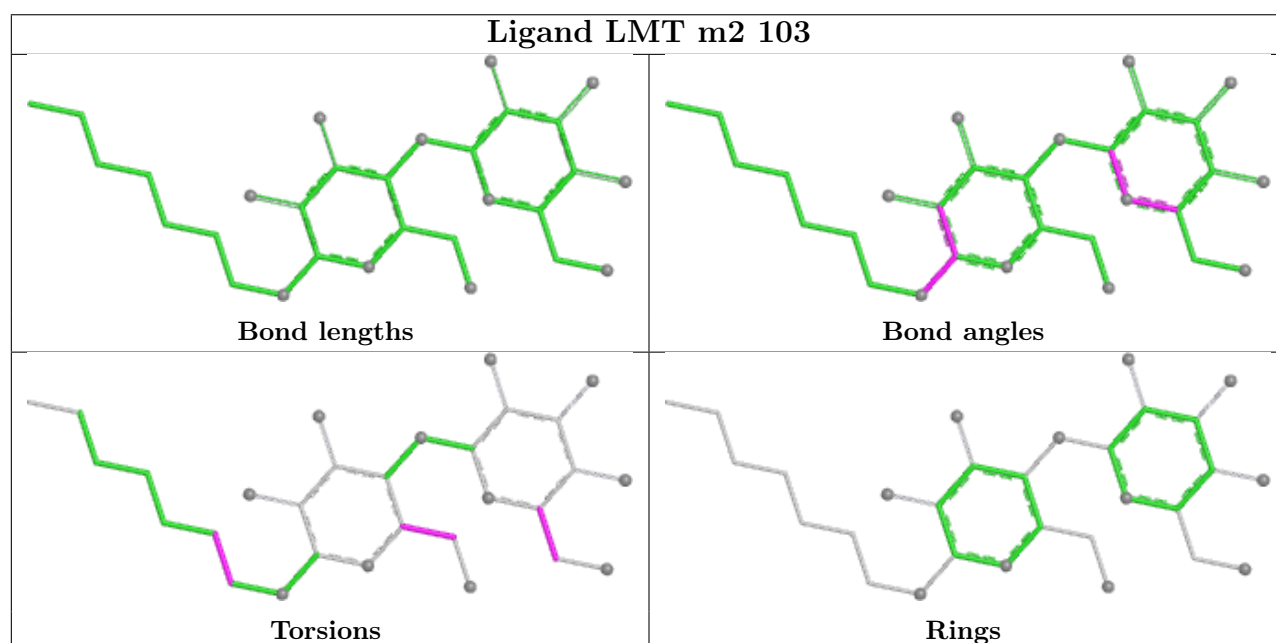
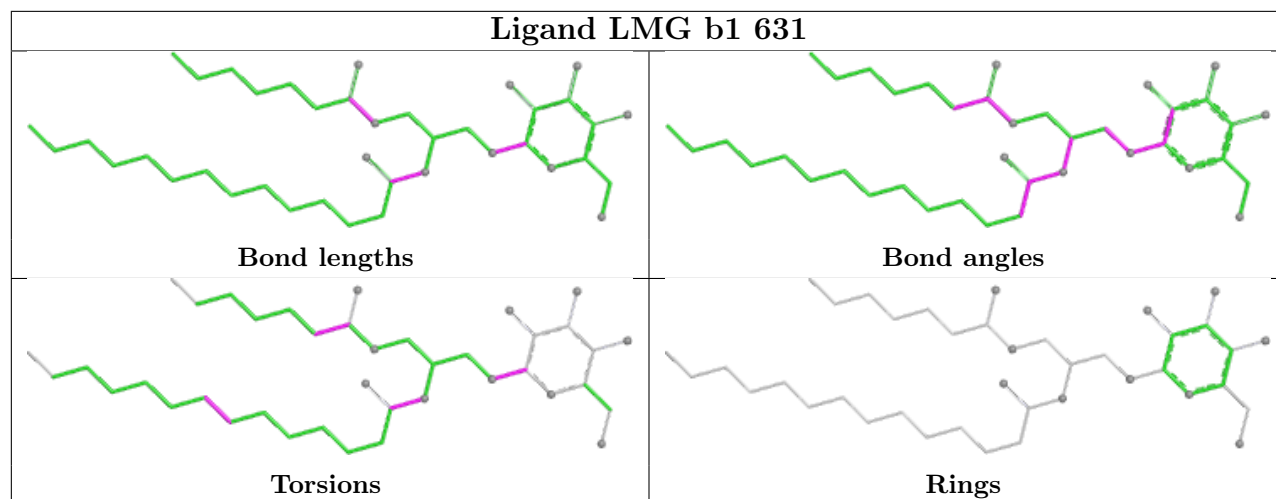
| Ligand CLA c1 510                                                                                       |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand CLA B2 618                                                                                       |                                                                                                         |
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCR B1 603                                                                                       |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

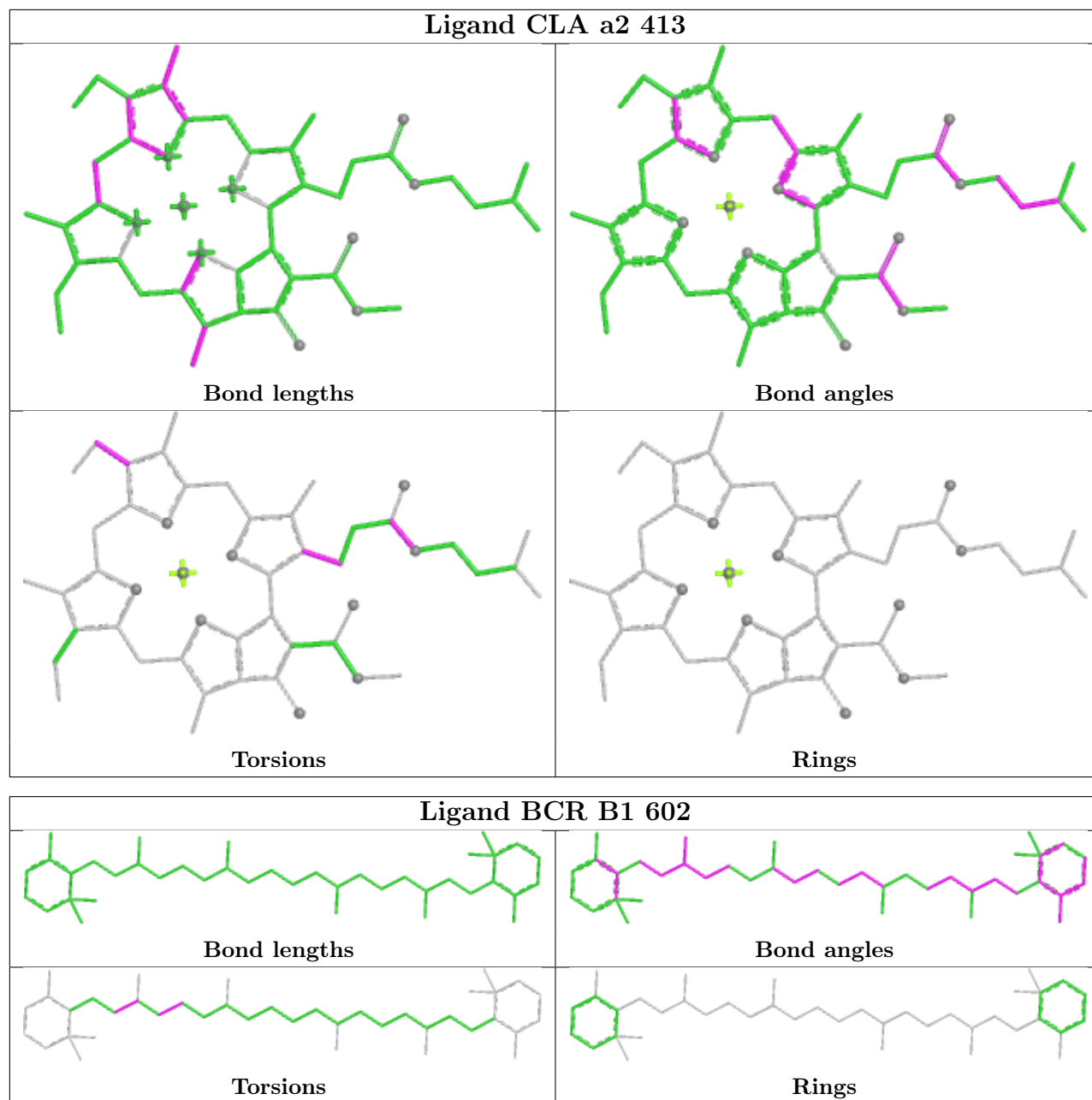


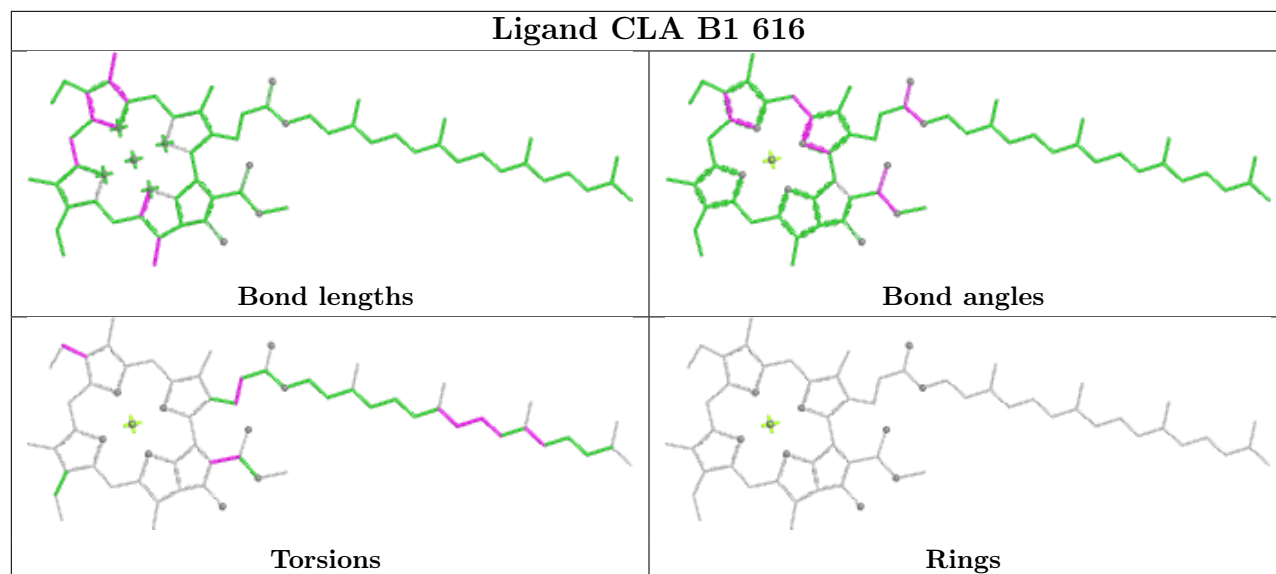
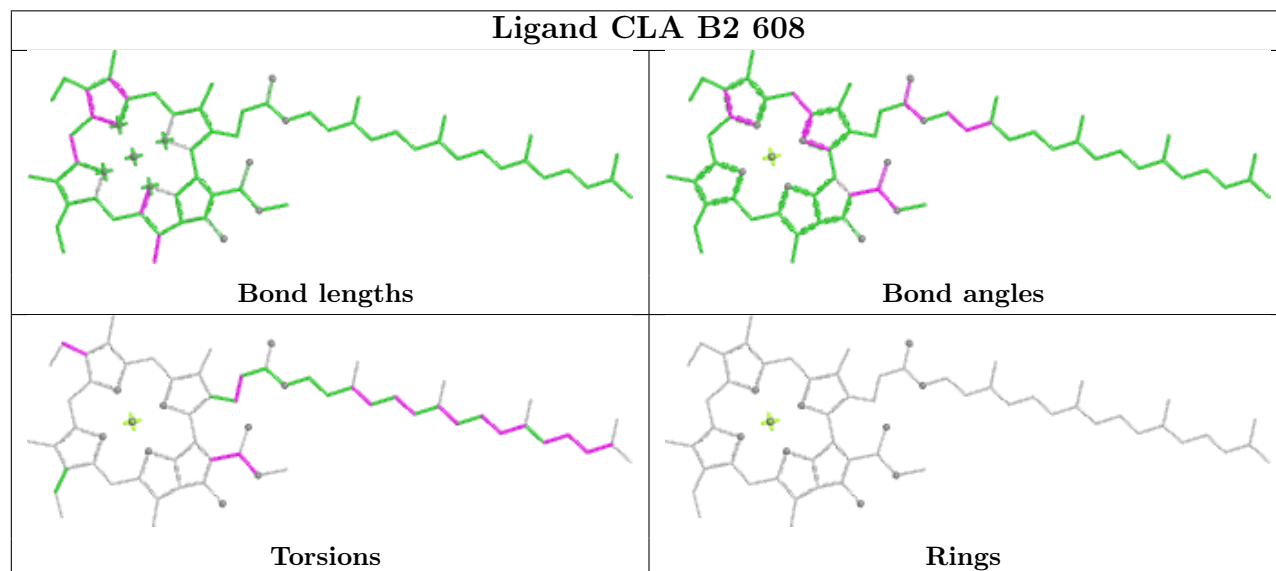


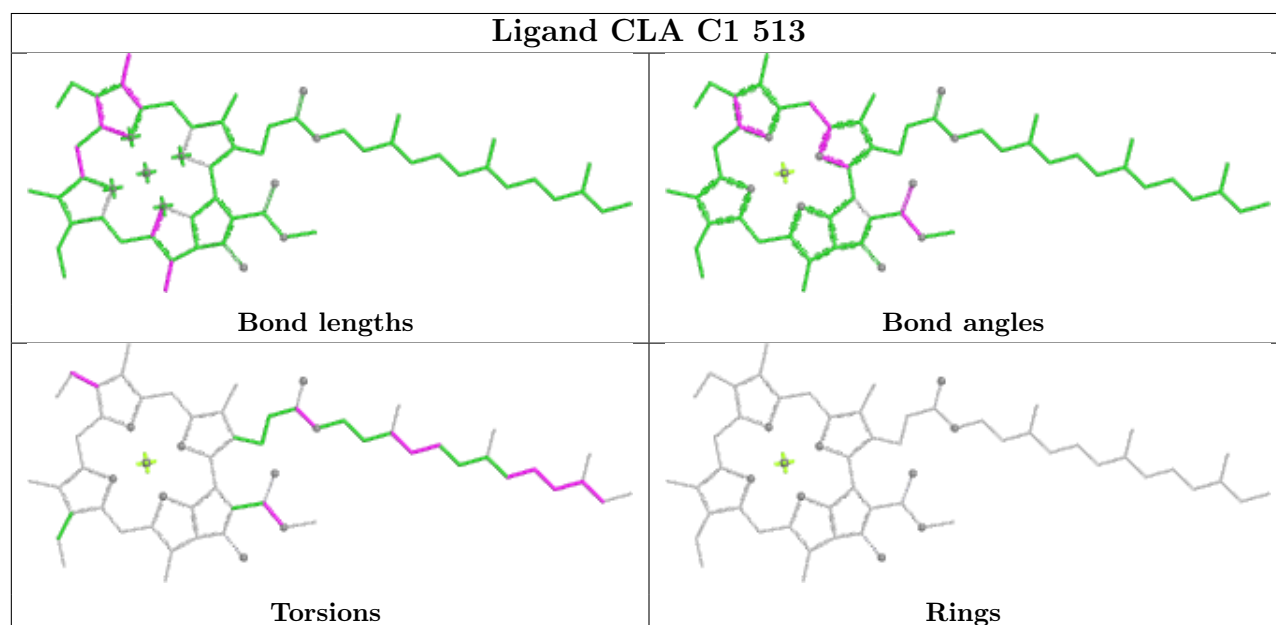
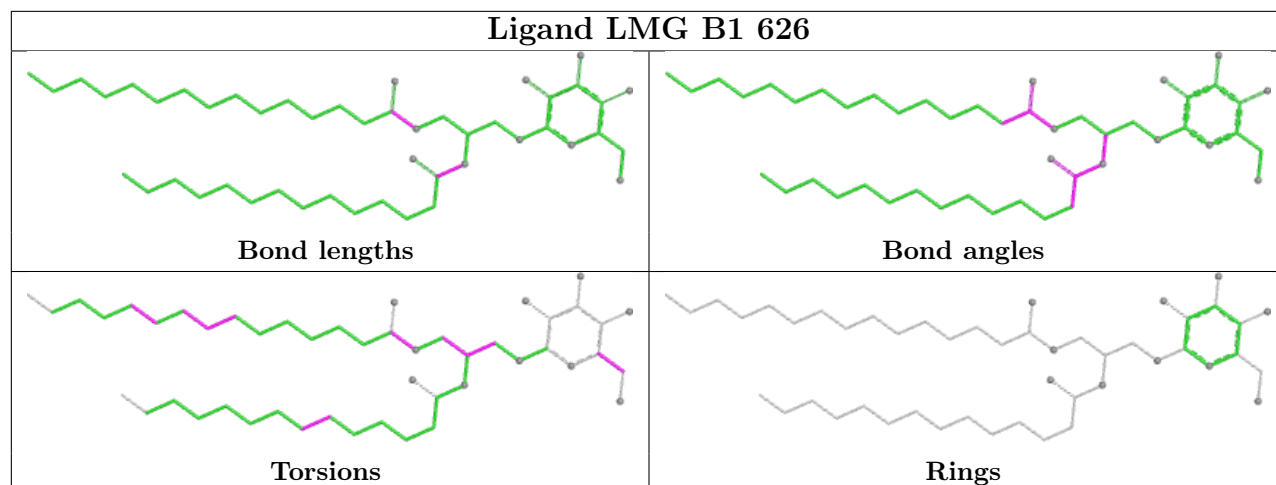
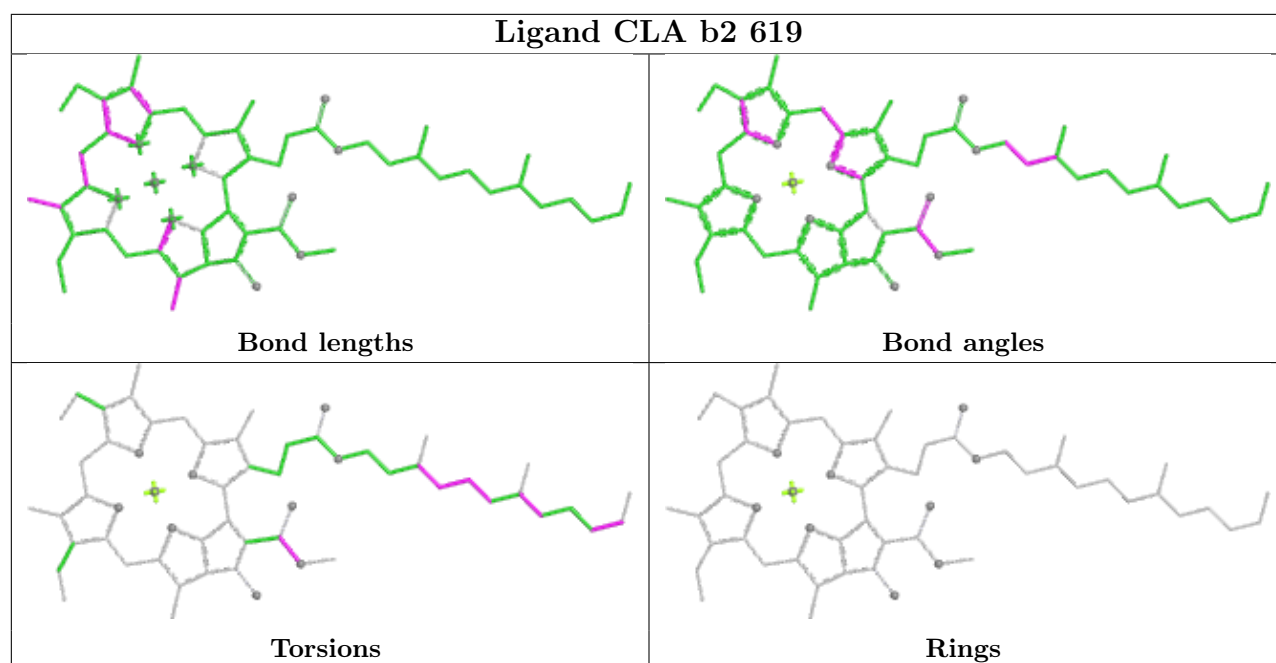


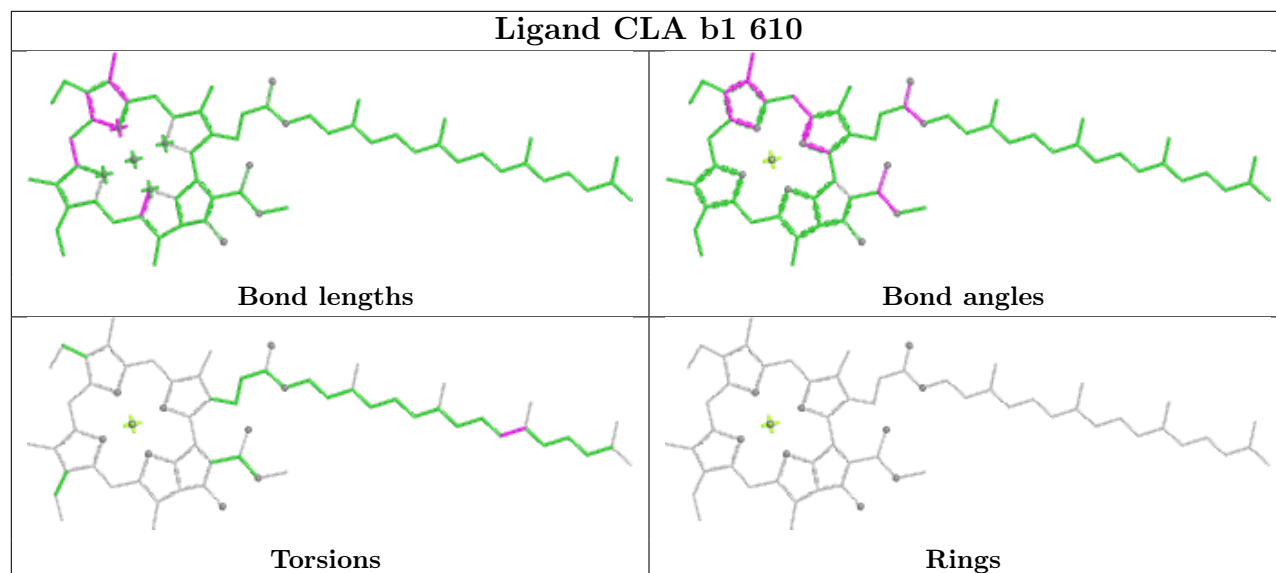
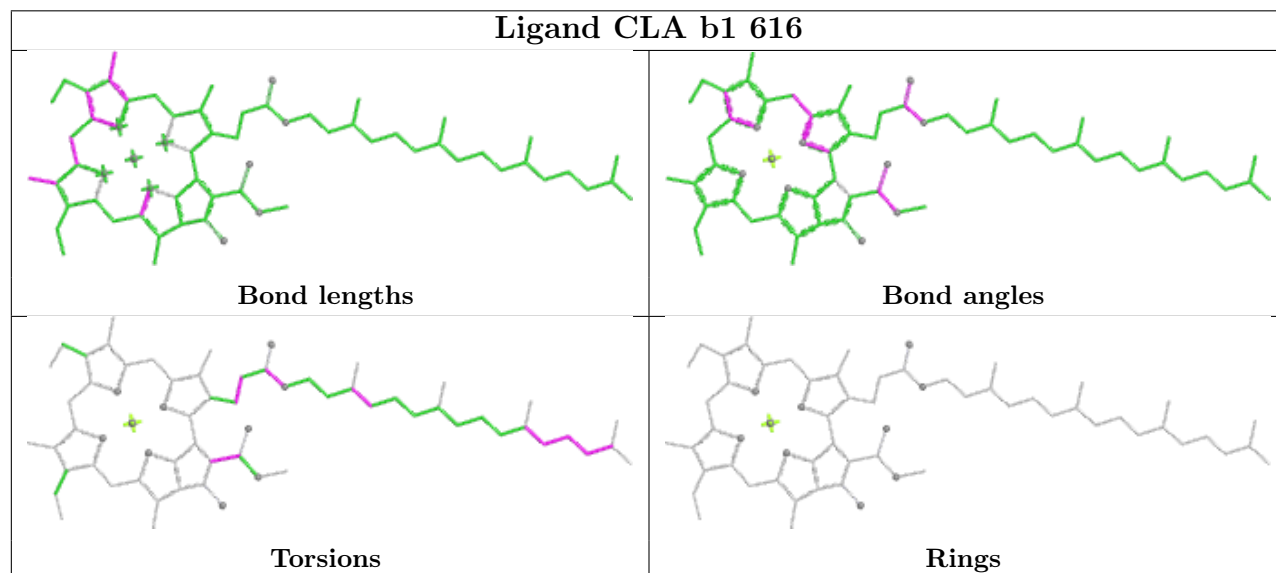
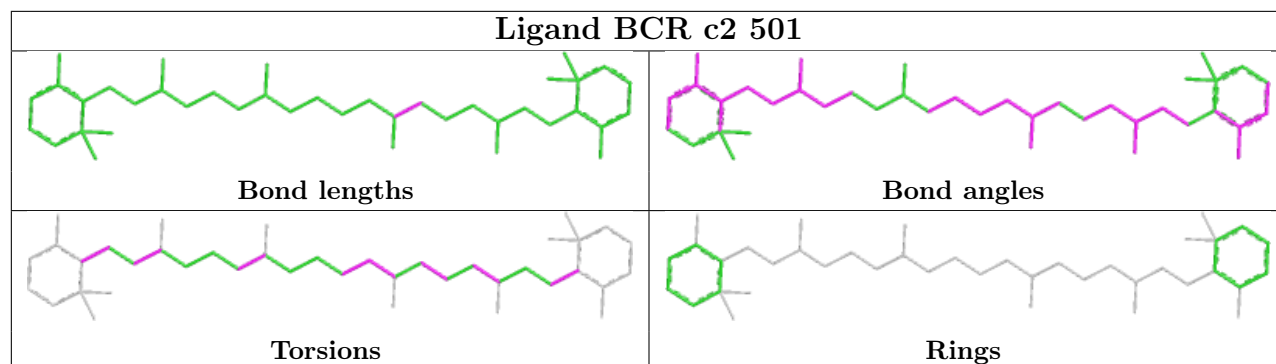


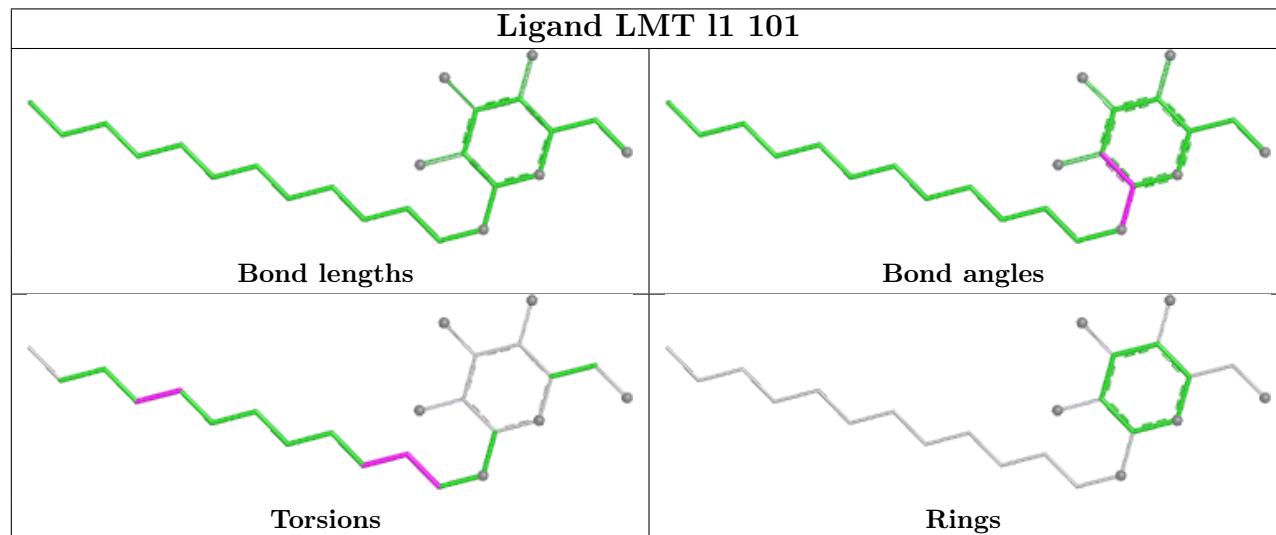
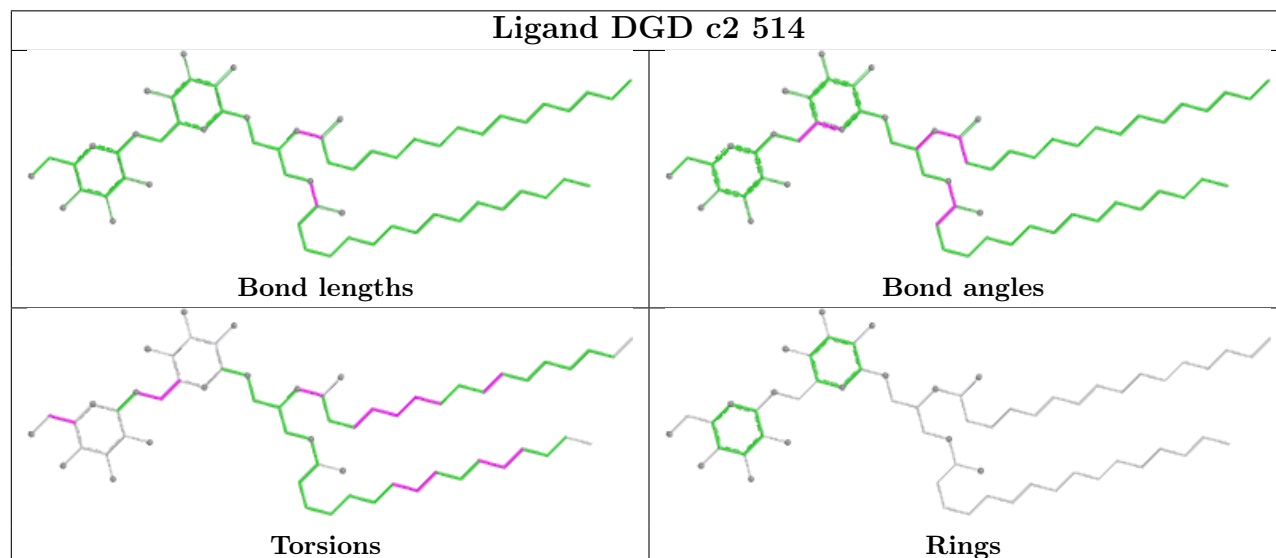
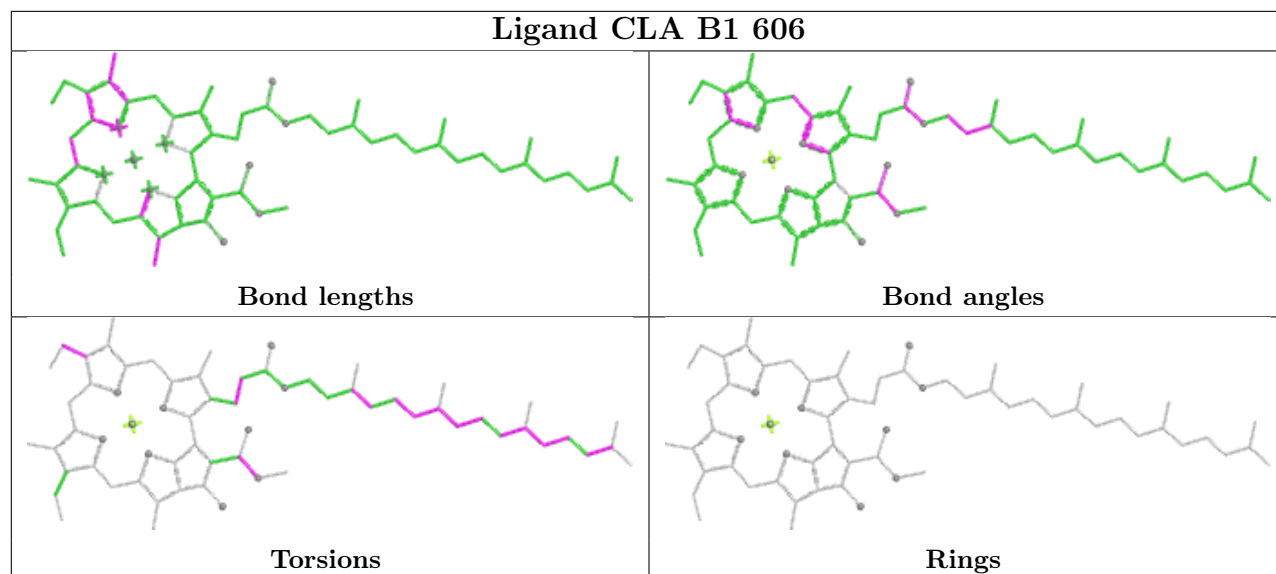


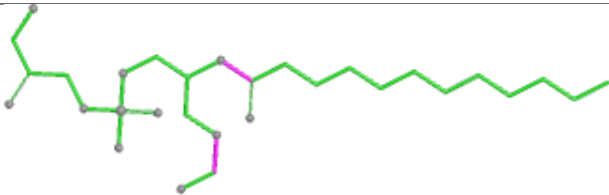
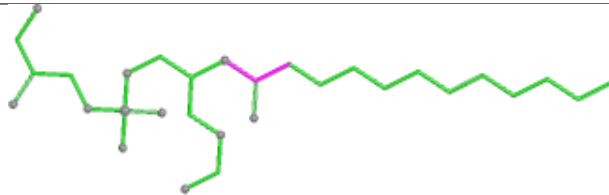
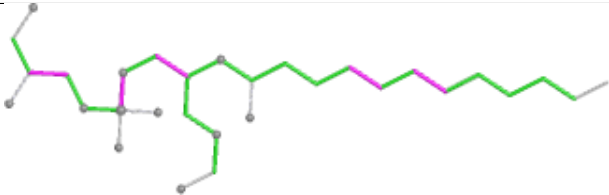
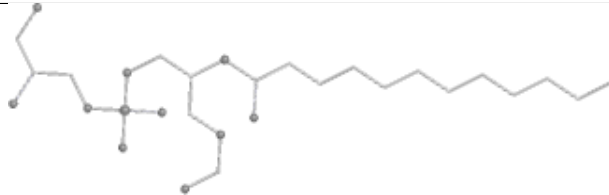


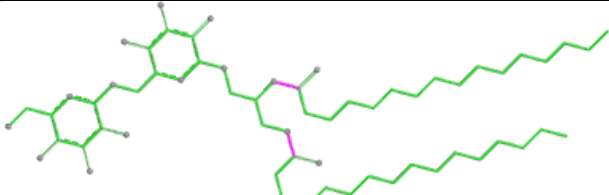
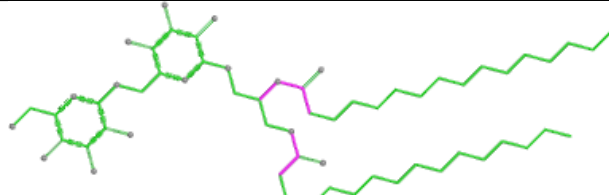
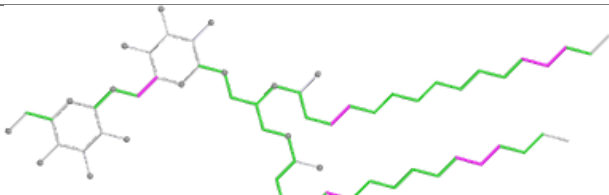
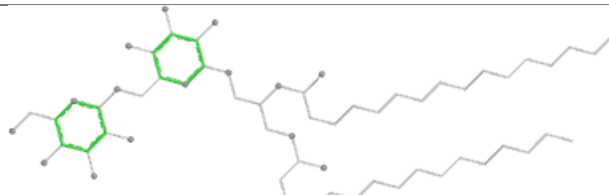
**Ligand CLA B1 616****Ligand CLA B2 608**

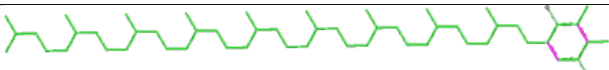
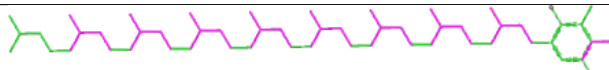
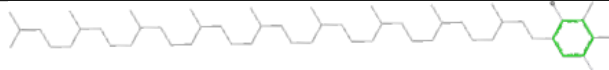






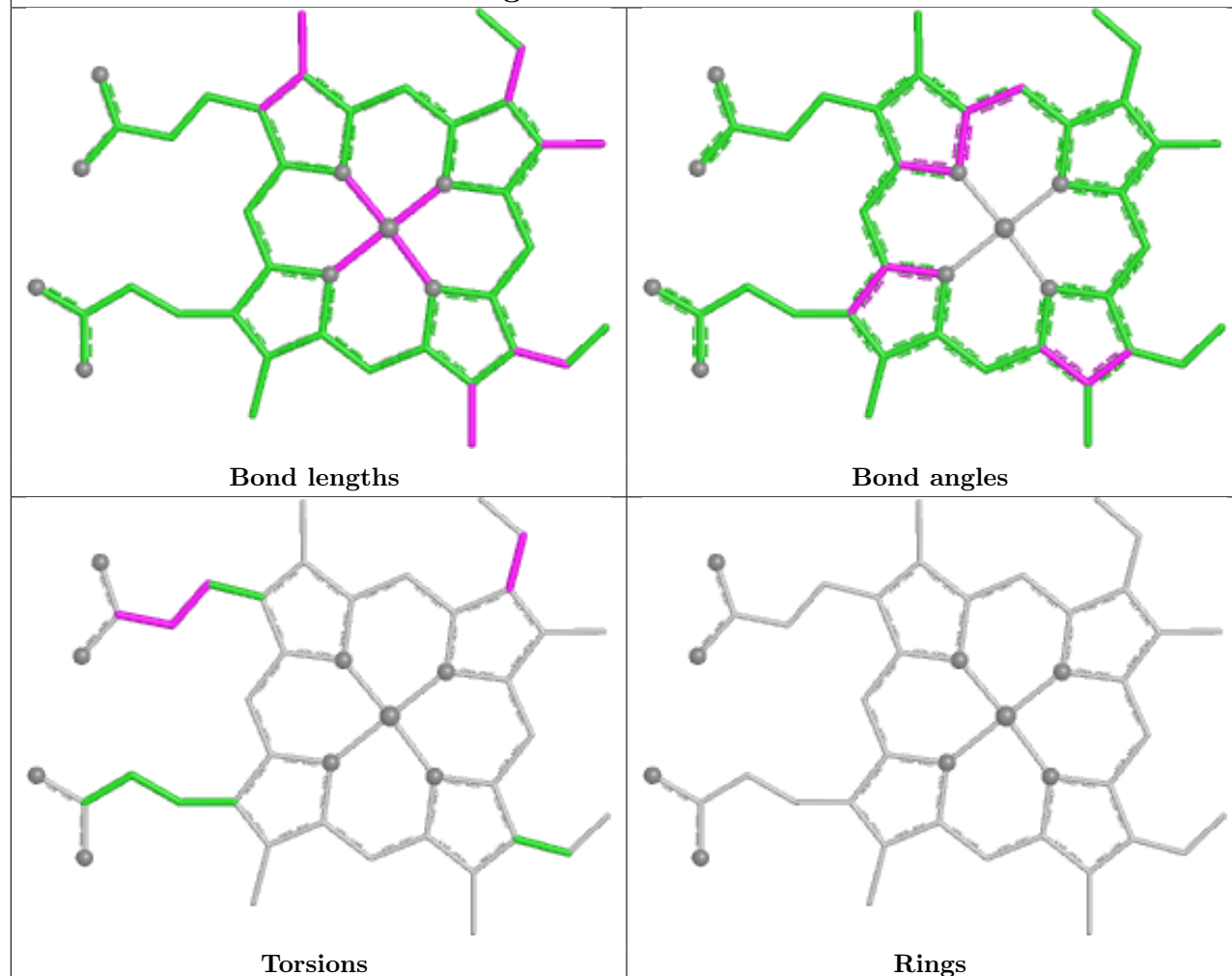
| Ligand LHG a2 407                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand DGD c2 517                                                                  |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

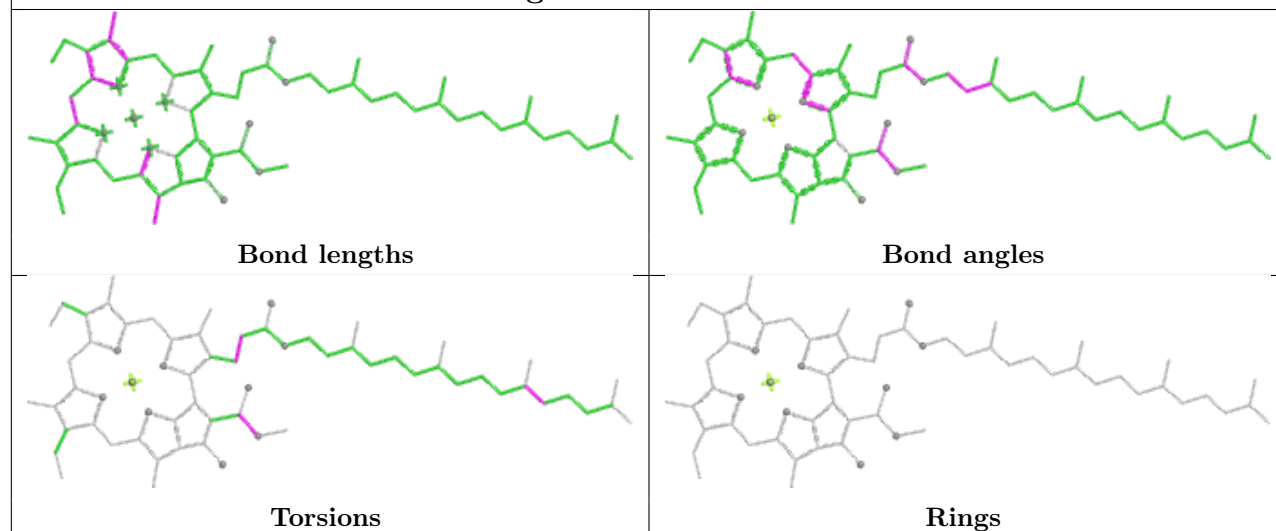
| Ligand PL9 D2 408                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



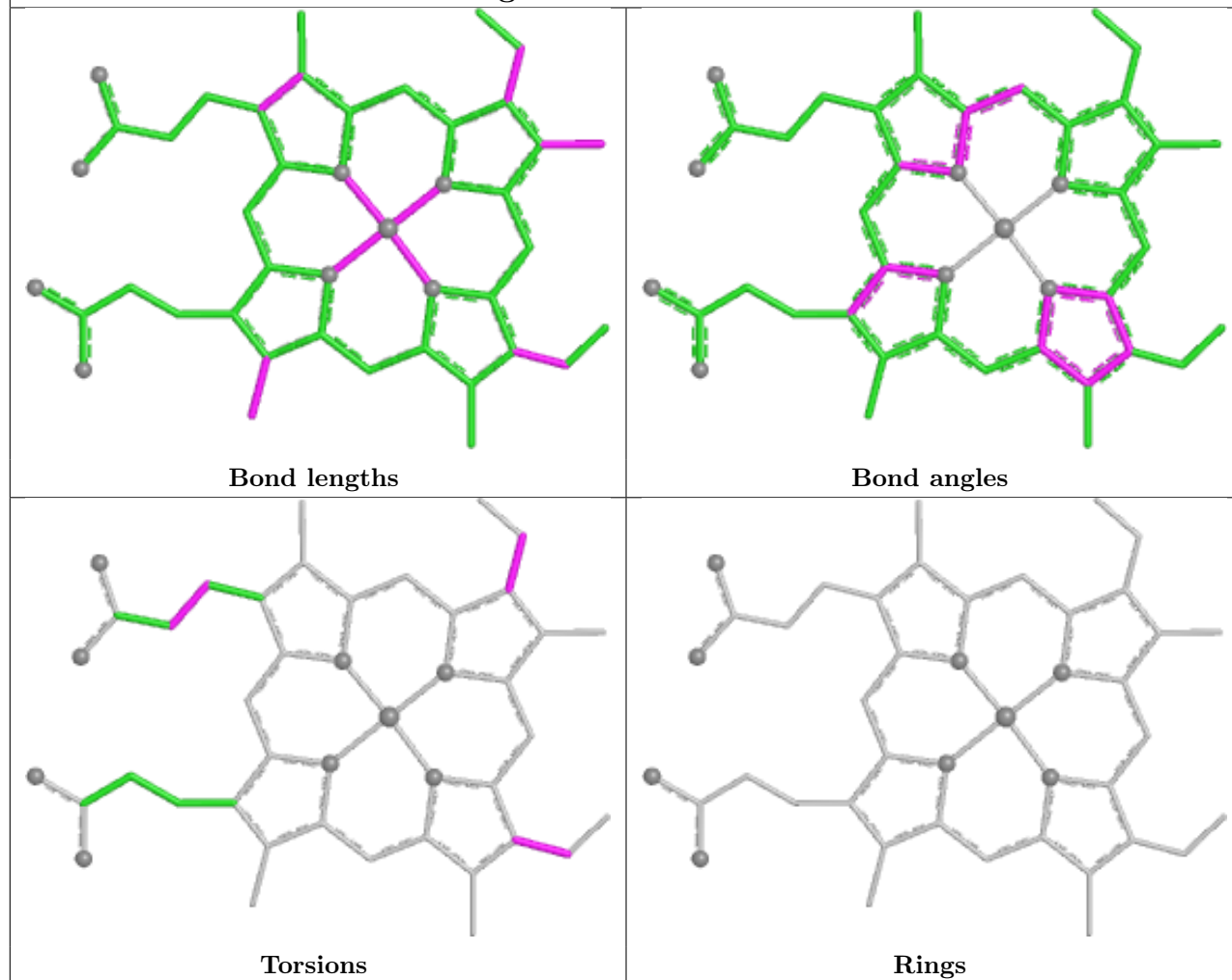
## Ligand HEM v1 201



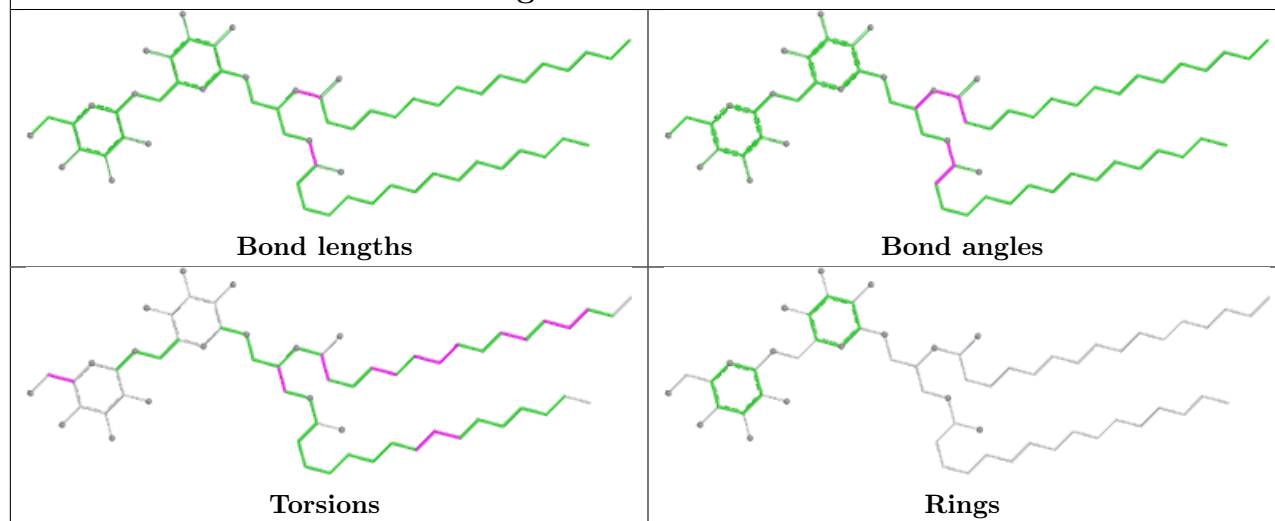
## Ligand CLA b2 613

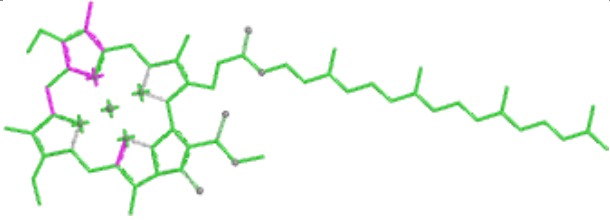
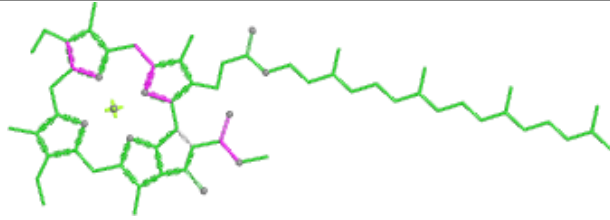
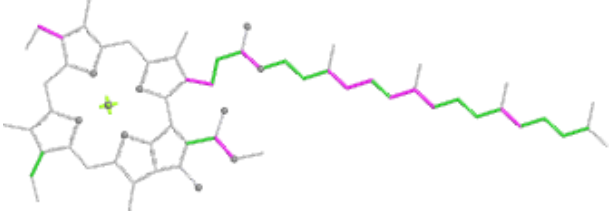
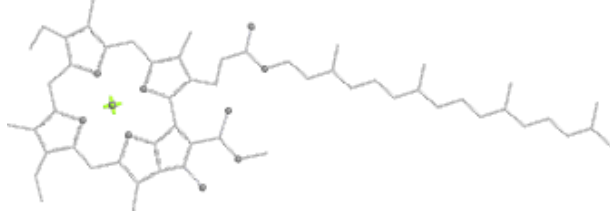
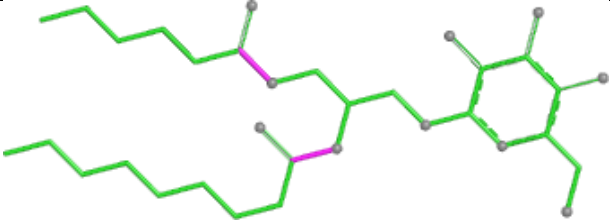
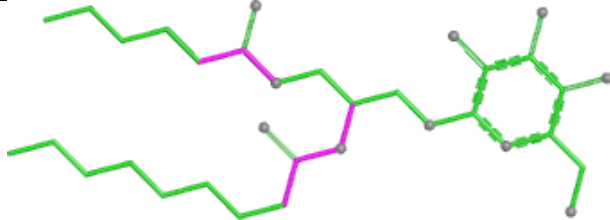
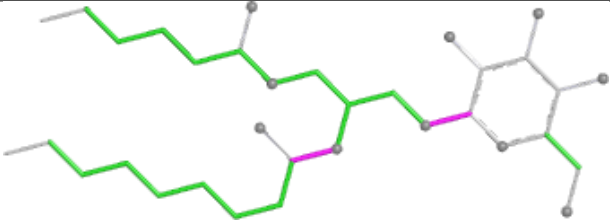
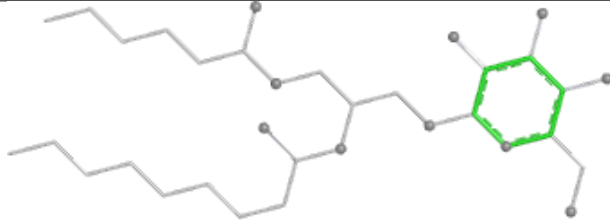
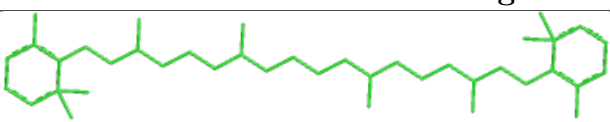
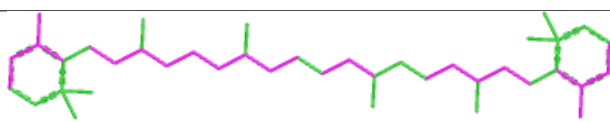
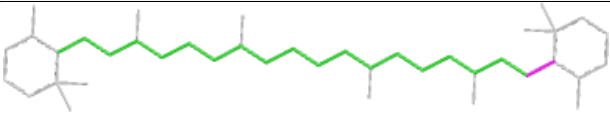
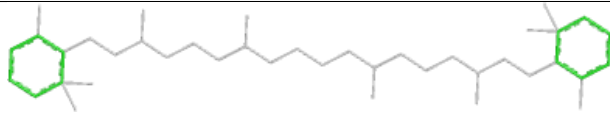


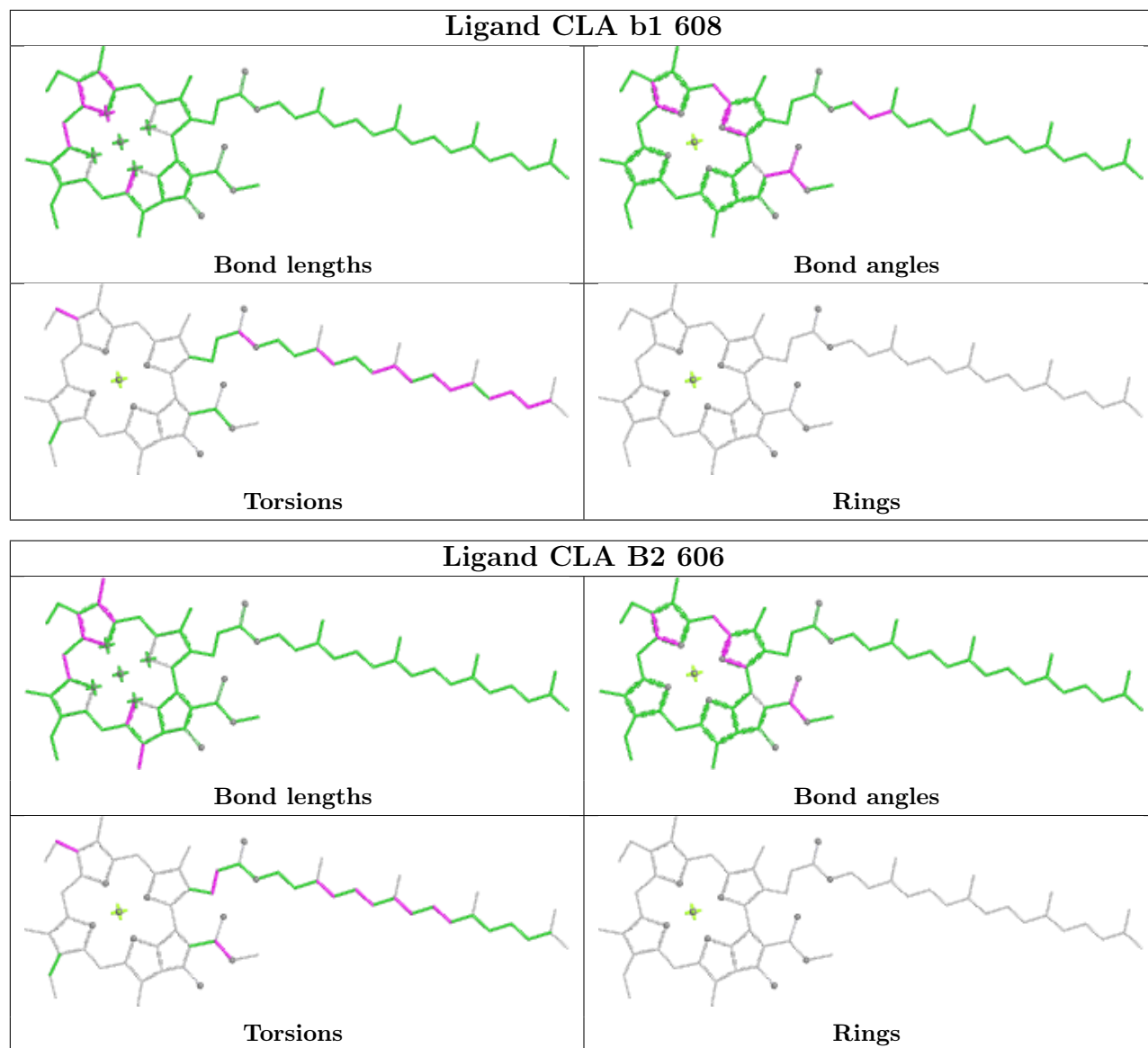
## Ligand HEM V2 201

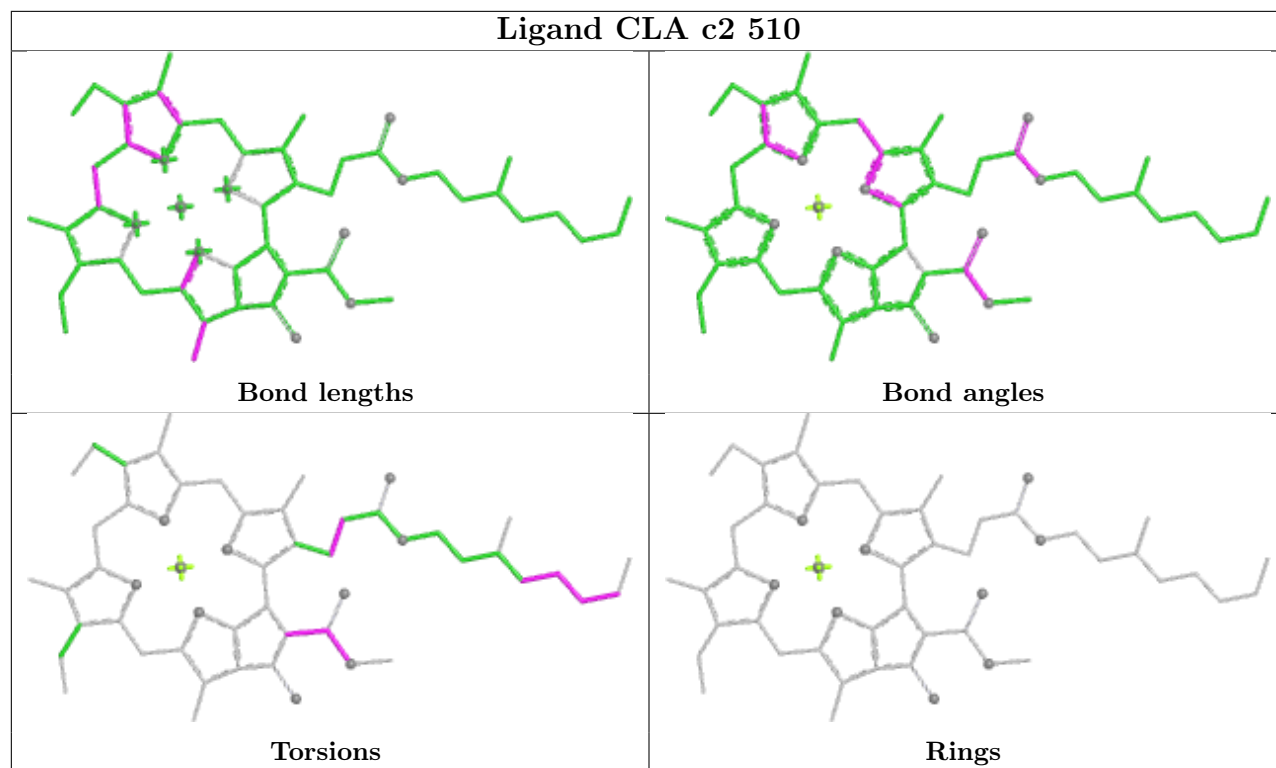


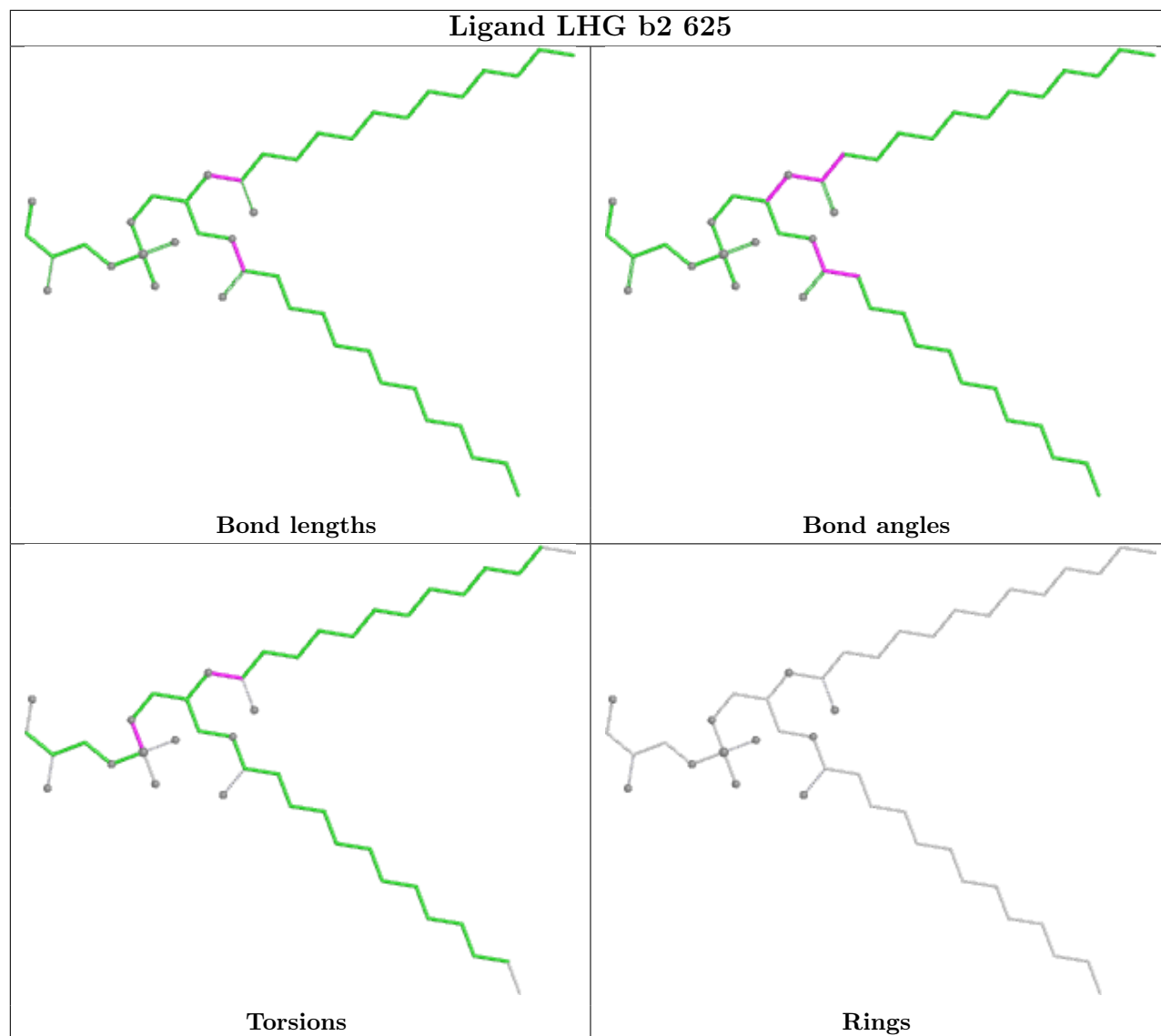
## Ligand DGD H1 101



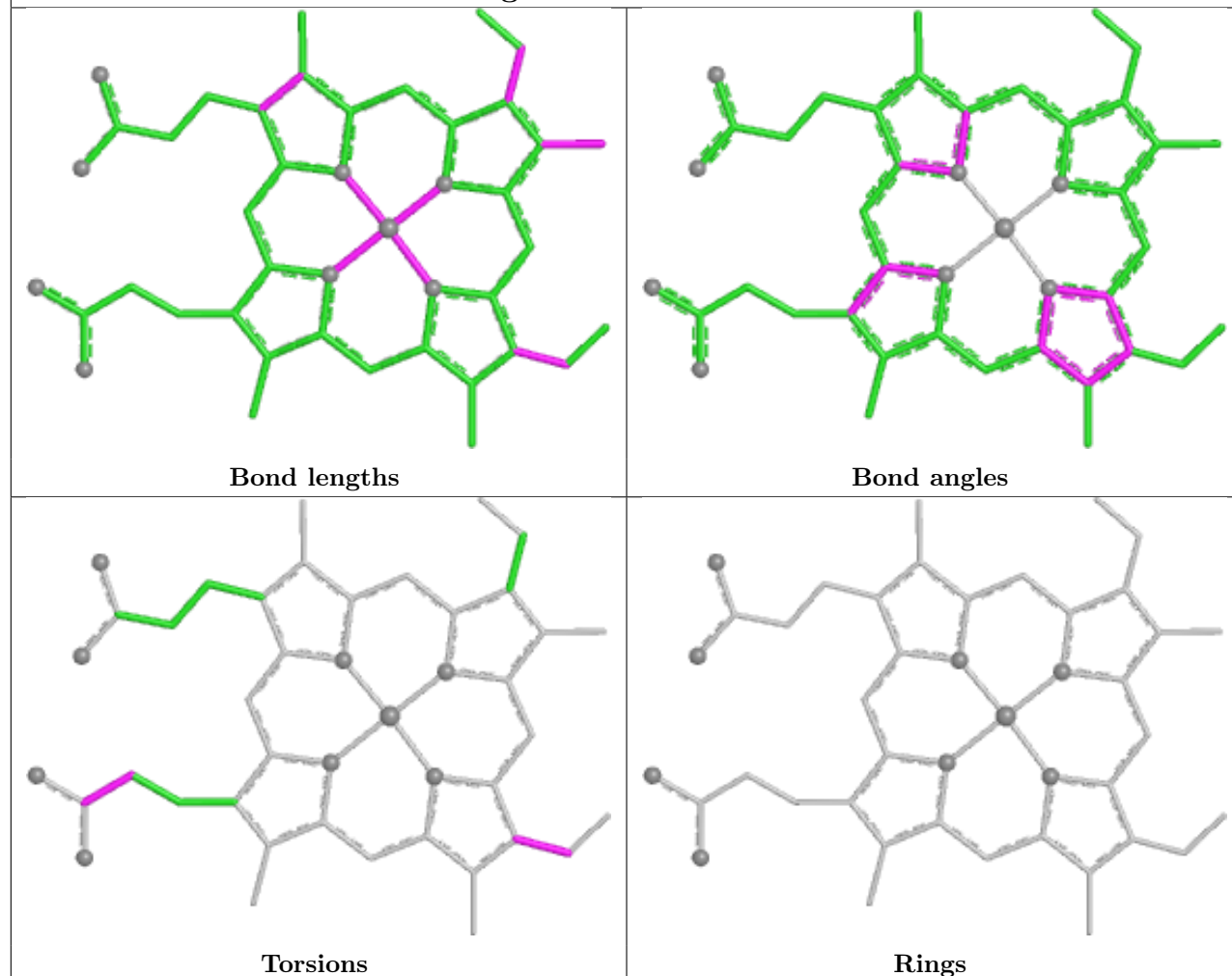
| Ligand CLA c2 503                                                                                       |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMG I2 101                                                                                       |                                                                                                         |
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCR B2 603                                                                                       |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |



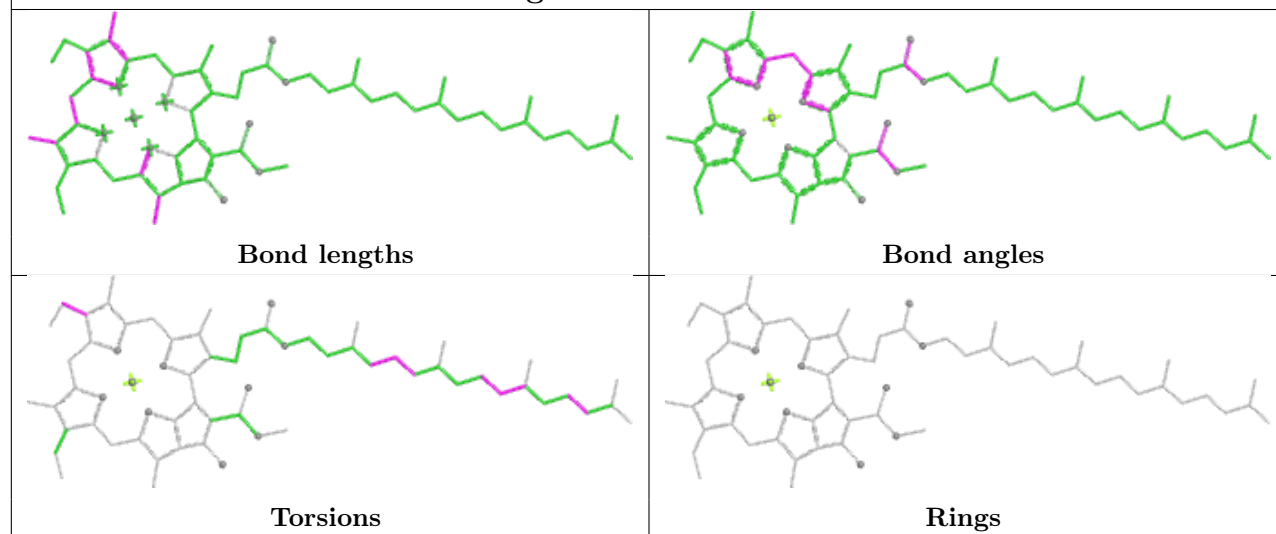


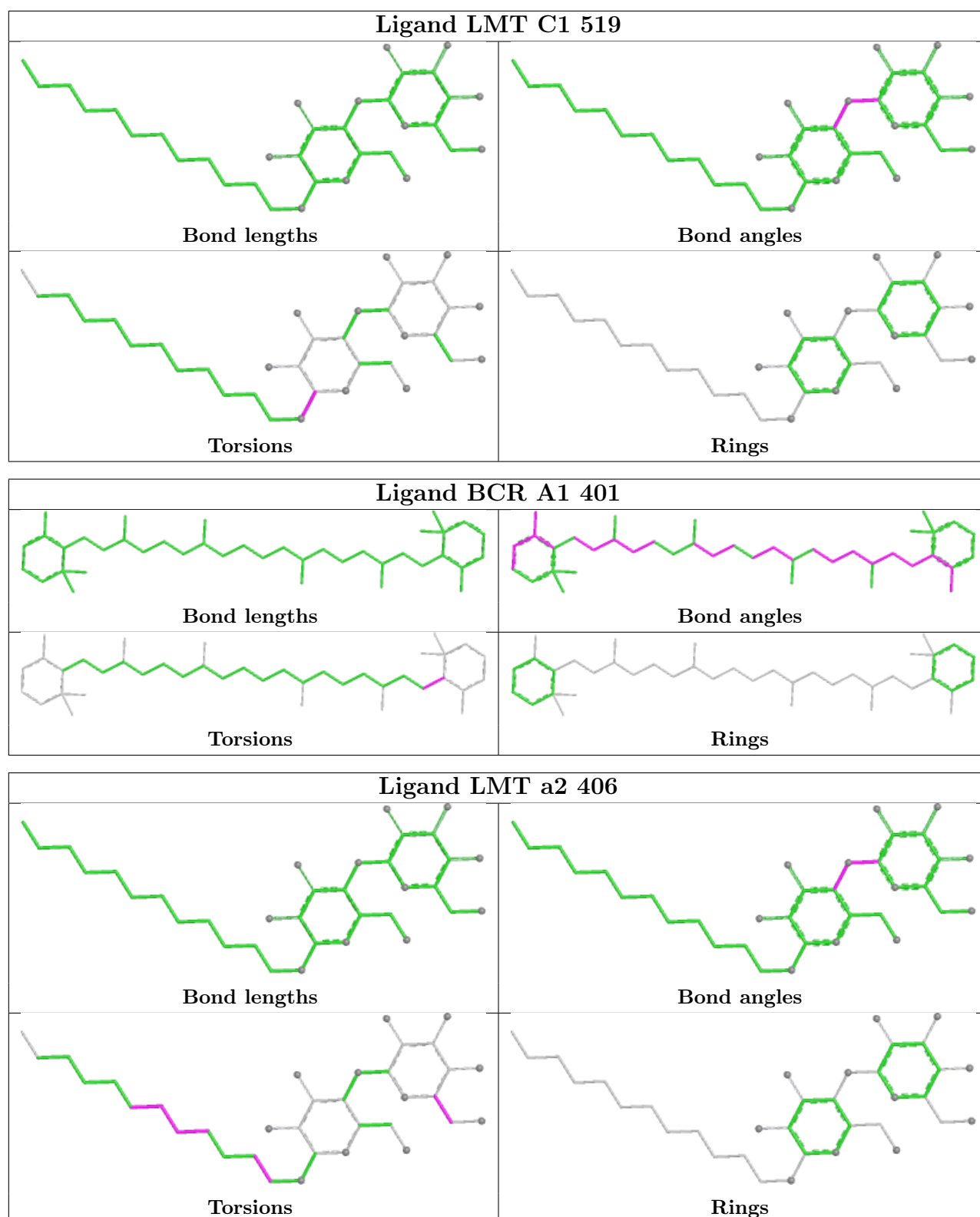


## Ligand HEM E1 101

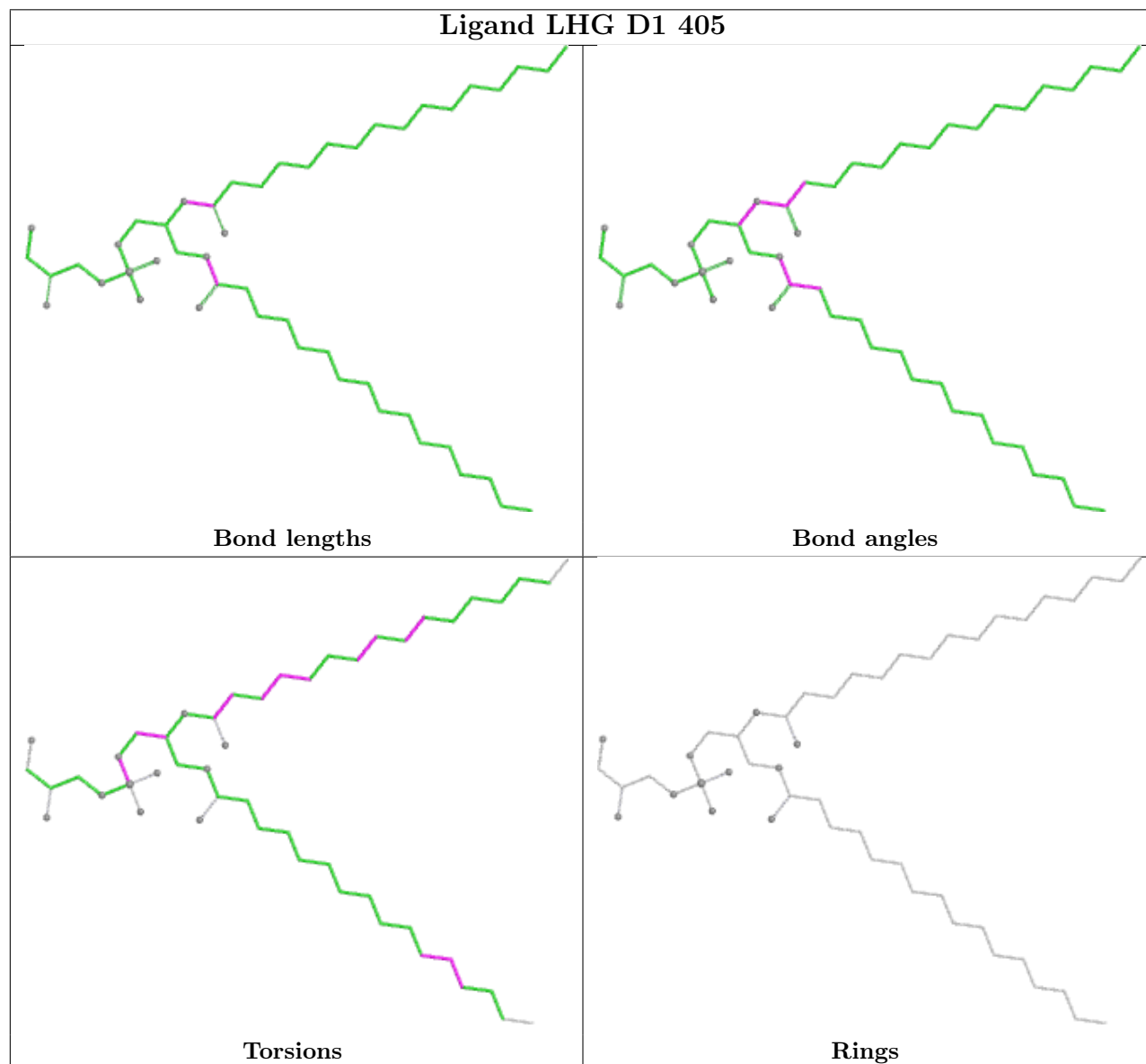
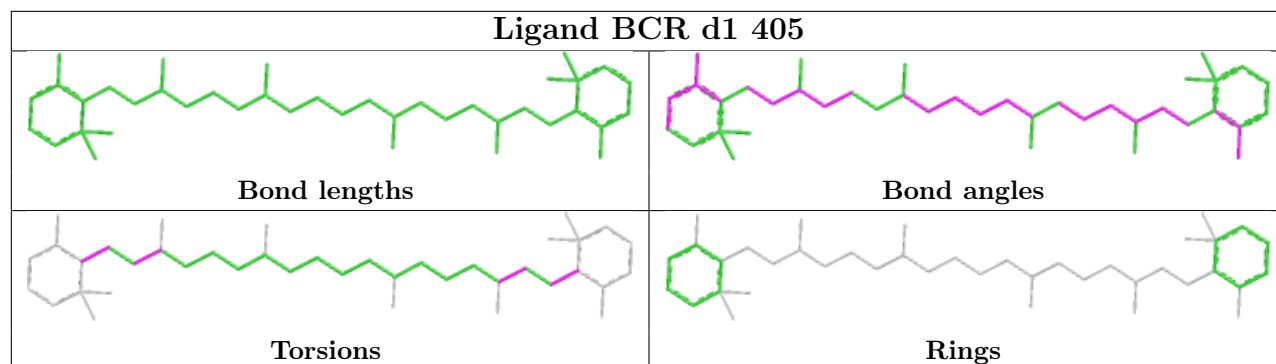


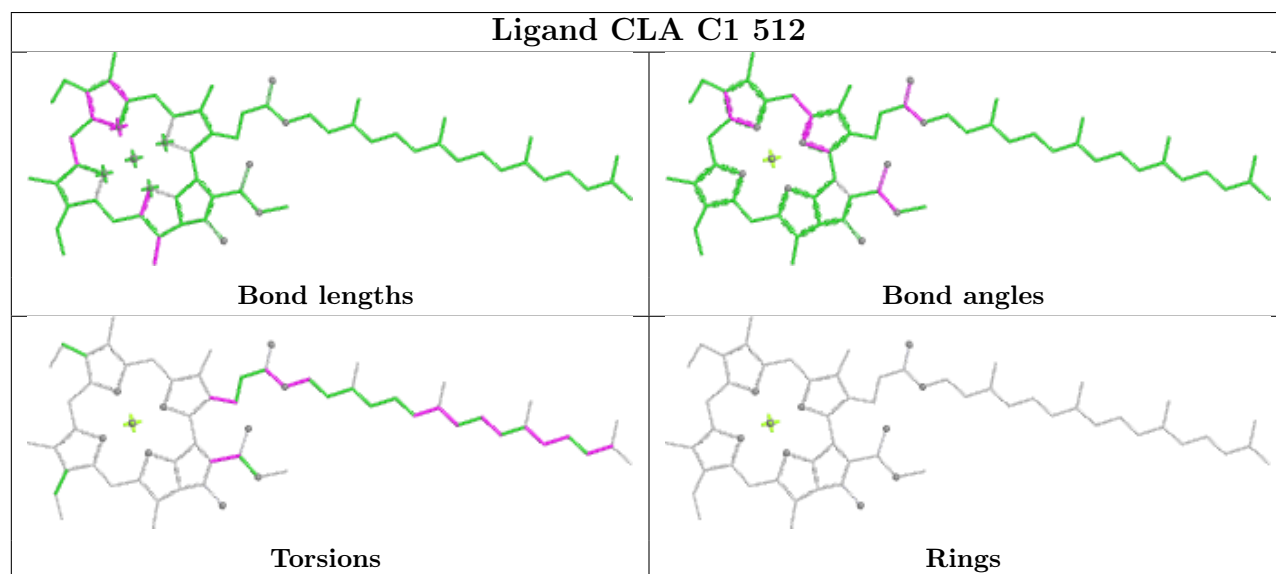
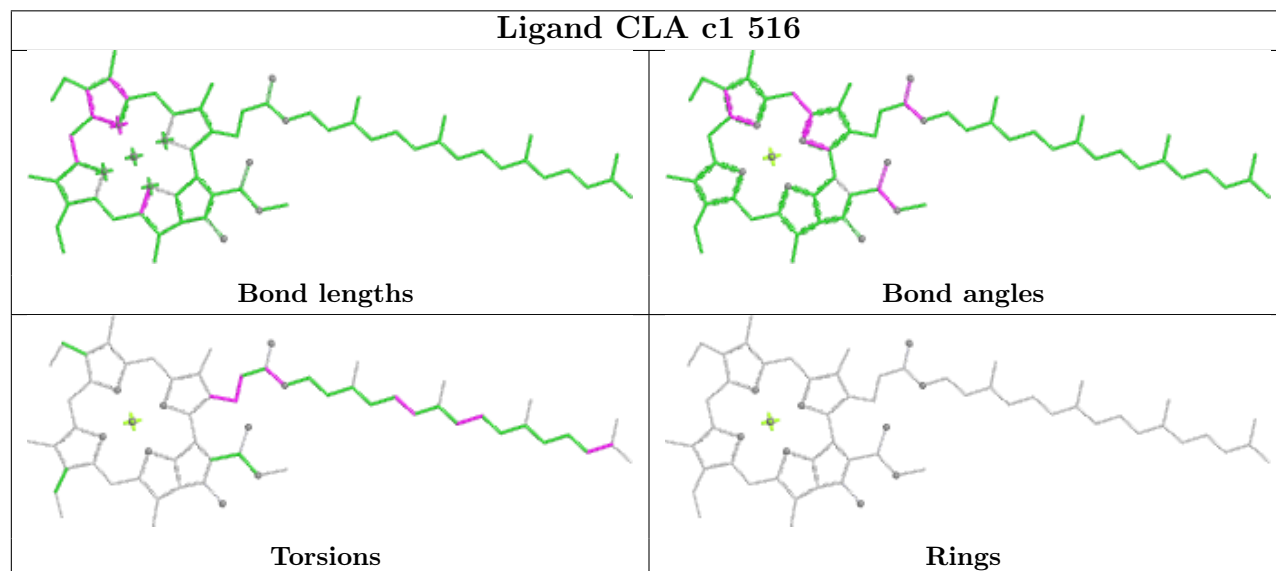
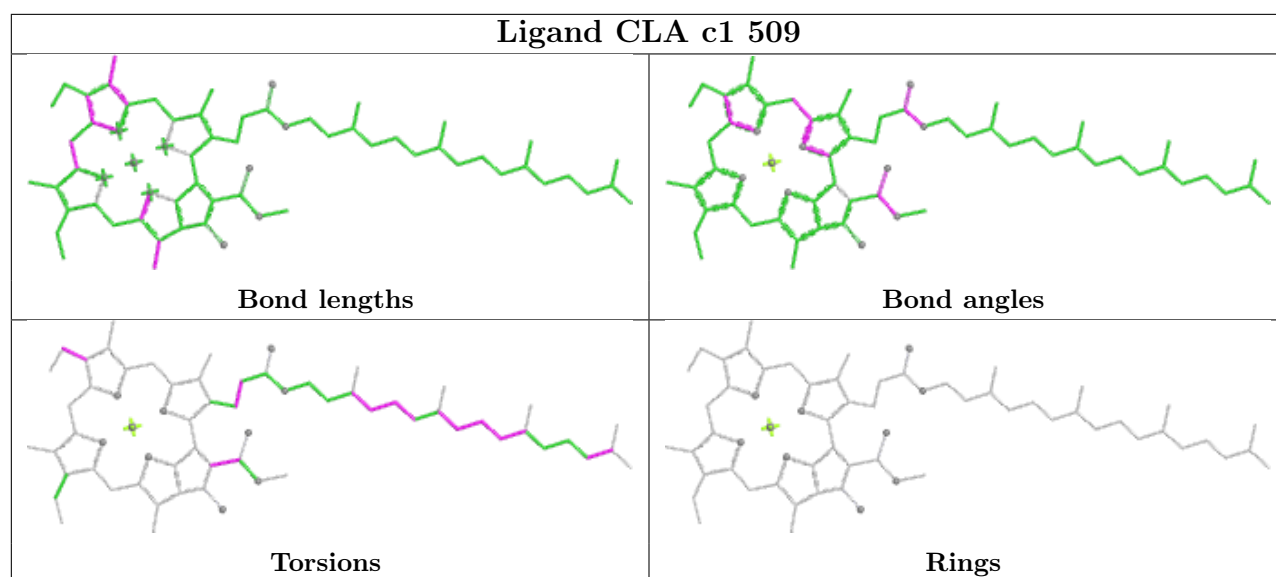
## Ligand CLA b1 613

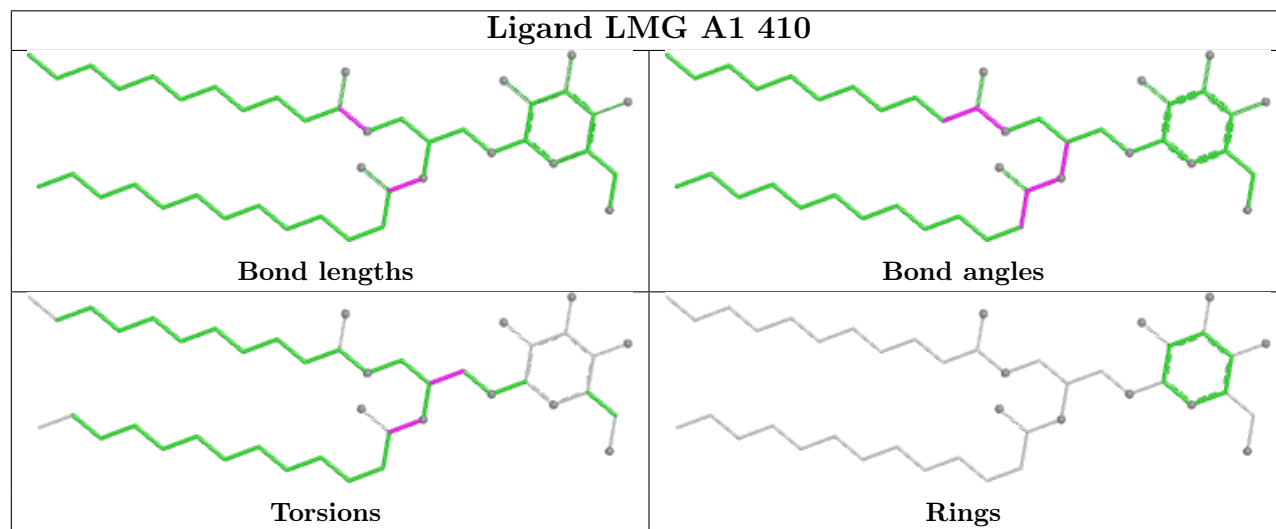
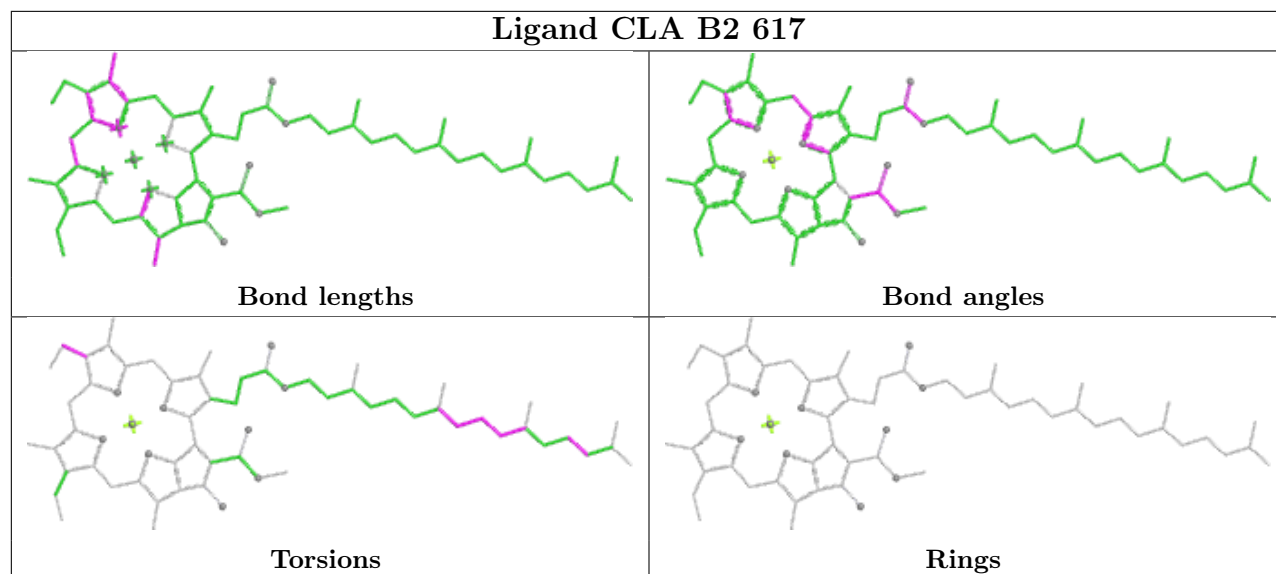


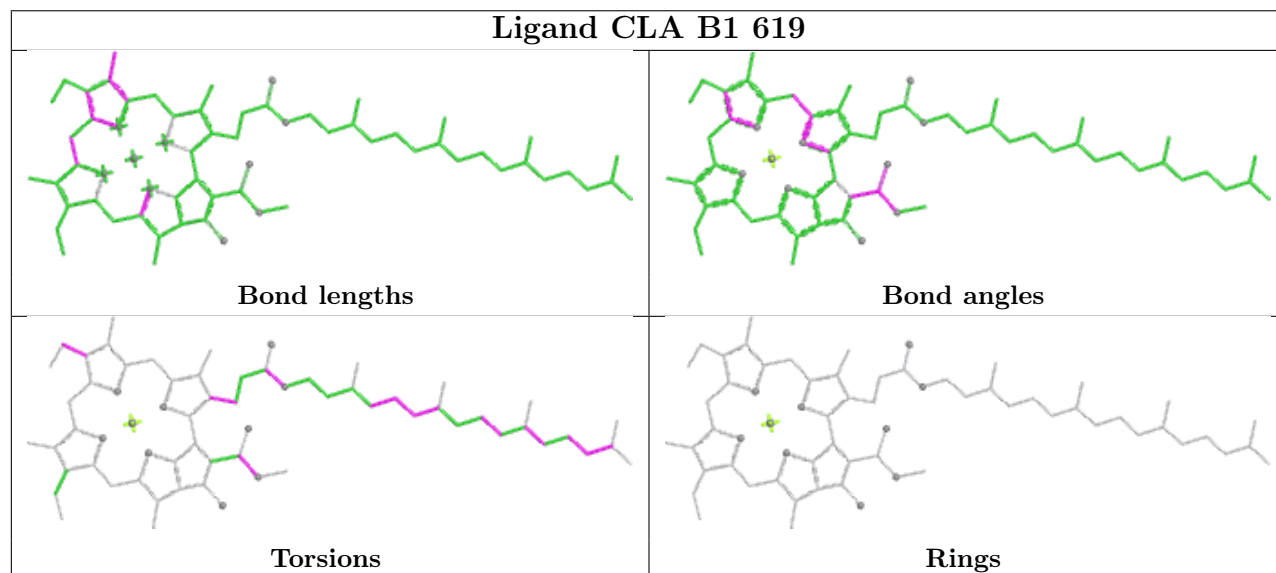
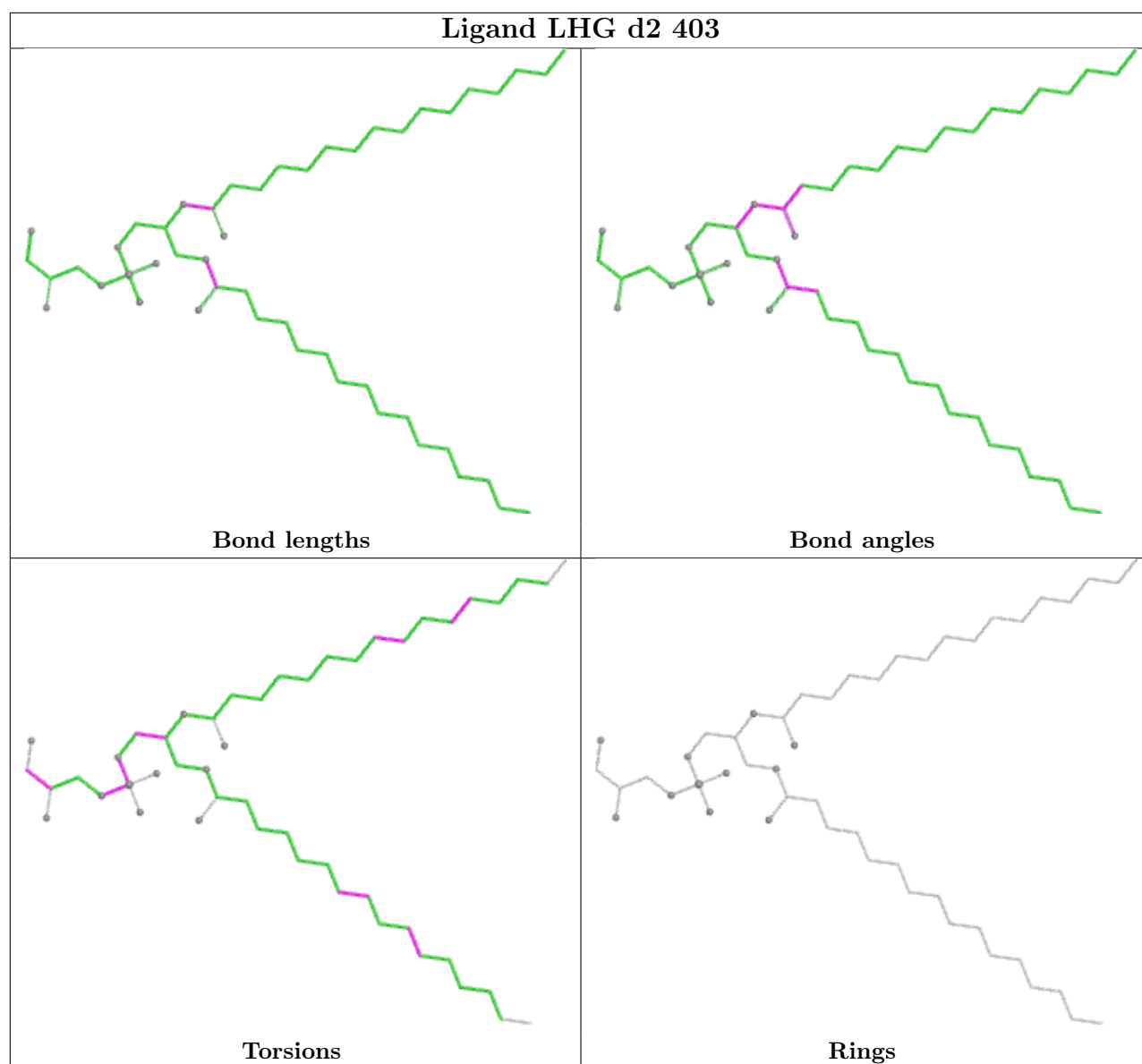


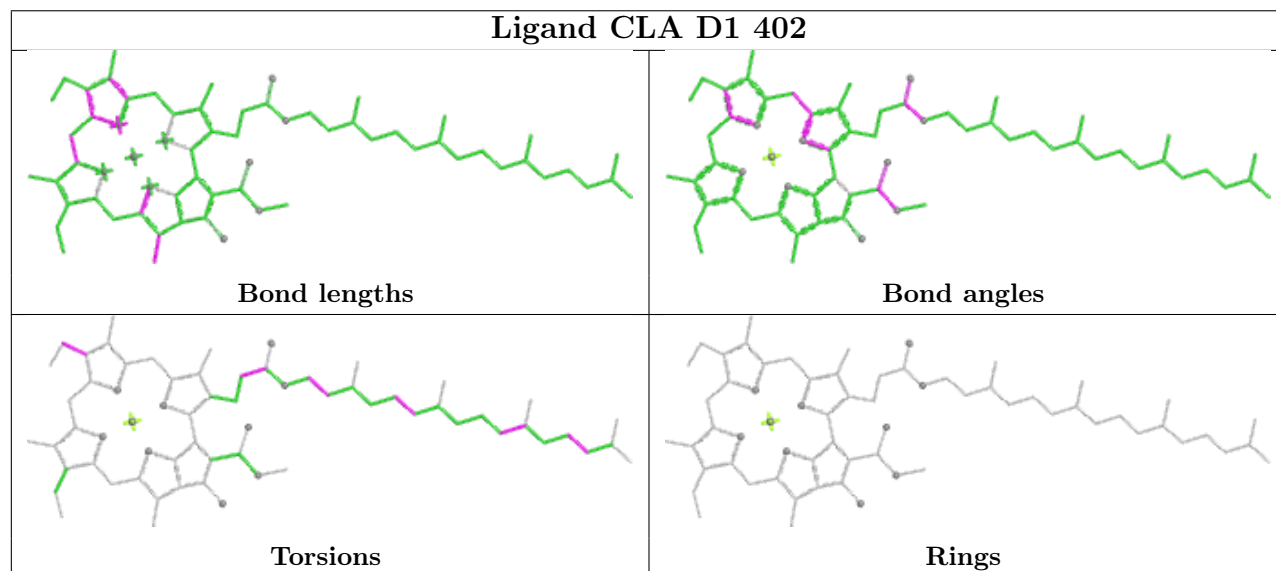
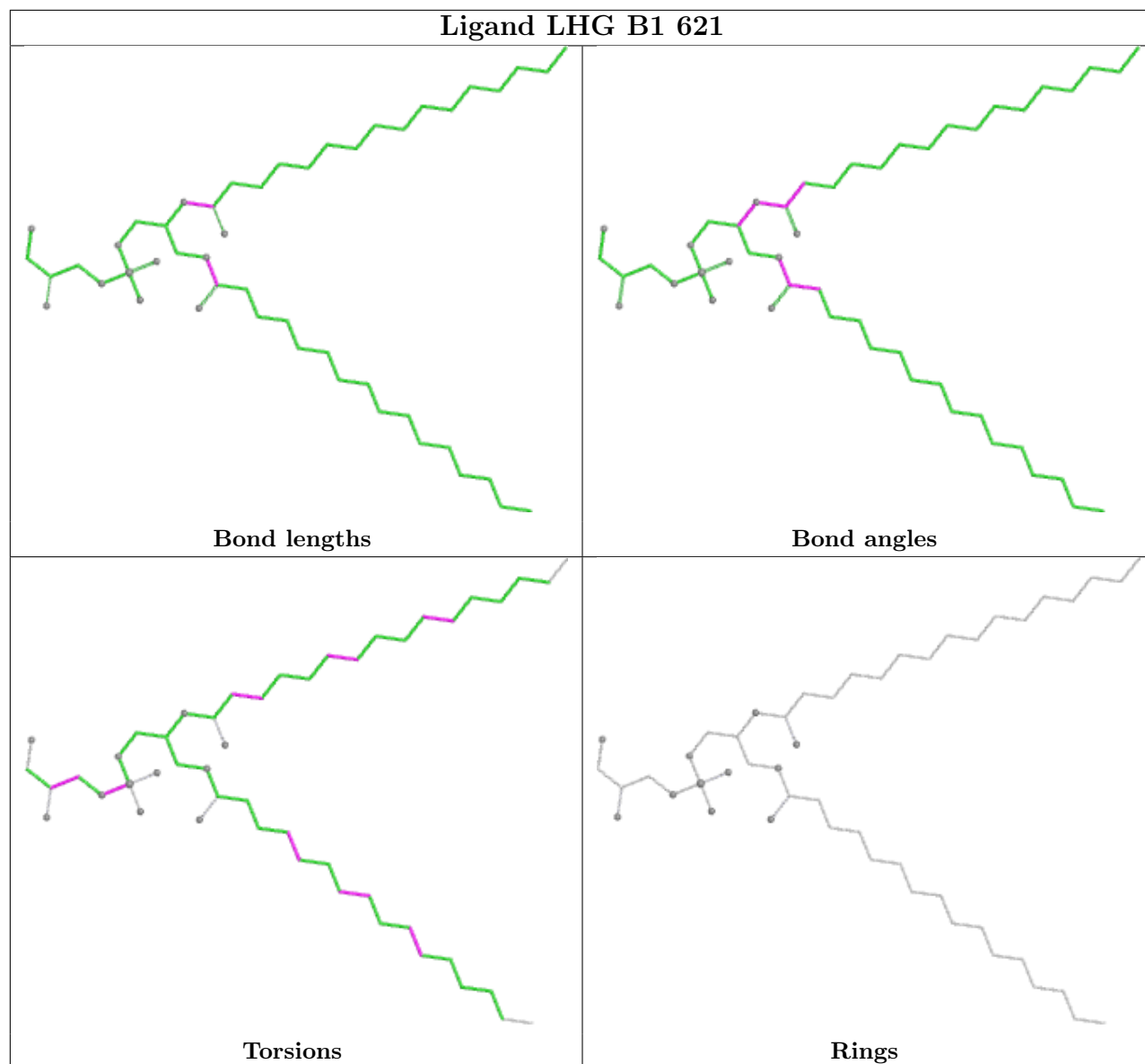


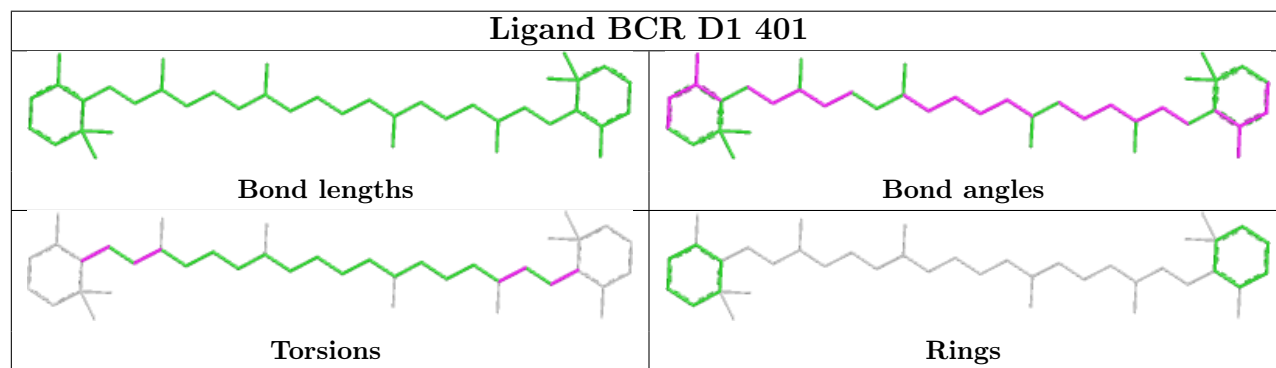
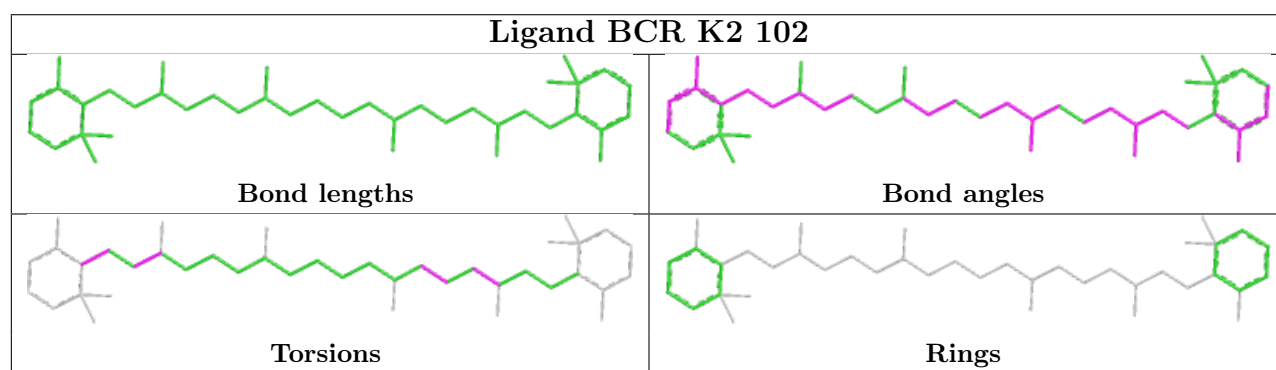
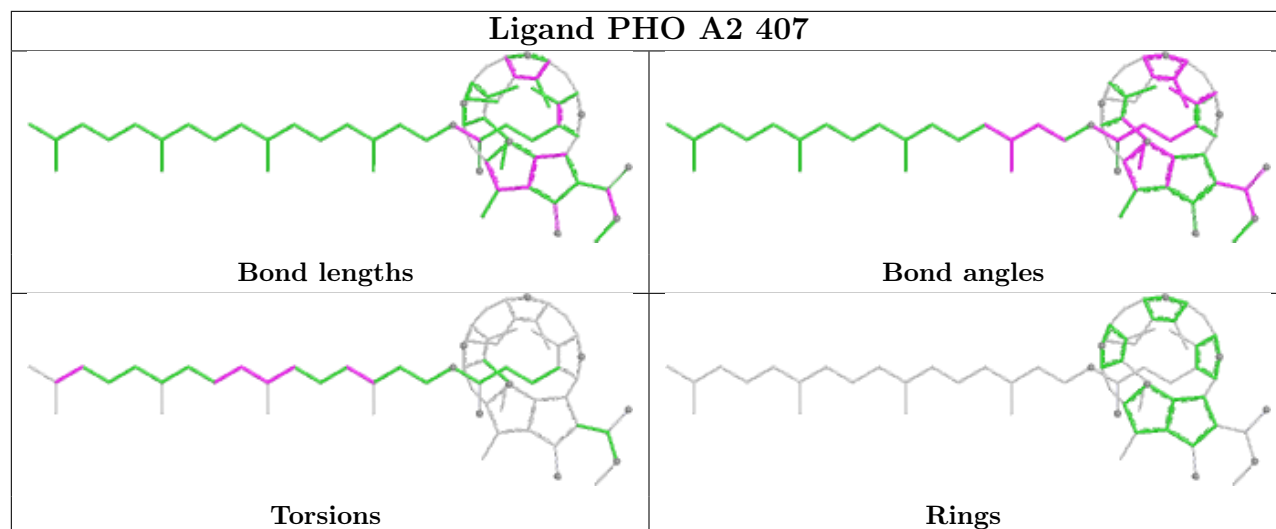


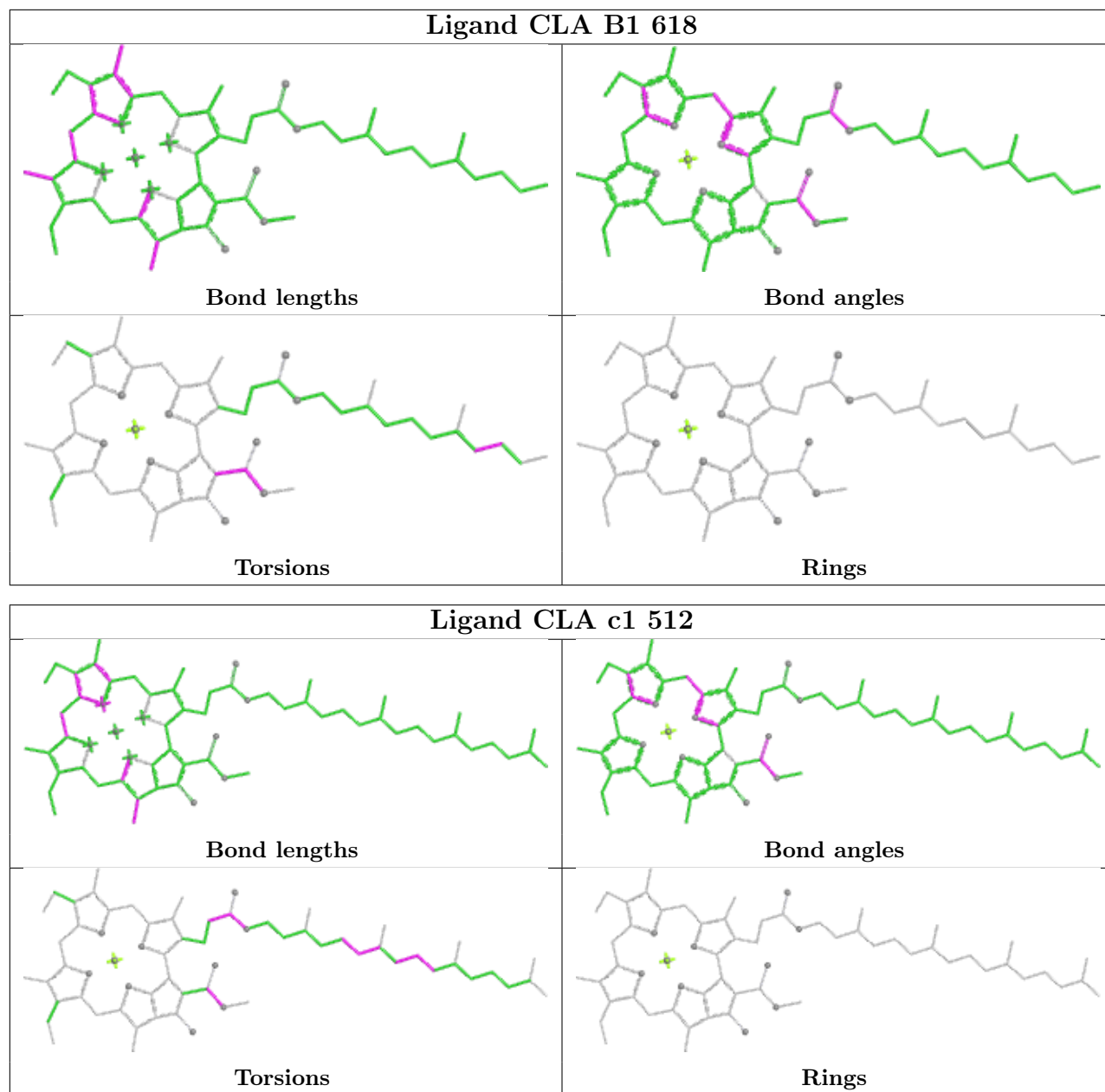


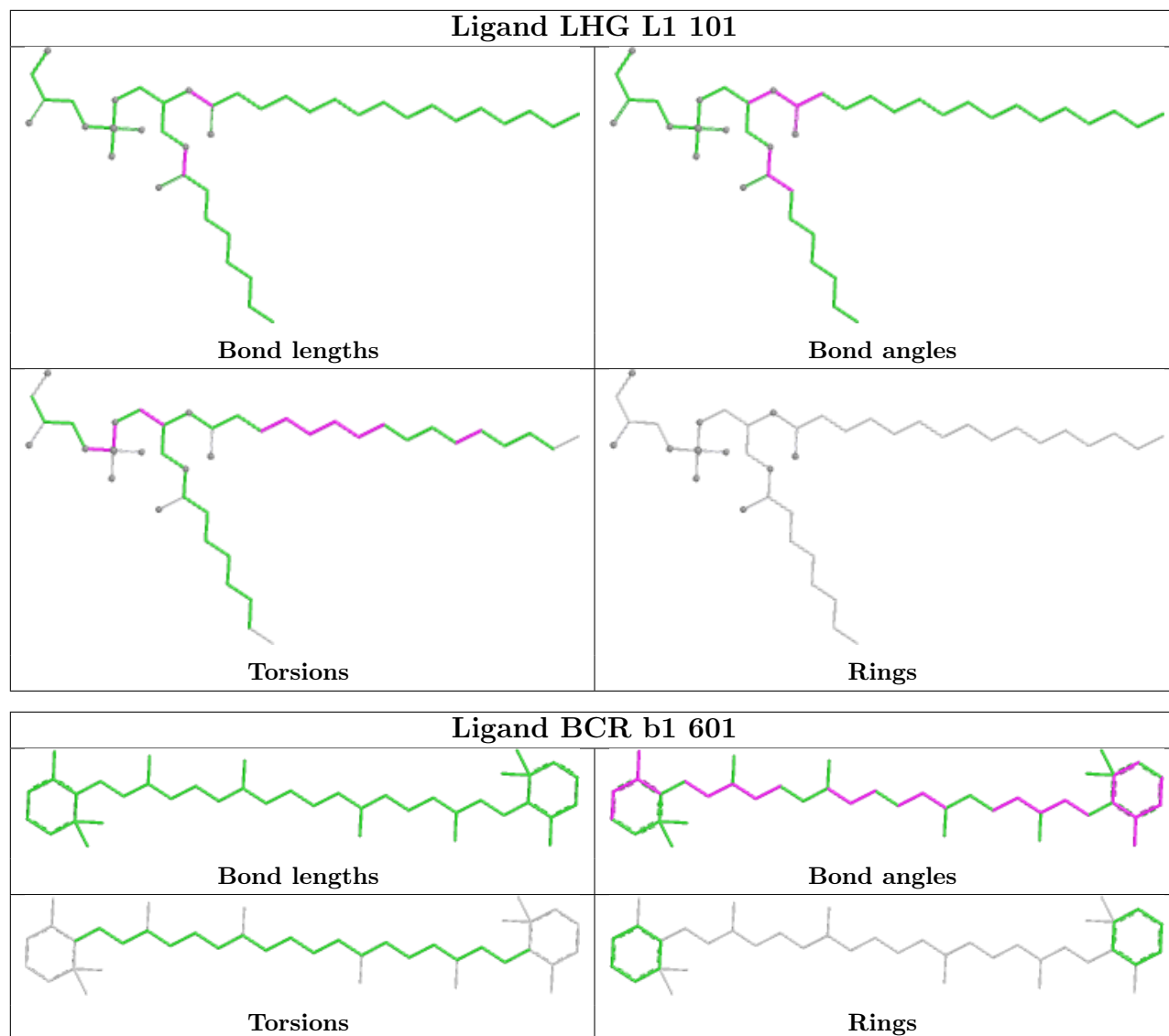




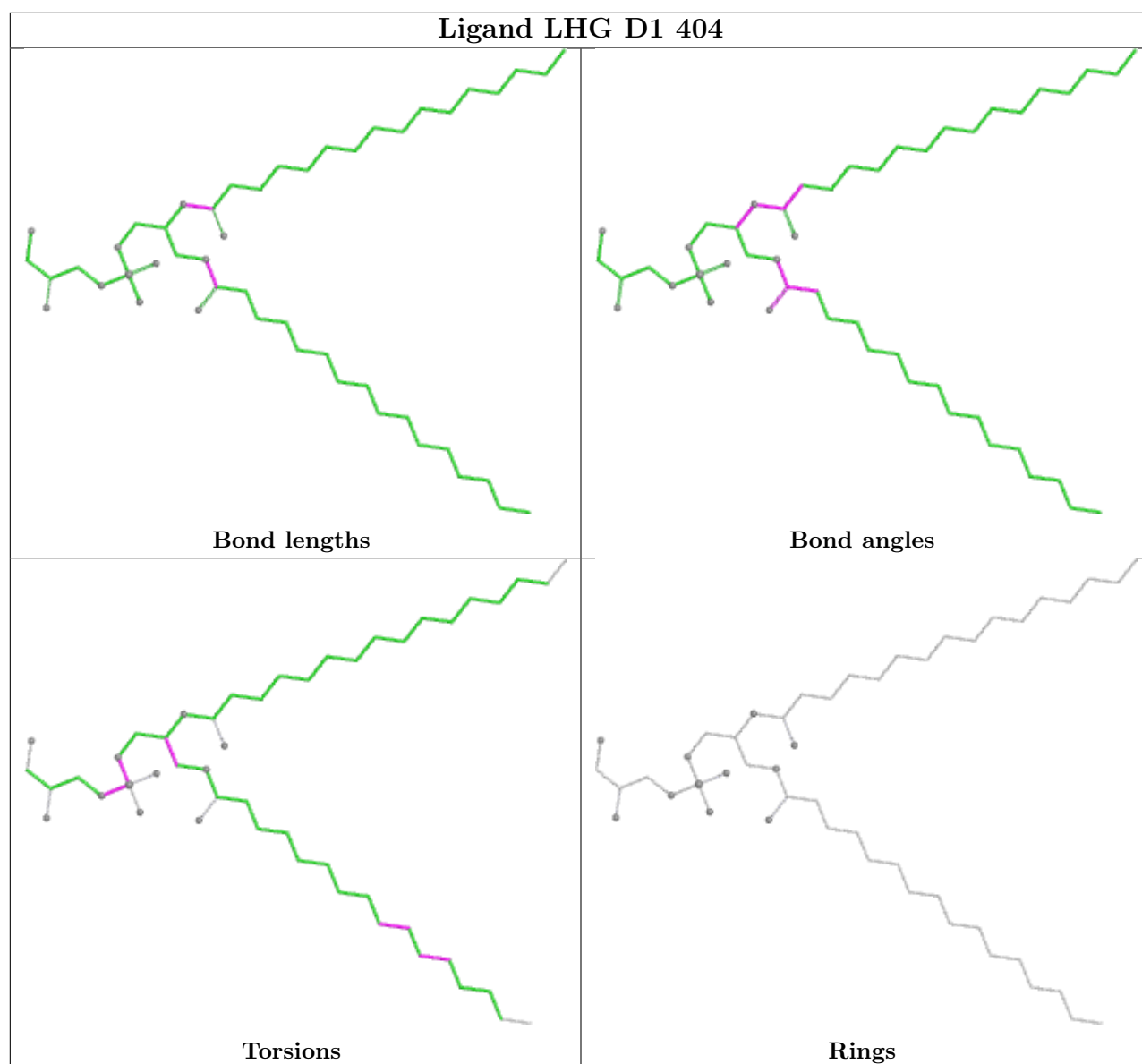


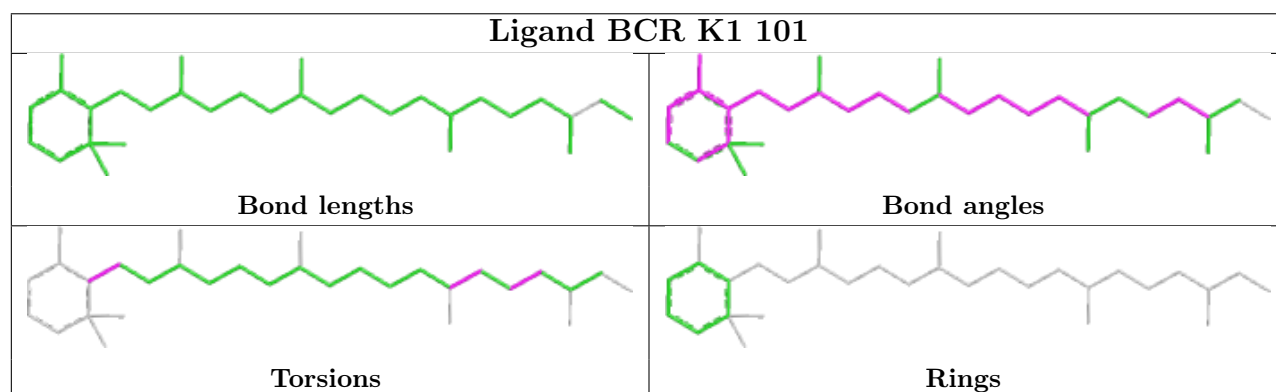
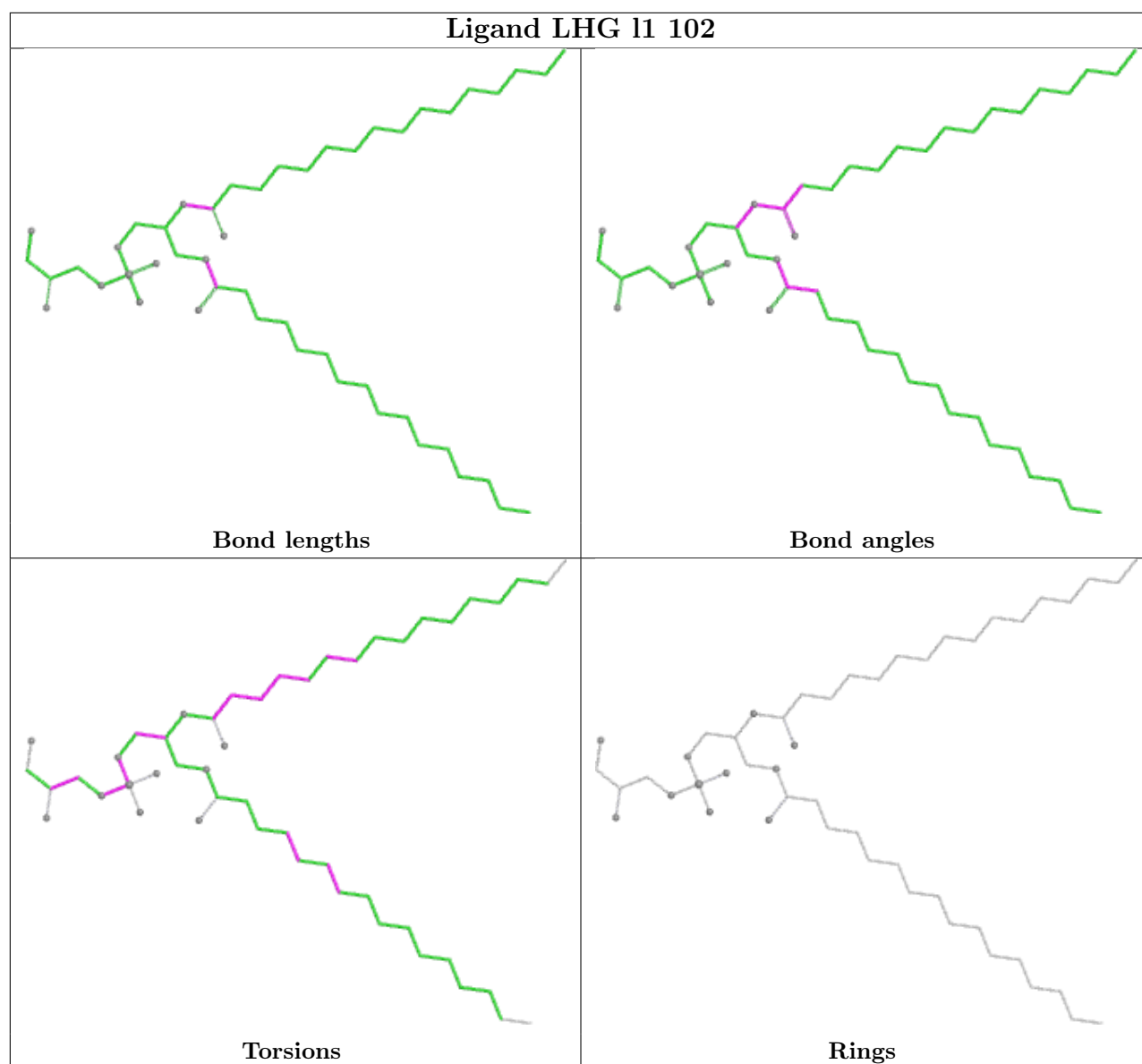


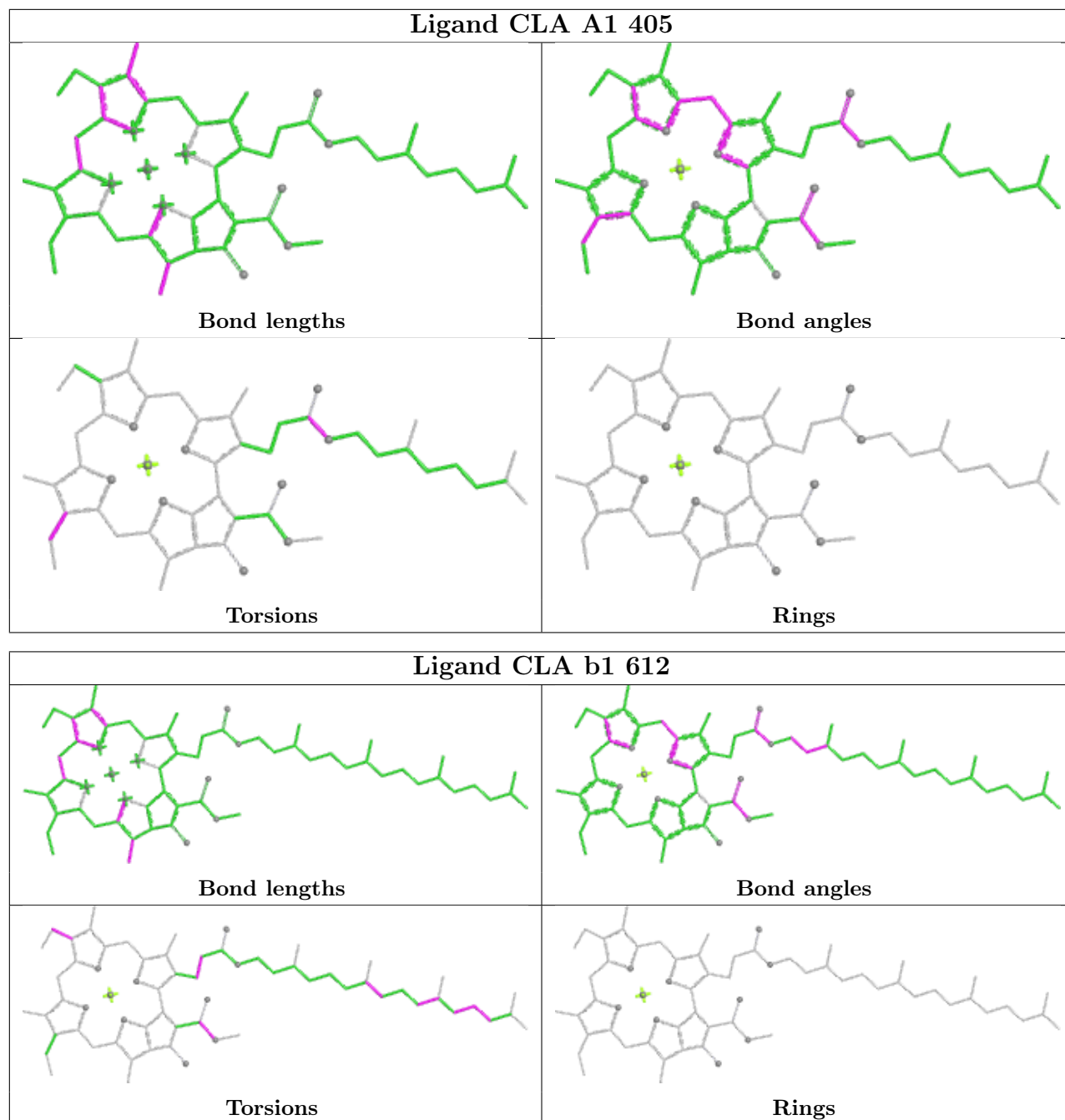


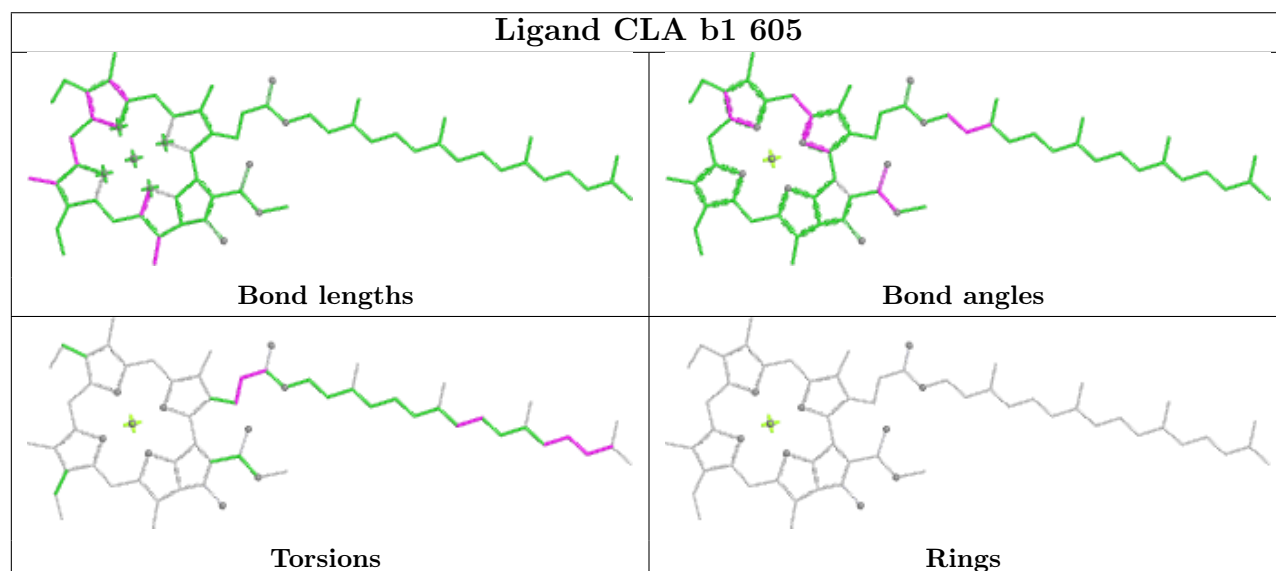
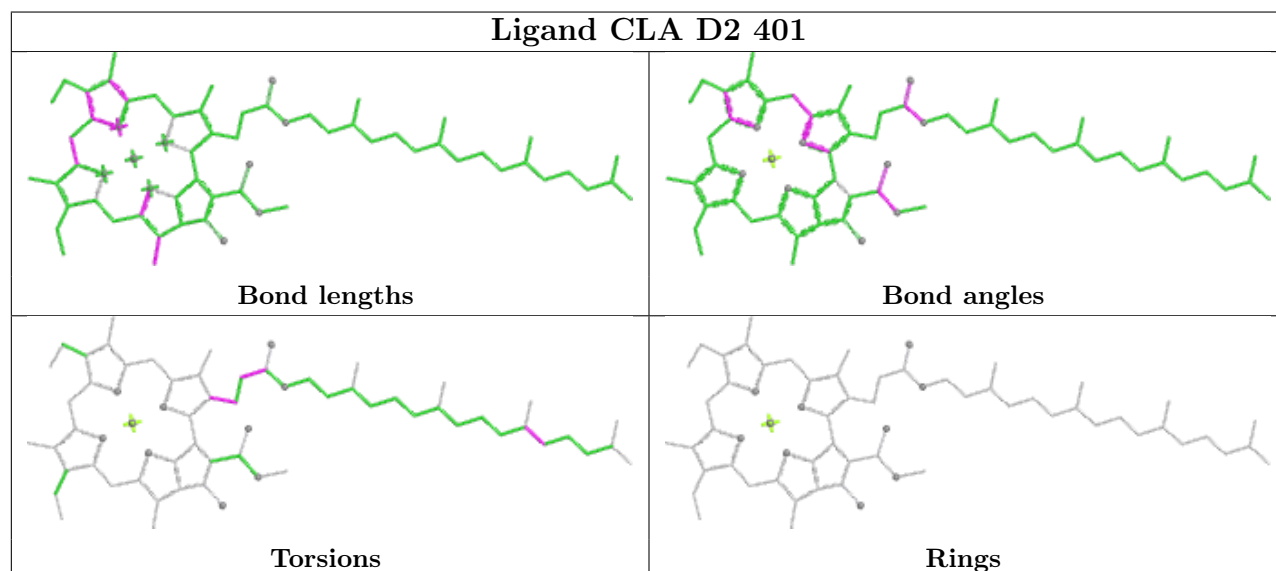
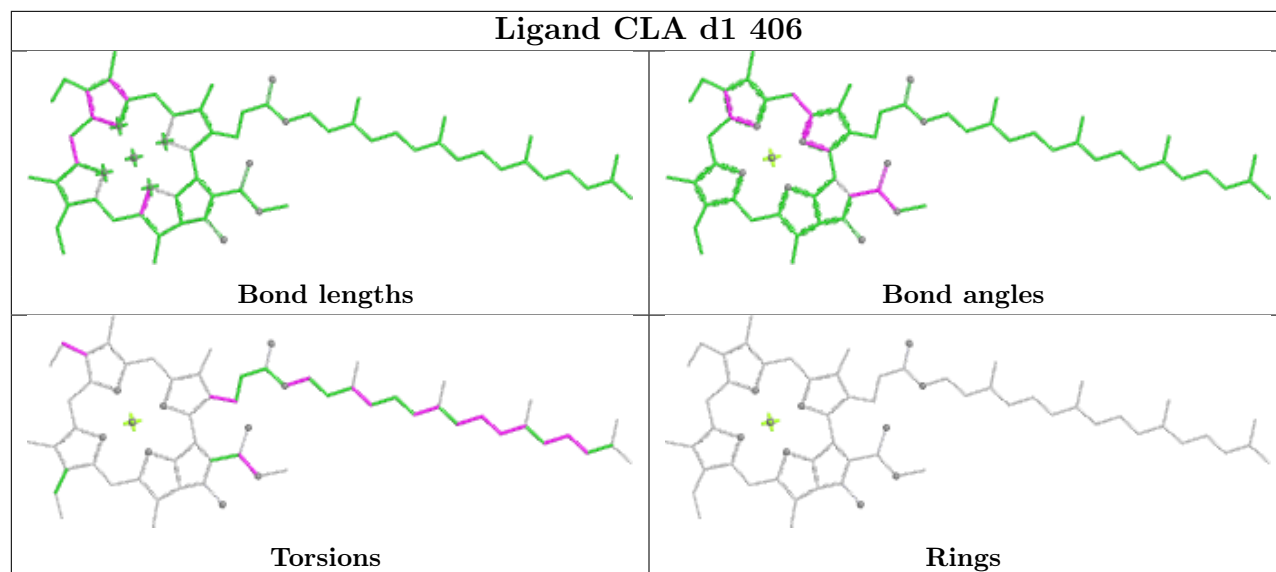




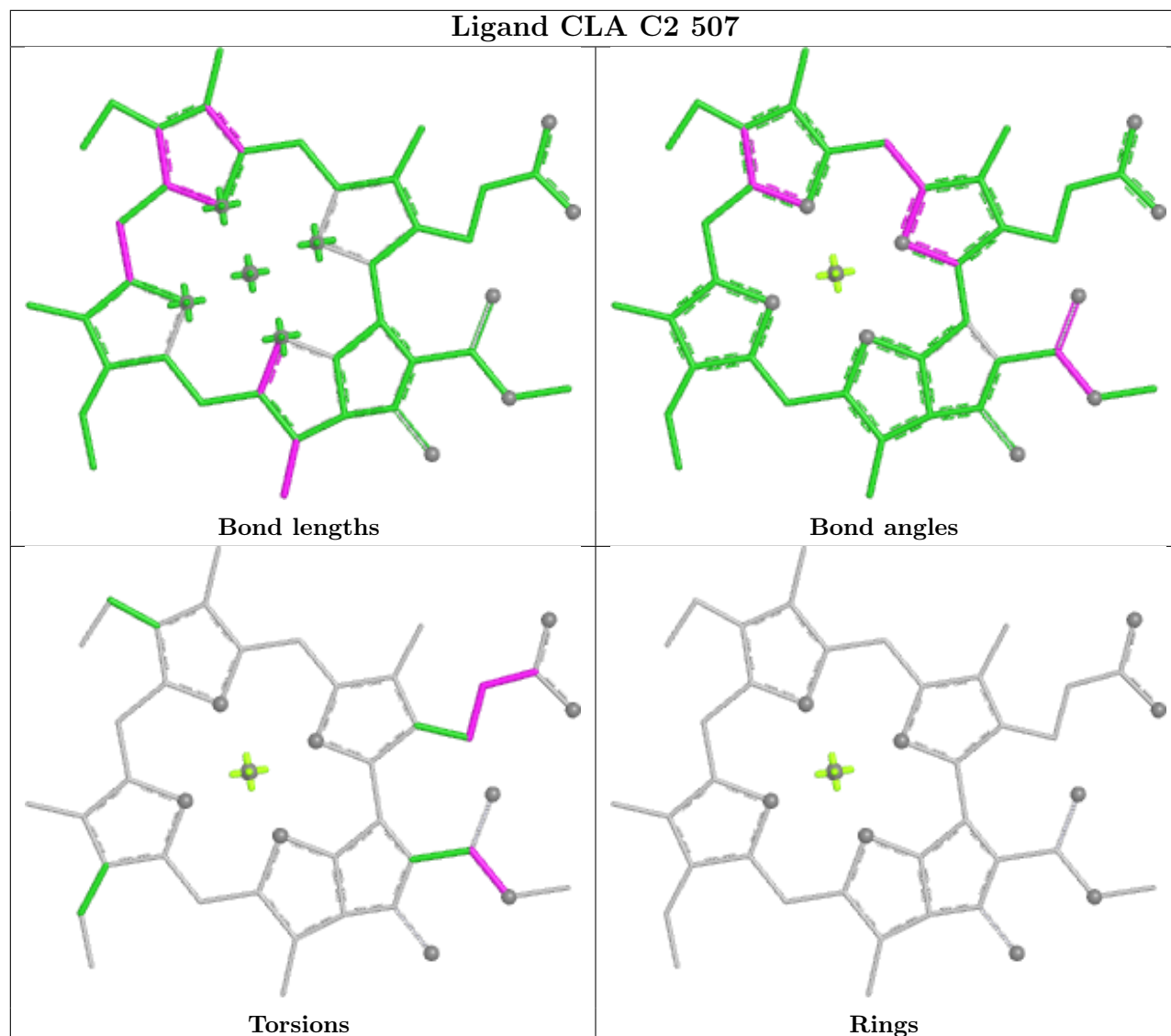




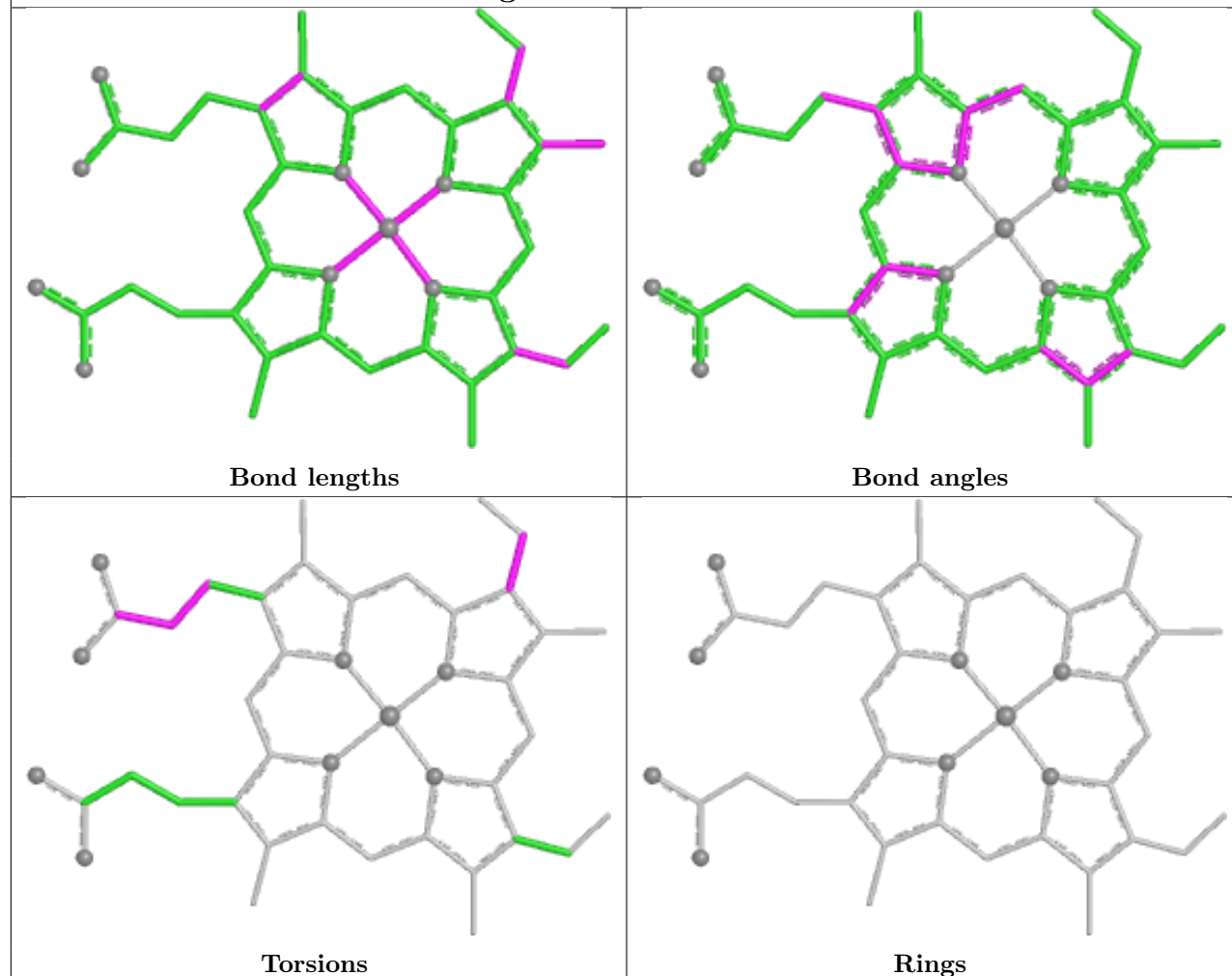




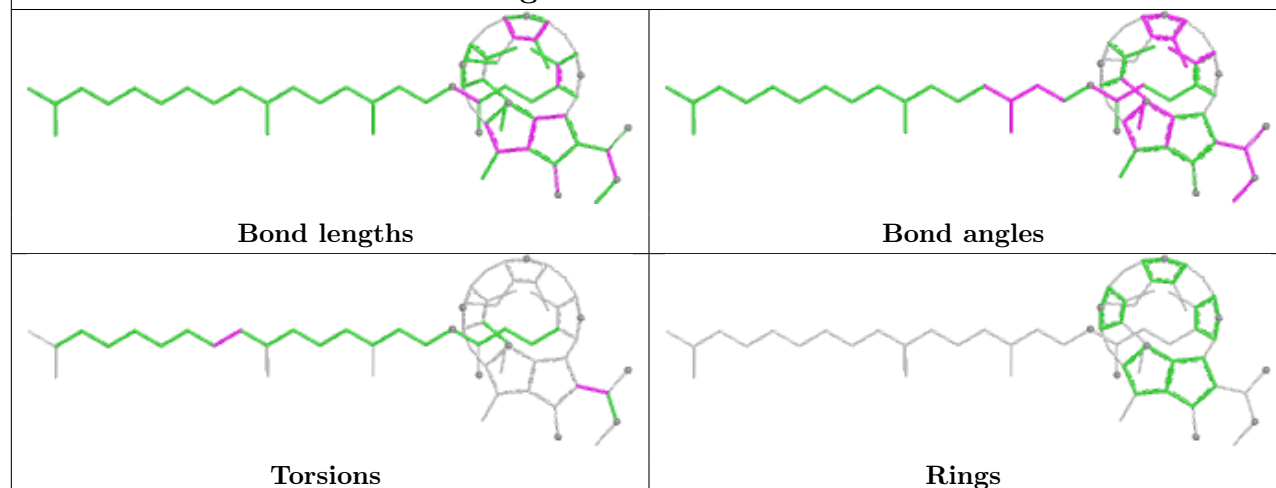
## Ligand CLA C2 507

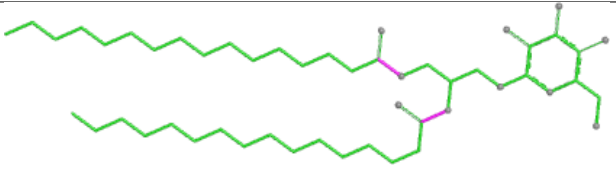
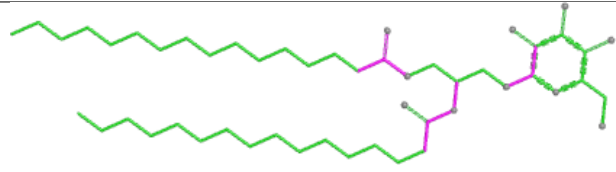
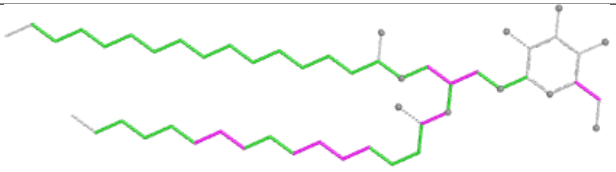
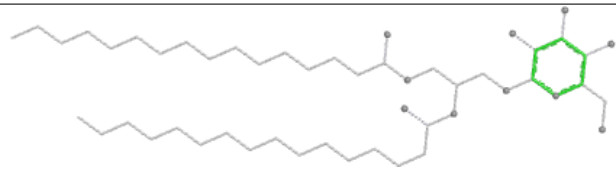


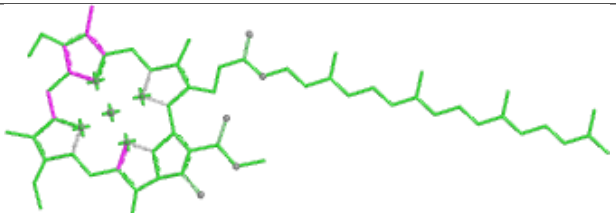
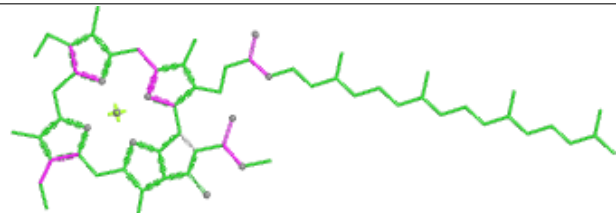
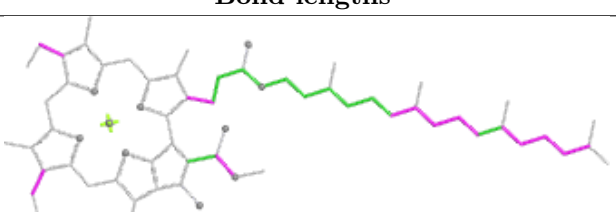
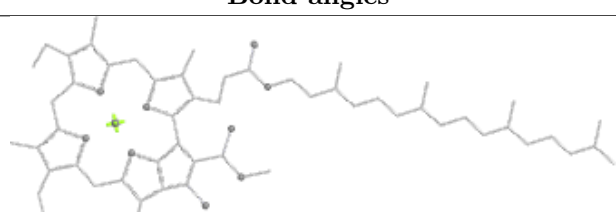
## Ligand HEM V1 201

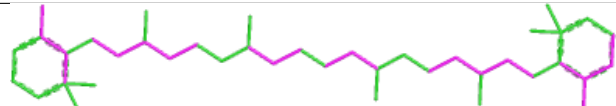
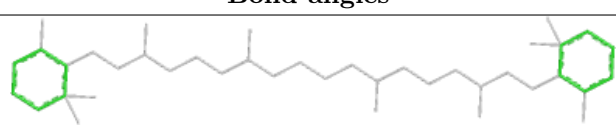


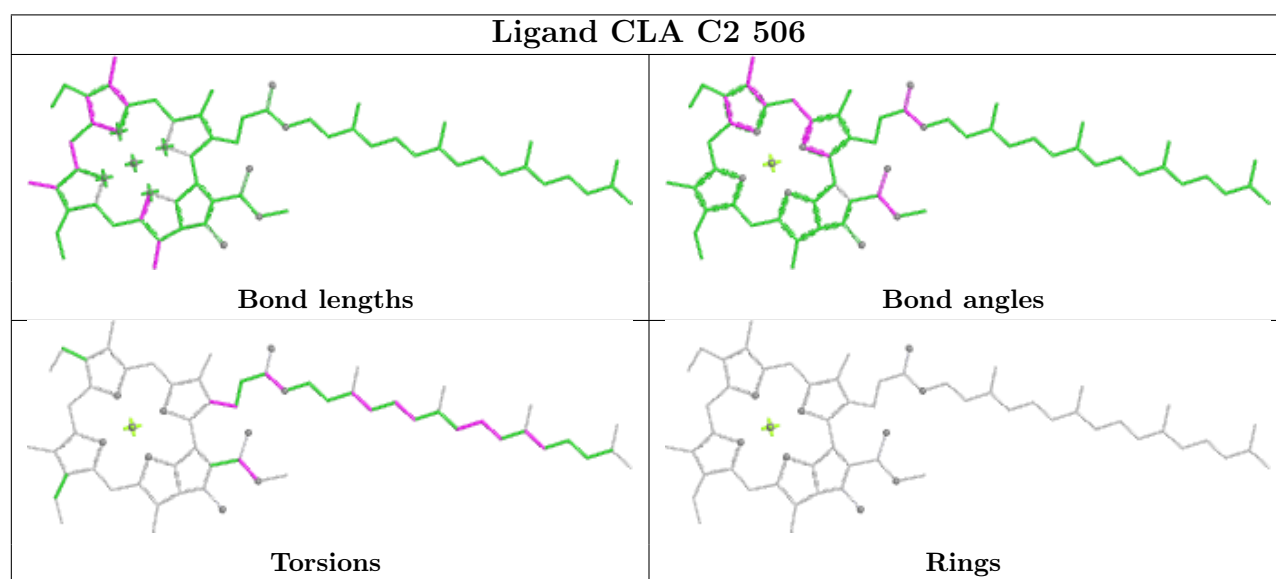
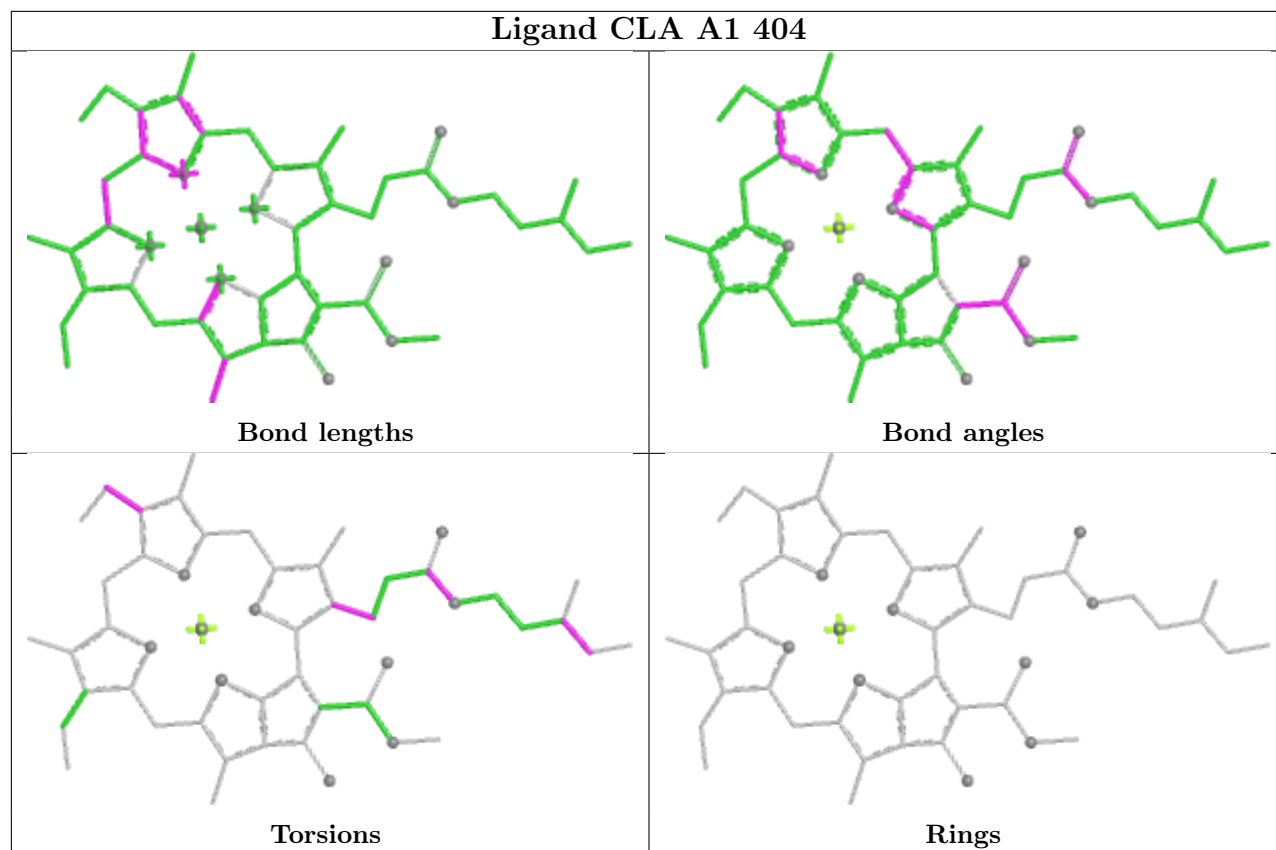
## Ligand PHO D1 407



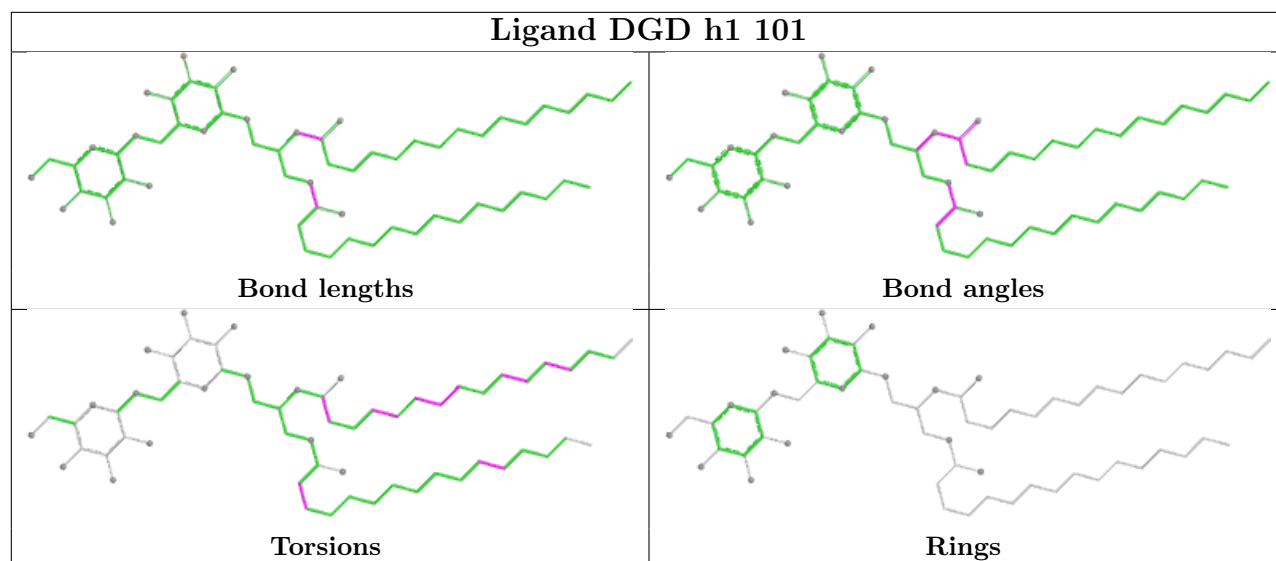
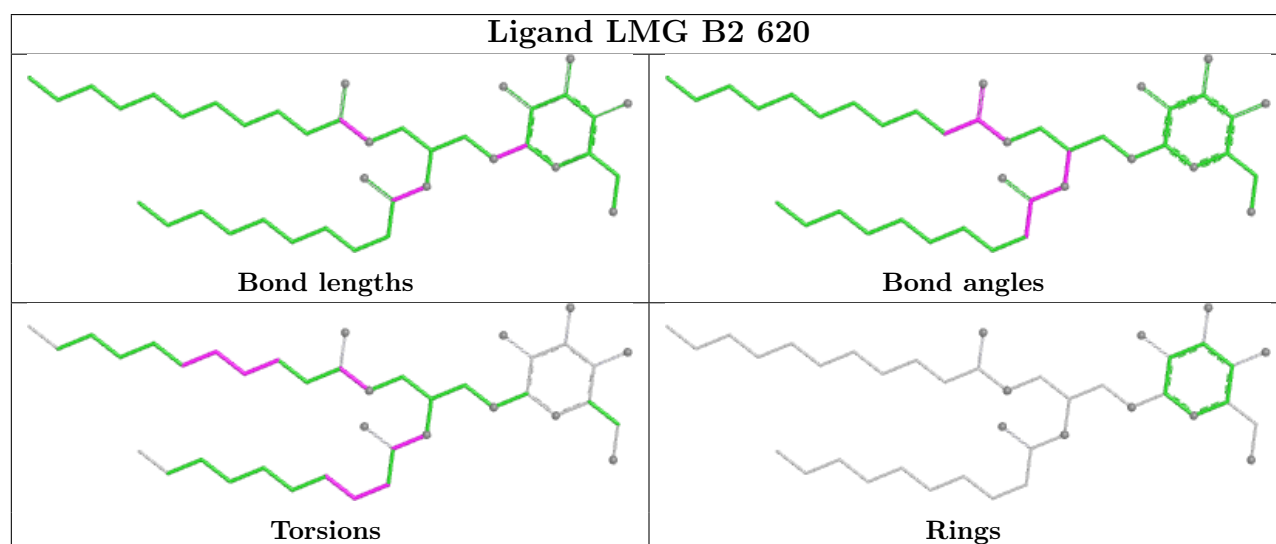
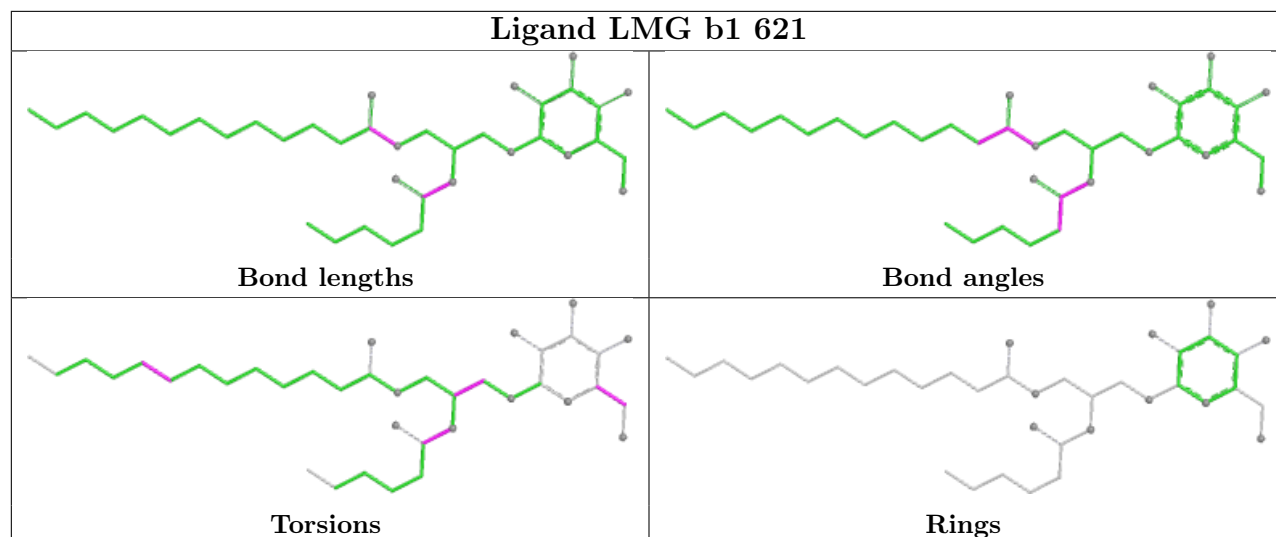
| Ligand LMG a1 412                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA a2 405                                                                  |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

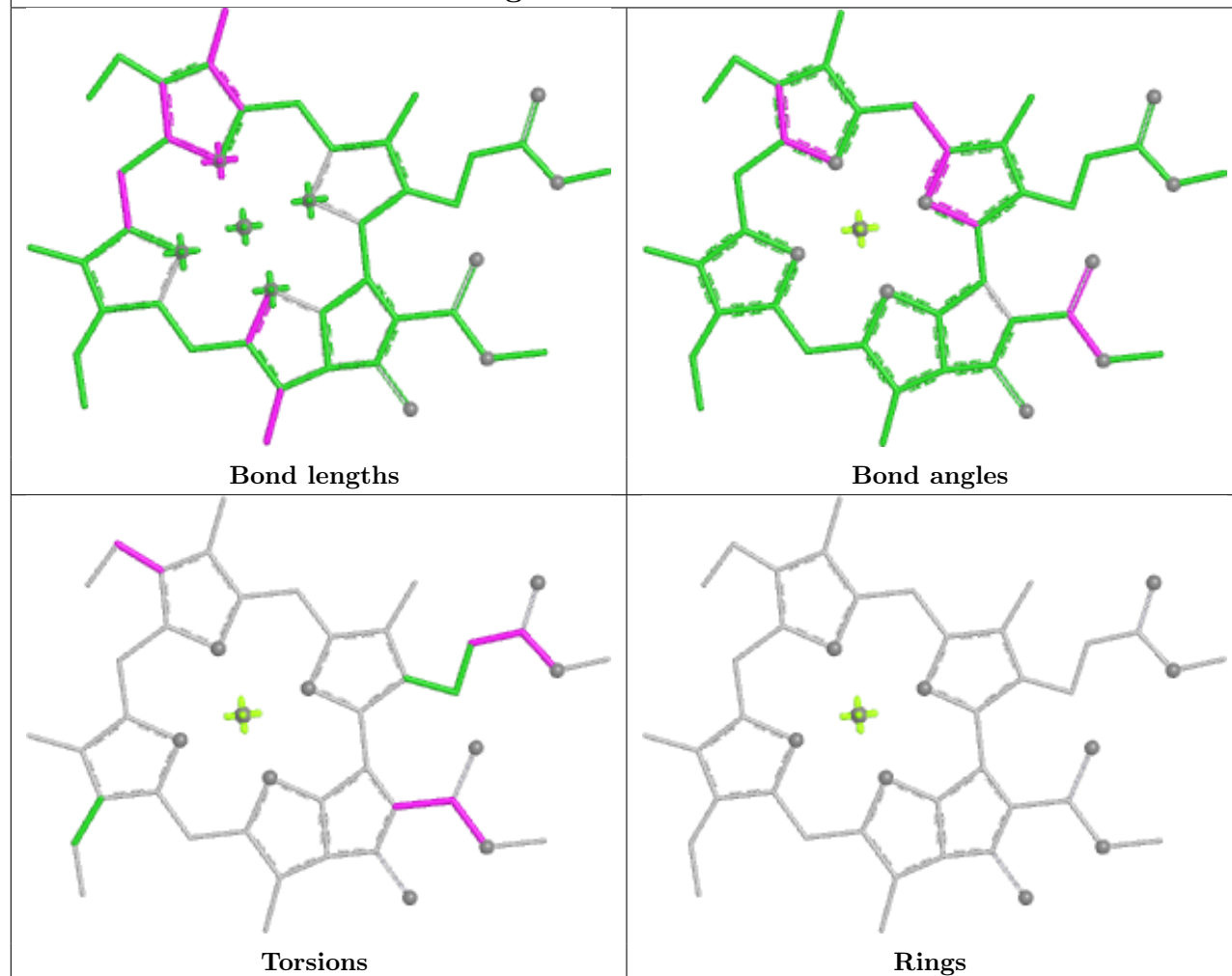
| Ligand BCR b1 603                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



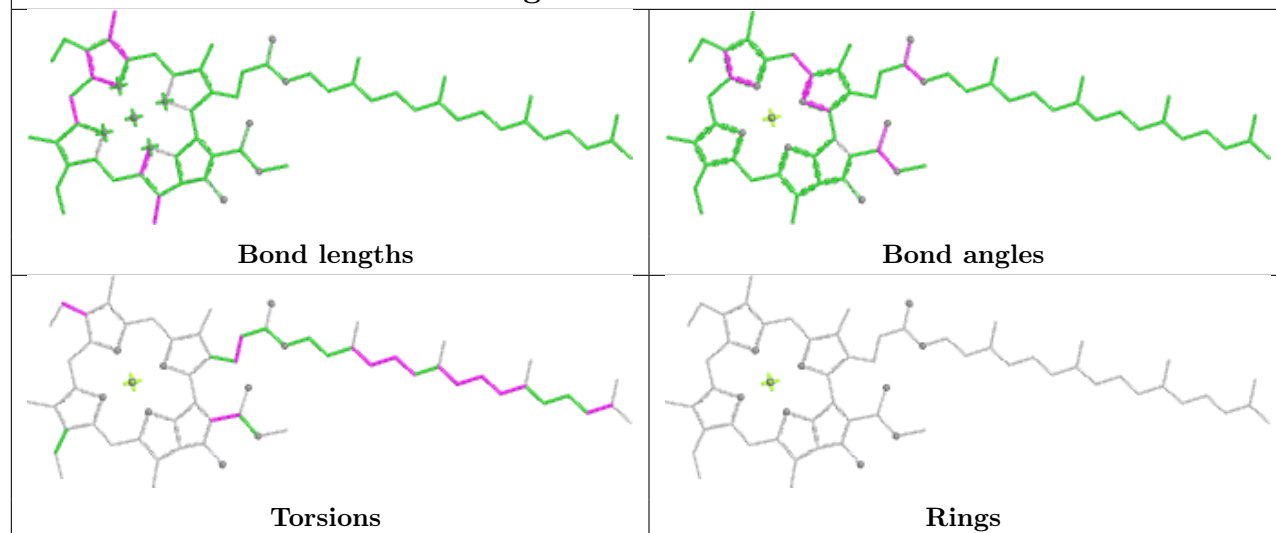


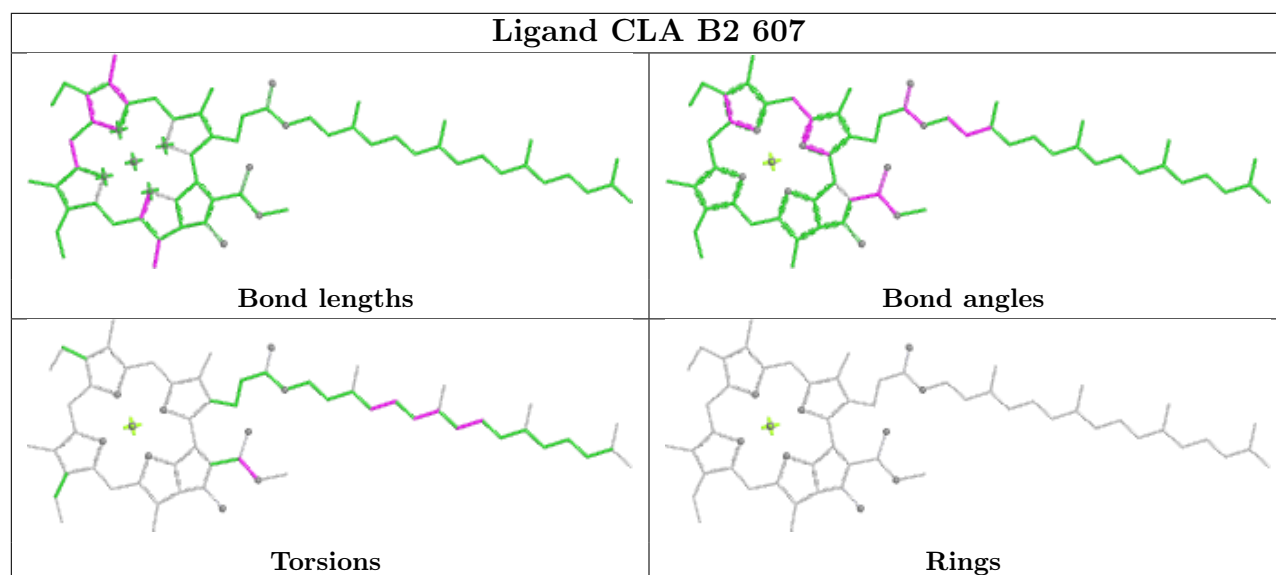
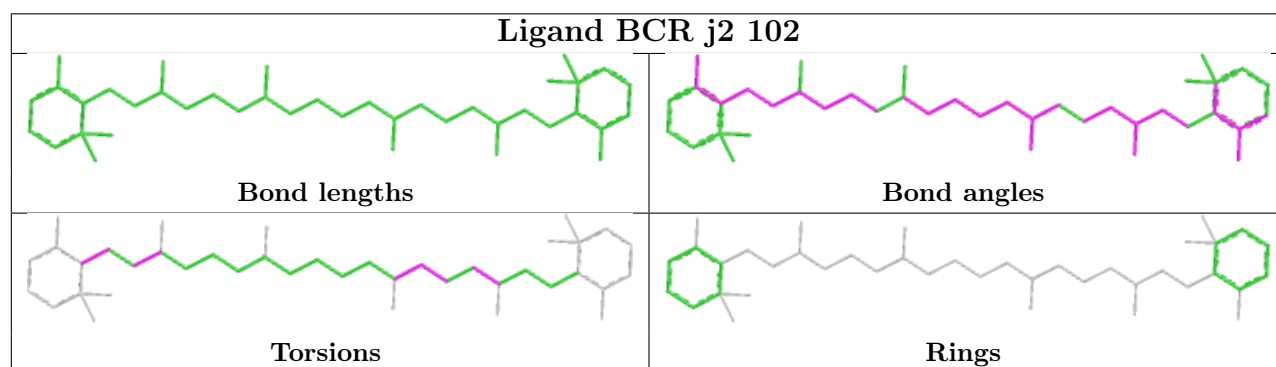
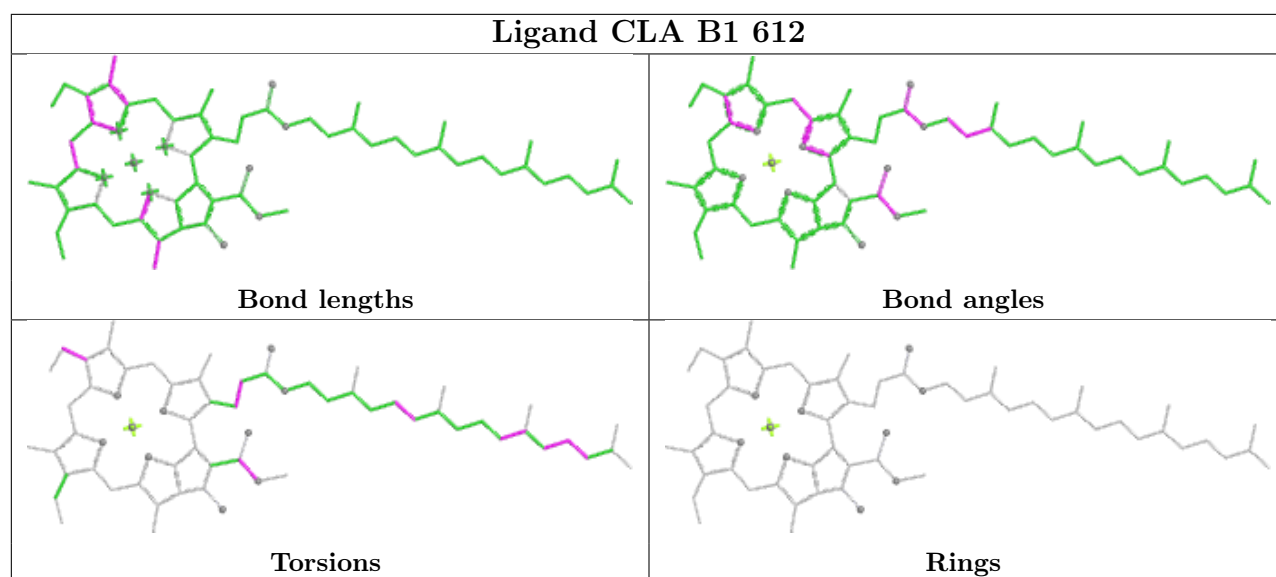


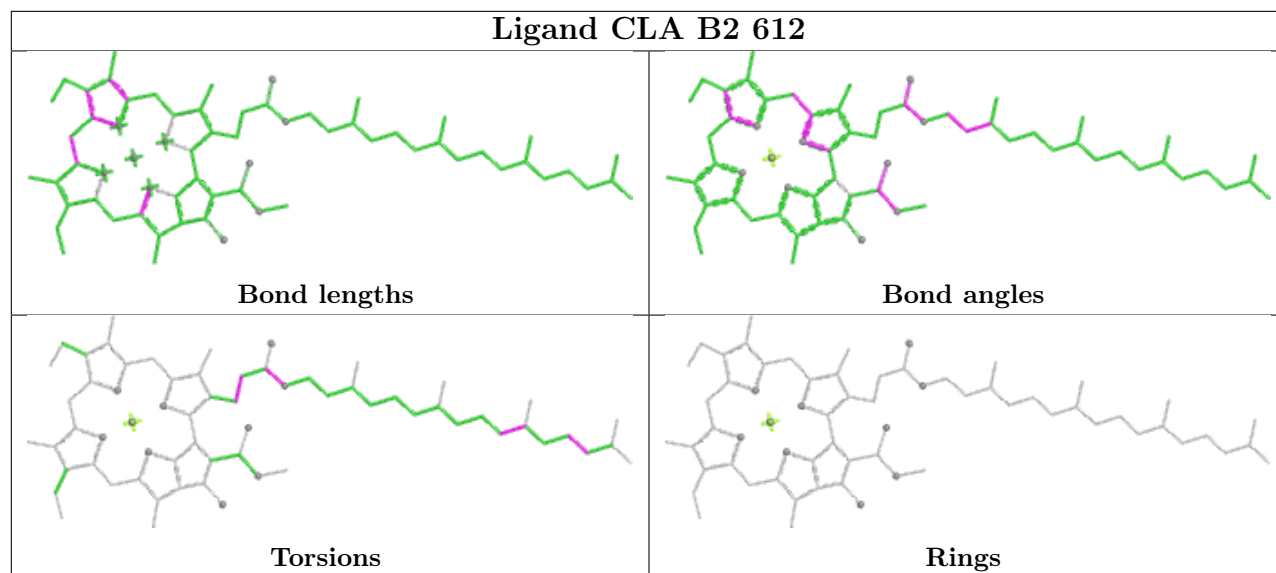
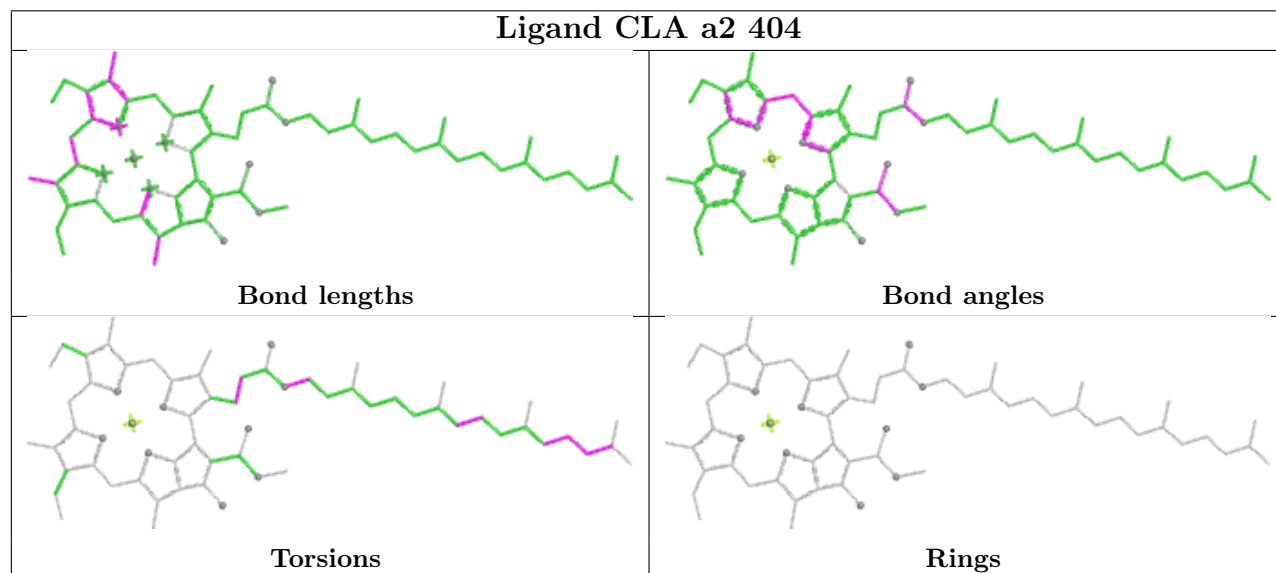
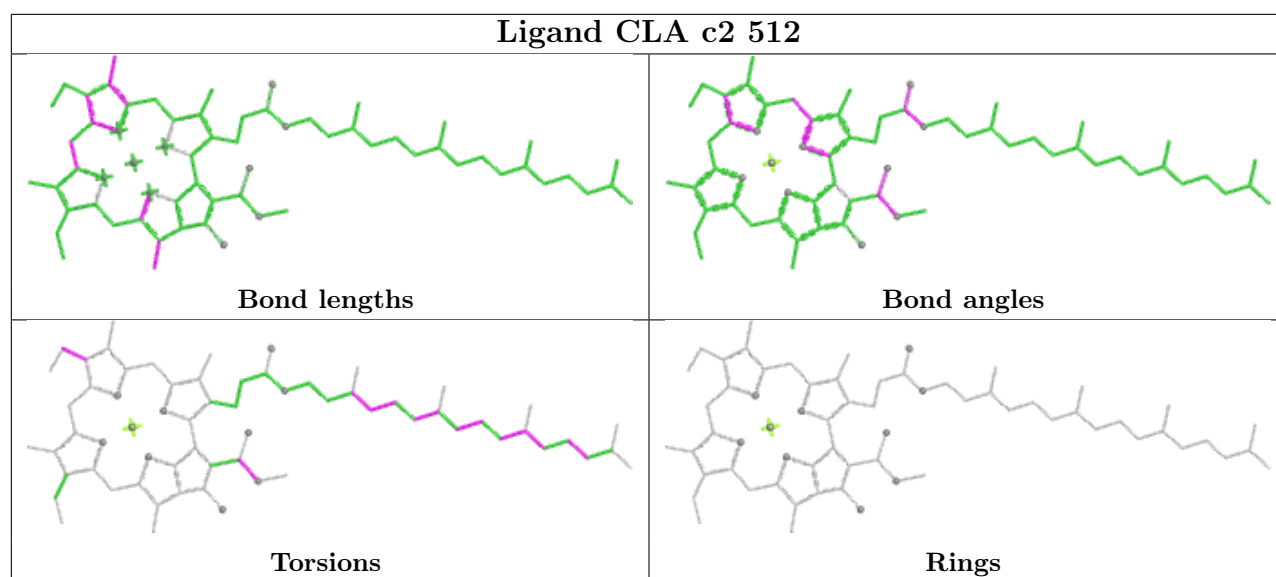
## Ligand CLA C2 516

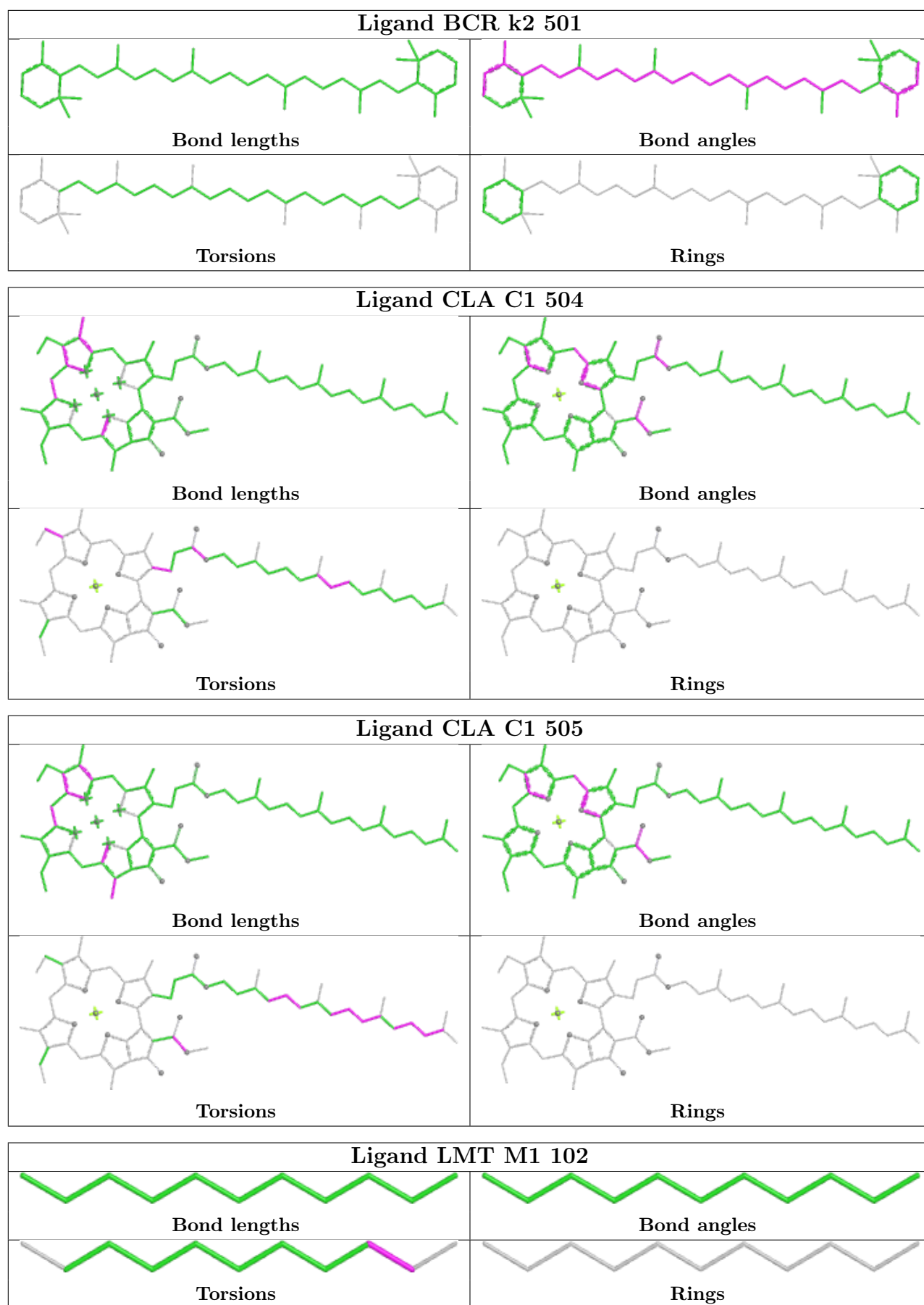


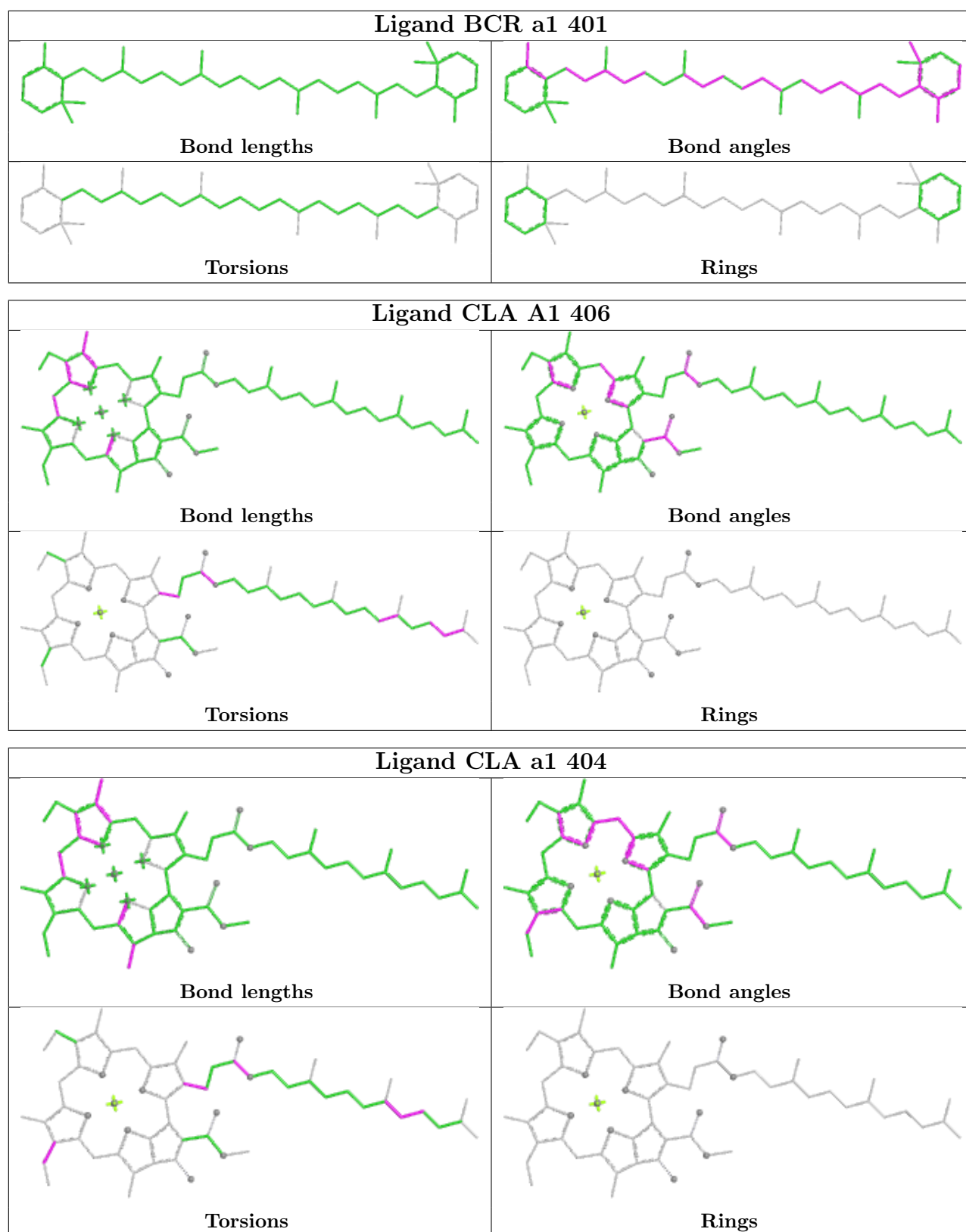
## Ligand CLA C2 509

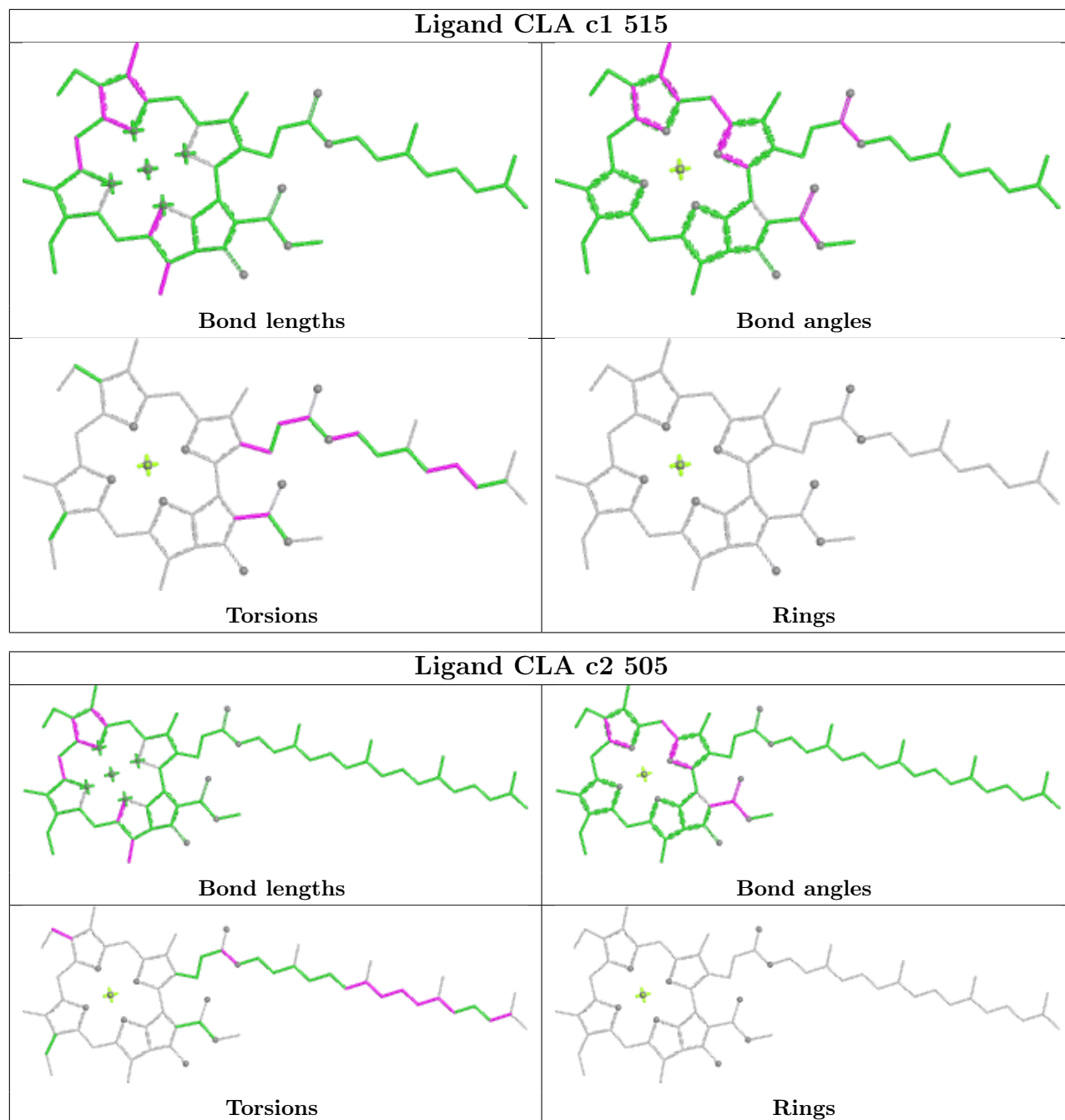


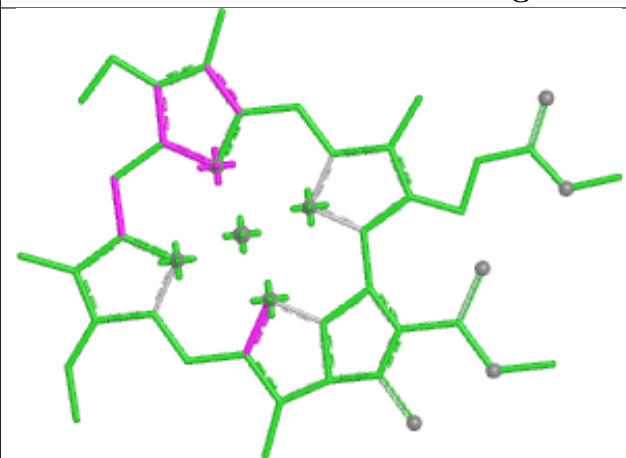
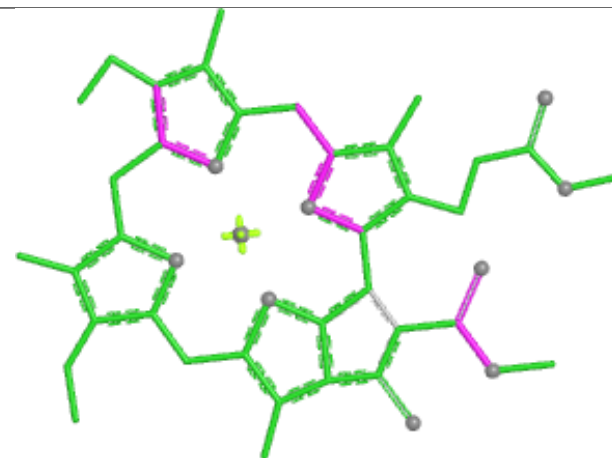
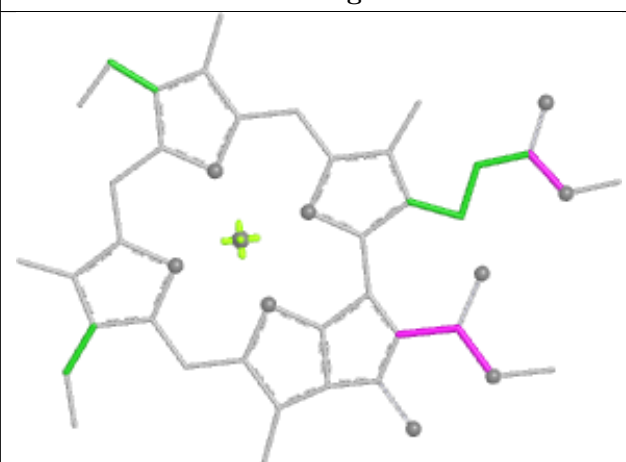
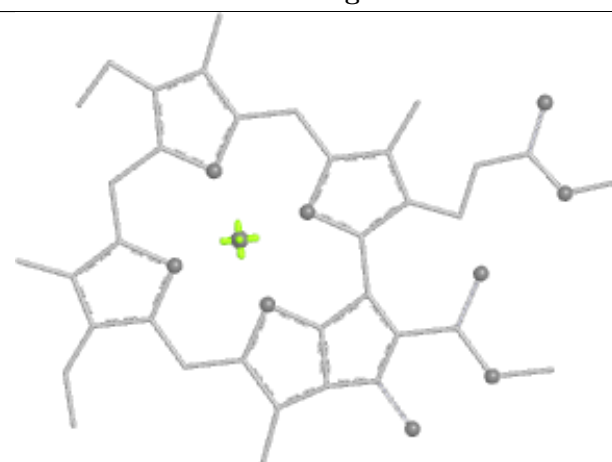
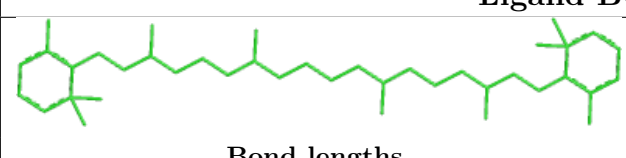
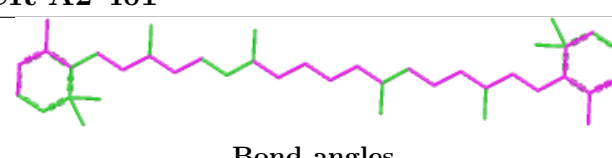
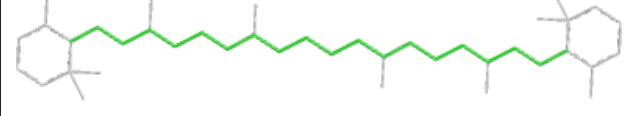
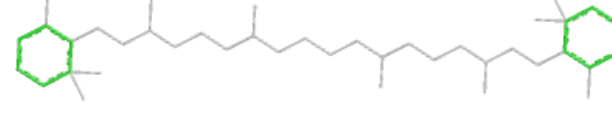




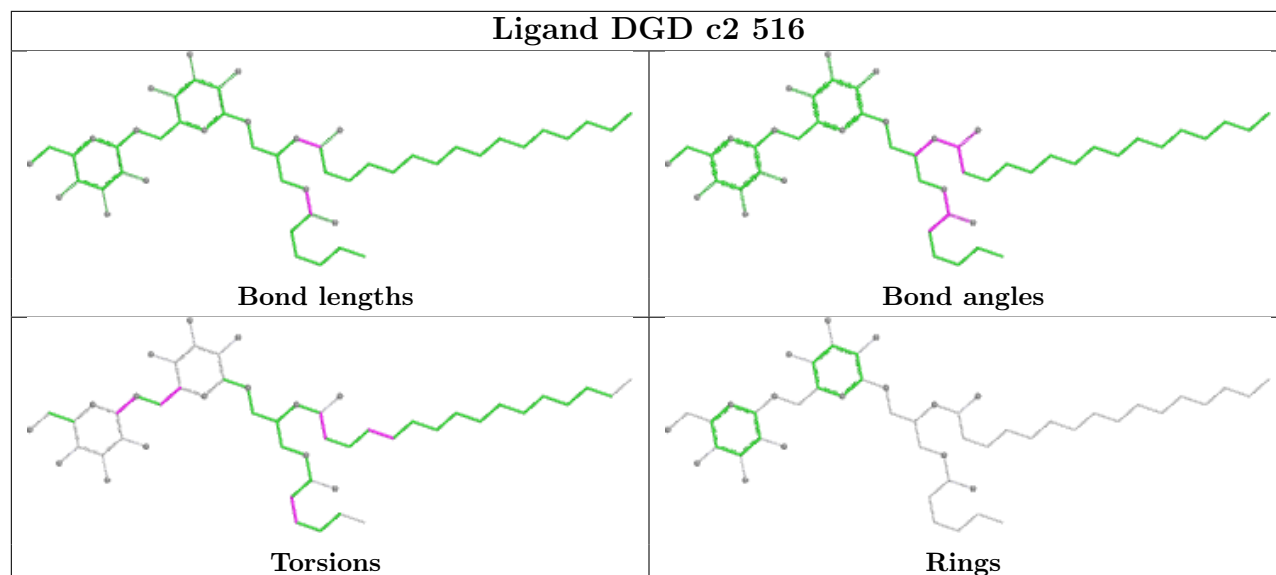
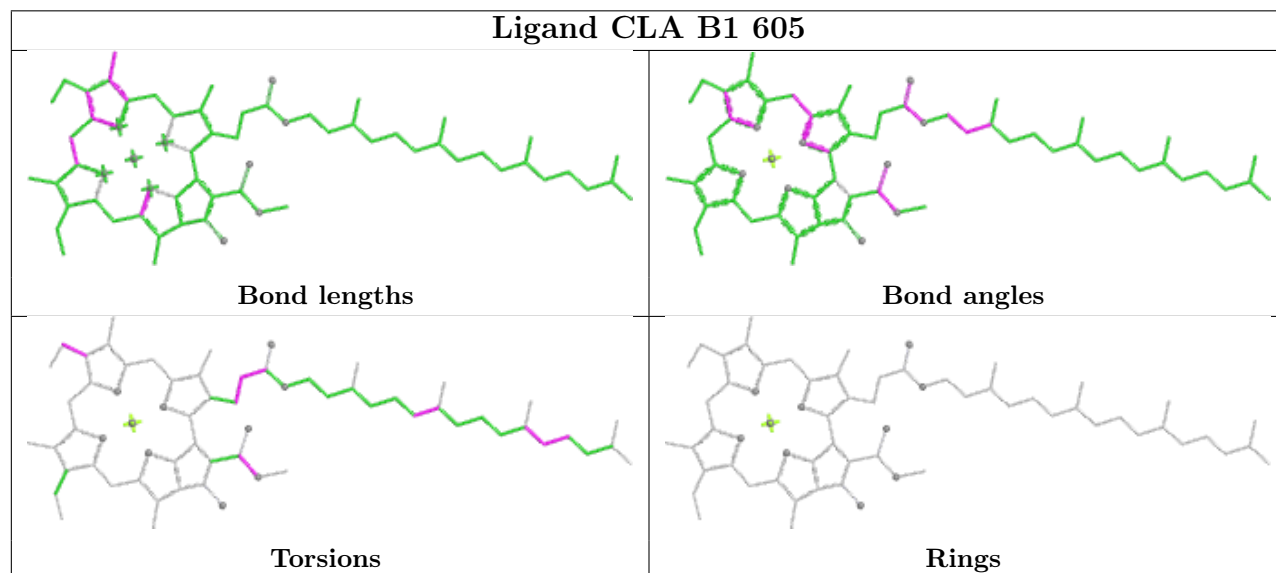
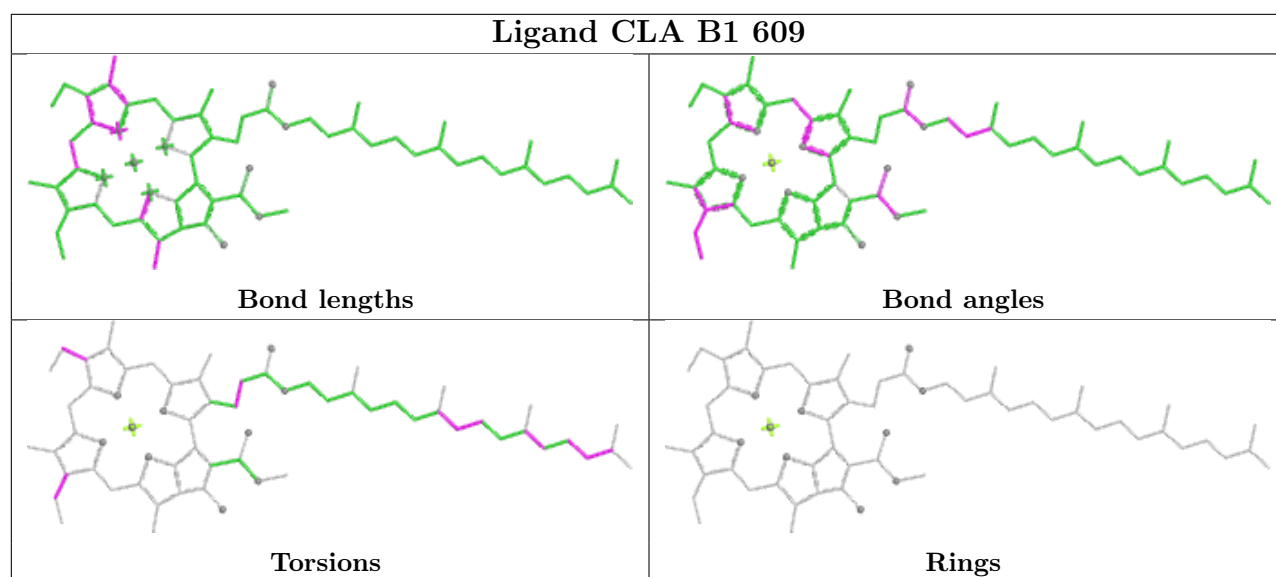


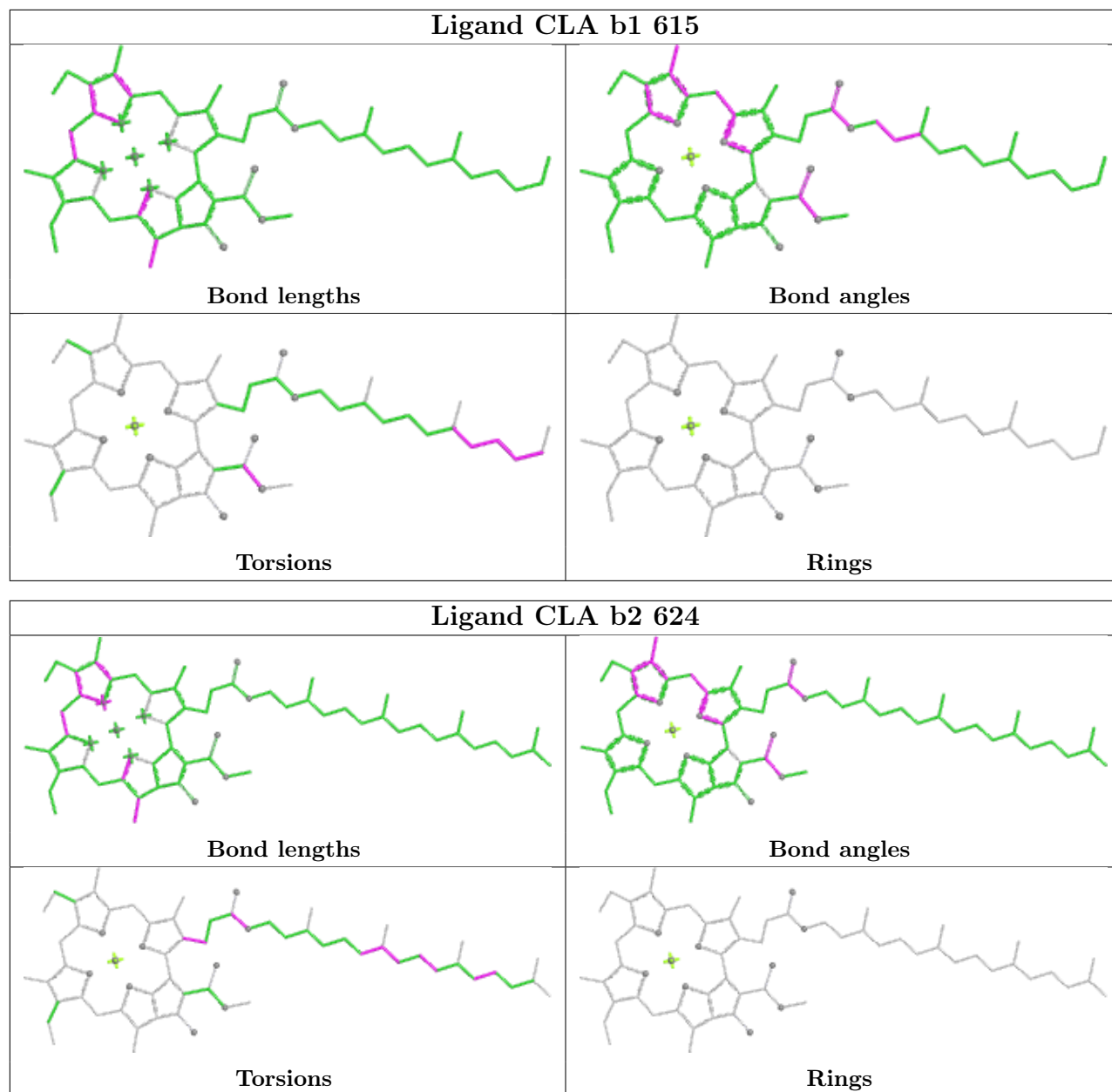


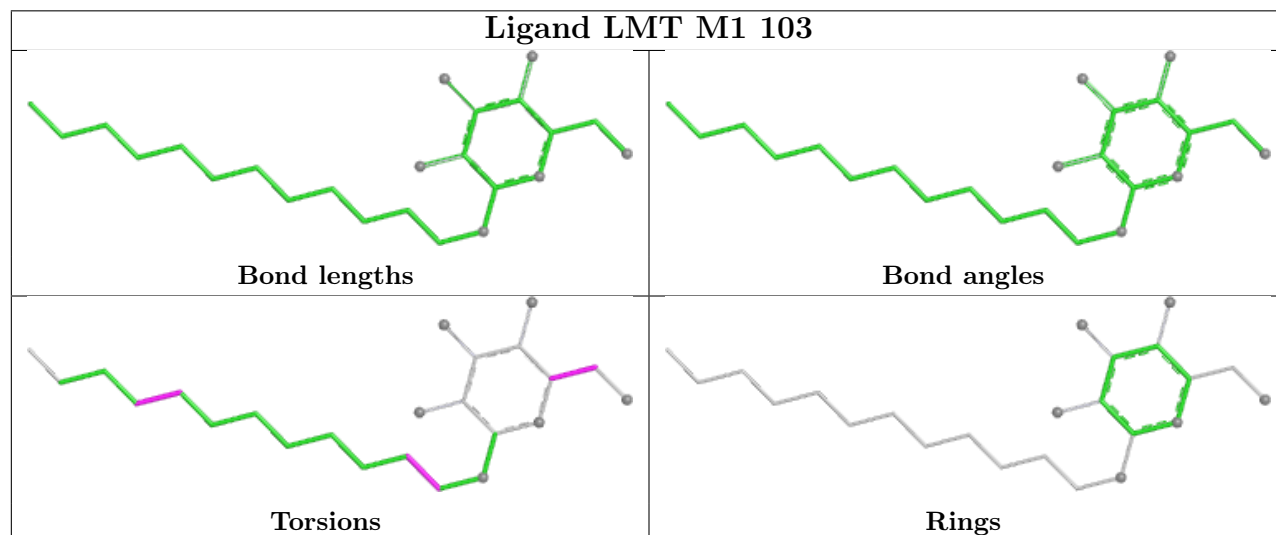
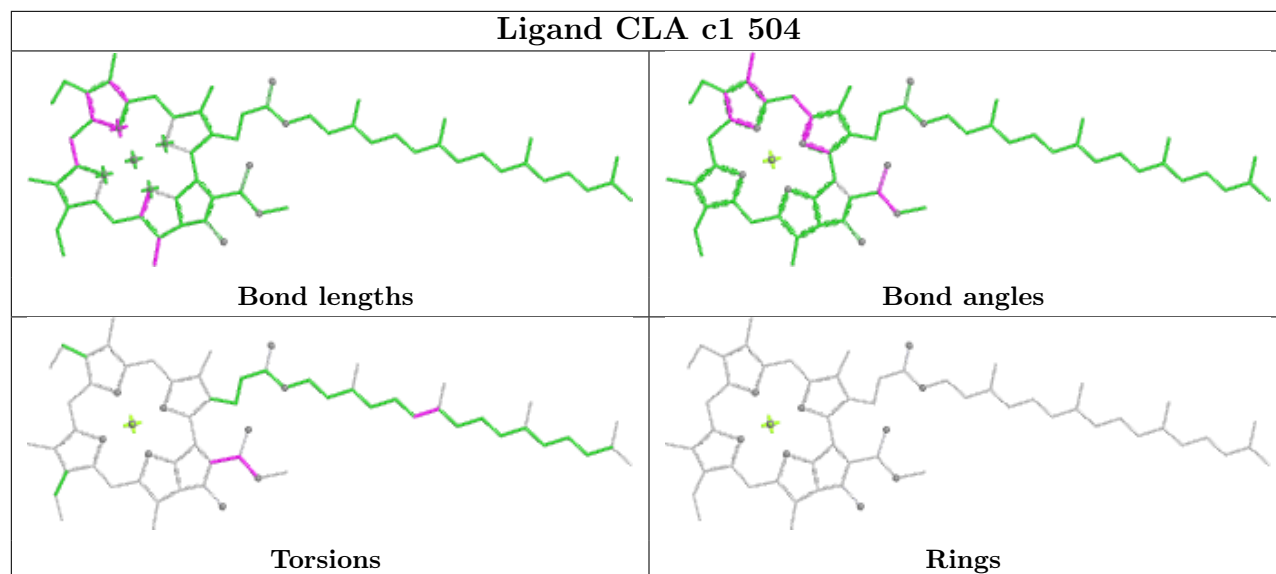


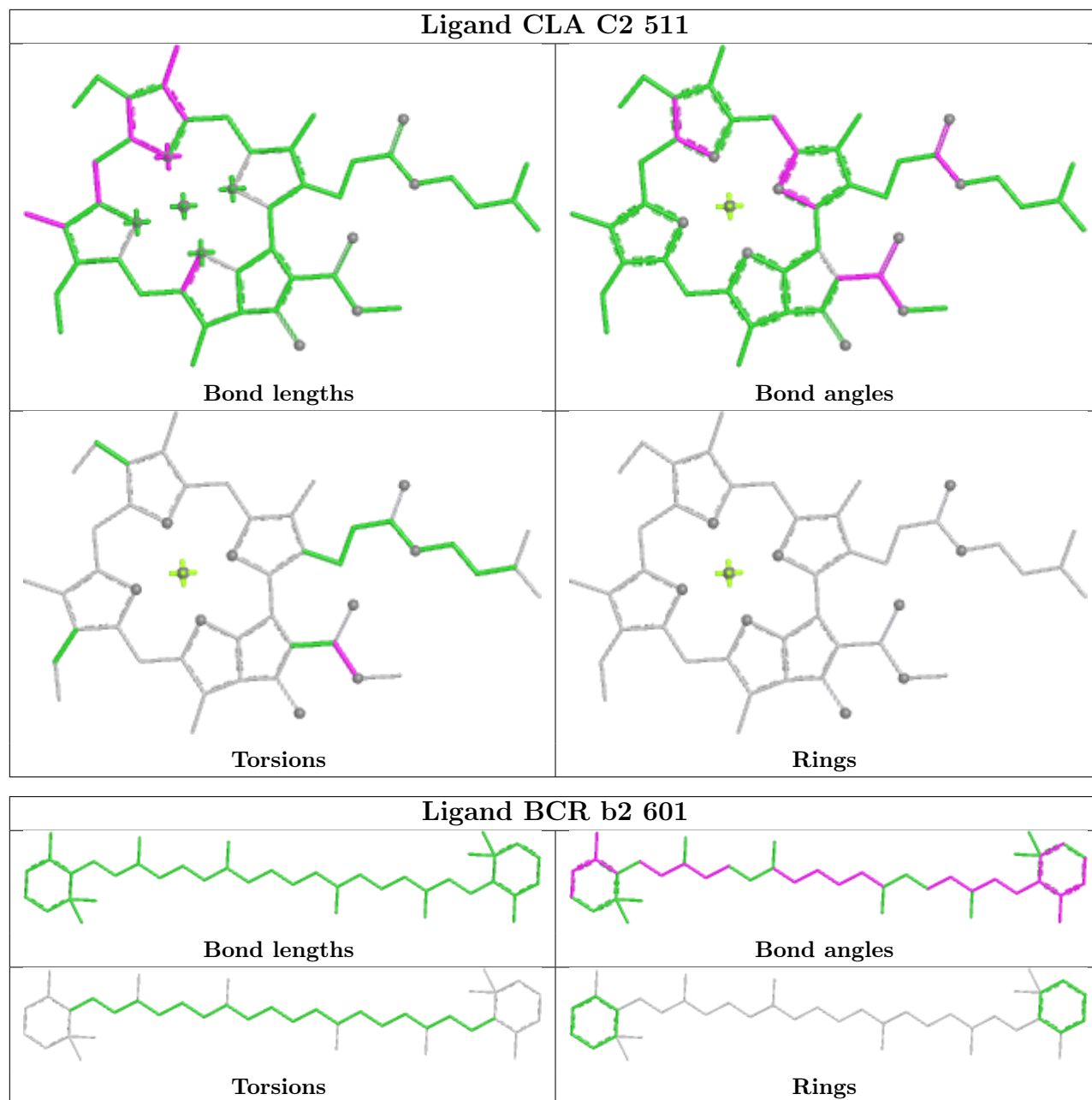
| Ligand CLA C2 504                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|   |   |
| Torsions                                                                            | Rings                                                                                |
| Ligand BCR A2 401                                                                   |                                                                                      |
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

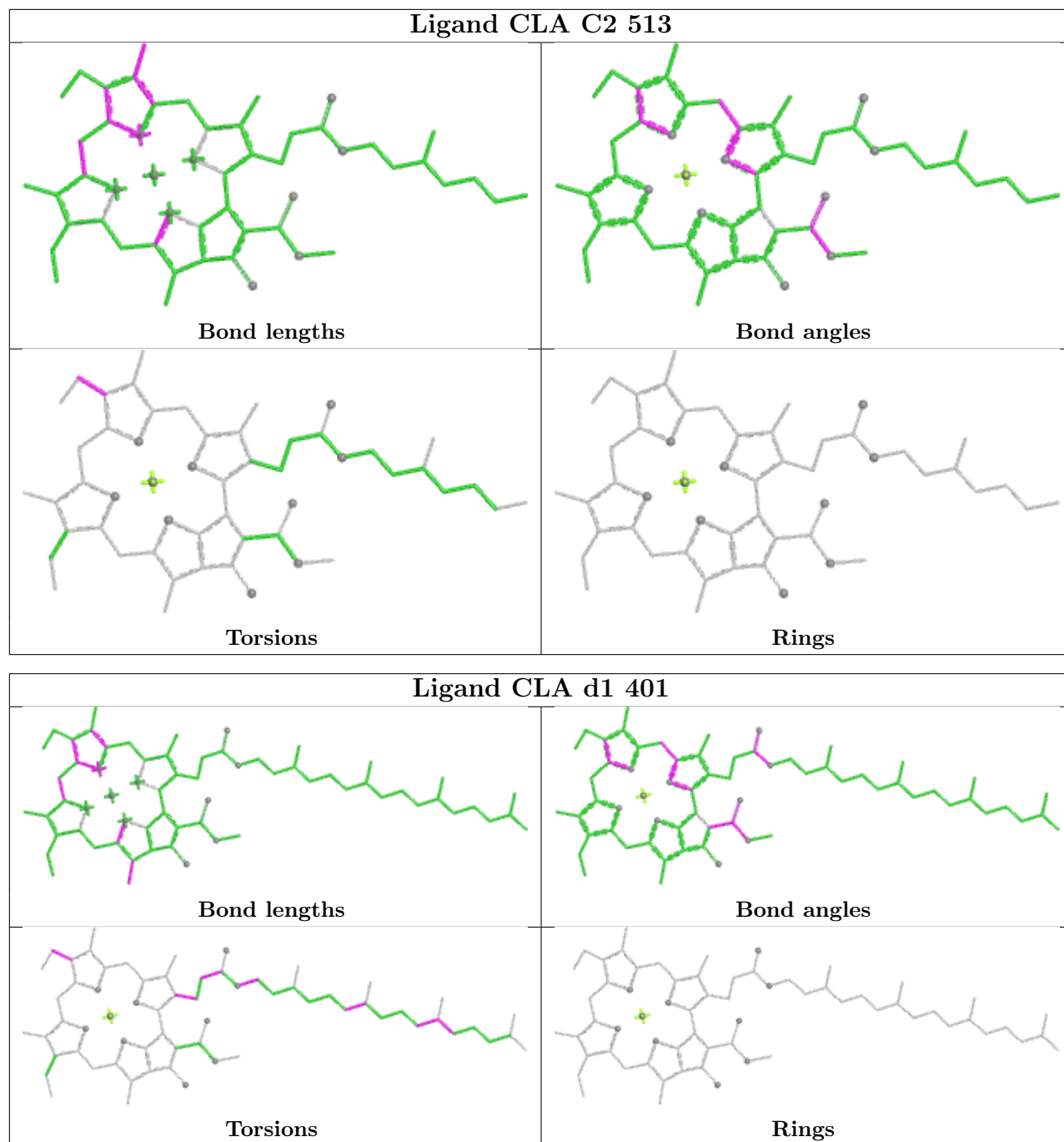




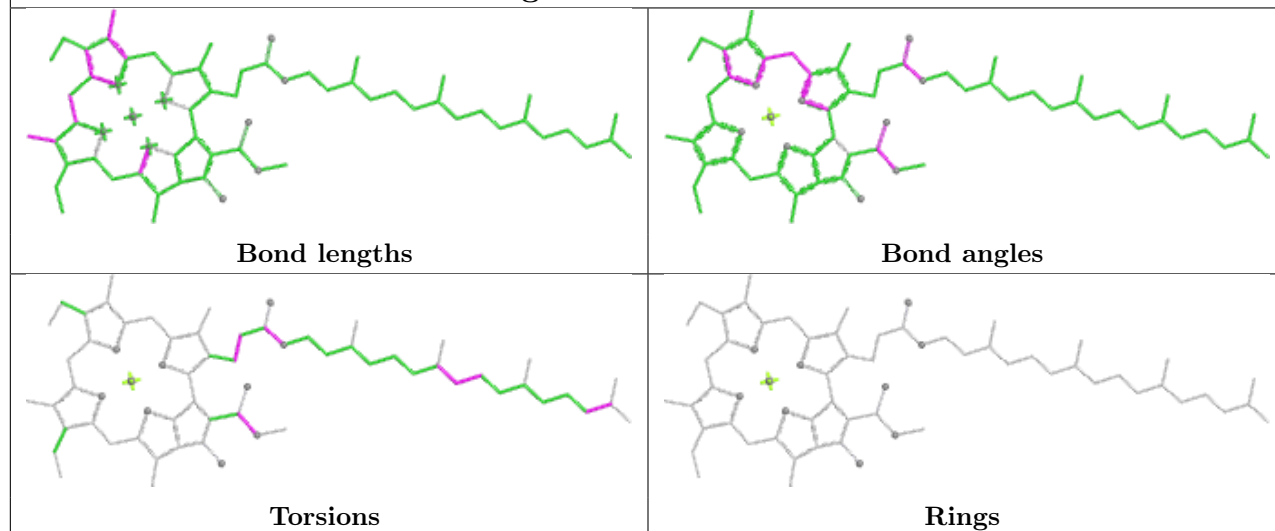




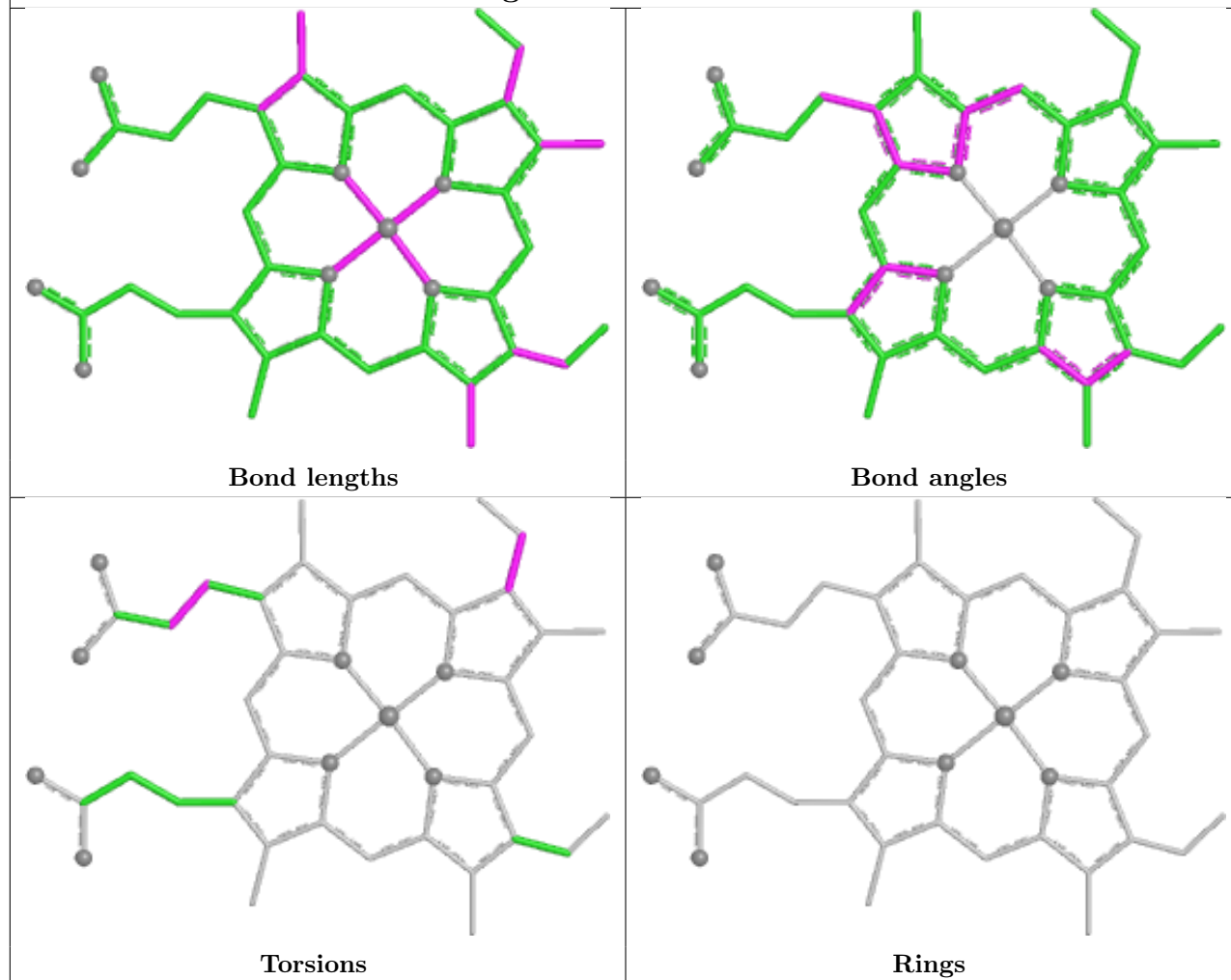


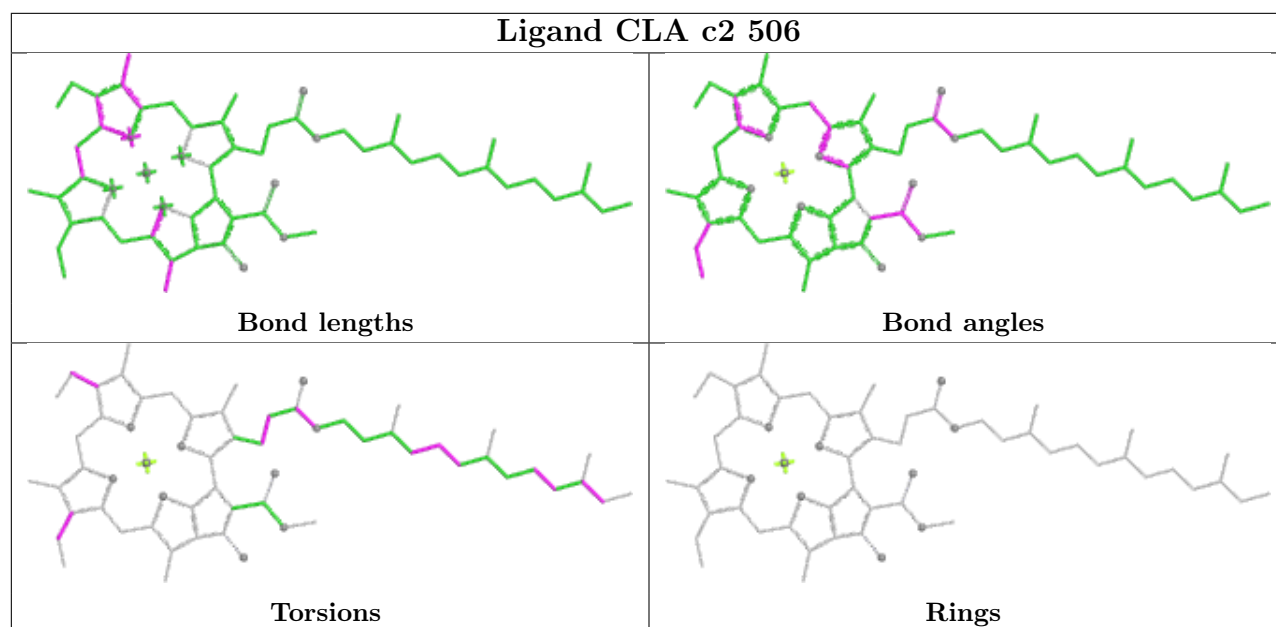
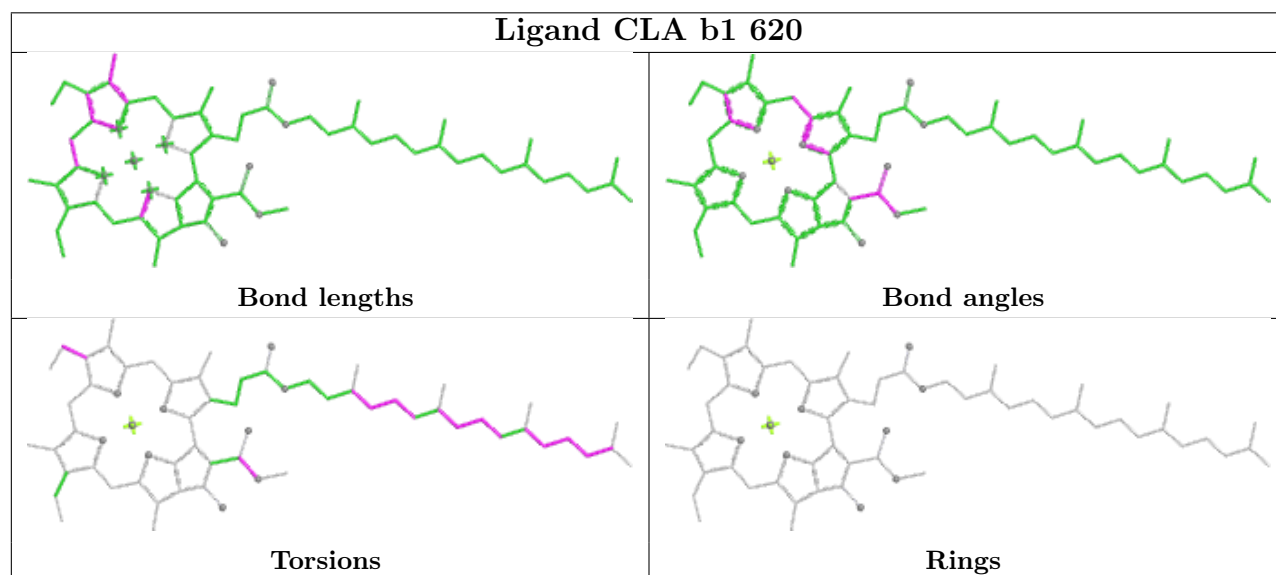
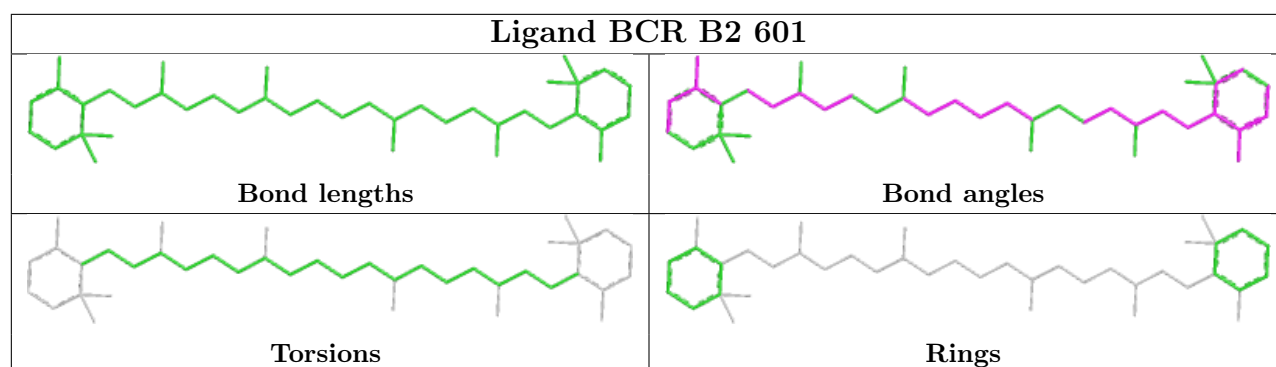


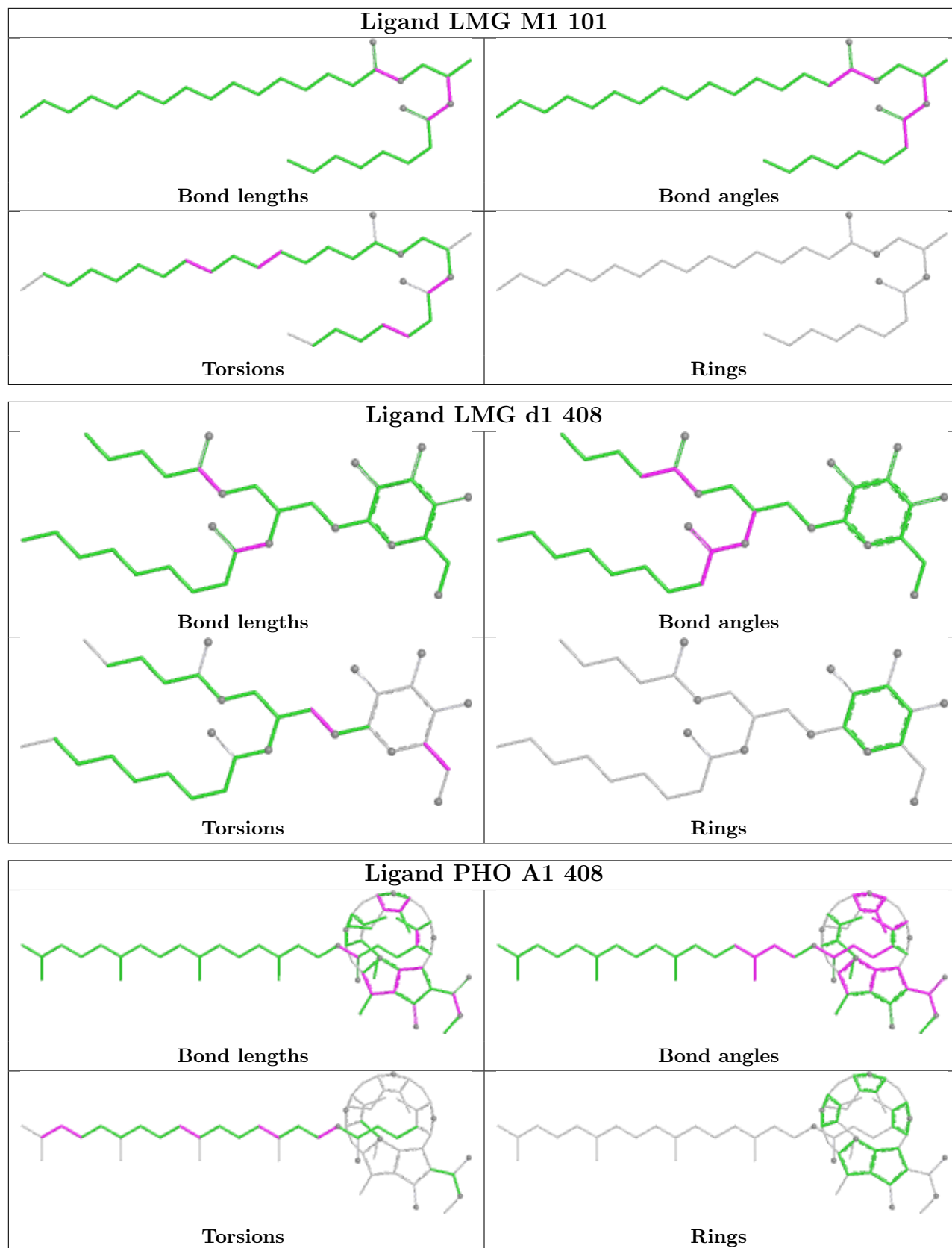
## Ligand CLA A2 402



## Ligand HEM v2 201

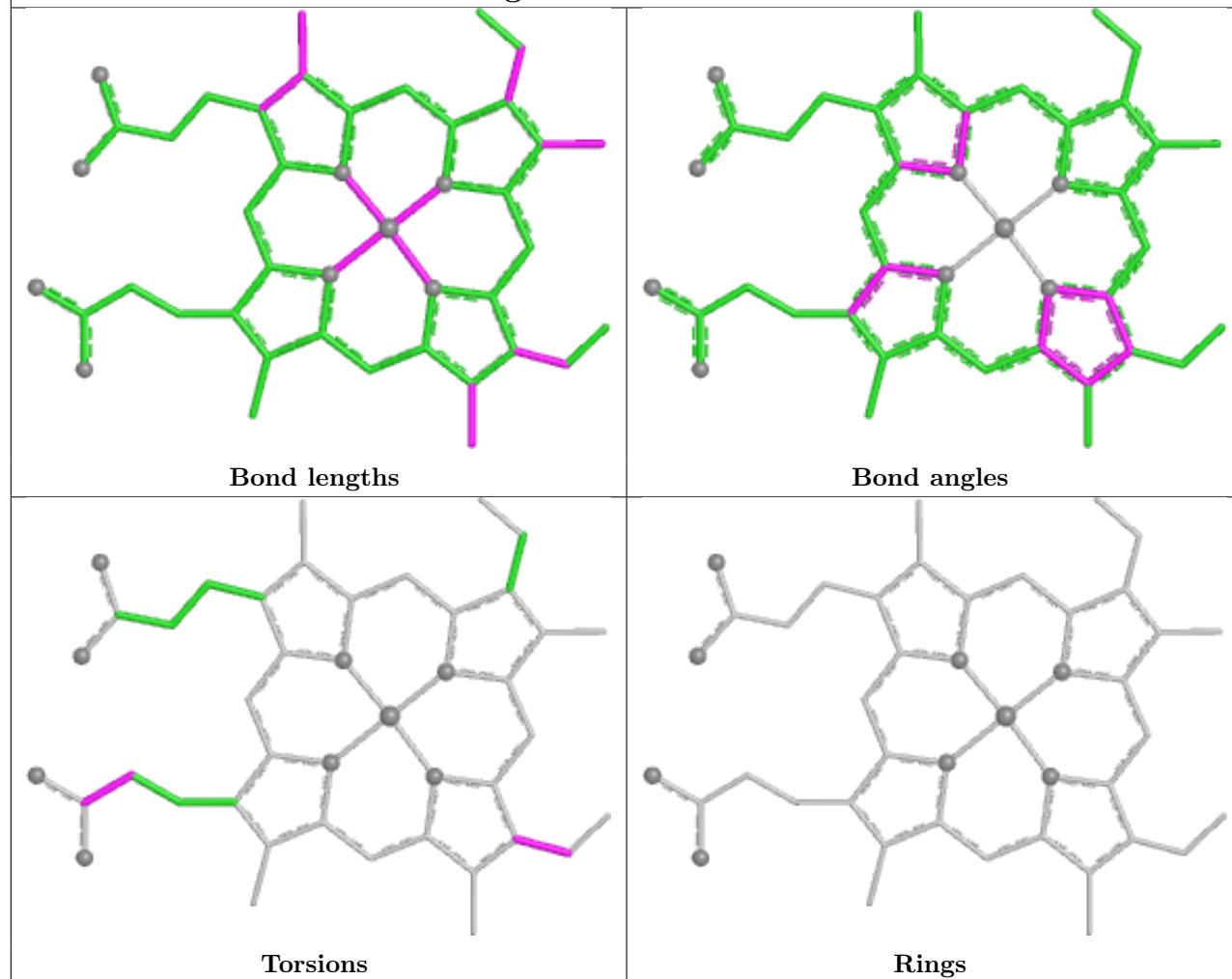




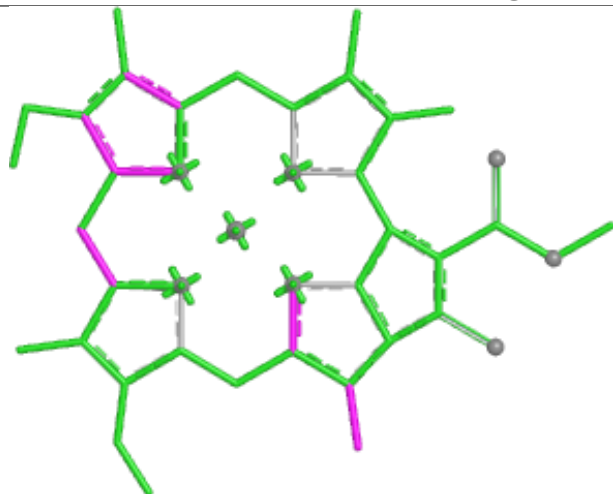




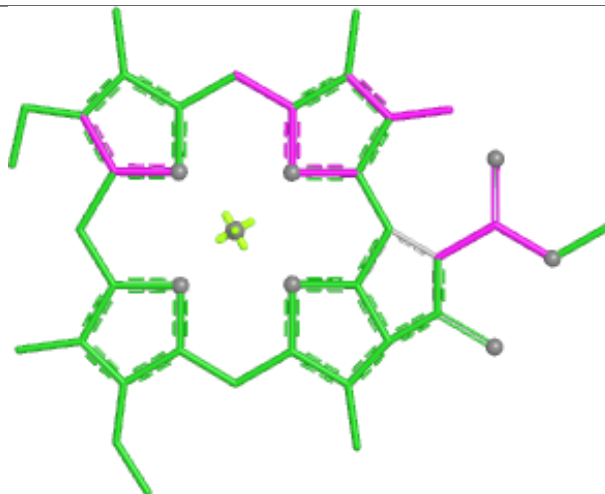
## Ligand HEM e2 101



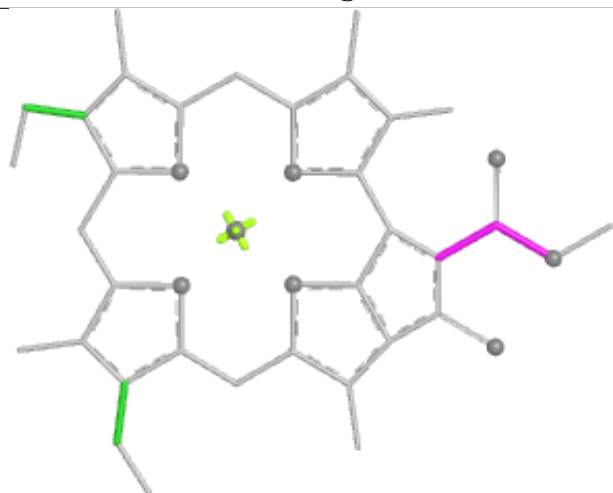
## Ligand CLA C2 518



Bond lengths



Bond angles

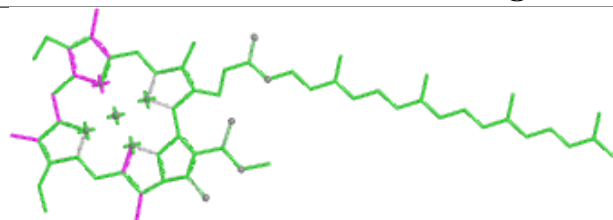


Torsions

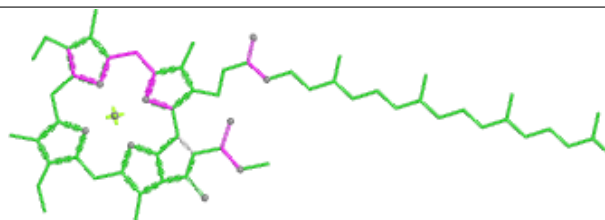


Rings

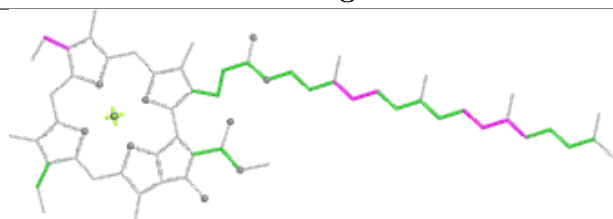
## Ligand CLA b2 612



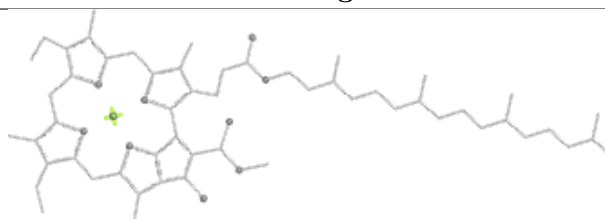
Bond lengths



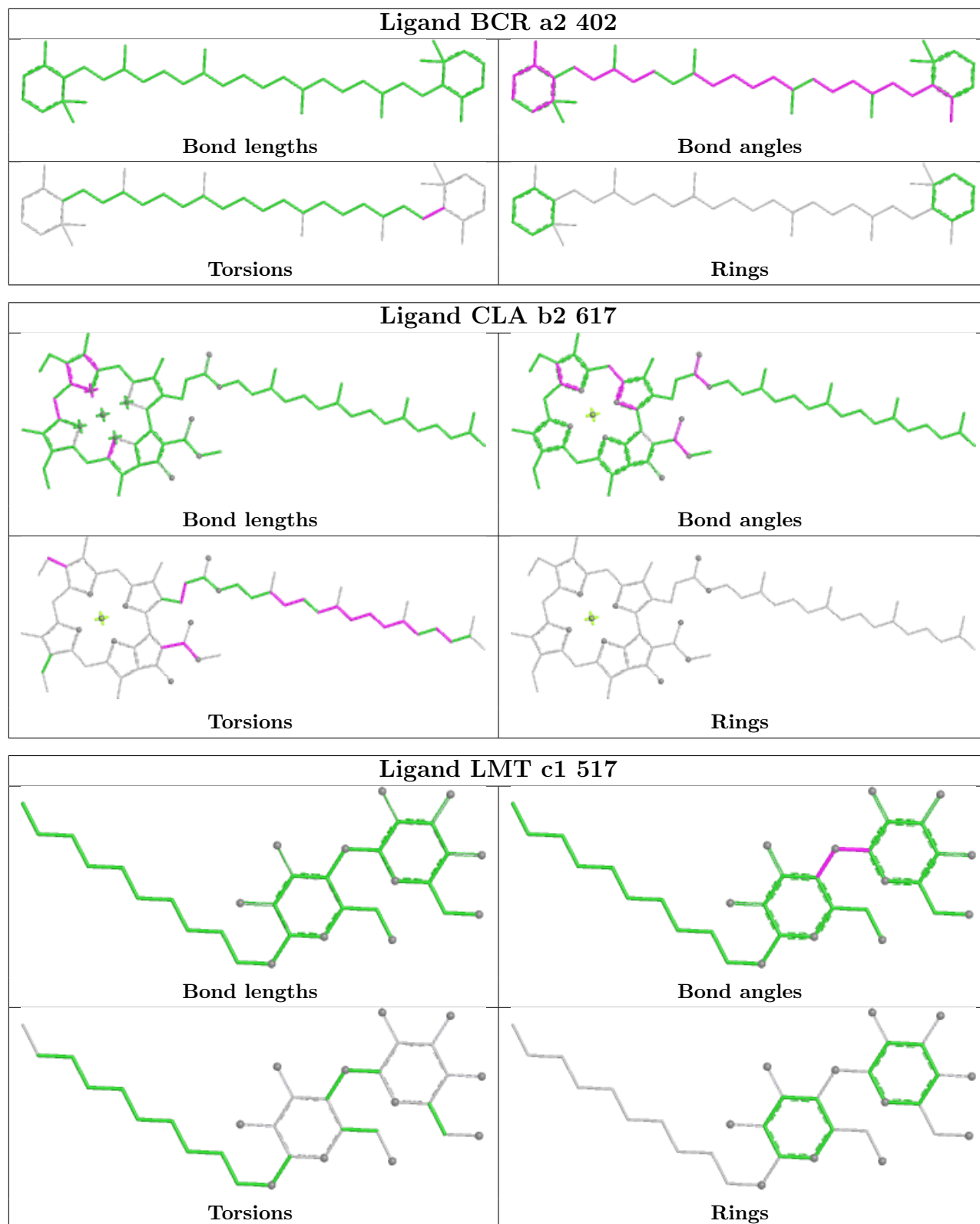
Bond angles

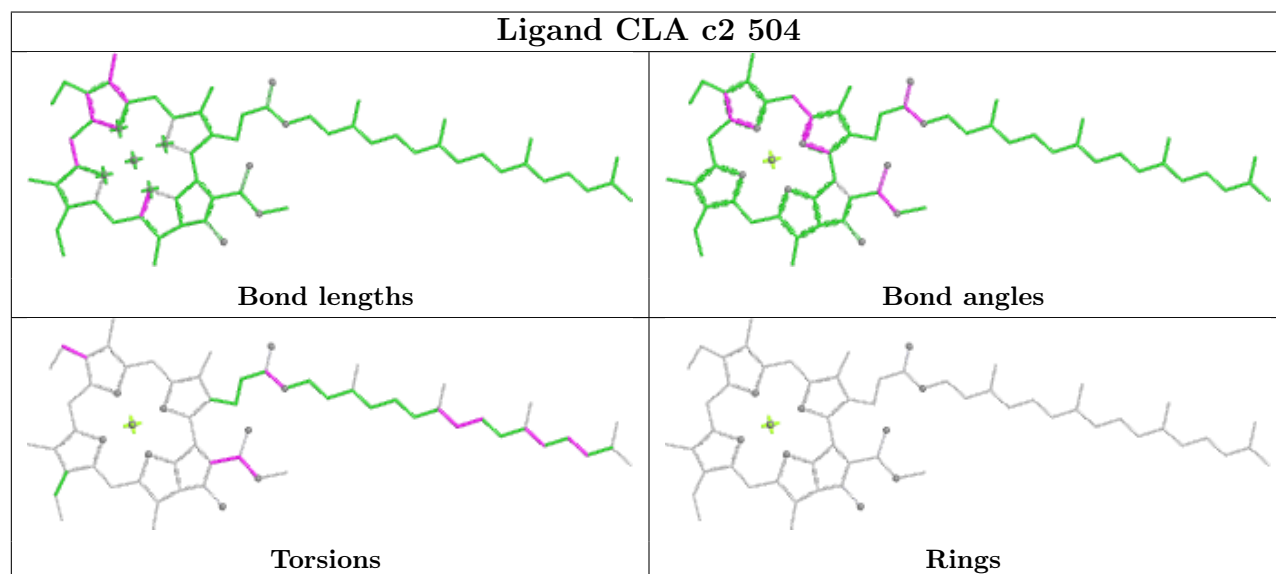
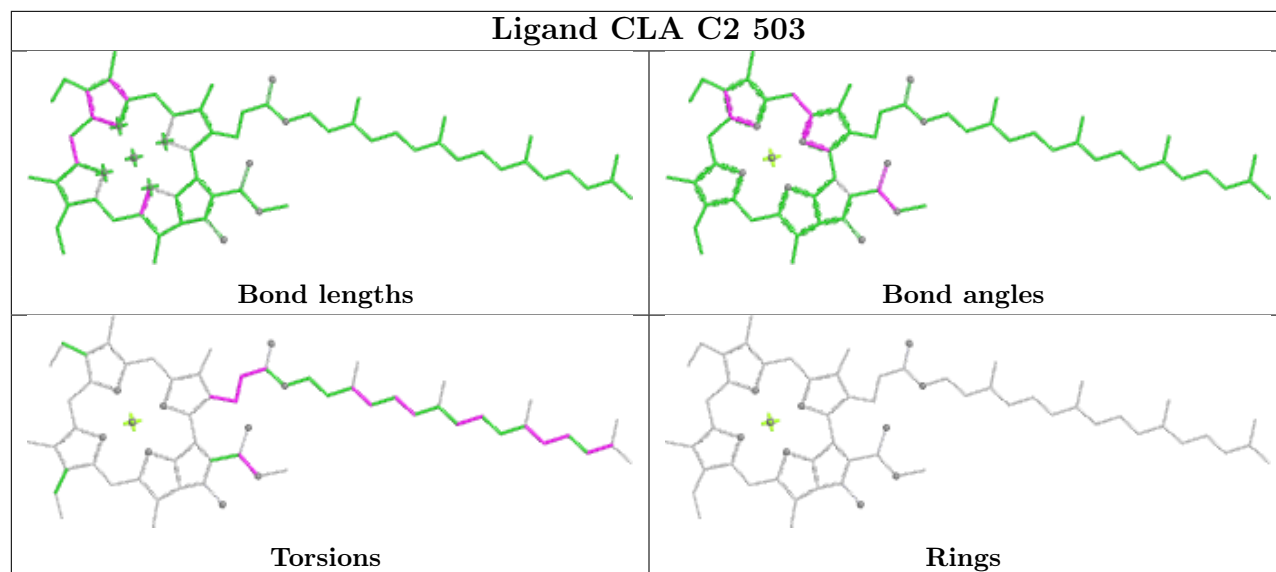


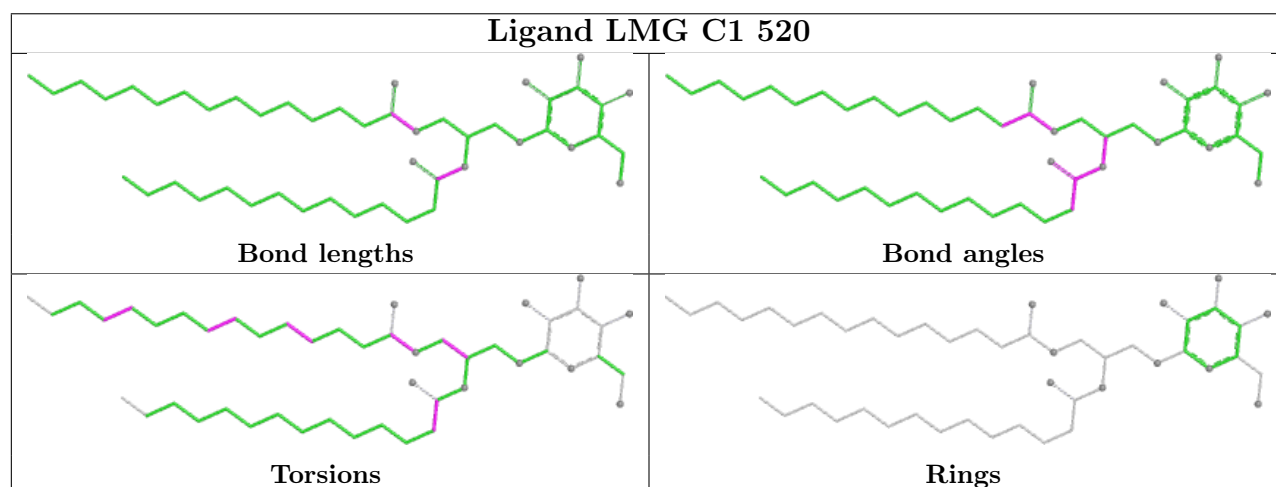
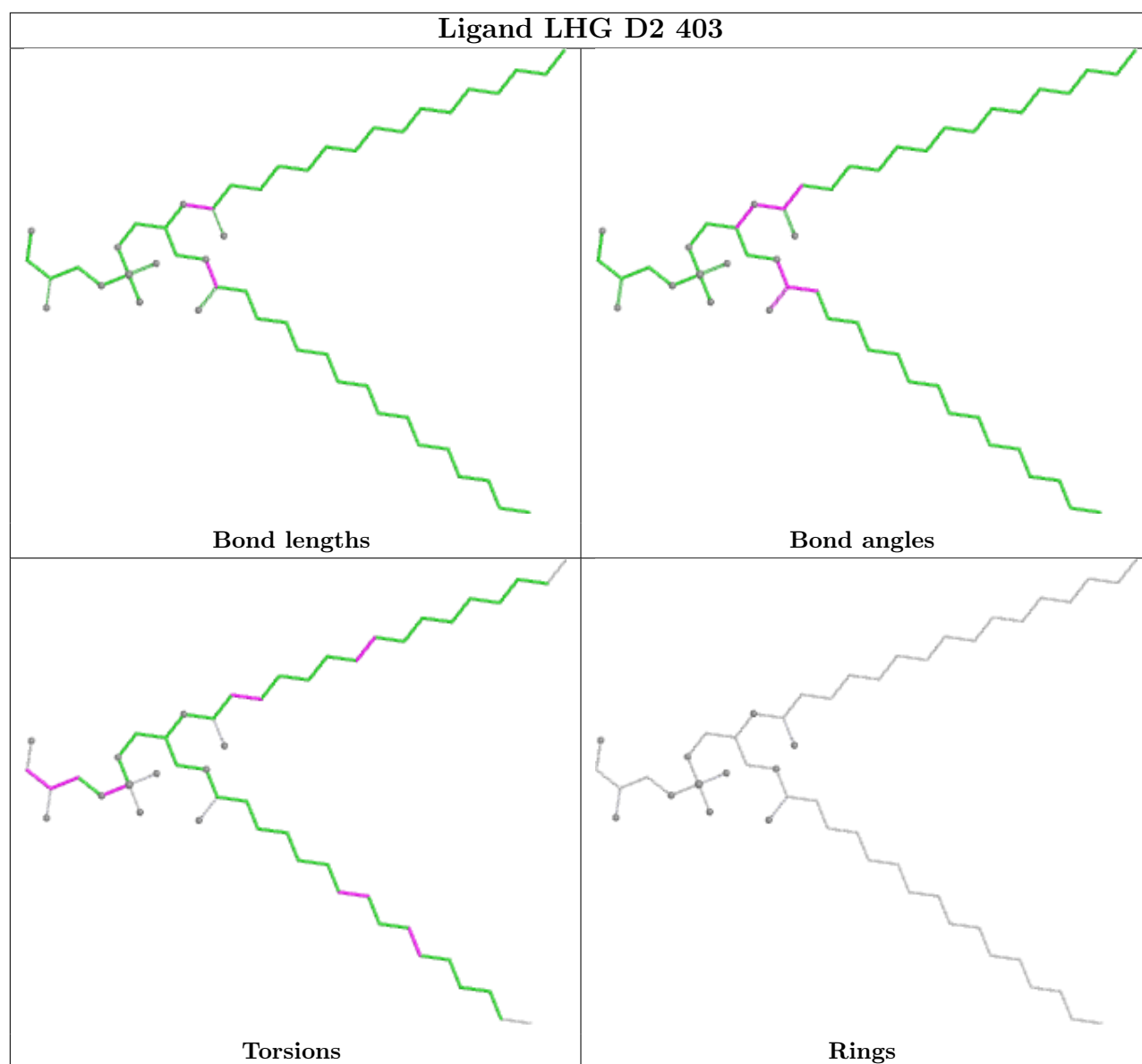
Torsions

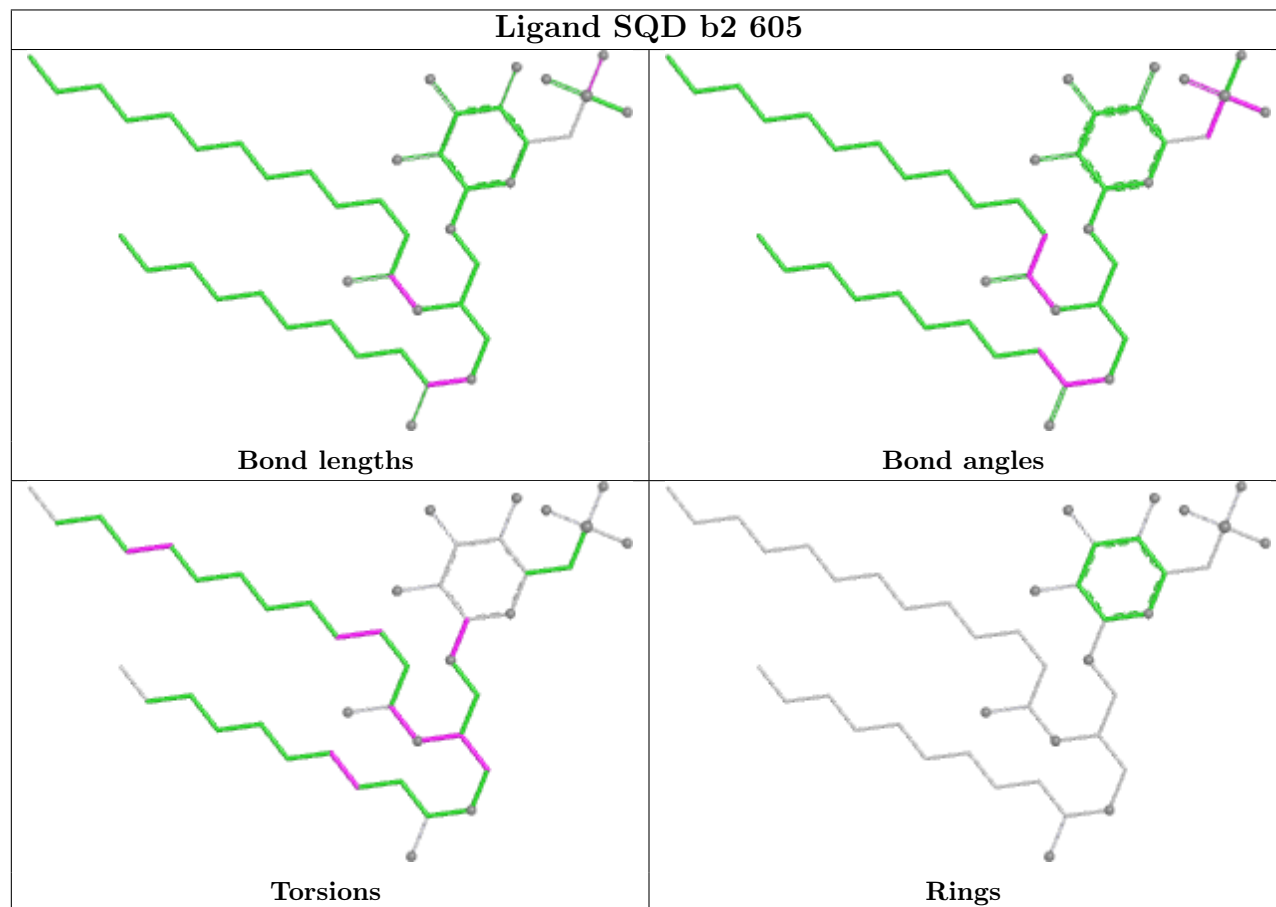
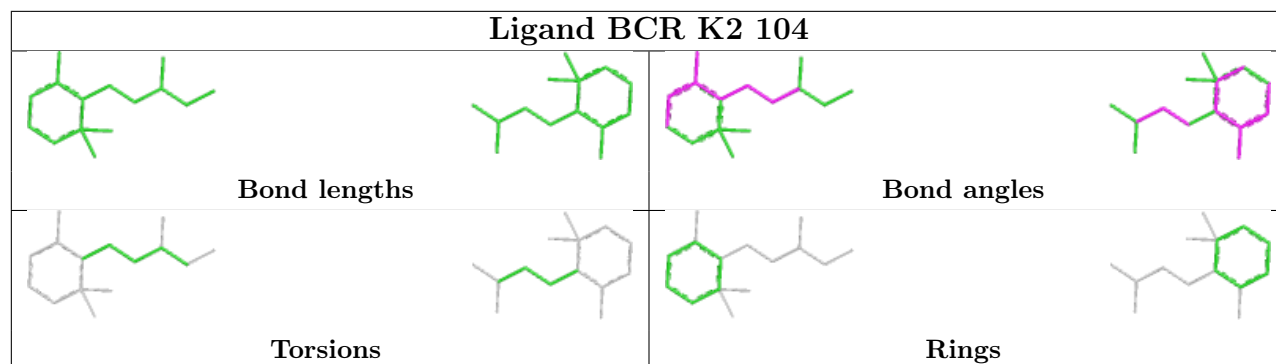


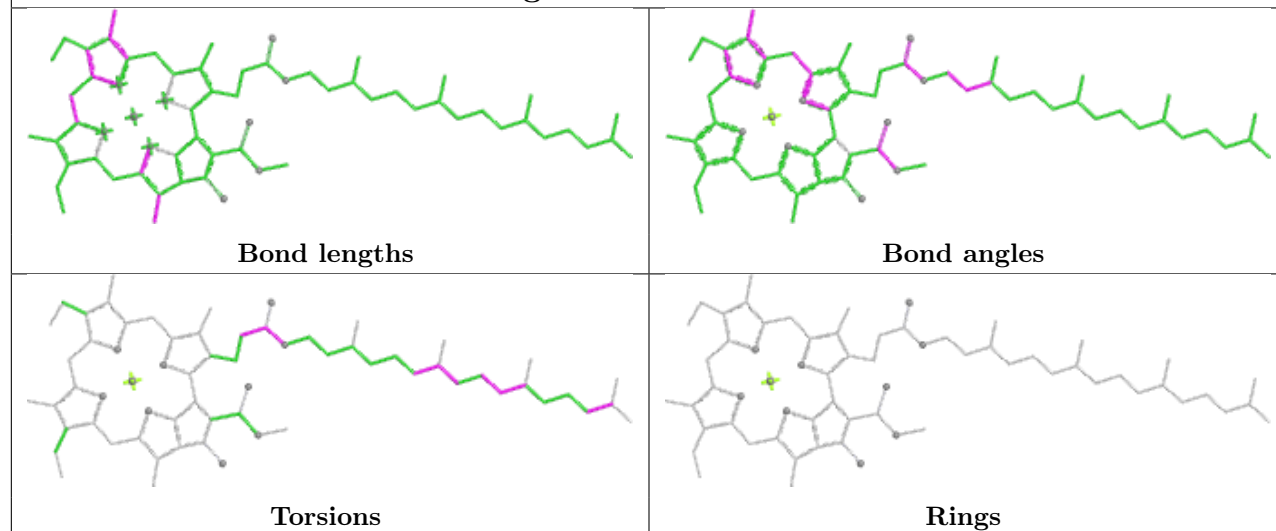
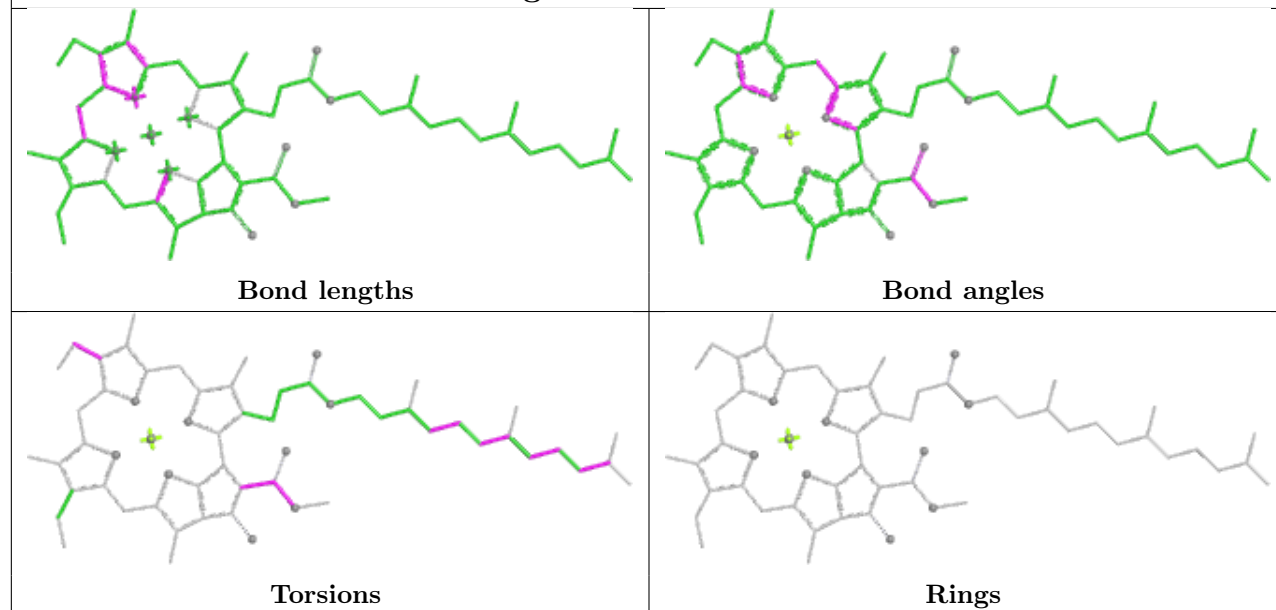
Rings

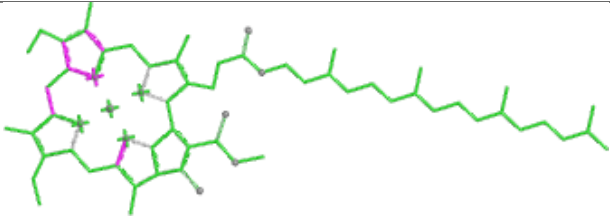
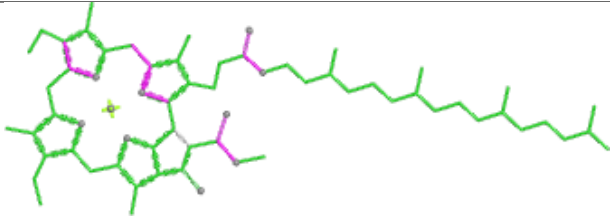
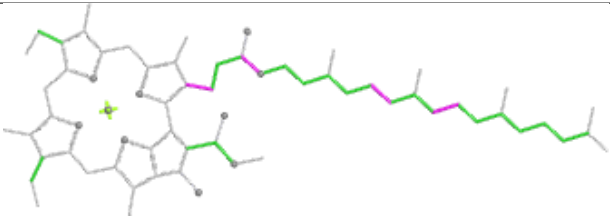
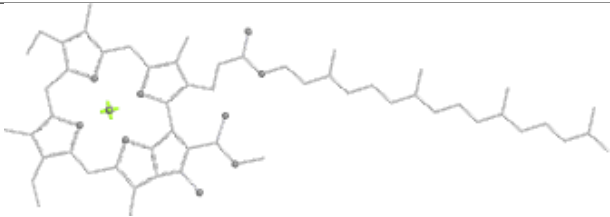
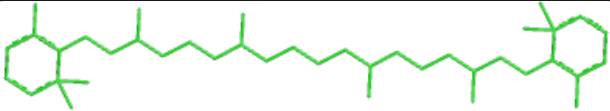
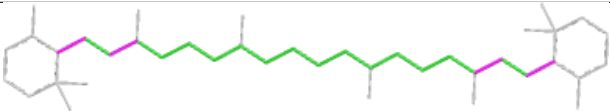
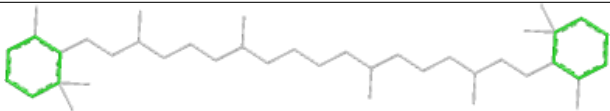






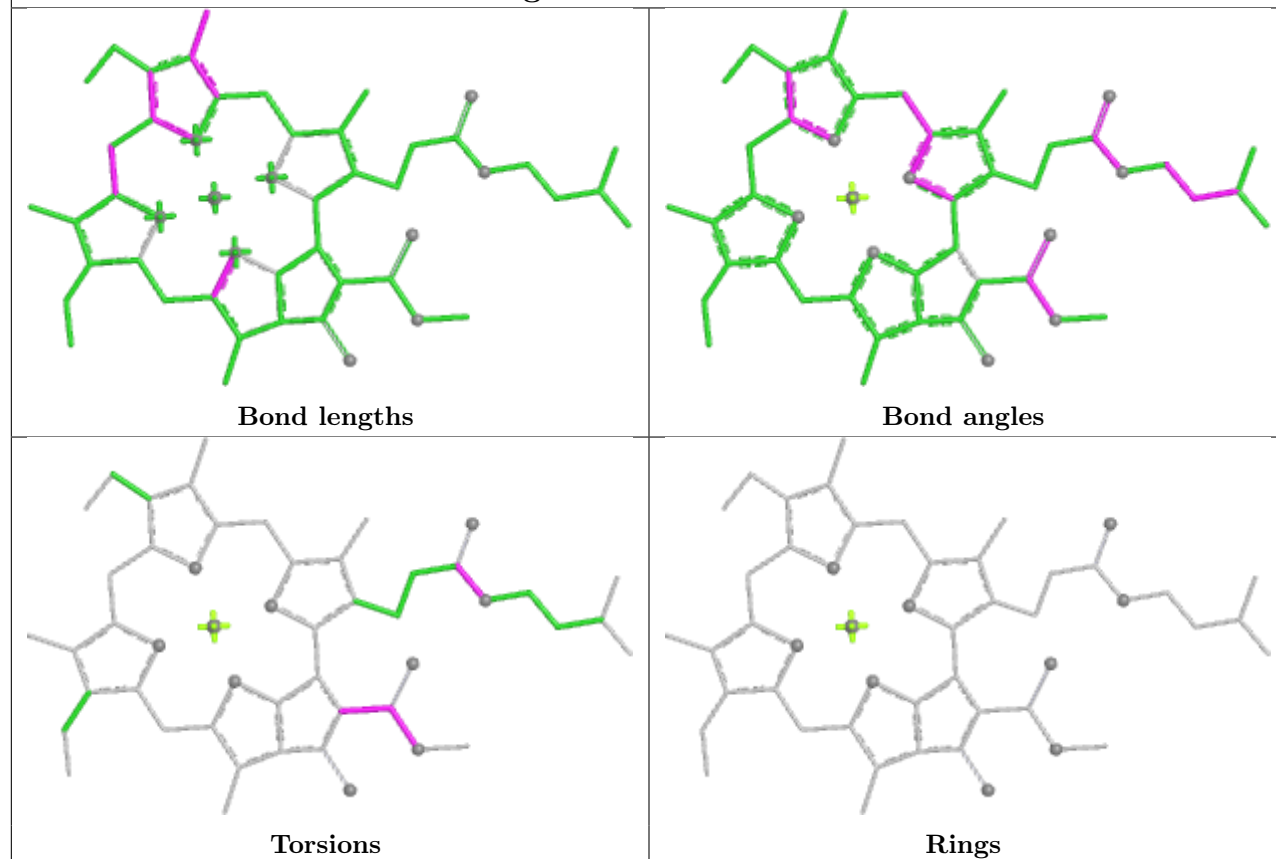


**Ligand CLA B1 614****Ligand CLA C1 503**

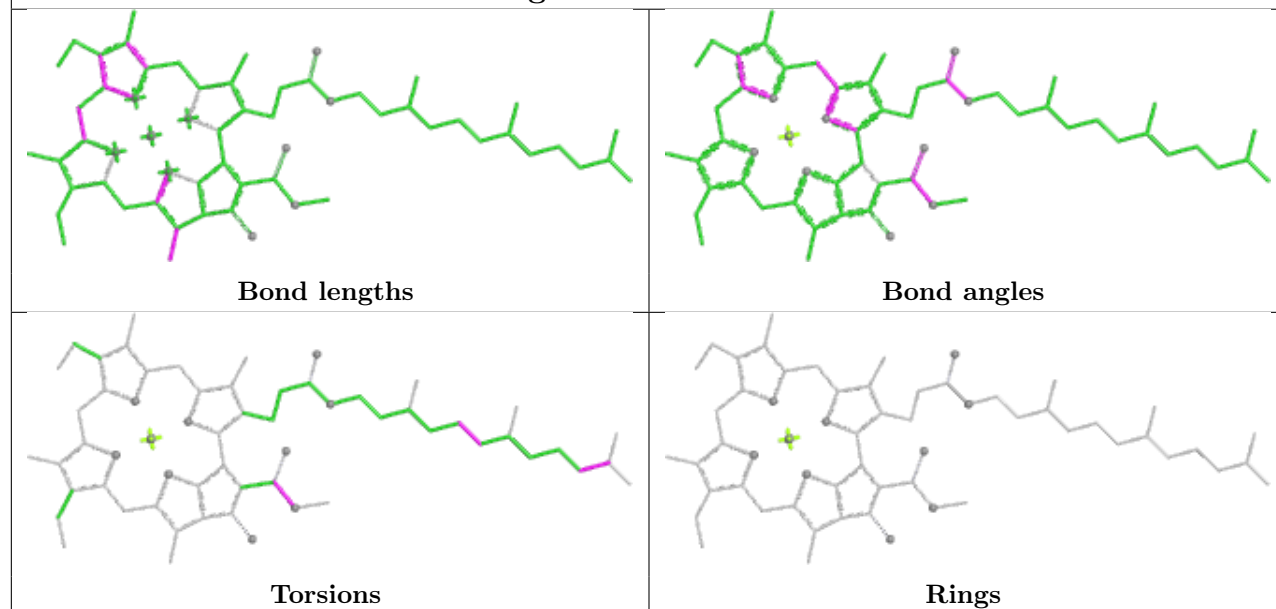
| Ligand CLA c1 505                                                                                     |                                                                                                       |
|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCR d2 401                                                                                     |                                                                                                       |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |

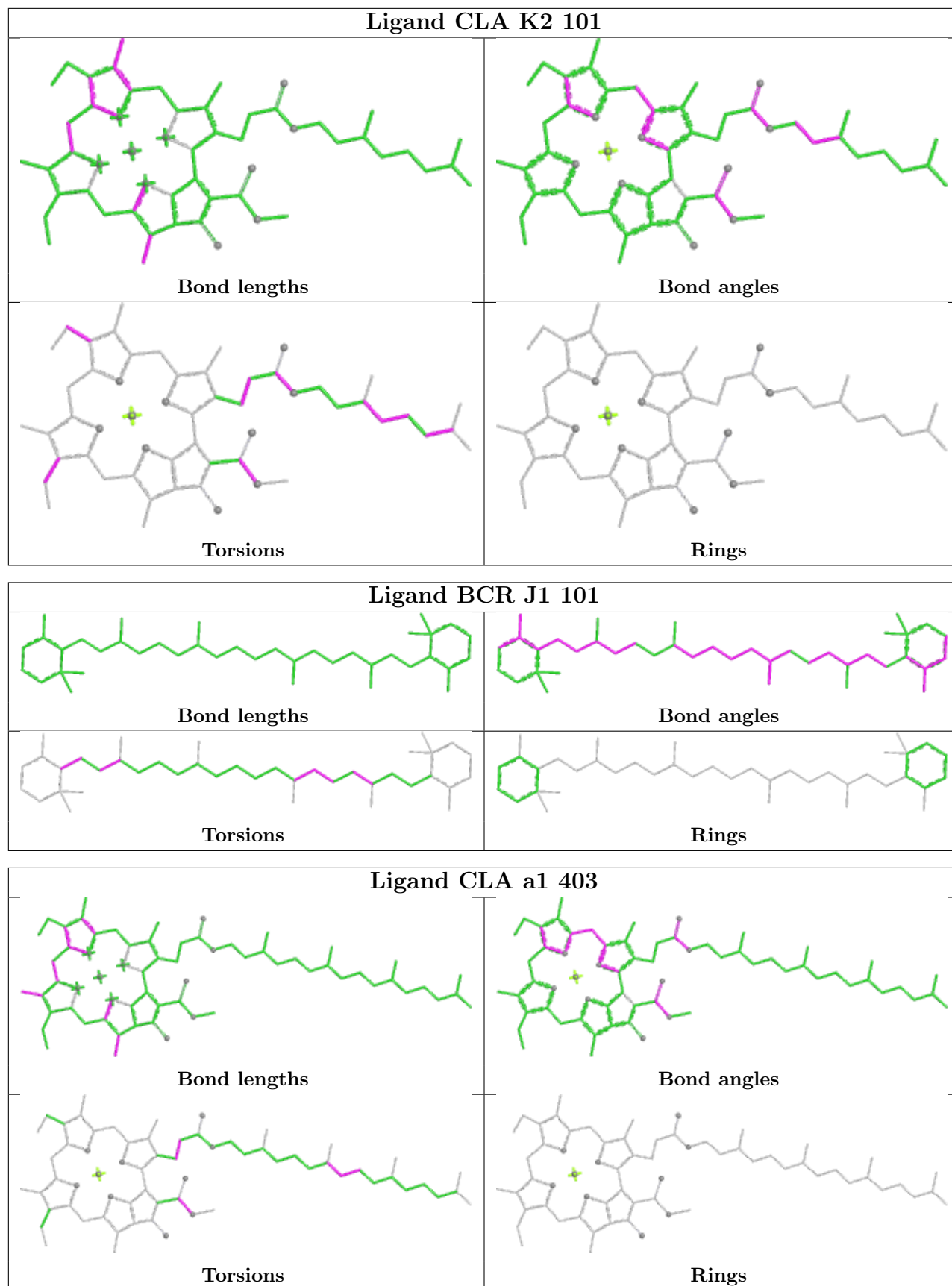


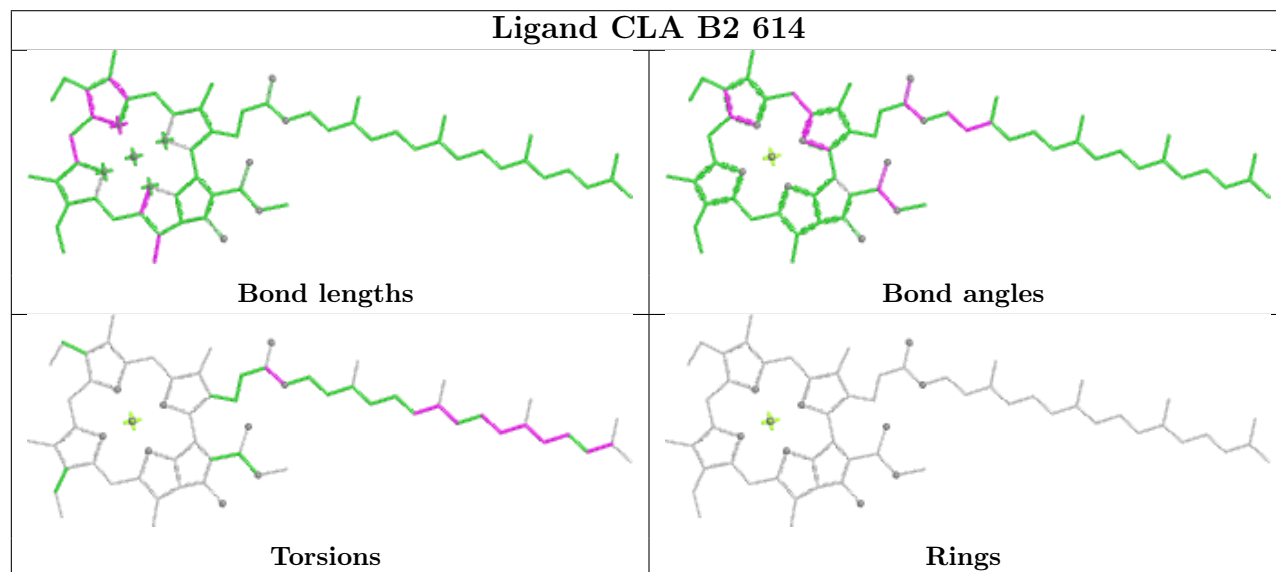
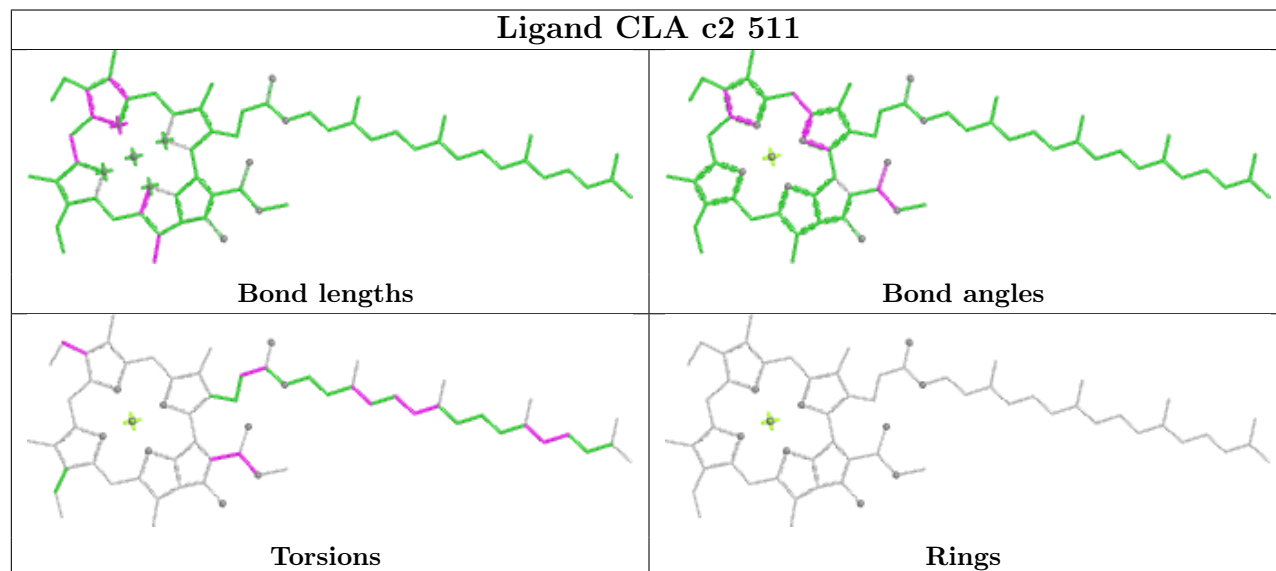
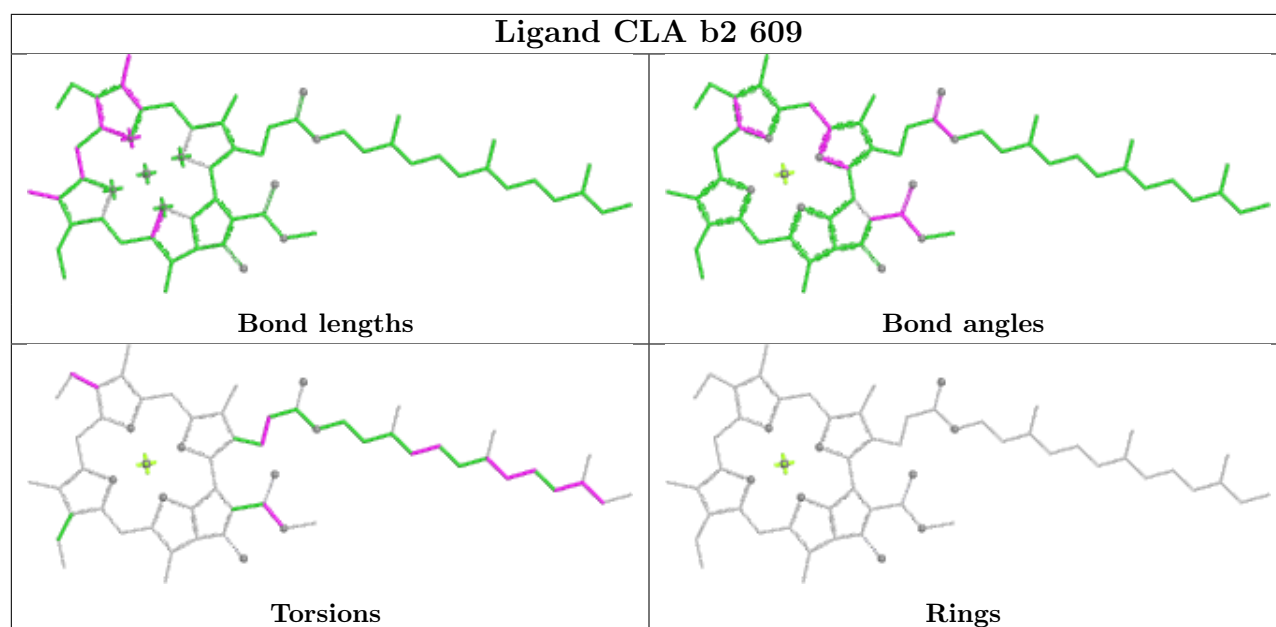
## Ligand CLA C2 508

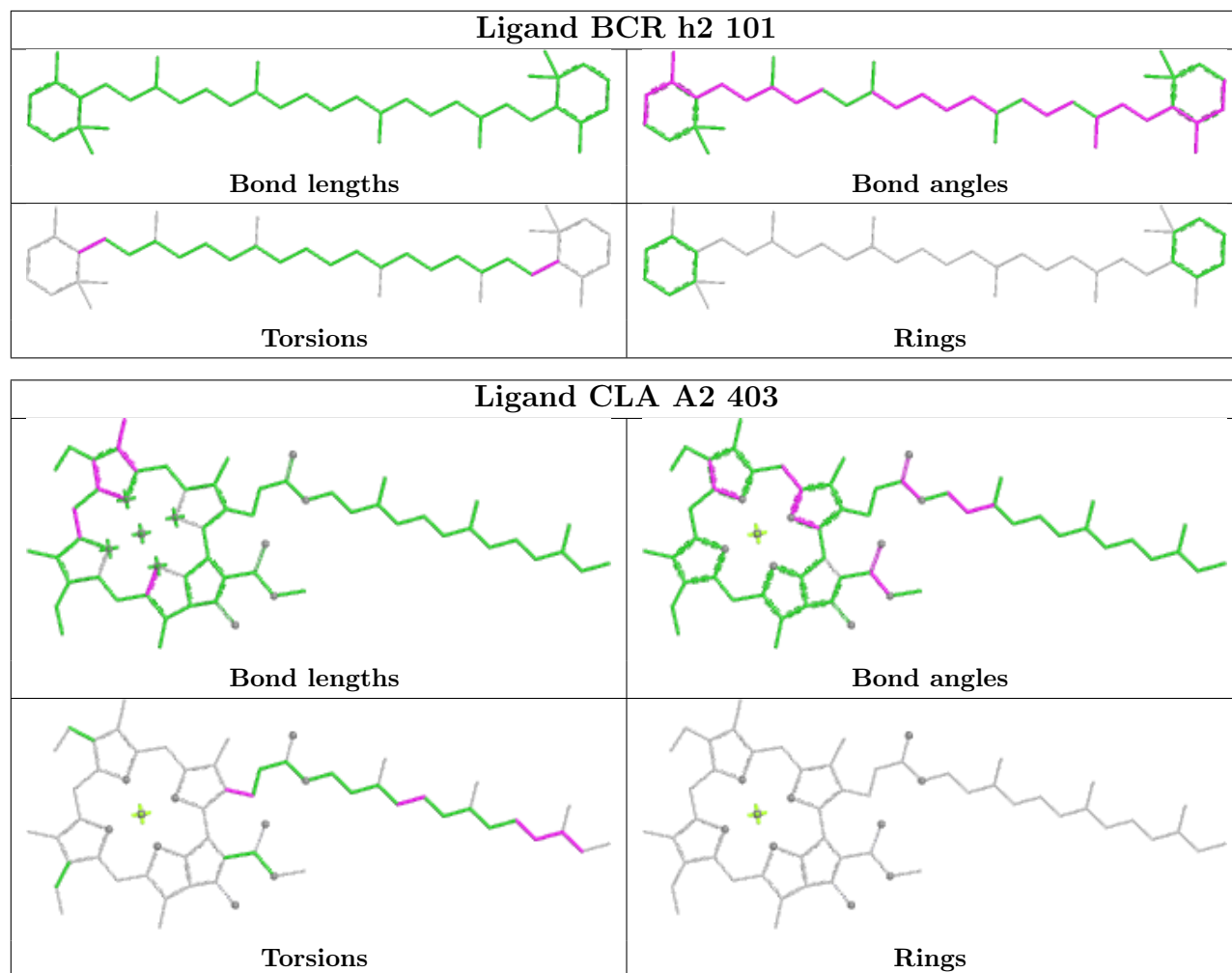


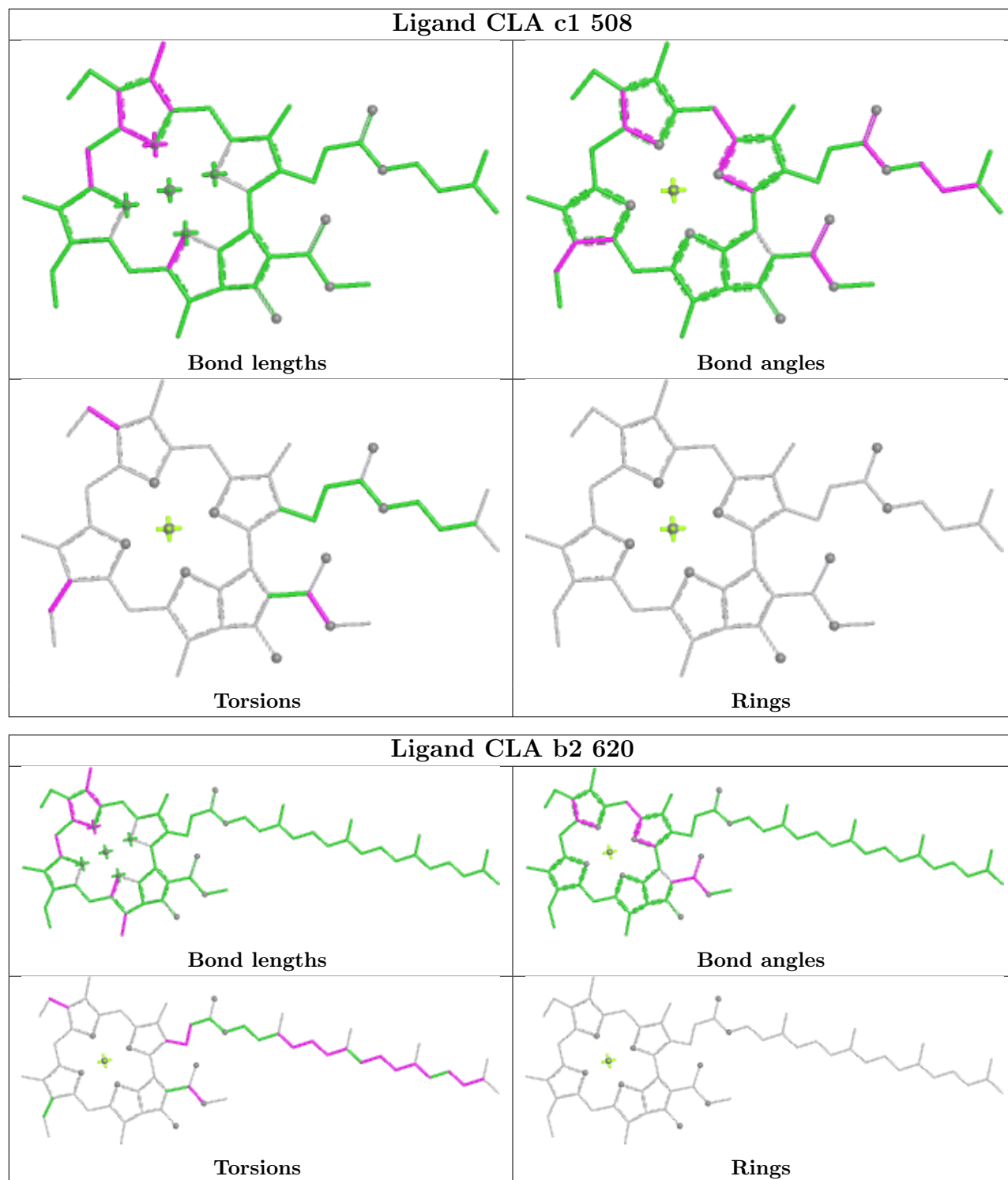
## Ligand CLA c1 513

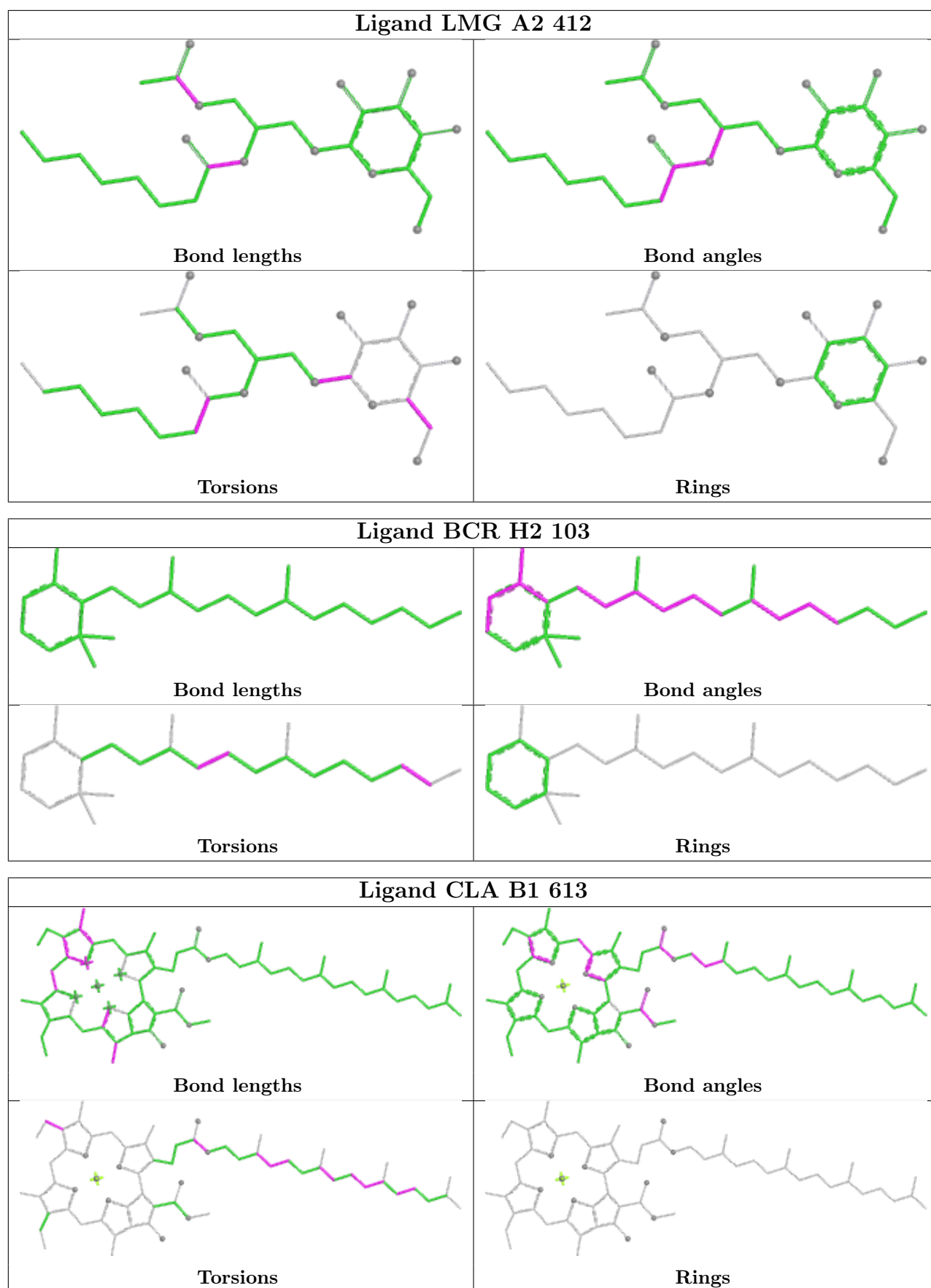


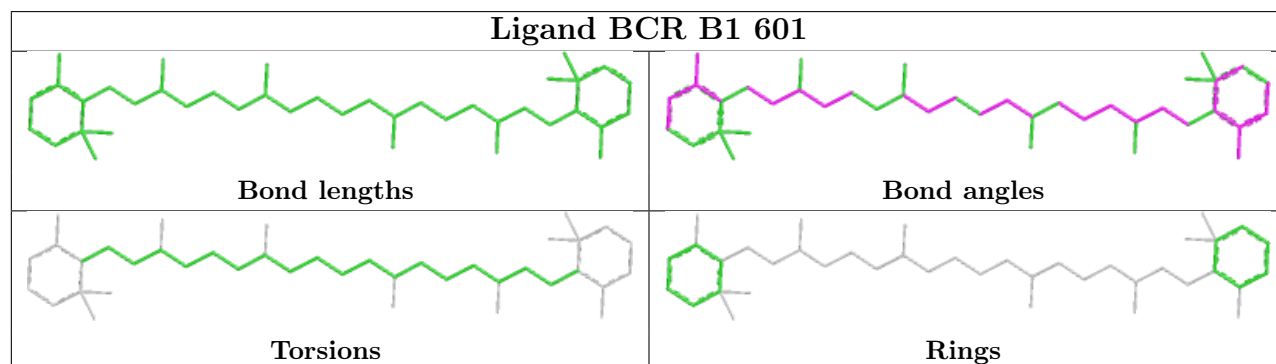
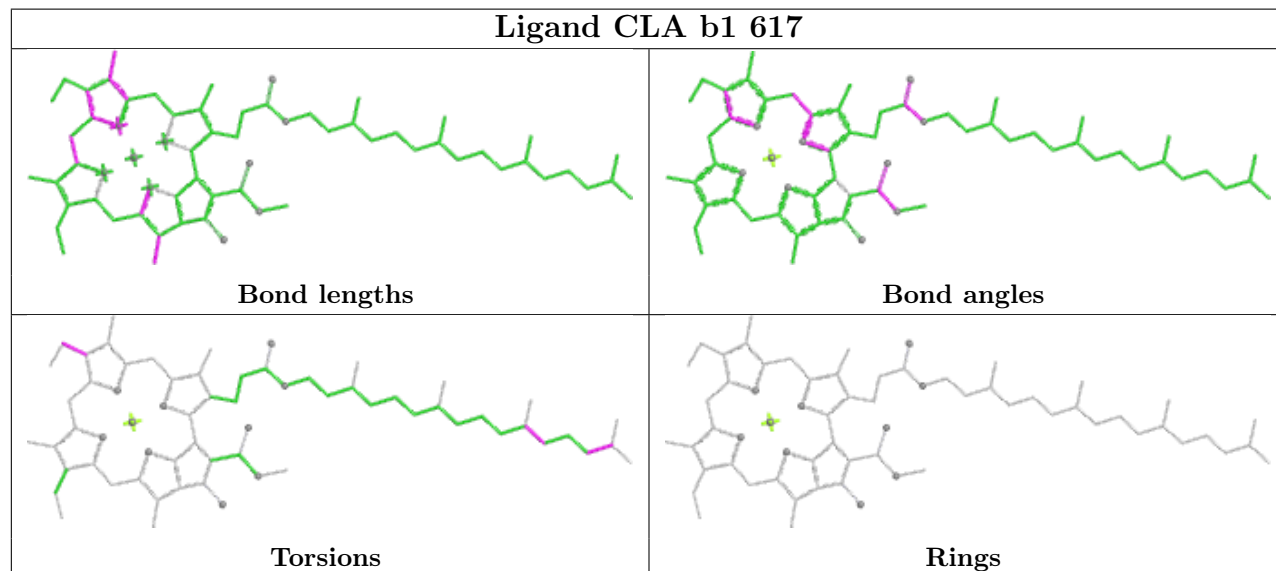
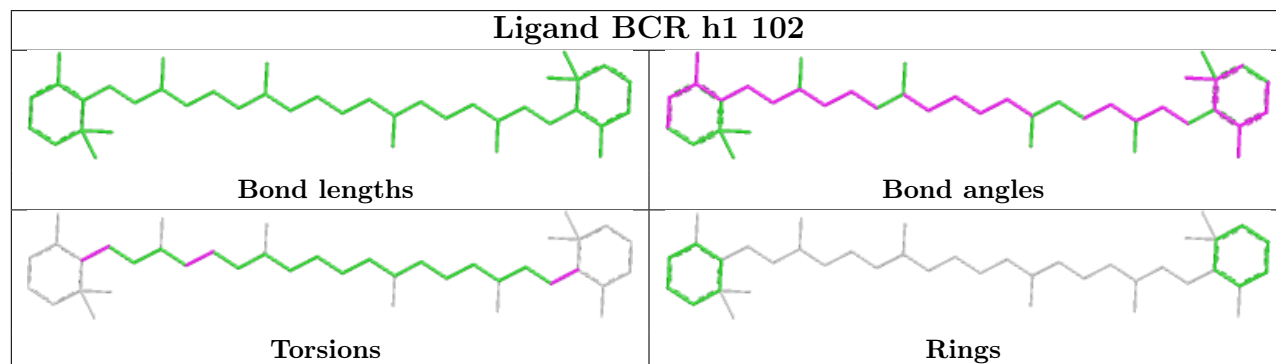
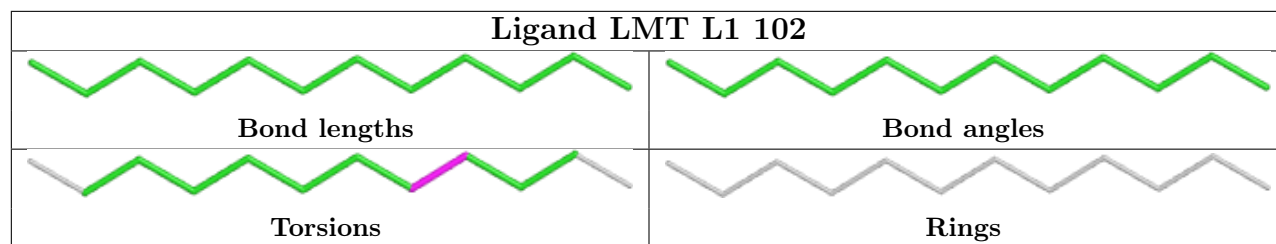


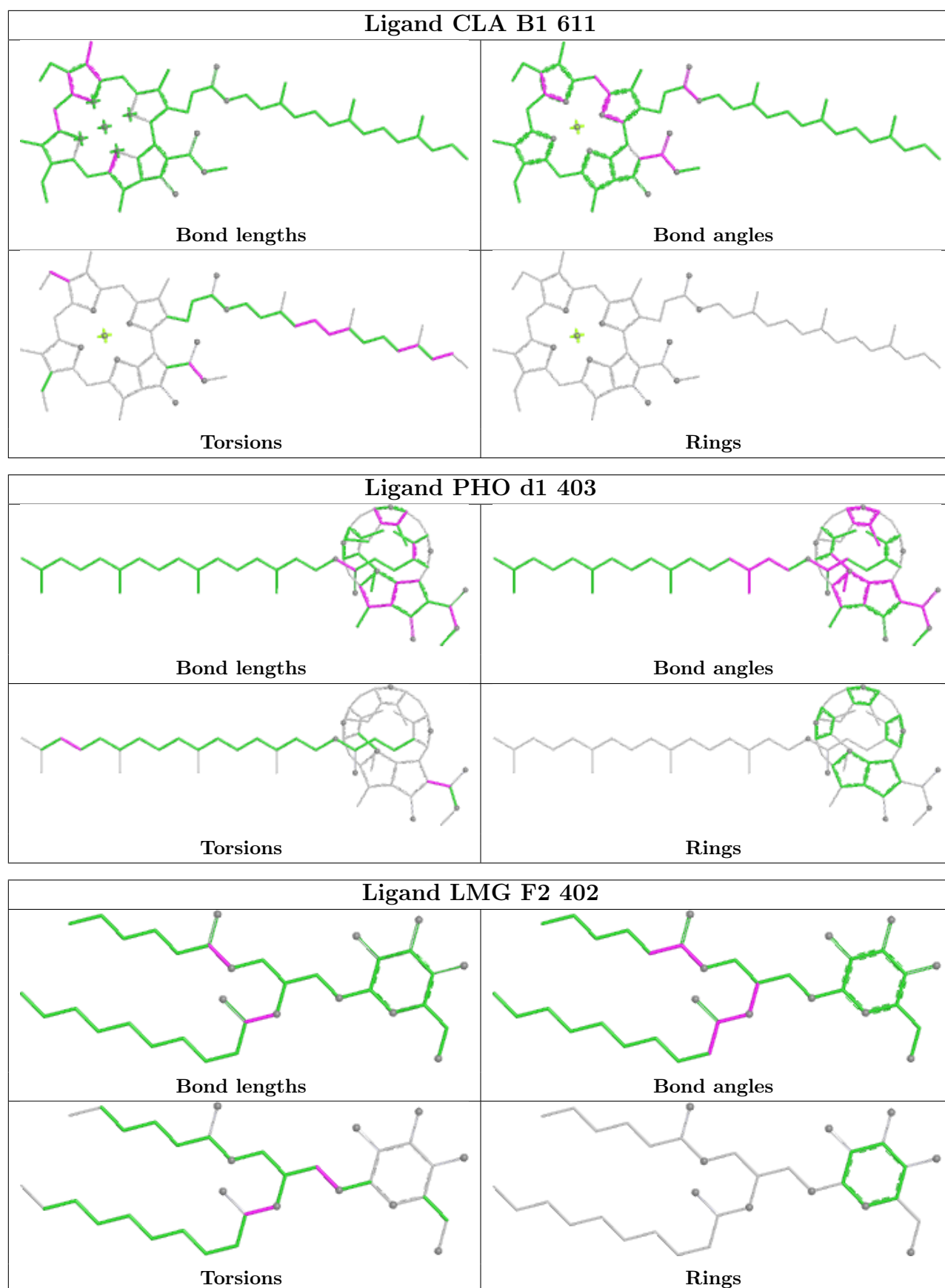




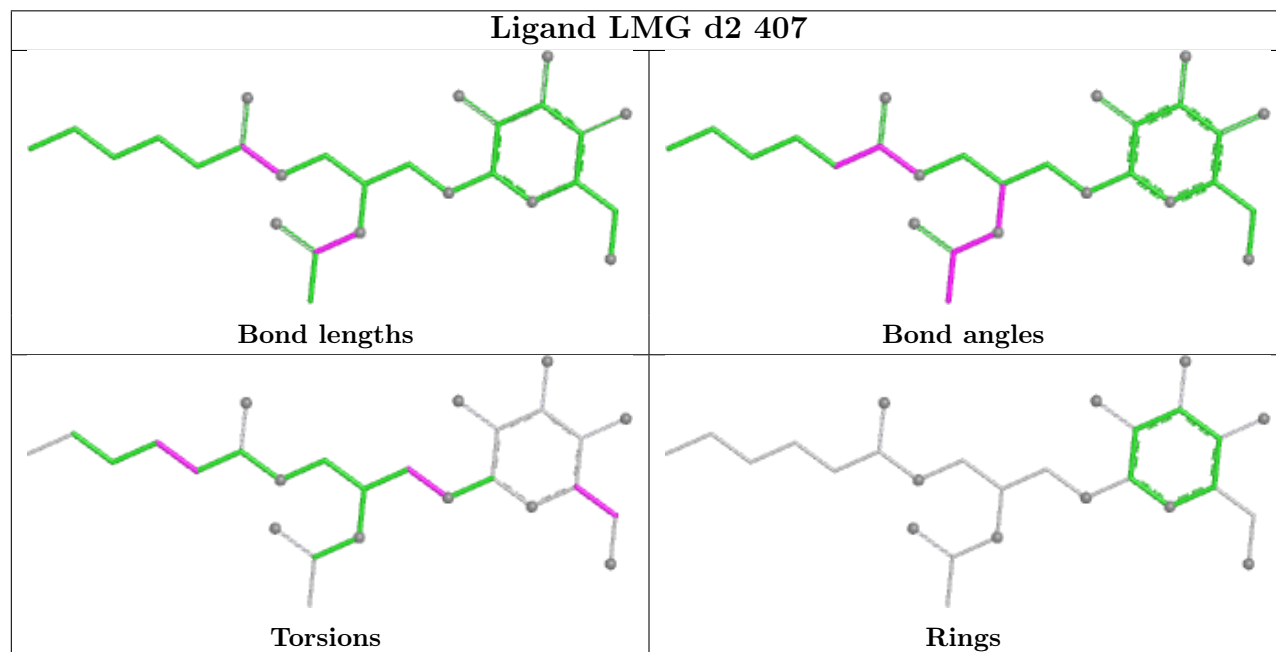
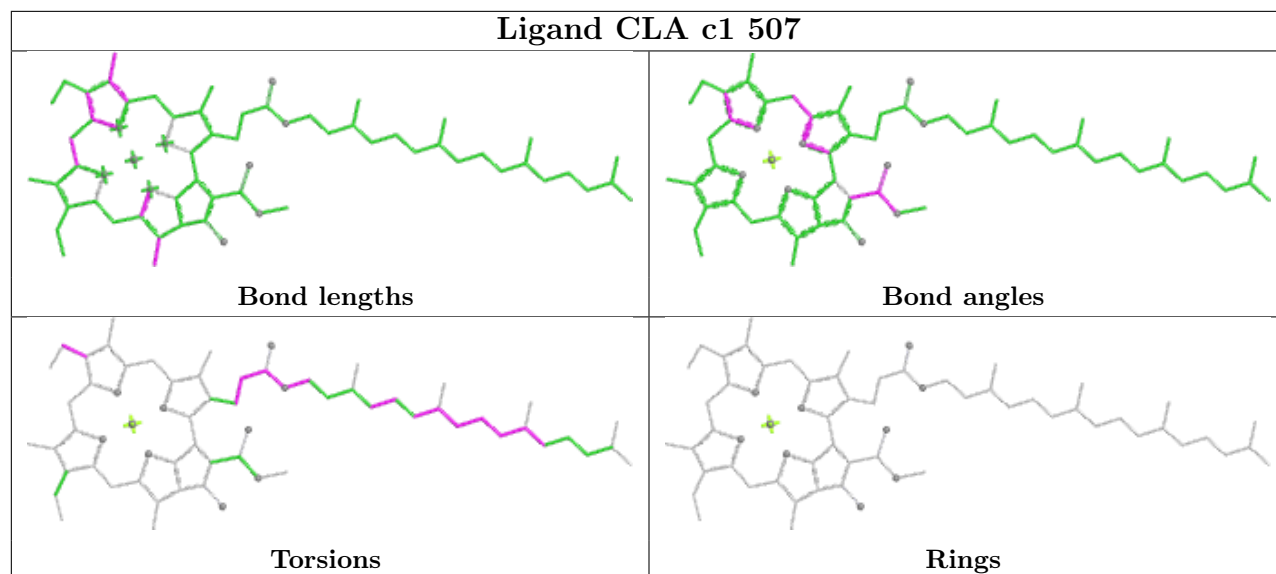


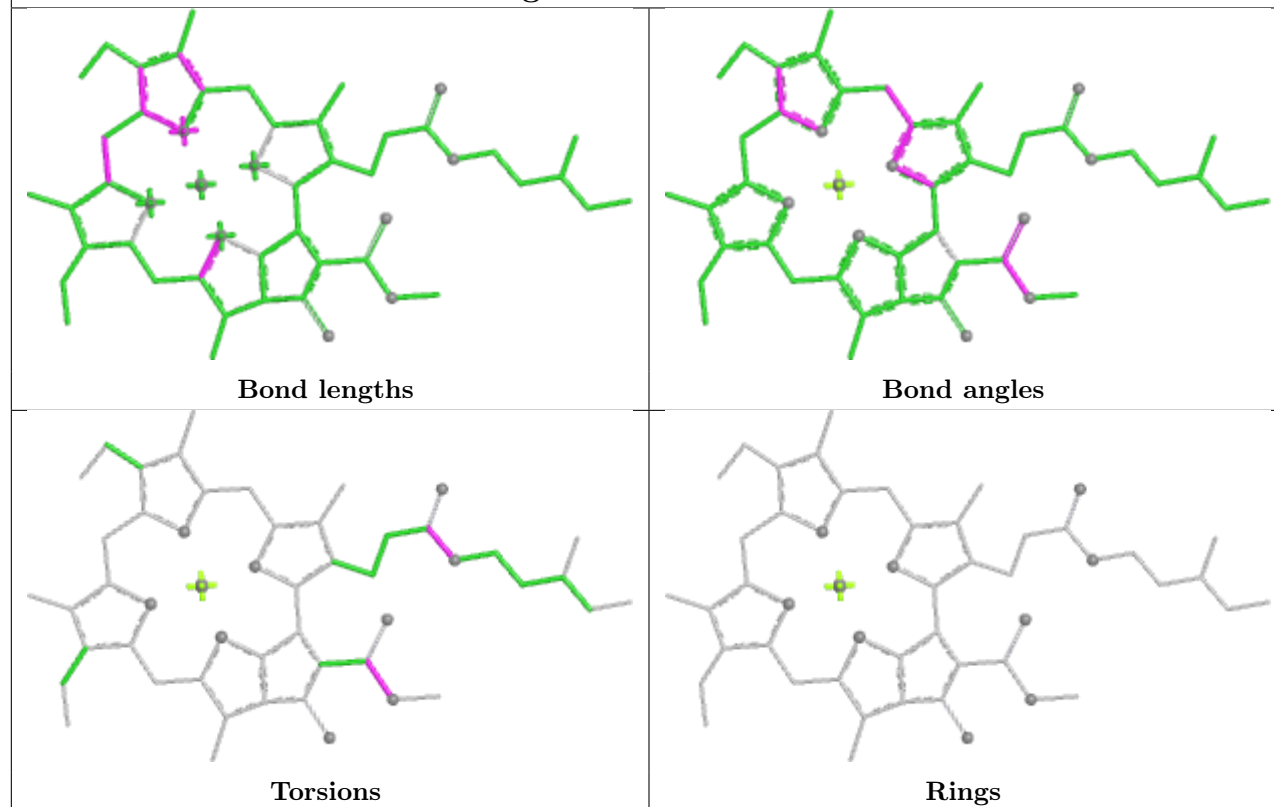
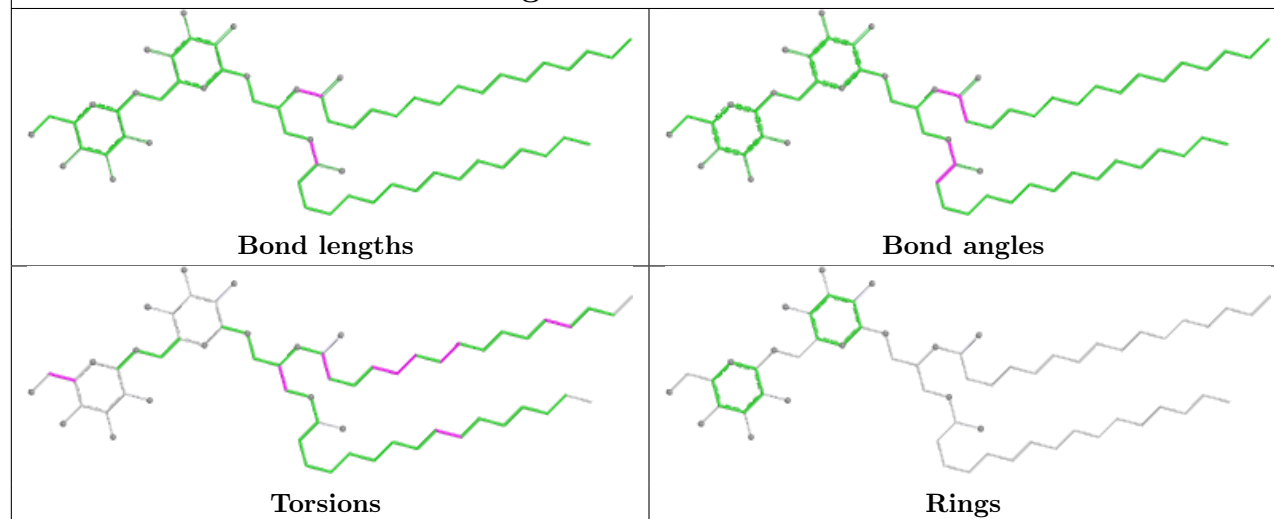


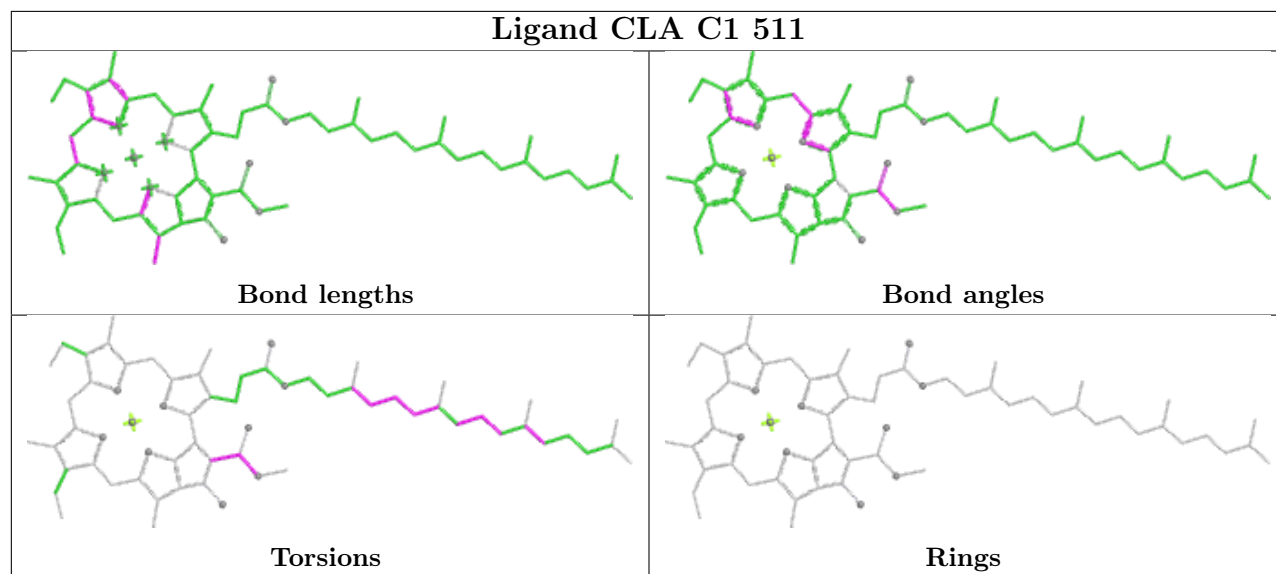
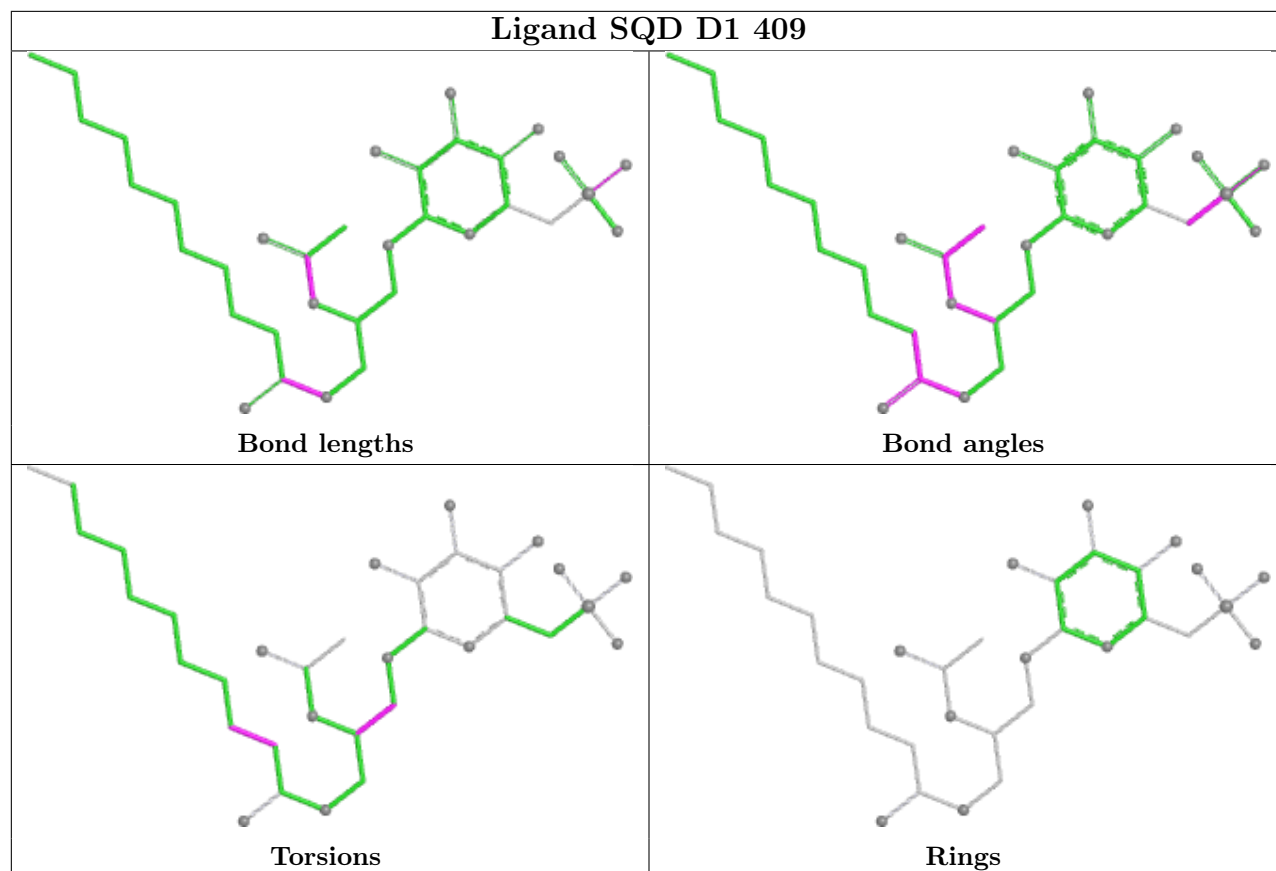


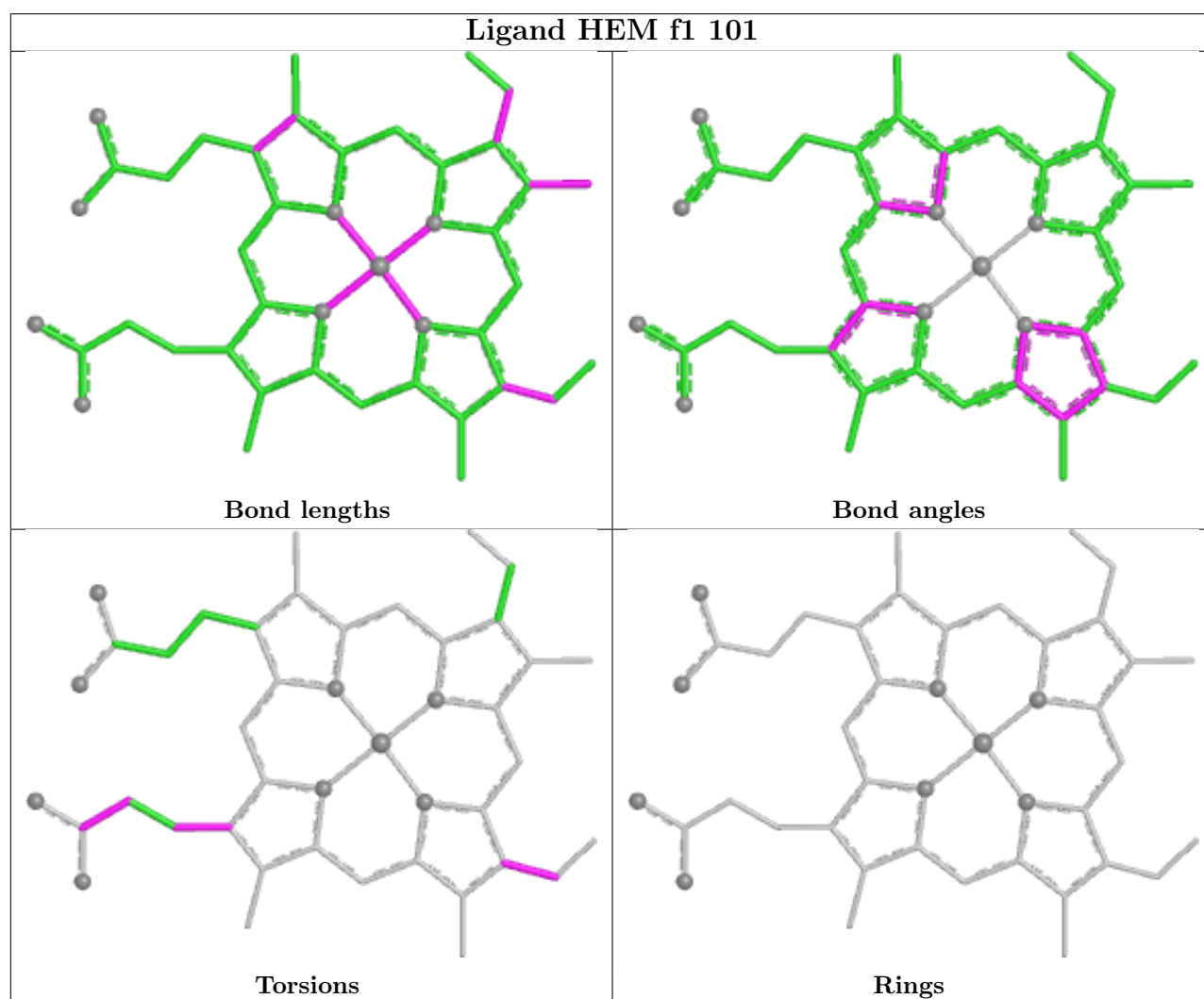
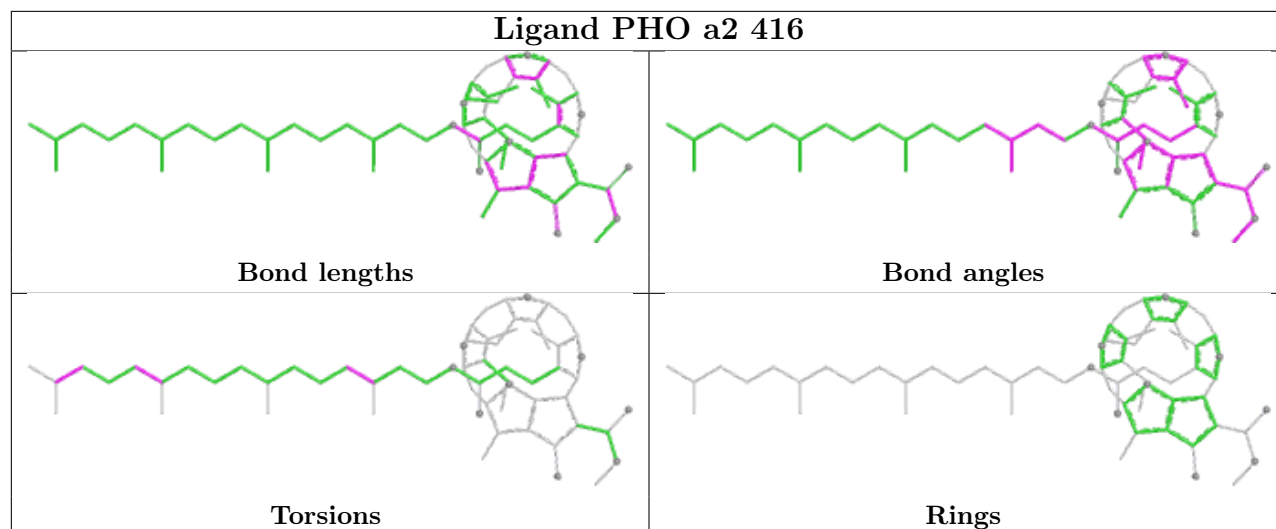


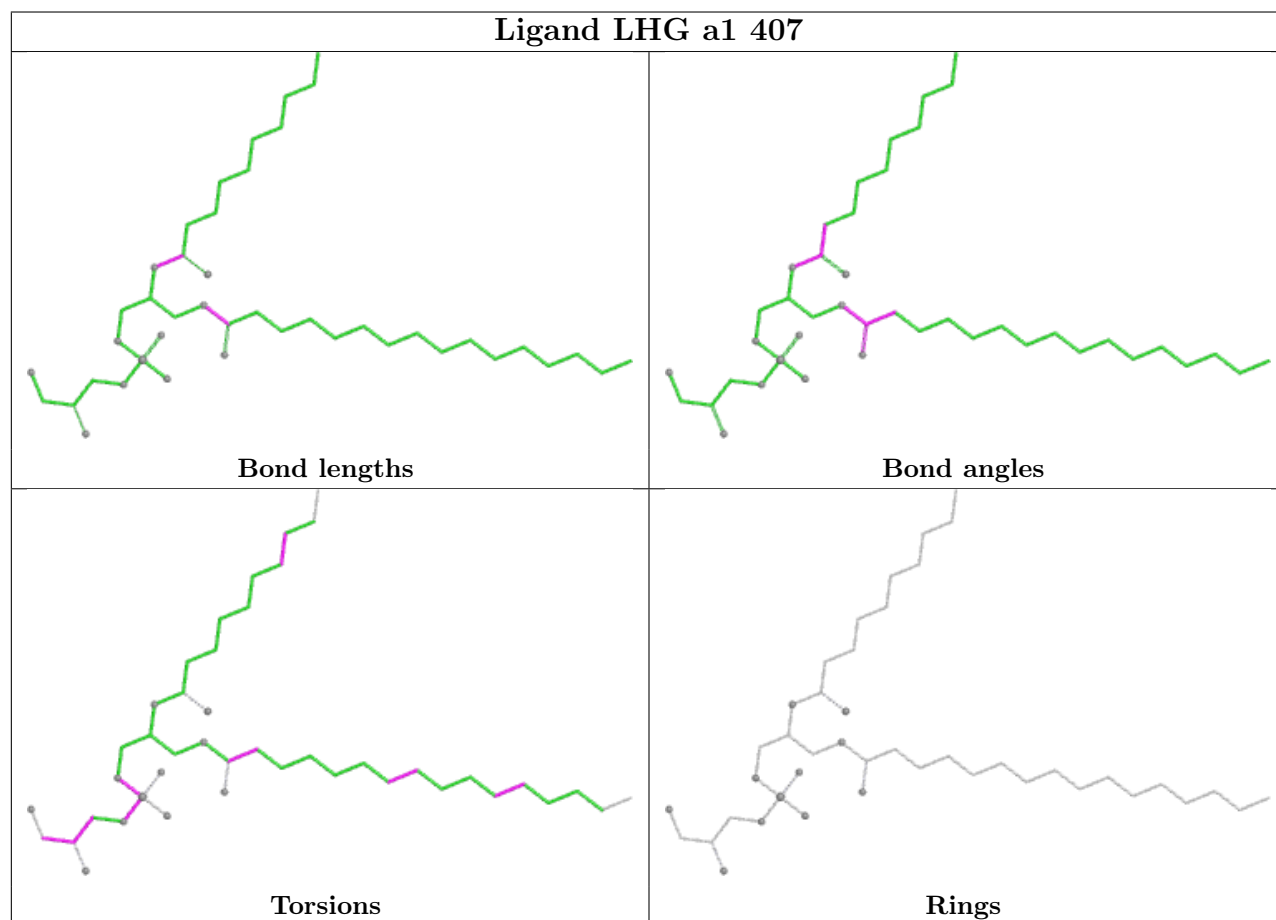
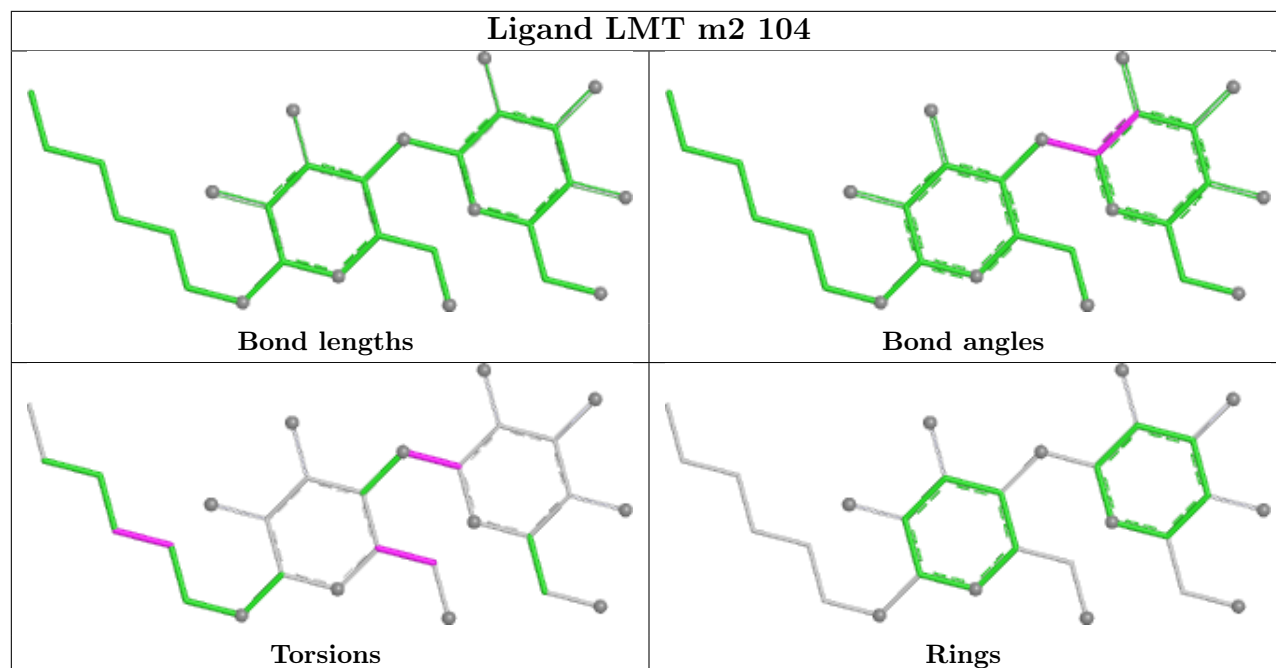


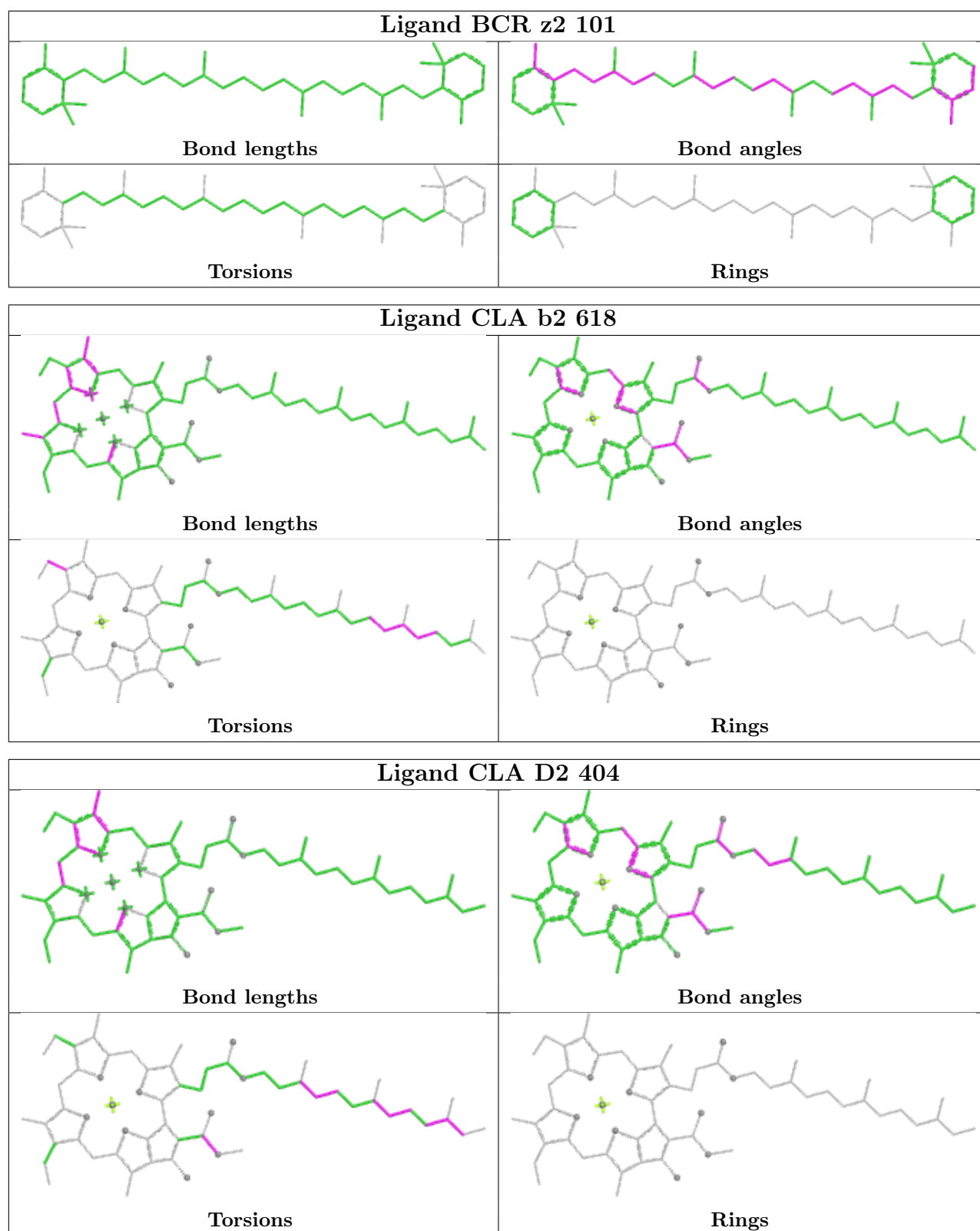


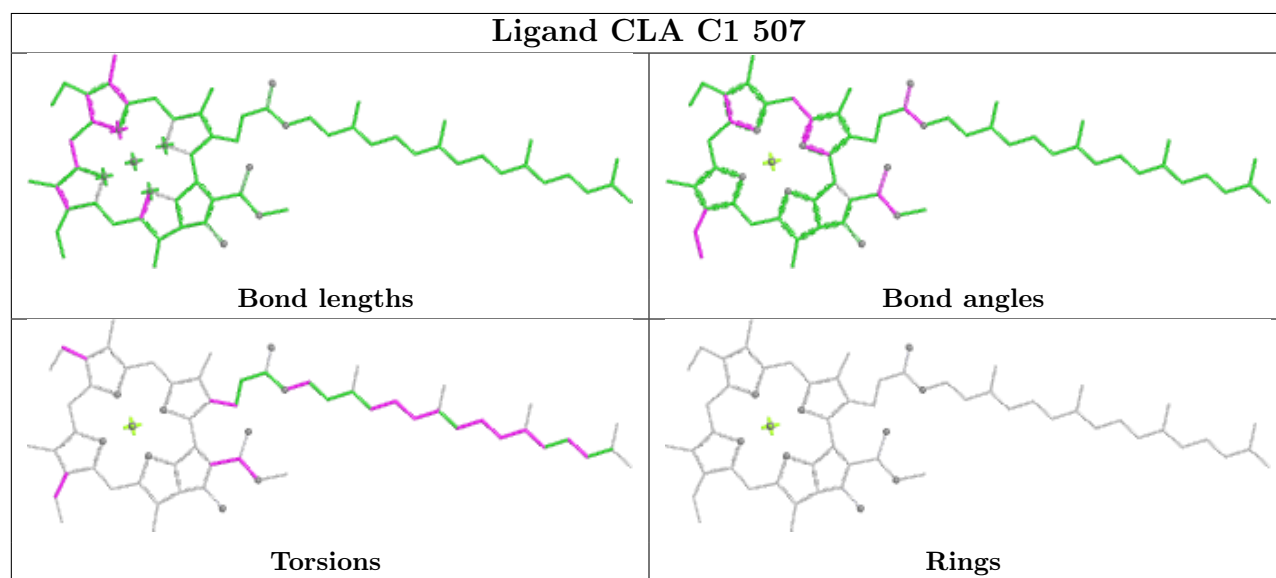
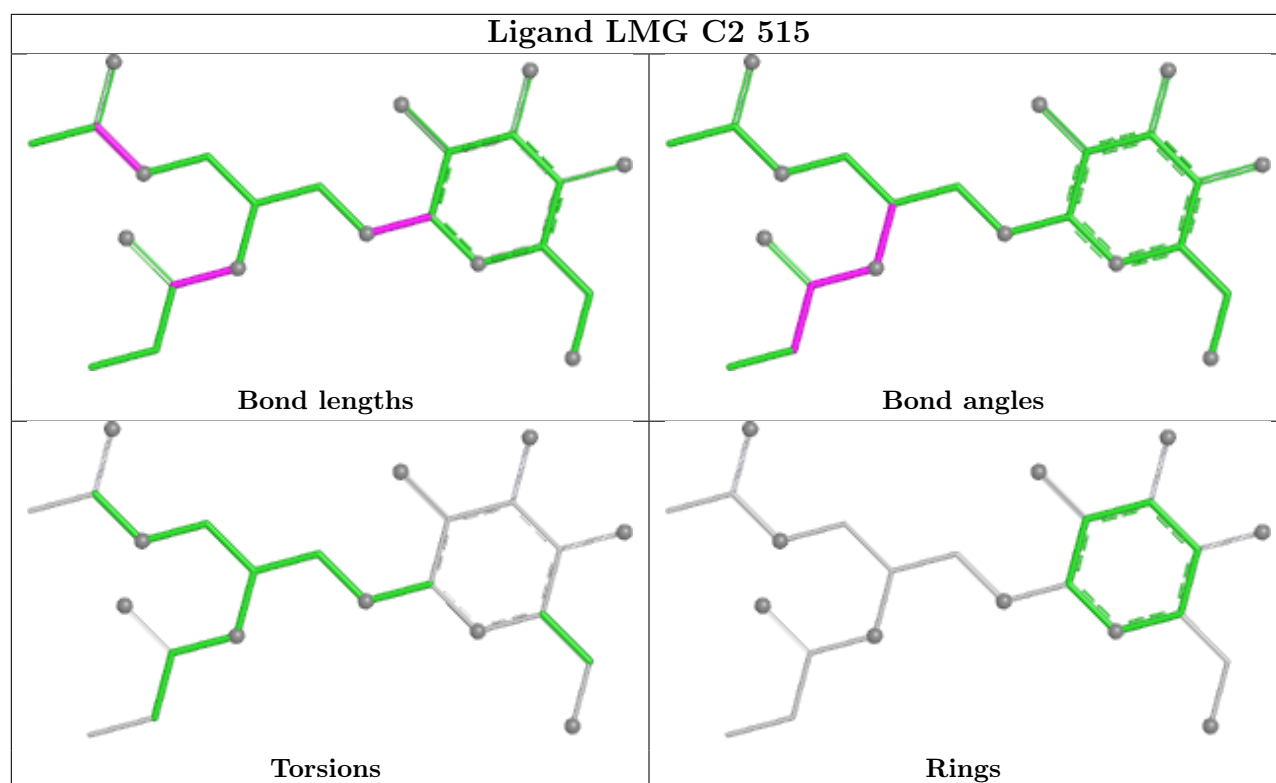
**Ligand CLA D1 403****Ligand DGD h2 102**

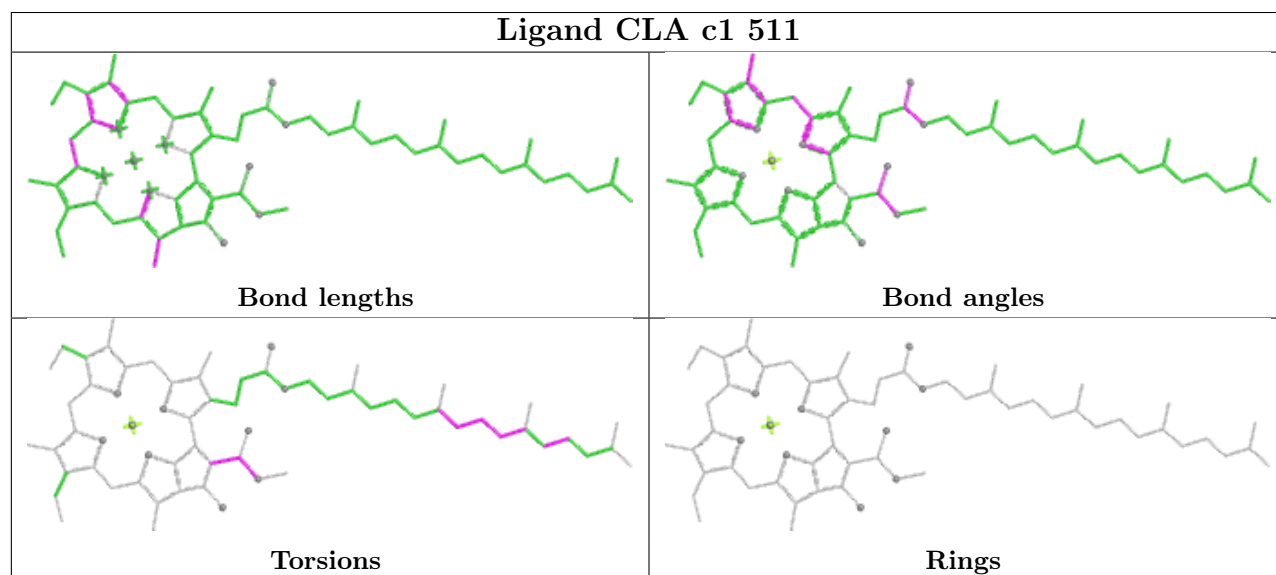
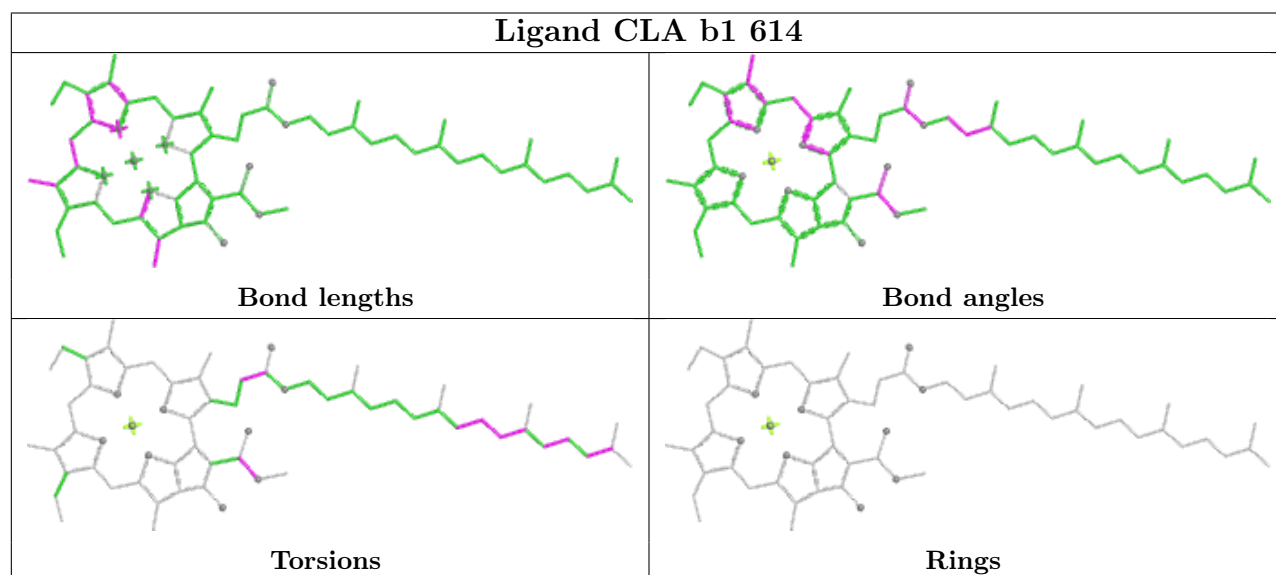
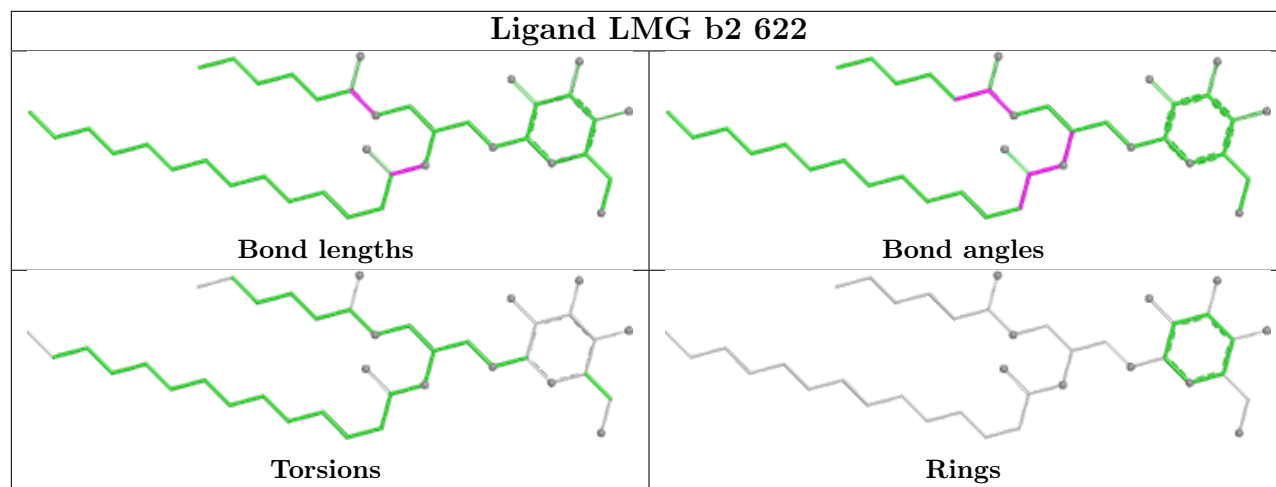




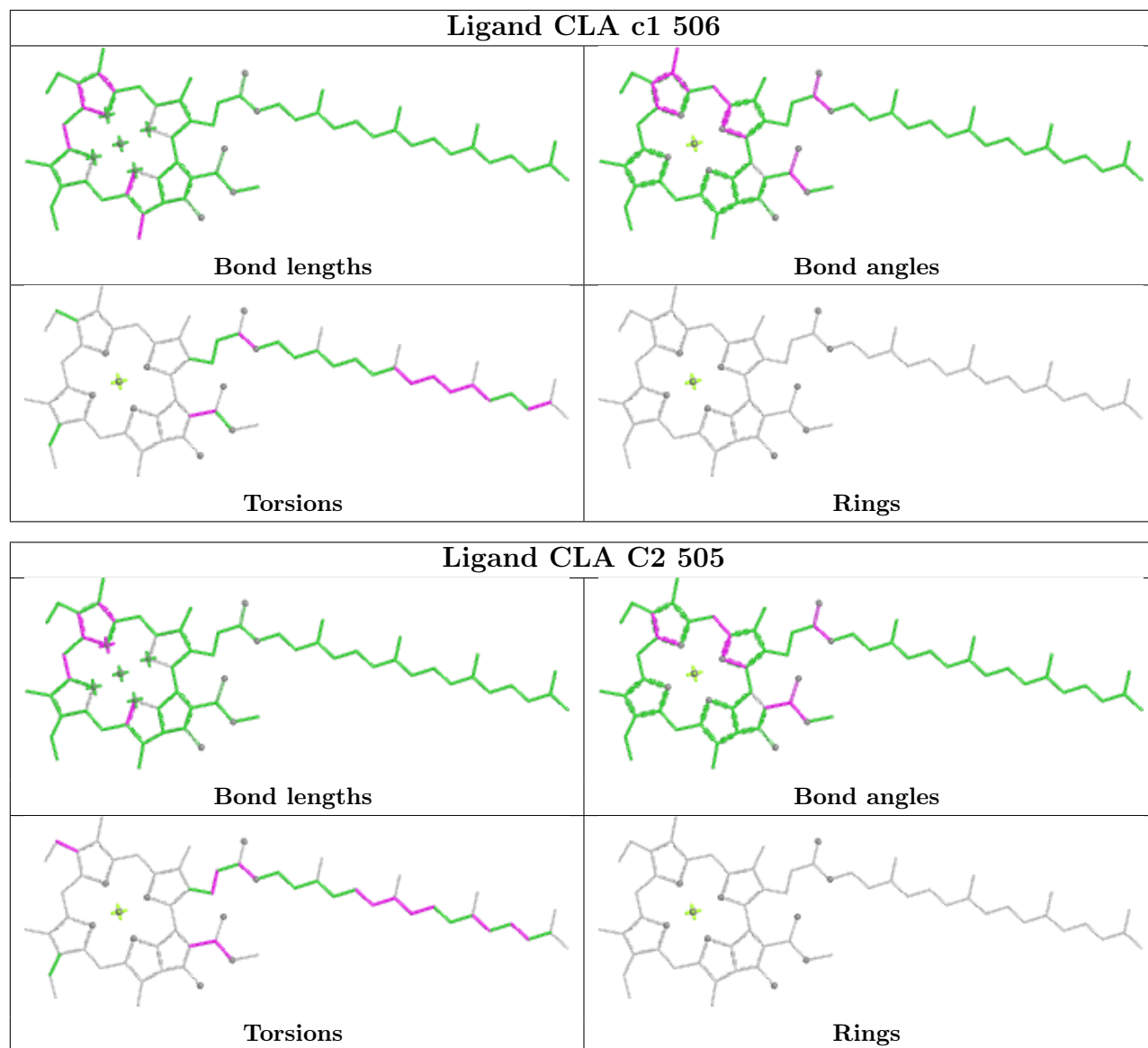


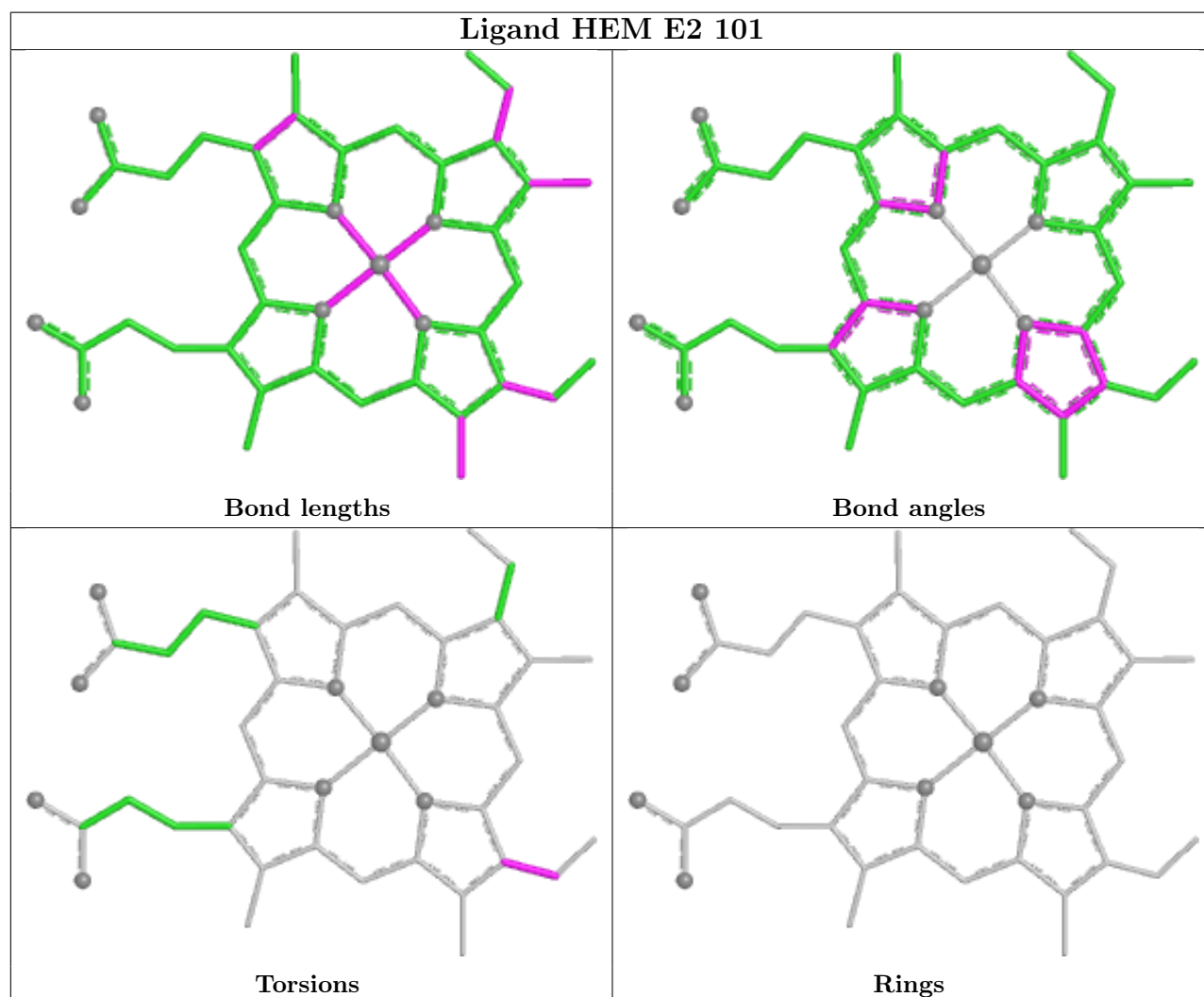
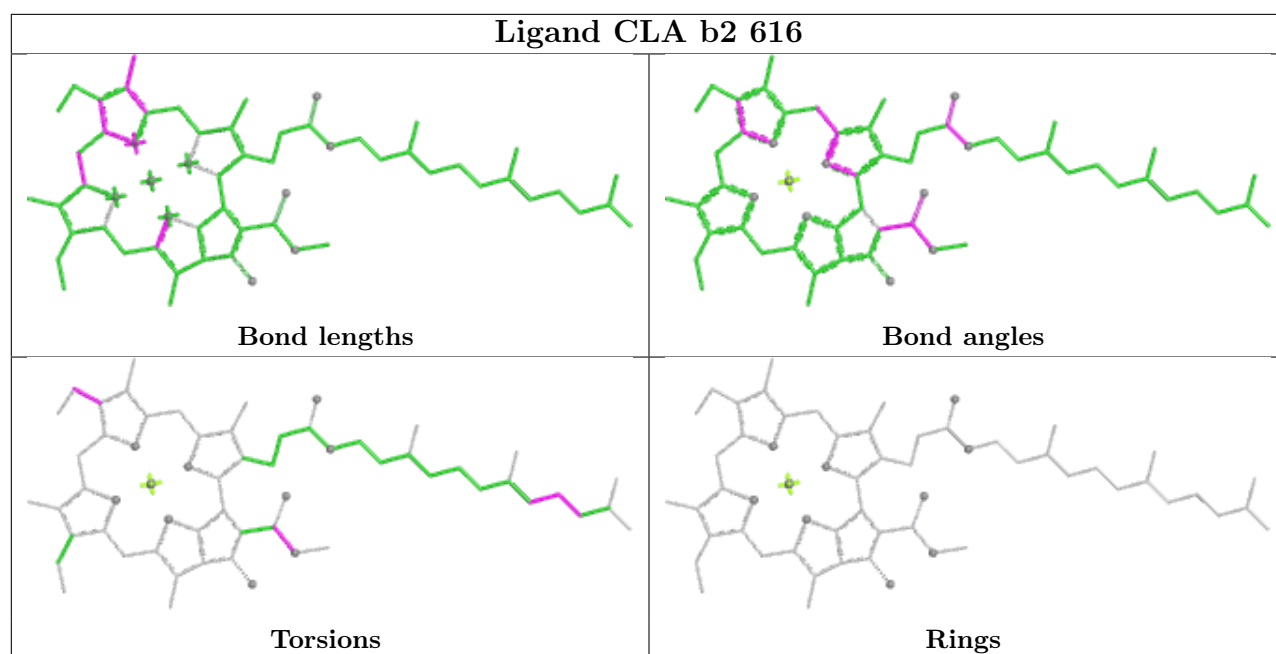


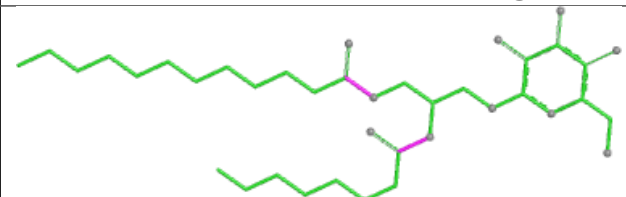
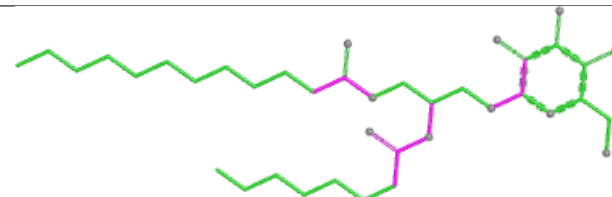
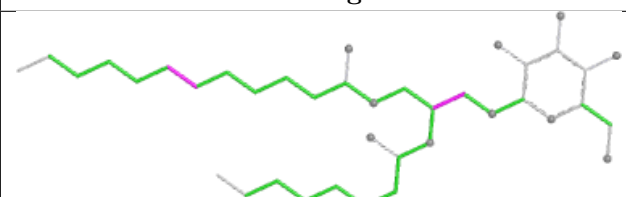
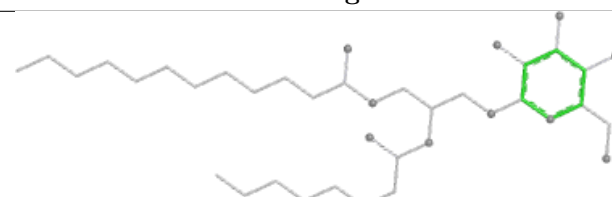


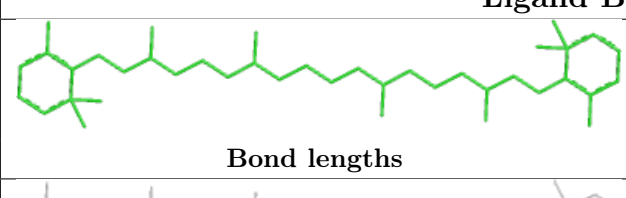
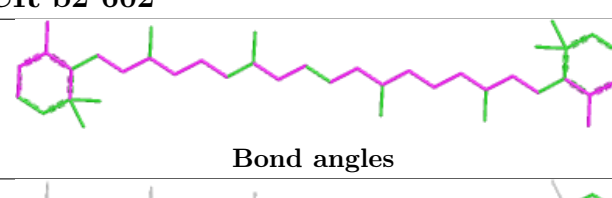
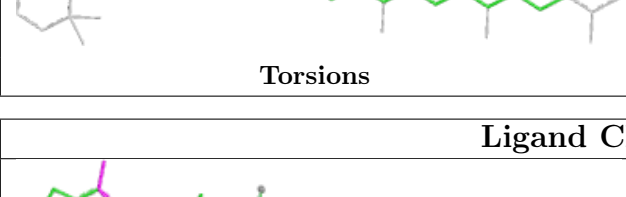
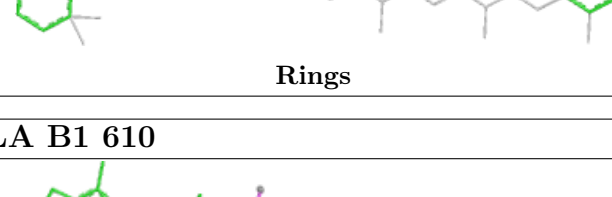


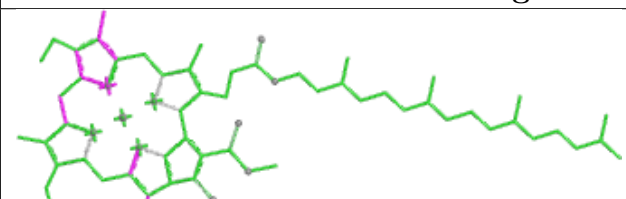
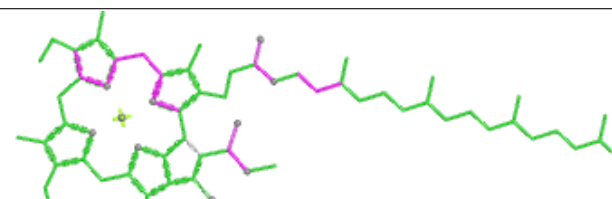
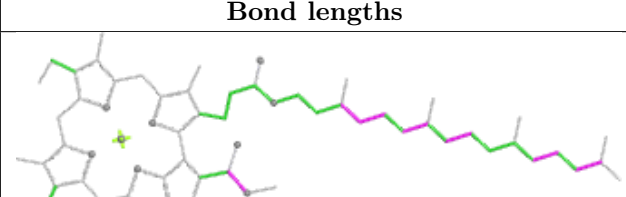
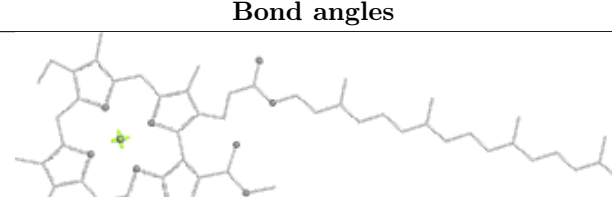


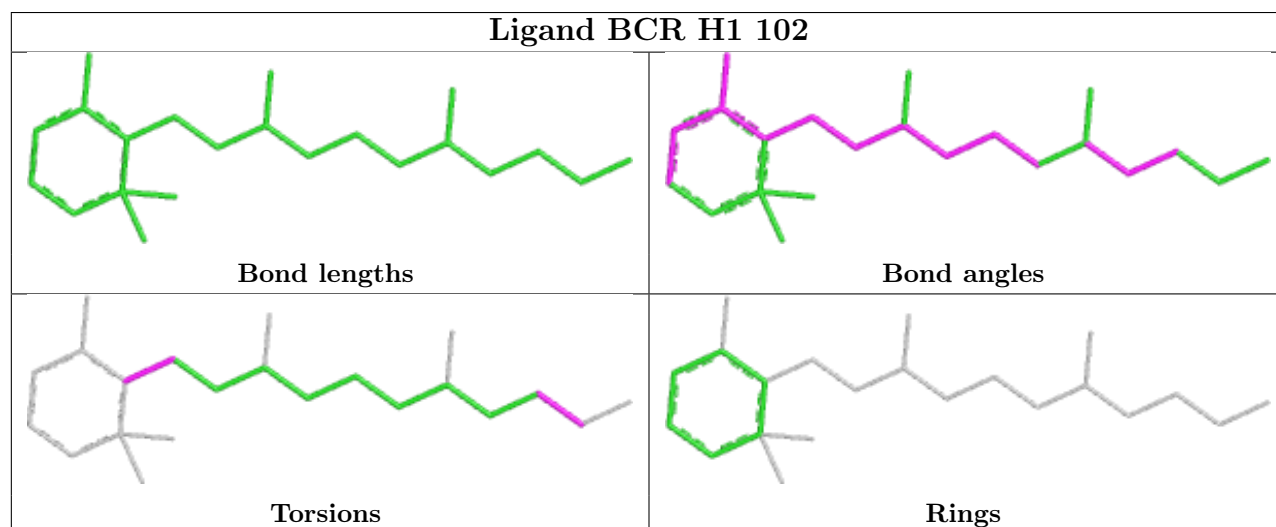
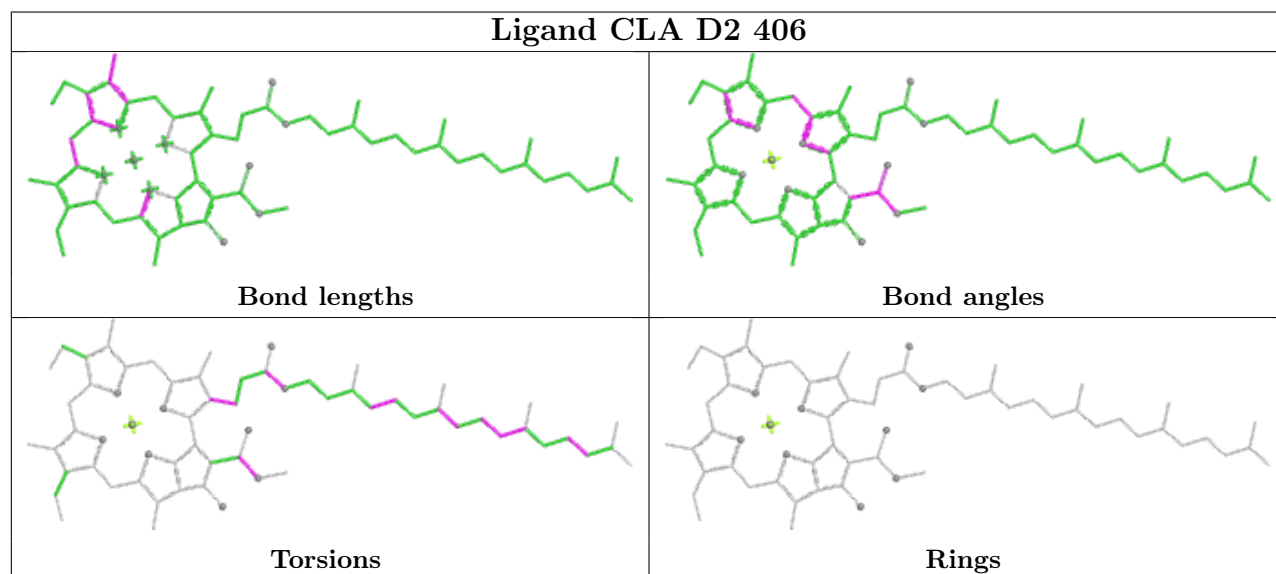
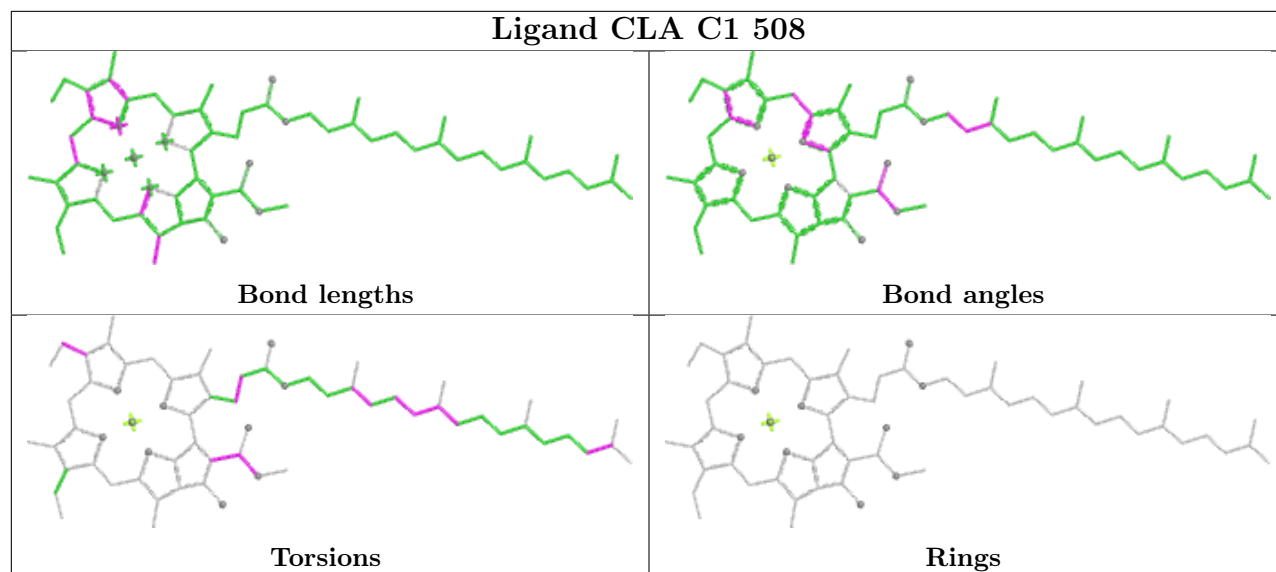


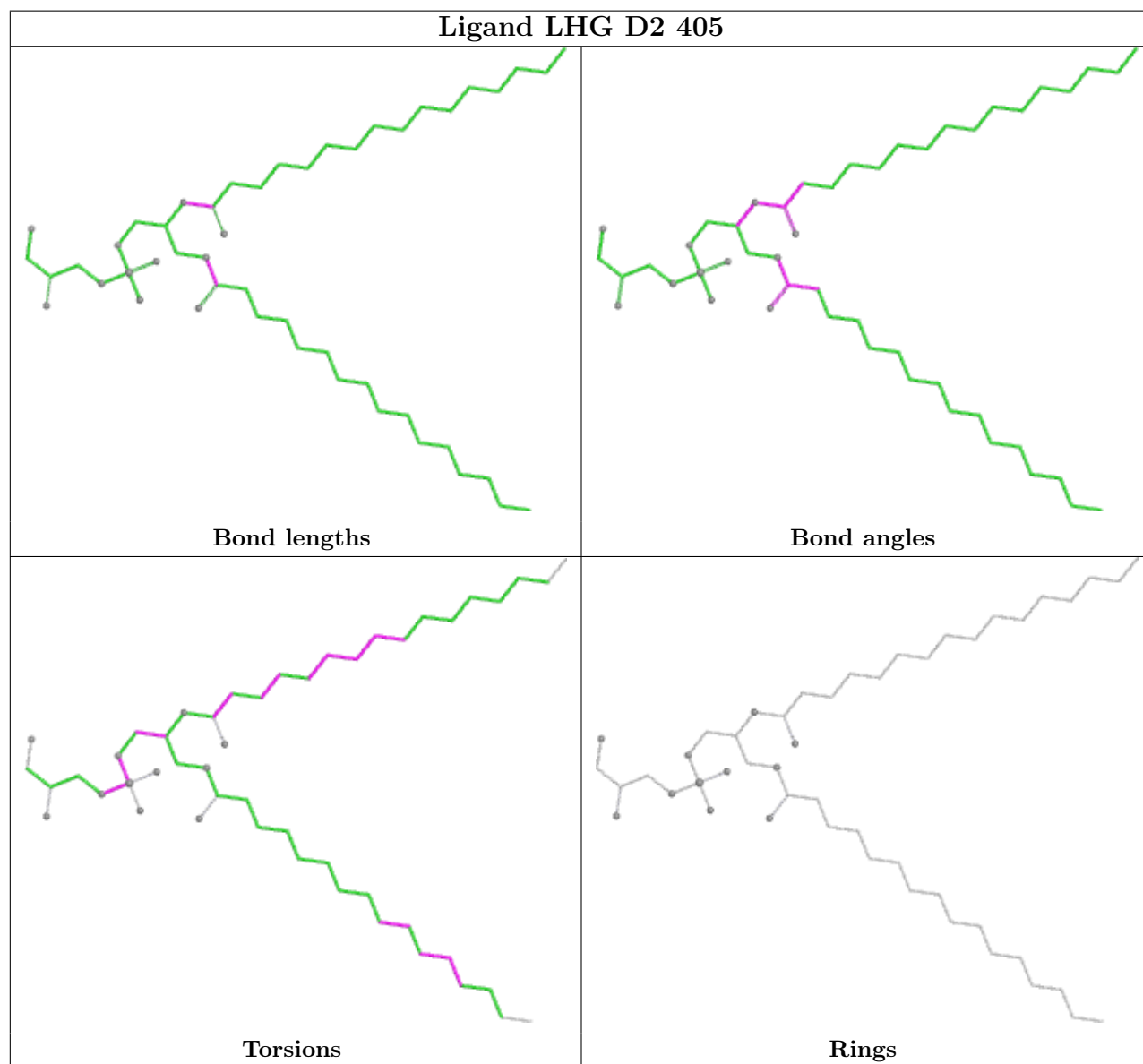
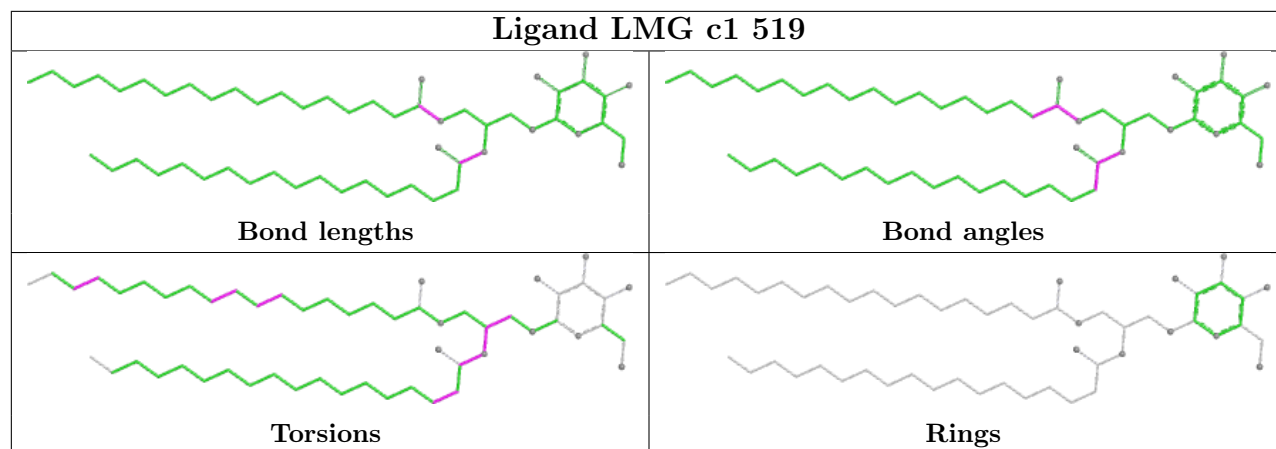


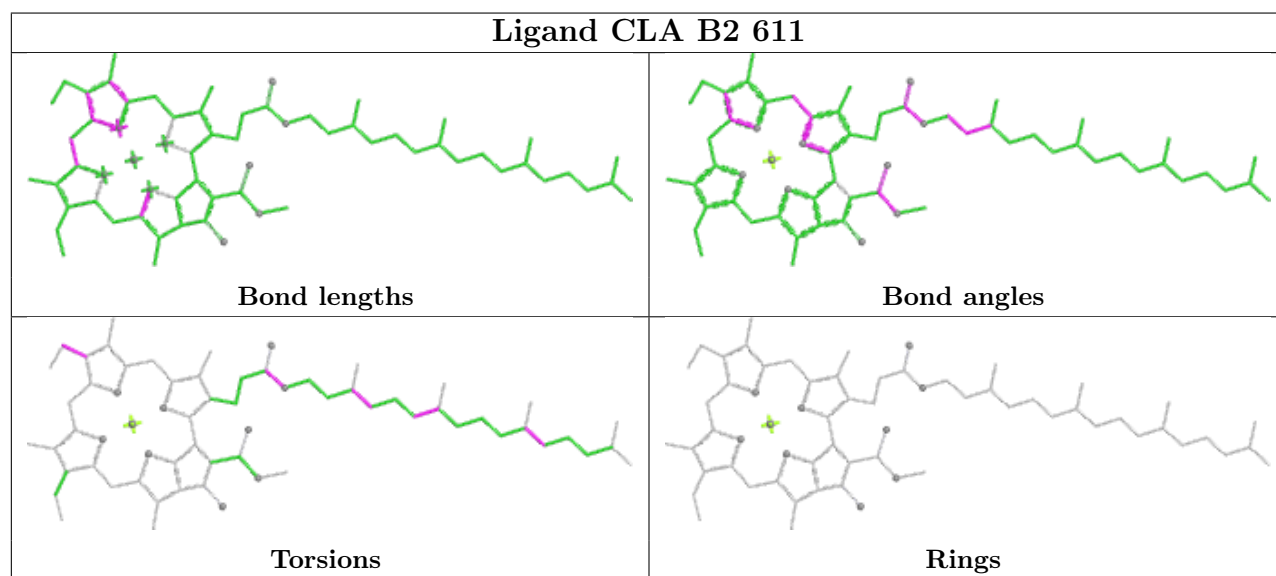
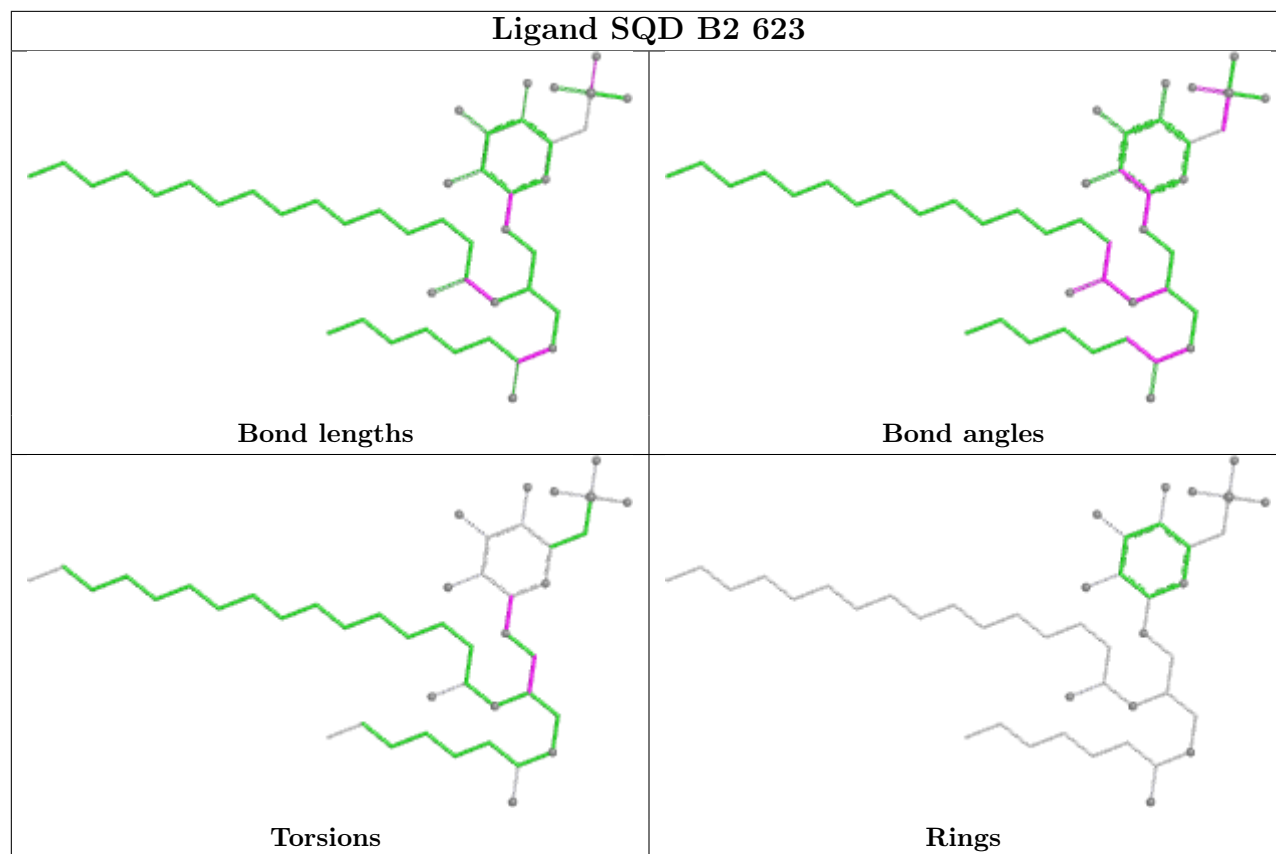
| Ligand LMG b1 624                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

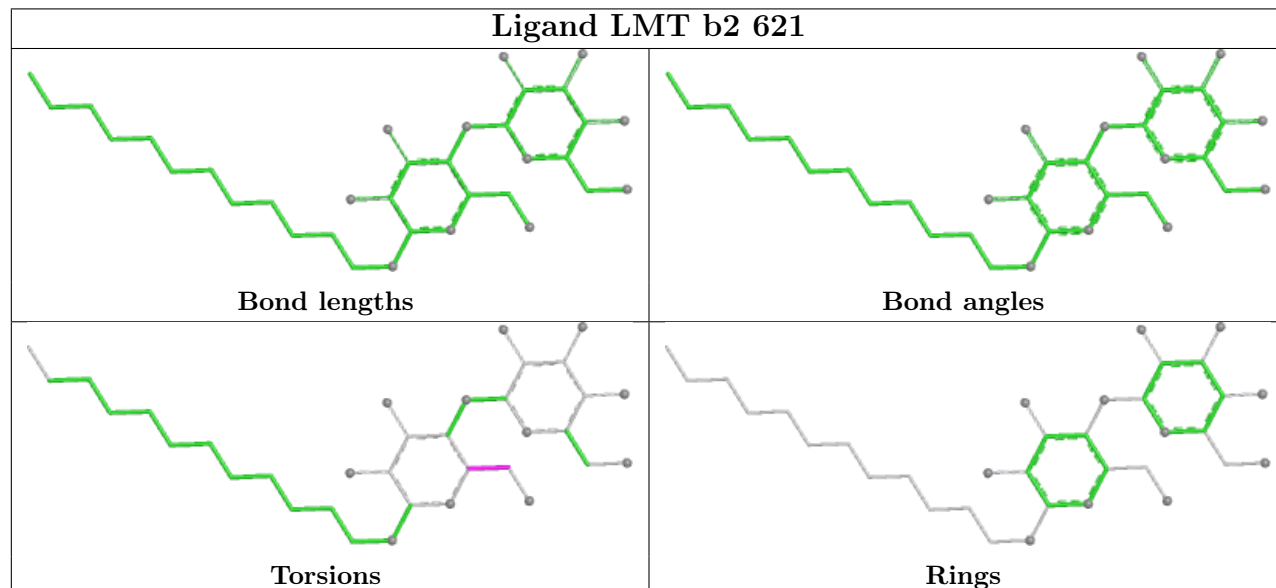
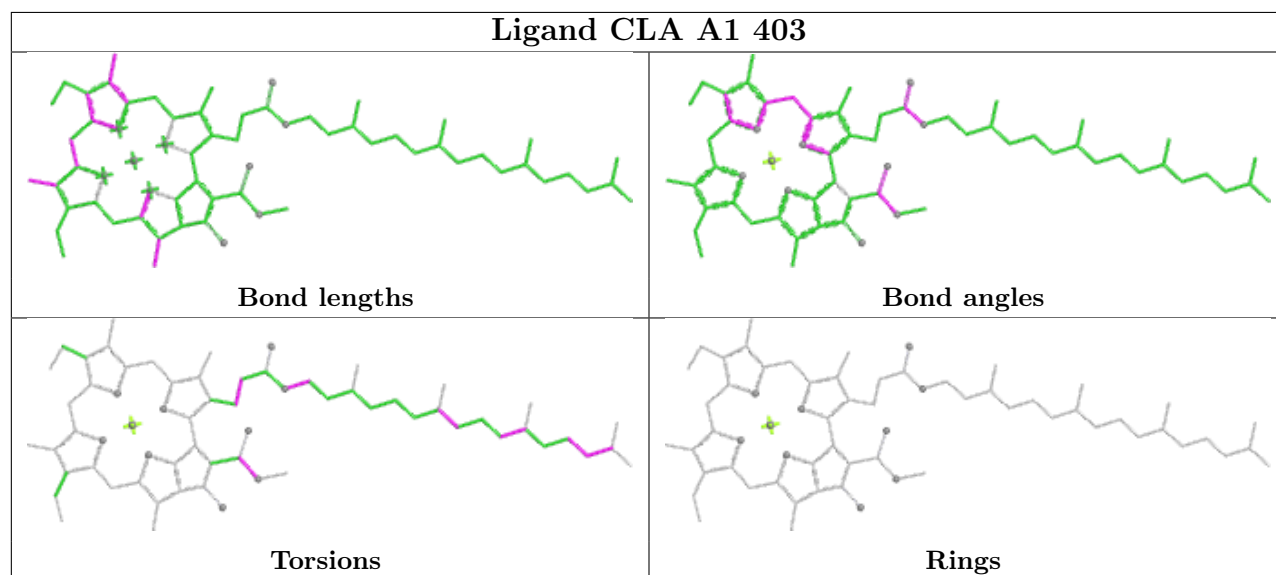
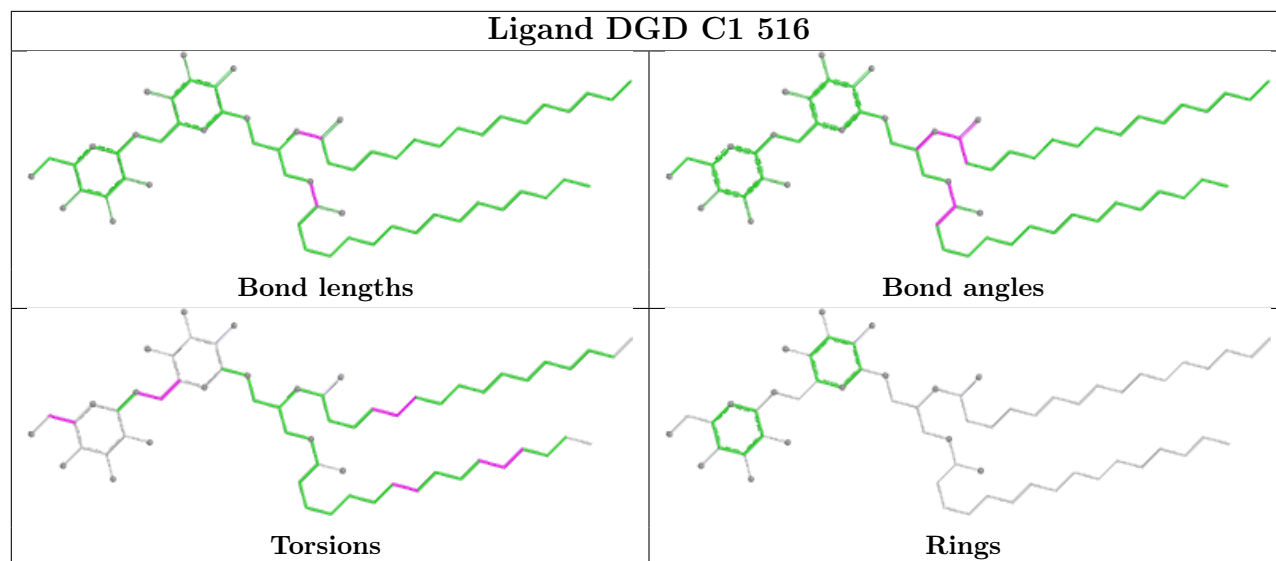
| Ligand BCR b2 602                                                                  |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

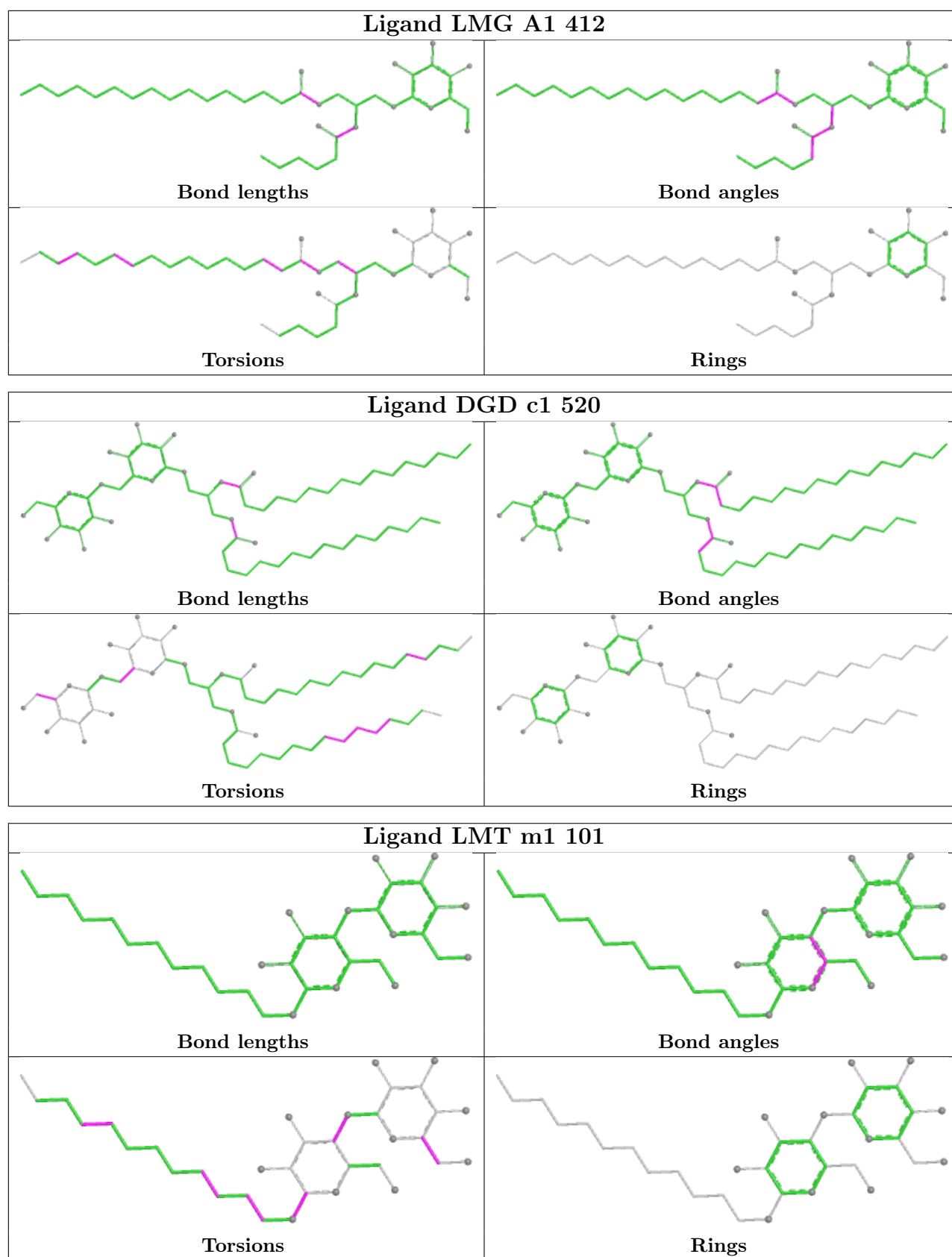
| Ligand CLA B1 610                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



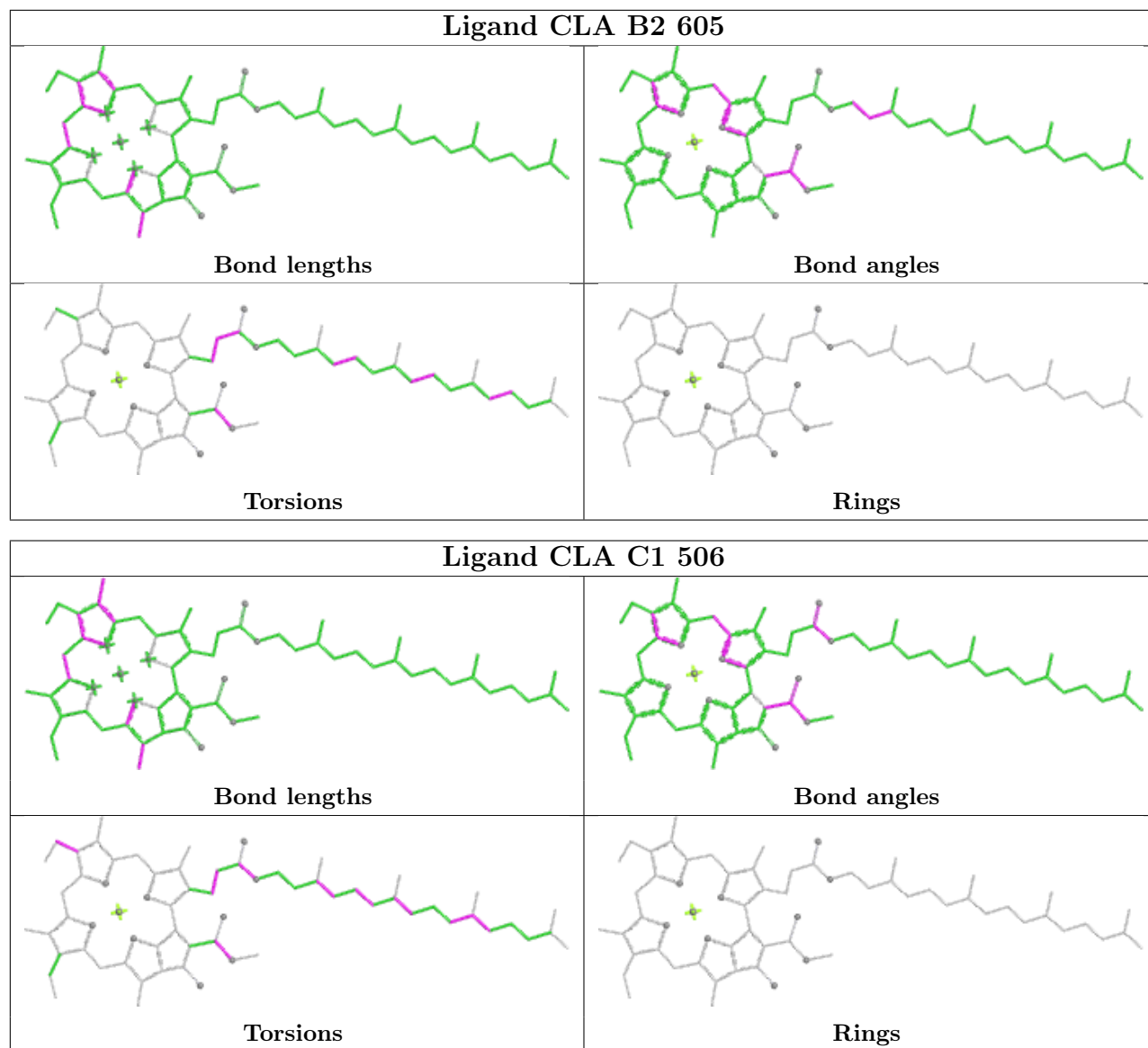




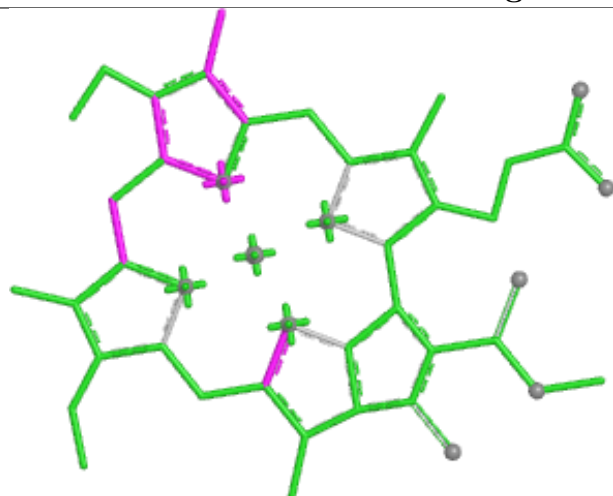




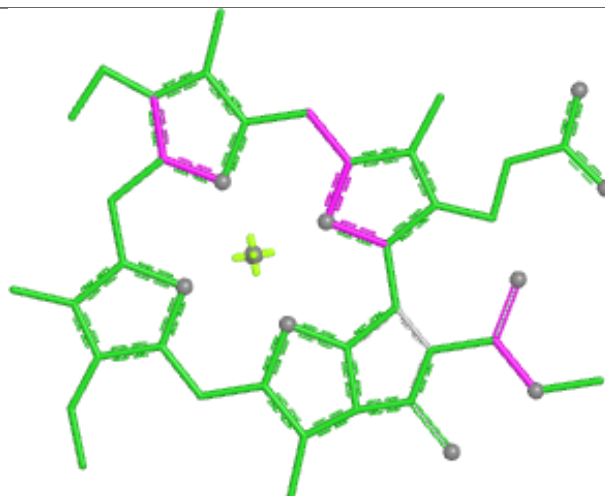




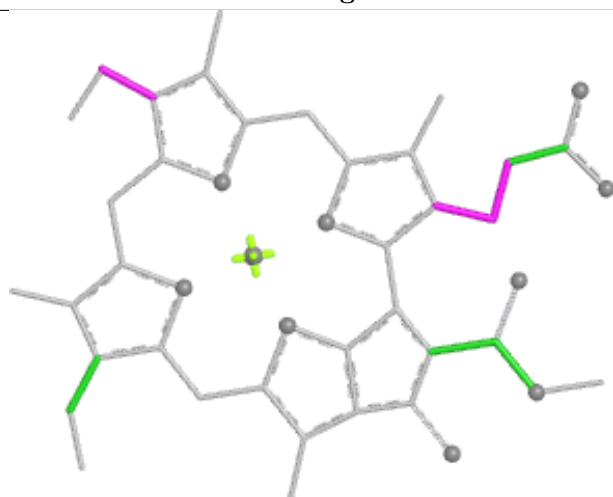
## Ligand CLA C1 514



Bond lengths



Bond angles

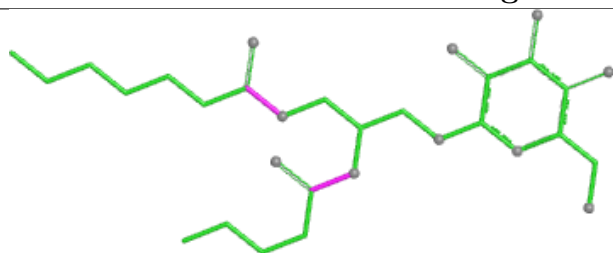


Torsions

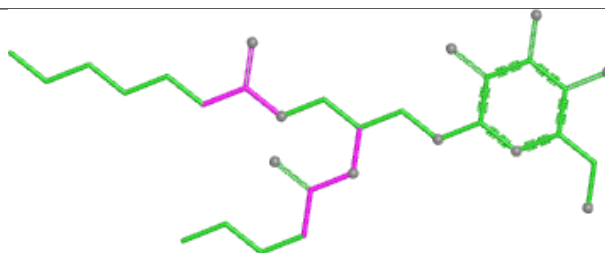


Rings

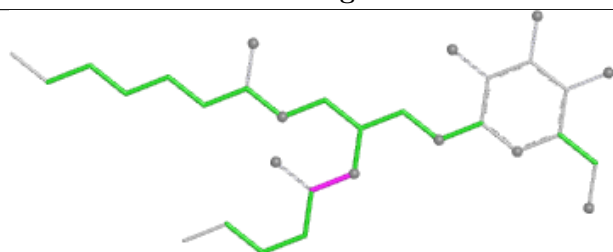
## Ligand LMG B1 622



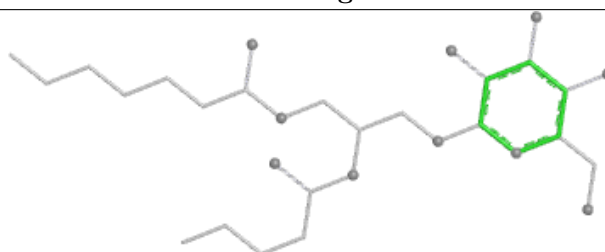
Bond lengths



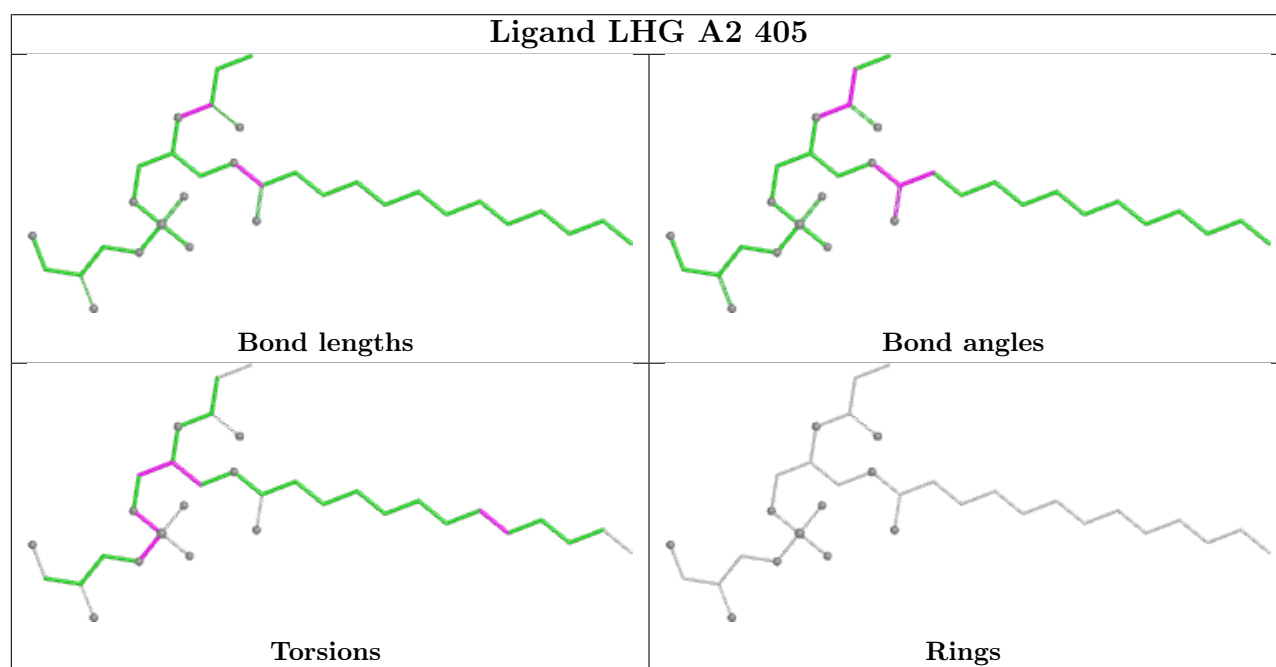
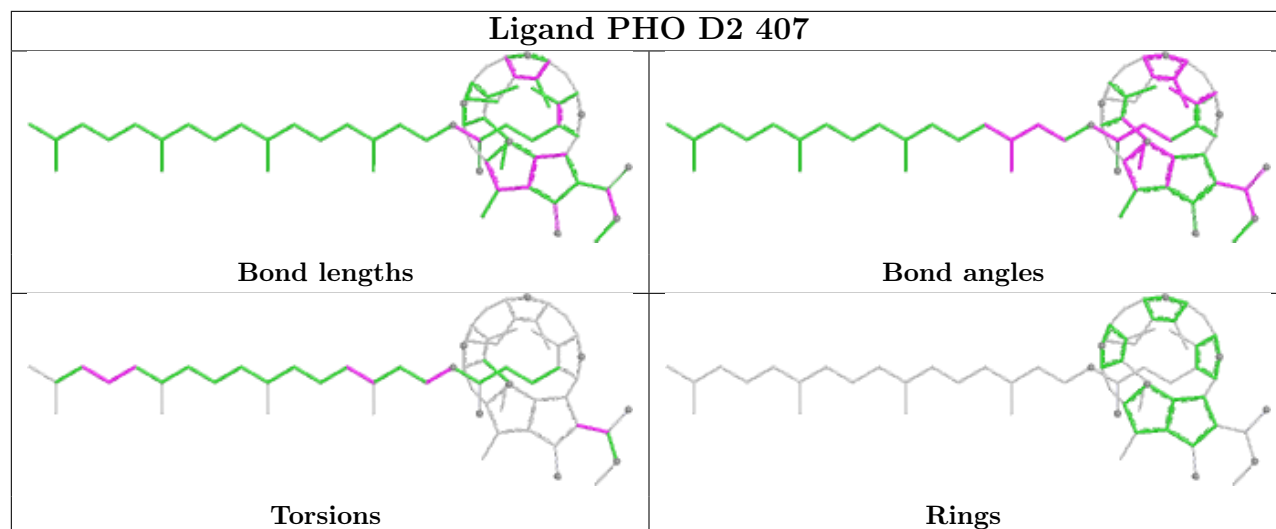
Bond angles

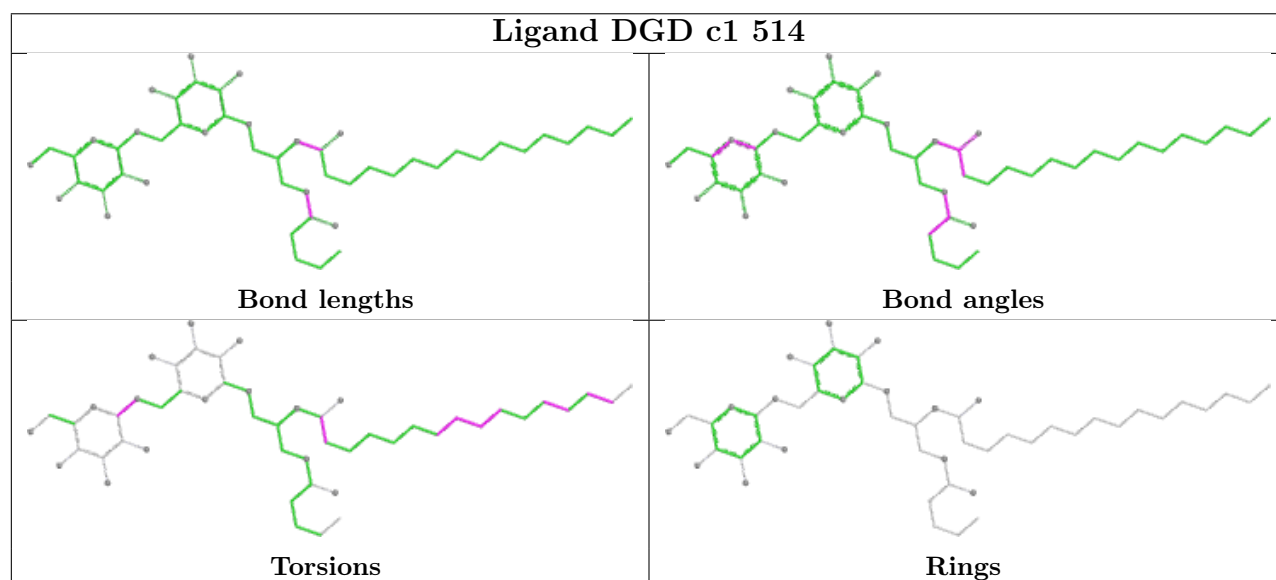
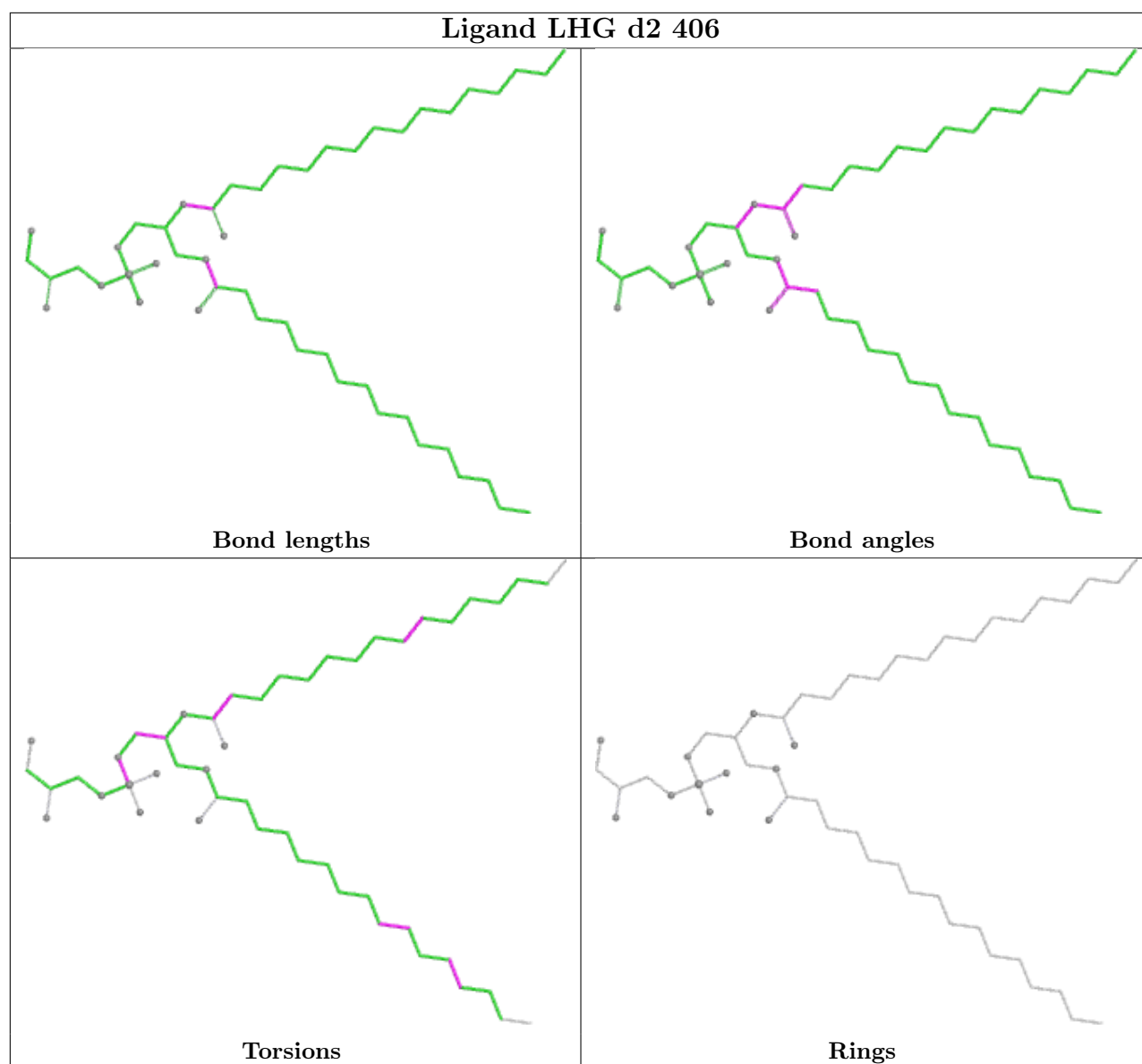


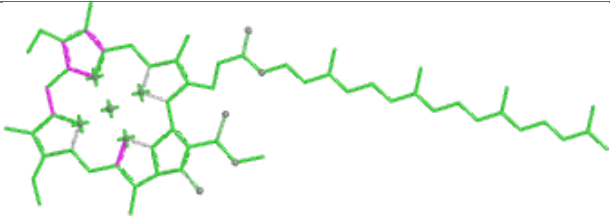
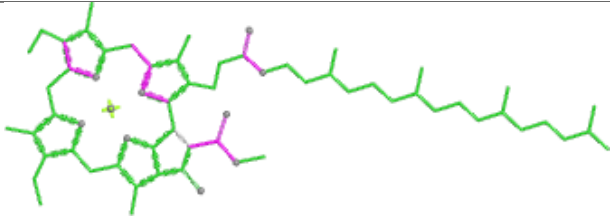
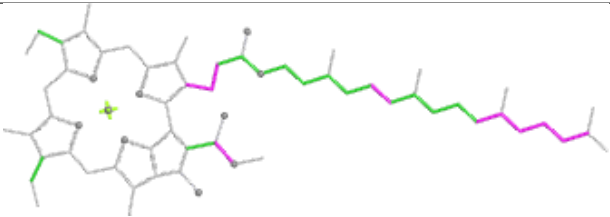
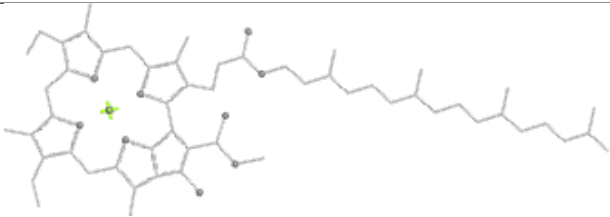
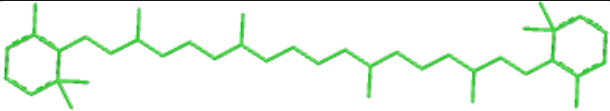
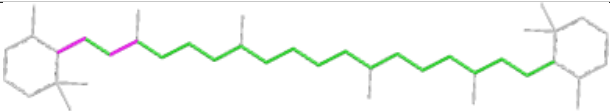
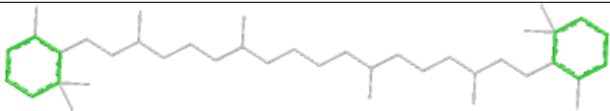
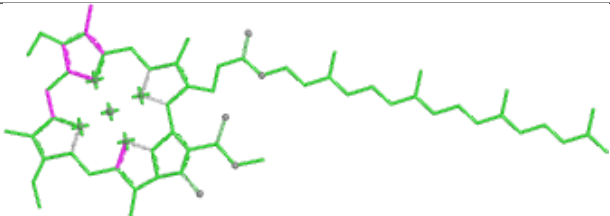
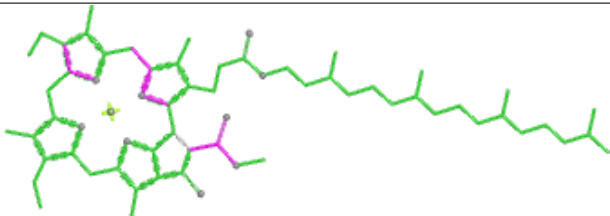
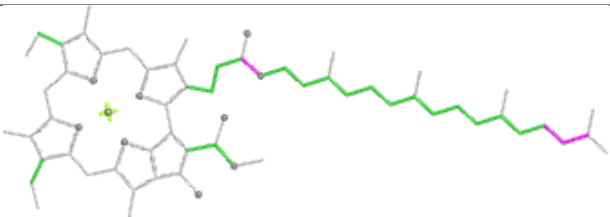
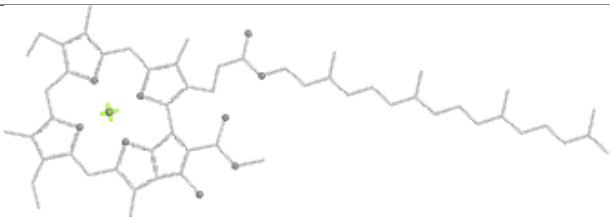
Torsions

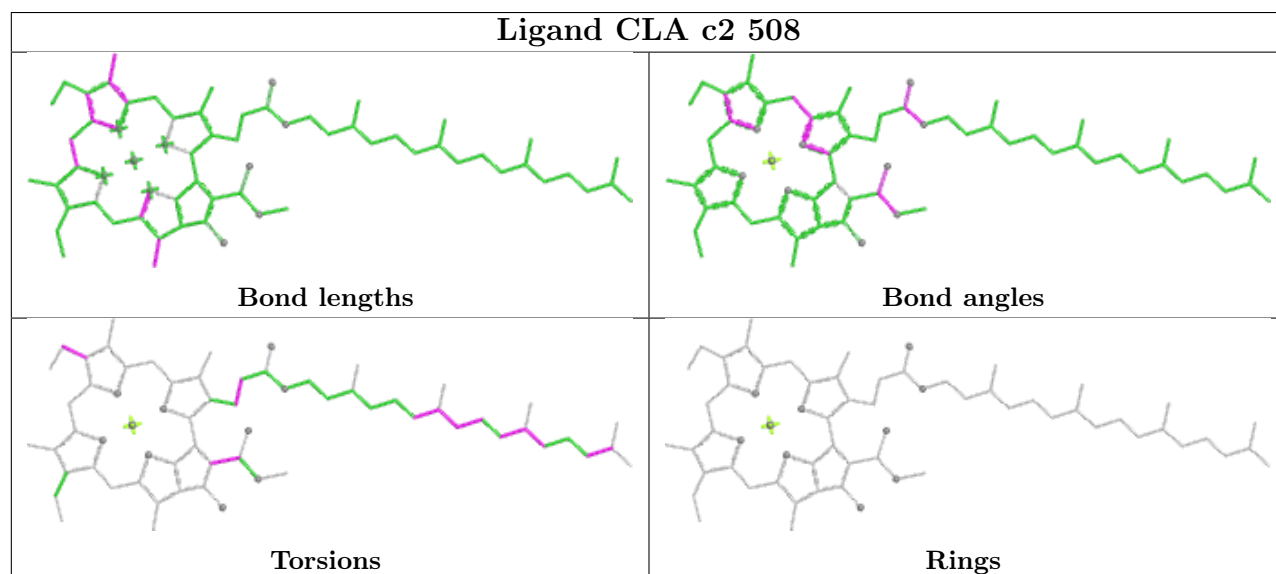
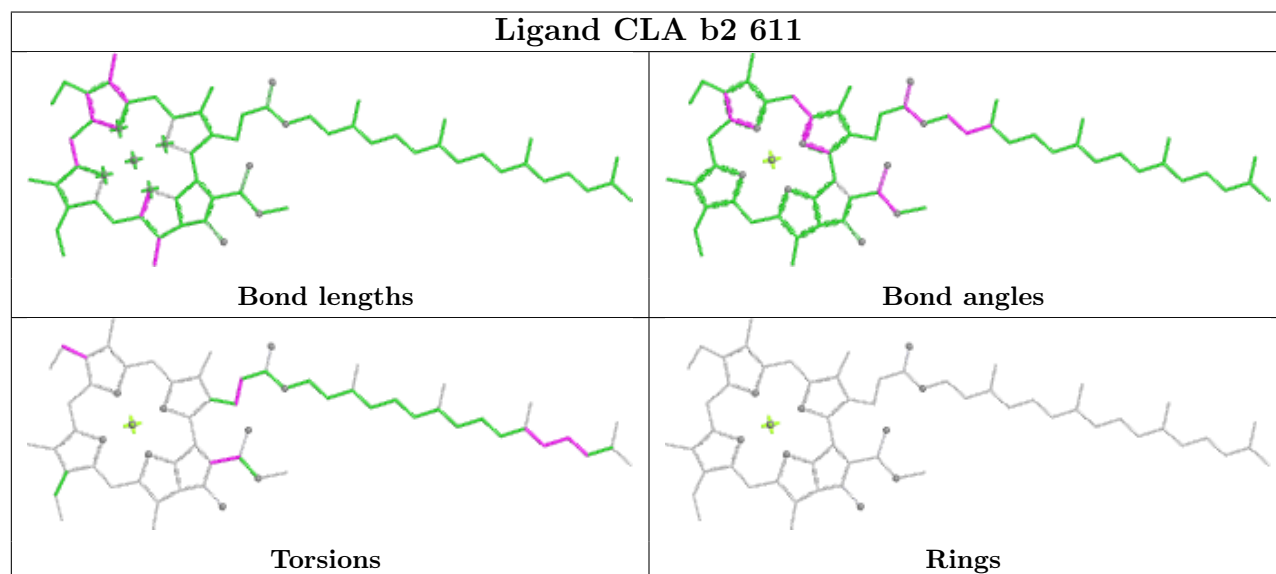
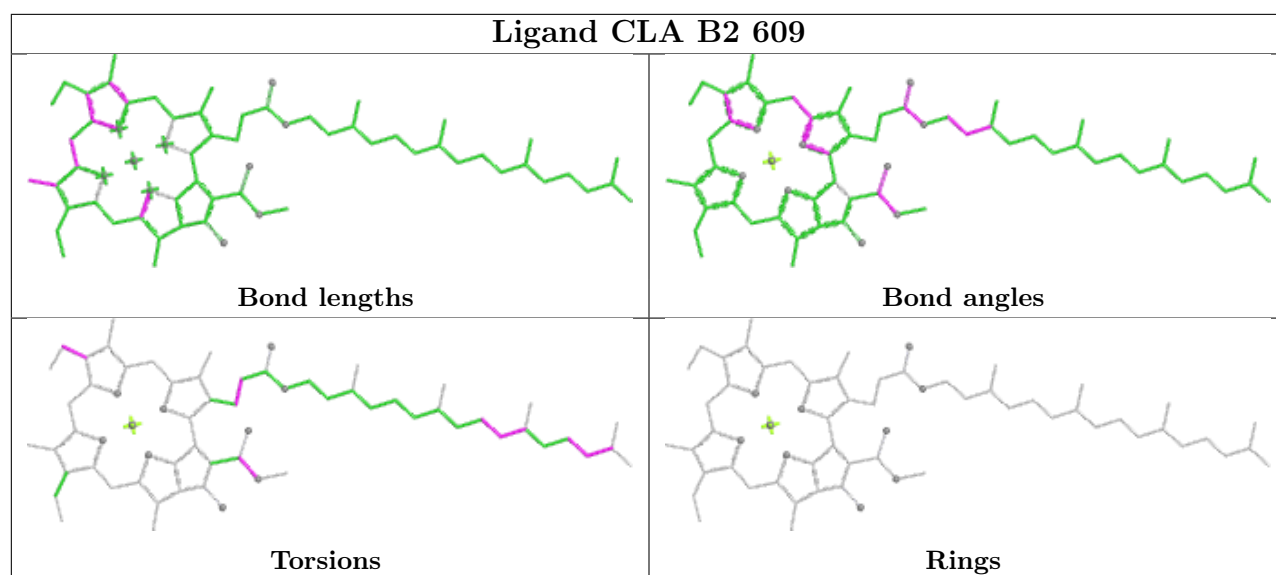


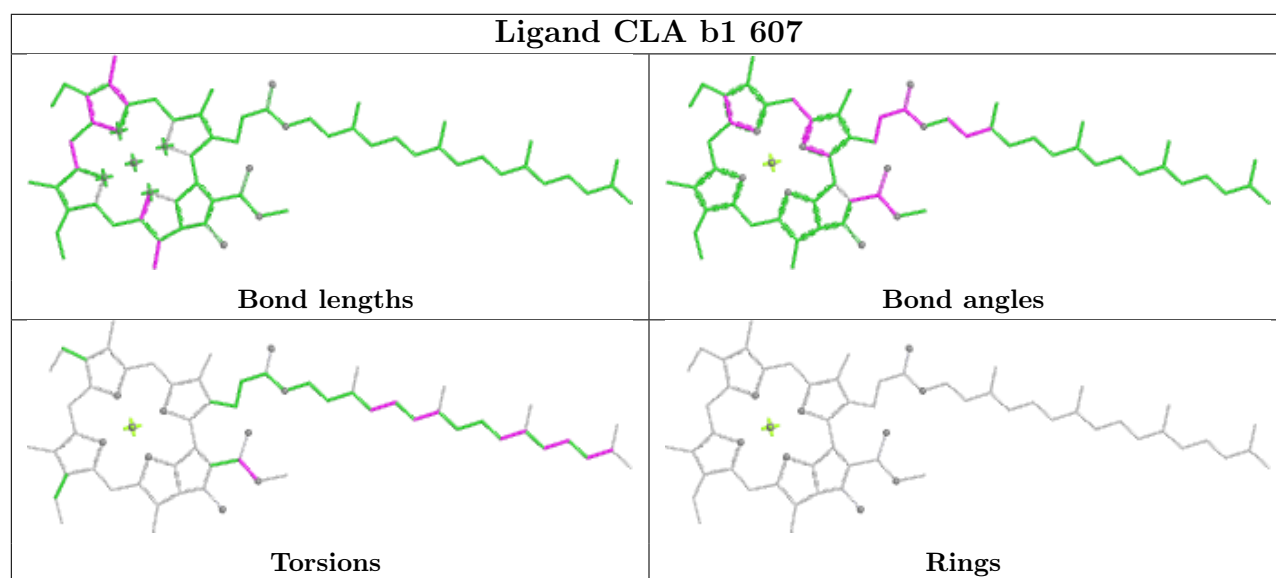
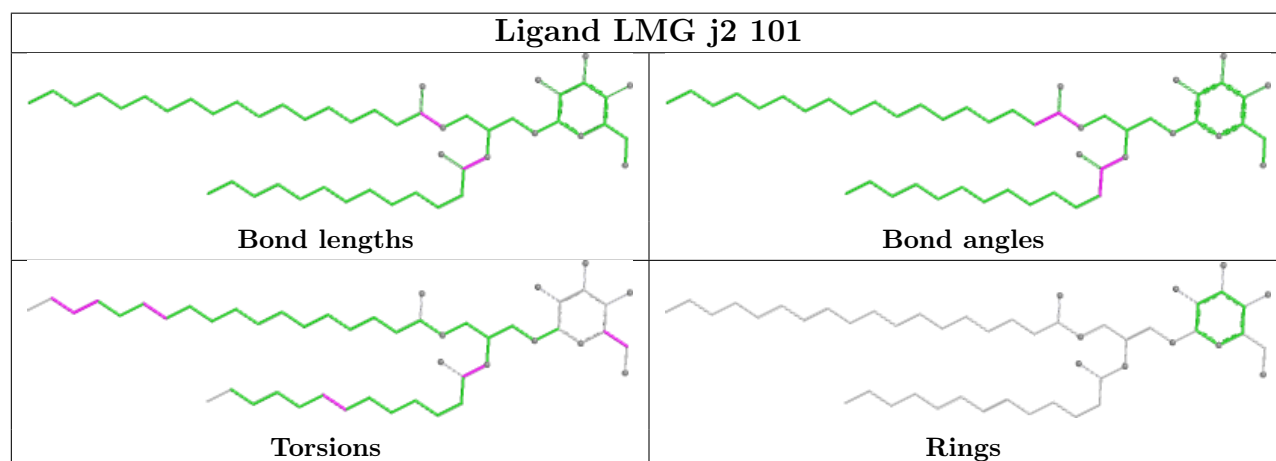
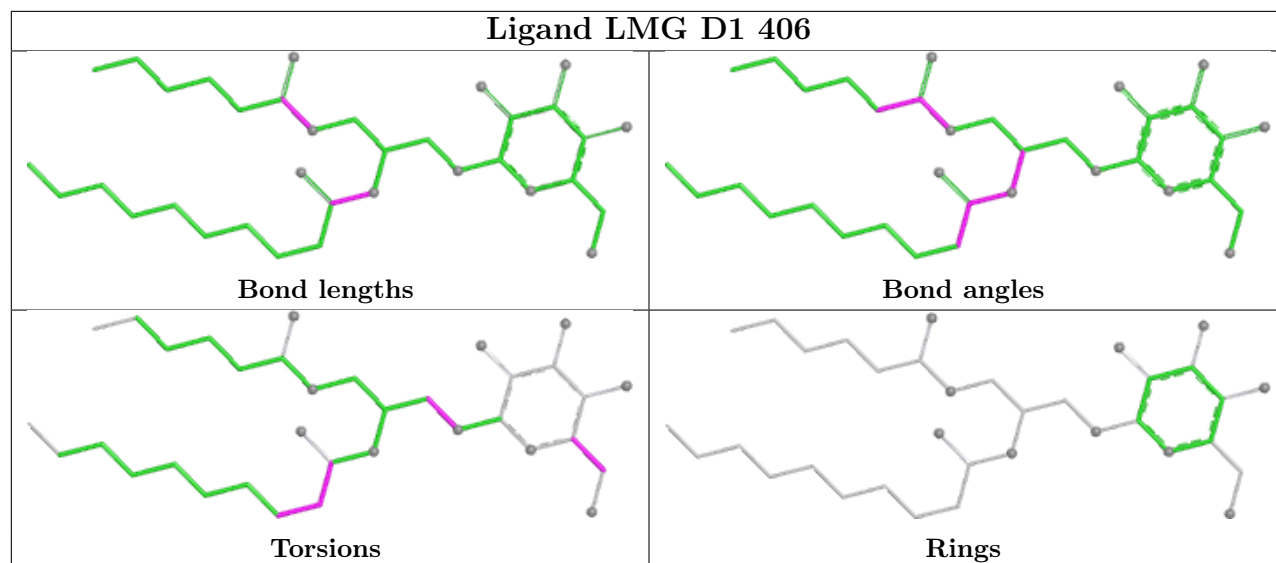
Rings

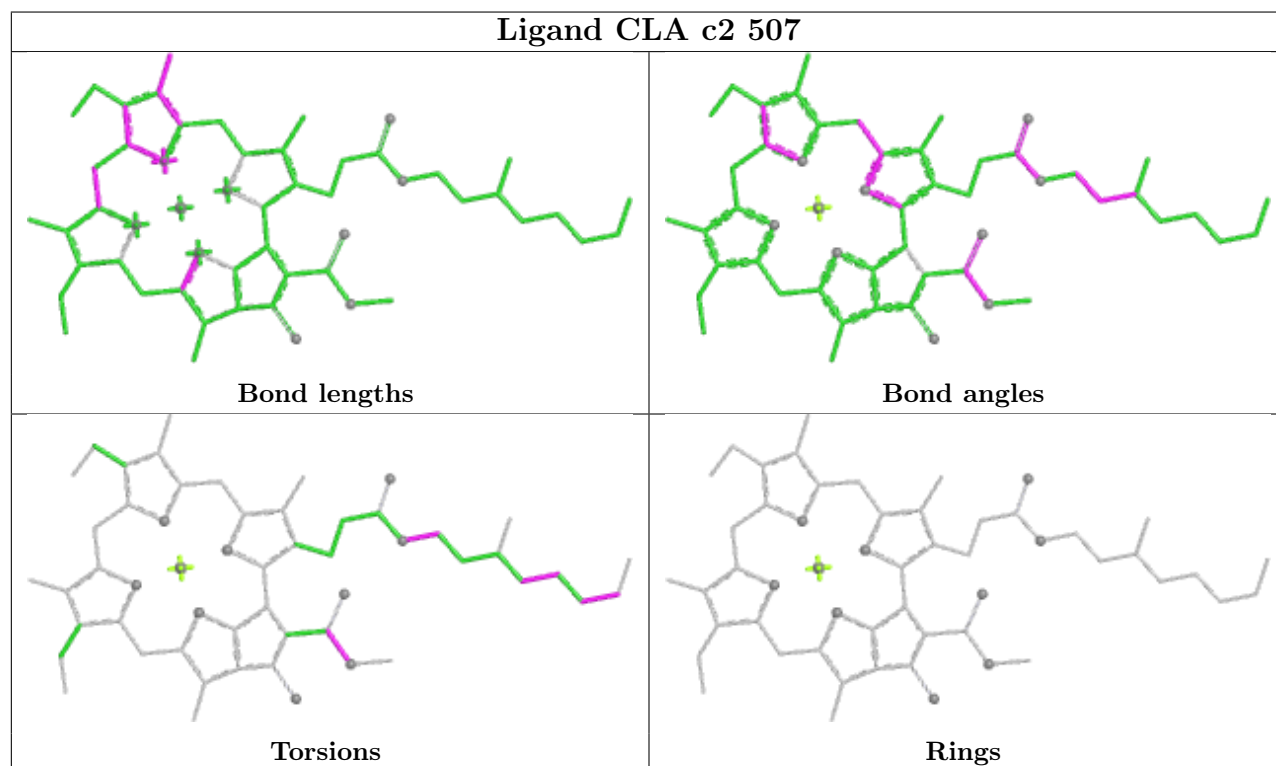
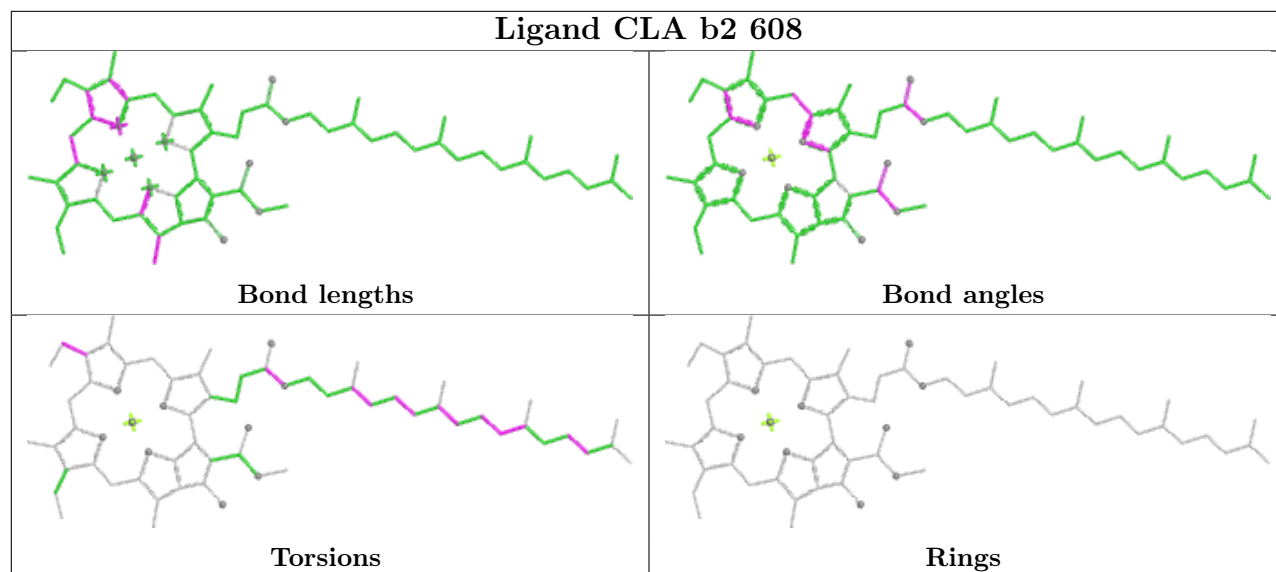




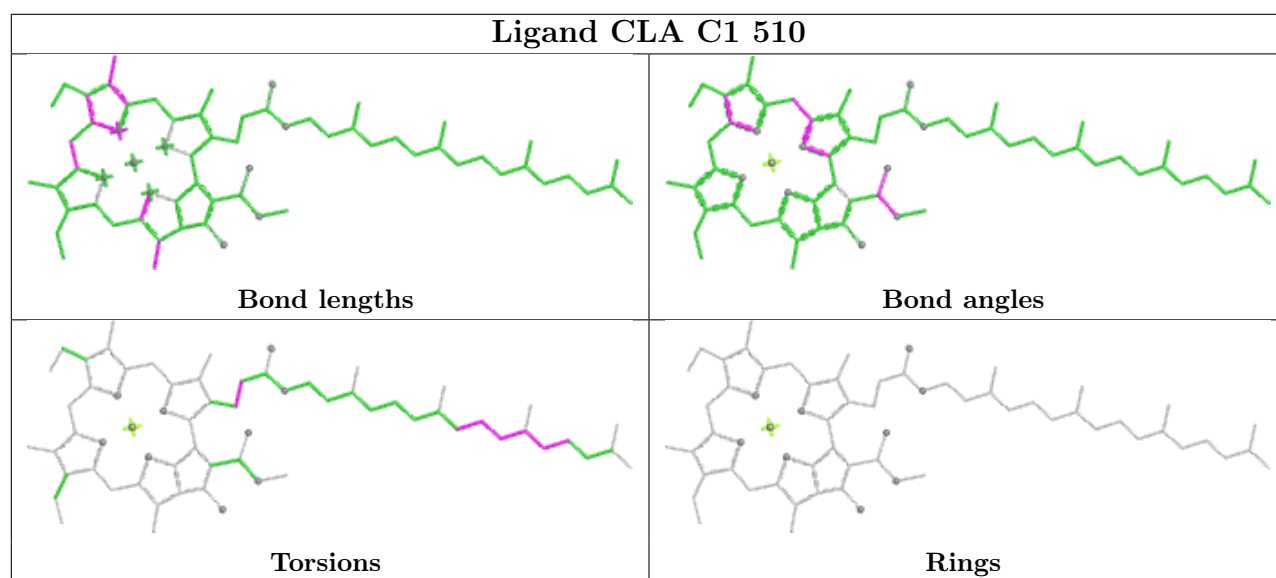
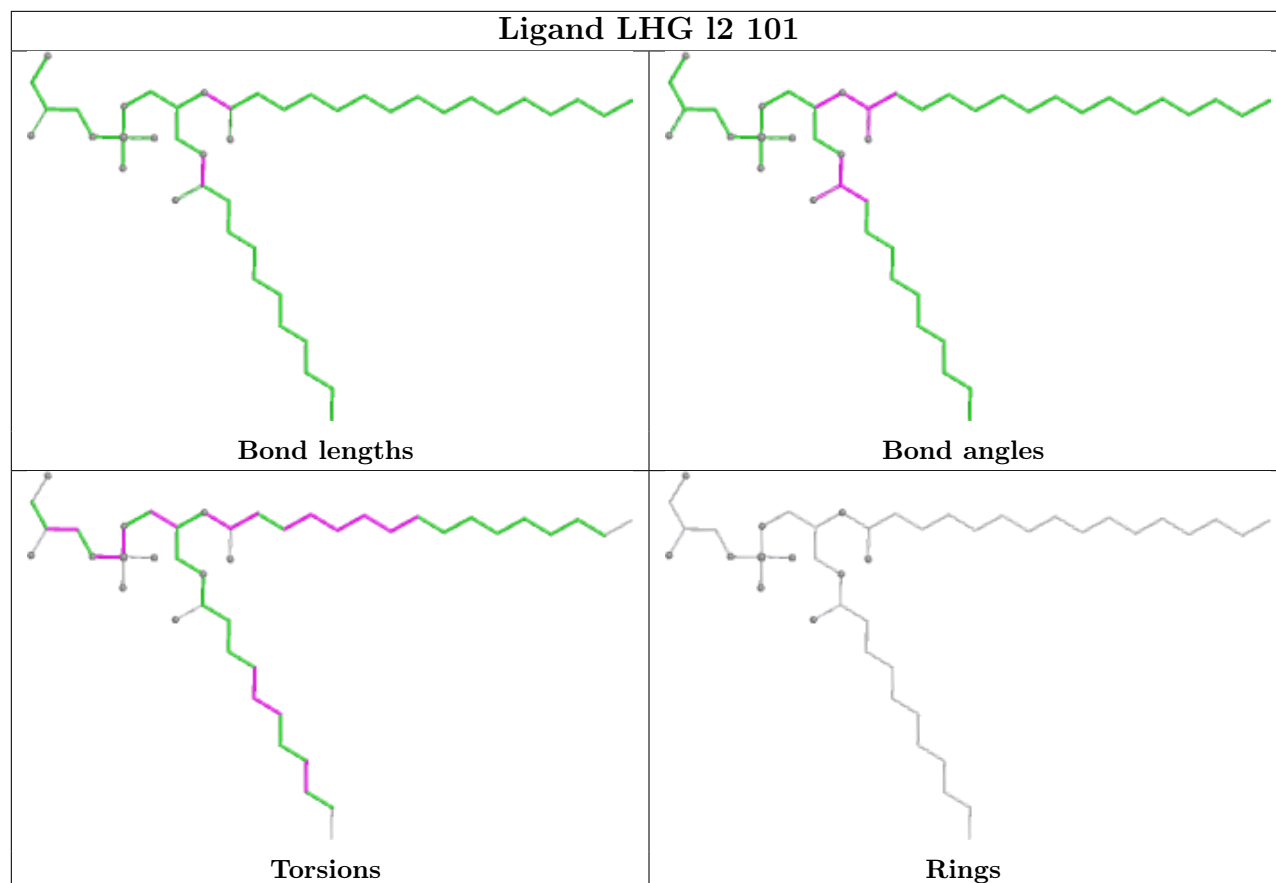
| Ligand CLA c2 502                                                                                       |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR C1 501                                                                                       |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand CLA d1 404                                                                                       |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

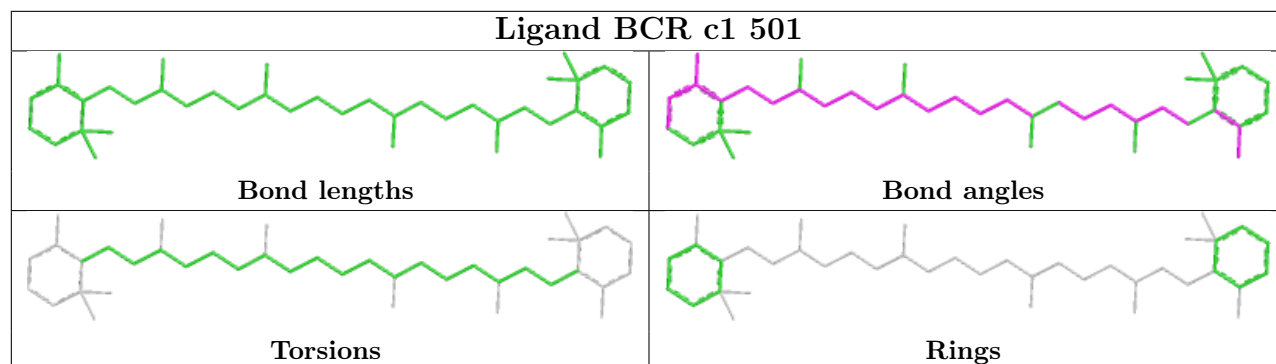
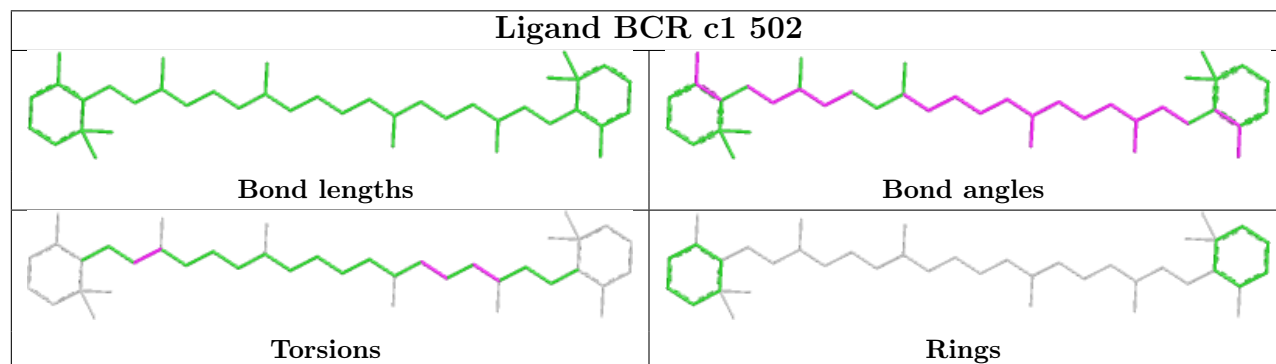
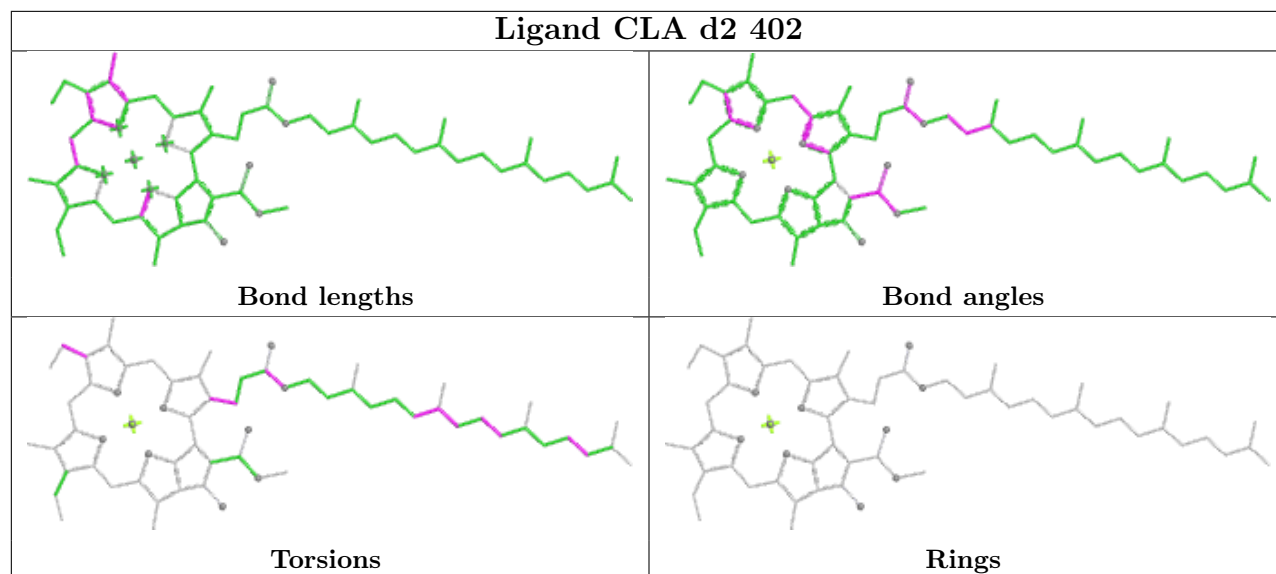


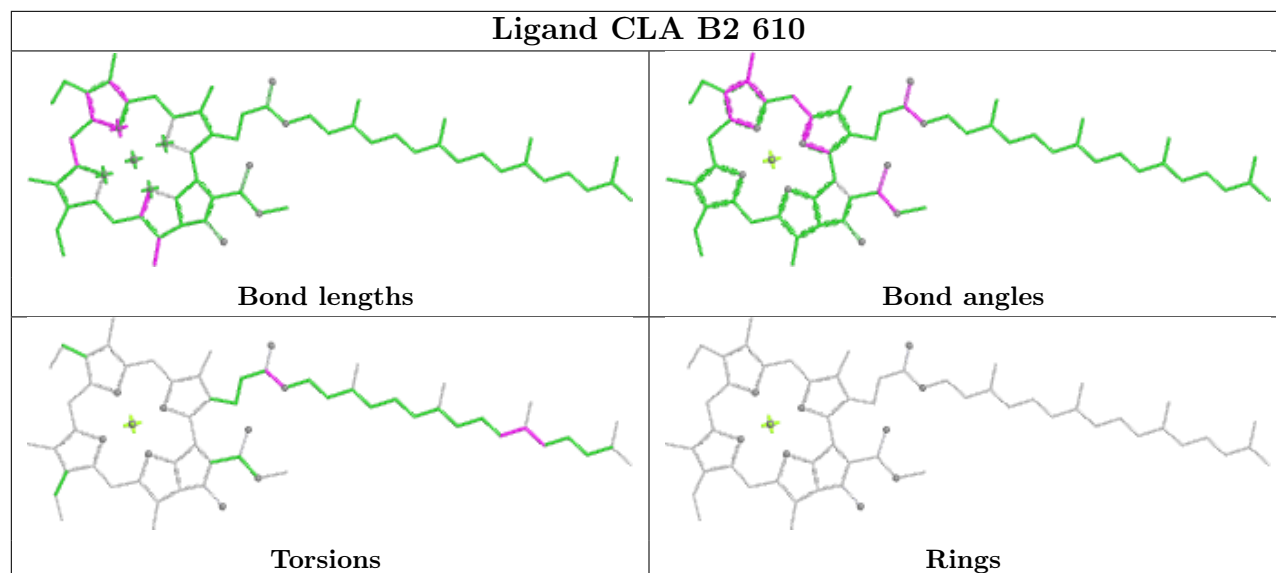
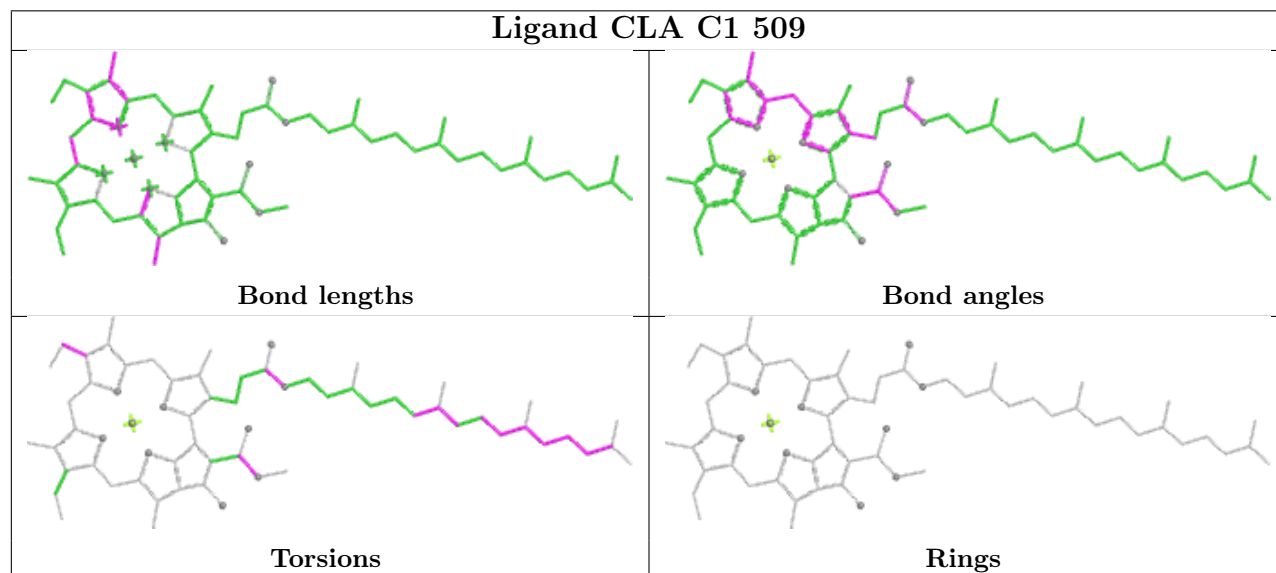
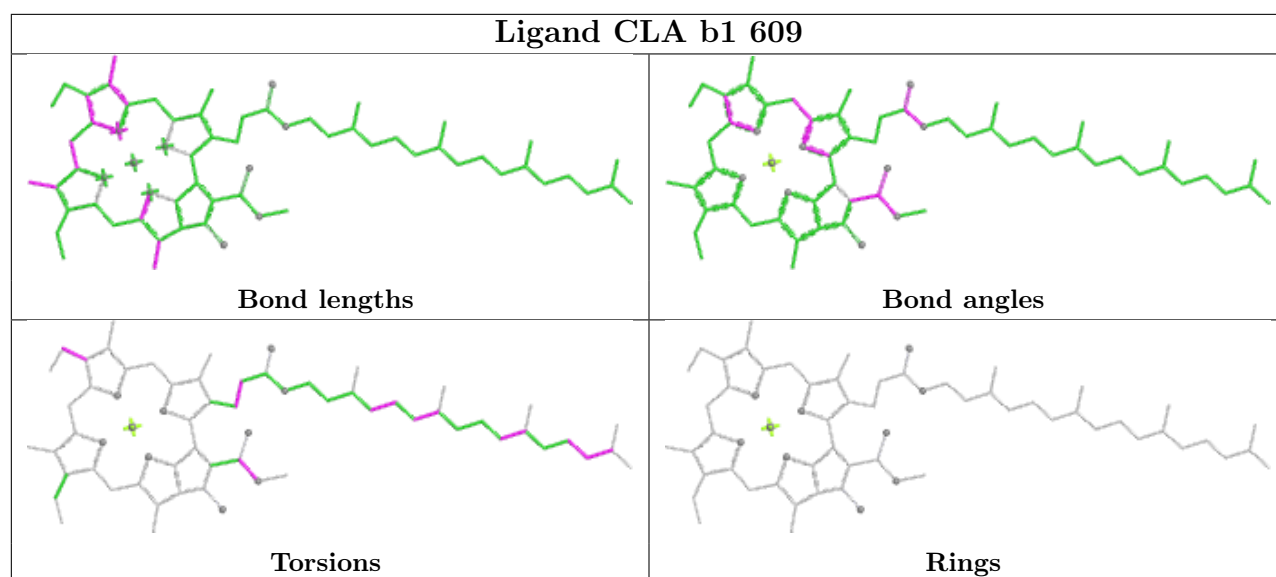


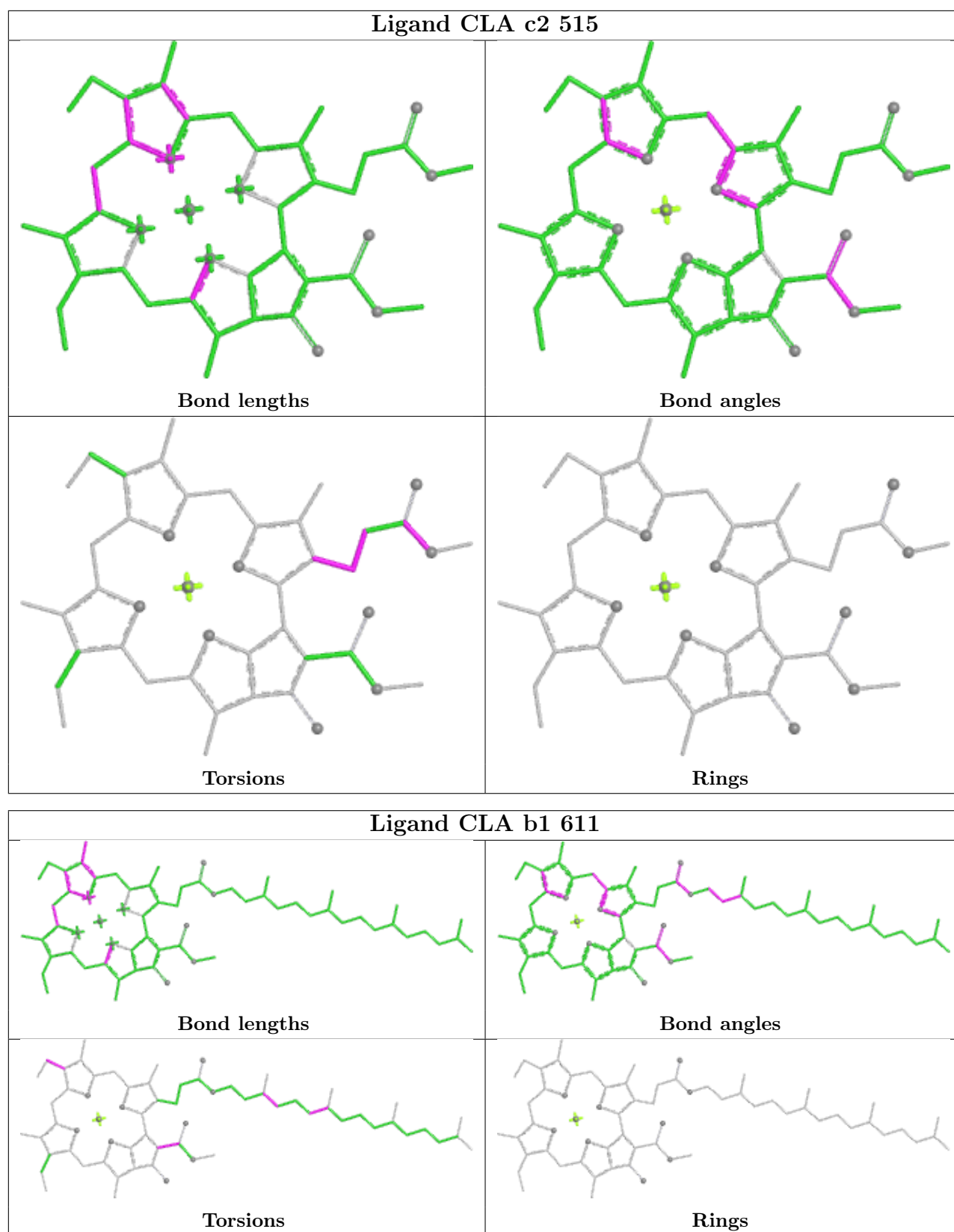


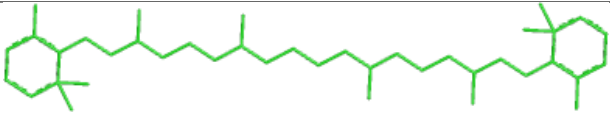
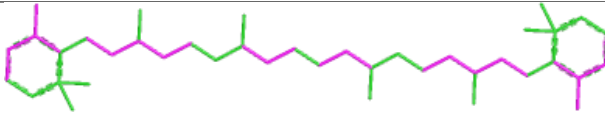
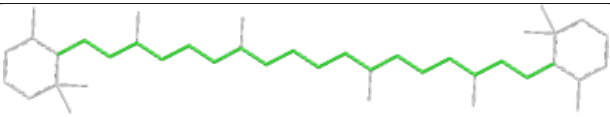
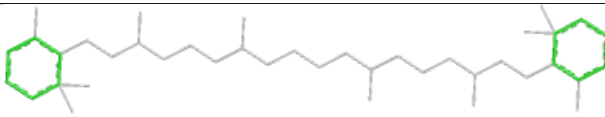
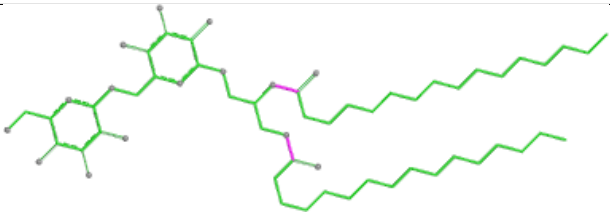
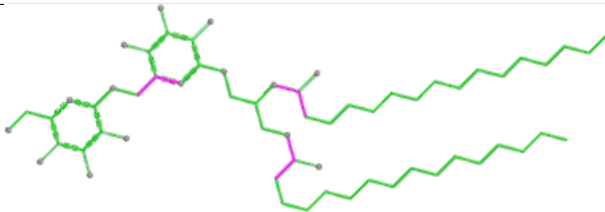
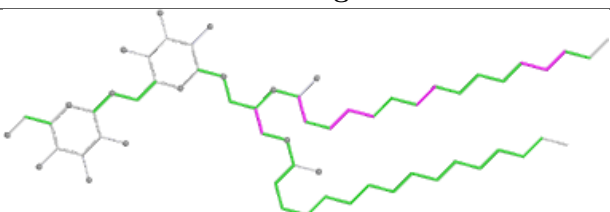
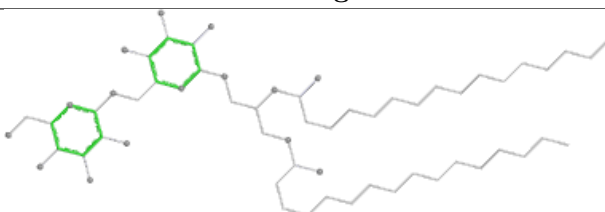
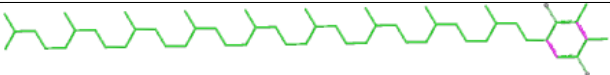
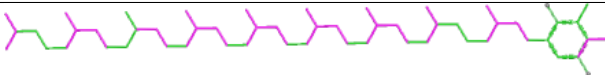
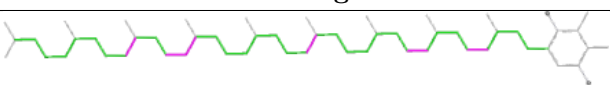
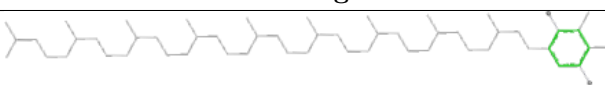


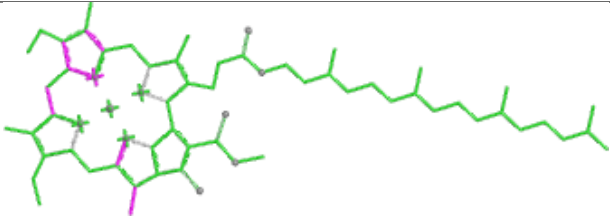
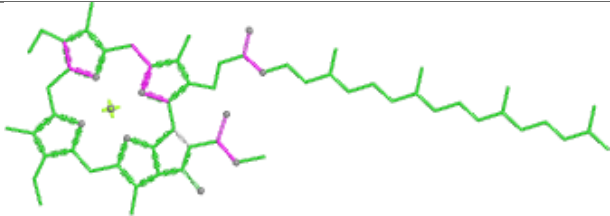
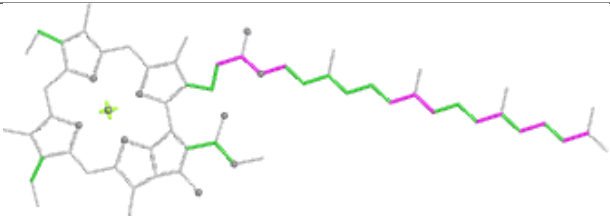
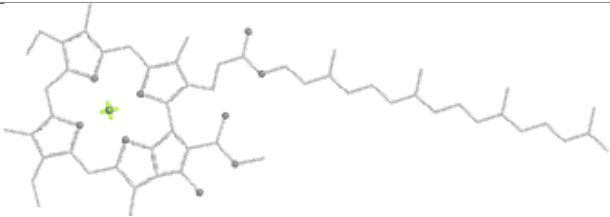
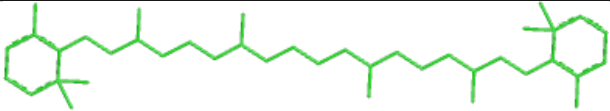
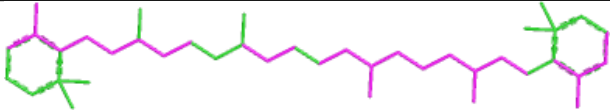
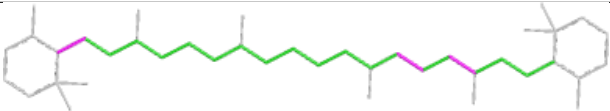
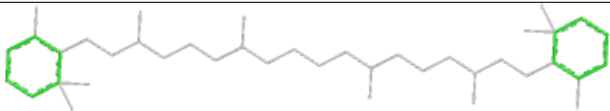




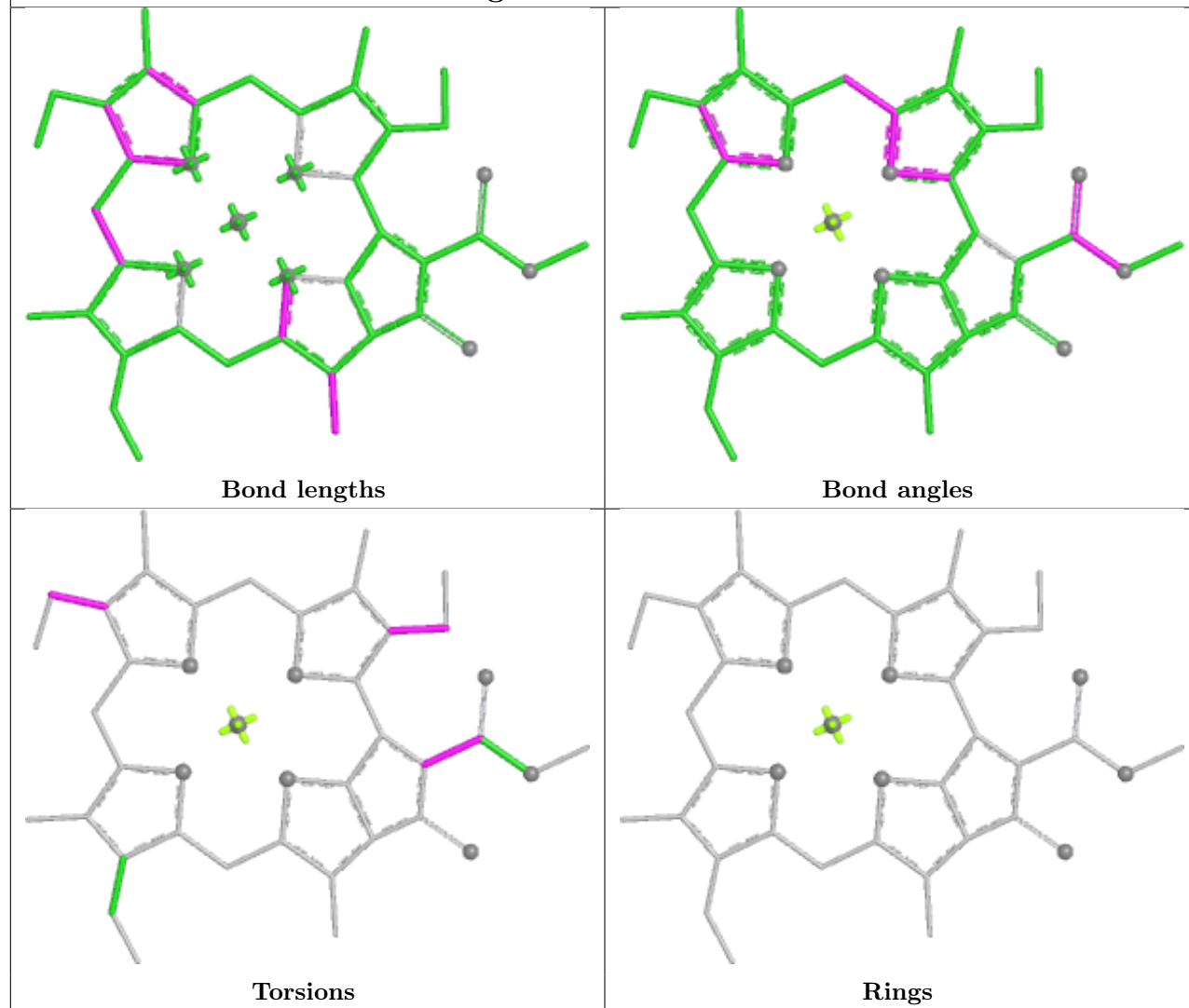




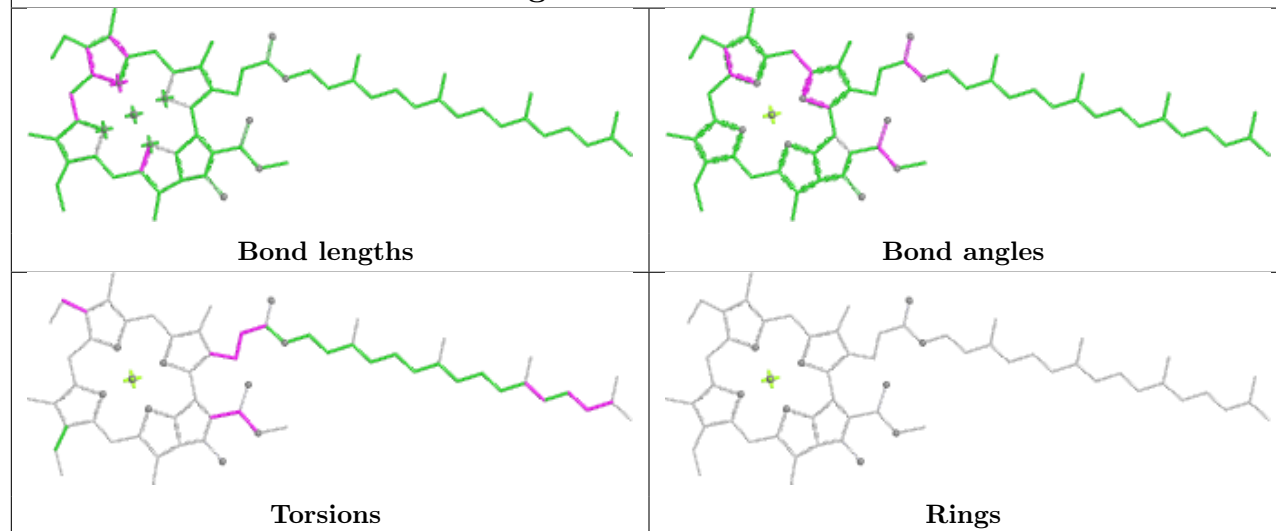
| Ligand BCR b2 603                                                                                       |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand DGD H2 101                                                                                       |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand PL9 d2 409                                                                                       |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

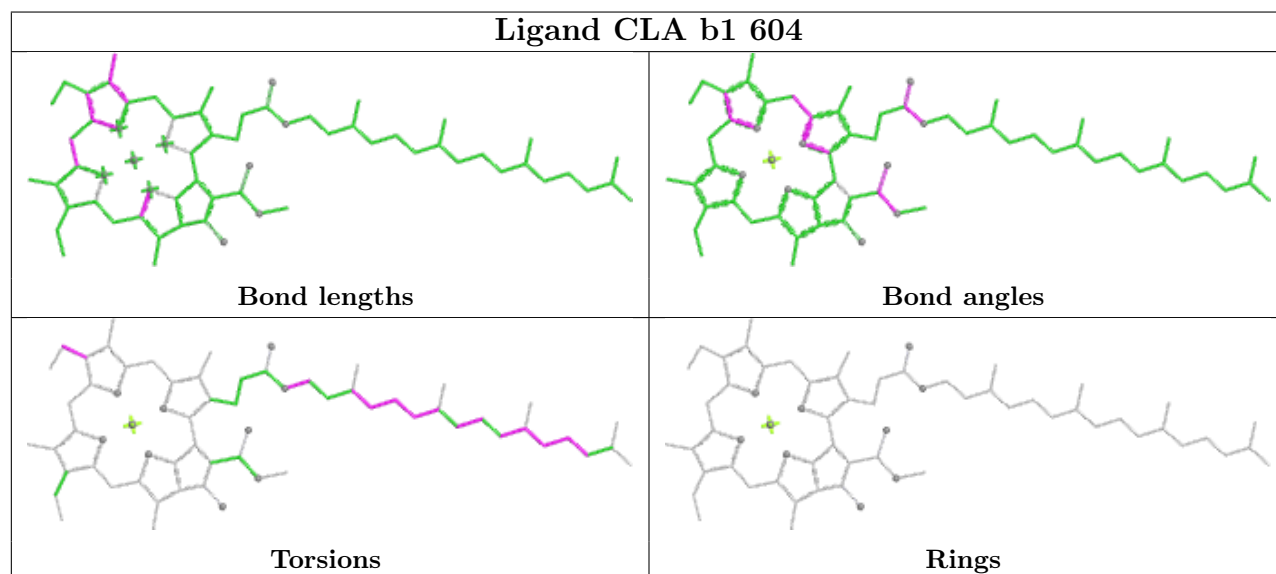
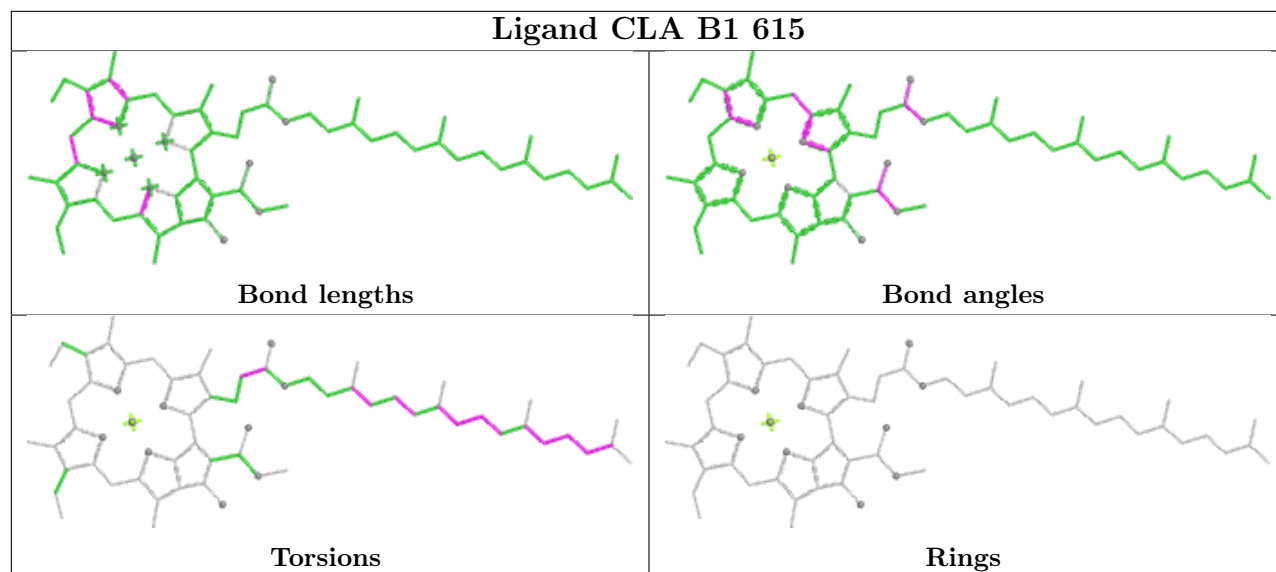
| Ligand CLA b2 614                                                                                     |                                                                                                       |
|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCR k1 101                                                                                     |                                                                                                       |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |

## Ligand CLA B1 604

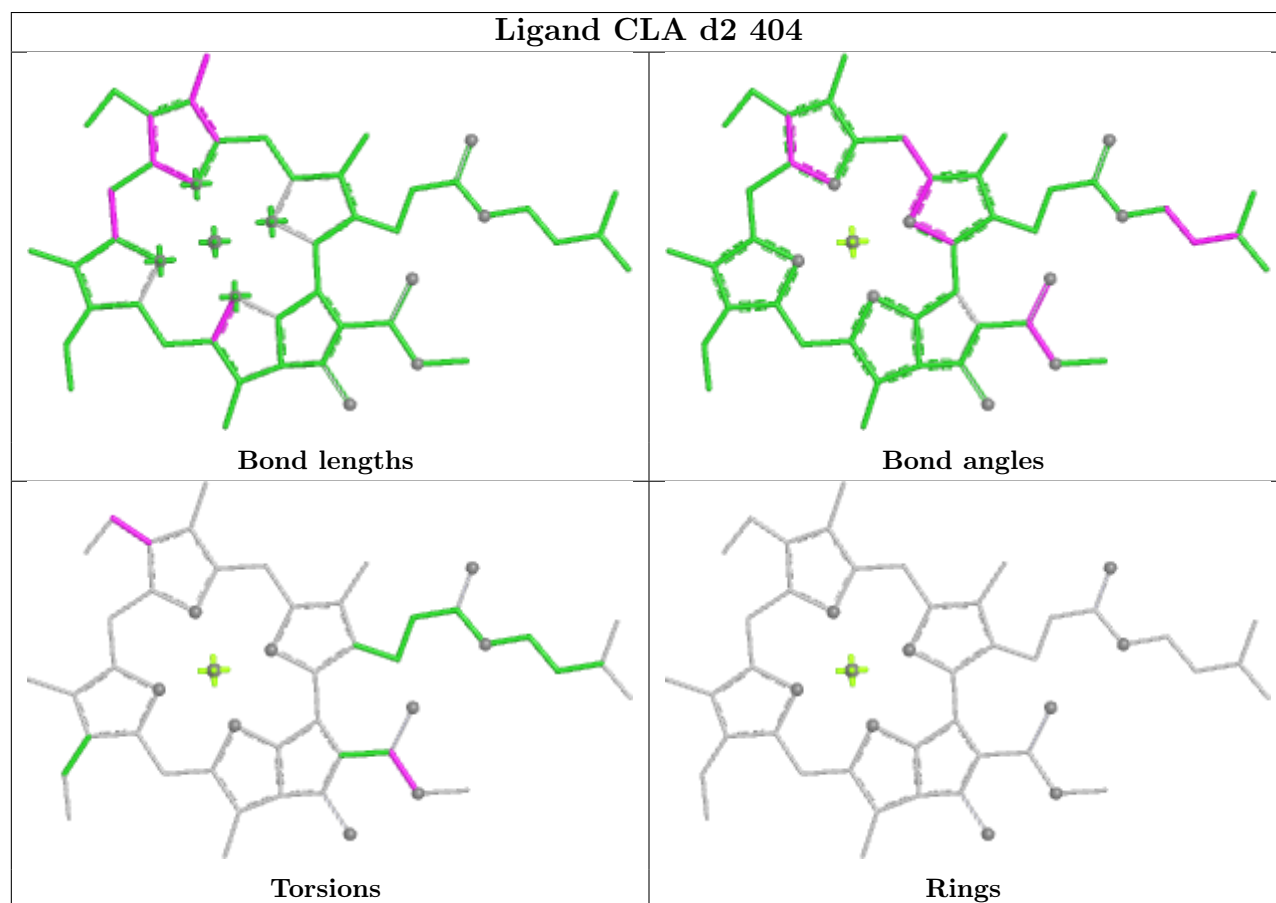
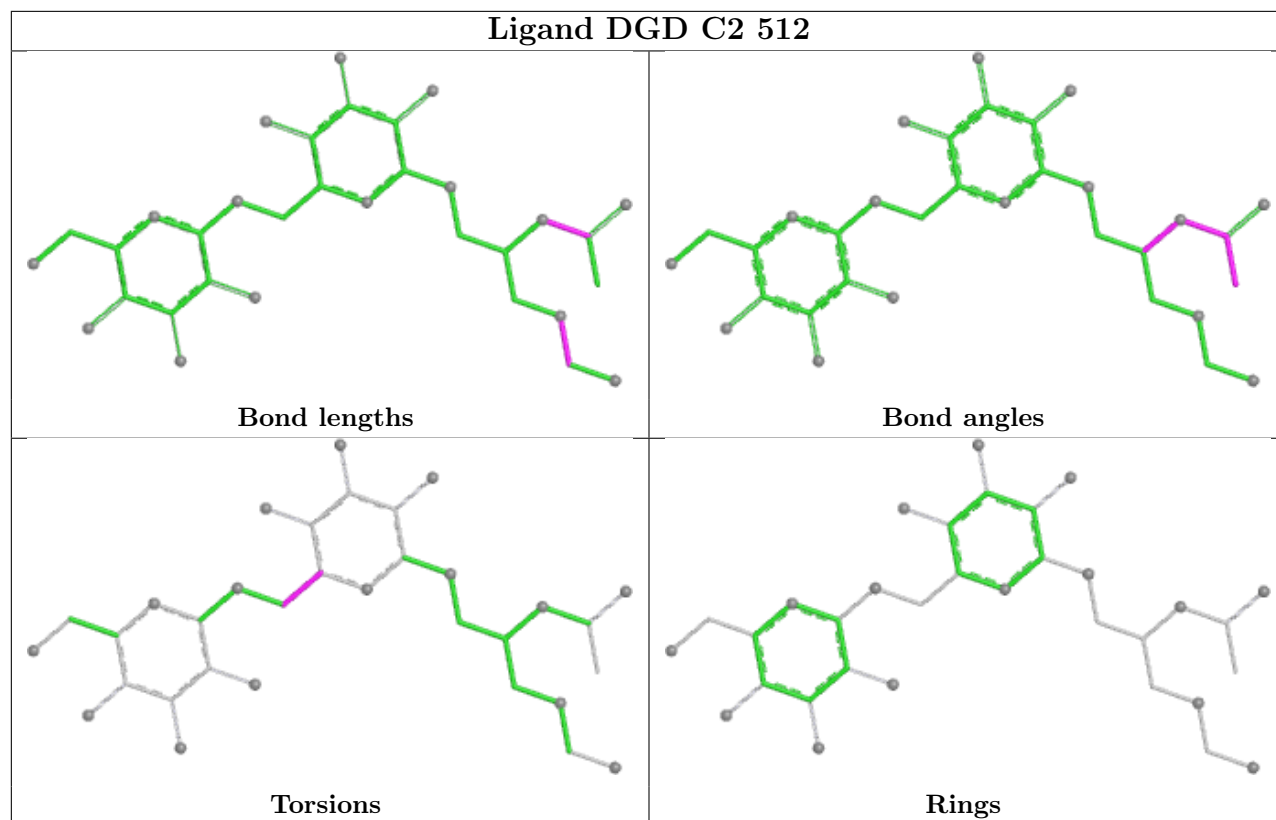


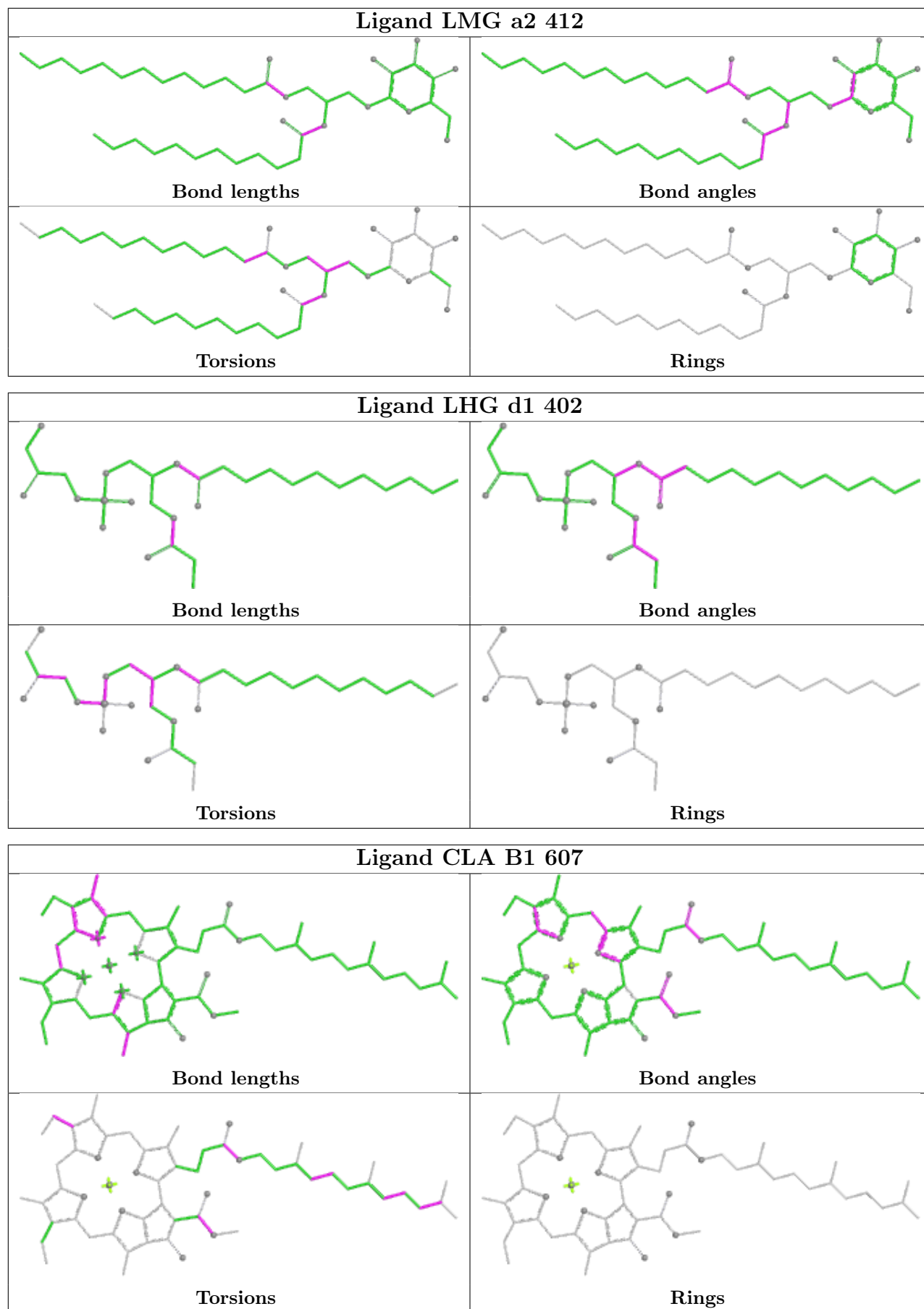
## Ligand CLA c1 503

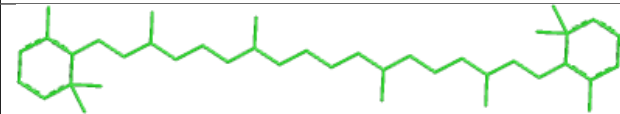
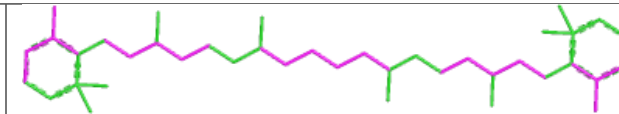
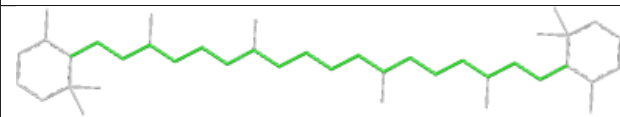
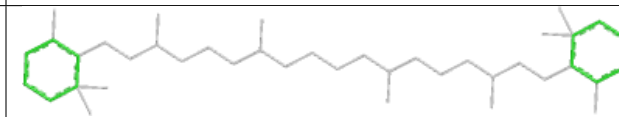


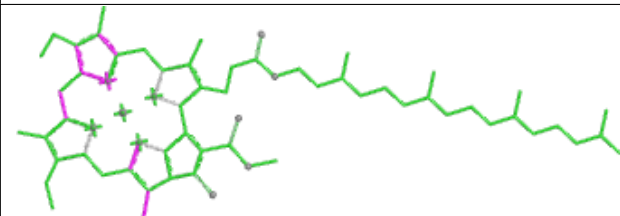
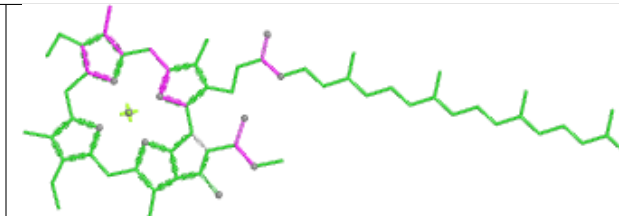
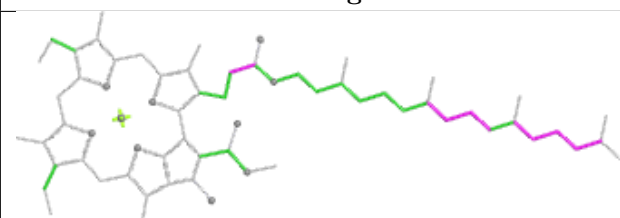
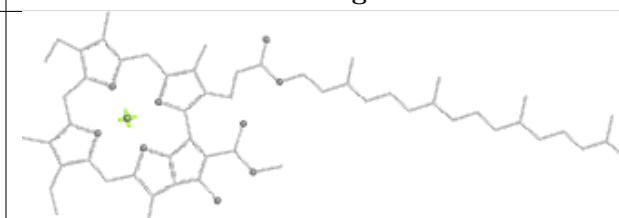


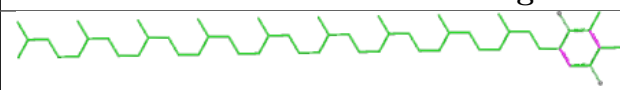
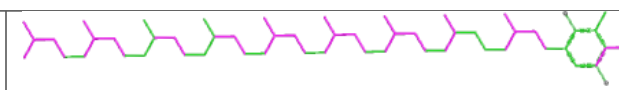
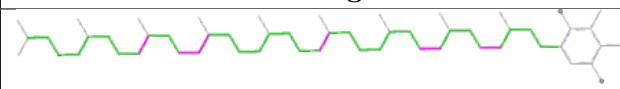
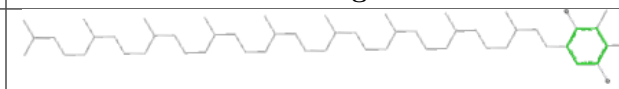


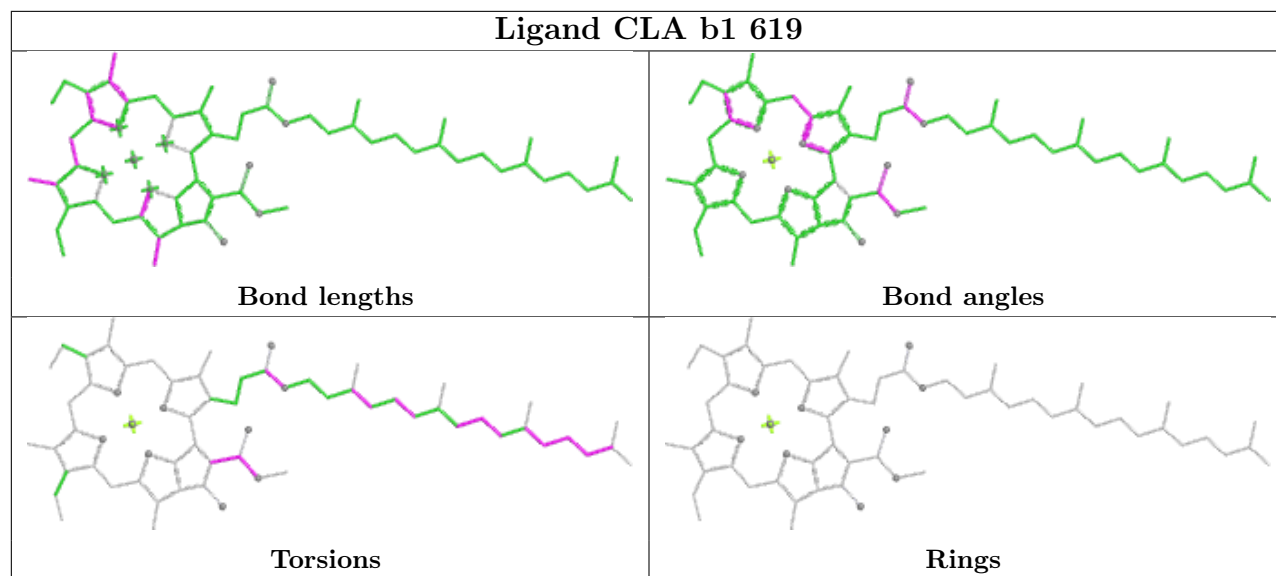




| Ligand BCR C2 502                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA B2 615                                                                  |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

| Ligand PL9 D1 408                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 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   | A1    | 344/344 (100%) | -0.17  | 3 (0%) 81 76  | 31, 48, 79, 104       | 0      |
| 1   | A2    | 332/344 (96%)  | 0.34   | 8 (2%) 59 52  | 48, 75, 91, 112       | 1 (0%) |
| 1   | a1    | 334/344 (97%)  | -0.20  | 2 (0%) 85 81  | 36, 48, 68, 105       | 0      |
| 1   | a2    | 334/344 (97%)  | -0.21  | 1 (0%) 90 88  | 34, 50, 83, 107       | 0      |
| 2   | B1    | 483/509 (94%)  | 0.11   | 6 (1%) 76 70  | 40, 63, 93, 108       | 0      |
| 2   | B2    | 503/509 (98%)  | 0.14   | 8 (1%) 70 63  | 46, 65, 93, 112       | 0      |
| 2   | b1    | 503/509 (98%)  | -0.11  | 1 (0%) 91 89  | 36, 53, 80, 99        | 1 (0%) |
| 2   | b2    | 481/509 (94%)  | 0.25   | 14 (2%) 53 46 | 43, 70, 99, 115       | 0      |
| 3   | C1    | 449/460 (97%)  | -0.04  | 8 (1%) 67 60  | 33, 59, 78, 93        | 0      |
| 3   | C2    | 444/460 (96%)  | 0.85   | 43 (9%) 13 10 | 73, 97, 117, 128      | 0      |
| 3   | c1    | 449/460 (97%)  | 0.14   | 4 (0%) 81 76  | 41, 62, 84, 101       | 2 (0%) |
| 3   | c2    | 448/460 (97%)  | 0.13   | 7 (1%) 70 63  | 39, 70, 93, 110       | 0      |
| 4   | D1    | 337/351 (96%)  | -0.14  | 2 (0%) 85 81  | 36, 56, 88, 94        | 0      |
| 4   | D2    | 340/351 (96%)  | 0.24   | 6 (1%) 67 60  | 51, 69, 85, 96        | 0      |
| 4   | d1    | 339/351 (96%)  | -0.30  | 2 (0%) 85 81  | 34, 45, 65, 94        | 0      |
| 4   | d2    | 340/351 (96%)  | -0.11  | 2 (0%) 85 81  | 36, 56, 88, 118       | 0      |
| 5   | E1    | 61/84 (72%)    | 0.56   | 7 (11%) 9 7   | 64, 87, 141, 158      | 0      |
| 5   | E2    | 63/84 (75%)    | 1.11   | 11 (17%) 4 3  | 77, 98, 131, 144      | 0      |
| 5   | e1    | 57/84 (67%)    | 0.26   | 2 (3%) 47 40  | 49, 65, 87, 91        | 0      |
| 5   | e2    | 60/84 (71%)    | 0.49   | 4 (6%) 24 19  | 59, 80, 144, 159      | 0      |
| 6   | F1    | 28/43 (65%)    | 0.28   | 1 (3%) 46 39  | 62, 75, 123, 131      | 0      |
| 6   | F2    | 31/43 (72%)    | 1.19   | 7 (22%) 2 1   | 81, 92, 144, 146      | 0      |
| 6   | f1    | 29/43 (67%)    | 0.08   | 1 (3%) 48 41  | 50, 60, 95, 108       | 0      |
| 6   | f2    | 29/43 (67%)    | 0.50   | 2 (6%) 23 18  | 64, 73, 128, 149      | 0      |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 7   | H1    | 60/67 (89%)   | 0.46   | 2 (3%) 49 42  | 70, 84, 93, 101       | 0     |
| 7   | H2    | 62/67 (92%)   | 0.36   | 0 100 100     | 63, 75, 92, 124       | 0     |
| 7   | h1    | 62/67 (92%)   | -0.10  | 0 100 100     | 47, 67, 78, 84        | 0     |
| 7   | h2    | 62/67 (92%)   | 0.55   | 6 (9%) 13 10  | 72, 87, 98, 122       | 0     |
| 8   | I1    | 34/38 (89%)   | -0.06  | 0 100 100     | 53, 61, 70, 71        | 0     |
| 8   | I2    | 35/38 (92%)   | 0.63   | 1 (2%) 53 46  | 82, 93, 105, 109      | 0     |
| 8   | i1    | 34/38 (89%)   | 0.03   | 0 100 100     | 54, 61, 71, 76        | 0     |
| 8   | i2    | 33/38 (86%)   | 0.15   | 0 100 100     | 60, 67, 75, 77        | 0     |
| 9   | J1    | 32/39 (82%)   | 0.16   | 1 (3%) 51 44  | 51, 65, 89, 105       | 0     |
| 9   | J2    | 35/39 (89%)   | 1.06   | 7 (20%) 3 2   | 75, 87, 125, 136      | 0     |
| 9   | j1    | 32/39 (82%)   | 0.10   | 0 100 100     | 49, 63, 74, 81        | 0     |
| 9   | j2    | 33/39 (84%)   | 0.23   | 1 (3%) 52 45  | 54, 70, 88, 110       | 0     |
| 10  | K1    | 37/41 (90%)   | 0.15   | 1 (2%) 56 48  | 56, 66, 78, 79        | 0     |
| 10  | K2    | 37/41 (90%)   | 1.06   | 6 (16%) 4 4   | 86, 96, 111, 117      | 0     |
| 10  | k1    | 37/41 (90%)   | 0.23   | 0 100 100     | 56, 67, 81, 81        | 0     |
| 10  | k2    | 37/41 (90%)   | 0.69   | 2 (5%) 31 26  | 67, 76, 89, 92        | 0     |
| 11  | L1    | 37/38 (97%)   | -0.26  | 0 100 100     | 39, 43, 67, 77        | 0     |
| 11  | L2    | 37/38 (97%)   | -0.03  | 0 100 100     | 49, 56, 61, 73        | 0     |
| 11  | l1    | 37/38 (97%)   | -0.16  | 0 100 100     | 36, 43, 63, 73        | 0     |
| 11  | l2    | 37/38 (97%)   | -0.15  | 0 100 100     | 43, 47, 73, 79        | 0     |
| 12  | M1    | 40/108 (37%)  | -0.11  | 0 100 100     | 32, 46, 62, 66        | 0     |
| 12  | M2    | 40/108 (37%)  | -0.10  | 0 100 100     | 45, 54, 67, 69        | 0     |
| 12  | m1    | 40/108 (37%)  | -0.05  | 1 (2%) 58 50  | 34, 44, 65, 67        | 0     |
| 12  | m2    | 40/108 (37%)  | -0.00  | 1 (2%) 58 50  | 44, 51, 65, 71        | 0     |
| 13  | O1    | 240/329 (72%) | 0.19   | 10 (4%) 40 34 | 38, 61, 96, 107       | 0     |
| 13  | O2    | 205/329 (62%) | 0.91   | 30 (14%) 6 5  | 54, 91, 119, 151      | 0     |
| 13  | o1    | 238/329 (72%) | 0.42   | 15 (6%) 26 21 | 38, 76, 121, 145      | 0     |
| 13  | o2    | 245/329 (74%) | 0.24   | 13 (5%) 32 26 | 41, 64, 103, 127      | 0     |
| 14  | T1    | 30/32 (93%)   | -0.24  | 1 (3%) 49 42  | 37, 44, 60, 68        | 0     |
| 14  | T2    | 30/32 (93%)   | 0.10   | 1 (3%) 49 42  | 54, 63, 76, 82        | 0     |
| 14  | t1    | 30/32 (93%)   | -0.23  | 0 100 100     | 40, 46, 60, 76        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-------------------|--------|----------------|-----------------------|--------|
| 14  | t2    | 29/32 (90%)       | -0.31  | 0 100 100      | 38, 48, 68, 84        | 0      |
| 15  | U1    | 93/155 (60%)      | -0.11  | 0 100 100      | 44, 59, 75, 104       | 0      |
| 15  | U2    | 90/155 (58%)      | 0.48   | 5 (5%) 30 25   | 74, 91, 104, 115      | 0      |
| 15  | u1    | 93/155 (60%)      | 0.03   | 1 (1%) 78 72   | 53, 68, 88, 95        | 0      |
| 15  | u2    | 93/155 (60%)      | -0.17  | 1 (1%) 78 72   | 44, 58, 71, 86        | 0      |
| 16  | V1    | 129/155 (83%)     | 0.15   | 1 (0%) 82 77   | 47, 62, 87, 93        | 0      |
| 16  | V2    | 129/155 (83%)     | 0.89   | 14 (10%) 10 8  | 75, 96, 114, 127      | 0      |
| 16  | v1    | 129/155 (83%)     | 0.37   | 5 (3%) 43 36   | 47, 69, 108, 124      | 0      |
| 16  | v2    | 129/155 (83%)     | 0.08   | 4 (3%) 51 44   | 47, 63, 90, 105       | 0      |
| 17  | Y1    | 27/35 (77%)       | 0.18   | 0 100 100      | 64, 74, 103, 118      | 0      |
| 17  | Y2    | 25/35 (71%)       | 1.00   | 1 (4%) 42 36   | 96, 100, 107, 109     | 0      |
| 17  | y1    | 27/35 (77%)       | 0.64   | 1 (3%) 45 38   | 64, 71, 105, 107      | 0      |
| 17  | y2    | 27/35 (77%)       | 0.52   | 0 100 100      | 72, 79, 92, 106       | 0      |
| 18  | X1    | 29/40 (72%)       | 1.32   | 5 (17%) 4 3    | 98, 113, 130, 135     | 0      |
| 18  | X2    | 31/40 (77%)       | 1.42   | 6 (19%) 3 2    | 83, 101, 114, 121     | 0      |
| 18  | x1    | 36/40 (90%)       | 0.90   | 6 (16%) 4 3    | 61, 83, 96, 102       | 0      |
| 18  | x2    | 32/40 (80%)       | 0.96   | 5 (15%) 5 4    | 83, 104, 122, 126     | 0      |
| 19  | S1    | 25/46 (54%)       | 0.63   | 1 (4%) 42 36   | 72, 79, 85, 98        | 0      |
| 19  | S2    | 30/46 (65%)       | 1.39   | 7 (23%) 2 1    | 98, 114, 120, 122     | 0      |
| 19  | s1    | 40/46 (86%)       | 0.75   | 2 (5%) 34 28   | 54, 78, 94, 95        | 0      |
| 19  | s2    | 46/46 (100%)      | 0.95   | 5 (10%) 10 8   | 75, 90, 106, 112      | 0      |
| 20  | W1    | 21/25 (84%)       | 0.64   | 1 (4%) 35 30   | 71, 79, 86, 90        | 0      |
| 20  | W2    | 21/25 (84%)       | 0.52   | 0 100 100      | 66, 76, 84, 89        | 0      |
| 20  | w1    | 25/25 (100%)      | 0.85   | 3 (12%) 9 7    | 73, 79, 96, 101       | 0      |
| 20  | w2    | 20/25 (80%)       | 0.88   | 3 (15%) 5 4    | 91, 96, 103, 111      | 0      |
| 21  | Q2    | 111/218 (50%)     | 1.29   | 24 (21%) 2 2   | 122, 132, 145, 151    | 0      |
| 21  | q1    | 105/218 (48%)     | 1.08   | 18 (17%) 4 3   | 103, 125, 138, 144    | 0      |
| 22  | Z2    | 59/62 (95%)       | 1.22   | 13 (22%) 2 2   | 108, 121, 134, 140    | 0      |
| 22  | z2    | 59/62 (95%)       | 0.87   | 4 (6%) 23 18   | 83, 101, 116, 127     | 0      |
| All | All   | 10516/12316 (85%) | 0.21   | 387 (3%) 45 38 | 31, 66, 113, 159      | 4 (0%) |

The worst 5 of 387 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C2    | 392 | ALA  | 8.1  |
| 13  | o2    | 195 | GLY  | 7.6  |
| 13  | o1    | 195 | GLY  | 6.6  |
| 18  | X2    | 17  | ALA  | 6.2  |
| 13  | O1    | 195 | GLY  | 6.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 28  | UNL  | I2    | 102 | 17/-  | 0.49 | 0.11 | 80,92,102,103              | 0     |
| 28  | UNL  | k2    | 505 | 6/-   | 0.51 | 0.10 | 70,80,84,87                | 0     |
| 28  | UNL  | I2    | 103 | 14/-  | 0.55 | 0.10 | 62,93,102,104              | 0     |
| 32  | GOL  | a1    | 406 | 6/6   | 0.55 | 0.11 | 68,75,86,90                | 0     |
| 28  | UNL  | a2    | 409 | 18/-  | 0.57 | 0.10 | 61,74,86,90                | 0     |
| 28  | UNL  | C2    | 501 | 6/-   | 0.57 | 0.10 | 72,74,78,87                | 0     |
| 28  | UNL  | J2    | 101 | 10/-  | 0.57 | 0.12 | 71,82,86,88                | 0     |
| 28  | UNL  | b1    | 623 | 11/-  | 0.58 | 0.12 | 59,74,83,84                | 0     |
| 23  | BCR  | K1    | 101 | 31/40 | 0.59 | 0.12 | 64,82,93,96                | 0     |
| 28  | UNL  | D1    | 410 | 6/-   | 0.59 | 0.14 | 59,62,66,66                | 0     |
| 28  | UNL  | F2    | 403 | 16/-  | 0.59 | 0.15 | 51,76,86,89                | 0     |
| 28  | UNL  | A2    | 409 | 10/-  | 0.60 | 0.14 | 72,82,85,87                | 0     |
| 28  | UNL  | c2    | 520 | 15/-  | 0.60 | 0.12 | 86,97,106,108              | 0     |
| 28  | UNL  | B1    | 624 | 18/-  | 0.61 | 0.10 | 43,71,79,81                | 0     |
| 28  | UNL  | H2    | 102 | 5/-   | 0.62 | 0.14 | 72,81,84,85                | 0     |
| 28  | UNL  | K2    | 103 | 5/-   | 0.63 | 0.16 | 79,83,88,90                | 0     |
| 25  | CLA  | b2    | 604 | 42/65 | 0.63 | 0.13 | 82,109,116,127             | 0     |
| 25  | CLA  | C2    | 518 | 41/65 | 0.63 | 0.12 | 105,121,127,134            | 0     |
| 28  | UNL  | d2    | 410 | 13/-  | 0.63 | 0.12 | 74,92,108,111              | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 28  | UNL  | C2    | 517 | 18/-  | 0.63 | 0.13 | 74,83,87,89                 | 0     |
| 28  | UNL  | b1    | 629 | 15/-  | 0.63 | 0.10 | 46,59,71,83                 | 0     |
| 28  | UNL  | m2    | 102 | 18/-  | 0.64 | 0.09 | 46,65,79,79                 | 0     |
| 29  | LMG  | C2    | 515 | 24/55 | 0.64 | 0.10 | 82,97,104,105               | 0     |
| 28  | UNL  | k2    | 502 | 9/-   | 0.64 | 0.09 | 72,78,84,86                 | 0     |
| 28  | UNL  | d1    | 410 | 12/-  | 0.65 | 0.13 | 49,72,77,79                 | 0     |
| 28  | UNL  | X2    | 101 | 7/-   | 0.65 | 0.24 | 83,85,91,93                 | 0     |
| 28  | UNL  | B2    | 626 | 15/-  | 0.66 | 0.10 | 79,83,92,95                 | 0     |
| 29  | LMG  | I2    | 101 | 34/55 | 0.66 | 0.13 | 82,103,109,114              | 0     |
| 25  | CLA  | C2    | 510 | 45/65 | 0.66 | 0.14 | 107,116,121,126             | 0     |
| 33  | LHG  | B2    | 627 | 42/49 | 0.66 | 0.10 | 67,88,120,132               | 0     |
| 35  | LMT  | m2    | 104 | 29/35 | 0.66 | 0.12 | 49,104,119,122              | 0     |
| 23  | BCR  | K2    | 102 | 40/40 | 0.67 | 0.13 | 84,99,113,115               | 0     |
| 33  | LHG  | b2    | 625 | 43/49 | 0.68 | 0.10 | 62,87,109,126               | 0     |
| 32  | GOL  | C1    | 518 | 6/6   | 0.68 | 0.11 | 65,73,77,81                 | 0     |
| 39  | CA   | o2    | 401 | 1/1   | 0.68 | 0.18 | 101,101,101,101             | 0     |
| 32  | GOL  | B1    | 620 | 6/6   | 0.69 | 0.10 | 63,75,81,82                 | 0     |
| 28  | UNL  | t1    | 101 | 18/-  | 0.69 | 0.10 | 43,60,66,67                 | 0     |
| 35  | LMT  | b2    | 621 | 35/35 | 0.69 | 0.11 | 69,110,123,123              | 0     |
| 28  | UNL  | B1    | 623 | 16/-  | 0.69 | 0.09 | 53,68,72,74                 | 0     |
| 33  | LHG  | d1    | 402 | 32/49 | 0.69 | 0.14 | 45,63,76,86                 | 0     |
| 29  | LMG  | j2    | 101 | 50/55 | 0.70 | 0.12 | 60,78,97,107                | 0     |
| 29  | LMG  | F2    | 402 | 35/55 | 0.70 | 0.11 | 68,81,91,92                 | 0     |
| 28  | UNL  | j1    | 101 | 17/-  | 0.70 | 0.11 | 60,69,71,77                 | 0     |
| 33  | LHG  | a2    | 407 | 30/49 | 0.70 | 0.13 | 55,75,94,102                | 0     |
| 28  | UNL  | a2    | 401 | 18/-  | 0.71 | 0.11 | 46,56,70,86                 | 0     |
| 24  | CL   | A2    | 410 | 1/1   | 0.71 | 0.09 | 87,87,87,87                 | 0     |
| 28  | UNL  | a2    | 410 | 8/-   | 0.71 | 0.10 | 61,68,70,76                 | 0     |
| 28  | UNL  | b2    | 607 | 12/-  | 0.71 | 0.12 | 64,75,80,87                 | 0     |
| 25  | CLA  | C2    | 503 | 65/65 | 0.71 | 0.12 | 94,104,112,116              | 0     |
| 25  | CLA  | D2    | 404 | 61/65 | 0.71 | 0.11 | 67,87,113,120               | 0     |
| 25  | CLA  | K2    | 101 | 55/65 | 0.71 | 0.10 | 86,98,104,109               | 0     |
| 28  | UNL  | k2    | 504 | 9/-   | 0.71 | 0.09 | 66,74,80,88                 | 0     |
| 28  | UNL  | i2    | 101 | 14/-  | 0.72 | 0.07 | 62,66,73,75                 | 0     |
| 28  | UNL  | M2    | 101 | 11/-  | 0.72 | 0.07 | 59,68,73,74                 | 0     |
| 35  | LMT  | c1    | 517 | 33/35 | 0.72 | 0.12 | 63,100,117,119              | 0     |
| 25  | CLA  | c2    | 513 | 54/65 | 0.73 | 0.10 | 75,94,102,105               | 0     |
| 23  | BCR  | c2    | 501 | 40/40 | 0.73 | 0.13 | 66,82,89,92                 | 0     |
| 28  | UNL  | b1    | 626 | 13/-  | 0.73 | 0.08 | 53,64,83,86                 | 0     |
| 32  | GOL  | C2    | 514 | 6/6   | 0.73 | 0.09 | 87,93,100,101               | 0     |
| 35  | LMT  | m2    | 103 | 30/35 | 0.73 | 0.14 | 52,89,111,113               | 0     |
| 23  | BCR  | K2    | 104 | 29/40 | 0.73 | 0.10 | 92,100,109,112              | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 28  | UNL  | b1    | 630 | 17/-  | 0.73 | 0.09 | 48,57,74,75                 | 0     |
| 29  | LMG  | d1    | 411 | 35/55 | 0.74 | 0.11 | 58,76,94,99                 | 0     |
| 23  | BCR  | z2    | 101 | 40/40 | 0.74 | 0.12 | 80,95,100,101               | 0     |
| 28  | UNL  | m2    | 101 | 18/-  | 0.74 | 0.09 | 44,57,79,85                 | 0     |
| 28  | UNL  | B2    | 625 | 18/-  | 0.74 | 0.09 | 37,56,68,68                 | 0     |
| 29  | LMG  | A1    | 412 | 41/55 | 0.74 | 0.11 | 50,75,96,100                | 0     |
| 29  | LMG  | b1    | 621 | 38/55 | 0.74 | 0.10 | 52,63,76,82                 | 0     |
| 23  | BCR  | F2    | 401 | 40/40 | 0.75 | 0.11 | 67,81,107,113               | 0     |
| 29  | LMG  | B2    | 621 | 37/55 | 0.75 | 0.10 | 53,68,80,96                 | 0     |
| 25  | CLA  | C2    | 505 | 65/65 | 0.75 | 0.12 | 78,100,112,118              | 0     |
| 28  | UNL  | A2    | 408 | 18/-  | 0.75 | 0.10 | 62,83,92,93                 | 0     |
| 23  | BCR  | B1    | 602 | 40/40 | 0.75 | 0.11 | 49,62,74,78                 | 0     |
| 33  | LHG  | A2    | 405 | 33/49 | 0.75 | 0.10 | 70,80,90,97                 | 0     |
| 23  | BCR  | C2    | 502 | 40/40 | 0.75 | 0.13 | 95,106,118,120              | 0     |
| 28  | UNL  | k2    | 503 | 6/-   | 0.76 | 0.09 | 67,76,79,80                 | 0     |
| 23  | BCR  | J1    | 101 | 40/40 | 0.76 | 0.10 | 50,70,86,88                 | 0     |
| 35  | LMT  | i2    | 102 | 7/35  | 0.76 | 0.08 | 68,71,76,79                 | 0     |
| 29  | LMG  | A2    | 412 | 29/55 | 0.76 | 0.10 | 86,94,100,102               | 0     |
| 32  | GOL  | b1    | 618 | 6/6   | 0.76 | 0.08 | 60,69,80,80                 | 0     |
| 25  | CLA  | C2    | 509 | 65/65 | 0.76 | 0.12 | 90,101,106,108              | 0     |
| 35  | LMT  | C1    | 519 | 35/35 | 0.77 | 0.10 | 57,76,85,93                 | 0     |
| 35  | LMT  | M1    | 103 | 24/35 | 0.77 | 0.10 | 42,68,97,101                | 0     |
| 35  | LMT  | T1    | 101 | 12/35 | 0.77 | 0.10 | 46,51,54,56                 | 0     |
| 25  | CLA  | C2    | 511 | 50/65 | 0.77 | 0.11 | 85,93,100,104               | 0     |
| 23  | BCR  | k1    | 101 | 40/40 | 0.77 | 0.11 | 56,70,82,85                 | 0     |
| 25  | CLA  | B1    | 604 | 42/65 | 0.77 | 0.11 | 83,98,107,113               | 0     |
| 28  | UNL  | B2    | 622 | 17/-  | 0.77 | 0.09 | 57,71,76,78                 | 0     |
| 25  | CLA  | C1    | 512 | 65/65 | 0.77 | 0.10 | 63,82,102,121               | 0     |
| 25  | CLA  | c1    | 516 | 65/65 | 0.77 | 0.11 | 66,82,104,109               | 0     |
| 35  | LMT  | a2    | 406 | 35/35 | 0.78 | 0.11 | 43,80,92,94                 | 0     |
| 28  | UNL  | b1    | 627 | 16/-  | 0.78 | 0.09 | 42,56,75,77                 | 0     |
| 25  | CLA  | B1    | 611 | 62/65 | 0.78 | 0.10 | 58,78,87,89                 | 0     |
| 25  | CLA  | c1    | 515 | 55/65 | 0.78 | 0.10 | 69,82,90,94                 | 0     |
| 29  | LMG  | b1    | 624 | 39/55 | 0.78 | 0.12 | 58,73,84,87                 | 0     |
| 37  | SQD  | D1    | 409 | 35/54 | 0.78 | 0.11 | 61,75,92,97                 | 0     |
| 28  | UNL  | W2    | 101 | 9/-   | 0.78 | 0.08 | 64,77,83,87                 | 0     |
| 25  | CLA  | C2    | 504 | 46/65 | 0.79 | 0.11 | 72,88,95,96                 | 0     |
| 25  | CLA  | C1    | 513 | 61/65 | 0.79 | 0.10 | 49,68,74,78                 | 0     |
| 28  | UNL  | a2    | 411 | 11/-  | 0.79 | 0.07 | 51,55,65,67                 | 0     |
| 25  | CLA  | C2    | 507 | 45/65 | 0.79 | 0.11 | 73,93,102,113               | 0     |
| 23  | BCR  | b2    | 603 | 40/40 | 0.80 | 0.10 | 60,74,102,104               | 0     |
| 23  | BCR  | H2    | 103 | 24/40 | 0.80 | 0.12 | 65,76,82,85                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 23  | BCR  | j2    | 102 | 40/40 | 0.80 | 0.11 | 59,75,86,87                 | 0     |
| 25  | CLA  | c2    | 515 | 46/65 | 0.80 | 0.11 | 81,100,104,109              | 0     |
| 29  | LMG  | C1    | 520 | 48/55 | 0.80 | 0.08 | 59,69,78,86                 | 0     |
| 29  | LMG  | a1    | 412 | 51/55 | 0.80 | 0.10 | 54,67,77,91                 | 0     |
| 25  | CLA  | C2    | 513 | 53/65 | 0.80 | 0.11 | 78,91,106,110               | 0     |
| 23  | BCR  | H1    | 102 | 22/40 | 0.80 | 0.12 | 75,88,95,100                | 0     |
| 23  | BCR  | D1    | 401 | 40/40 | 0.80 | 0.10 | 54,67,89,95                 | 0     |
| 23  | BCR  | b2    | 602 | 40/40 | 0.81 | 0.10 | 51,70,78,82                 | 0     |
| 25  | CLA  | C2    | 506 | 65/65 | 0.81 | 0.10 | 78,90,97,100                | 0     |
| 23  | BCR  | b1    | 602 | 40/40 | 0.81 | 0.10 | 35,57,65,73                 | 0     |
| 25  | CLA  | C2    | 508 | 50/65 | 0.81 | 0.13 | 87,103,112,115              | 0     |
| 34  | DGD  | H2    | 101 | 62/66 | 0.81 | 0.09 | 51,74,83,85                 | 0     |
| 25  | CLA  | C2    | 516 | 46/65 | 0.81 | 0.10 | 70,92,97,100                | 0     |
| 28  | UNL  | d2    | 411 | 12/-  | 0.81 | 0.08 | 55,67,73,79                 | 0     |
| 39  | CA   | O1    | 401 | 1/1   | 0.81 | 0.06 | 82,82,82,82                 | 0     |
| 29  | LMG  | b2    | 622 | 39/55 | 0.81 | 0.10 | 47,60,85,90                 | 0     |
| 32  | GOL  | c2    | 518 | 6/6   | 0.82 | 0.11 | 50,55,59,64                 | 0     |
| 25  | CLA  | d2    | 404 | 50/65 | 0.82 | 0.10 | 57,74,83,88                 | 0     |
| 35  | LMT  | m1    | 101 | 35/35 | 0.82 | 0.11 | 44,80,103,112               | 0     |
| 25  | CLA  | B2    | 604 | 41/65 | 0.82 | 0.09 | 68,79,92,97                 | 0     |
| 28  | UNL  | x1    | 101 | 15/-  | 0.82 | 0.09 | 55,73,79,82                 | 0     |
| 25  | CLA  | c2    | 509 | 65/65 | 0.82 | 0.08 | 54,70,82,85                 | 0     |
| 23  | BCR  | C1    | 521 | 40/40 | 0.82 | 0.10 | 59,68,80,84                 | 0     |
| 34  | DGD  | C2    | 512 | 33/66 | 0.82 | 0.10 | 63,77,83,93                 | 0     |
| 29  | LMG  | B1    | 622 | 31/55 | 0.82 | 0.11 | 66,74,81,83                 | 0     |
| 37  | SQD  | B2    | 623 | 45/54 | 0.82 | 0.10 | 58,79,89,96                 | 0     |
| 37  | SQD  | b2    | 605 | 45/54 | 0.82 | 0.08 | 54,83,114,124               | 0     |
| 29  | LMG  | B1    | 626 | 48/55 | 0.82 | 0.09 | 55,70,89,94                 | 0     |
| 25  | CLA  | C1    | 514 | 45/65 | 0.82 | 0.10 | 73,84,92,96                 | 0     |
| 23  | BCR  | B2    | 602 | 40/40 | 0.83 | 0.10 | 47,59,80,86                 | 0     |
| 29  | LMG  | B2    | 620 | 40/55 | 0.83 | 0.09 | 62,74,97,98                 | 0     |
| 25  | CLA  | c1    | 503 | 65/65 | 0.83 | 0.10 | 55,66,71,75                 | 0     |
| 25  | CLA  | C1    | 502 | 65/65 | 0.83 | 0.09 | 51,63,68,70                 | 0     |
| 35  | LMT  | b2    | 623 | 35/35 | 0.83 | 0.08 | 63,90,98,101                | 0     |
| 28  | UNL  | B1    | 625 | 7/-   | 0.83 | 0.08 | 45,52,55,63                 | 0     |
| 25  | CLA  | b2    | 618 | 65/65 | 0.83 | 0.10 | 68,82,90,92                 | 0     |
| 23  | BCR  | h2    | 101 | 40/40 | 0.83 | 0.10 | 71,85,107,109               | 0     |
| 28  | UNL  | b1    | 625 | 10/-  | 0.83 | 0.10 | 50,62,68,69                 | 0     |
| 23  | BCR  | c1    | 502 | 40/40 | 0.83 | 0.10 | 57,66,72,72                 | 0     |
| 29  | LMG  | b1    | 631 | 40/55 | 0.83 | 0.10 | 29,52,85,92                 | 0     |
| 38  | HEM  | E1    | 101 | 43/43 | 0.83 | 0.13 | 108,134,152,155             | 0     |
| 29  | LMG  | c1    | 519 | 55/55 | 0.83 | 0.08 | 47,70,84,91                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | CLA  | B2    | 611 | 65/65 | 0.83 | 0.10 | 51,73,81,86                 | 0     |
| 28  | UNL  | a1    | 409 | 11/-  | 0.84 | 0.06 | 43,51,60,63                 | 0     |
| 25  | CLA  | c2    | 512 | 65/65 | 0.84 | 0.09 | 61,76,86,93                 | 0     |
| 23  | BCR  | d2    | 401 | 40/40 | 0.84 | 0.09 | 48,67,81,85                 | 0     |
| 25  | CLA  | B2    | 606 | 65/65 | 0.84 | 0.09 | 53,67,75,78                 | 0     |
| 23  | BCR  | k2    | 501 | 40/40 | 0.84 | 0.09 | 61,84,95,98                 | 0     |
| 25  | CLA  | b2    | 610 | 65/65 | 0.84 | 0.09 | 60,82,90,92                 | 0     |
| 25  | CLA  | b1    | 604 | 65/65 | 0.84 | 0.10 | 52,78,110,115               | 0     |
| 37  | SQD  | D2    | 402 | 25/54 | 0.84 | 0.09 | 85,90,96,98                 | 0     |
| 25  | CLA  | c2    | 502 | 65/65 | 0.84 | 0.09 | 60,78,85,90                 | 0     |
| 35  | LMT  | l1    | 101 | 24/35 | 0.84 | 0.08 | 42,55,89,90                 | 0     |
| 38  | HEM  | V2    | 201 | 43/43 | 0.84 | 0.12 | 83,98,102,107               | 0     |
| 38  | HEM  | e2    | 101 | 43/43 | 0.84 | 0.11 | 126,145,163,171             | 0     |
| 25  | CLA  | A2    | 403 | 61/65 | 0.84 | 0.11 | 80,89,98,102                | 0     |
| 28  | UNL  | m1    | 102 | 6/-   | 0.84 | 0.08 | 54,55,63,66                 | 0     |
| 29  | LMG  | a2    | 412 | 44/55 | 0.85 | 0.09 | 55,70,78,93                 | 0     |
| 25  | CLA  | b2    | 609 | 61/65 | 0.85 | 0.10 | 77,89,95,100                | 0     |
| 25  | CLA  | A2    | 404 | 51/65 | 0.85 | 0.08 | 47,58,70,73                 | 0     |
| 25  | CLA  | C1    | 509 | 65/65 | 0.85 | 0.09 | 48,59,71,80                 | 0     |
| 28  | UNL  | B2    | 624 | 8/-   | 0.85 | 0.07 | 46,51,54,55                 | 0     |
| 25  | CLA  | b2    | 619 | 59/65 | 0.85 | 0.10 | 71,80,106,109               | 0     |
| 23  | BCR  | c1    | 501 | 40/40 | 0.85 | 0.08 | 56,66,79,82                 | 0     |
| 32  | GOL  | i1    | 101 | 6/6   | 0.85 | 0.12 | 55,57,60,64                 | 0     |
| 25  | CLA  | c2    | 506 | 61/65 | 0.85 | 0.10 | 55,70,77,83                 | 0     |
| 32  | GOL  | a2    | 415 | 6/6   | 0.85 | 0.14 | 47,55,59,63                 | 0     |
| 25  | CLA  | c2    | 508 | 65/65 | 0.85 | 0.10 | 68,78,84,88                 | 0     |
| 28  | UNL  | b1    | 628 | 10/-  | 0.85 | 0.08 | 51,57,61,67                 | 0     |
| 25  | CLA  | B2    | 610 | 65/65 | 0.85 | 0.09 | 44,59,82,86                 | 0     |
| 25  | CLA  | c1    | 508 | 50/65 | 0.85 | 0.10 | 57,66,77,81                 | 0     |
| 25  | CLA  | c1    | 510 | 65/65 | 0.85 | 0.08 | 41,54,62,72                 | 0     |
| 25  | CLA  | c1    | 513 | 60/65 | 0.85 | 0.07 | 49,59,71,72                 | 0     |
| 34  | DGD  | c1    | 520 | 62/66 | 0.85 | 0.09 | 36,59,73,87                 | 0     |
| 25  | CLA  | B1    | 609 | 65/65 | 0.85 | 0.10 | 54,71,81,90                 | 0     |
| 25  | CLA  | C1    | 506 | 65/65 | 0.85 | 0.09 | 49,62,70,73                 | 0     |
| 25  | CLA  | D1    | 403 | 51/65 | 0.85 | 0.09 | 64,74,88,90                 | 0     |
| 34  | DGD  | c2    | 517 | 62/66 | 0.86 | 0.08 | 45,57,70,75                 | 0     |
| 25  | CLA  | c1    | 509 | 65/65 | 0.86 | 0.10 | 51,62,68,72                 | 0     |
| 29  | LMG  | A1    | 410 | 43/55 | 0.86 | 0.08 | 52,59,65,76                 | 0     |
| 25  | CLA  | a2    | 405 | 65/65 | 0.86 | 0.09 | 51,60,81,87                 | 0     |
| 25  | CLA  | c1    | 505 | 65/65 | 0.86 | 0.09 | 47,70,79,88                 | 0     |
| 28  | UNL  | t1    | 102 | 9/-   | 0.86 | 0.08 | 45,57,68,69                 | 0     |
| 34  | DGD  | C1    | 517 | 64/66 | 0.86 | 0.08 | 38,55,75,92                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 38  | HEM  | E2    | 101 | 43/43 | 0.86 | 0.13 | 116,132,146,152             | 0     |
| 25  | CLA  | B1    | 606 | 65/65 | 0.86 | 0.10 | 60,71,77,82                 | 0     |
| 29  | LMG  | d2    | 407 | 27/55 | 0.86 | 0.09 | 49,60,64,70                 | 0     |
| 25  | CLA  | c2    | 504 | 65/65 | 0.86 | 0.10 | 46,78,92,100                | 0     |
| 34  | DGD  | c2    | 516 | 52/66 | 0.86 | 0.10 | 37,63,71,75                 | 0     |
| 23  | BCR  | b2    | 601 | 40/40 | 0.87 | 0.09 | 51,61,69,72                 | 0     |
| 34  | DGD  | c1    | 514 | 51/66 | 0.87 | 0.09 | 46,54,62,64                 | 0     |
| 25  | CLA  | b1    | 609 | 65/65 | 0.87 | 0.10 | 42,58,84,104                | 0     |
| 25  | CLA  | b2    | 624 | 65/65 | 0.87 | 0.08 | 47,60,75,82                 | 0     |
| 25  | CLA  | b1    | 619 | 65/65 | 0.87 | 0.10 | 48,62,81,85                 | 0     |
| 27  | PHO  | D2    | 407 | 64/64 | 0.87 | 0.08 | 58,68,81,83                 | 0     |
| 25  | CLA  | b2    | 606 | 65/65 | 0.87 | 0.11 | 68,77,84,90                 | 0     |
| 25  | CLA  | C1    | 511 | 65/65 | 0.87 | 0.10 | 45,56,62,68                 | 0     |
| 35  | LMT  | L1    | 102 | 12/35 | 0.87 | 0.07 | 35,45,59,62                 | 0     |
| 29  | LMG  | M1    | 101 | 31/55 | 0.87 | 0.09 | 41,52,63,70                 | 0     |
| 25  | CLA  | c2    | 507 | 54/65 | 0.87 | 0.10 | 76,81,86,92                 | 0     |
| 25  | CLA  | B1    | 618 | 58/65 | 0.87 | 0.10 | 53,64,80,86                 | 0     |
| 29  | LMG  | c2    | 519 | 26/55 | 0.87 | 0.07 | 58,67,73,74                 | 0     |
| 28  | UNL  | l1    | 103 | 12/-  | 0.87 | 0.08 | 35,47,53,55                 | 0     |
| 25  | CLA  | b2    | 613 | 65/65 | 0.87 | 0.10 | 59,84,96,99                 | 0     |
| 25  | CLA  | c1    | 507 | 65/65 | 0.88 | 0.09 | 49,62,72,80                 | 0     |
| 23  | BCR  | B2    | 603 | 40/40 | 0.88 | 0.08 | 46,59,76,81                 | 0     |
| 25  | CLA  | B2    | 612 | 65/65 | 0.88 | 0.10 | 58,64,71,83                 | 0     |
| 25  | CLA  | c2    | 511 | 65/65 | 0.88 | 0.10 | 54,65,72,75                 | 0     |
| 25  | CLA  | B2    | 619 | 65/65 | 0.88 | 0.07 | 46,55,63,71                 | 0     |
| 25  | CLA  | B1    | 605 | 65/65 | 0.88 | 0.09 | 60,75,87,88                 | 0     |
| 25  | CLA  | C1    | 505 | 65/65 | 0.88 | 0.08 | 43,55,64,68                 | 0     |
| 34  | DGD  | C1    | 515 | 52/66 | 0.88 | 0.09 | 36,58,67,71                 | 0     |
| 25  | CLA  | c1    | 512 | 65/65 | 0.88 | 0.10 | 36,50,57,60                 | 0     |
| 36  | PL9  | D2    | 408 | 55/55 | 0.88 | 0.09 | 43,59,64,74                 | 0     |
| 27  | PHO  | D1    | 407 | 63/64 | 0.88 | 0.08 | 40,56,63,67                 | 0     |
| 23  | BCR  | C1    | 501 | 40/40 | 0.88 | 0.08 | 47,61,72,75                 | 0     |
| 25  | CLA  | C1    | 507 | 65/65 | 0.88 | 0.09 | 46,67,86,105                | 0     |
| 25  | CLA  | b2    | 616 | 60/65 | 0.88 | 0.09 | 51,64,82,82                 | 0     |
| 25  | CLA  | b1    | 616 | 65/65 | 0.88 | 0.09 | 39,46,57,69                 | 0     |
| 23  | BCR  | A2    | 401 | 40/40 | 0.88 | 0.12 | 58,84,90,91                 | 0     |
| 23  | BCR  | d1    | 405 | 40/40 | 0.88 | 0.09 | 38,51,94,99                 | 0     |
| 25  | CLA  | B1    | 617 | 65/65 | 0.88 | 0.08 | 59,67,74,75                 | 0     |
| 25  | CLA  | B2    | 605 | 65/65 | 0.88 | 0.07 | 63,71,77,82                 | 0     |
| 25  | CLA  | c1    | 506 | 65/65 | 0.88 | 0.08 | 40,54,68,73                 | 0     |
| 25  | CLA  | B2    | 614 | 65/65 | 0.89 | 0.08 | 46,58,66,68                 | 0     |
| 25  | CLA  | B2    | 616 | 54/65 | 0.89 | 0.08 | 43,51,57,59                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 34  | DGD  | c1    | 518 | 62/66 | 0.89 | 0.07 | 41,61,69,79                 | 0     |
| 25  | CLA  | B2    | 617 | 65/65 | 0.89 | 0.08 | 52,63,70,74                 | 0     |
| 25  | CLA  | B2    | 618 | 60/65 | 0.89 | 0.08 | 59,65,80,85                 | 0     |
| 36  | PL9  | d1    | 409 | 55/55 | 0.89 | 0.09 | 28,41,50,61                 | 0     |
| 25  | CLA  | b2    | 617 | 65/65 | 0.89 | 0.08 | 47,58,65,72                 | 0     |
| 36  | PL9  | d2    | 409 | 55/55 | 0.89 | 0.09 | 33,44,56,57                 | 0     |
| 25  | CLA  | B1    | 610 | 65/65 | 0.89 | 0.09 | 46,58,73,76                 | 0     |
| 25  | CLA  | a1    | 404 | 60/65 | 0.89 | 0.10 | 49,57,82,89                 | 0     |
| 23  | BCR  | B1    | 603 | 40/40 | 0.89 | 0.07 | 45,56,78,85                 | 0     |
| 33  | LHG  | D1    | 404 | 49/49 | 0.89 | 0.09 | 48,60,84,90                 | 0     |
| 25  | CLA  | B1    | 607 | 60/65 | 0.89 | 0.09 | 45,56,68,72                 | 0     |
| 28  | UNL  | A1    | 409 | 14/-  | 0.89 | 0.06 | 44,48,57,68                 | 0     |
| 23  | BCR  | B1    | 601 | 40/40 | 0.89 | 0.08 | 41,55,65,65                 | 0     |
| 25  | CLA  | c2    | 505 | 65/65 | 0.89 | 0.08 | 48,61,71,80                 | 0     |
| 25  | CLA  | d1    | 406 | 65/65 | 0.89 | 0.08 | 44,58,94,99                 | 0     |
| 25  | CLA  | C1    | 508 | 65/65 | 0.89 | 0.09 | 47,66,76,80                 | 0     |
| 25  | CLA  | c2    | 503 | 65/65 | 0.90 | 0.10 | 53,62,83,89                 | 0     |
| 23  | BCR  | B2    | 601 | 40/40 | 0.90 | 0.07 | 41,56,66,68                 | 0     |
| 29  | LMG  | D1    | 406 | 35/55 | 0.90 | 0.08 | 50,57,71,74                 | 0     |
| 33  | LHG  | D2    | 405 | 49/49 | 0.90 | 0.07 | 52,60,66,68                 | 0     |
| 33  | LHG  | L2    | 101 | 49/49 | 0.90 | 0.08 | 42,57,70,78                 | 0     |
| 25  | CLA  | B1    | 616 | 65/65 | 0.90 | 0.08 | 39,49,58,66                 | 0     |
| 23  | BCR  | b1    | 603 | 40/40 | 0.90 | 0.08 | 40,58,69,77                 | 0     |
| 33  | LHG  | d2    | 403 | 49/49 | 0.90 | 0.08 | 42,59,69,73                 | 0     |
| 25  | CLA  | b2    | 611 | 65/65 | 0.90 | 0.10 | 66,72,80,83                 | 0     |
| 34  | DGD  | C1    | 516 | 62/66 | 0.90 | 0.07 | 44,53,60,61                 | 0     |
| 31  | BCT  | a1    | 413 | 4/4   | 0.90 | 0.07 | 43,48,48,50                 | 0     |
| 34  | DGD  | H1    | 101 | 62/66 | 0.90 | 0.08 | 50,71,84,89                 | 0     |
| 25  | CLA  | b2    | 612 | 65/65 | 0.90 | 0.08 | 39,54,64,70                 | 0     |
| 25  | CLA  | A1    | 405 | 55/65 | 0.90 | 0.08 | 38,46,59,65                 | 0     |
| 25  | CLA  | c2    | 510 | 54/65 | 0.90 | 0.10 | 64,69,77,79                 | 0     |
| 25  | CLA  | B2    | 607 | 65/65 | 0.90 | 0.08 | 49,59,73,78                 | 0     |
| 25  | CLA  | B2    | 609 | 65/65 | 0.90 | 0.08 | 51,67,76,82                 | 0     |
| 34  | DGD  | c2    | 514 | 62/66 | 0.90 | 0.07 | 47,59,67,69                 | 0     |
| 25  | CLA  | b1    | 611 | 65/65 | 0.90 | 0.08 | 37,59,68,73                 | 0     |
| 25  | CLA  | B1    | 619 | 65/65 | 0.90 | 0.08 | 32,50,57,73                 | 0     |
| 25  | CLA  | A2    | 402 | 65/65 | 0.90 | 0.09 | 47,57,69,77                 | 0     |
| 33  | LHG  | B1    | 621 | 49/49 | 0.90 | 0.08 | 41,57,67,73                 | 0     |
| 25  | CLA  | b1    | 617 | 65/65 | 0.90 | 0.07 | 47,56,65,68                 | 0     |
| 25  | CLA  | b2    | 614 | 65/65 | 0.91 | 0.08 | 51,66,73,75                 | 0     |
| 25  | CLA  | d1    | 401 | 65/65 | 0.91 | 0.08 | 30,36,44,47                 | 0     |
| 25  | CLA  | B2    | 615 | 65/65 | 0.91 | 0.07 | 44,56,73,86                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | CLA  | d2    | 405 | 65/65 | 0.91 | 0.08 | 34,44,61,77                 | 0     |
| 25  | CLA  | B1    | 615 | 65/65 | 0.91 | 0.08 | 35,47,73,80                 | 0     |
| 33  | LHG  | d2    | 406 | 49/49 | 0.91 | 0.07 | 36,50,59,66                 | 0     |
| 25  | CLA  | c1    | 504 | 65/65 | 0.91 | 0.09 | 36,53,83,98                 | 0     |
| 25  | CLA  | b2    | 620 | 65/65 | 0.91 | 0.09 | 42,56,63,72                 | 0     |
| 25  | CLA  | D2    | 401 | 65/65 | 0.91 | 0.08 | 43,53,71,76                 | 0     |
| 23  | BCR  | a1    | 401 | 40/40 | 0.91 | 0.08 | 47,56,64,65                 | 0     |
| 36  | PL9  | D1    | 408 | 55/55 | 0.91 | 0.08 | 28,42,52,63                 | 0     |
| 25  | CLA  | D2    | 406 | 65/65 | 0.91 | 0.07 | 45,57,65,67                 | 0     |
| 24  | CL   | a1    | 402 | 1/1   | 0.91 | 0.05 | 49,49,49,49                 | 0     |
| 23  | BCR  | h1    | 102 | 40/40 | 0.91 | 0.08 | 53,60,67,69                 | 0     |
| 25  | CLA  | b1    | 606 | 65/65 | 0.91 | 0.09 | 44,53,61,63                 | 0     |
| 29  | LMG  | d1    | 408 | 33/55 | 0.91 | 0.08 | 41,50,61,63                 | 0     |
| 25  | CLA  | A1    | 404 | 51/65 | 0.91 | 0.07 | 37,48,58,70                 | 0     |
| 25  | CLA  | C1    | 510 | 65/65 | 0.91 | 0.09 | 47,59,77,82                 | 0     |
| 25  | CLA  | B1    | 612 | 65/65 | 0.91 | 0.10 | 52,66,71,77                 | 0     |
| 38  | HEM  | f1    | 101 | 43/43 | 0.91 | 0.11 | 62,82,124,136               | 0     |
| 38  | HEM  | v1    | 201 | 43/43 | 0.91 | 0.10 | 60,66,72,75                 | 0     |
| 34  | DGD  | h2    | 102 | 62/66 | 0.91 | 0.08 | 47,67,82,96                 | 0     |
| 25  | CLA  | C1    | 503 | 60/65 | 0.91 | 0.07 | 38,53,67,73                 | 0     |
| 25  | CLA  | C1    | 504 | 65/65 | 0.91 | 0.07 | 49,64,74,77                 | 0     |
| 35  | LMT  | M1    | 102 | 11/35 | 0.91 | 0.08 | 47,52,56,58                 | 0     |
| 25  | CLA  | b1    | 620 | 65/65 | 0.91 | 0.08 | 31,43,56,60                 | 0     |
| 33  | LHG  | D2    | 403 | 49/49 | 0.92 | 0.07 | 45,60,68,73                 | 0     |
| 25  | CLA  | b2    | 608 | 65/65 | 0.92 | 0.08 | 65,77,85,86                 | 0     |
| 25  | CLA  | d1    | 404 | 65/65 | 0.92 | 0.07 | 31,43,49,51                 | 0     |
| 27  | PHO  | d1    | 403 | 64/64 | 0.92 | 0.07 | 32,41,50,54                 | 0     |
| 27  | PHO  | A2    | 407 | 64/64 | 0.92 | 0.08 | 53,64,72,80                 | 0     |
| 32  | GOL  | c1    | 521 | 6/6   | 0.92 | 0.08 | 54,56,60,65                 | 0     |
| 25  | CLA  | b1    | 615 | 59/65 | 0.92 | 0.08 | 31,43,58,64                 | 0     |
| 27  | PHO  | d2    | 408 | 64/64 | 0.92 | 0.08 | 45,56,62,64                 | 0     |
| 25  | CLA  | b1    | 607 | 65/65 | 0.92 | 0.08 | 33,46,69,76                 | 0     |
| 23  | BCR  | a2    | 402 | 40/40 | 0.92 | 0.07 | 33,51,62,67                 | 0     |
| 25  | CLA  | b1    | 610 | 65/65 | 0.92 | 0.07 | 37,47,56,63                 | 0     |
| 25  | CLA  | B1    | 613 | 65/65 | 0.92 | 0.08 | 38,49,57,64                 | 0     |
| 33  | LHG  | b1    | 622 | 49/49 | 0.92 | 0.09 | 36,49,57,69                 | 0     |
| 25  | CLA  | B2    | 613 | 65/65 | 0.92 | 0.07 | 41,52,68,70                 | 0     |
| 34  | DGD  | h1    | 101 | 62/66 | 0.92 | 0.07 | 37,48,59,65                 | 0     |
| 25  | CLA  | b1    | 612 | 65/65 | 0.92 | 0.07 | 45,54,60,68                 | 0     |
| 31  | BCT  | A2    | 413 | 4/4   | 0.92 | 0.07 | 65,69,71,72                 | 0     |
| 25  | CLA  | c1    | 511 | 65/65 | 0.93 | 0.08 | 38,53,71,78                 | 0     |
| 31  | BCT  | A1    | 413 | 4/4   | 0.93 | 0.06 | 54,60,62,63                 | 0     |

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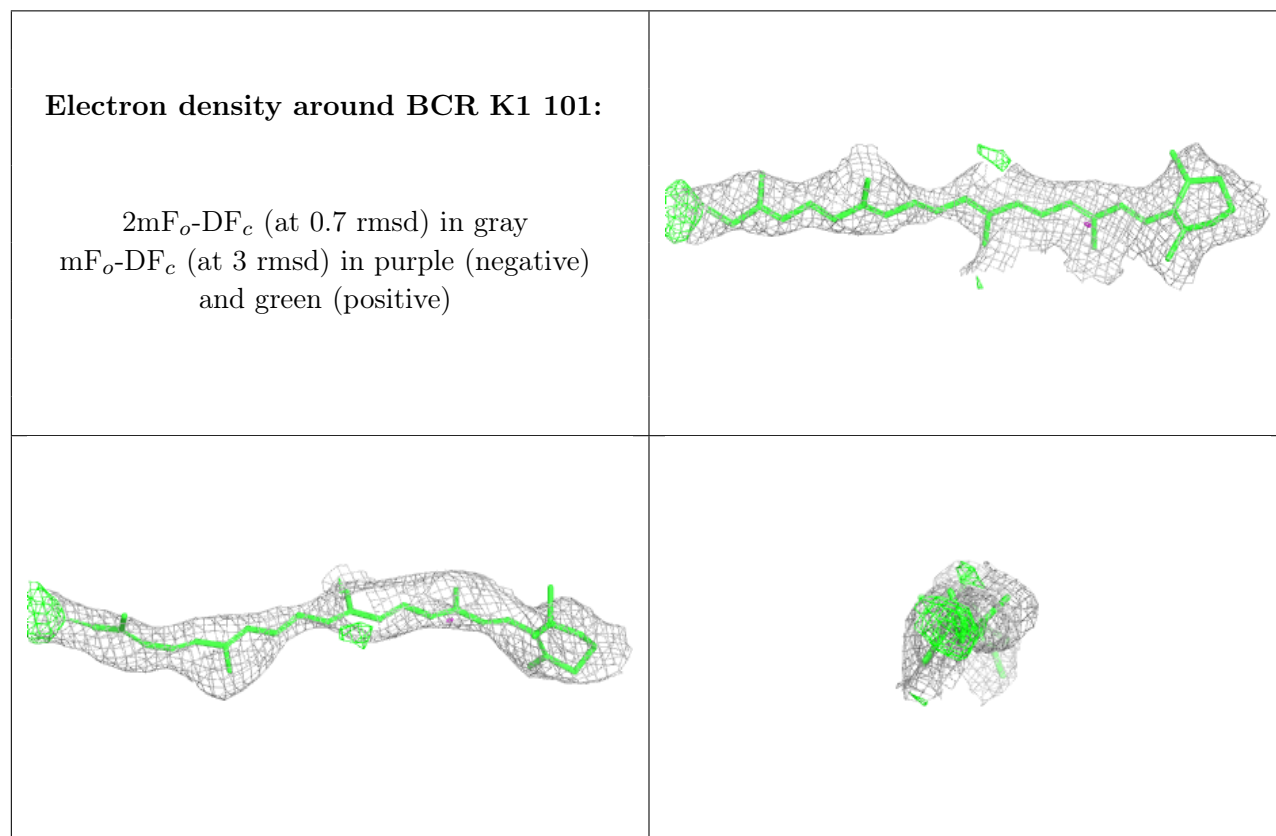
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 33  | LHG  | d1    | 407 | 49/49 | 0.93 | 0.07 | 34,44,53,67                 | 0     |
| 26  | OEX  | A2    | 406 | 10/10 | 0.93 | 0.09 | 68,84,93,94                 | 0     |
| 25  | CLA  | a1    | 405 | 50/65 | 0.93 | 0.07 | 25,33,49,55                 | 0     |
| 23  | BCR  | b1    | 601 | 40/40 | 0.93 | 0.07 | 36,47,56,57                 | 0     |
| 25  | CLA  | b1    | 613 | 65/65 | 0.93 | 0.07 | 36,44,54,68                 | 0     |
| 25  | CLA  | a2    | 404 | 65/65 | 0.93 | 0.07 | 30,42,52,53                 | 0     |
| 27  | PHO  | a2    | 416 | 64/64 | 0.93 | 0.07 | 35,46,53,62                 | 0     |
| 25  | CLA  | b1    | 605 | 65/65 | 0.93 | 0.07 | 38,52,60,66                 | 0     |
| 25  | CLA  | a2    | 413 | 50/65 | 0.93 | 0.06 | 33,46,57,66                 | 0     |
| 24  | CL   | A1    | 402 | 1/1   | 0.93 | 0.12 | 39,39,39,39                 | 0     |
| 38  | HEM  | V1    | 201 | 43/43 | 0.93 | 0.08 | 35,61,66,71                 | 0     |
| 33  | LHG  | l2    | 101 | 44/49 | 0.93 | 0.06 | 36,53,66,72                 | 0     |
| 25  | CLA  | B2    | 608 | 65/65 | 0.93 | 0.07 | 43,53,70,76                 | 0     |
| 25  | CLA  | D1    | 402 | 65/65 | 0.93 | 0.06 | 31,40,58,63                 | 0     |
| 23  | BCR  | A1    | 401 | 40/40 | 0.93 | 0.07 | 36,48,54,58                 | 0     |
| 25  | CLA  | B1    | 614 | 65/65 | 0.93 | 0.07 | 43,55,62,67                 | 0     |
| 33  | LHG  | L1    | 101 | 41/49 | 0.93 | 0.06 | 30,46,61,85                 | 0     |
| 33  | LHG  | a1    | 407 | 43/49 | 0.93 | 0.06 | 36,52,66,70                 | 0     |
| 25  | CLA  | d2    | 402 | 65/65 | 0.94 | 0.06 | 24,37,48,52                 | 0     |
| 25  | CLA  | b2    | 615 | 60/65 | 0.94 | 0.07 | 45,54,67,74                 | 0     |
| 25  | CLA  | a1    | 403 | 65/65 | 0.94 | 0.07 | 29,37,48,51                 | 0     |
| 25  | CLA  | A1    | 406 | 65/65 | 0.94 | 0.07 | 28,37,46,55                 | 0     |
| 33  | LHG  | l1    | 102 | 49/49 | 0.94 | 0.07 | 25,43,67,75                 | 0     |
| 27  | PHO  | A1    | 408 | 64/64 | 0.94 | 0.07 | 30,42,50,56                 | 0     |
| 25  | CLA  | B1    | 608 | 65/65 | 0.94 | 0.07 | 46,58,71,81                 | 0     |
| 27  | PHO  | a1    | 411 | 64/64 | 0.94 | 0.06 | 33,41,47,50                 | 0     |
| 38  | HEM  | v2    | 201 | 43/43 | 0.94 | 0.09 | 47,60,66,78                 | 0     |
| 33  | LHG  | D1    | 405 | 49/49 | 0.94 | 0.06 | 35,45,54,56                 | 0     |
| 25  | CLA  | b1    | 614 | 65/65 | 0.94 | 0.08 | 35,45,54,56                 | 0     |
| 25  | CLA  | A1    | 403 | 65/65 | 0.95 | 0.06 | 27,37,49,54                 | 0     |
| 25  | CLA  | b1    | 608 | 65/65 | 0.95 | 0.07 | 37,48,58,63                 | 0     |
| 31  | BCT  | a2    | 417 | 4/4   | 0.96 | 0.05 | 59,65,67,73                 | 0     |
| 26  | OEX  | A1    | 407 | 10/10 | 0.97 | 0.08 | 45,49,63,68                 | 0     |
| 30  | FE   | A1    | 411 | 1/1   | 0.97 | 0.02 | 52,52,52,52                 | 0     |
| 30  | FE   | a1    | 410 | 1/1   | 0.98 | 0.07 | 49,49,49,49                 | 0     |
| 30  | FE   | a2    | 414 | 1/1   | 0.98 | 0.03 | 57,57,57,57                 | 0     |
| 26  | OEX  | a2    | 408 | 10/10 | 0.98 | 0.07 | 42,49,58,61                 | 0     |
| 26  | OEX  | a1    | 408 | 10/10 | 0.98 | 0.08 | 39,49,62,70                 | 0     |
| 24  | CL   | a2    | 403 | 1/1   | 0.98 | 0.03 | 37,37,37,37                 | 0     |
| 30  | FE   | A2    | 411 | 1/1   | 0.99 | 0.04 | 63,63,63,63                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

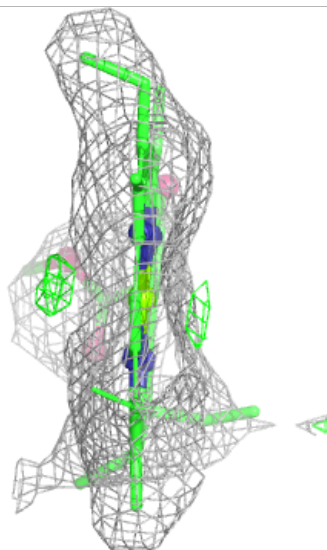
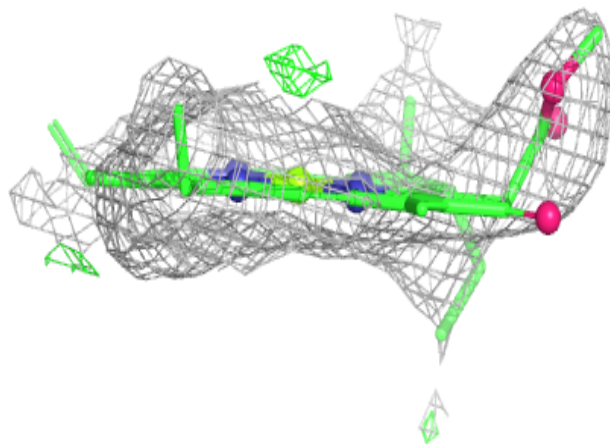
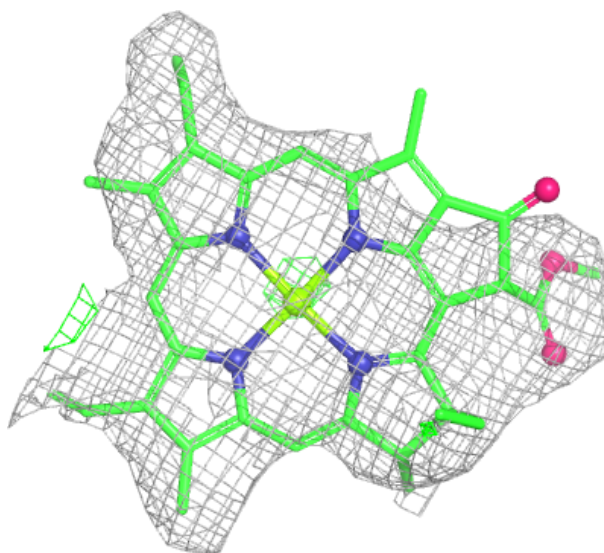


as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



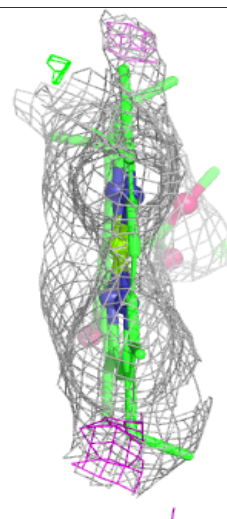
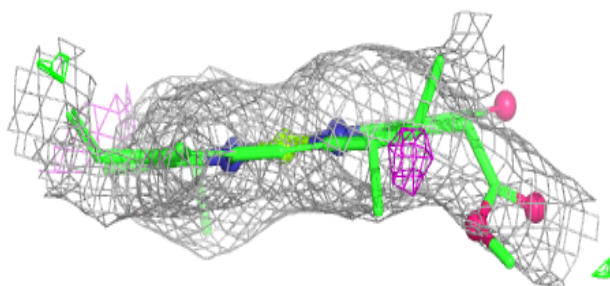
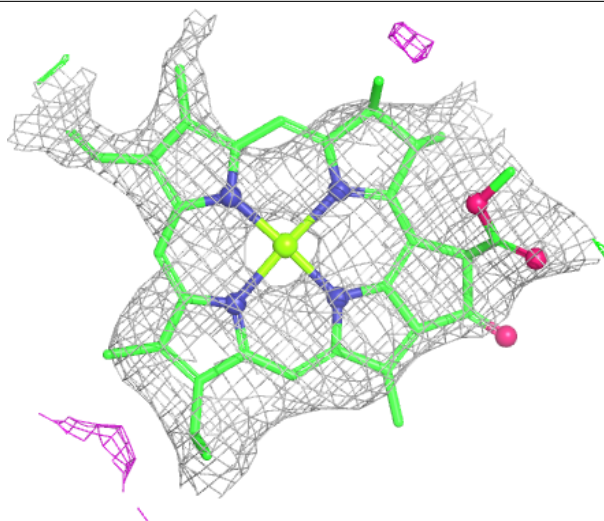
**Electron density around CLA b2 604:**

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



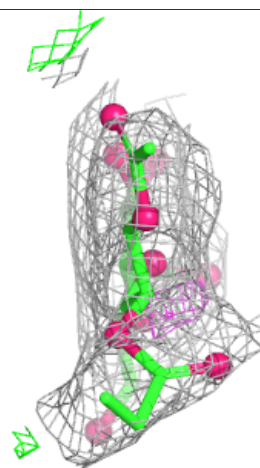
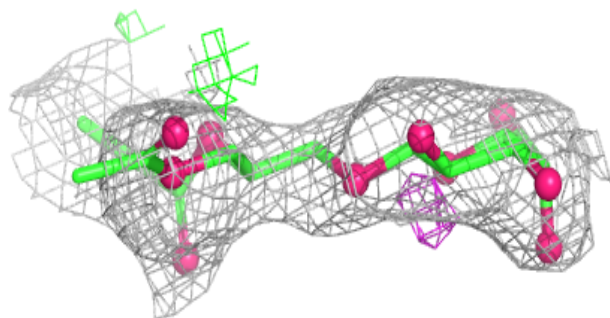
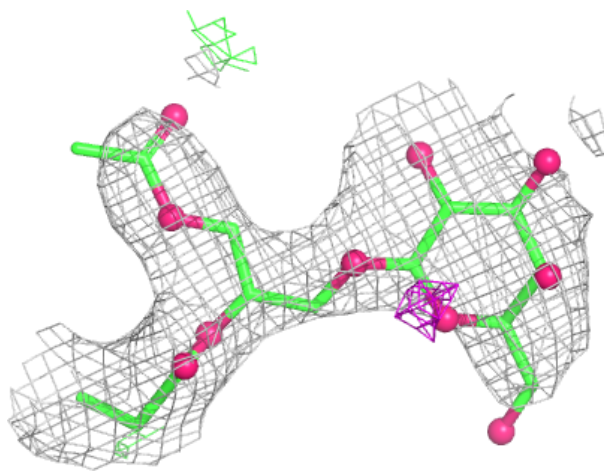
**Electron density around CLA C2 518:**

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



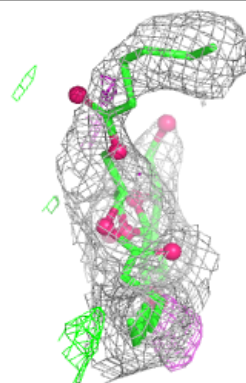
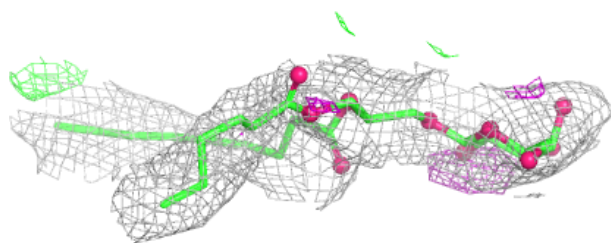
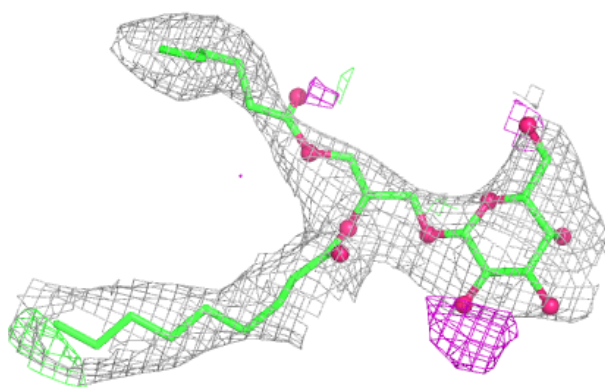
**Electron density around LMG C2 515:**

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



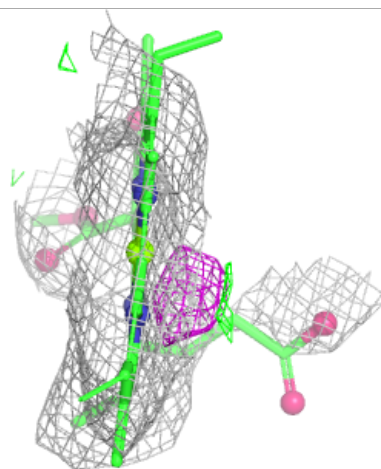
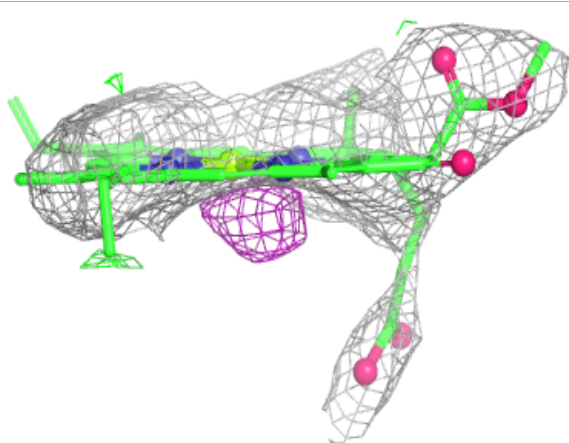
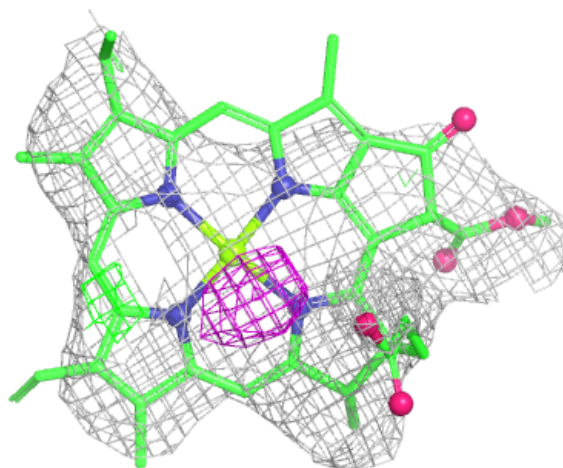
**Electron density around LMG I2 101:**

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



**Electron density around CLA C2 510:**

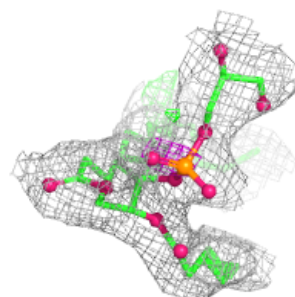
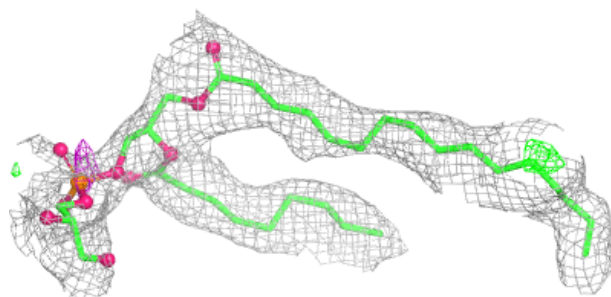
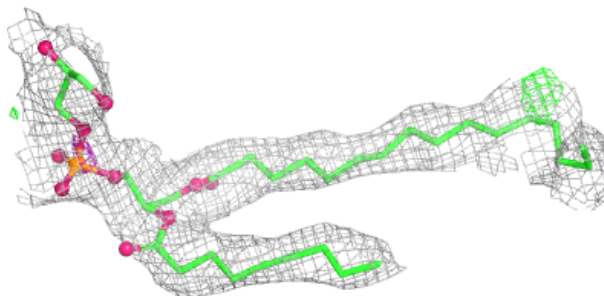
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



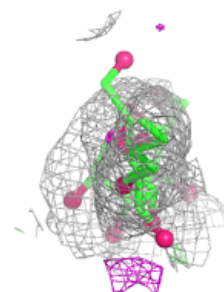
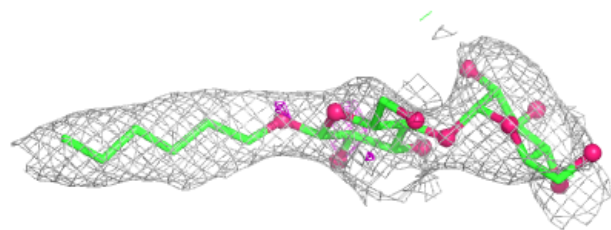
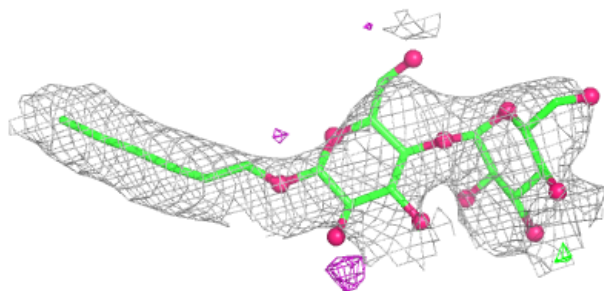


**Electron density around LHG B2 627:**

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

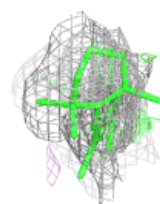
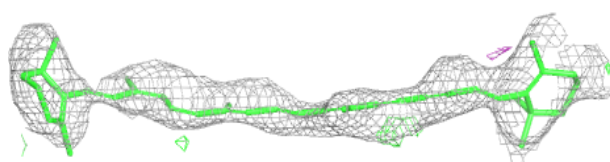
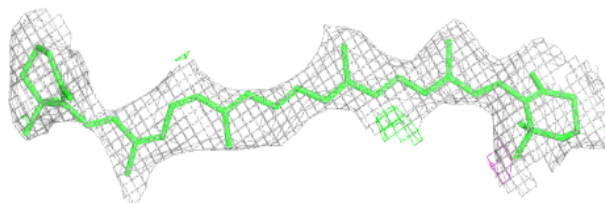
**Electron density around LMT m2 104:**

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

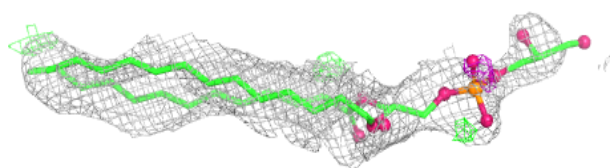
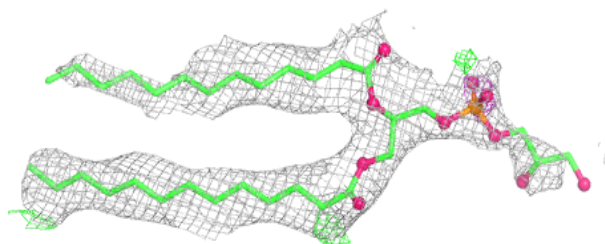


**Electron density around BCR K2 102:**

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

**Electron density around LHG b2 625:**

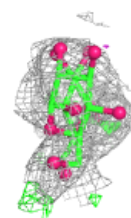
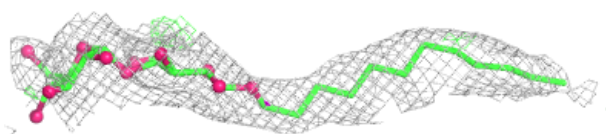
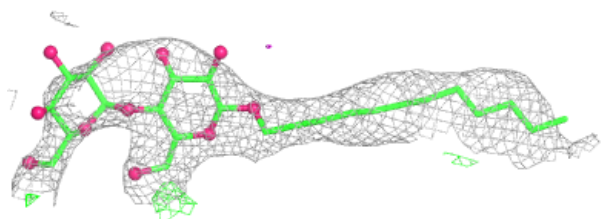
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



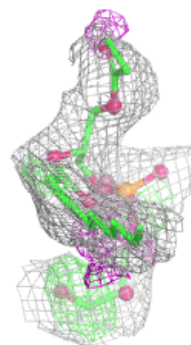
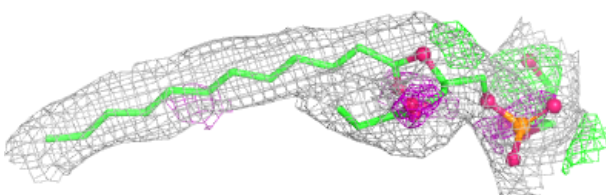
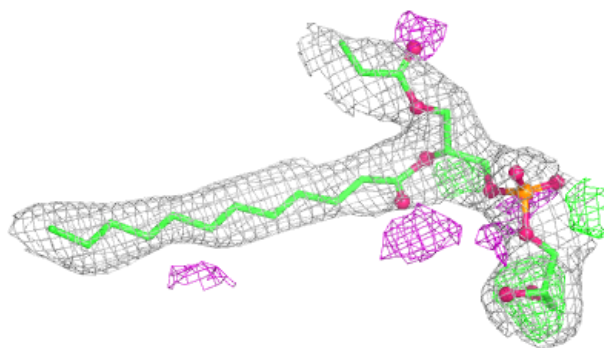


**Electron density around LMT b2 621:**

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

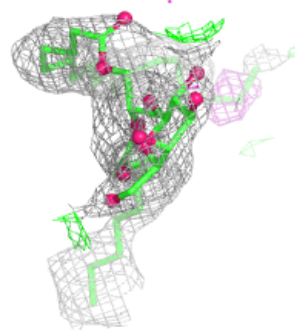
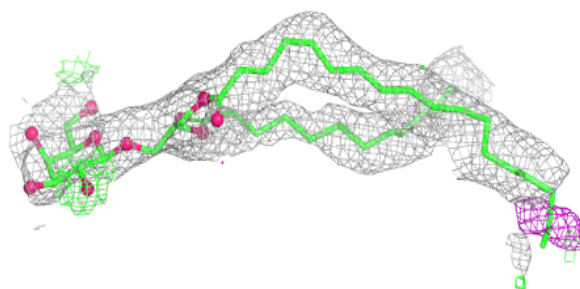
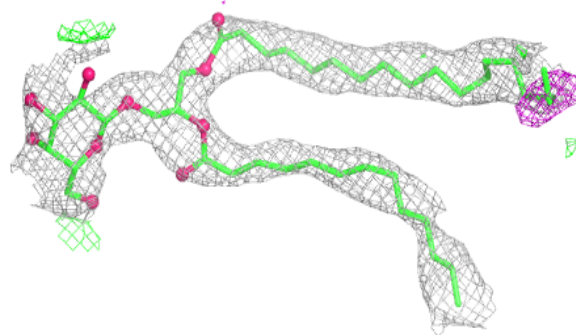
**Electron density around LHG d1 402:**

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

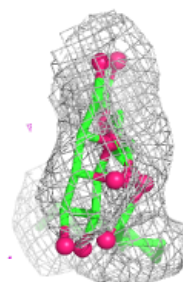
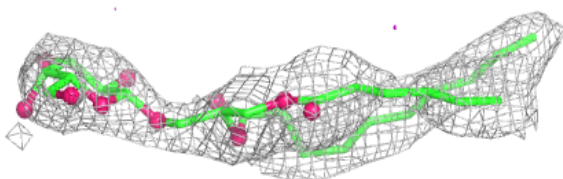
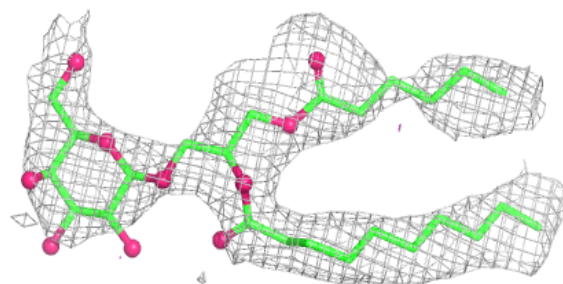


**Electron density around LMG j2 101:**

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

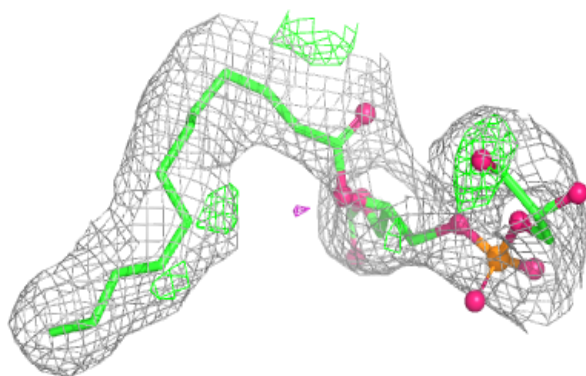
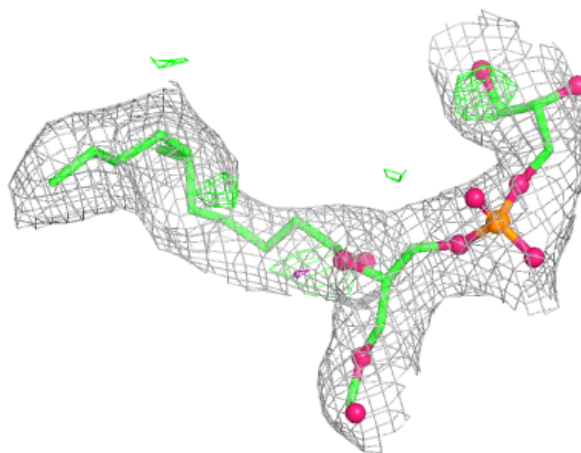
**Electron density around LMG F2 402:**

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



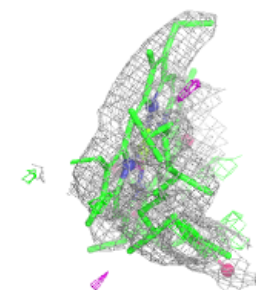
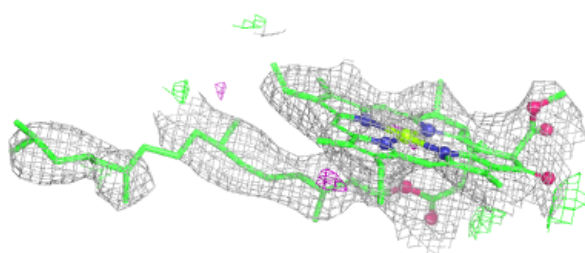
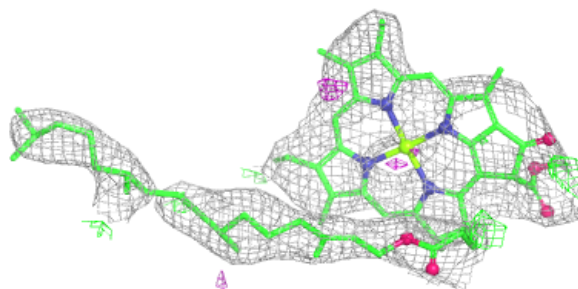
**Electron density around LHG a2 407:**

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

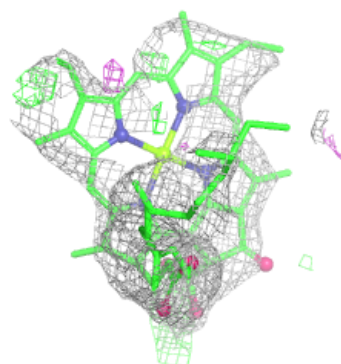
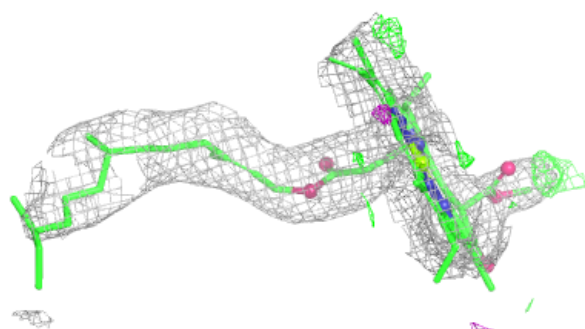
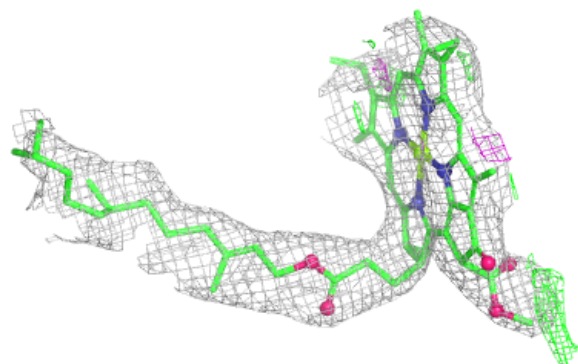


**Electron density around CLA C2 503:**

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

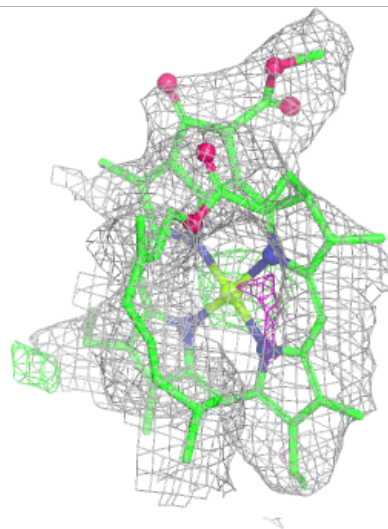
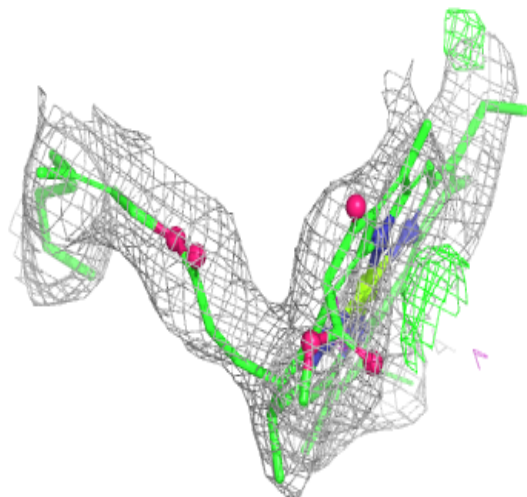
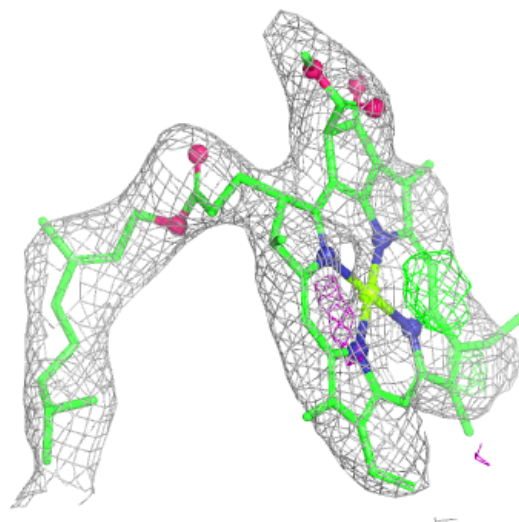
**Electron density around CLA D2 404:**

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



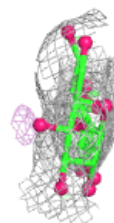
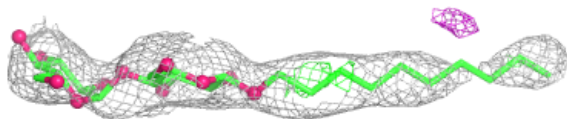
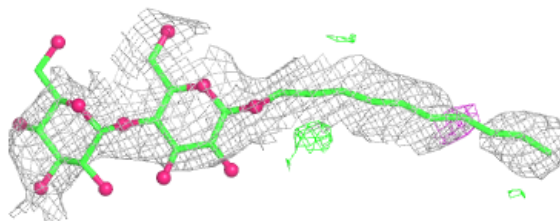
**Electron density around CLA K2 101:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LMT c1 517:**

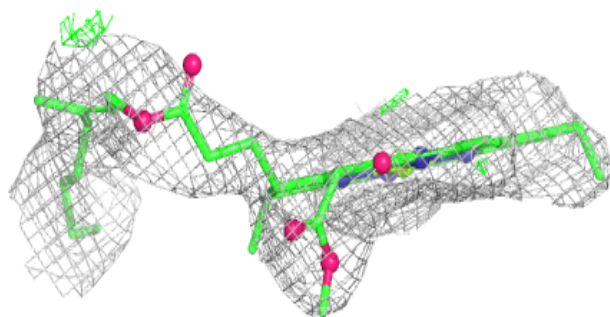
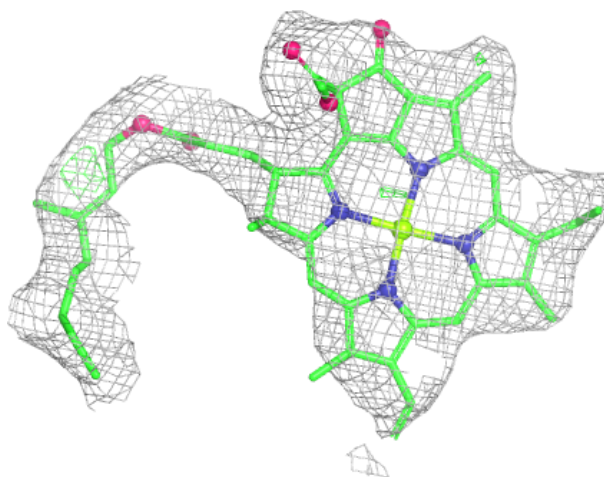
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





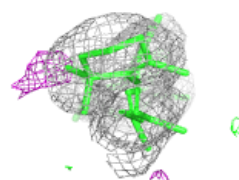
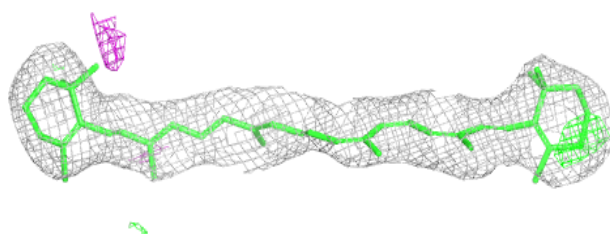
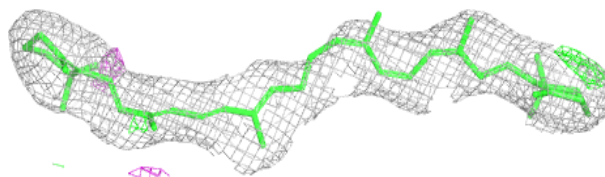
**Electron density around CLA c2 513:**

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

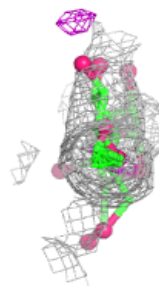
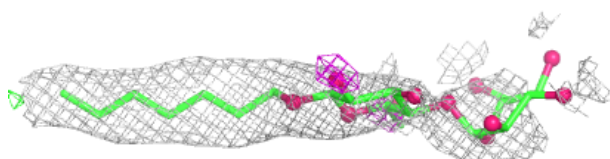
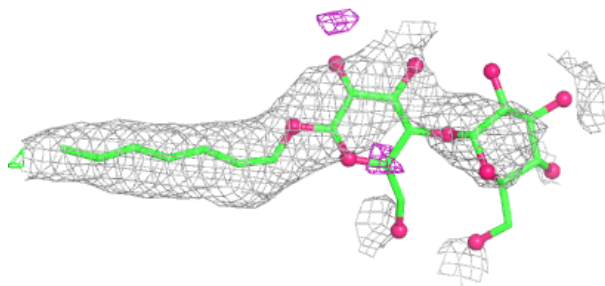


**Electron density around BCR c2 501:**

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

**Electron density around LMT m2 103:**

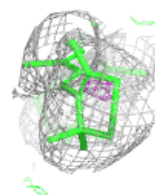
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



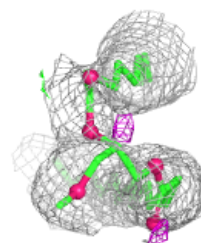
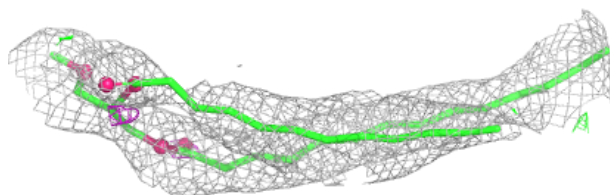
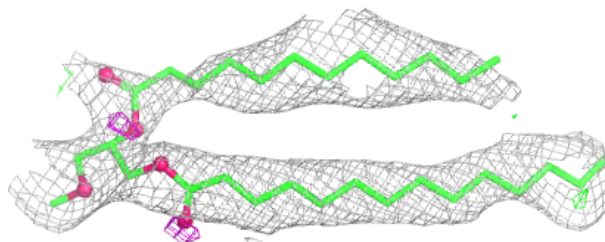


**Electron density around BCR K2 104:**

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

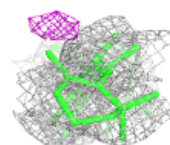
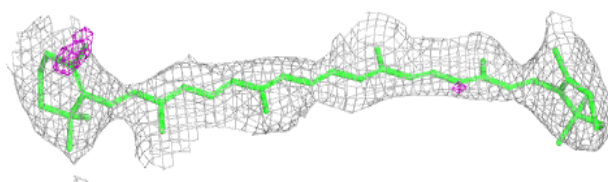
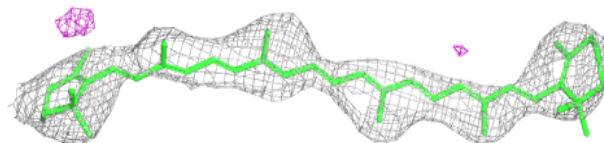
**Electron density around LMG d1 411:**

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

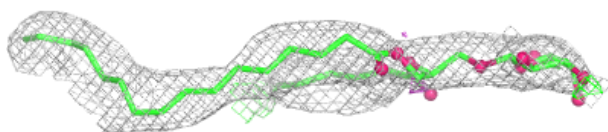
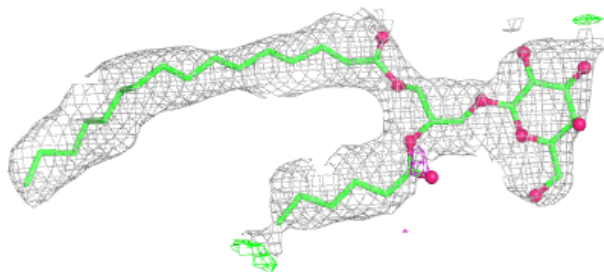


**Electron density around BCR z2 101:**

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

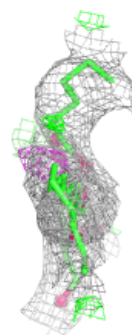
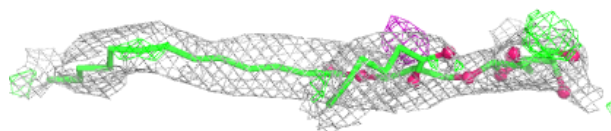
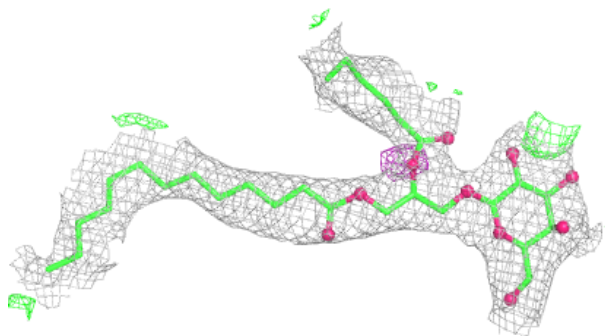
**Electron density around LMG A1 412:**

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

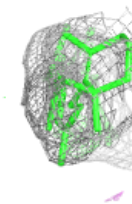
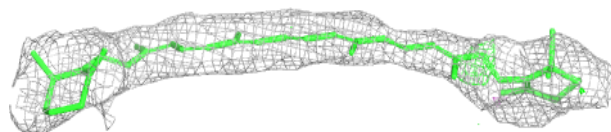
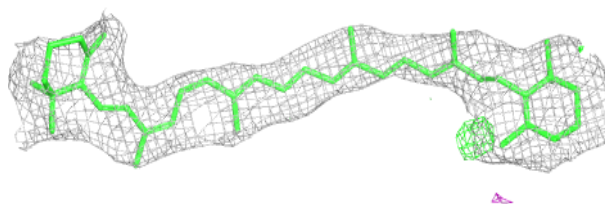


**Electron density around LMG b1 621:**

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

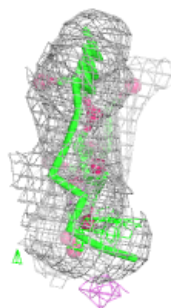
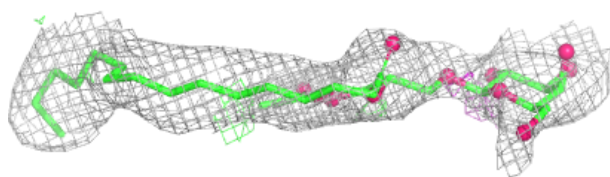
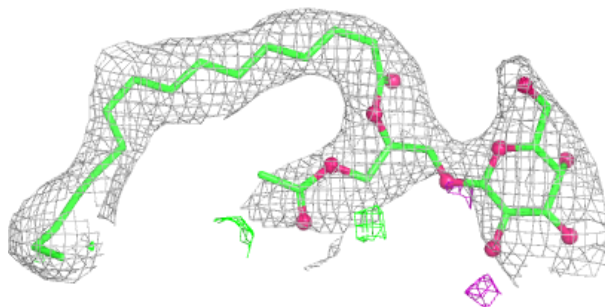
**Electron density around BCR F2 401:**

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



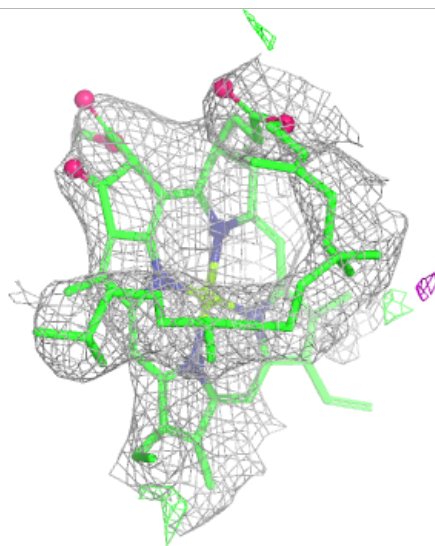
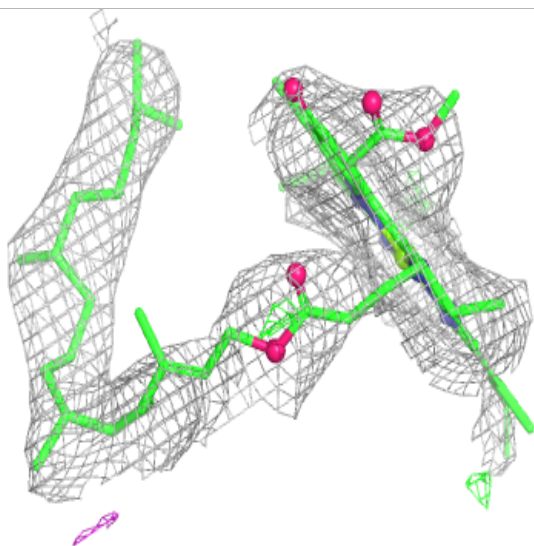
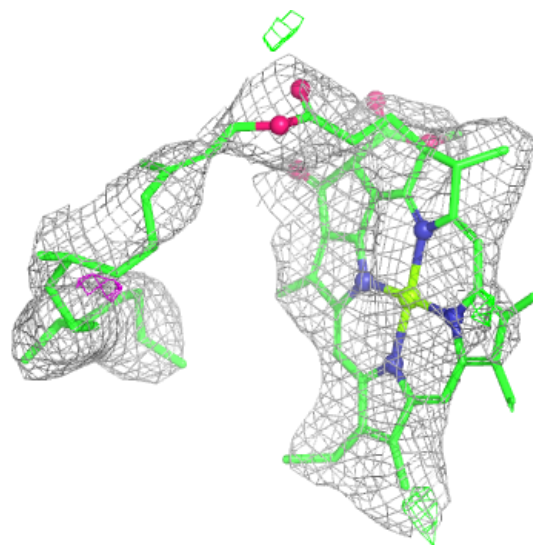
**Electron density around LMG B2 621:**

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



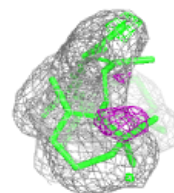
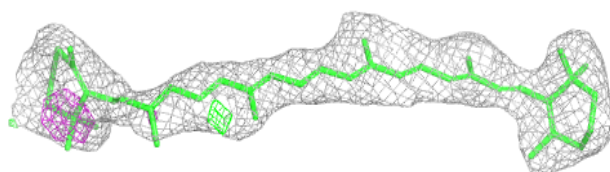
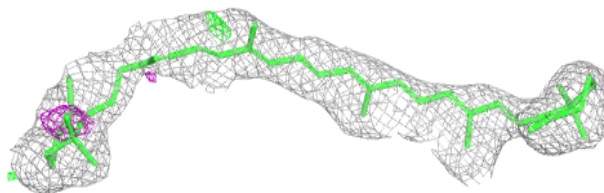
**Electron density around CLA C2 505:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



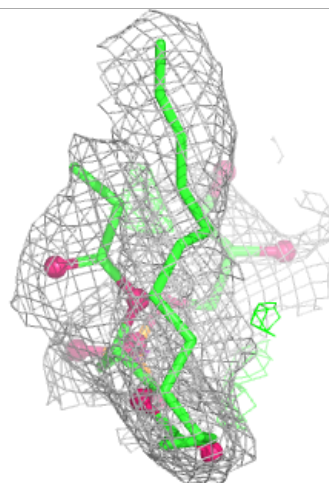
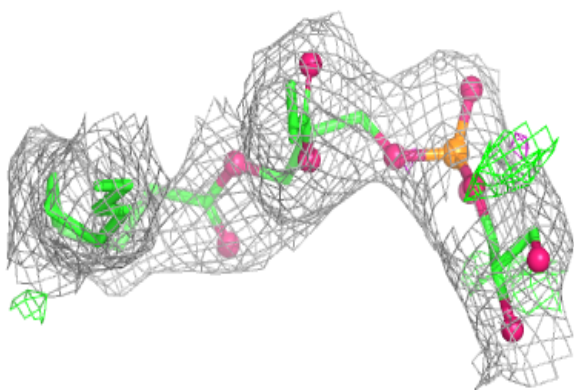
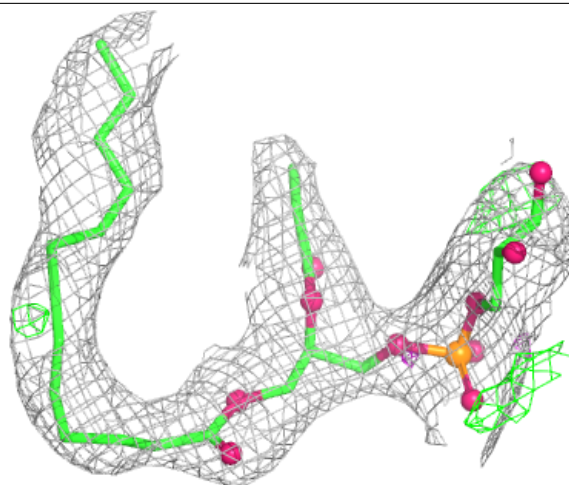
**Electron density around BCR B1 602:**

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



**Electron density around LHG A2 405:**

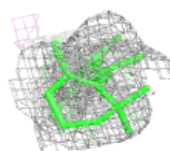
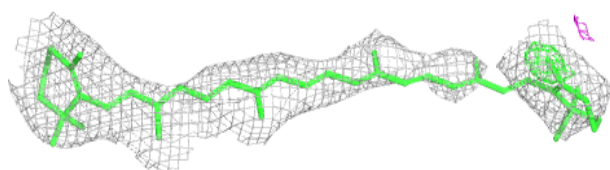
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



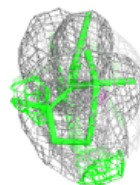
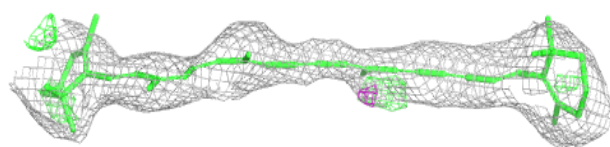
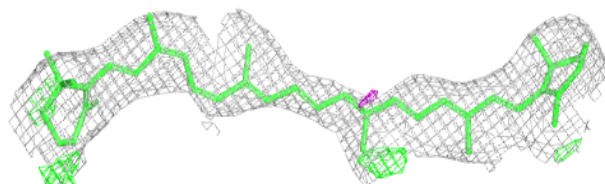


**Electron density around BCR C2 502:**

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

**Electron density around BCR J1 101:**

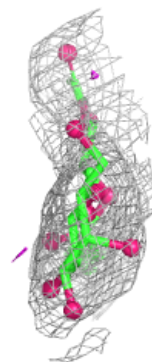
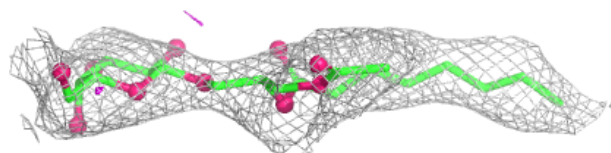
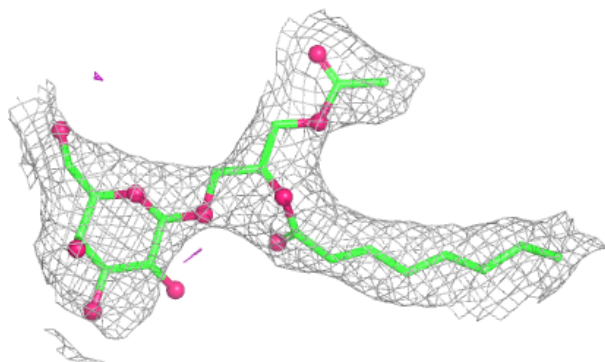
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





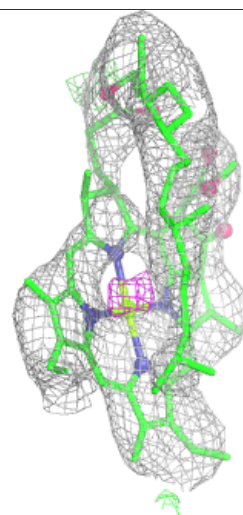
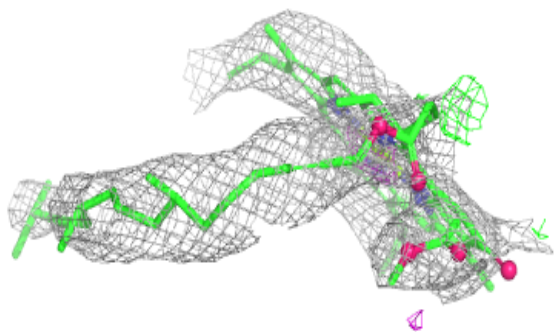
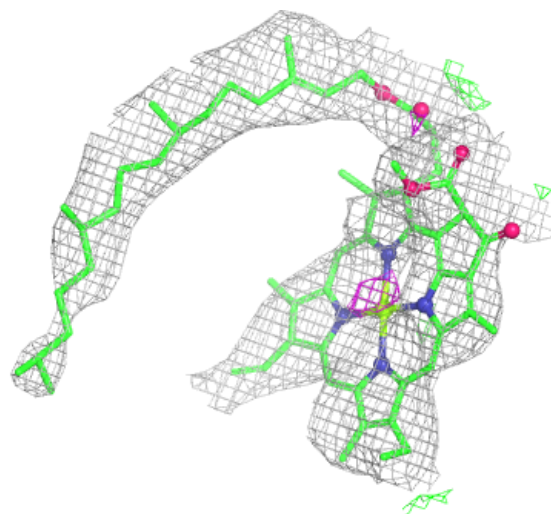
**Electron density around LMG A2 412:**

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



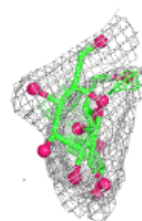
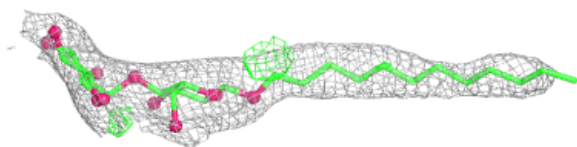
**Electron density around CLA C2 509:**

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

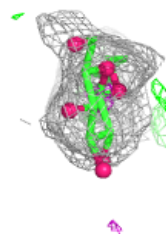
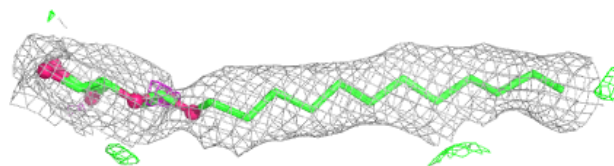
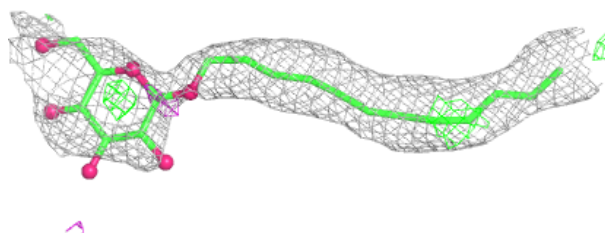


**Electron density around LMT C1 519:**

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

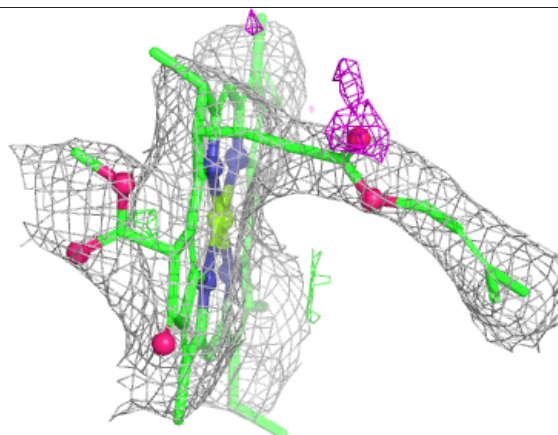
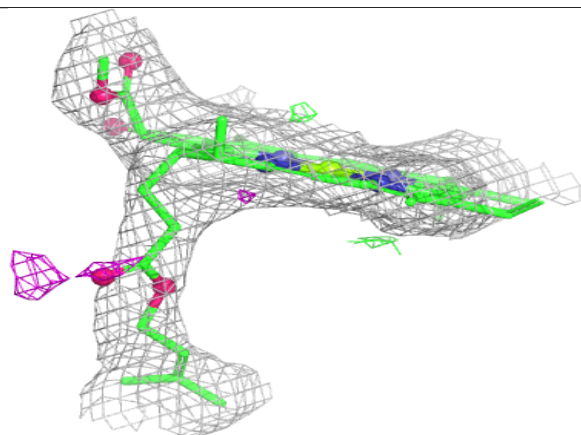
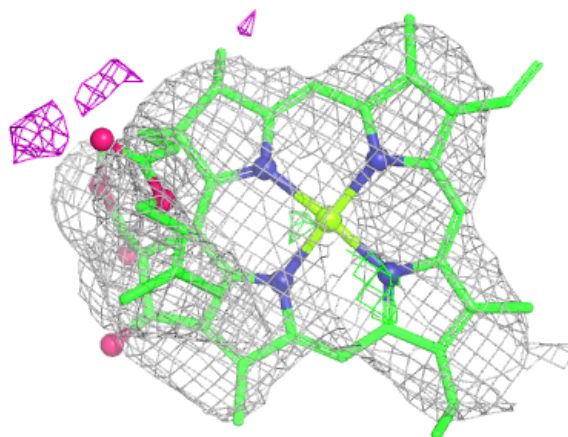
**Electron density around LMT M1 103:**

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

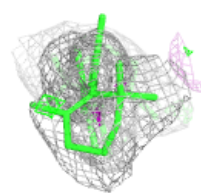
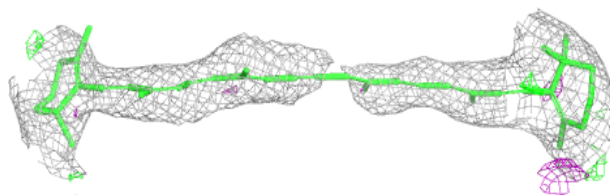
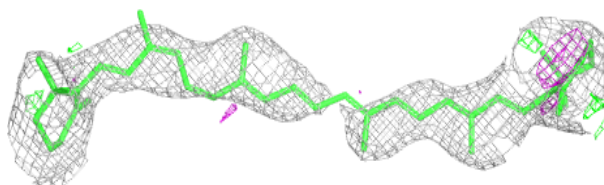


**Electron density around CLA C2 511:**

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

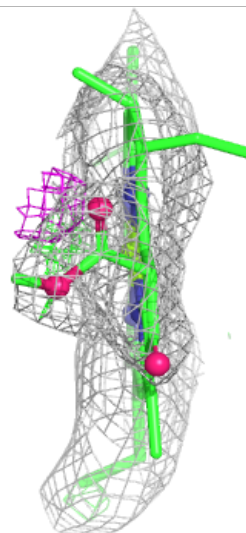
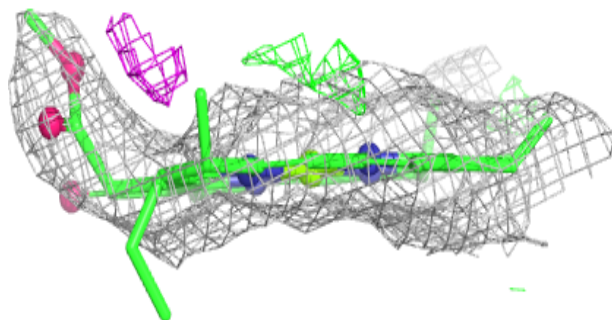
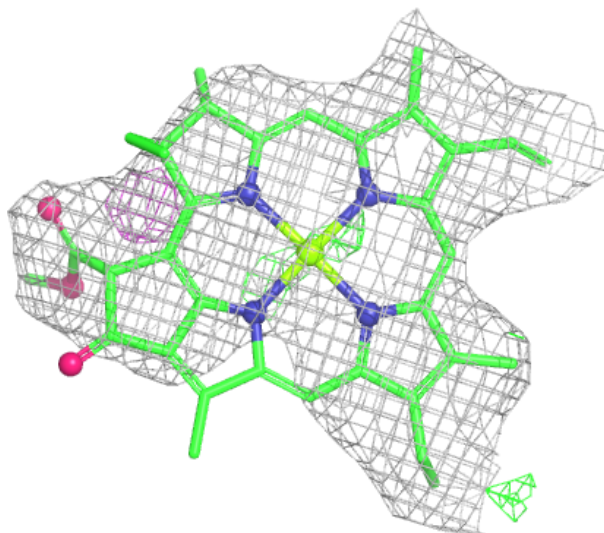
**Electron density around BCR k1 101:**

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



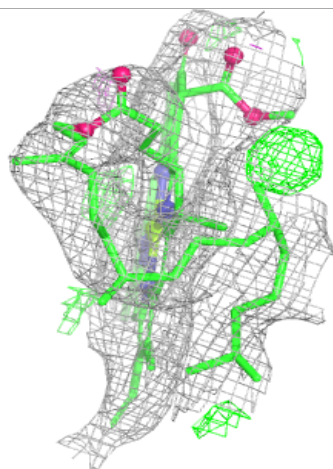
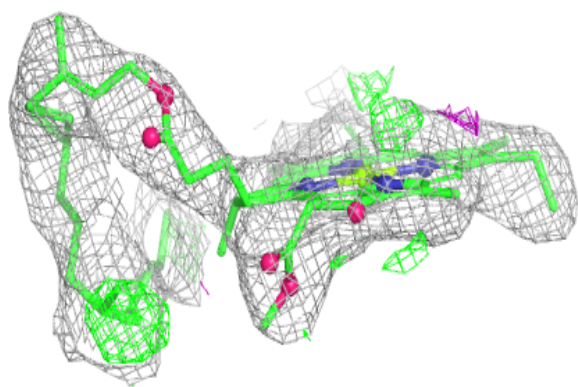
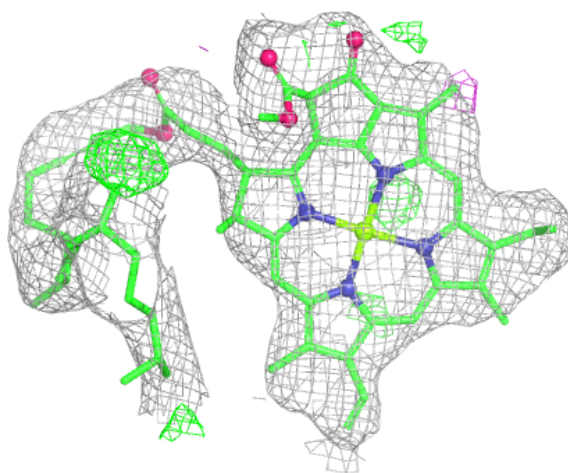
**Electron density around CLA B1 604:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA C1 512:**

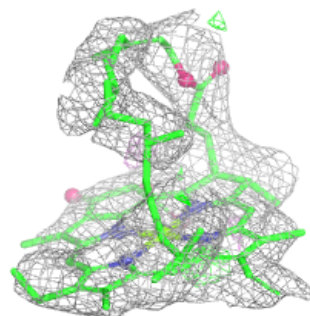
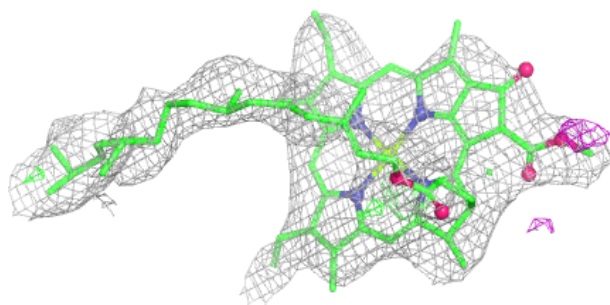
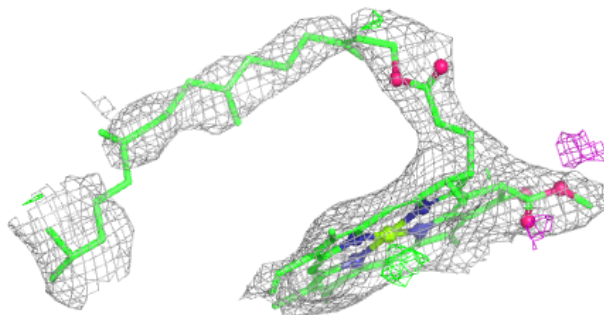
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



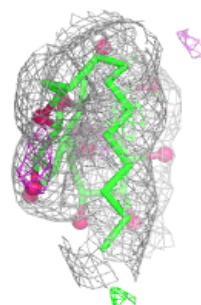
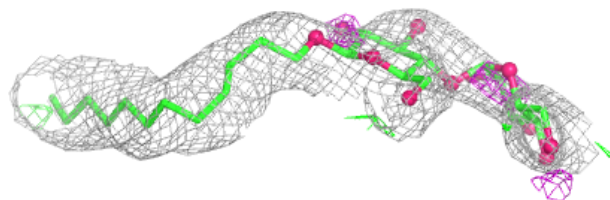
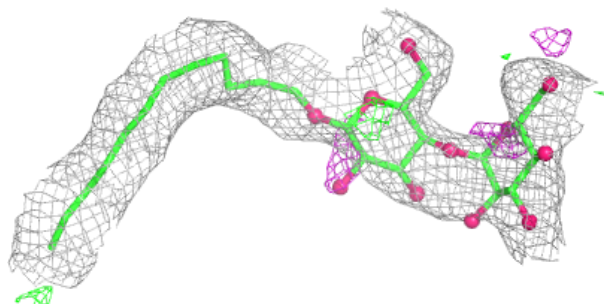


**Electron density around CLA c1 516:**

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

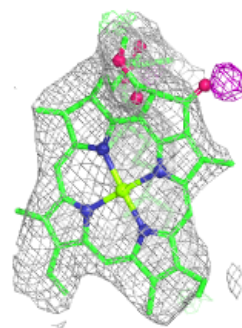
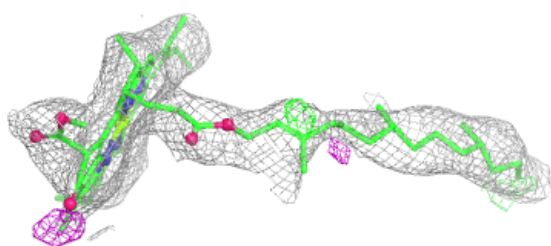
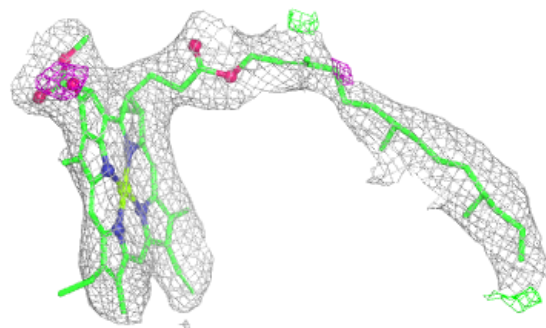
**Electron density around LMT a2 406:**

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



**Electron density around CLA B1 611:**

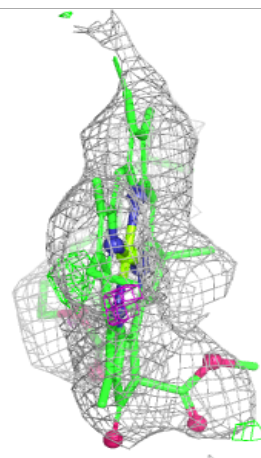
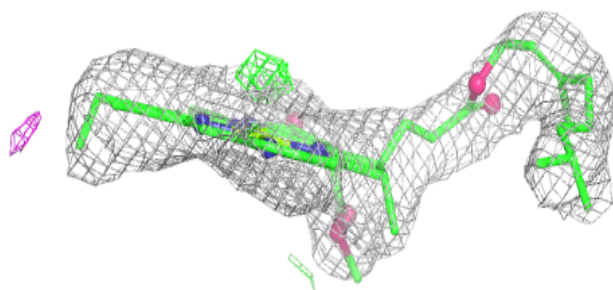
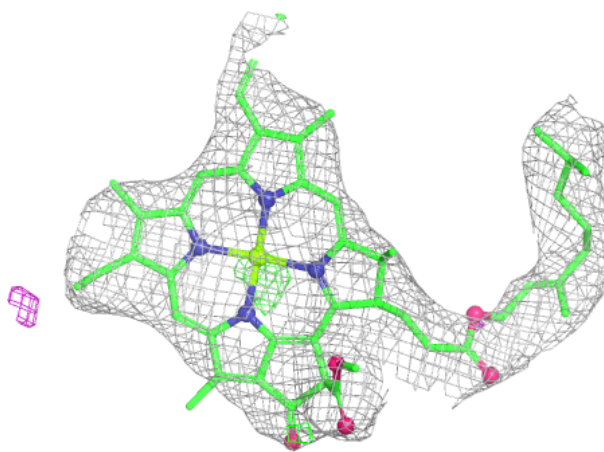
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





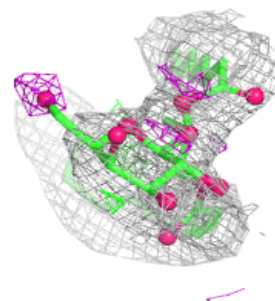
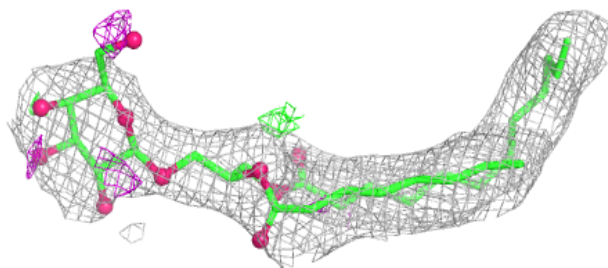
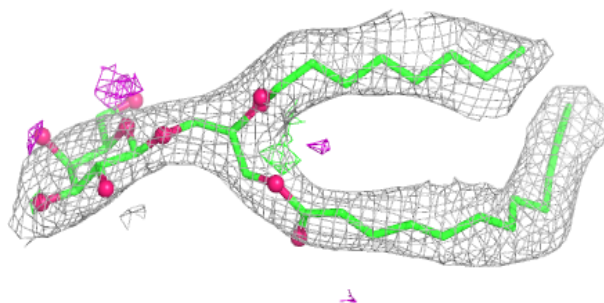
**Electron density around CLA c1 515:**

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

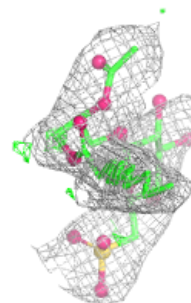
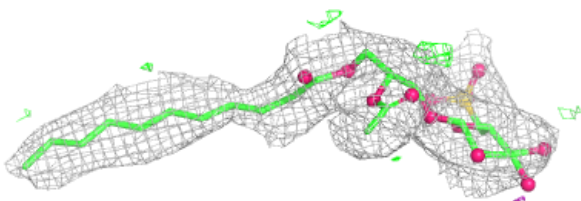
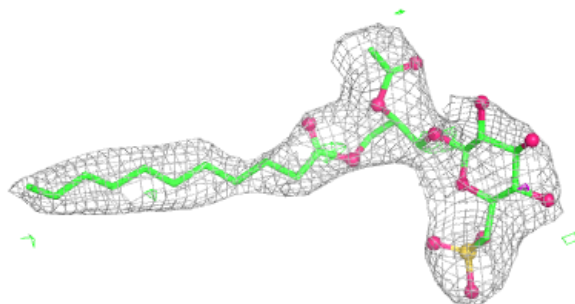


**Electron density around LMG b1 624:**

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

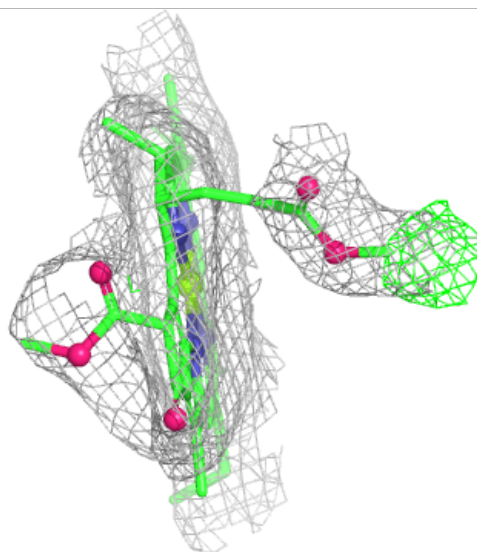
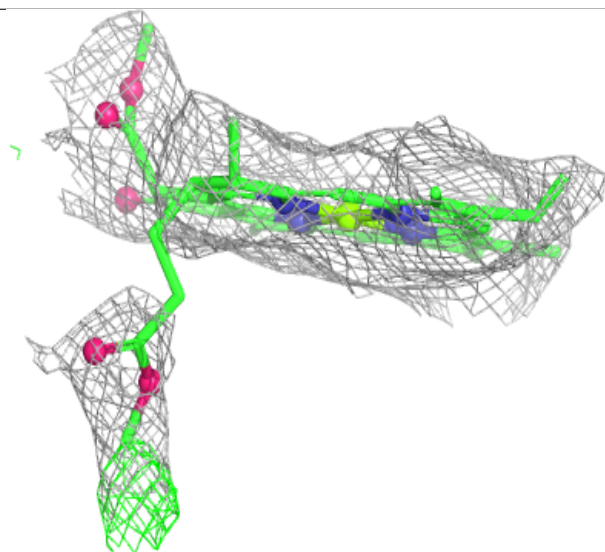
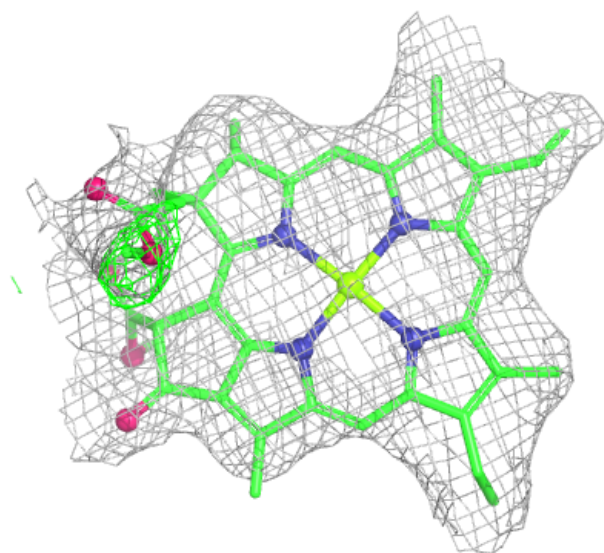
**Electron density around SQD D1 409:**

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



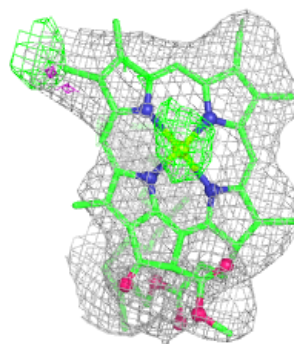
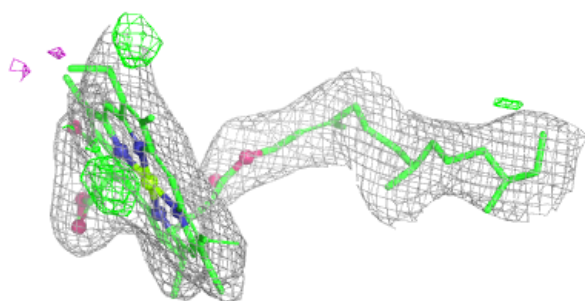
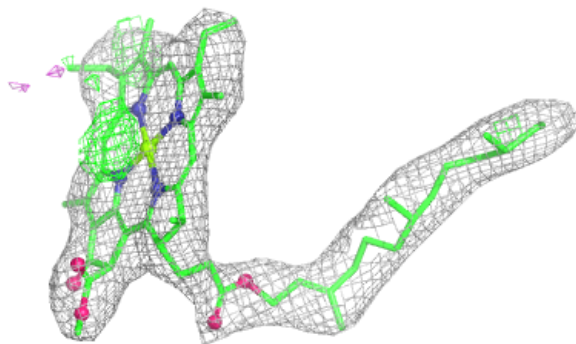
**Electron density around CLA C2 504:**

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



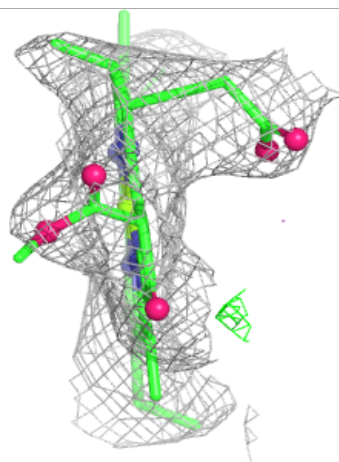
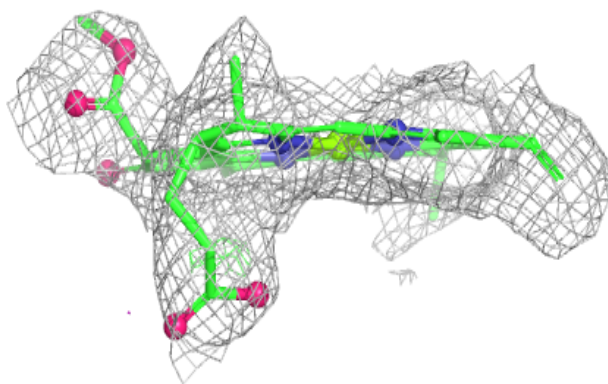
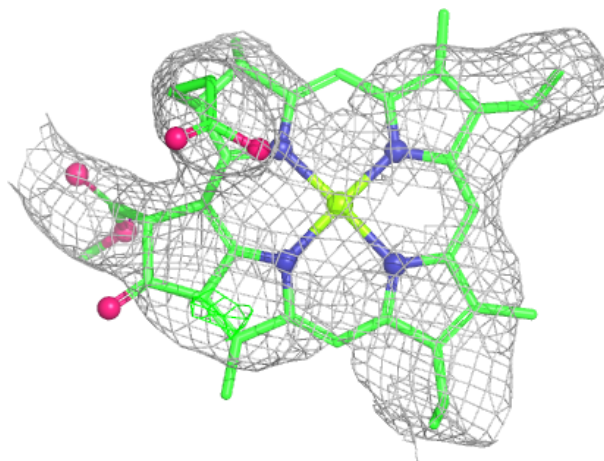
**Electron density around CLA C1 513:**

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



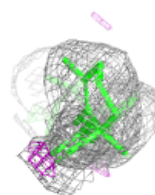
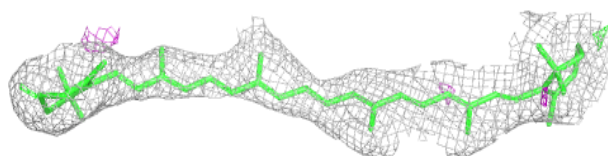
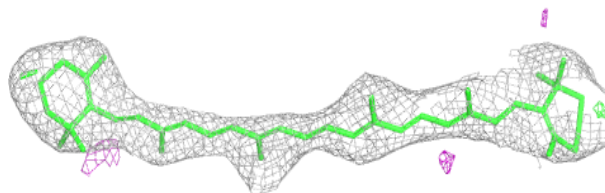
**Electron density around CLA C2 507:**

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

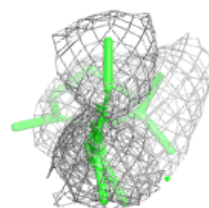
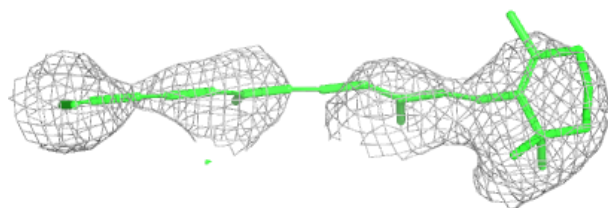
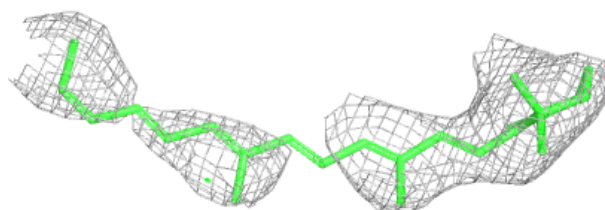


**Electron density around BCR b2 603:**

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

**Electron density around BCR H2 103:**

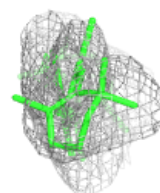
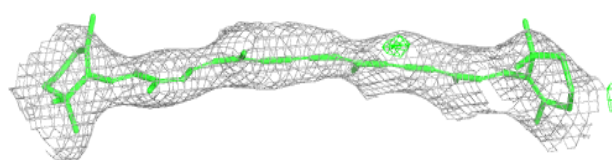
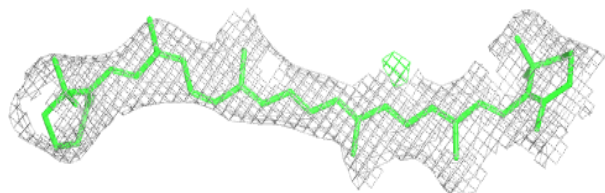
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



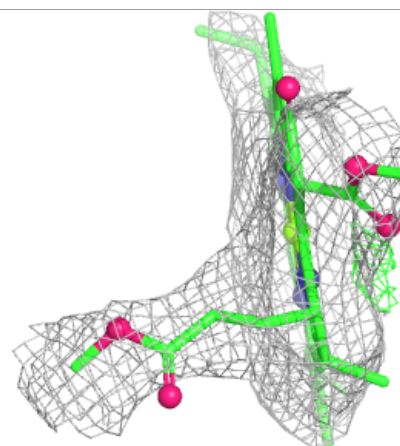
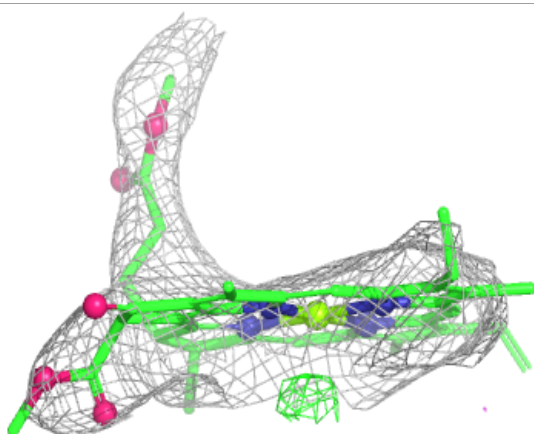
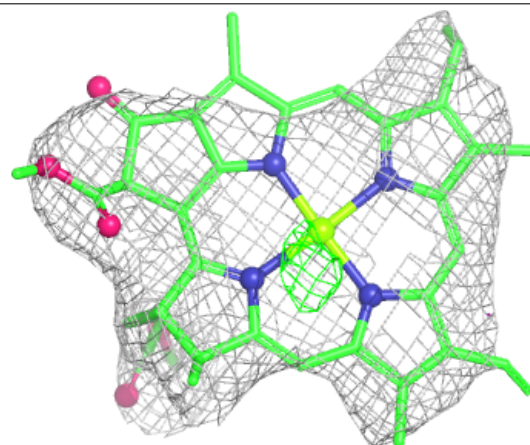


**Electron density around BCR j2 102:**

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

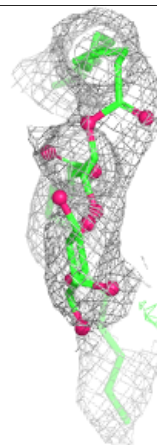
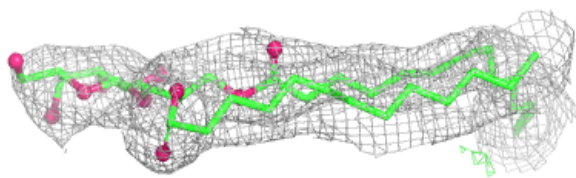
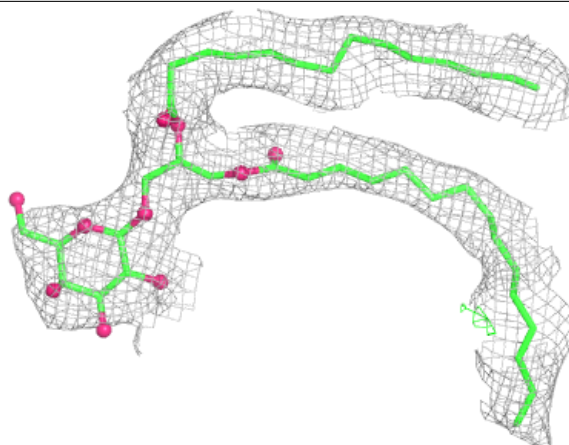
**Electron density around CLA c2 515:**

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

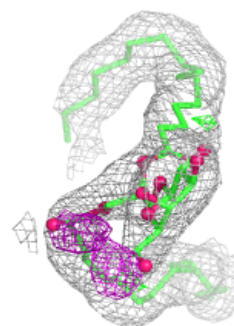
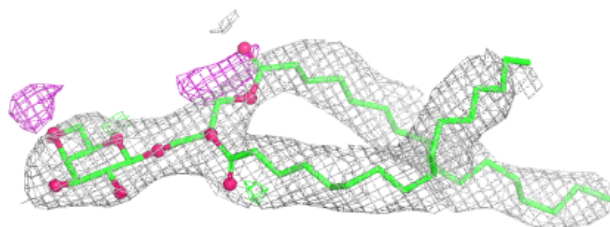
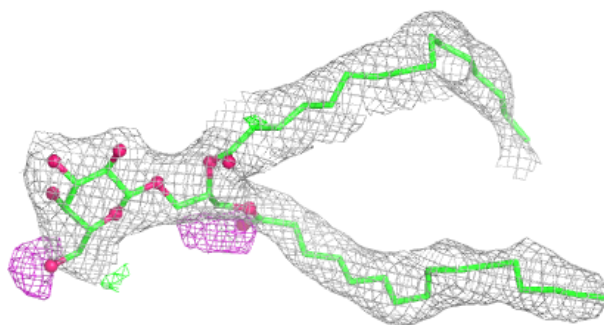


**Electron density around LMG C1 520:**

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

**Electron density around LMG a1 412:**

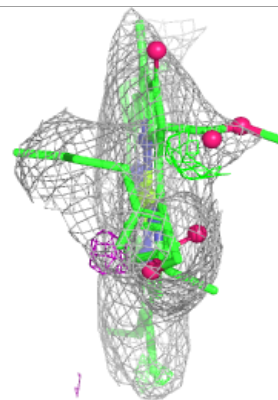
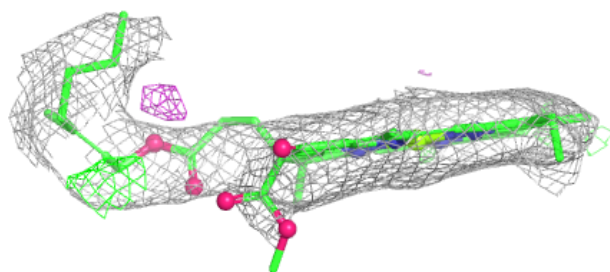
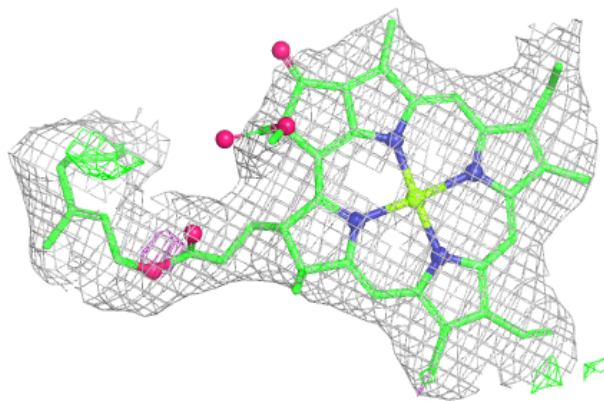
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



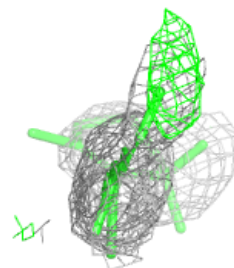
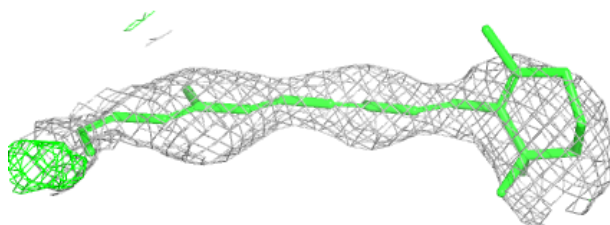
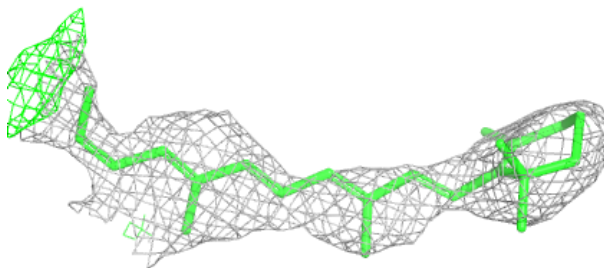


**Electron density around CLA C2 513:**

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

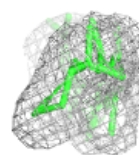
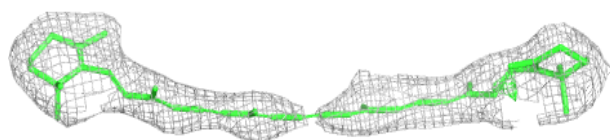
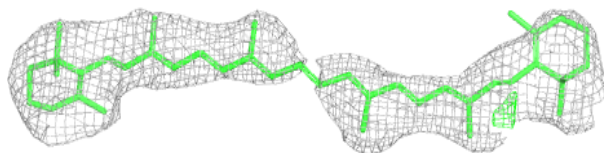
**Electron density around BCR H1 102:**

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

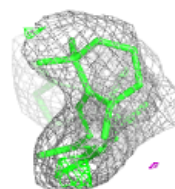
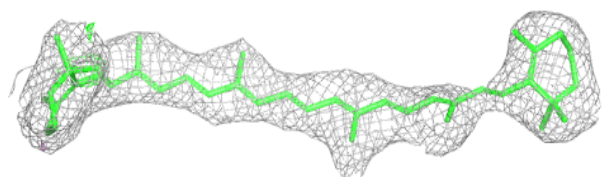
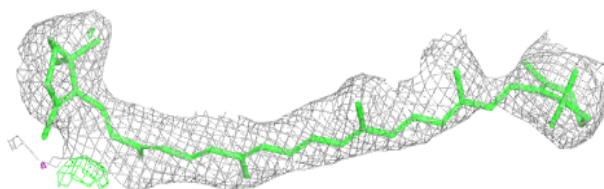


**Electron density around BCR D1 401:**

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

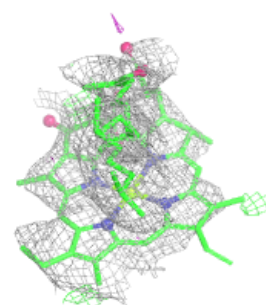
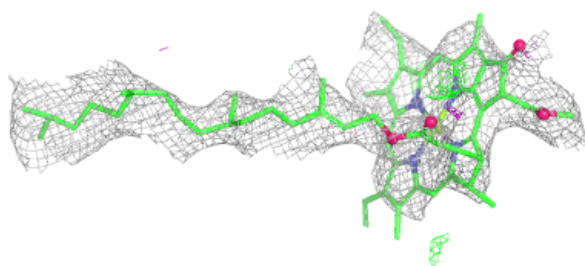
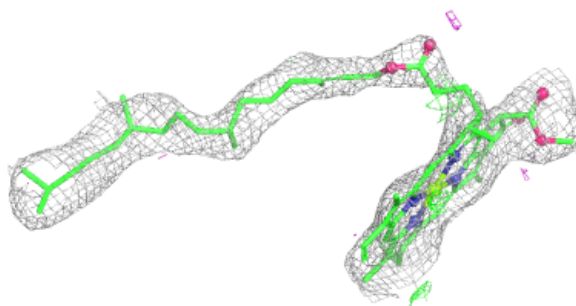
**Electron density around BCR b2 602:**

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

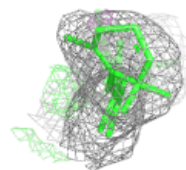
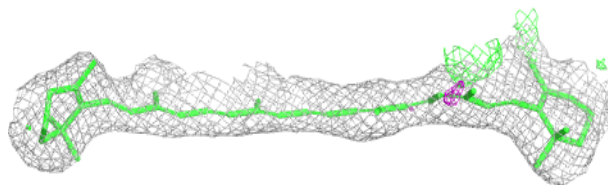
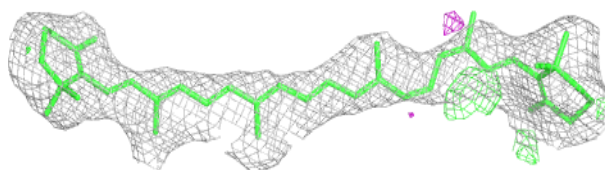


**Electron density around CLA C2 506:**

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

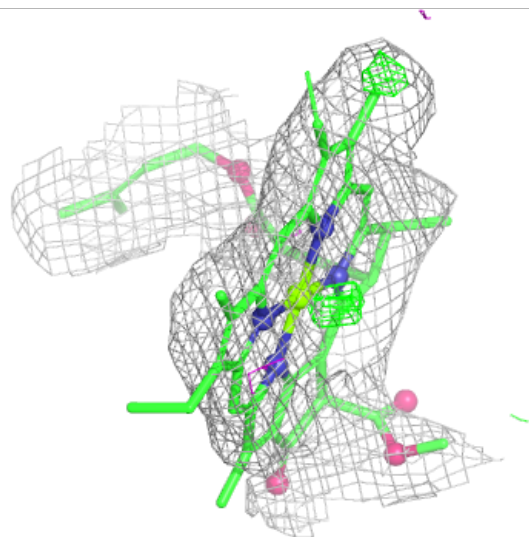
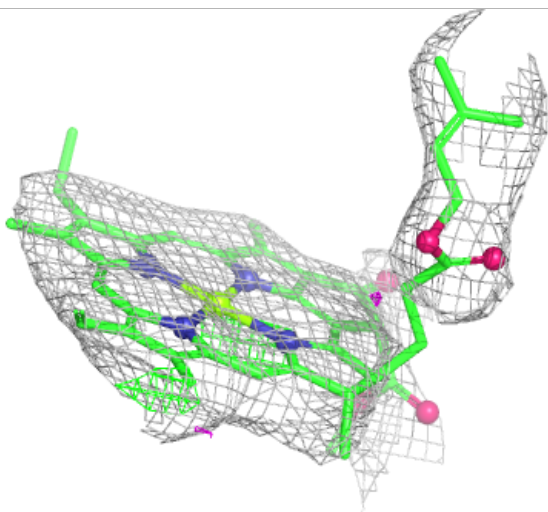
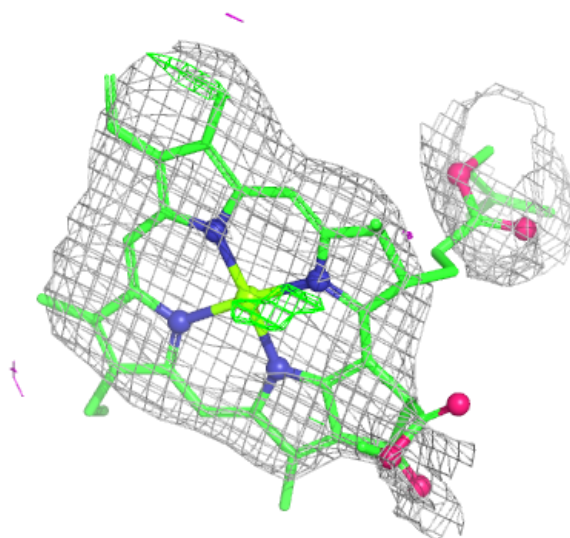
**Electron density around BCR b1 602:**

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



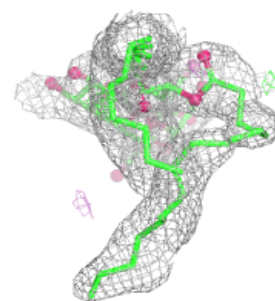
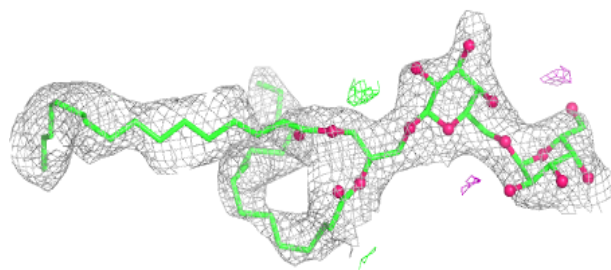
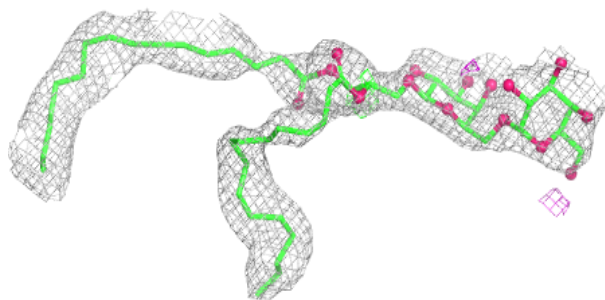
**Electron density around CLA C2 508:**

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



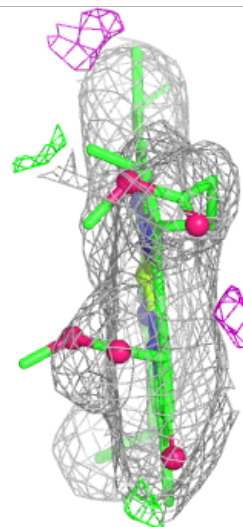
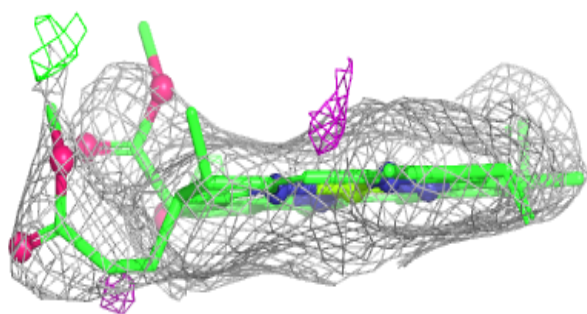
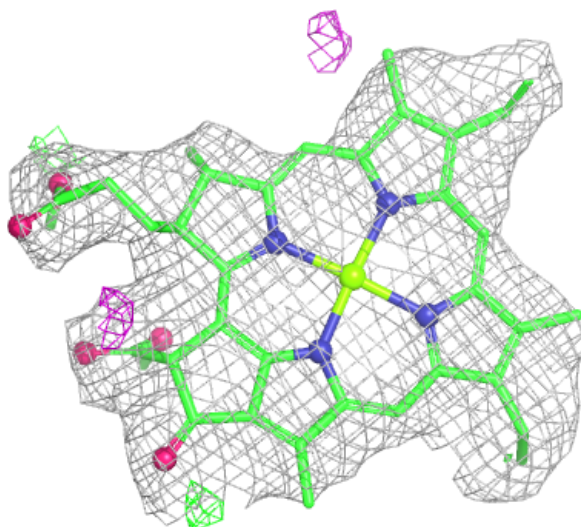
**Electron density around DGD H2 101:**

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



**Electron density around CLA C2 516:**

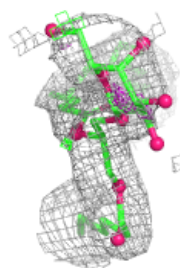
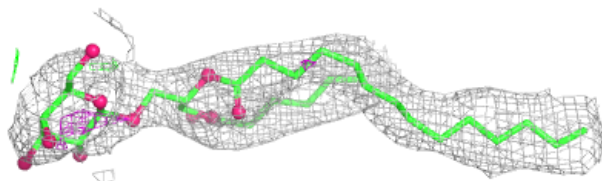
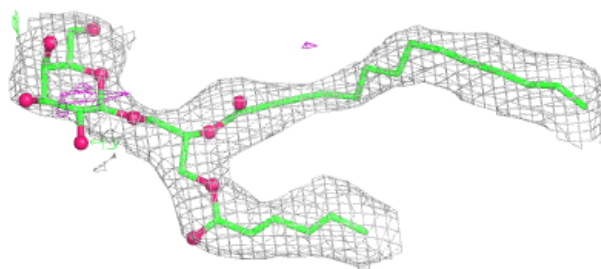
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





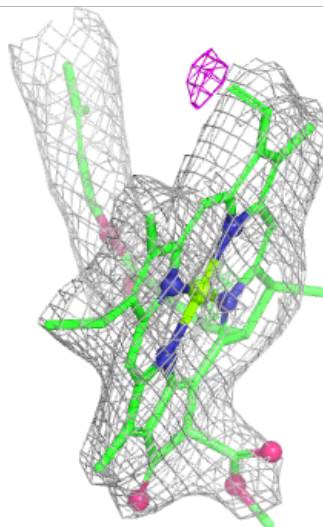
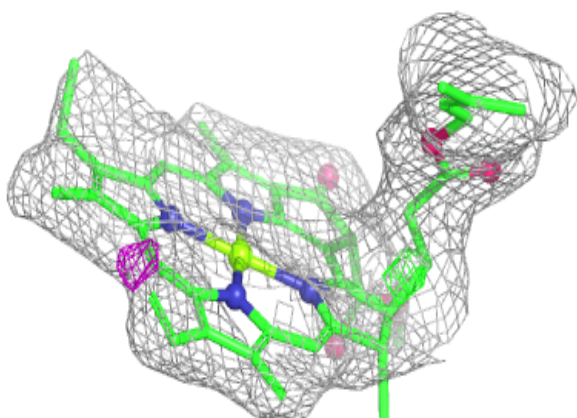
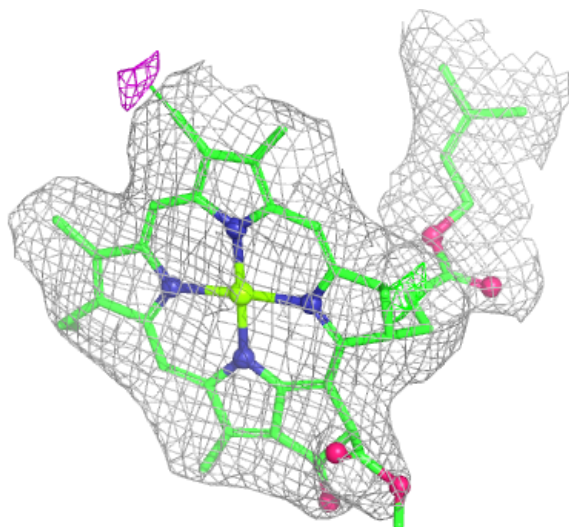
**Electron density around LMG b2 622:**

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



**Electron density around CLA d2 404:**

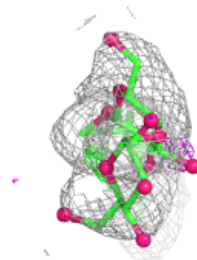
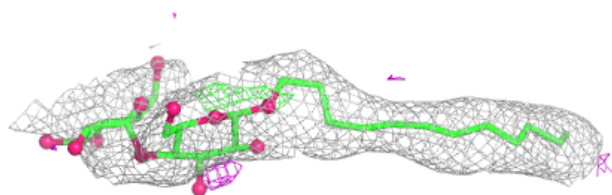
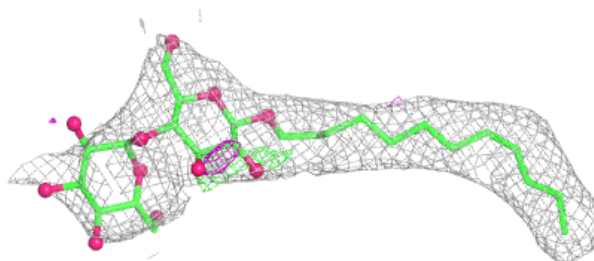
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





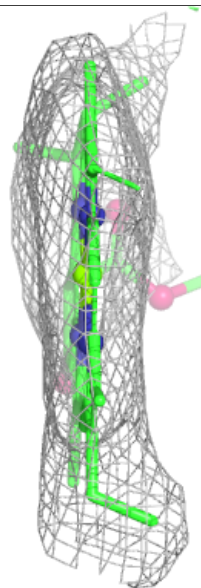
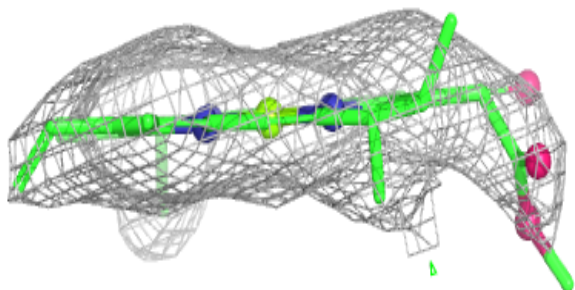
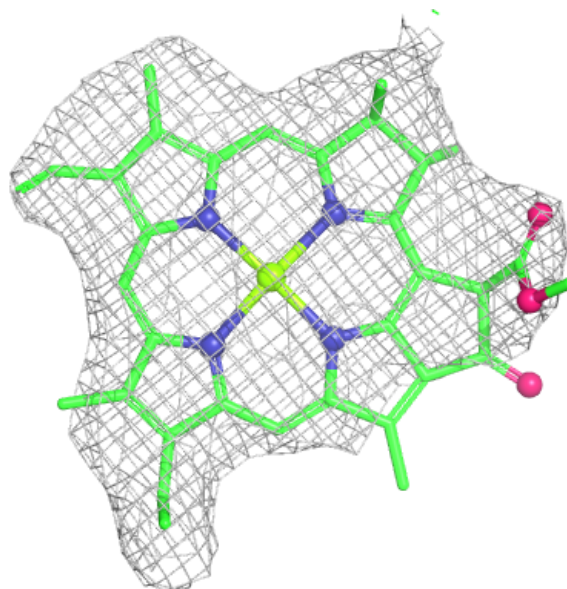
**Electron density around LMT m1 101:**

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



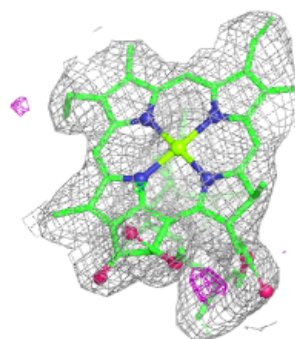
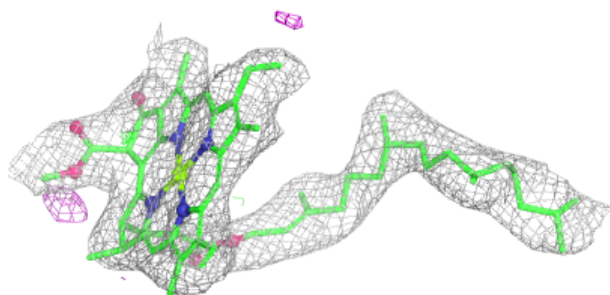
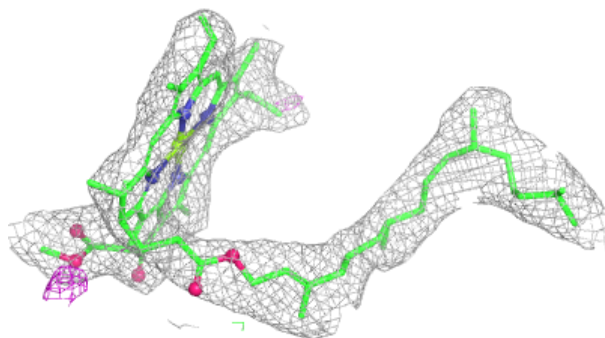
**Electron density around CLA B2 604:**

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

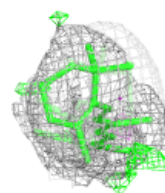
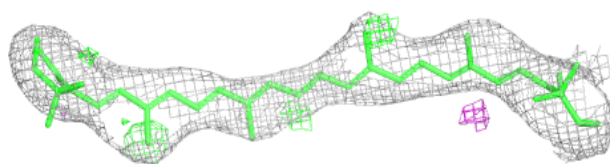
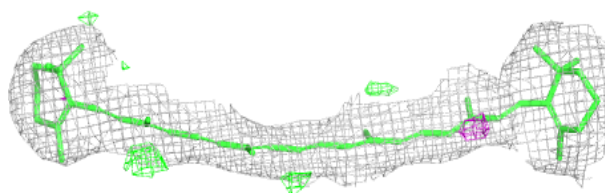


**Electron density around CLA c2 509:**

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

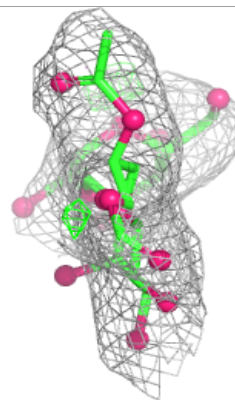
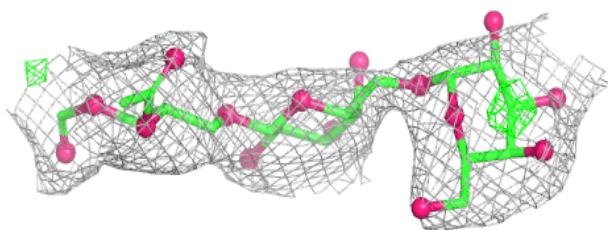
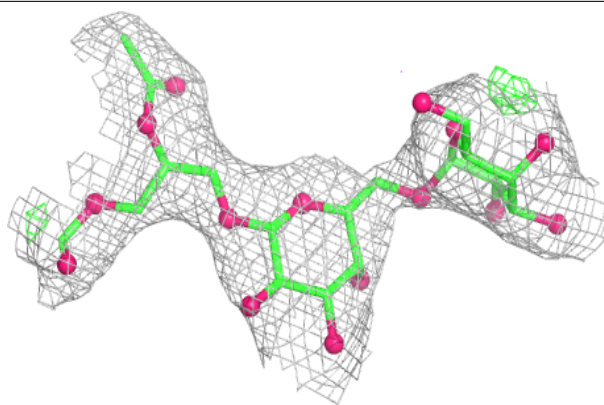
**Electron density around BCR C1 521:**

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

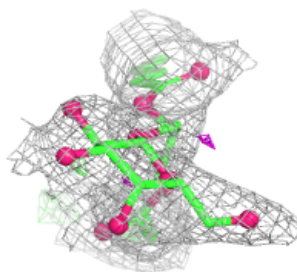
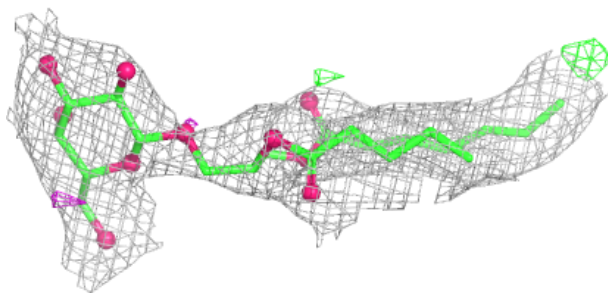
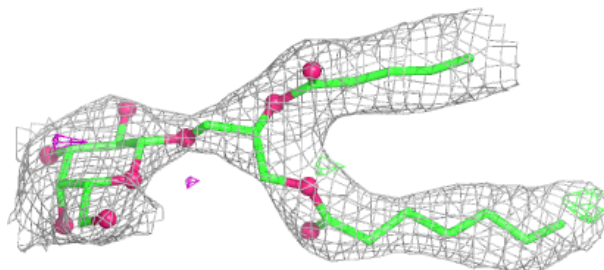


**Electron density around DGD C2 512:**

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

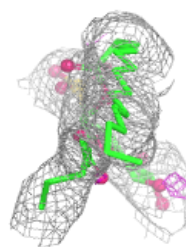
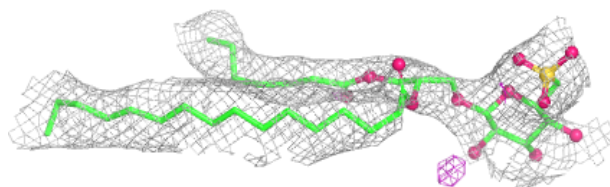
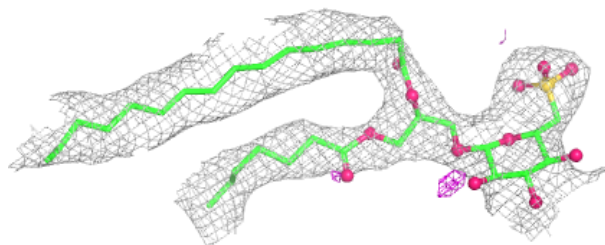
**Electron density around LMG B1 622:**

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

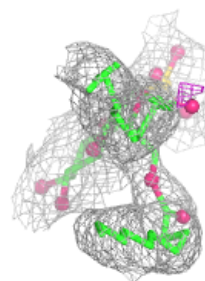
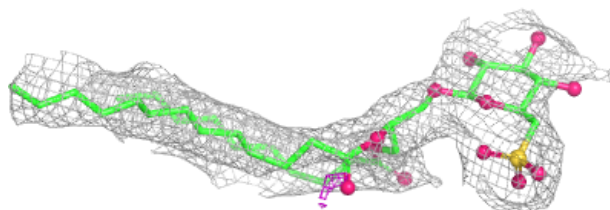
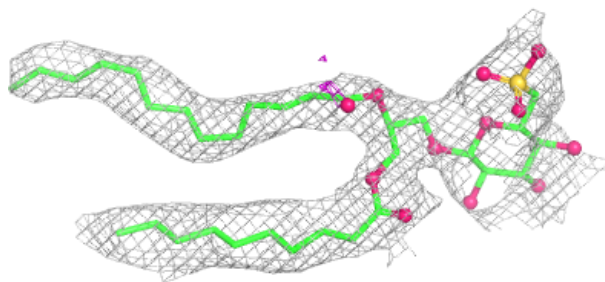


**Electron density around SQD B2 623:**

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

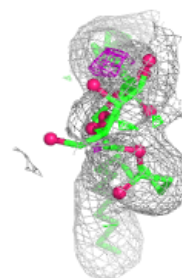
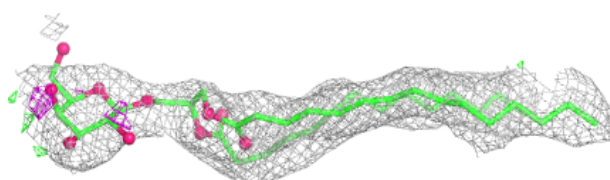
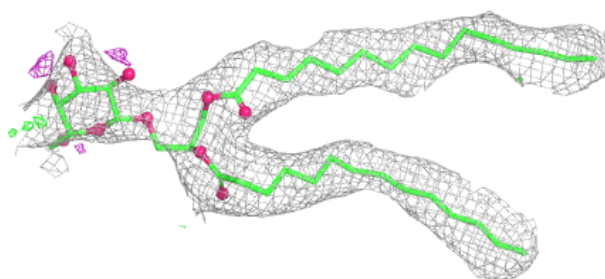
**Electron density around SQD b2 605:**

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



**Electron density around LMG B1 626:**

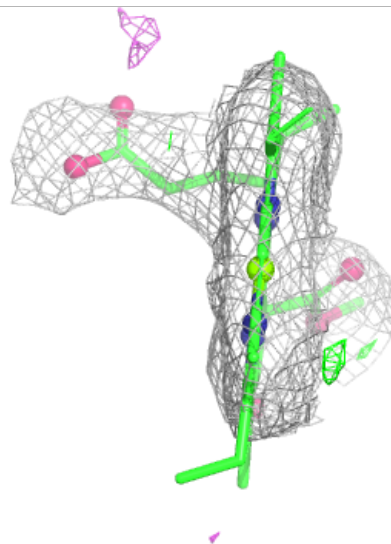
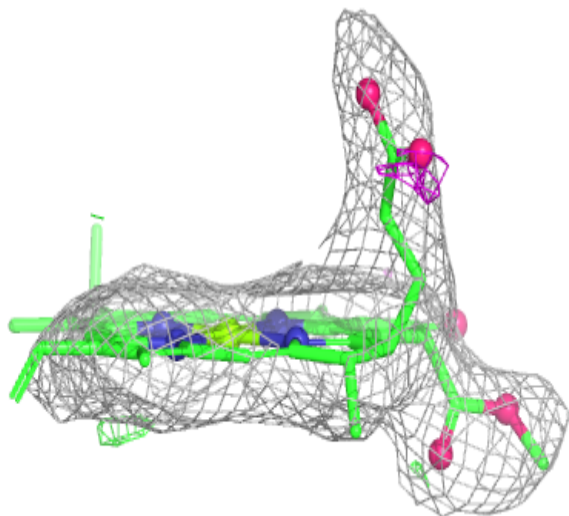
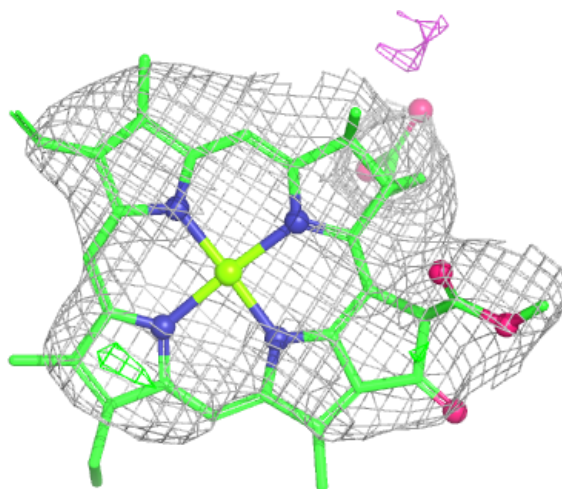
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





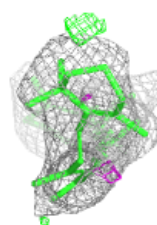
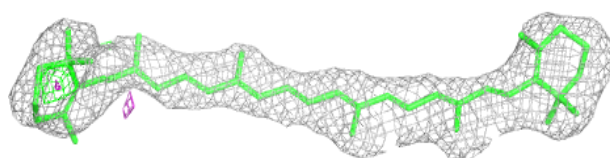
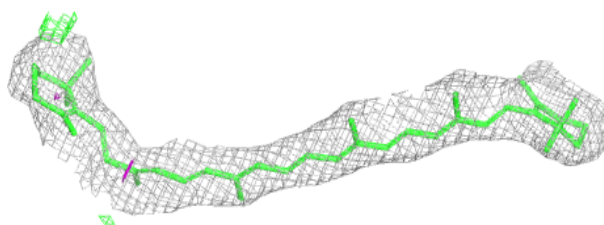
**Electron density around CLA C1 514:**

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

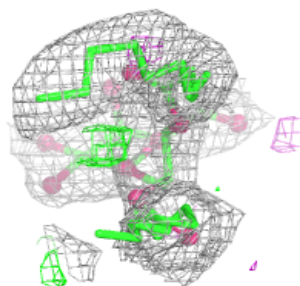
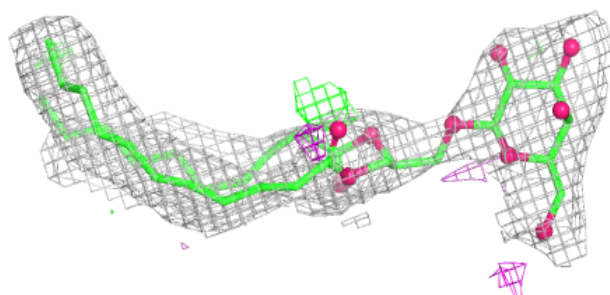
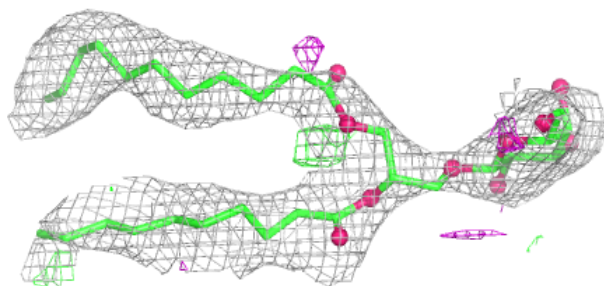


**Electron density around BCR B2 602:**

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

**Electron density around LMG B2 620:**

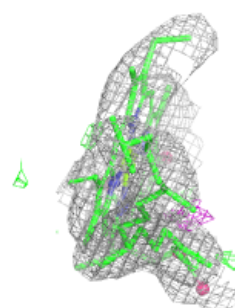
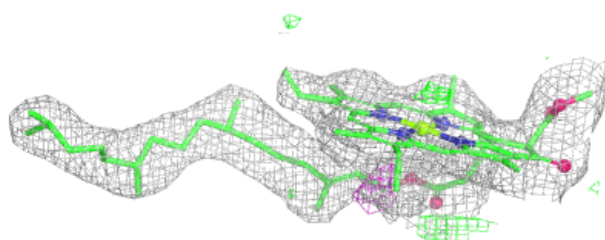
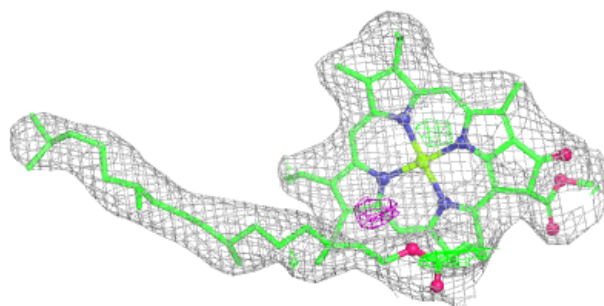
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



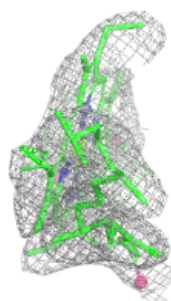
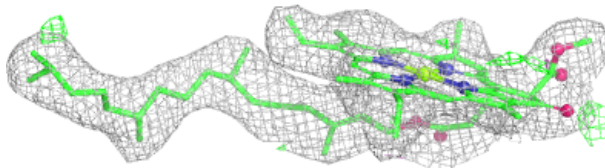
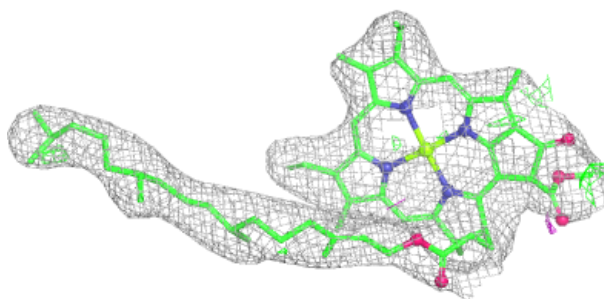


**Electron density around CLA c1 503:**

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

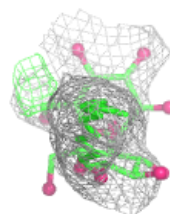
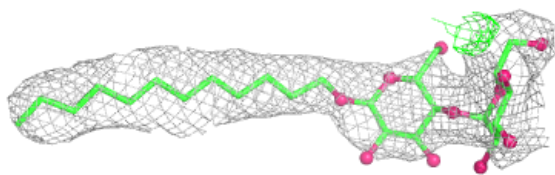
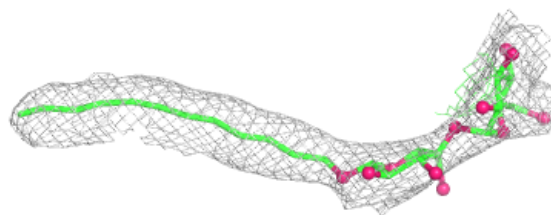
**Electron density around CLA C1 502:**

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



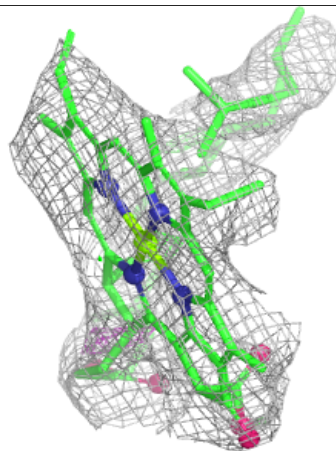
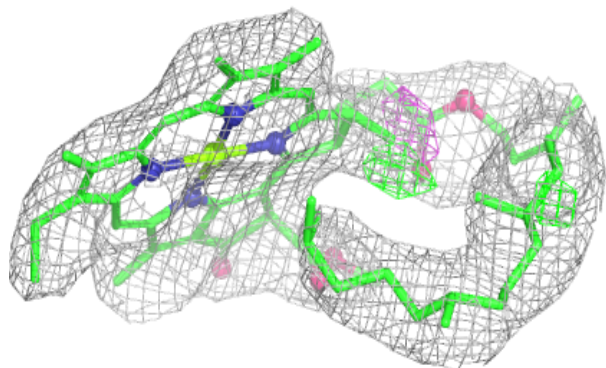
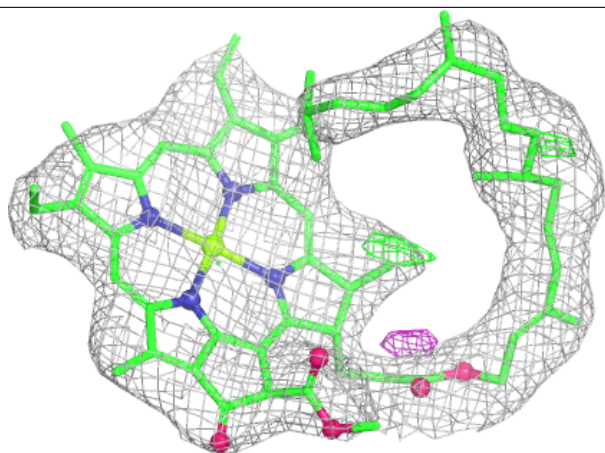
**Electron density around LMT b2 623:**

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

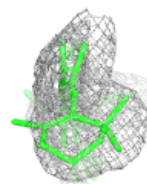
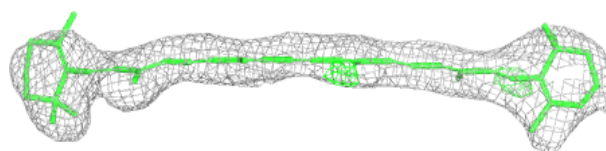
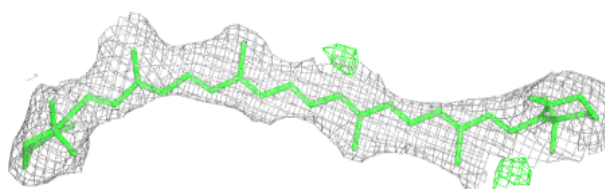


**Electron density around CLA b2 618:**

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

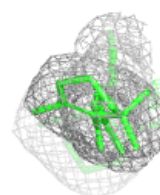
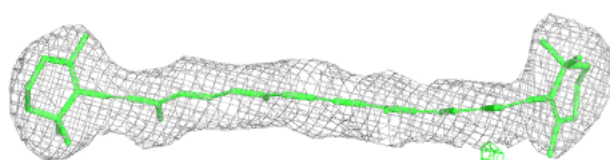
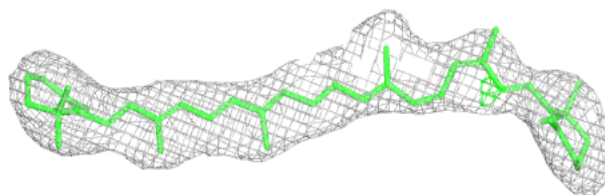
**Electron density around BCR h2 101:**

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

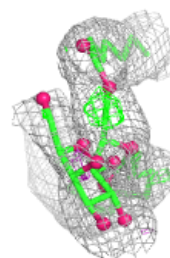
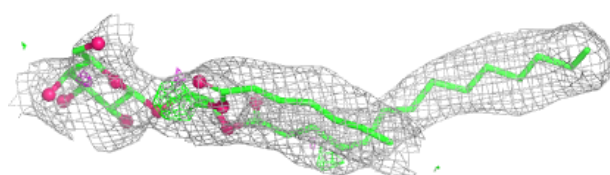
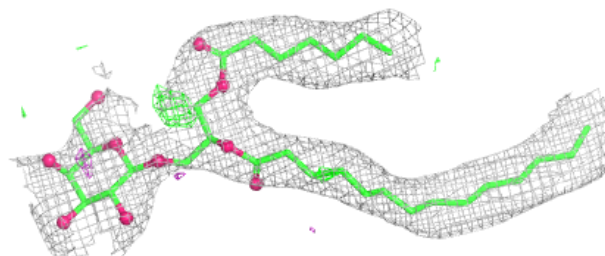


**Electron density around BCR c1 502:**

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

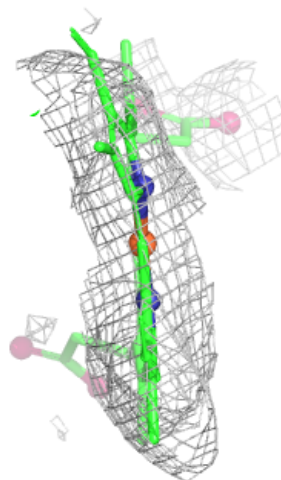
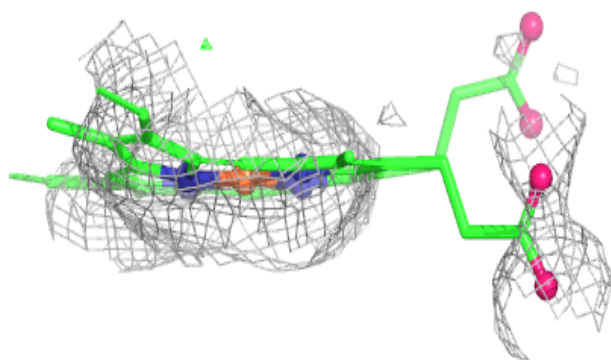
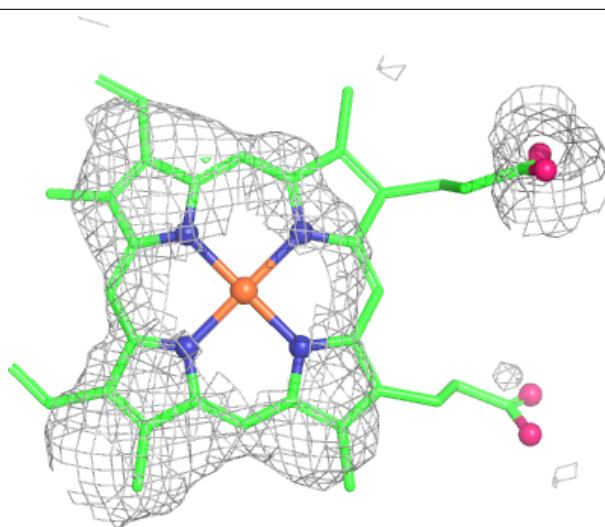
**Electron density around LMG b1 631:**

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



**Electron density around HEM E1 101:**

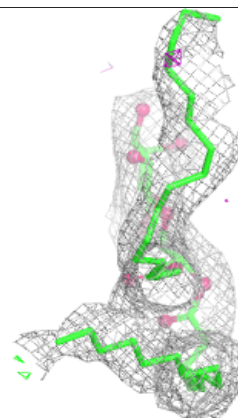
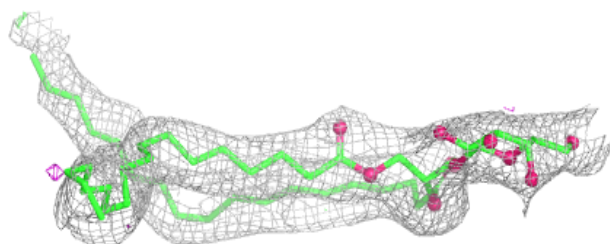
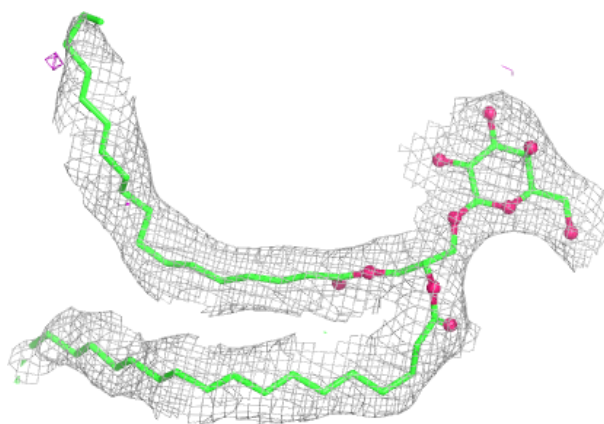
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



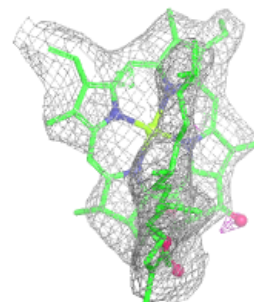
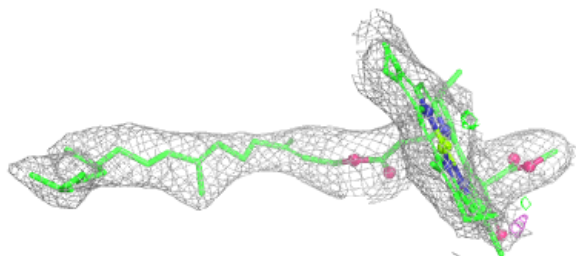
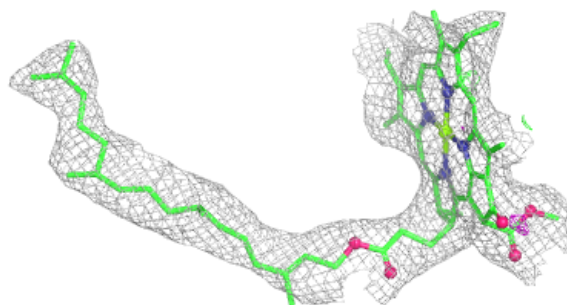


**Electron density around LMG c1 519:**

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

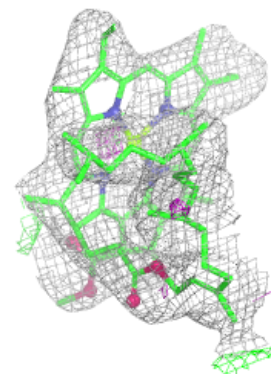
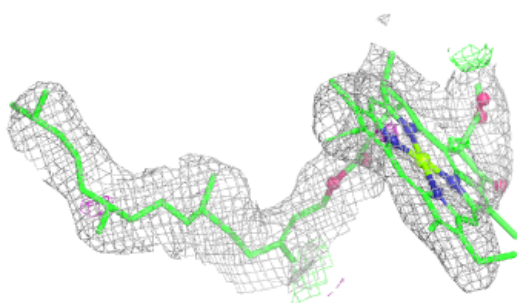
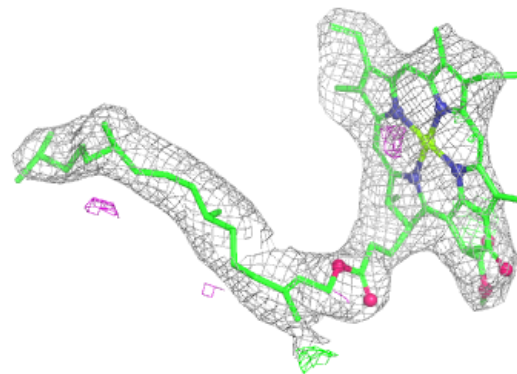
**Electron density around CLA B2 611:**

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

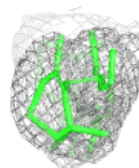
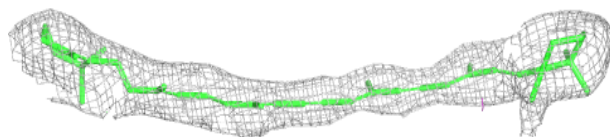
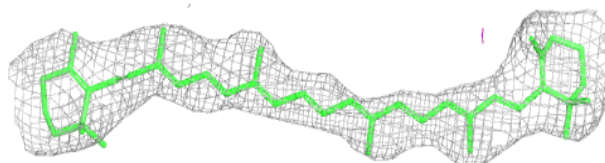


**Electron density around CLA c2 512:**

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

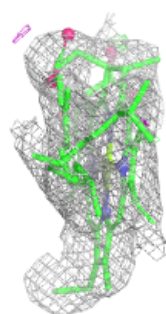
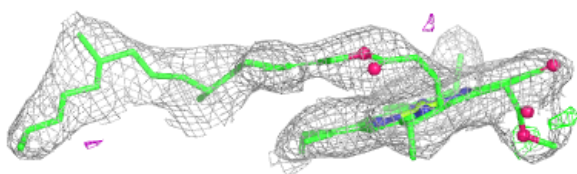
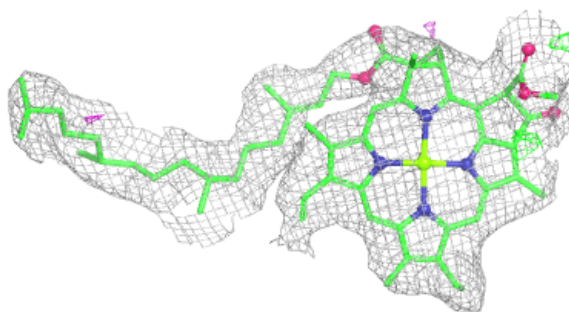
**Electron density around BCR d2 401:**

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

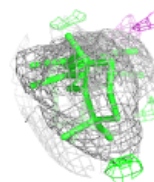
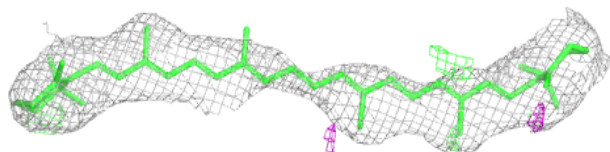
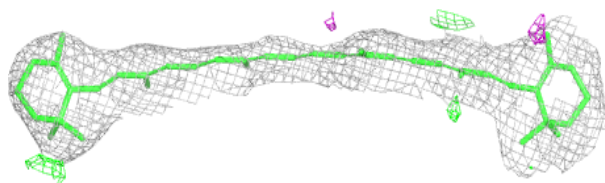


**Electron density around CLA B2 606:**

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

**Electron density around BCR k2 501:**

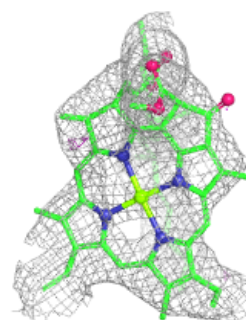
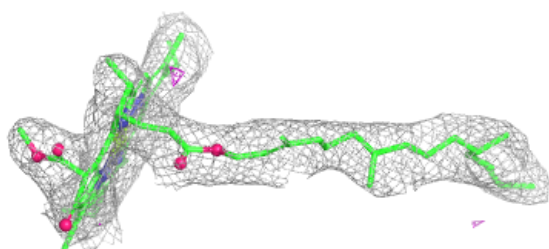
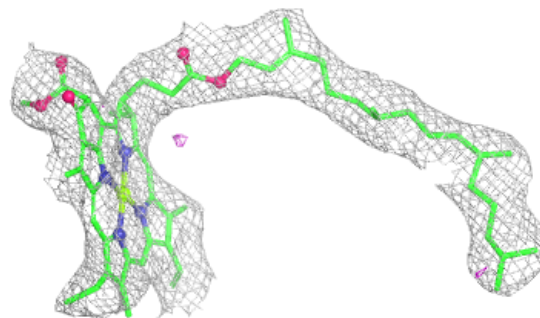
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



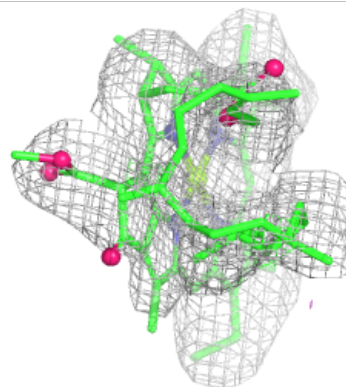
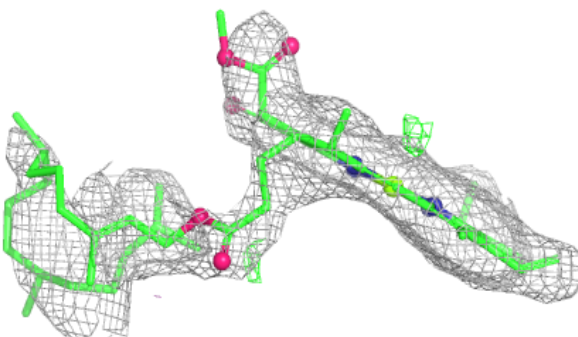
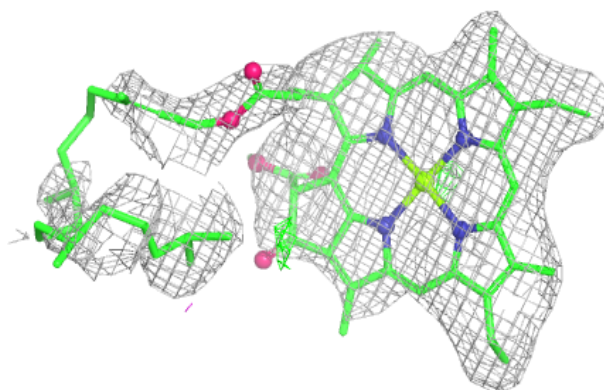


**Electron density around CLA b2 610:**

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

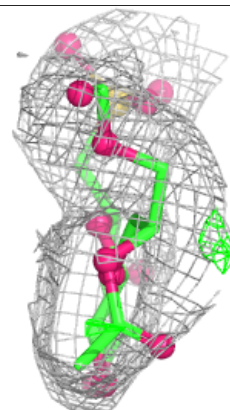
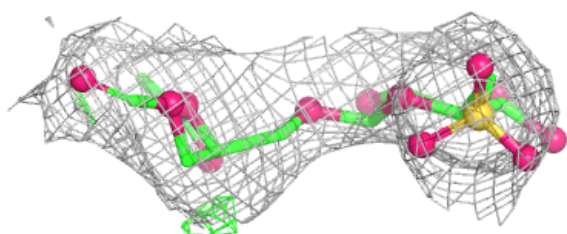
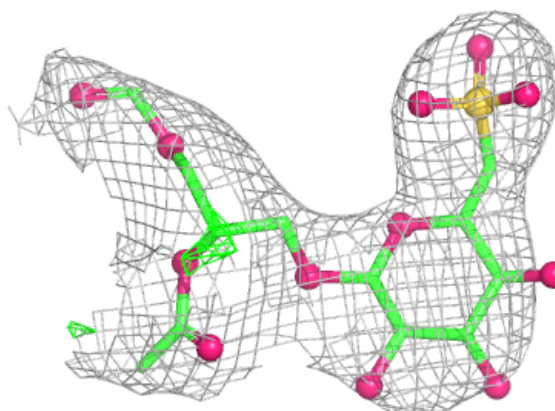
**Electron density around CLA b1 604:**

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

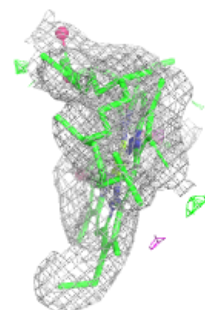
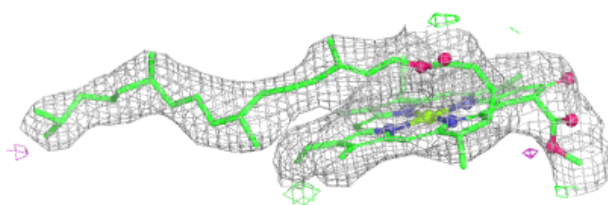
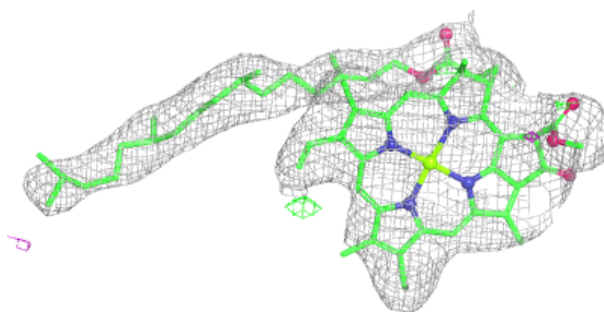


**Electron density around SQD D2 402:**

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

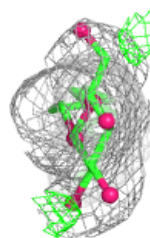
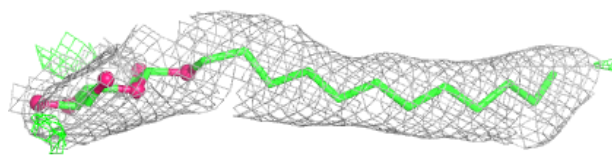
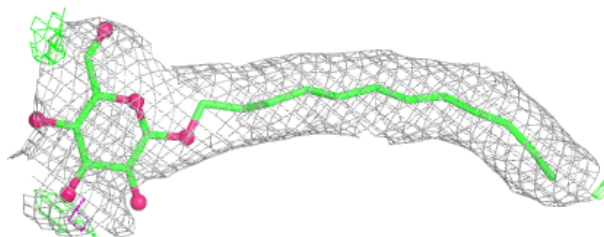
**Electron density around CLA c2 502:**

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



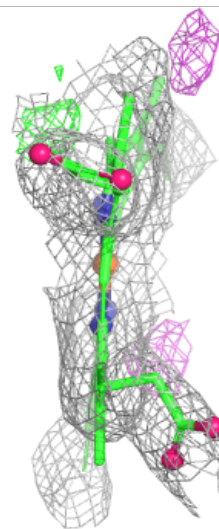
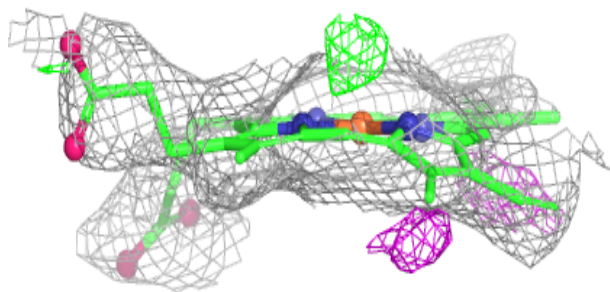
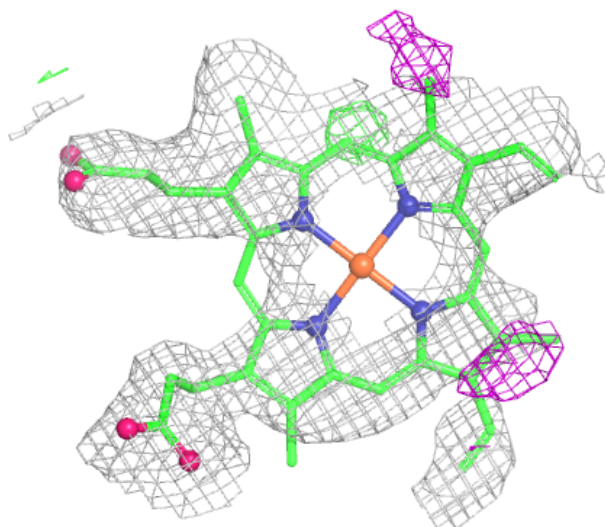
**Electron density around LMT 11 101:**

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



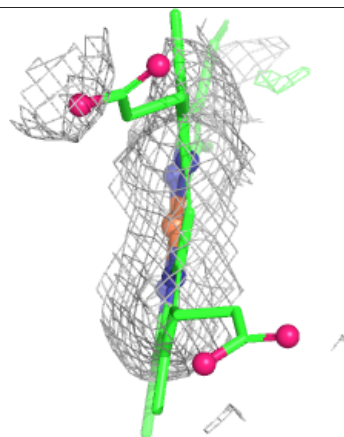
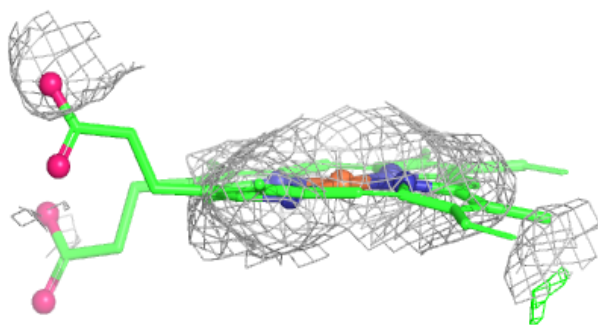
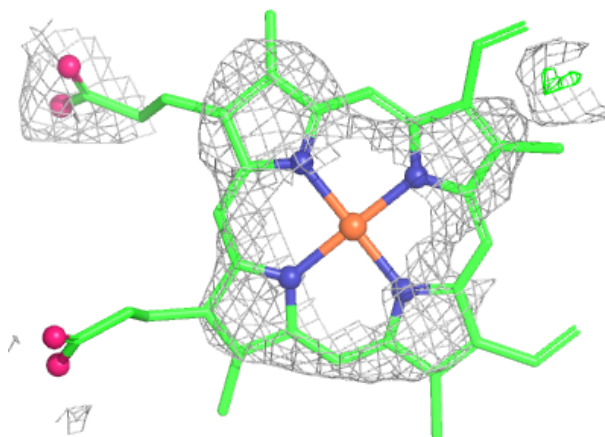
**Electron density around HEM V2 201:**

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



**Electron density around HEM e2 101:**

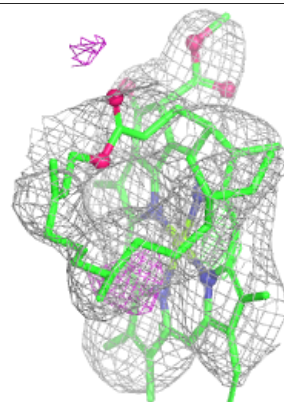
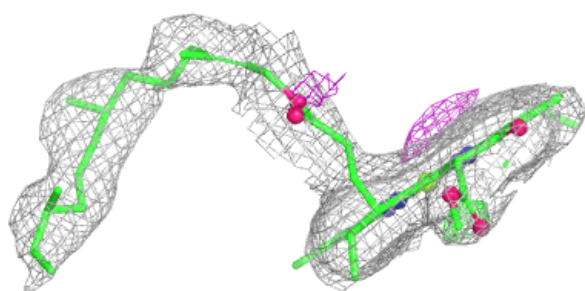
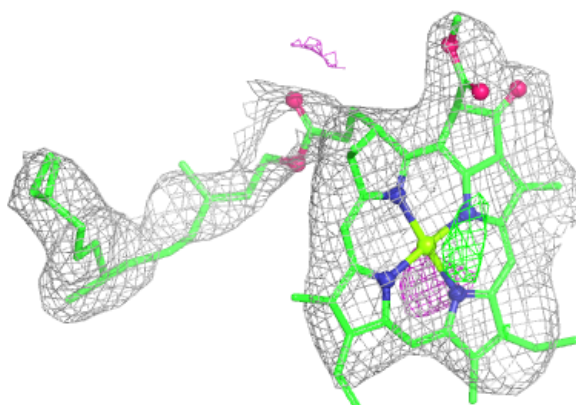
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



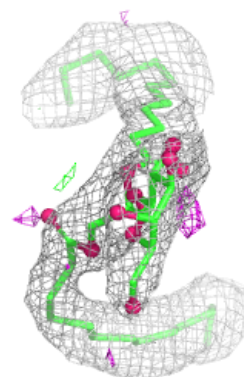
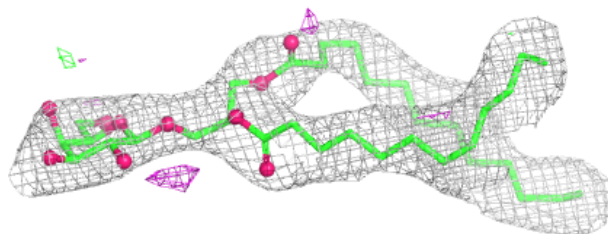
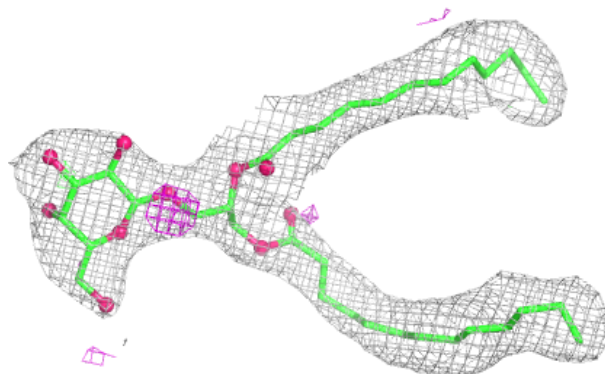


**Electron density around CLA A2 403:**

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

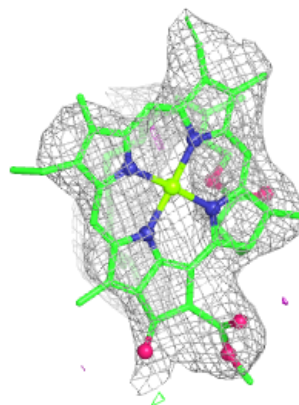
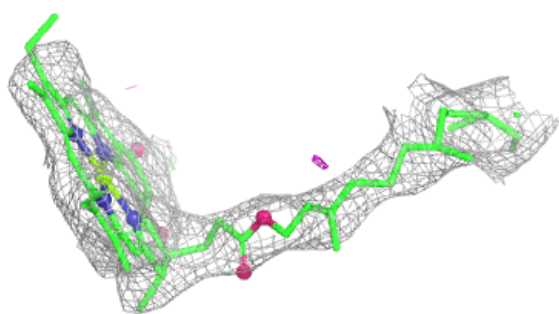
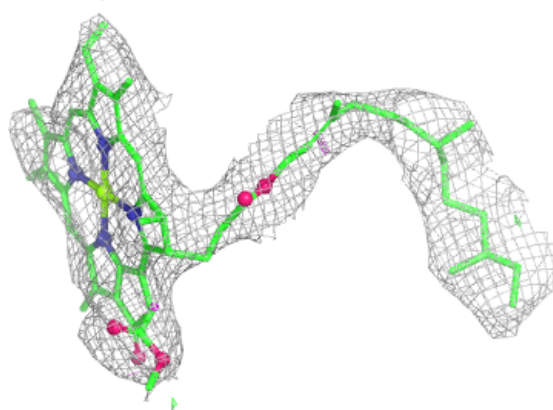
**Electron density around LMG a2 412:**

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



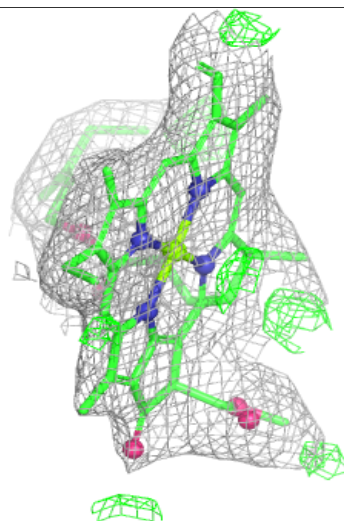
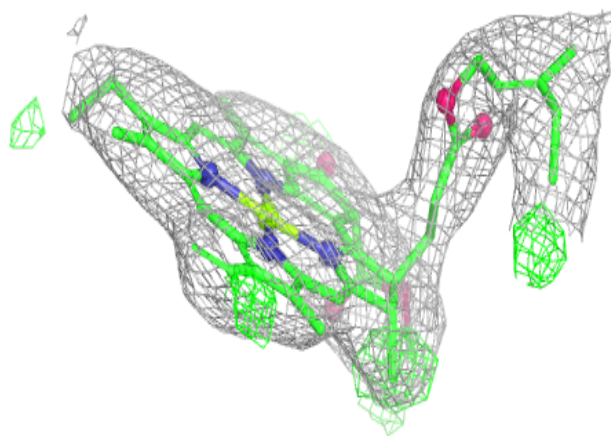
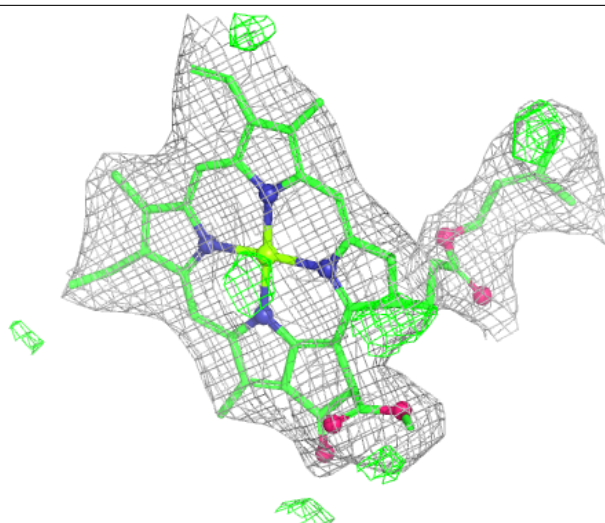
**Electron density around CLA b2 609:**

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



**Electron density around CLA A2 404:**

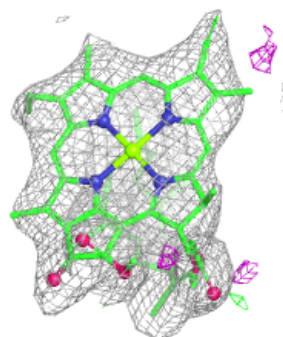
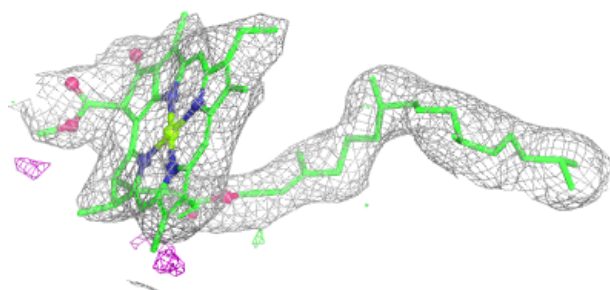
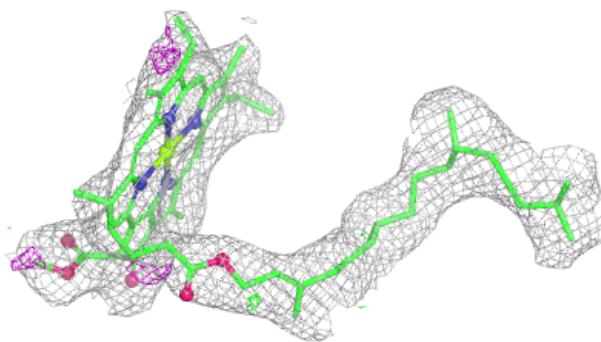
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



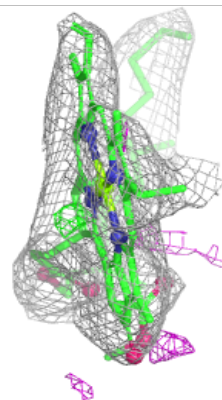
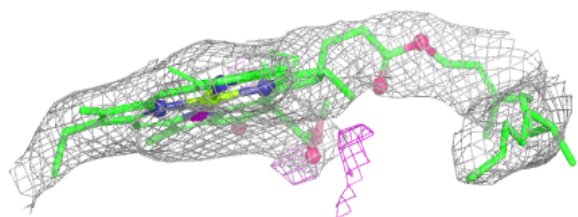
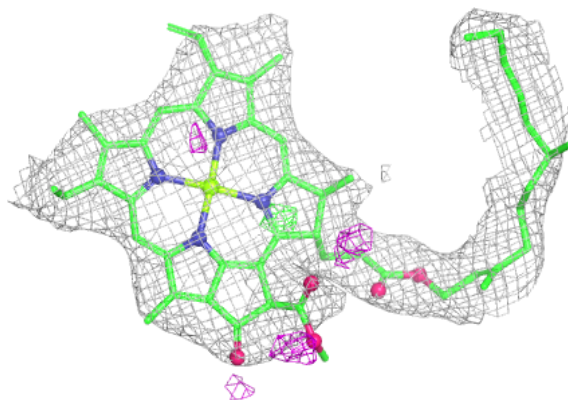


**Electron density around CLA C1 509:**

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

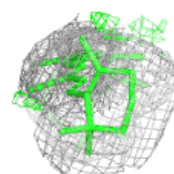
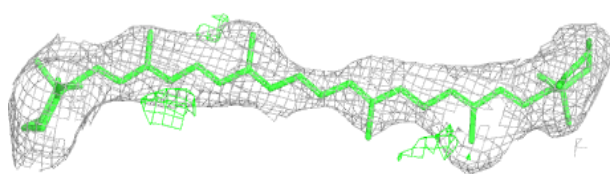
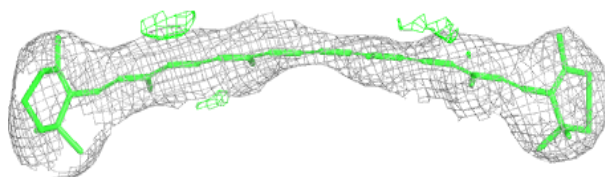
**Electron density around CLA b2 619:**

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

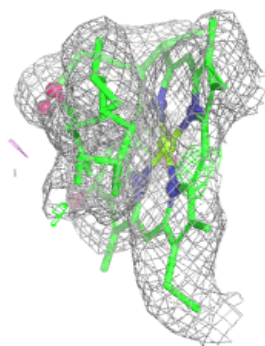
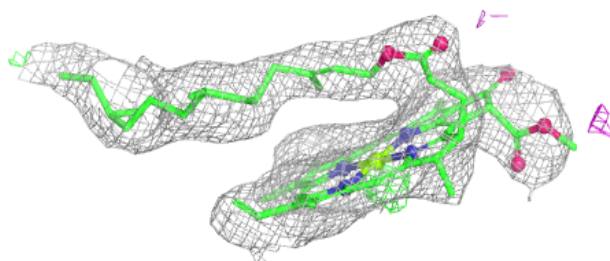
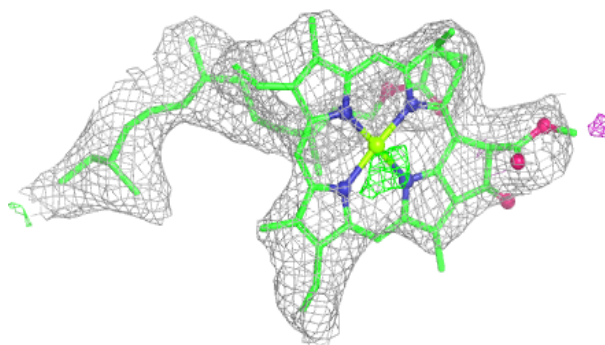


**Electron density around BCR c1 501:**

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

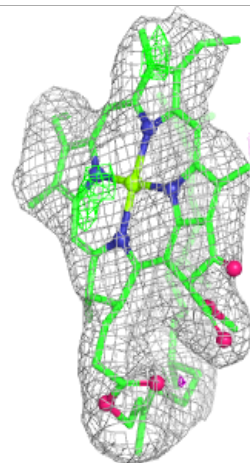
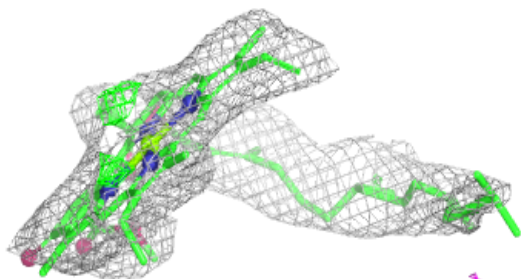
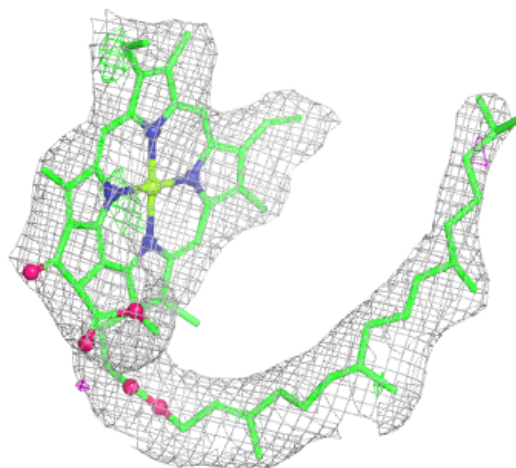
**Electron density around CLA c2 506:**

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



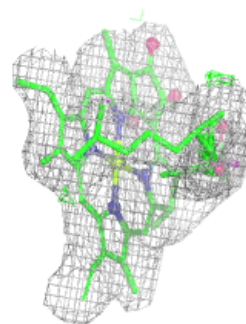
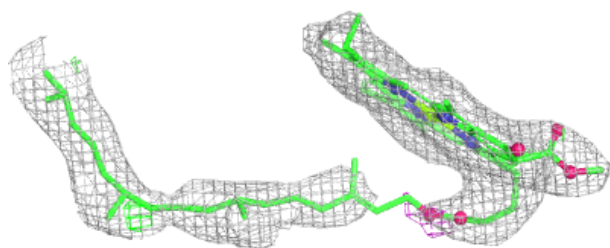
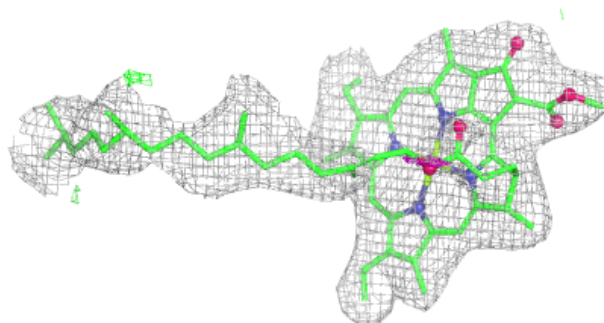
**Electron density around CLA c2 508:**

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



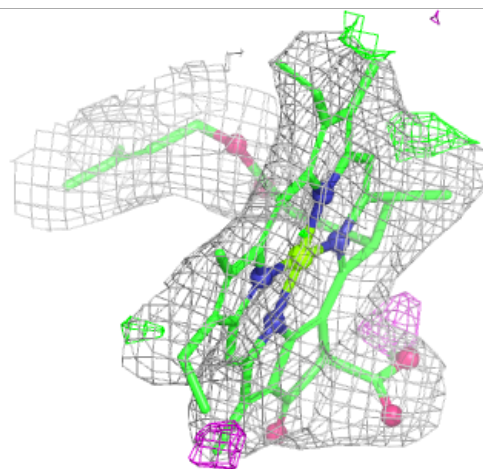
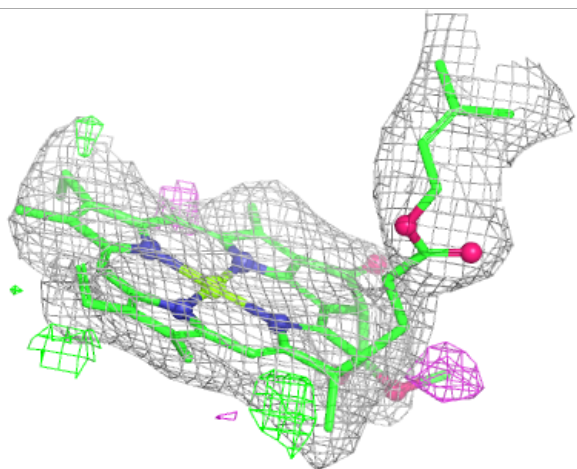
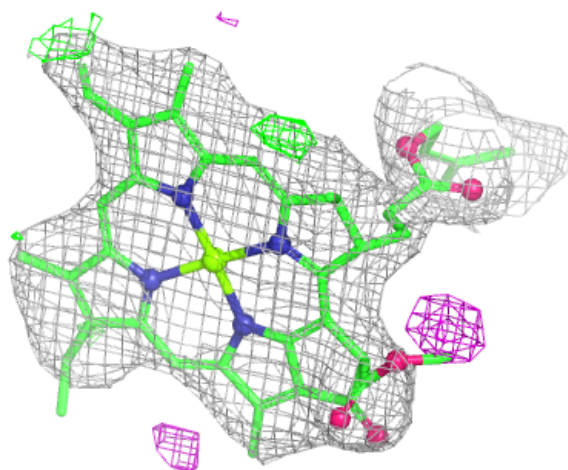
**Electron density around CLA B2 610:**

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



**Electron density around CLA c1 508:**

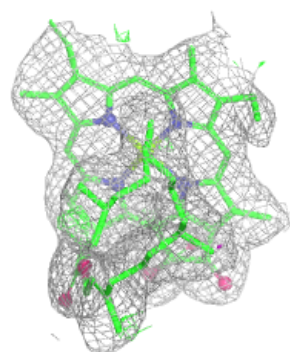
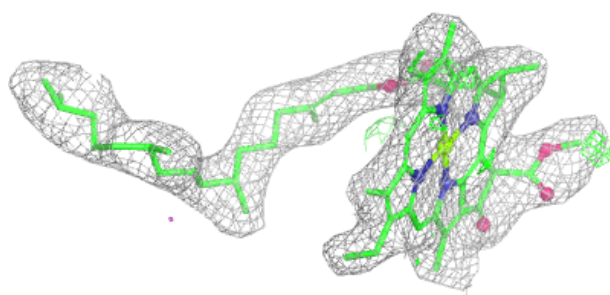
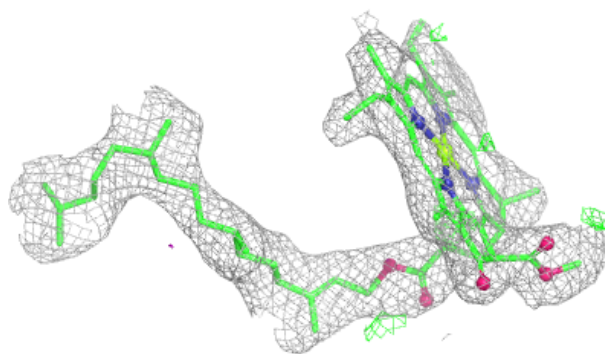
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



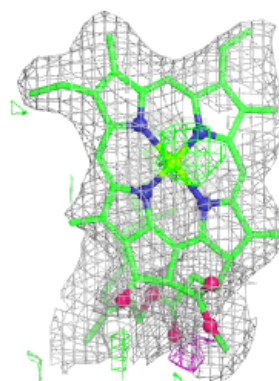
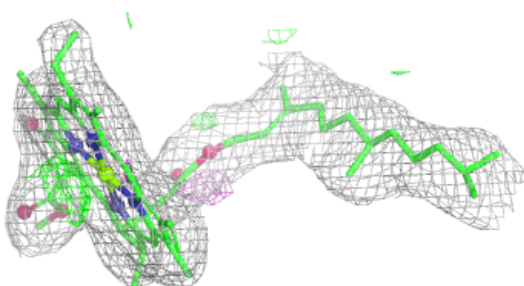
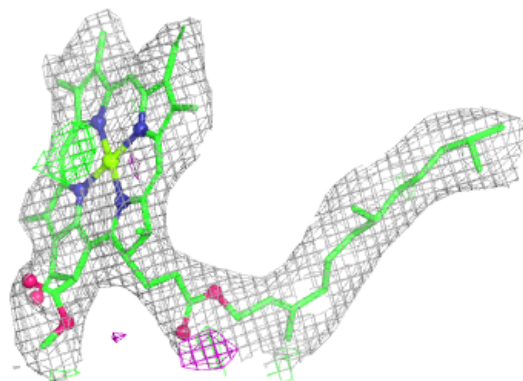


**Electron density around CLA c1 510:**

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

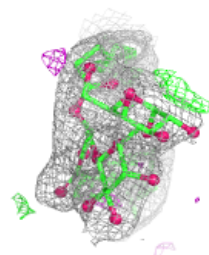
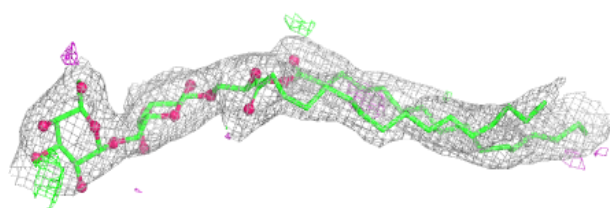
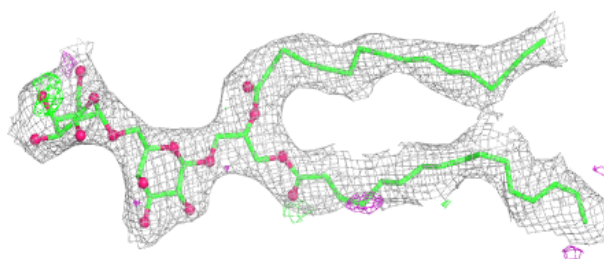
**Electron density around CLA c1 513:**

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

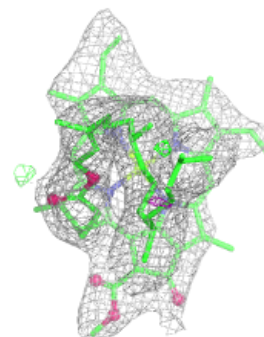
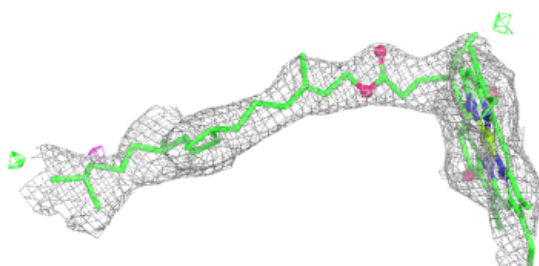
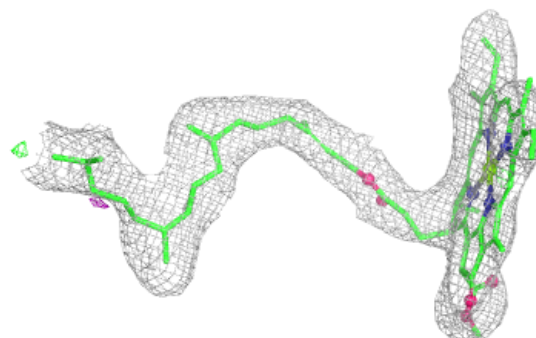


**Electron density around DGD c1 520:**

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

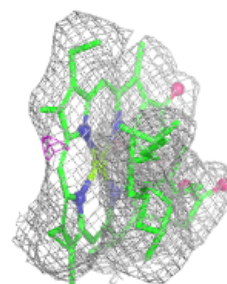
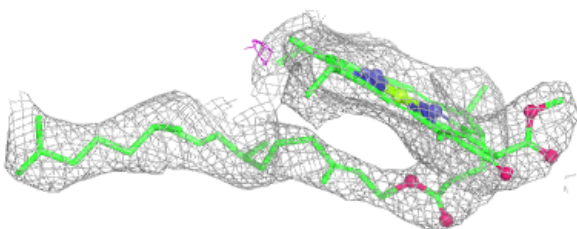
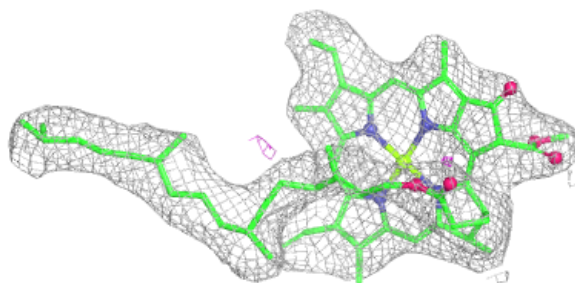
**Electron density around CLA B1 609:**

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



**Electron density around CLA C1 506:**

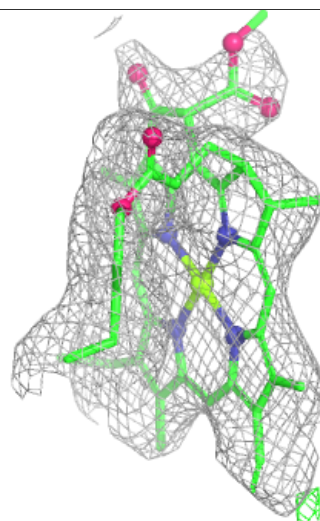
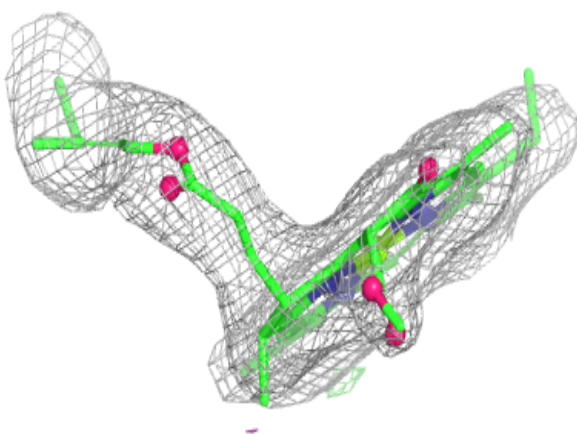
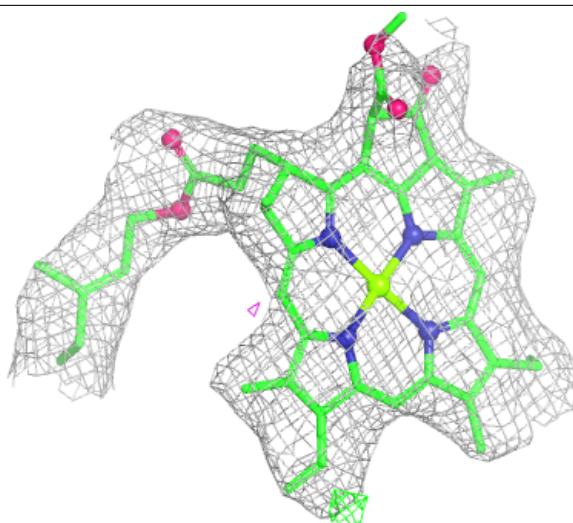
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





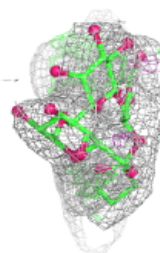
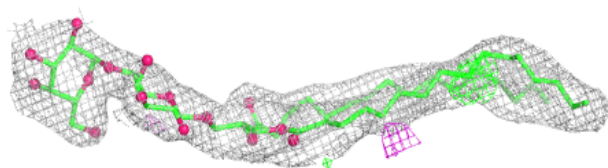
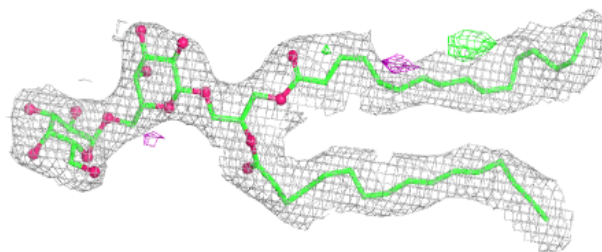
**Electron density around CLA D1 403:**

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



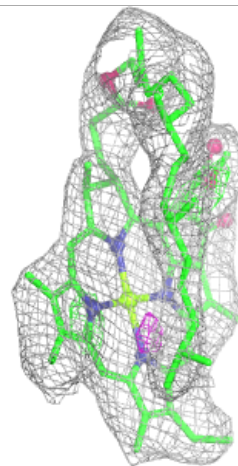
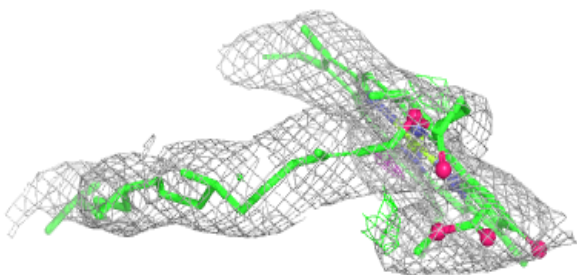
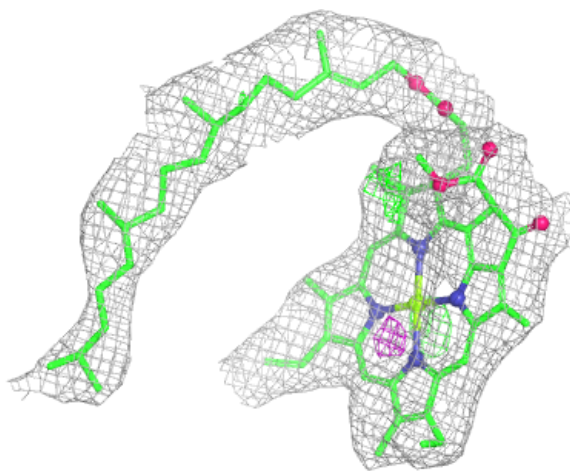
**Electron density around DGD c2 517:**

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



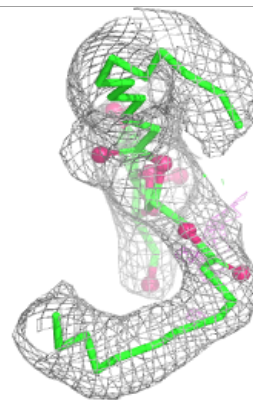
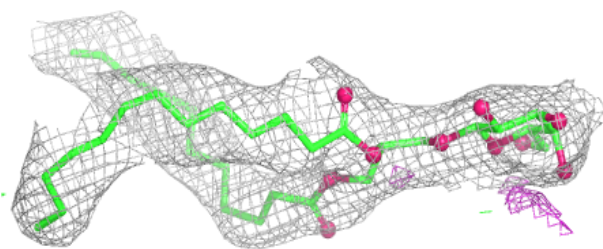
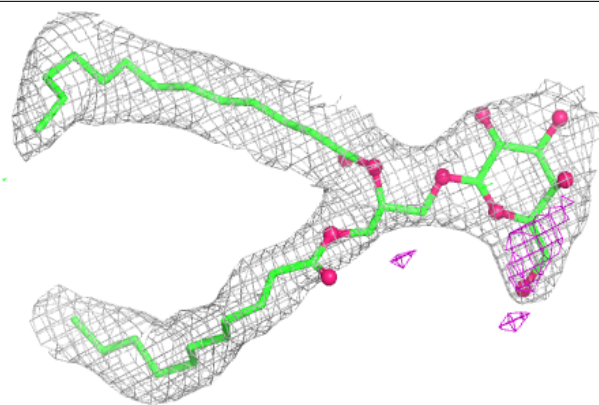
**Electron density around CLA c1 509:**

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

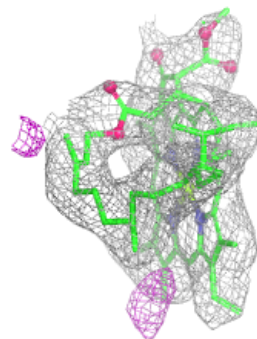
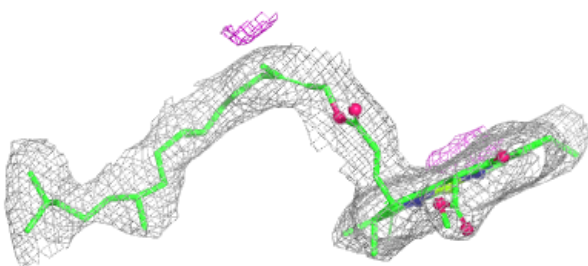
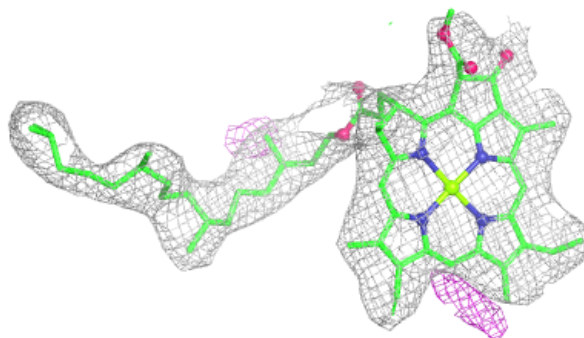


**Electron density around LMG A1 410:**

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

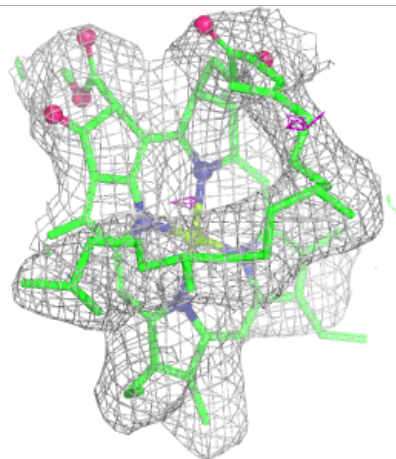
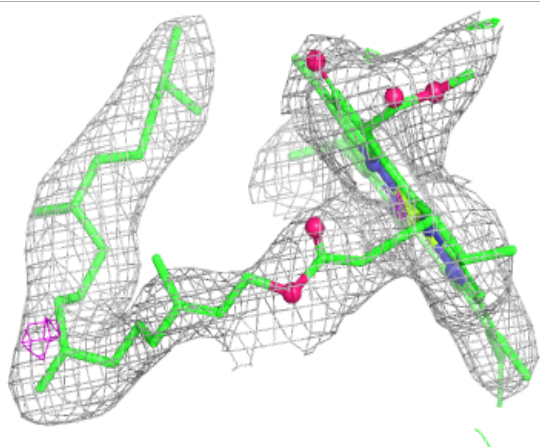
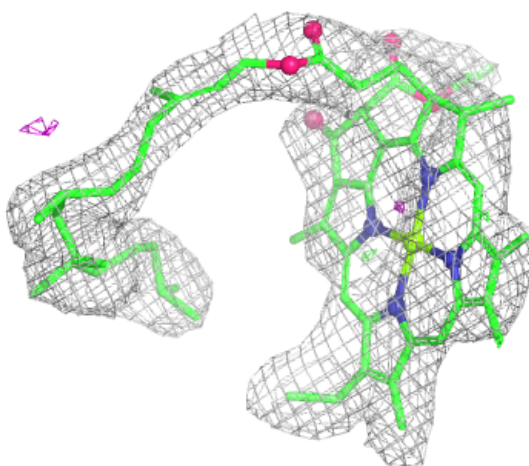
**Electron density around CLA a2 405:**

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



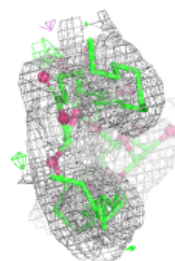
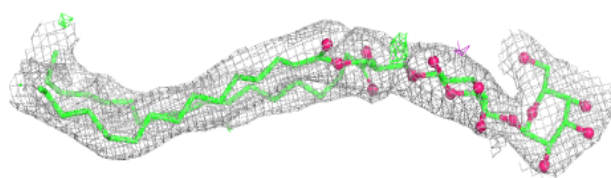
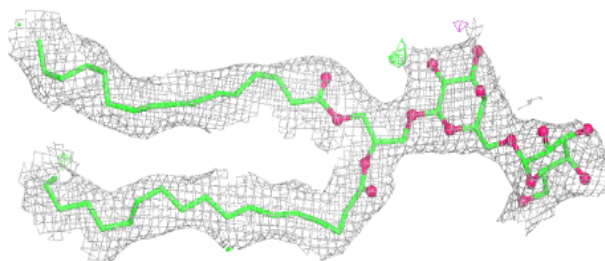
**Electron density around CLA c1 505:**

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



**Electron density around DGD C1 517:**

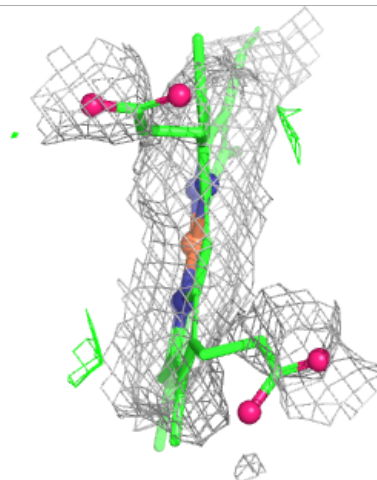
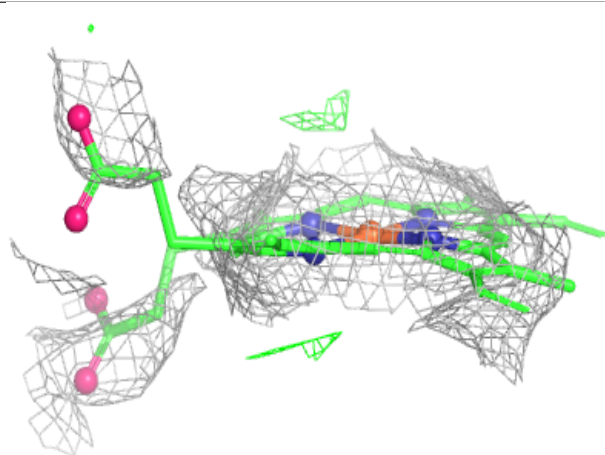
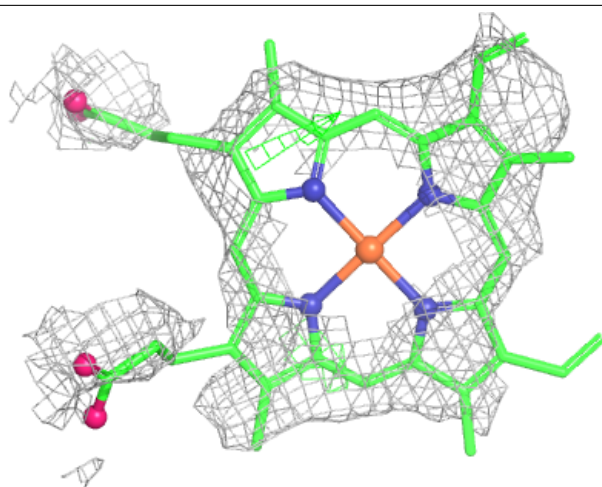
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





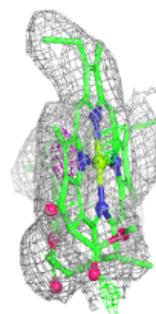
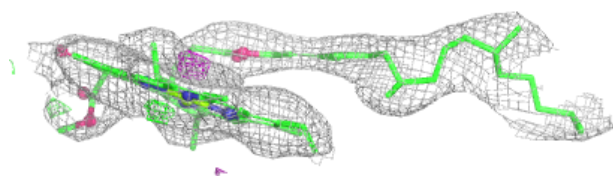
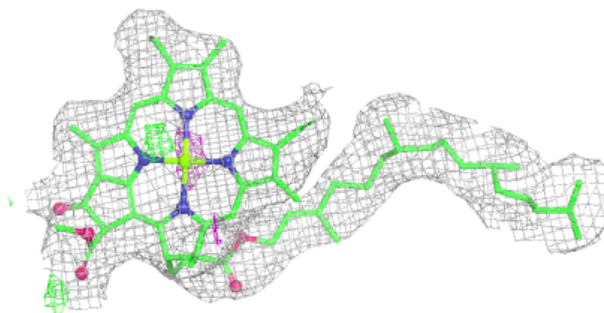
**Electron density around HEM E2 101:**

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

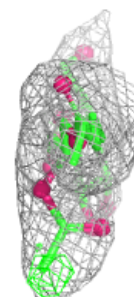
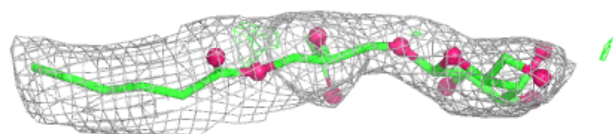
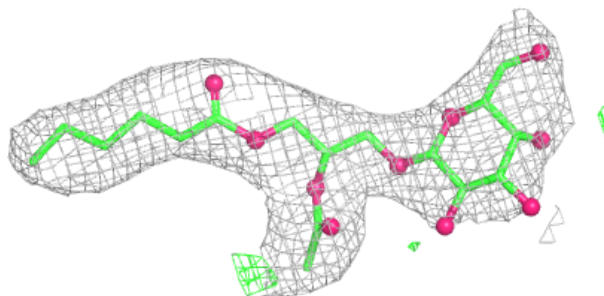


**Electron density around CLA B1 606:**

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

**Electron density around LMG d2 407:**

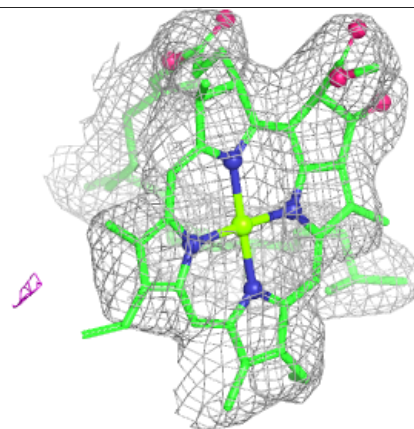
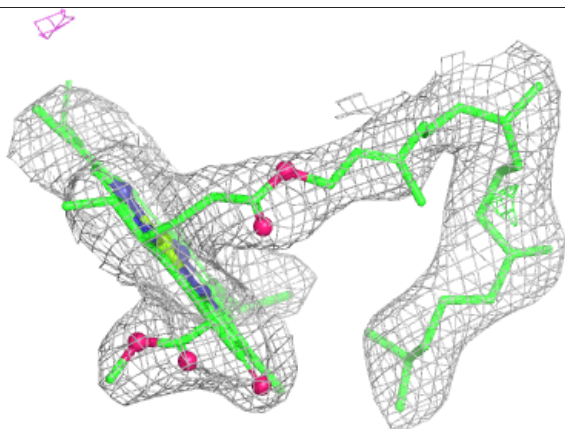
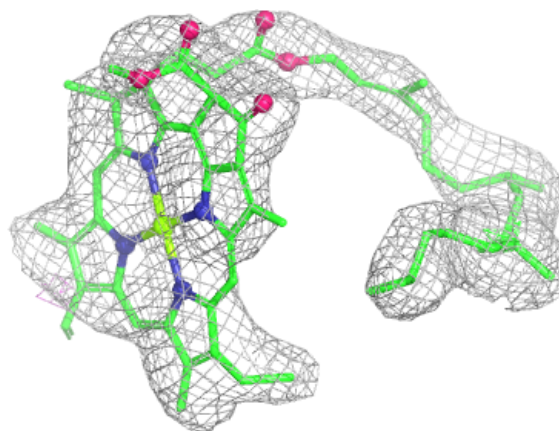
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





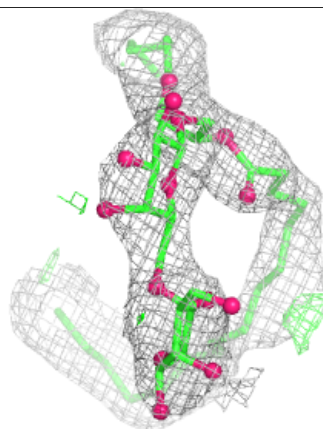
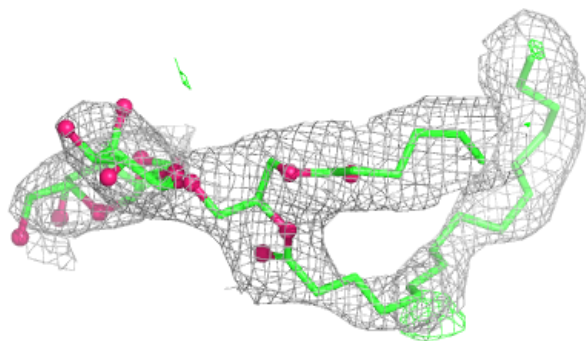
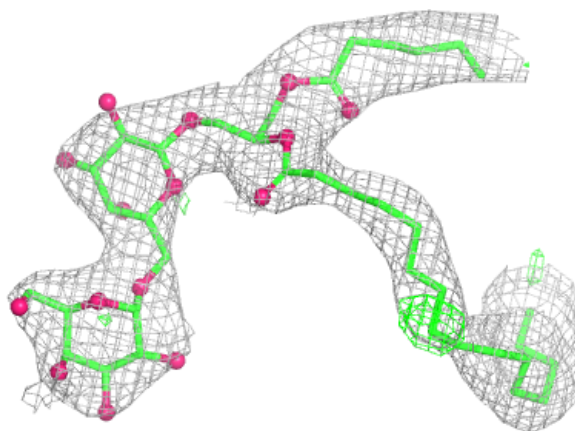
**Electron density around CLA c2 504:**

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

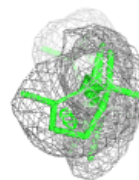
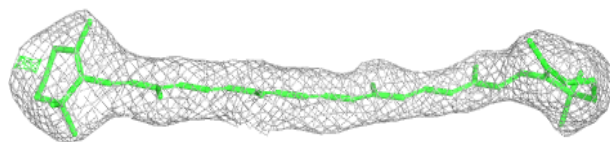
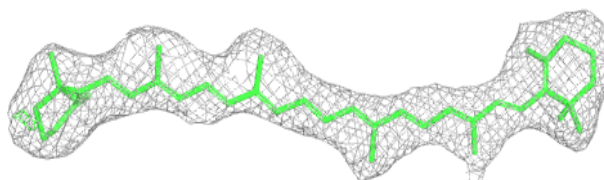


**Electron density around DGD c2 516:**

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

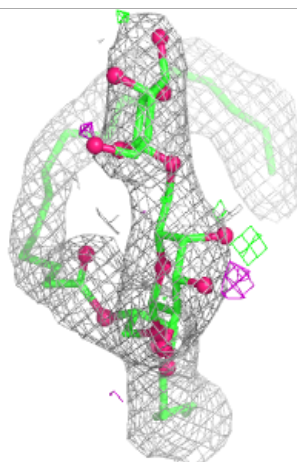
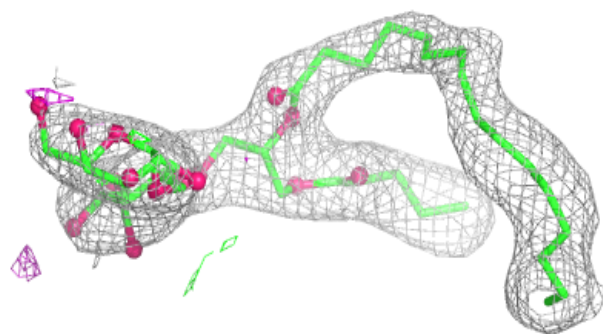
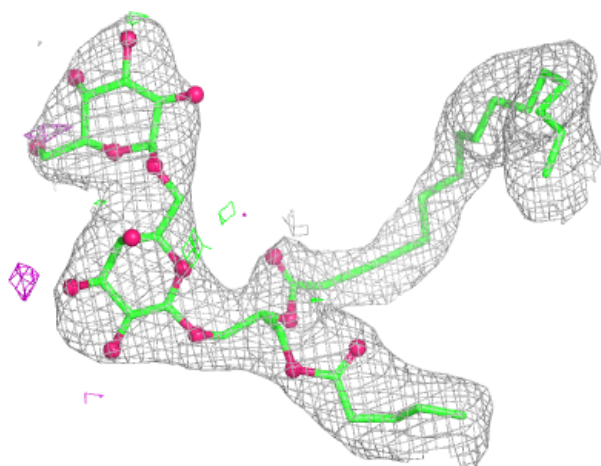
**Electron density around BCR b2 601:**

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



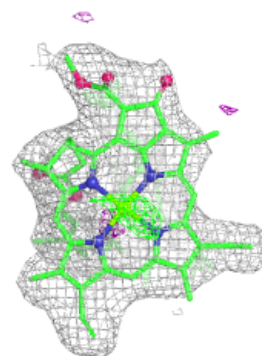
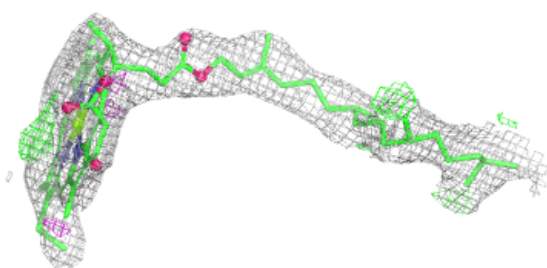
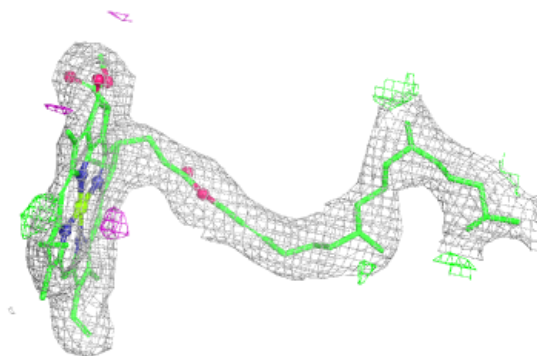
**Electron density around DGD c1 514:**

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

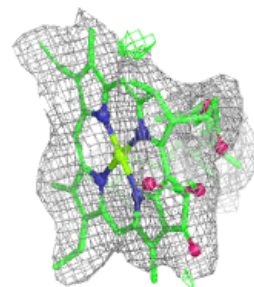
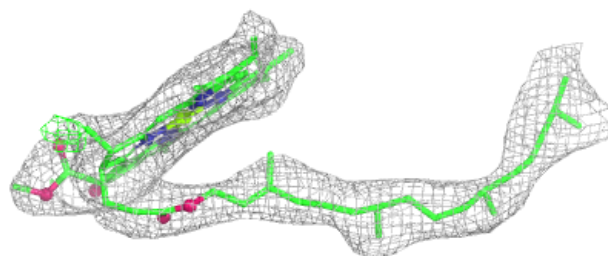
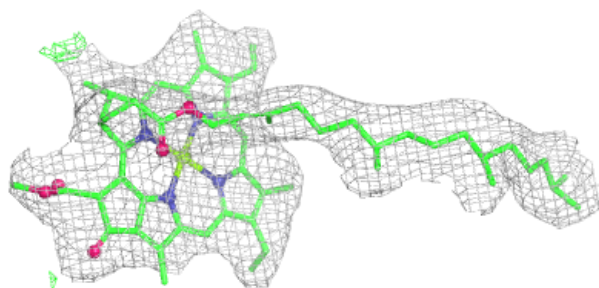


**Electron density around CLA b1 609:**

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

**Electron density around CLA b2 624:**

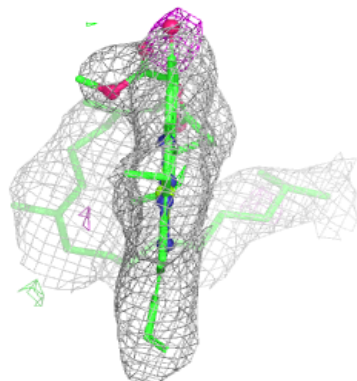
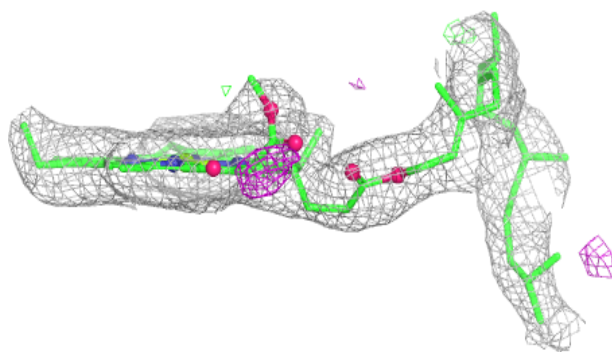
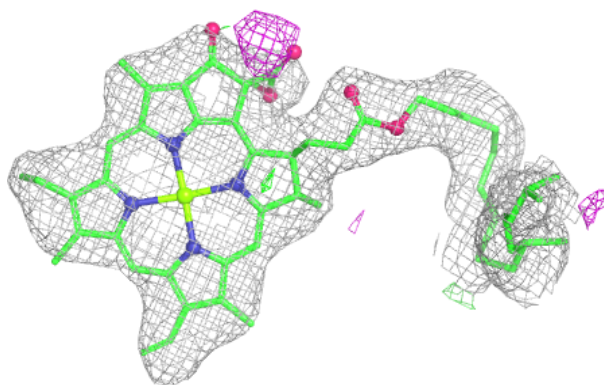
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



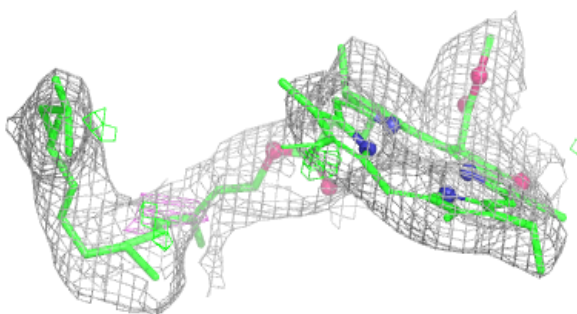
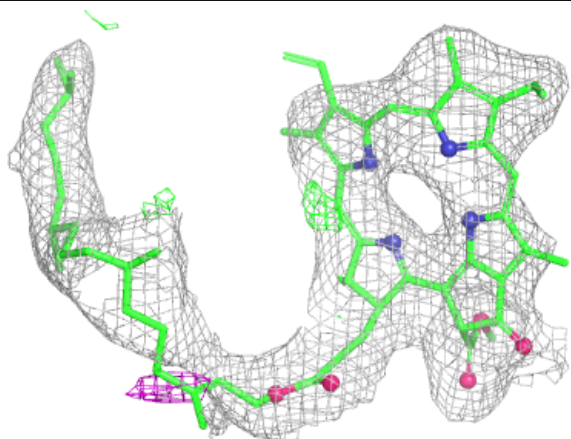


**Electron density around CLA b1 619:**

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

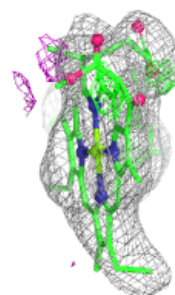
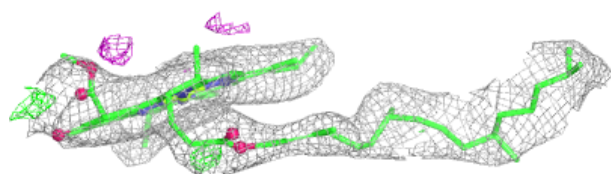
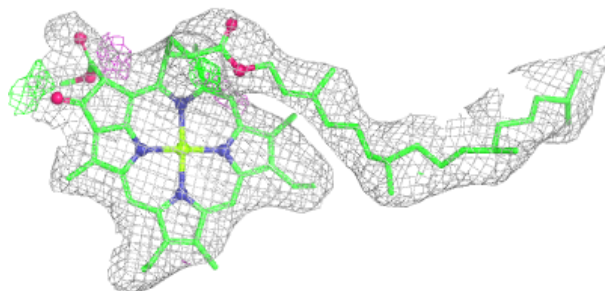
**Electron density around PHO D2 407:**

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



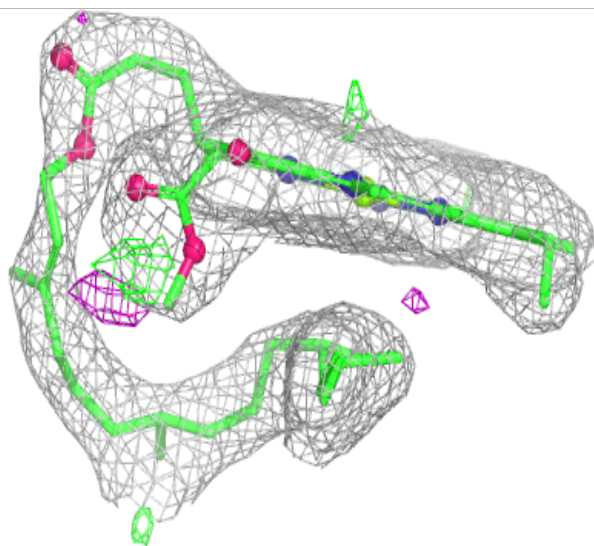
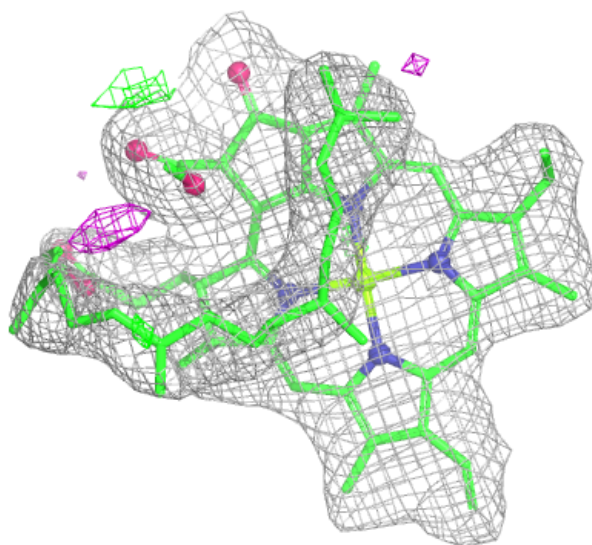
**Electron density around CLA b2 606:**

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



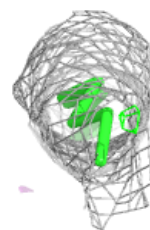
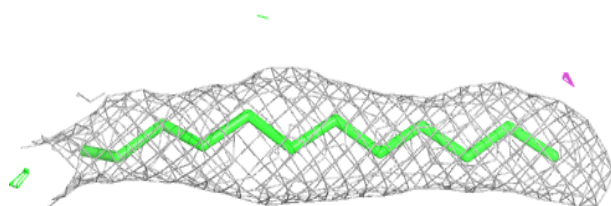
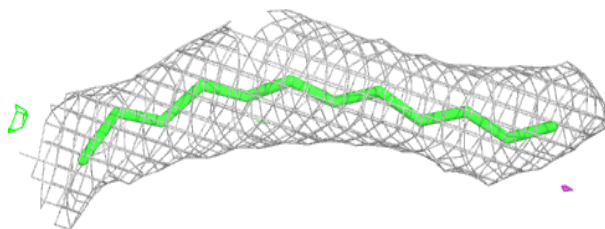
**Electron density around CLA C1 511:**

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

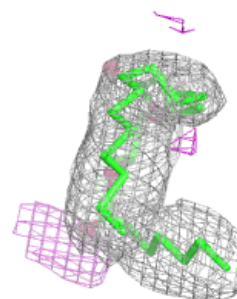
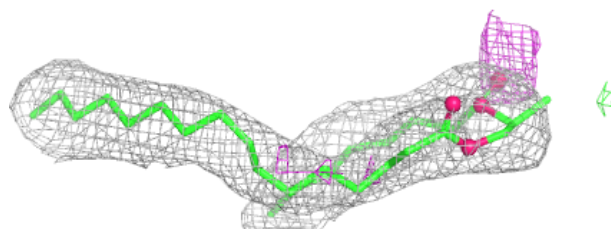
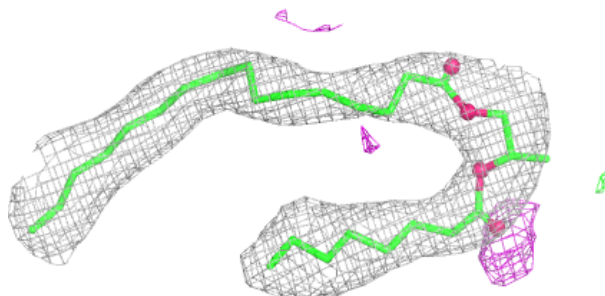


**Electron density around LMT L1 102:**

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

**Electron density around LMG M1 101:**

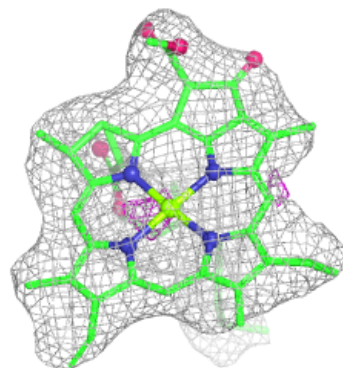
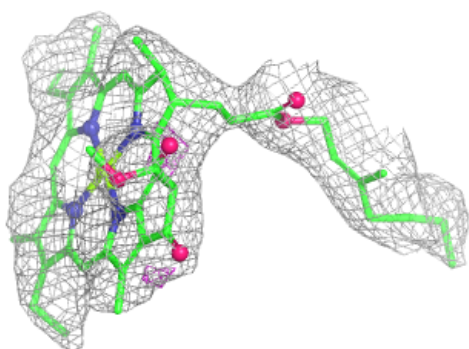
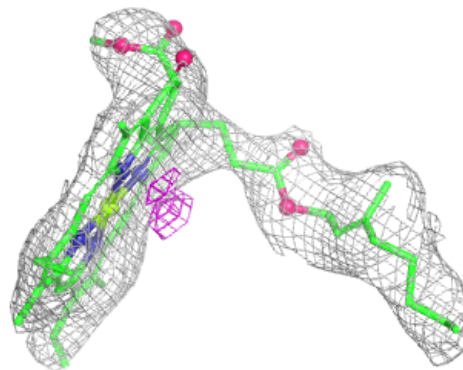
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



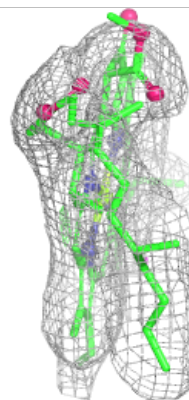
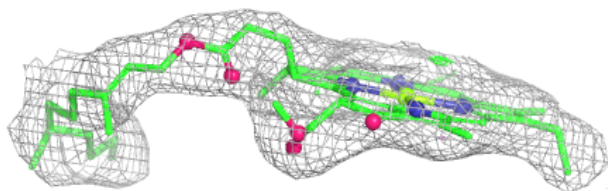
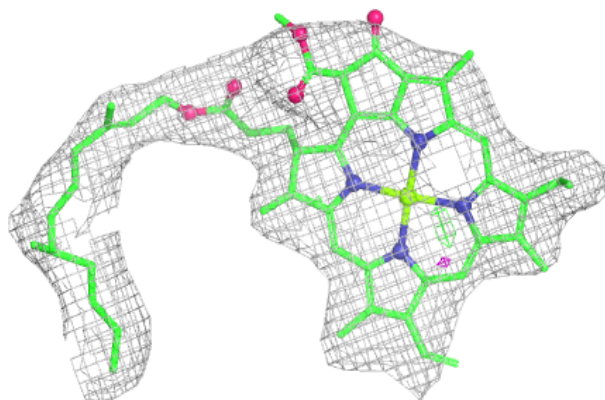


**Electron density around CLA c2 507:**

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

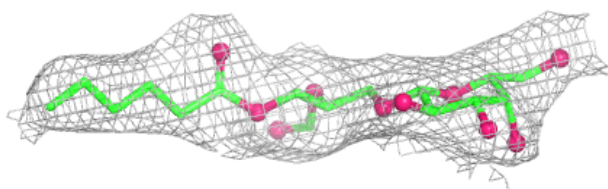
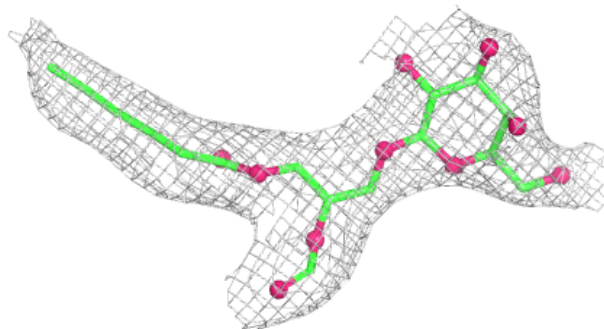
**Electron density around CLA B1 618:**

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

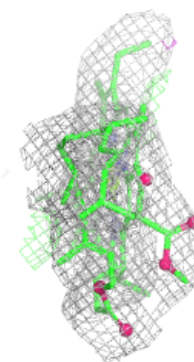
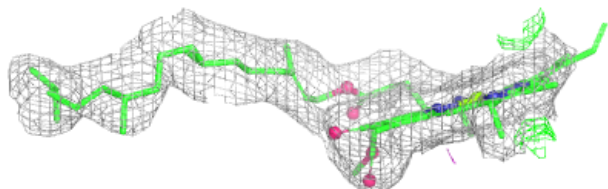
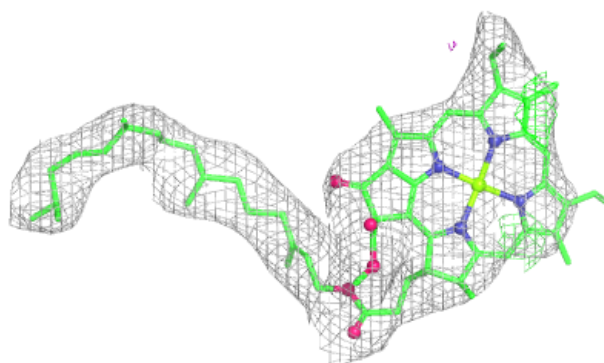


**Electron density around LMG c2 519:**

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

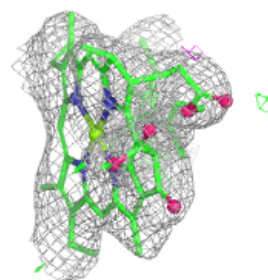
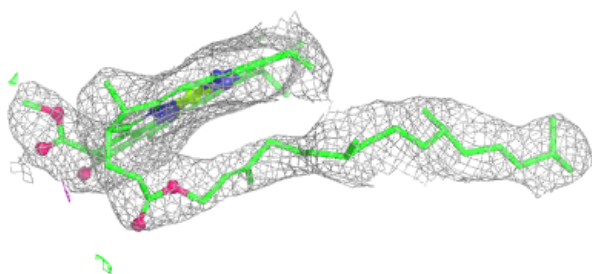
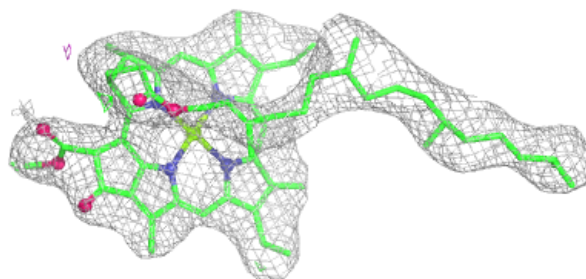
**Electron density around CLA b2 613:**

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

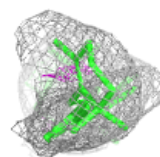
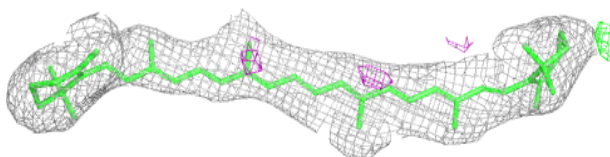
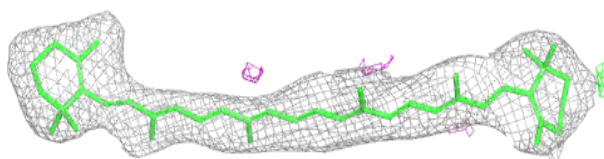


**Electron density around CLA c1 507:**

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

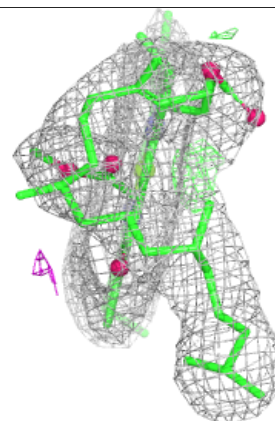
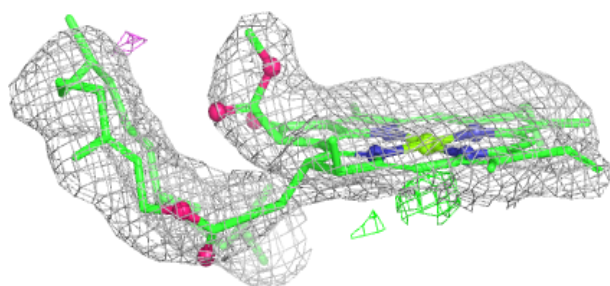
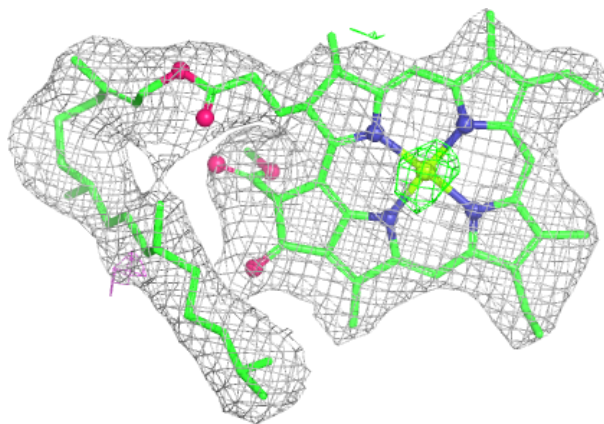
**Electron density around BCR B2 603:**

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



**Electron density around CLA B2 612:**

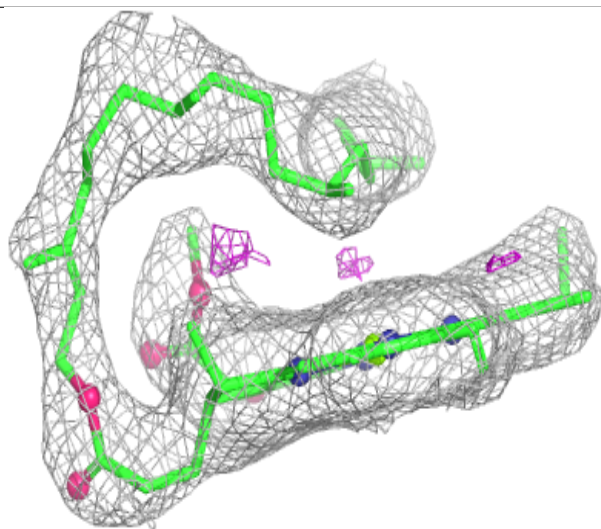
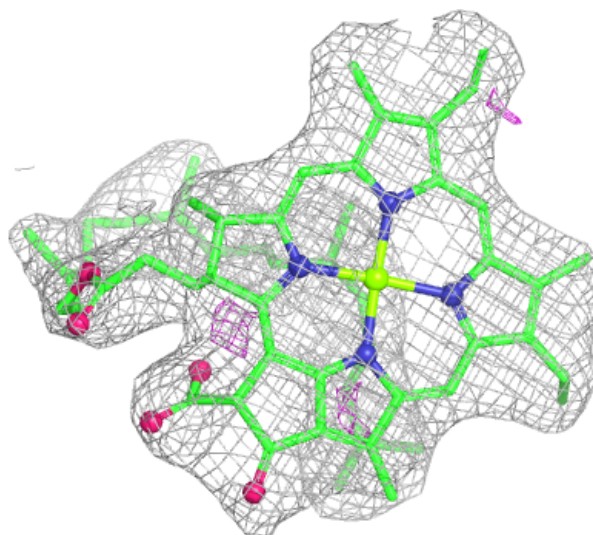
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





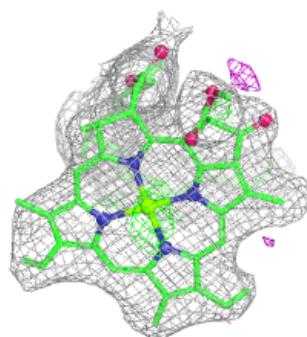
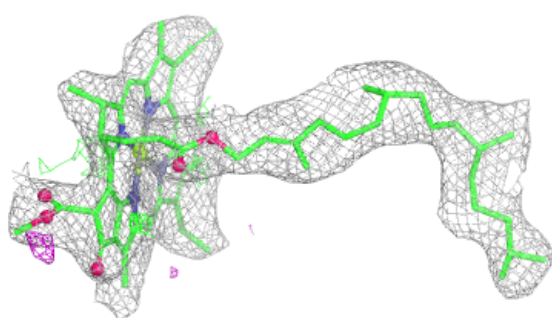
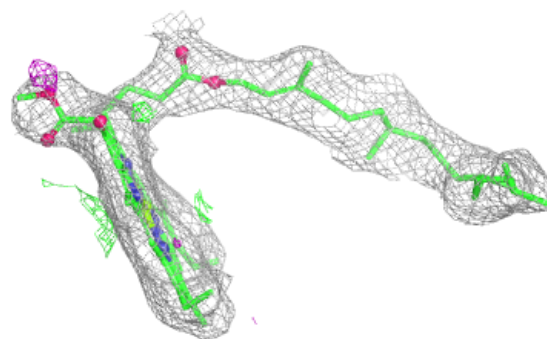
**Electron density around CLA c2 511:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

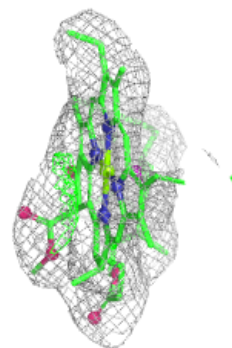
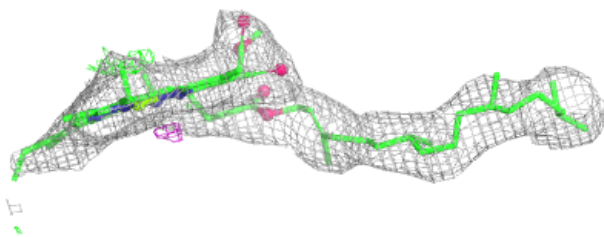
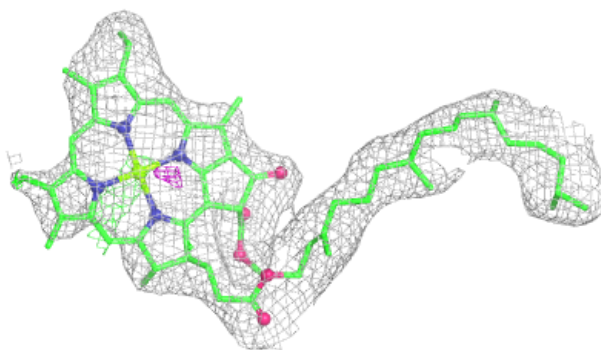


**Electron density around CLA B2 619:**

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

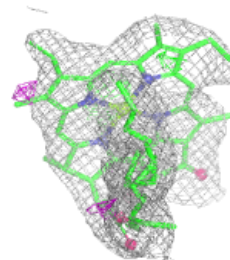
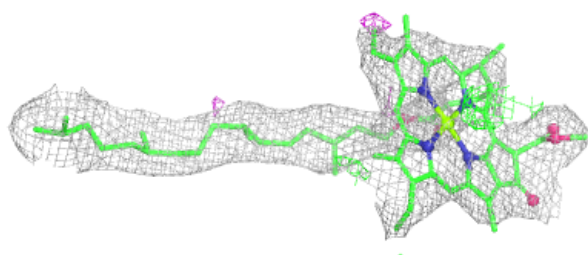
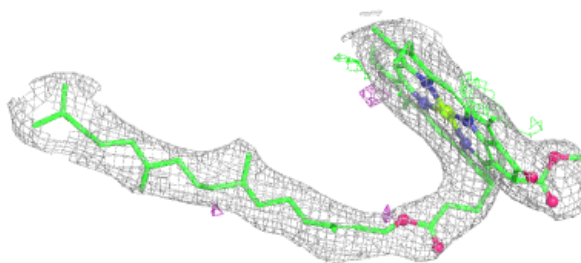
**Electron density around CLA B1 605:**

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



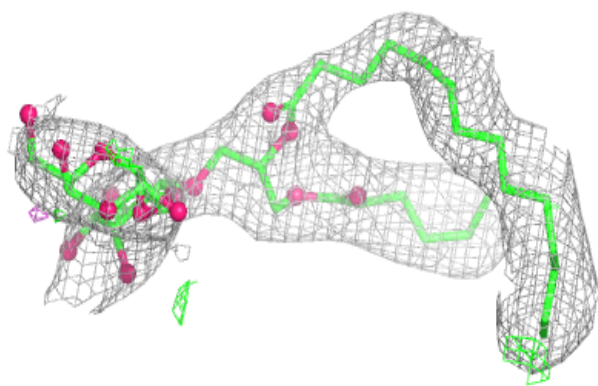
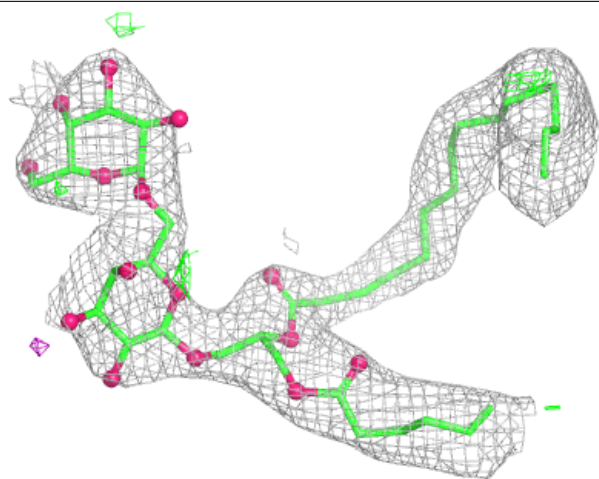
**Electron density around CLA C1 505:**

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



**Electron density around DGD C1 515:**

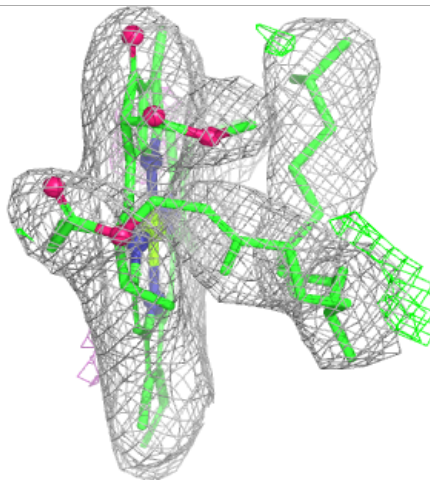
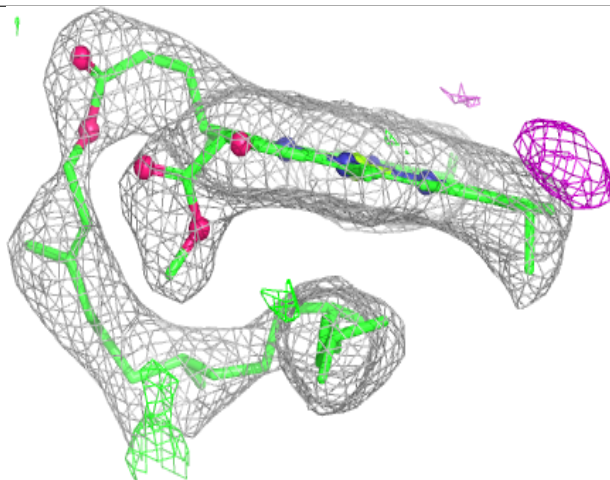
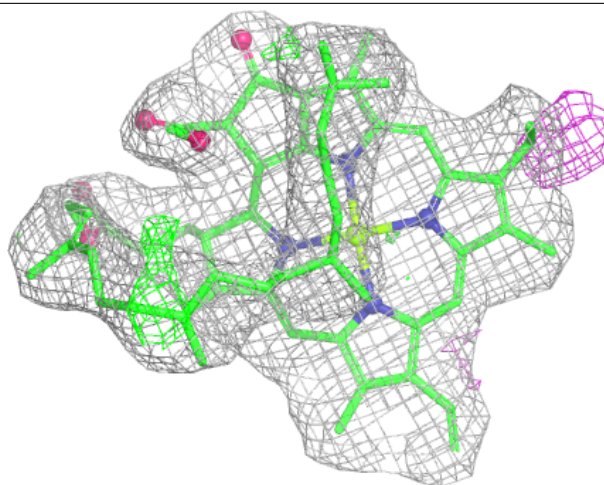
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





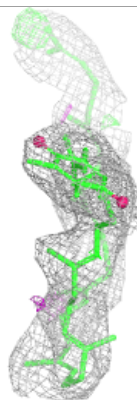
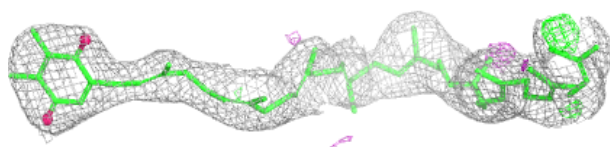
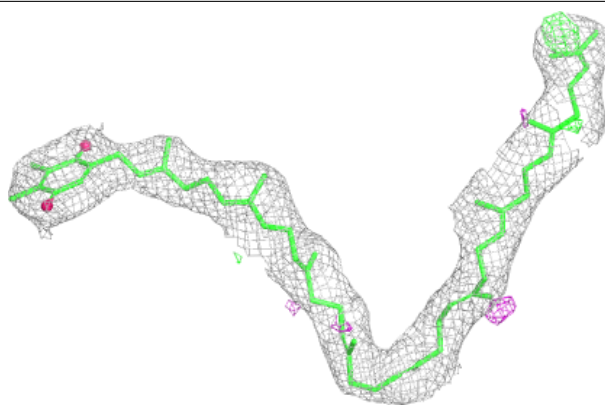
**Electron density around CLA c1 512:**

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

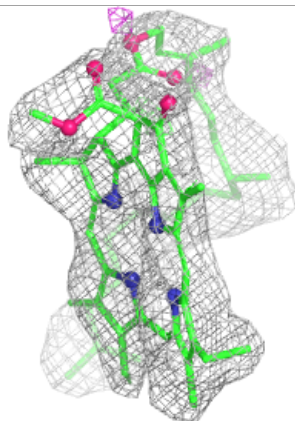
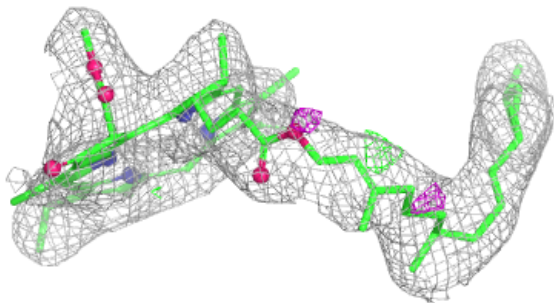
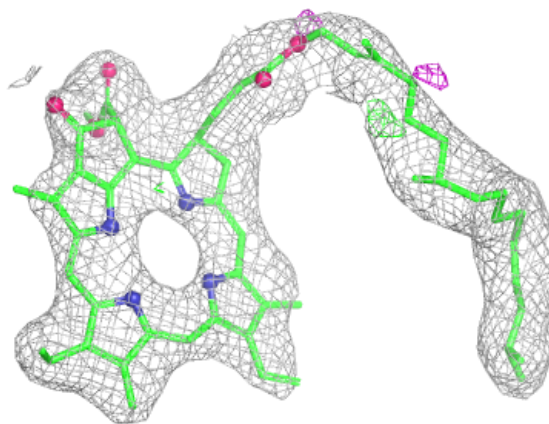


**Electron density around PL9 D2 408:**

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

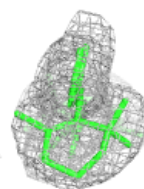
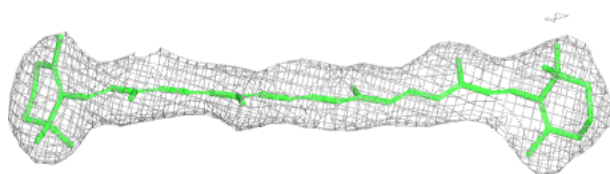
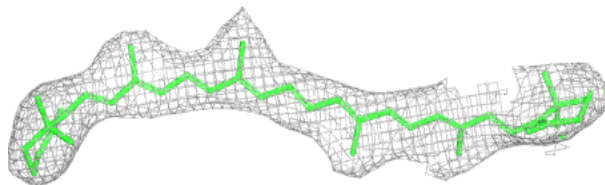
**Electron density around PHO D1 407:**

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

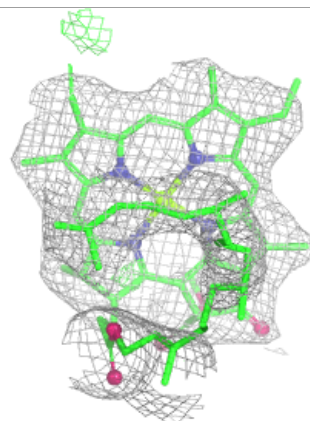
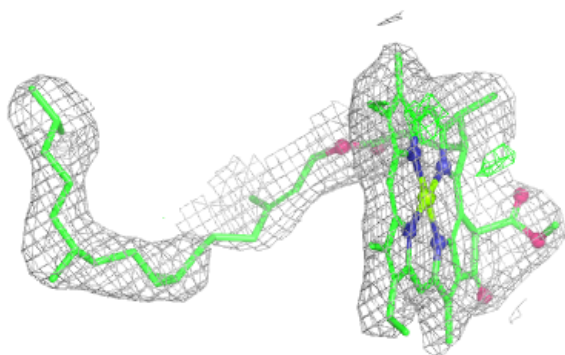
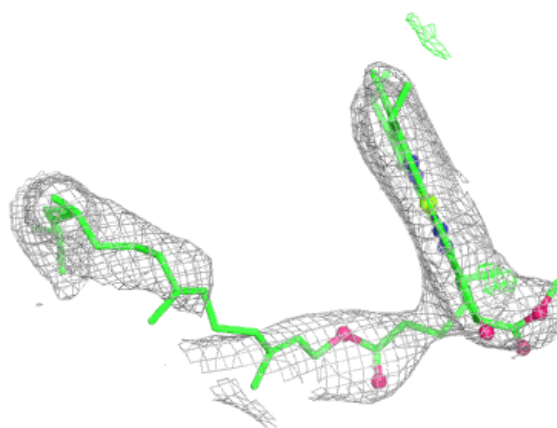


**Electron density around BCR C1 501:**

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

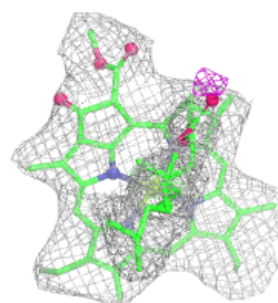
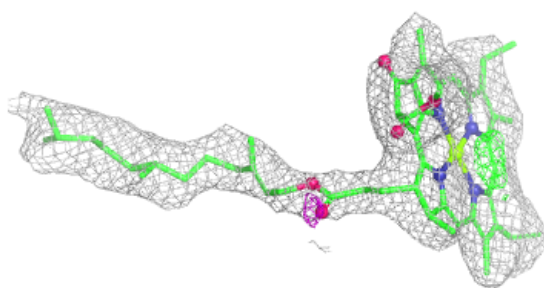
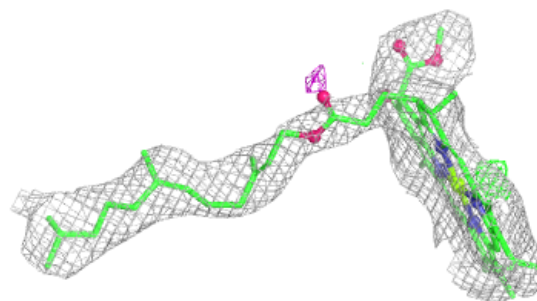
**Electron density around CLA C1 507:**

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

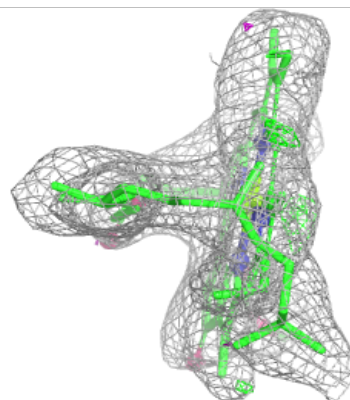
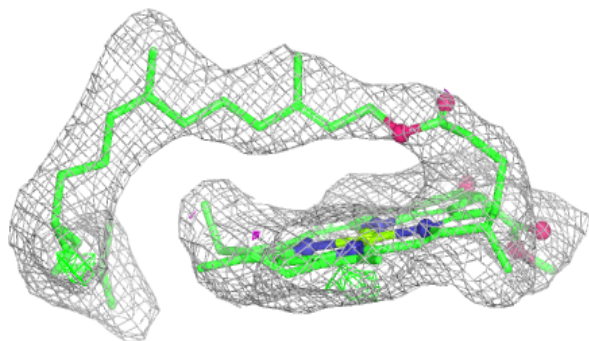
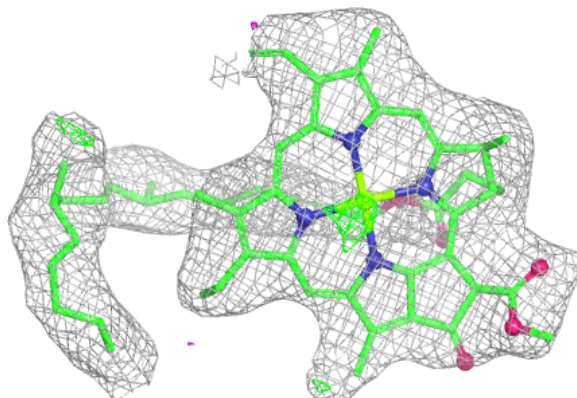


**Electron density around CLA b2 616:**

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

**Electron density around CLA b1 616:**

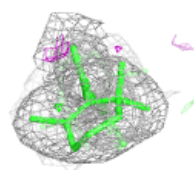
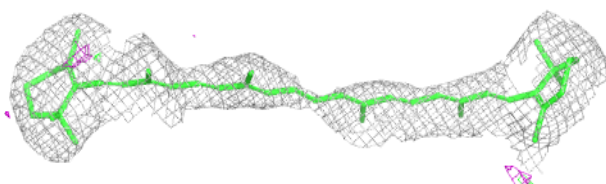
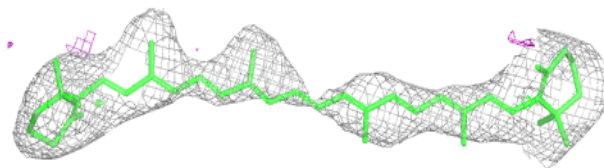
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



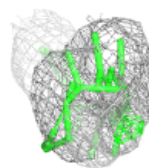
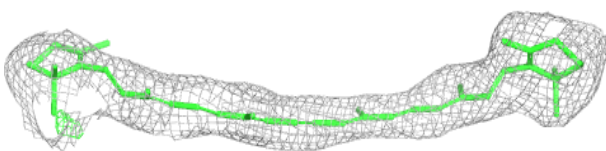
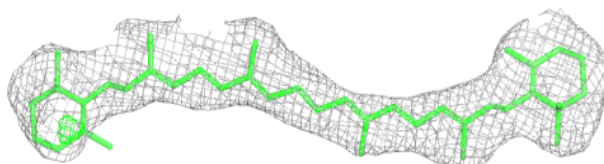


**Electron density around BCR A2 401:**

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

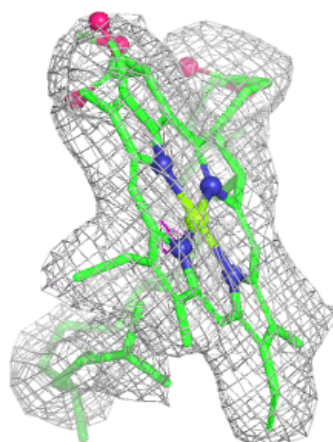
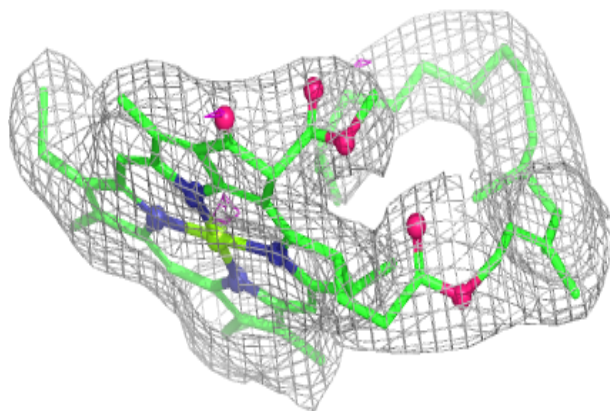
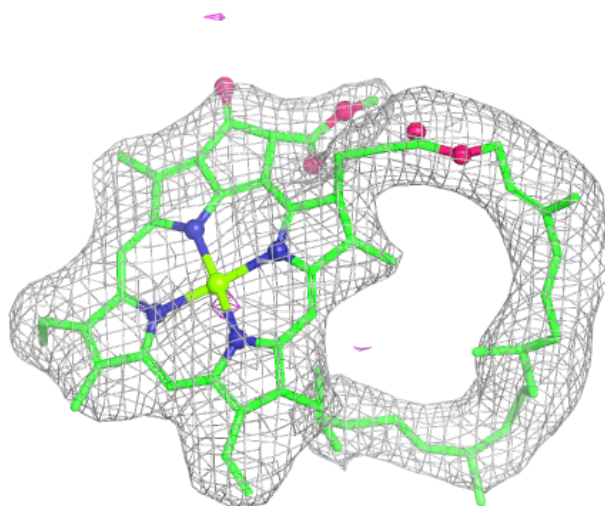
**Electron density around BCR d1 405:**

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



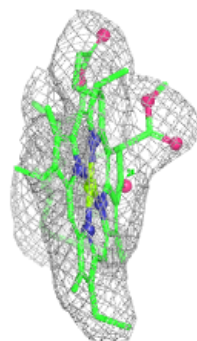
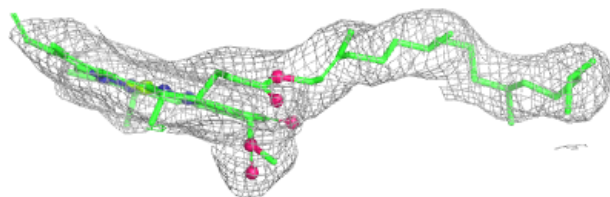
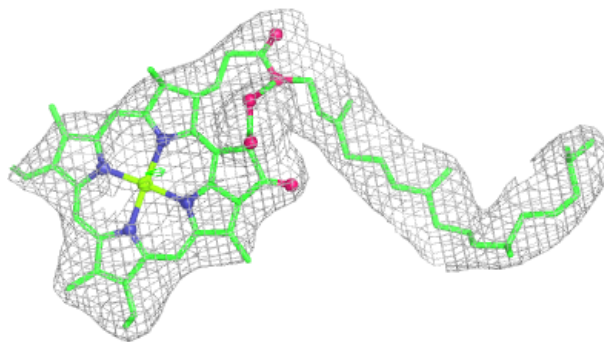
**Electron density around CLA B1 617:**

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

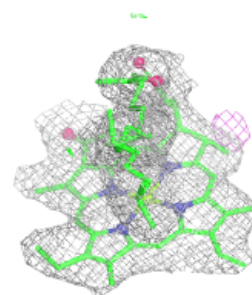
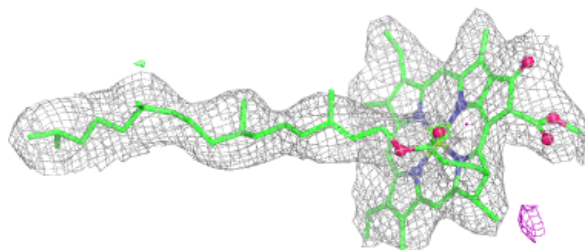
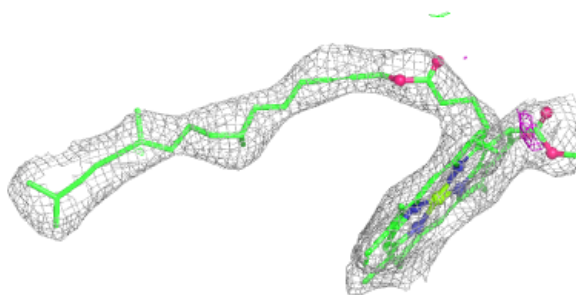


**Electron density around CLA B2 605:**

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

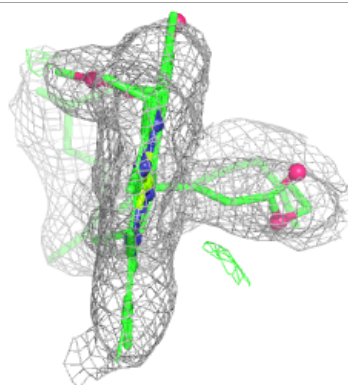
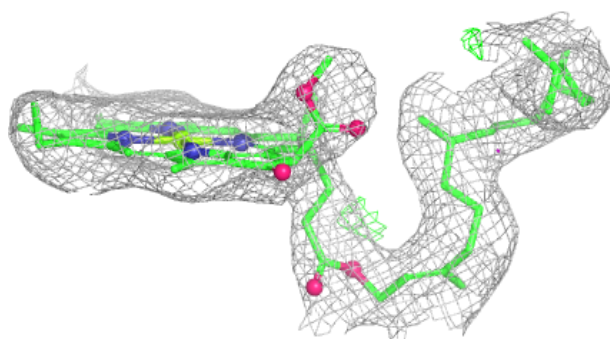
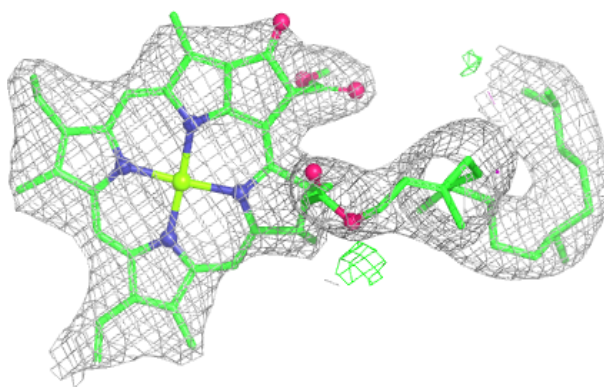
**Electron density around CLA c1 506:**

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

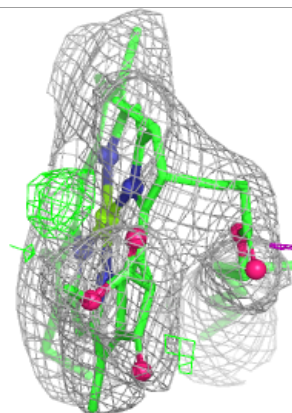
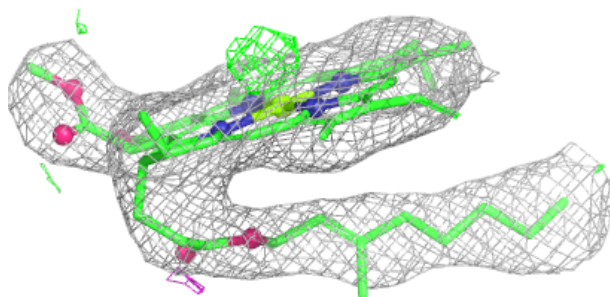
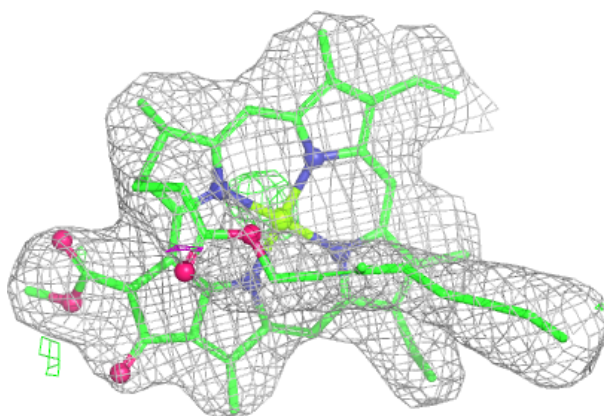


**Electron density around CLA B2 614:**

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

**Electron density around CLA B2 616:**

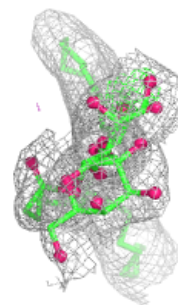
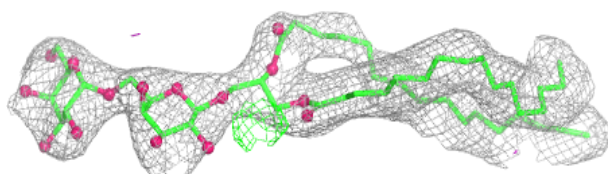
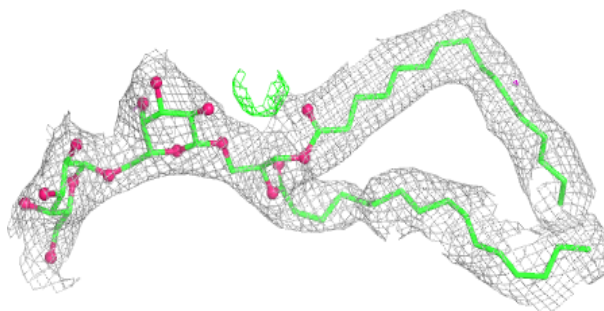
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





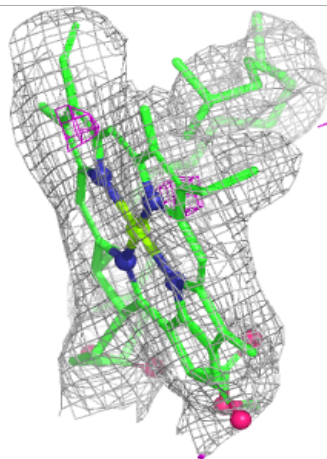
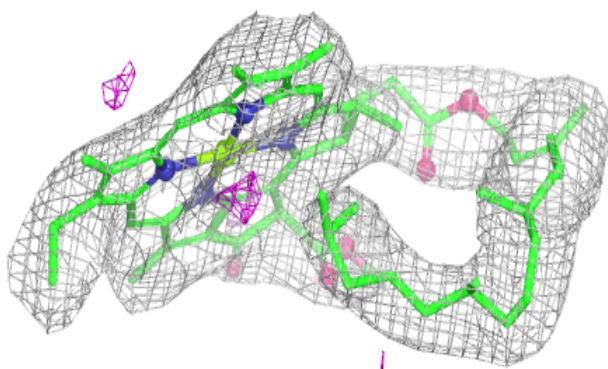
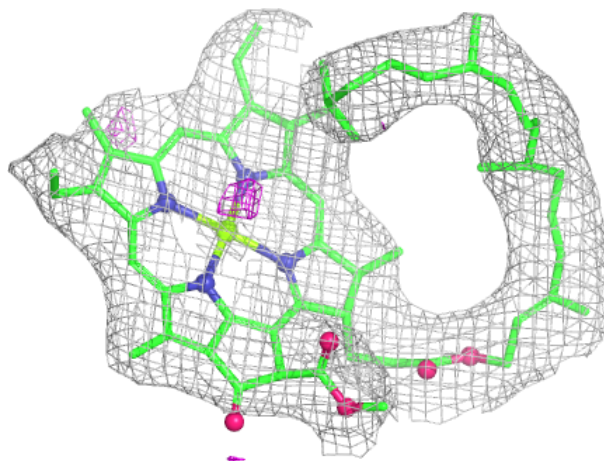
**Electron density around DGD c1 518:**

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



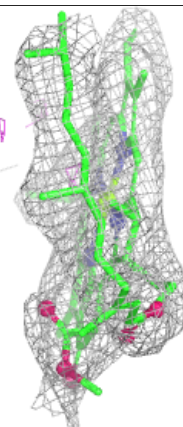
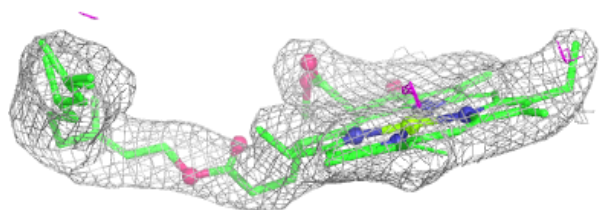
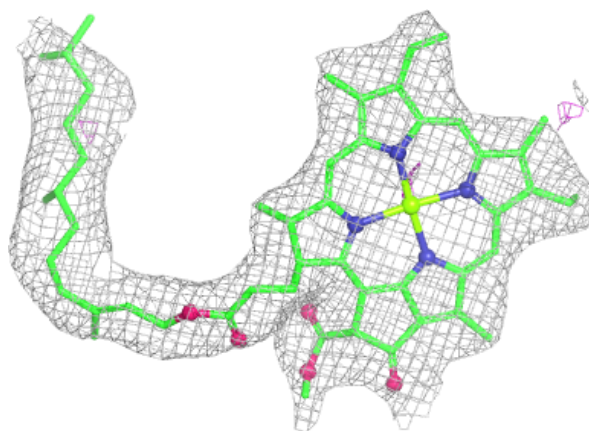
**Electron density around CLA B2 617:**

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

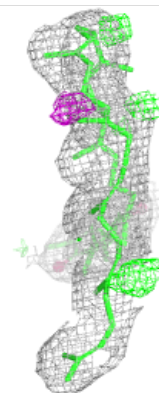
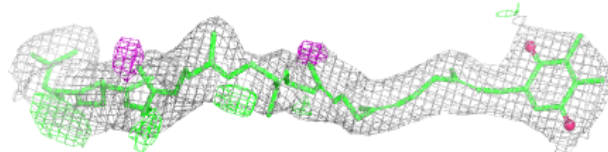
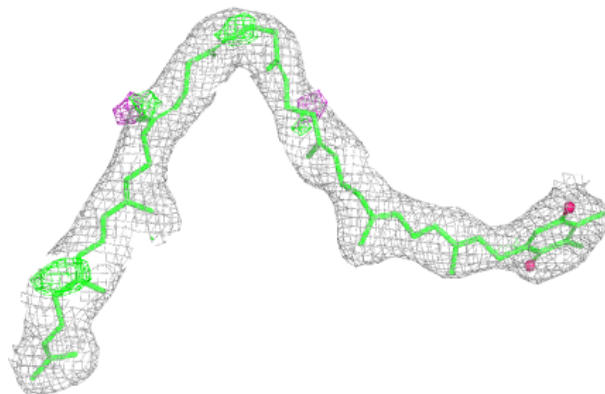


**Electron density around CLA B2 618:**

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

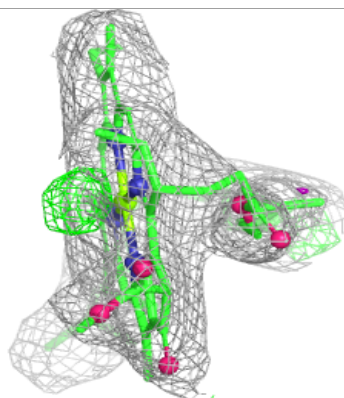
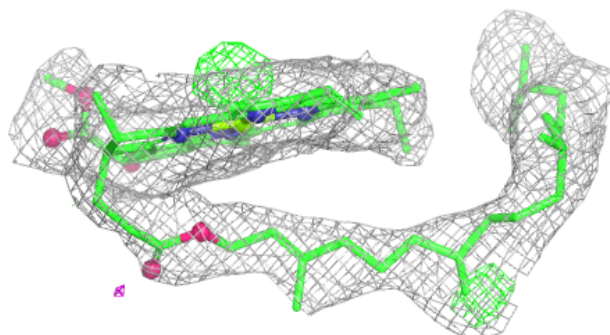
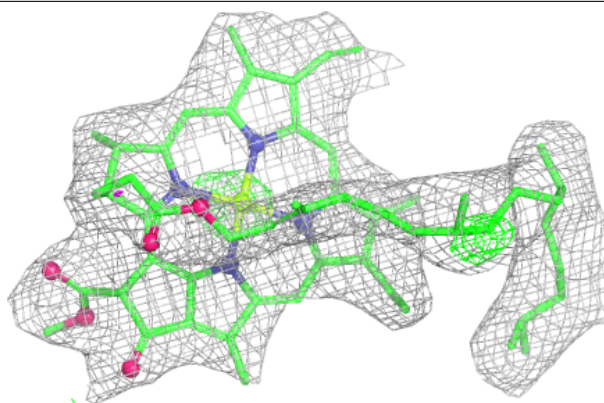
**Electron density around PL9 d1 409:**

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

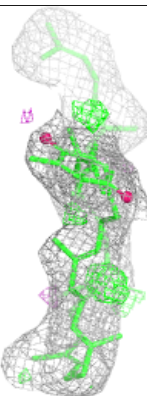
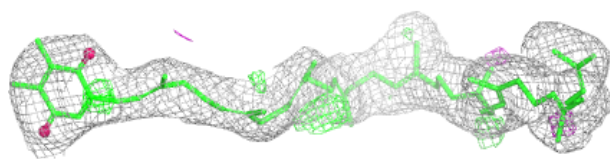
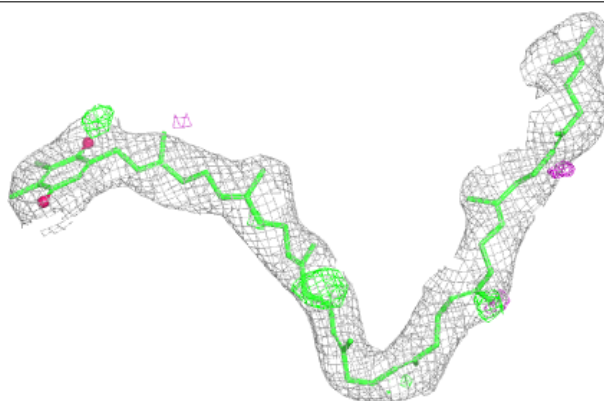


**Electron density around CLA b2 617:**

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

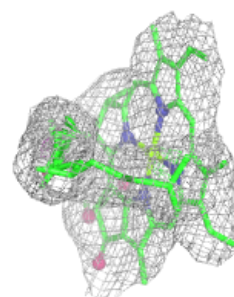
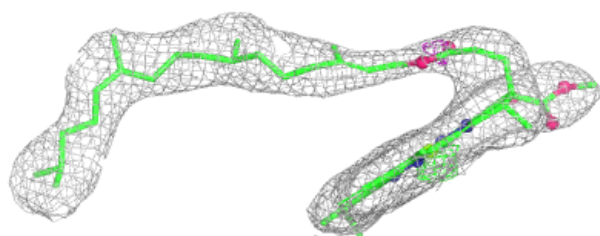
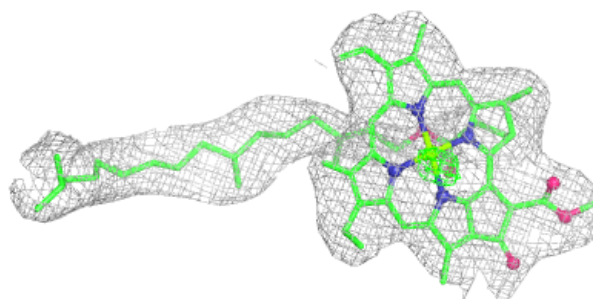
**Electron density around PL9 d2 409:**

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

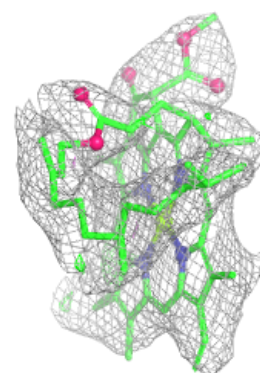
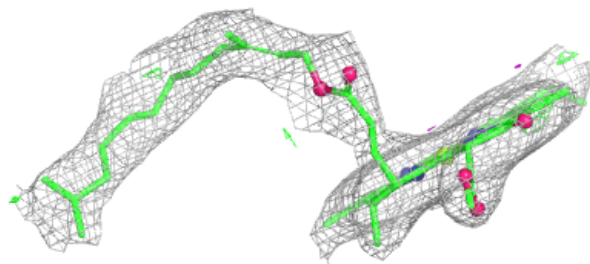
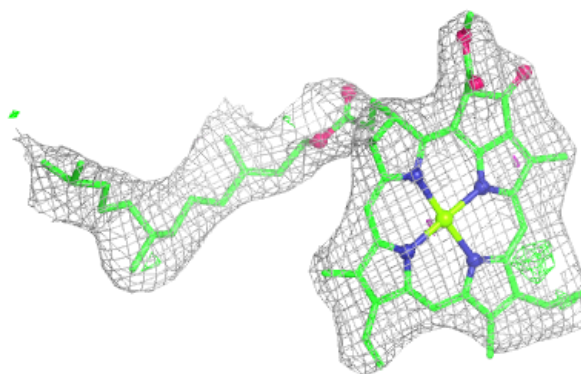


**Electron density around CLA B1 610:**

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

**Electron density around CLA a1 404:**

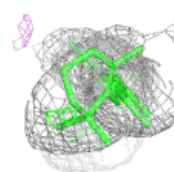
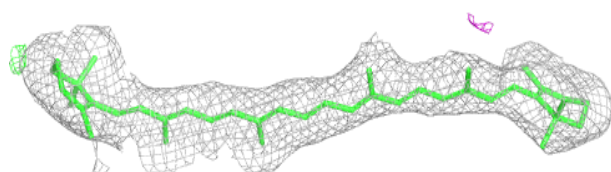
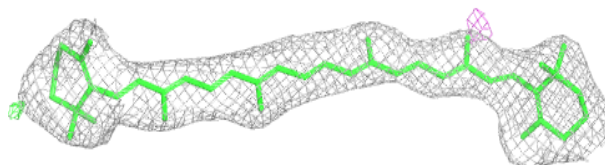
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



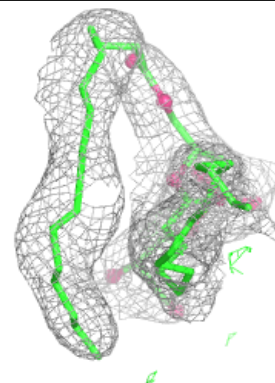
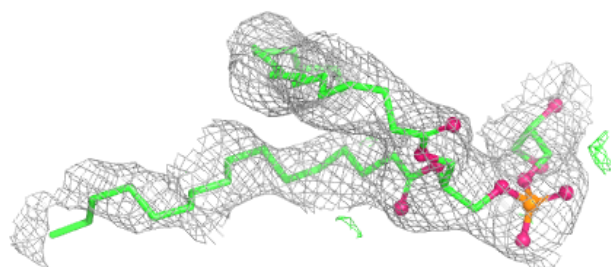
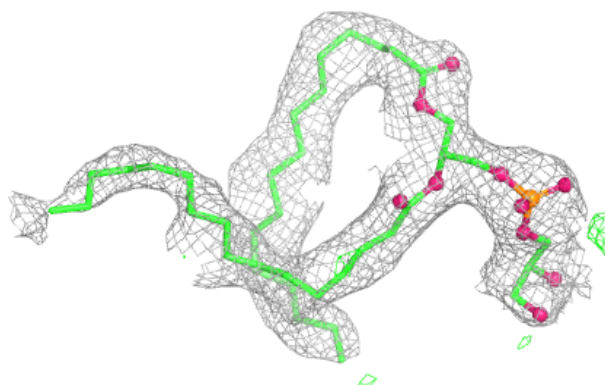


**Electron density around BCR B1 603:**

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

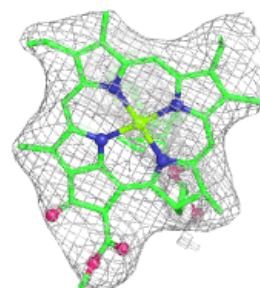
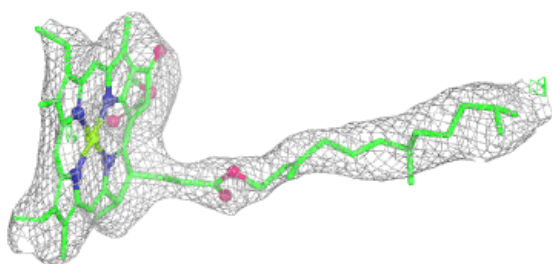
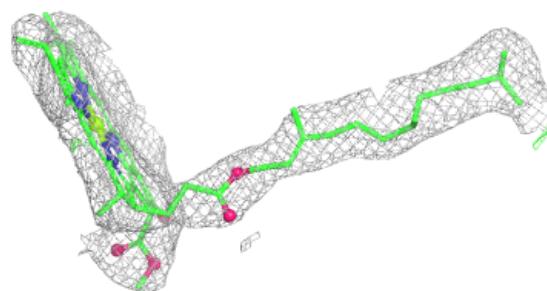
**Electron density around LHG D1 404:**

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

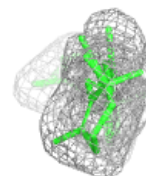
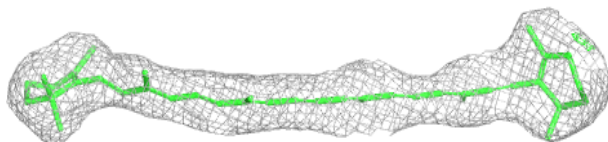
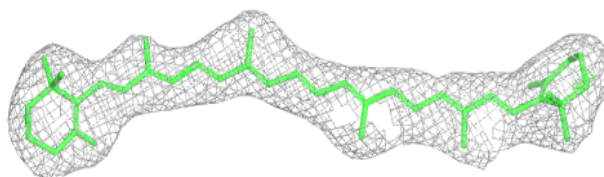


**Electron density around CLA B1 607:**

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

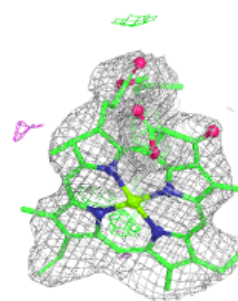
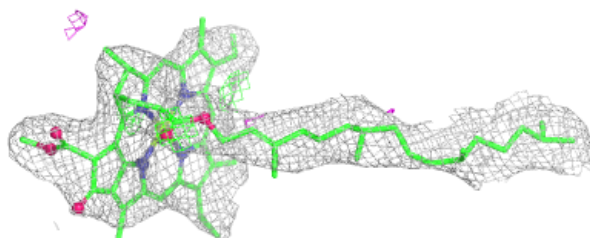
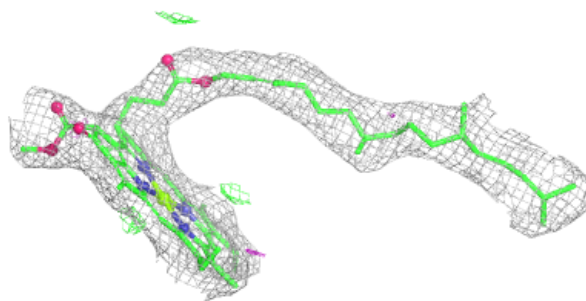
**Electron density around BCR B1 601:**

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

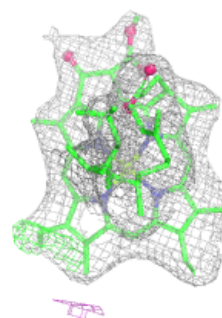
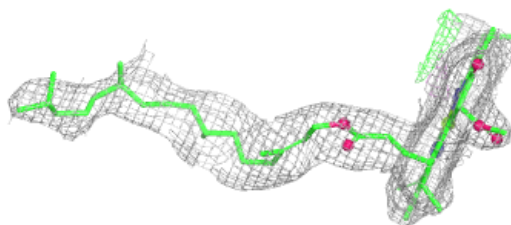
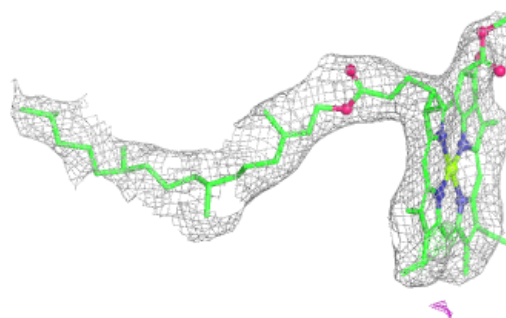


**Electron density around CLA c2 505:**

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

**Electron density around CLA d1 406:**

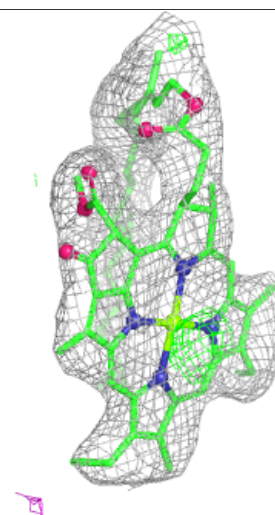
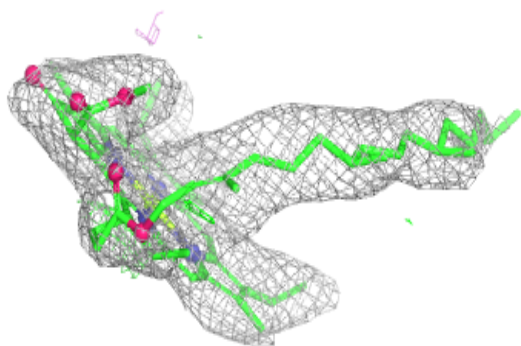
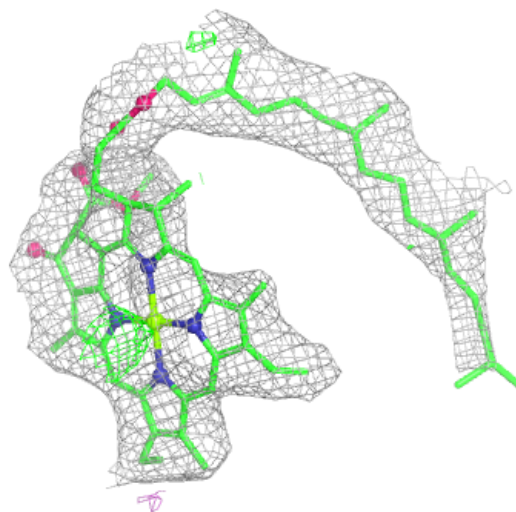
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





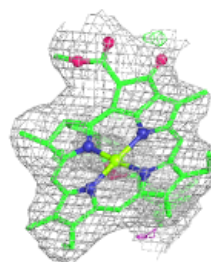
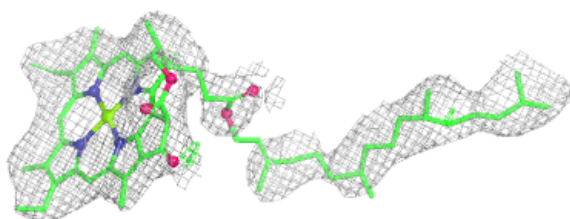
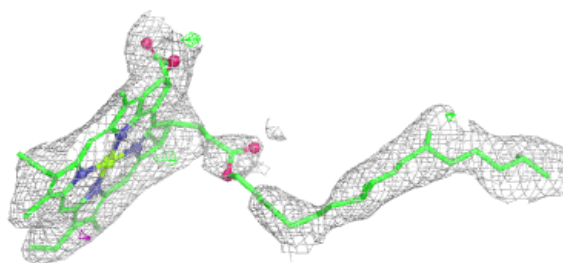
**Electron density around CLA C1 508:**

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

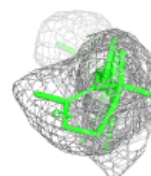
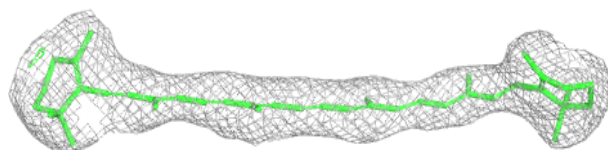
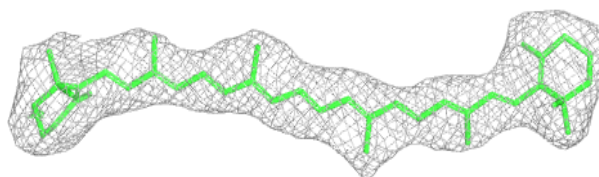


**Electron density around CLA c2 503:**

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

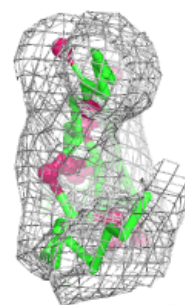
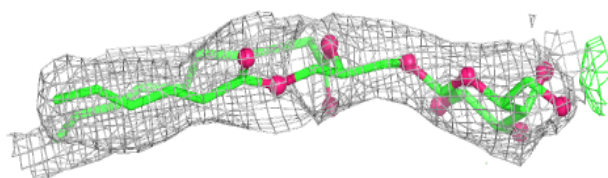
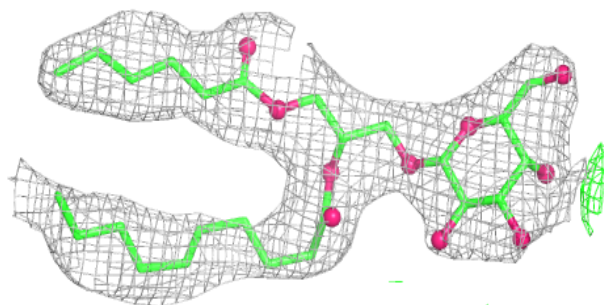
**Electron density around BCR B2 601:**

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

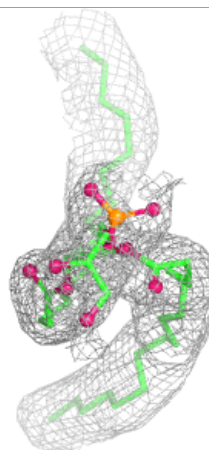
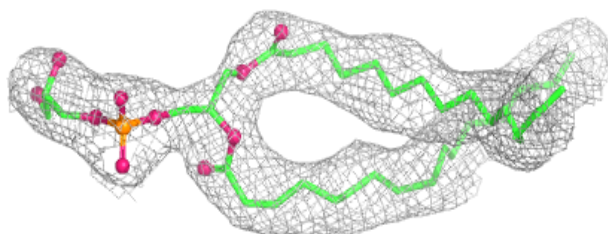
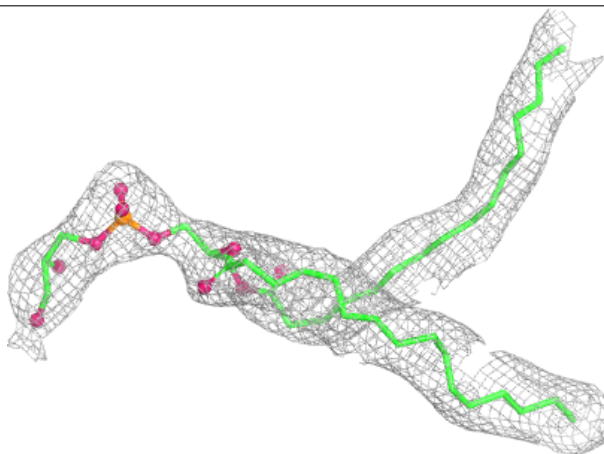


**Electron density around LMG D1 406:**

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

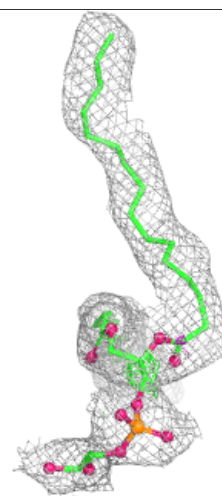
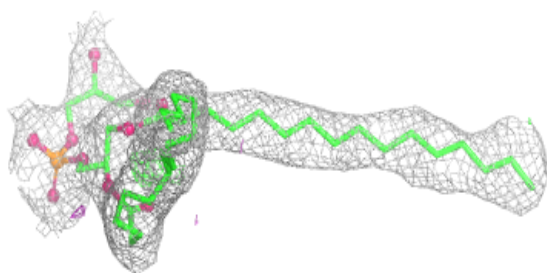
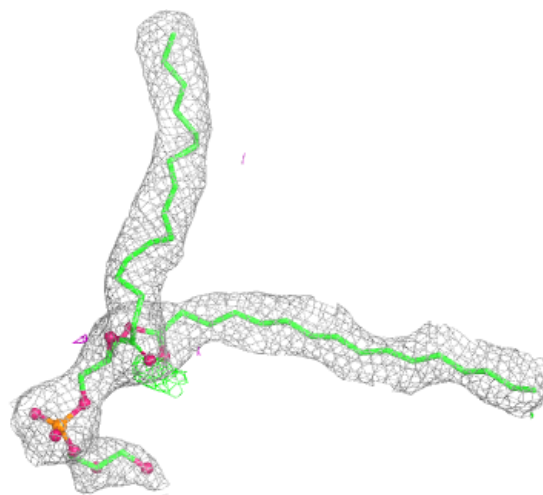
**Electron density around LHG D2 405:**

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



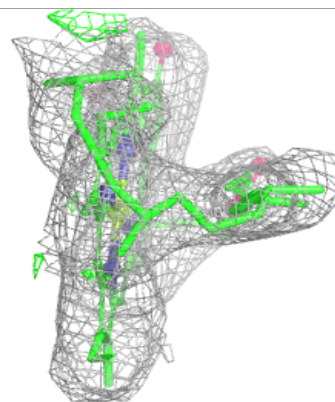
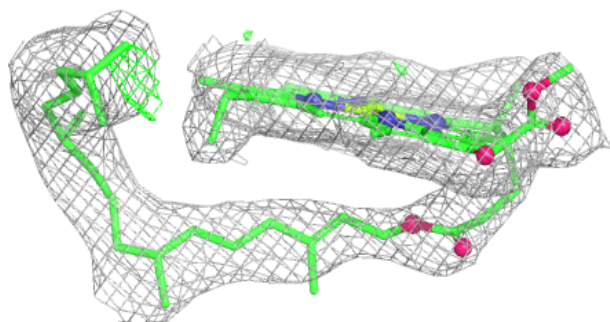
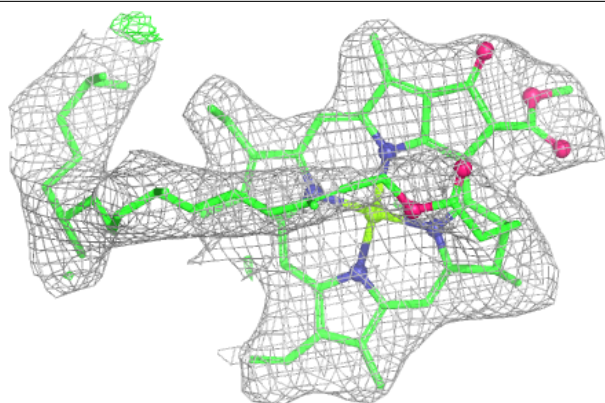
**Electron density around LHG L2 101:**

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

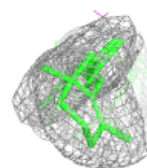
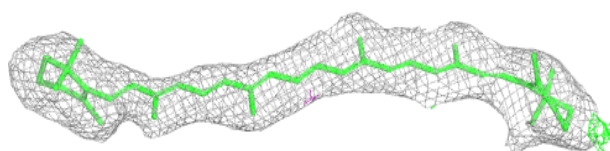
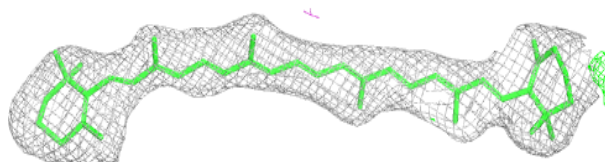


**Electron density around CLA B1 616:**

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

**Electron density around BCR b1 603:**

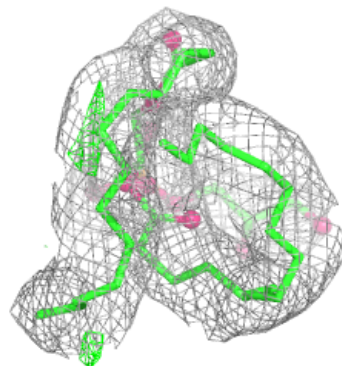
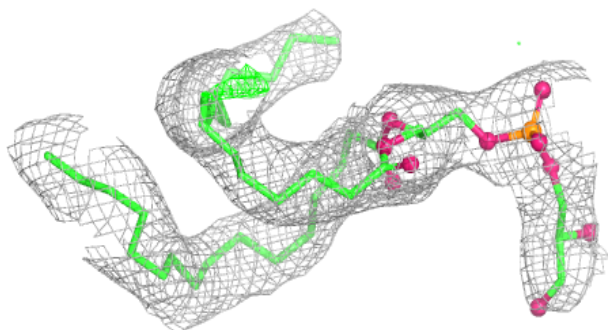
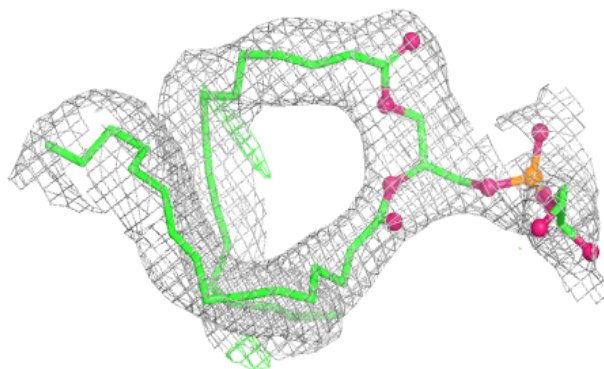
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



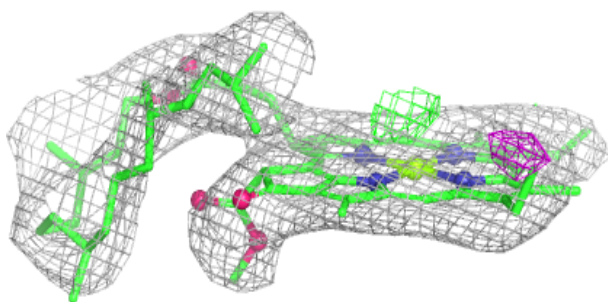
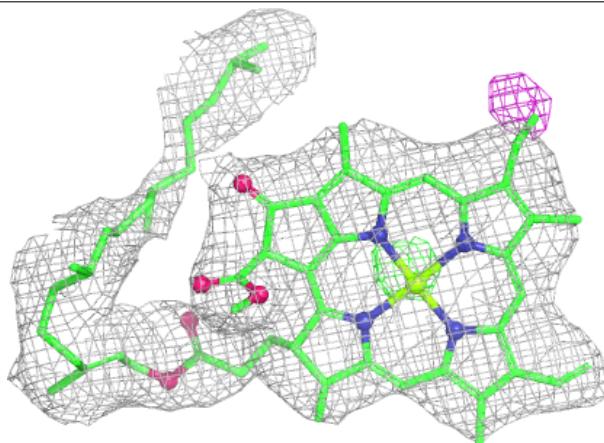


**Electron density around LHG d2 403:**

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

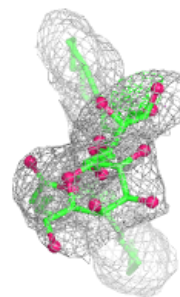
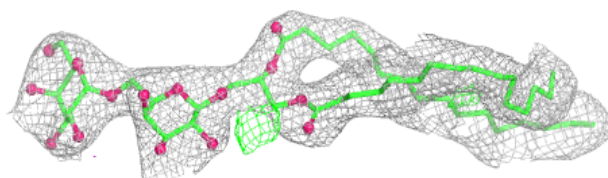
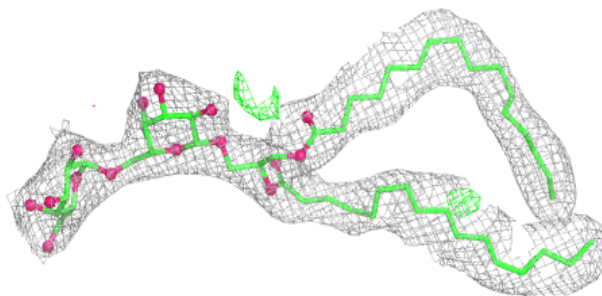
**Electron density around CLA b2 611:**

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

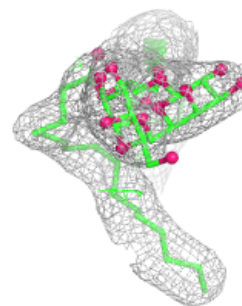
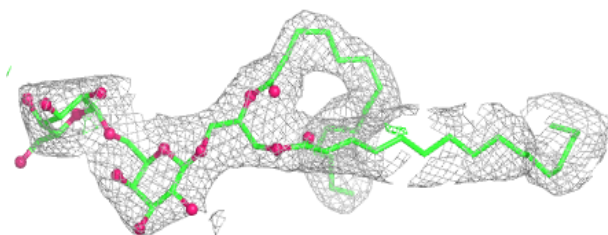
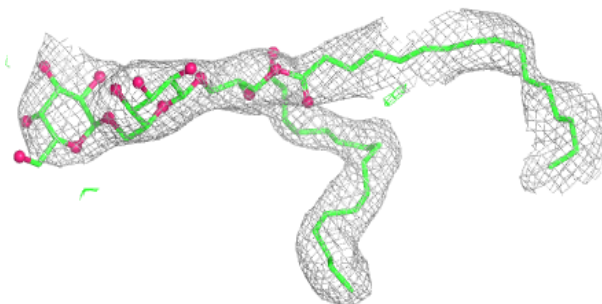


**Electron density around DGD C1 516:**

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

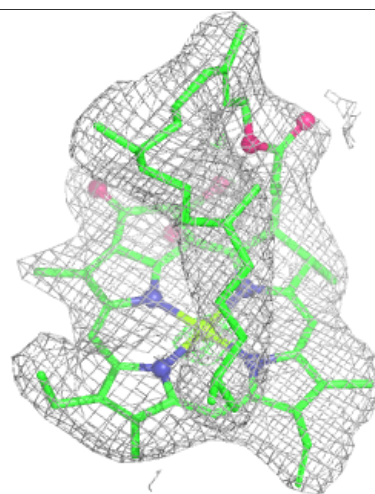
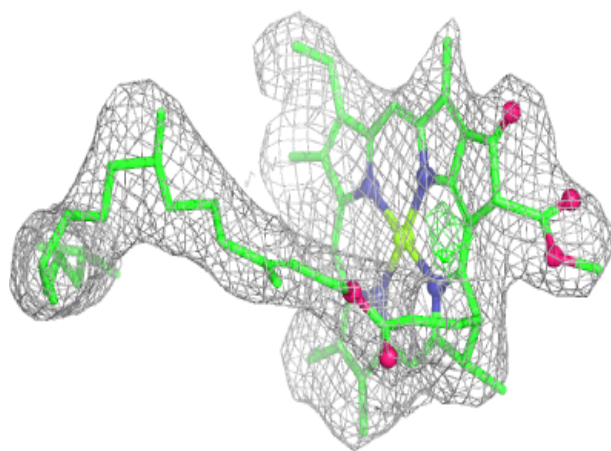
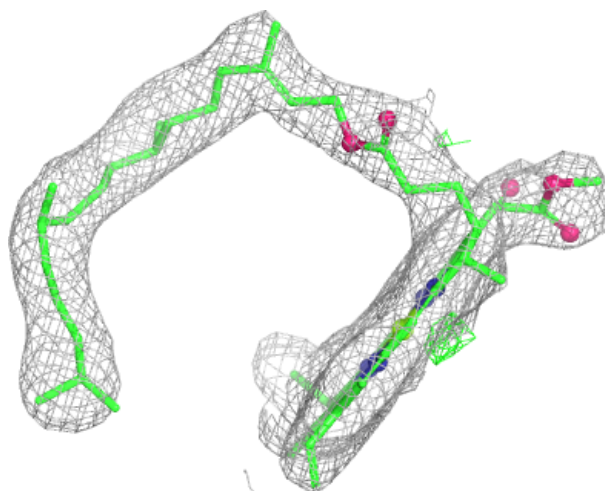
**Electron density around DGD H1 101:**

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



**Electron density around CLA b2 612:**

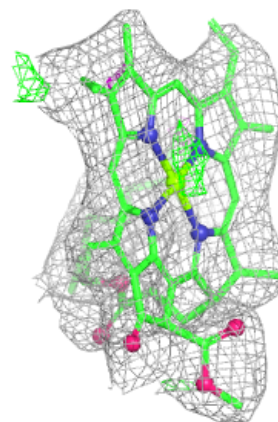
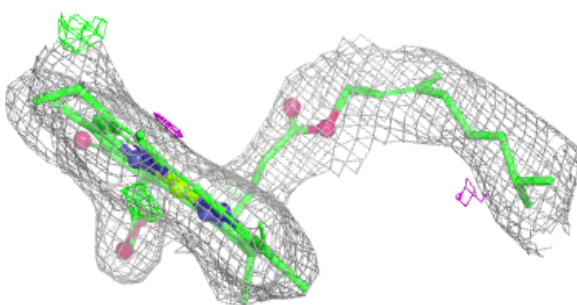
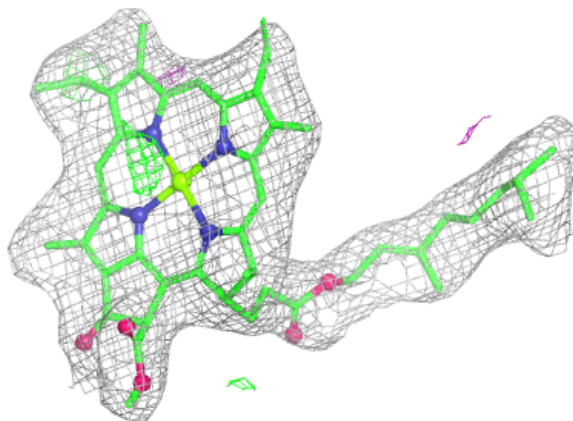
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



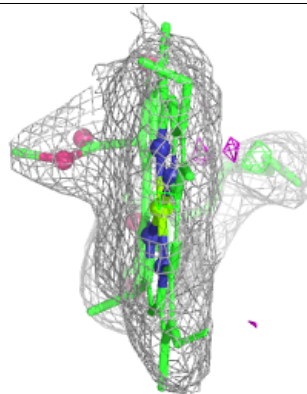
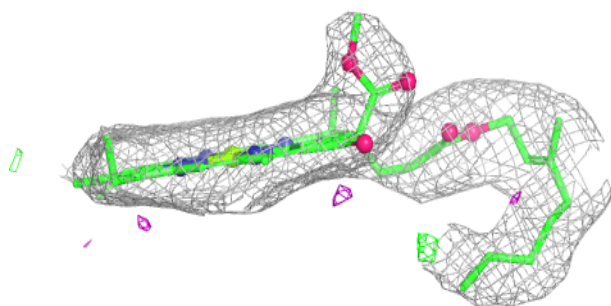
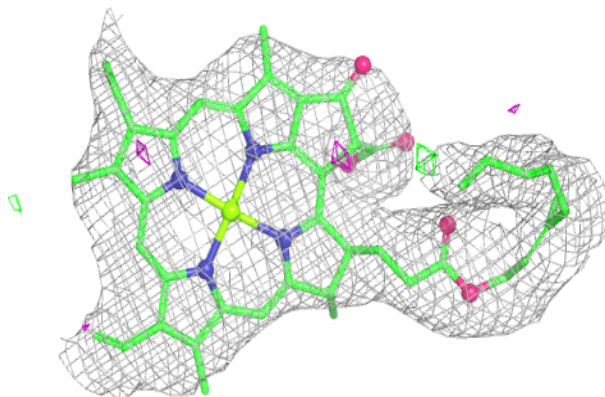


**Electron density around CLA A1 405:**

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

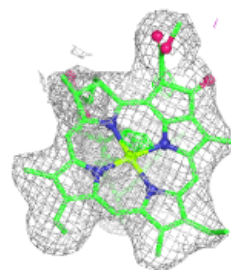
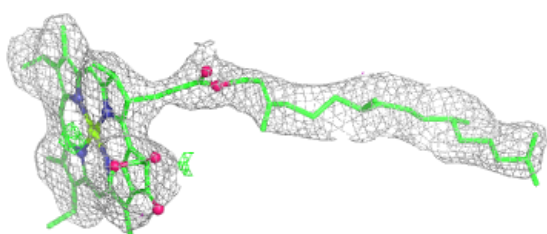
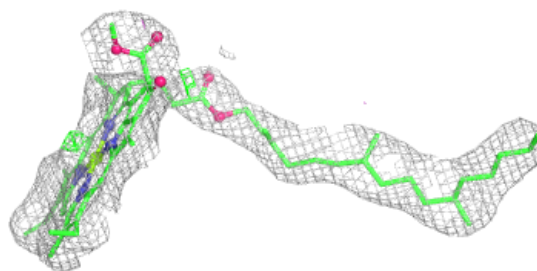
**Electron density around CLA c2 510:**

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

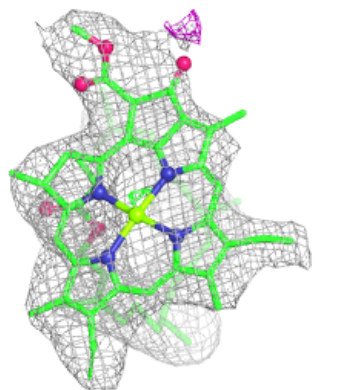
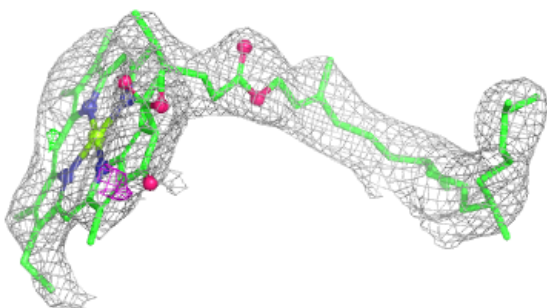
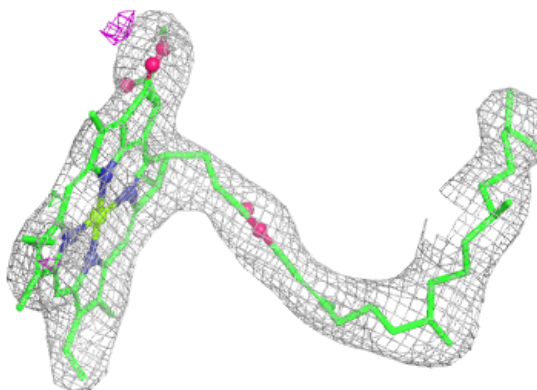


**Electron density around CLA B2 607:**

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

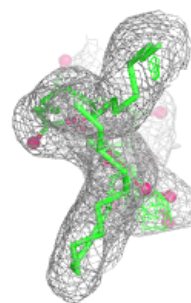
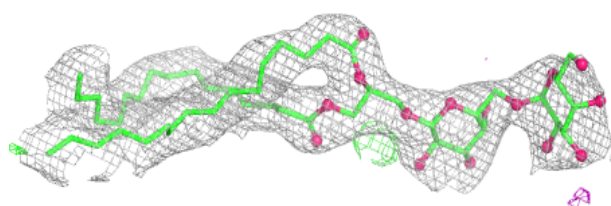
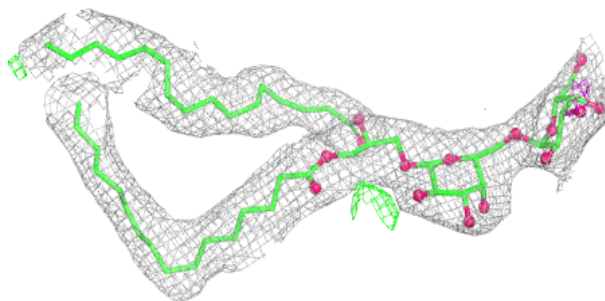
**Electron density around CLA B2 609:**

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

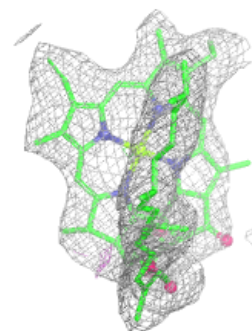
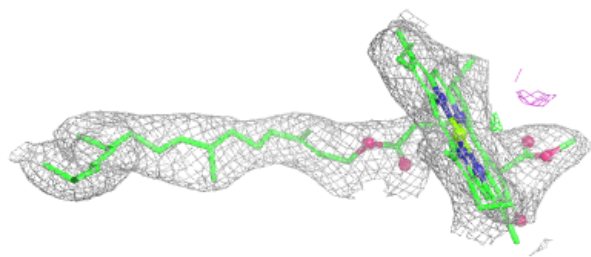
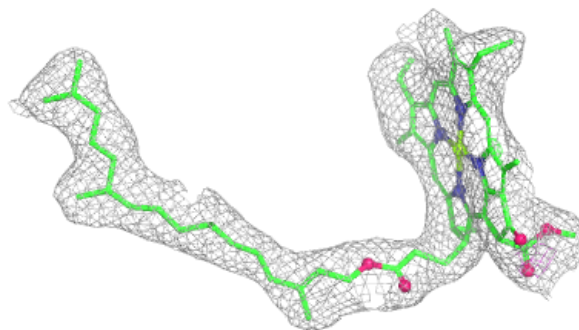


**Electron density around DGD c2 514:**

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

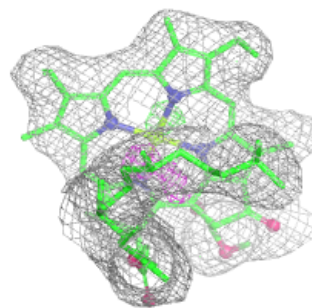
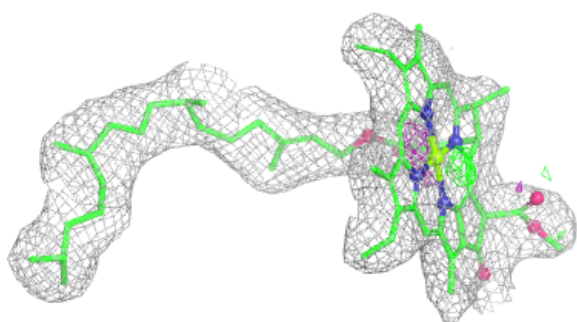
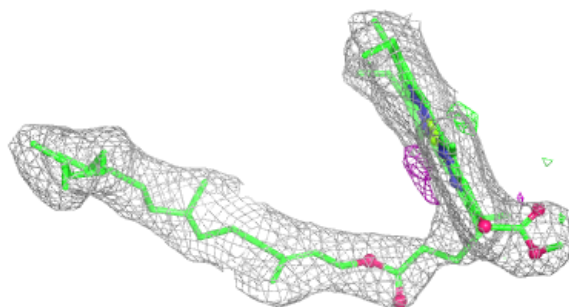
**Electron density around CLA b1 611:**

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

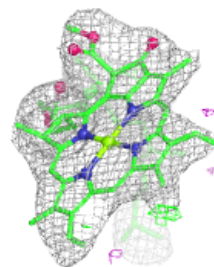
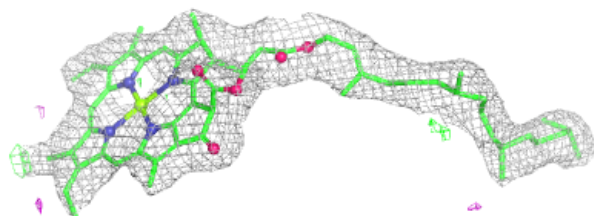
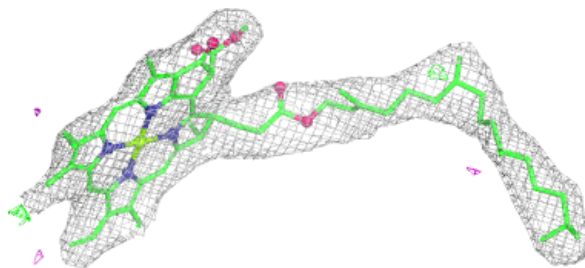


**Electron density around CLA B1 619:**

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

**Electron density around CLA A2 402:**

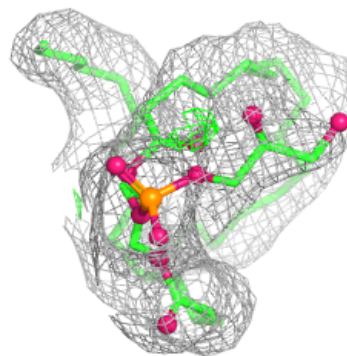
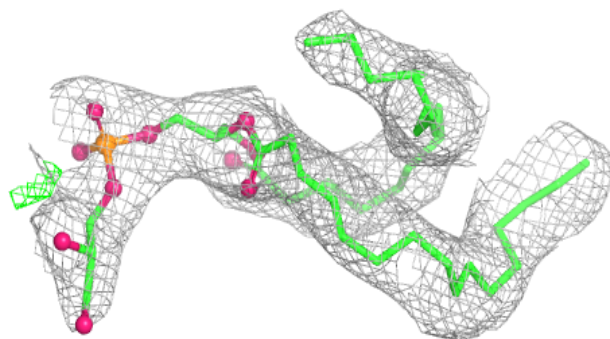
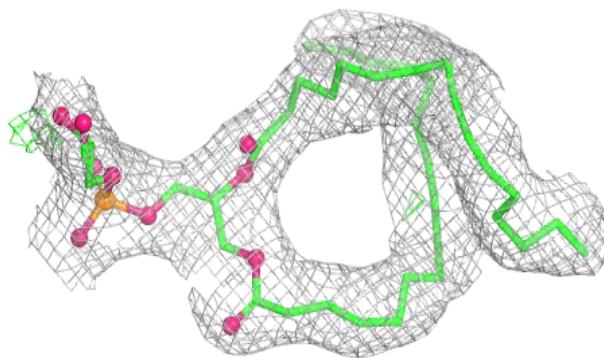
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





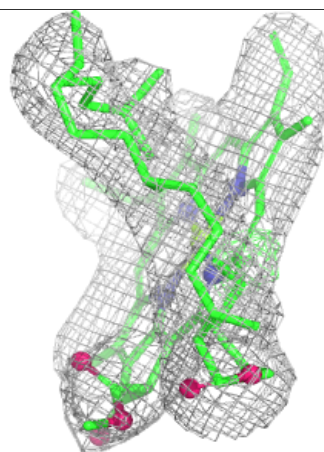
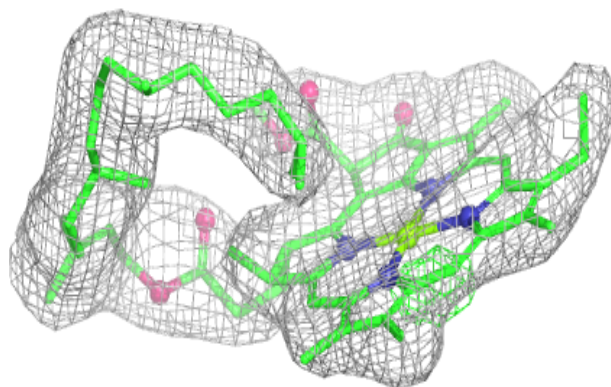
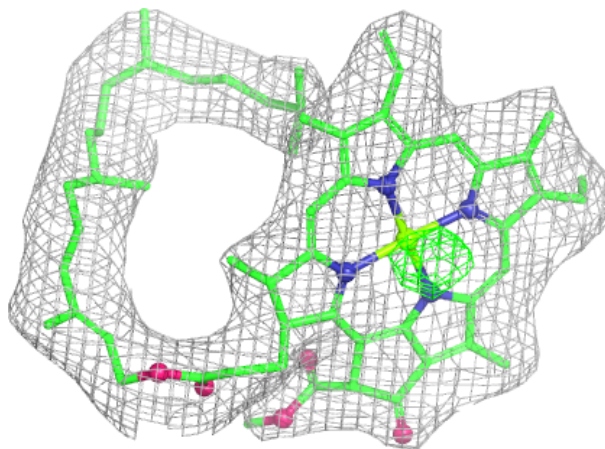
**Electron density around LHG B1 621:**

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



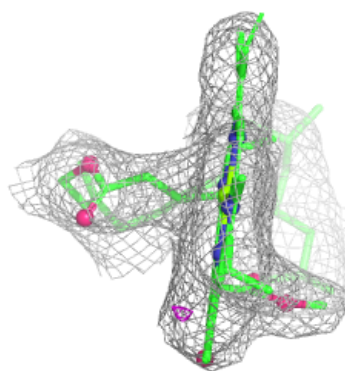
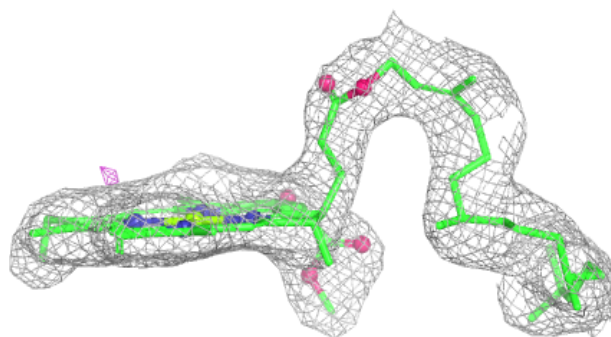
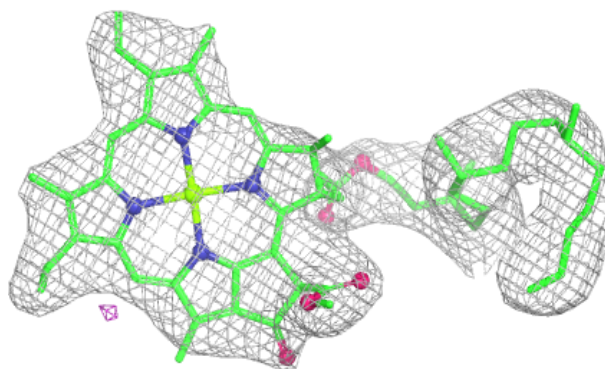
**Electron density around CLA b1 617:**

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

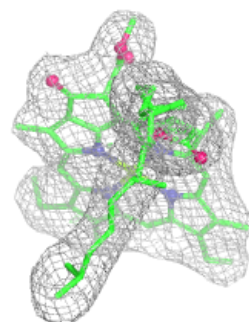
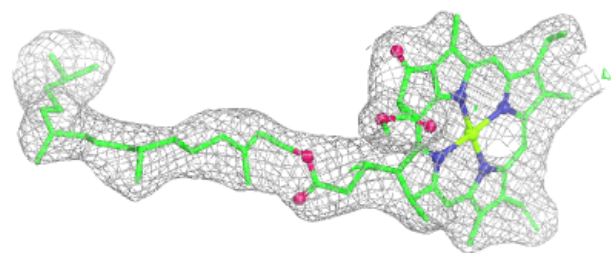
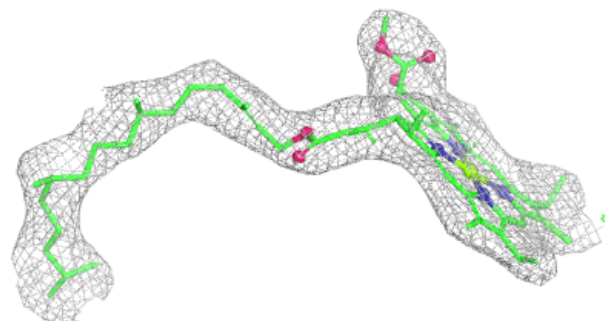


**Electron density around CLA b2 614:**

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

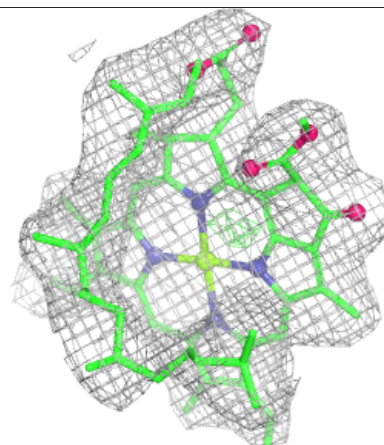
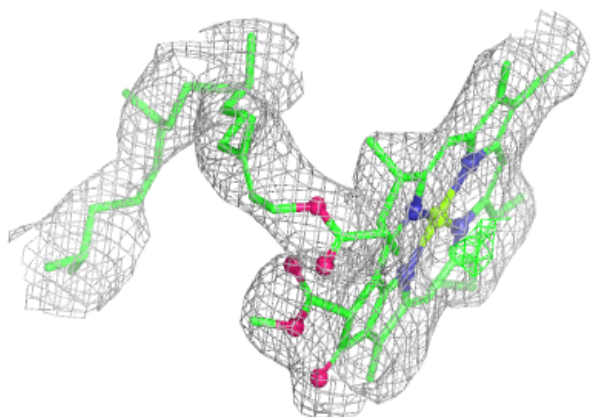
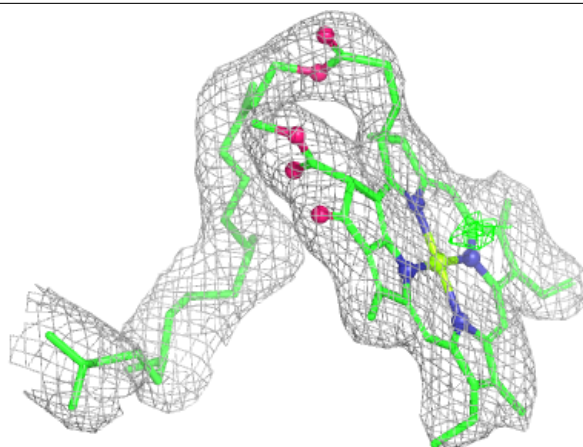
**Electron density around CLA d1 401:**

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



**Electron density around CLA B2 615:**

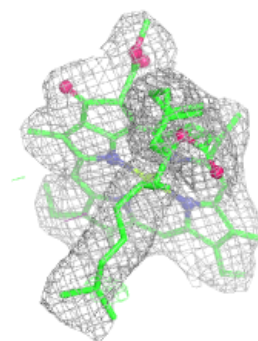
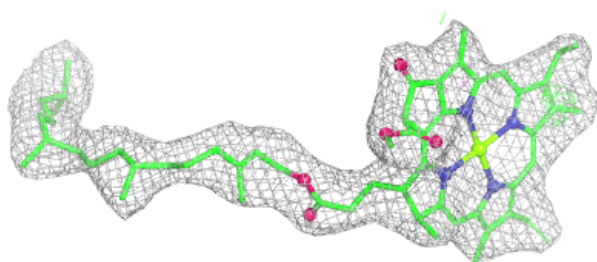
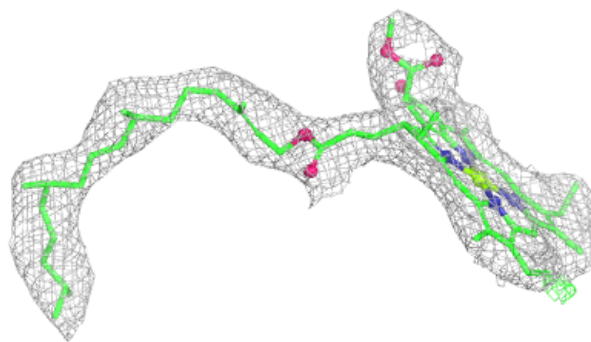
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





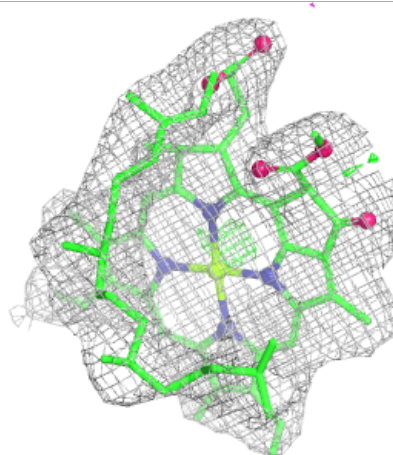
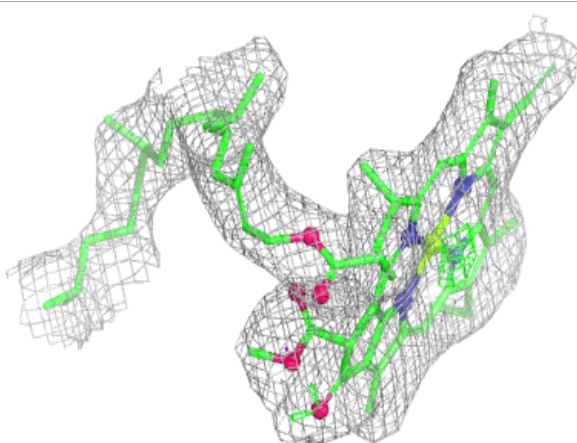
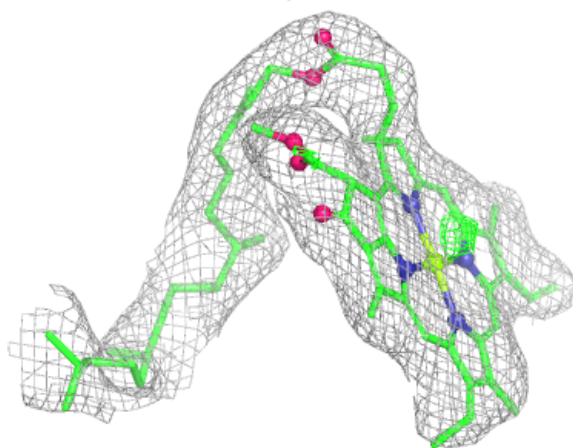
**Electron density around CLA d2 405:**

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



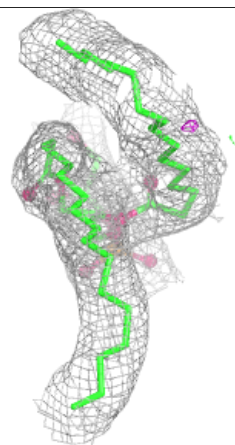
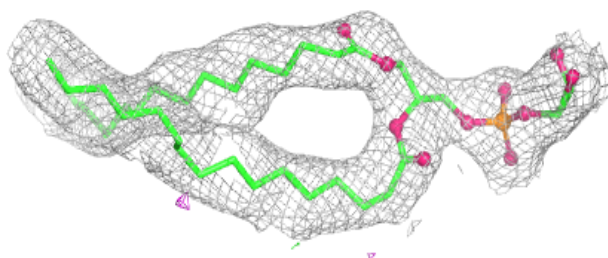
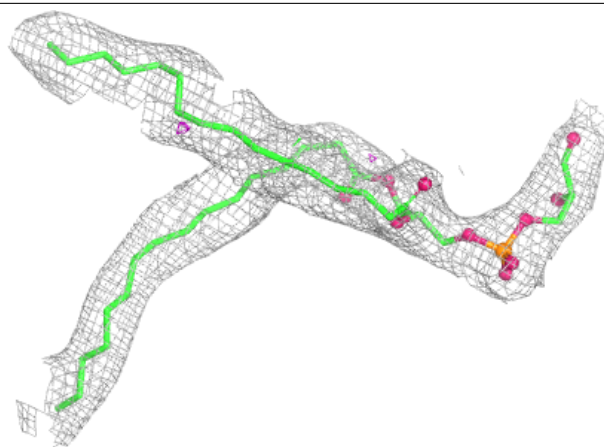
**Electron density around CLA B1 615:**

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



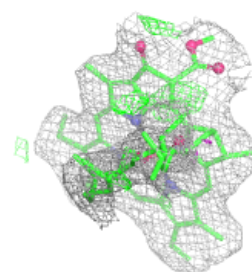
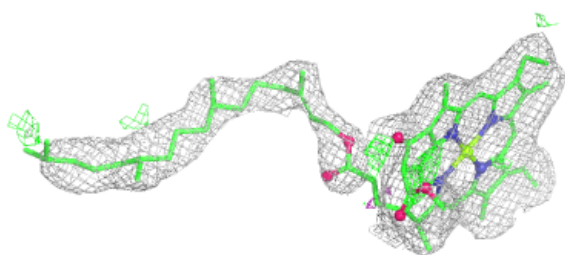
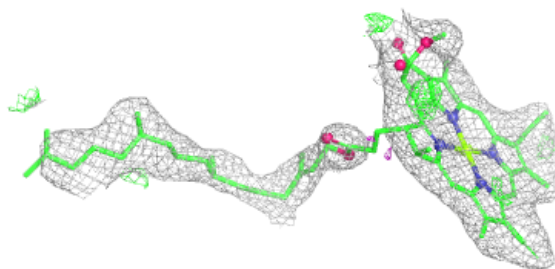
**Electron density around LHG d2 406:**

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

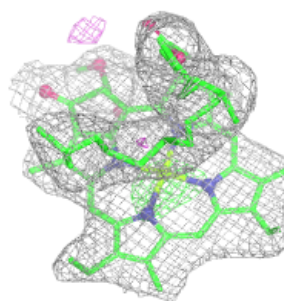
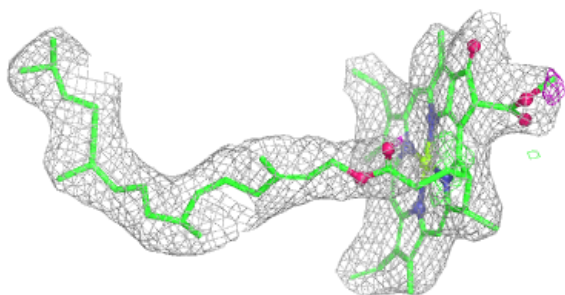
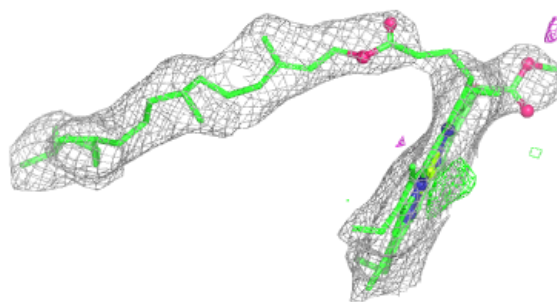


**Electron density around CLA c1 504:**

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

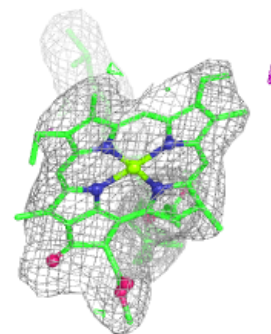
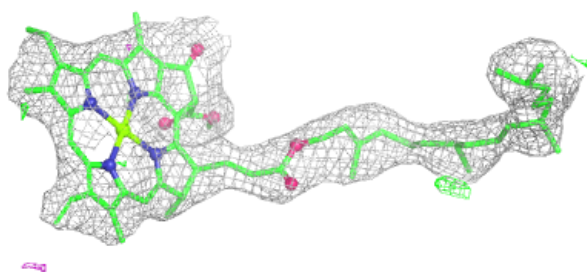
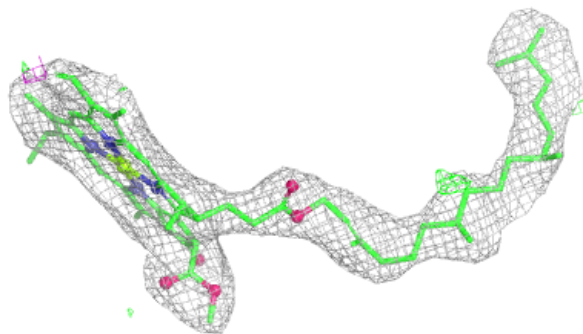
**Electron density around CLA b2 620:**

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

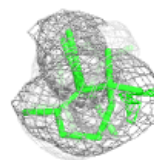
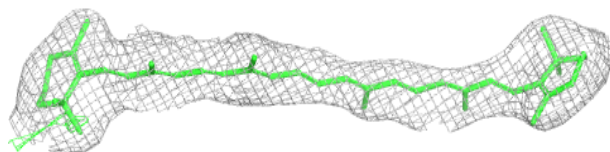
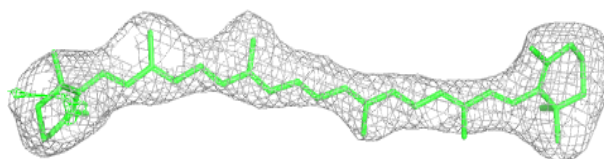


**Electron density around CLA D2 401:**

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

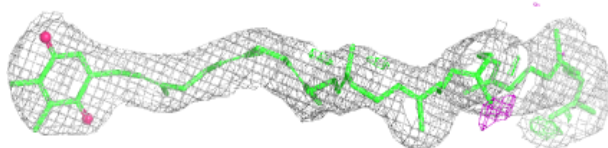
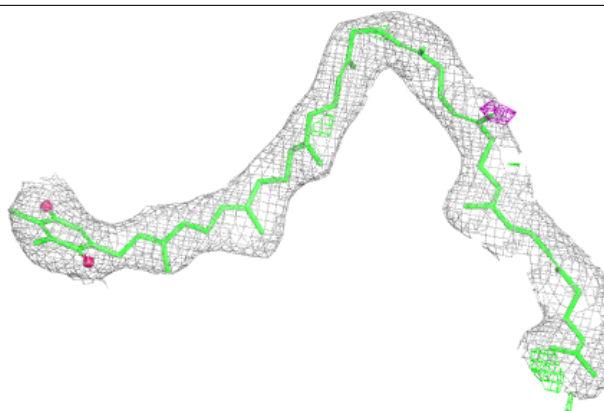
**Electron density around BCR a1 401:**

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

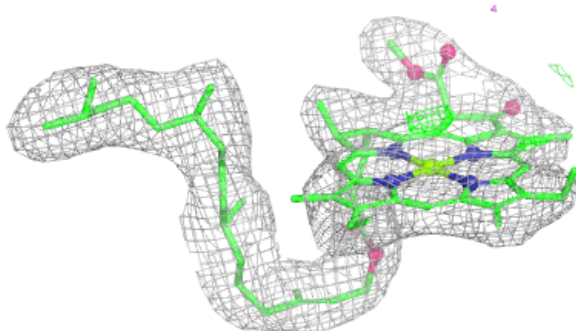
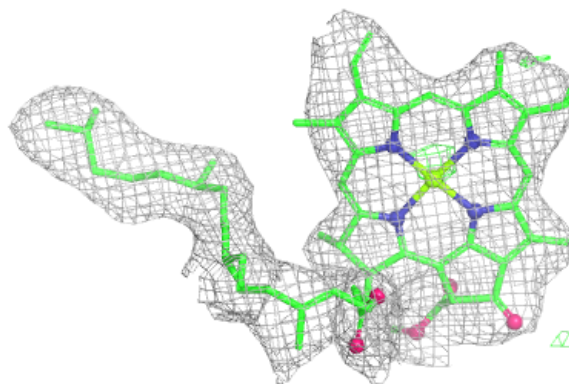


**Electron density around PL9 D1 408:**

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

**Electron density around CLA D2 406:**

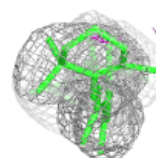
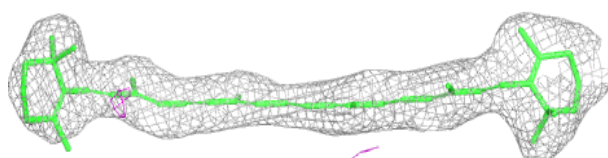
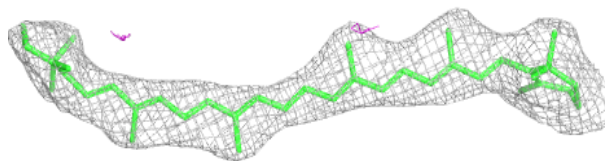
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



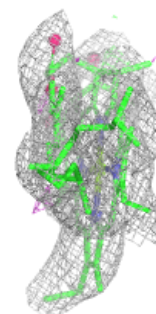
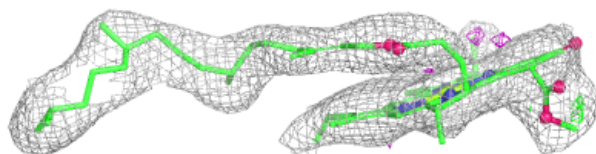
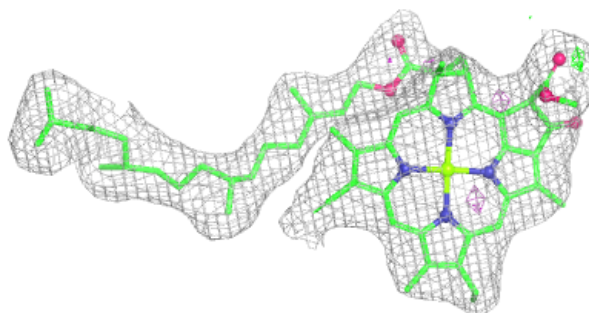


**Electron density around BCR h1 102:**

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

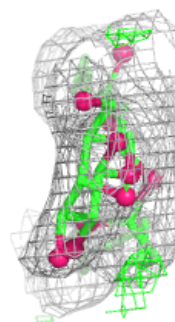
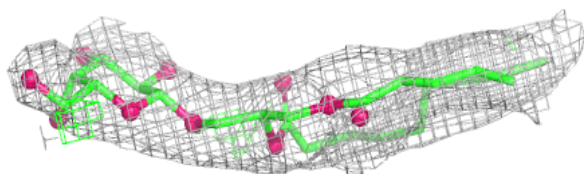
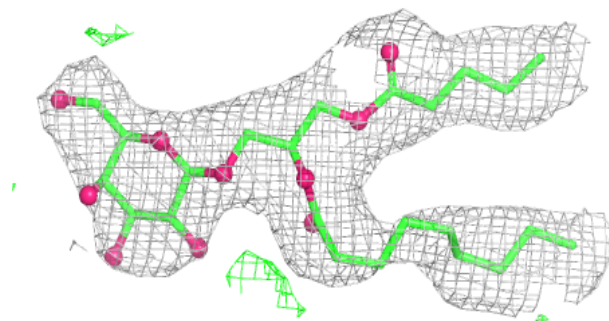
**Electron density around CLA b1 606:**

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



**Electron density around LMG d1 408:**

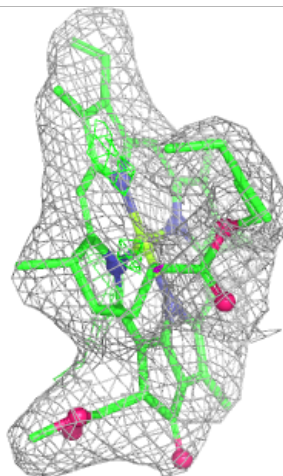
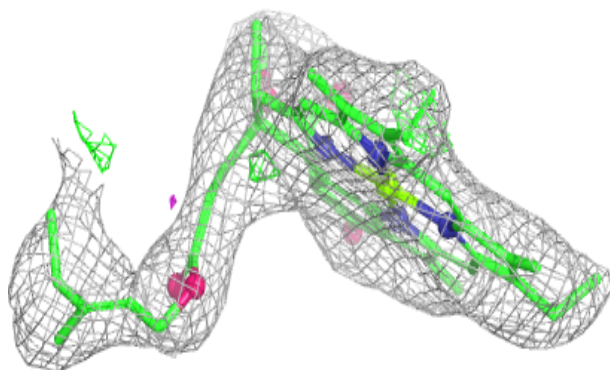
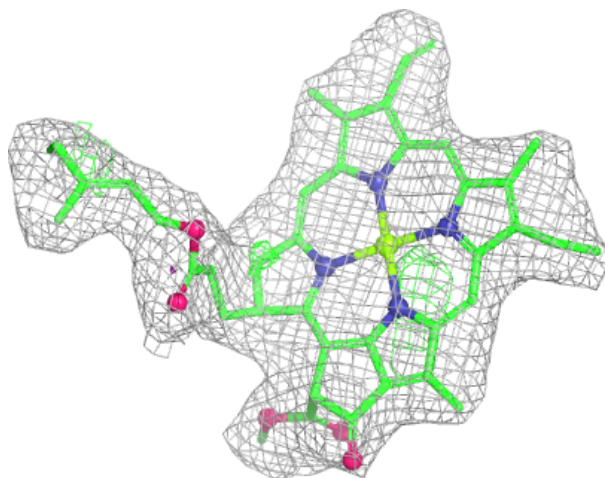
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





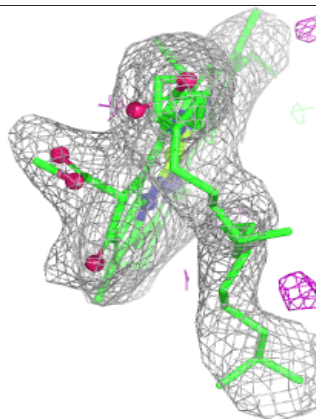
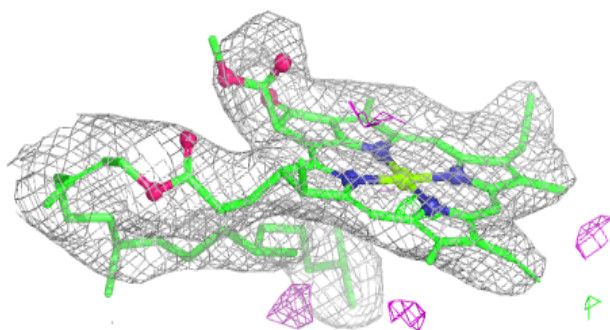
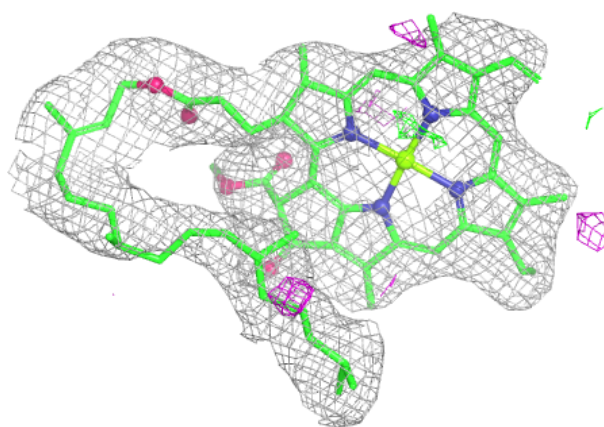
**Electron density around CLA A1 404:**

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



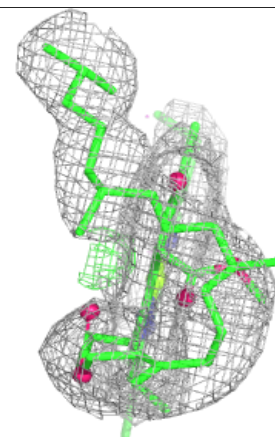
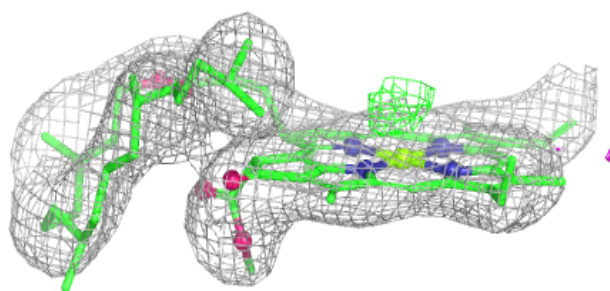
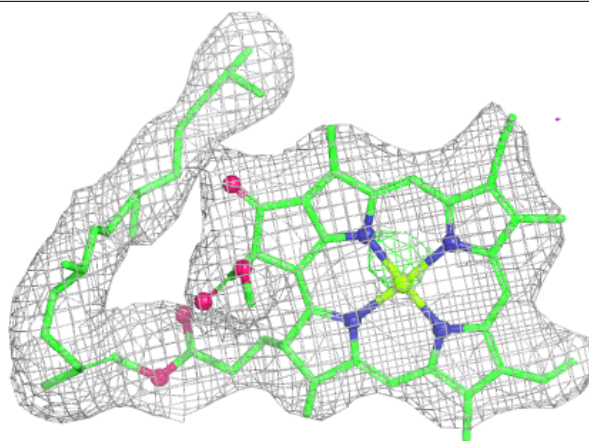
**Electron density around CLA C1 510:**

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



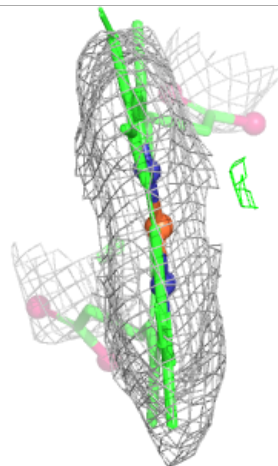
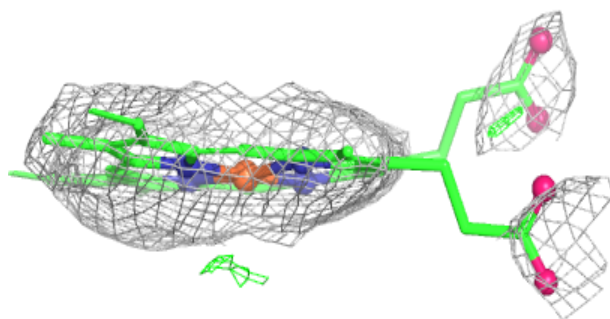
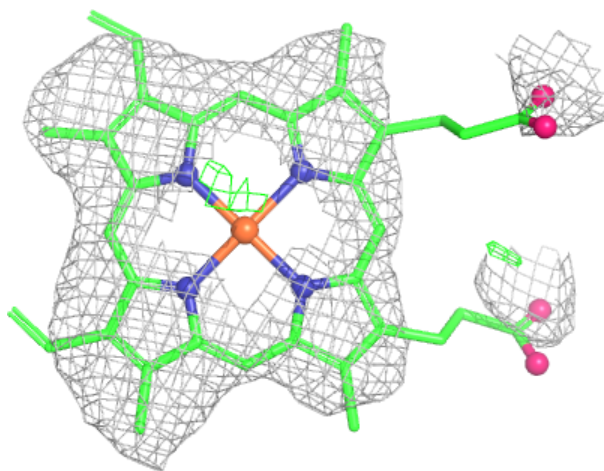
**Electron density around CLA B1 612:**

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



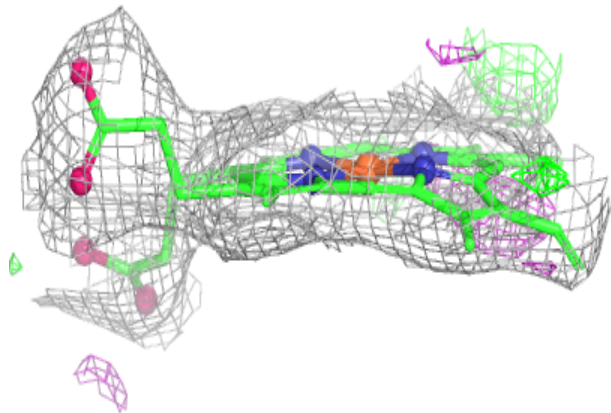
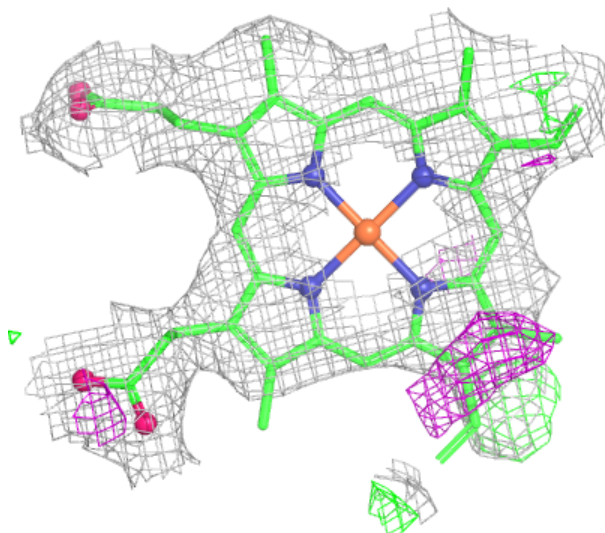
**Electron density around HEM f1 101:**

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



**Electron density around HEM v1 201:**

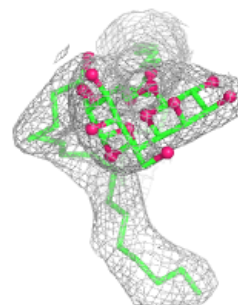
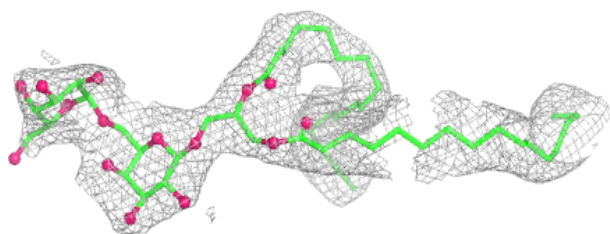
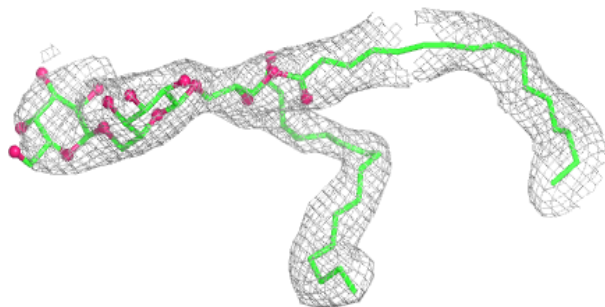
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



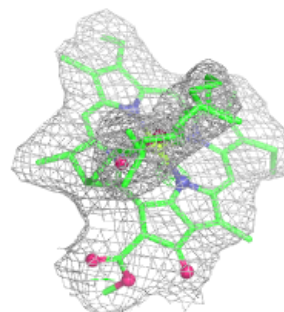
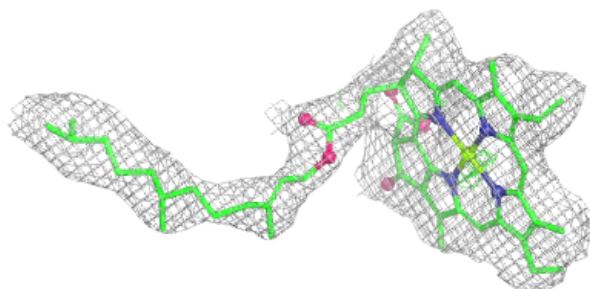
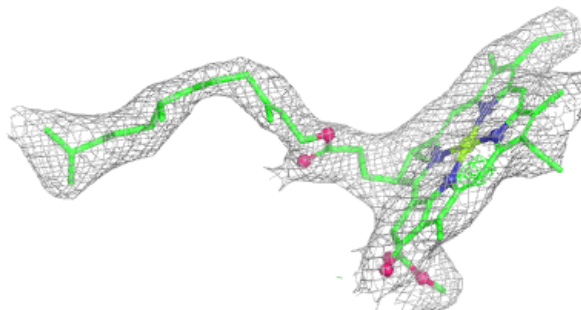


**Electron density around DGD h2 102:**

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

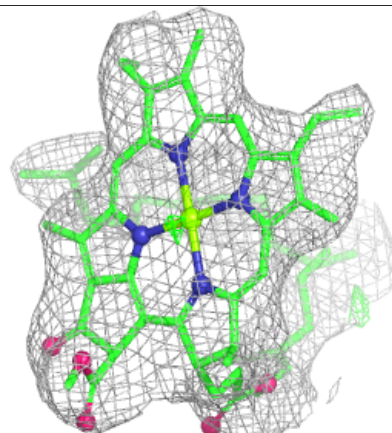
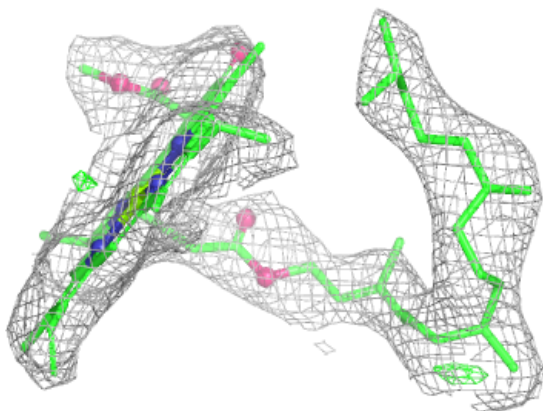
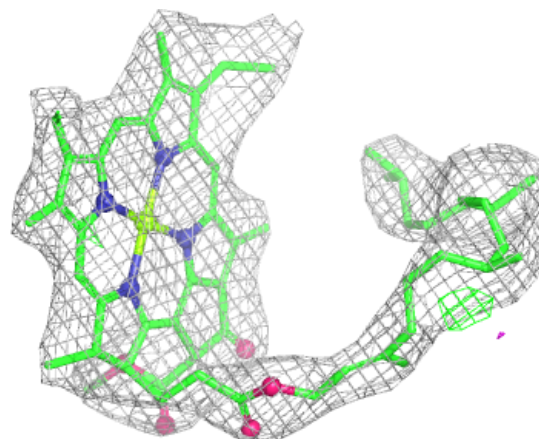
**Electron density around CLA C1 503:**

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

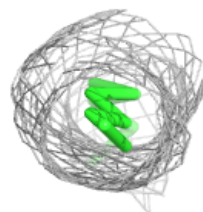
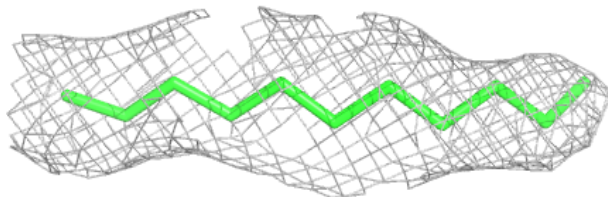
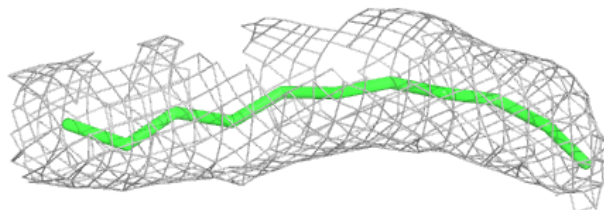


**Electron density around CLA C1 504:**

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

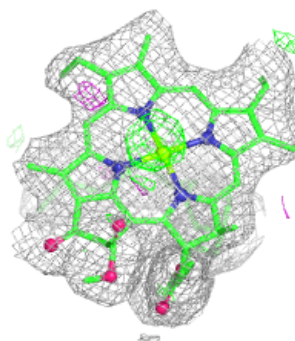
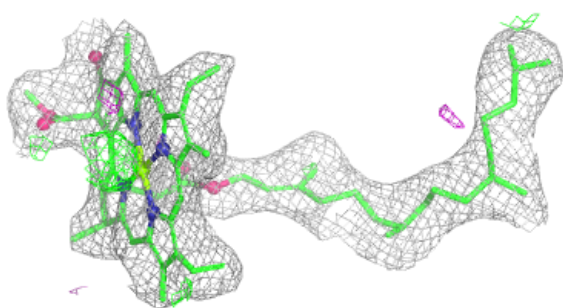
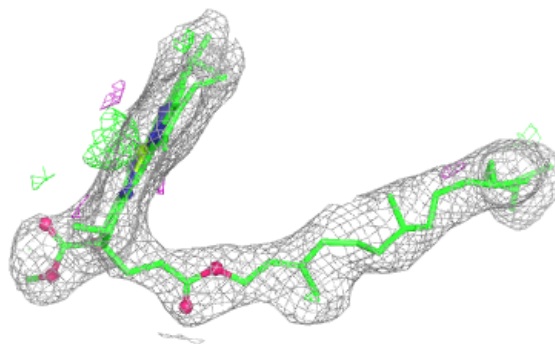
**Electron density around LMT M1 102:**

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

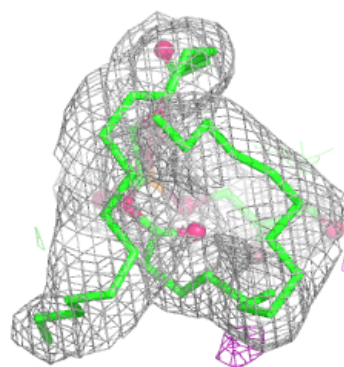
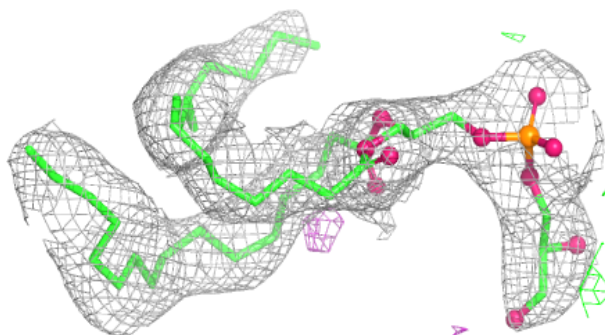
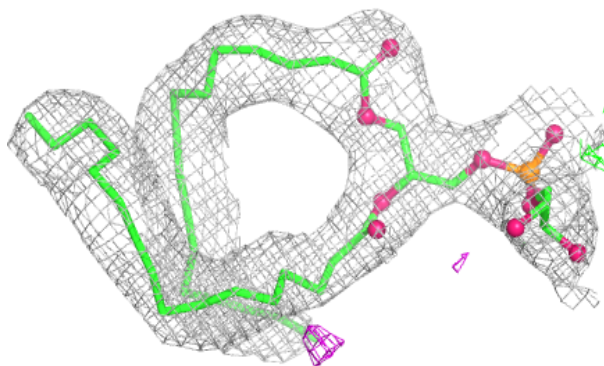


**Electron density around CLA b1 620:**

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

**Electron density around LHG D2 403:**

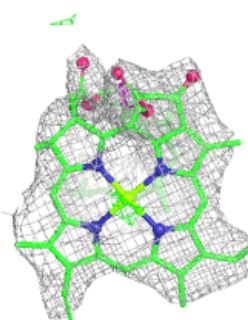
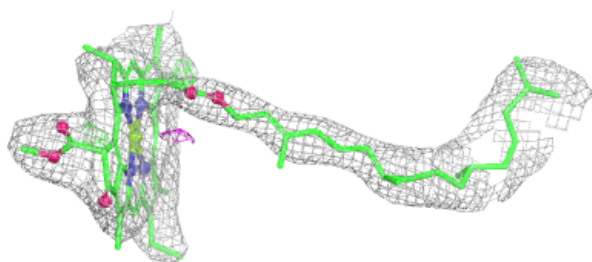
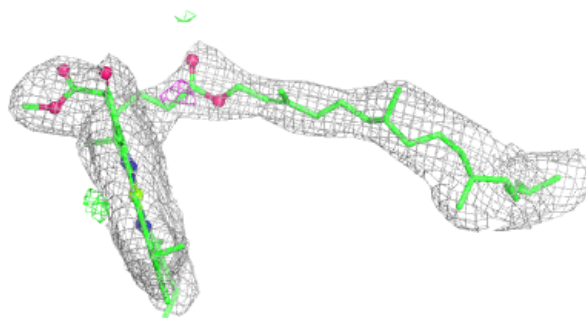
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



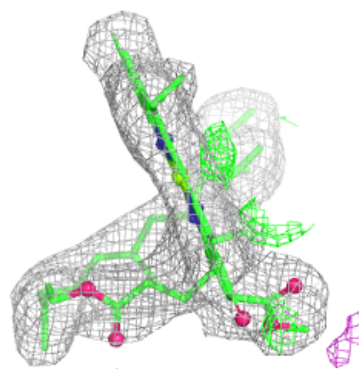
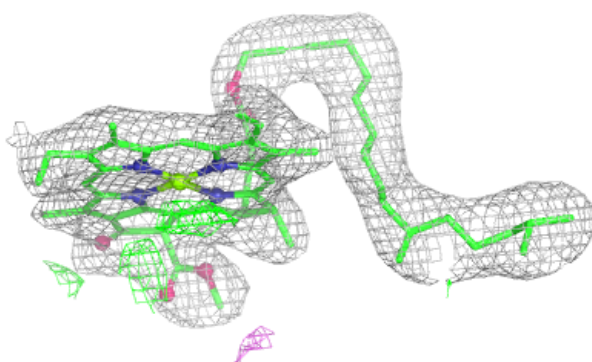
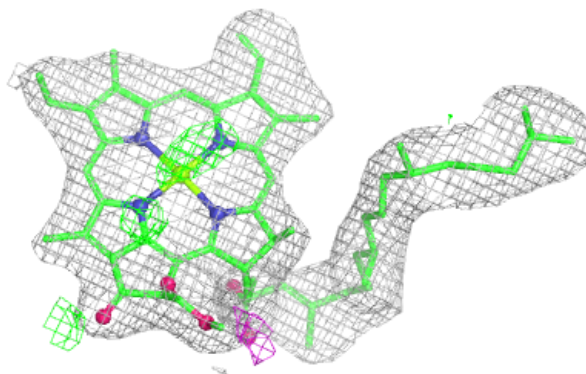


**Electron density around CLA b2 608:**

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

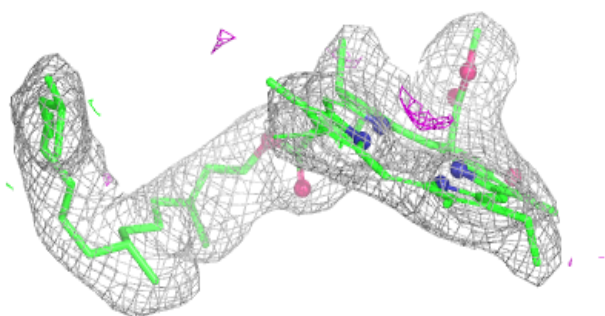
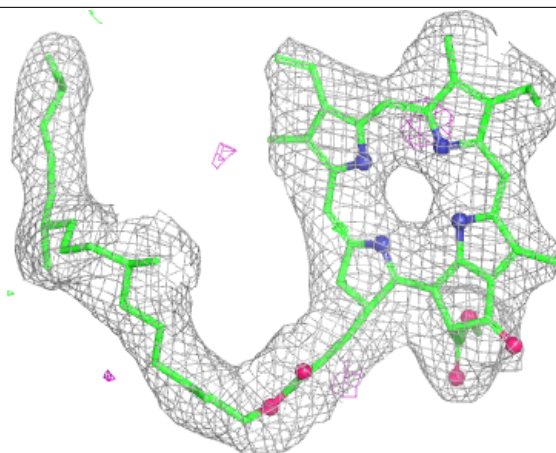
**Electron density around CLA d1 404:**

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

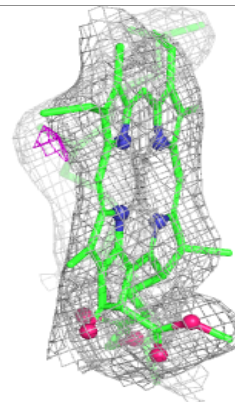
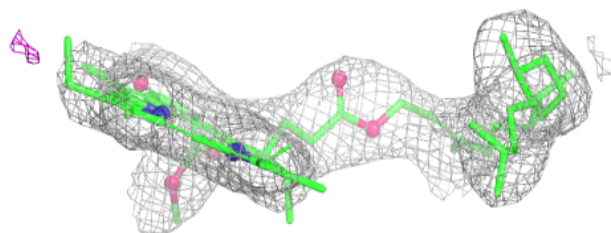
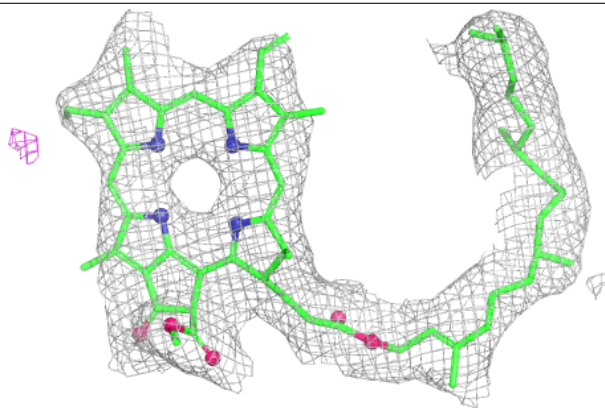


**Electron density around PHO d1 403:**

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

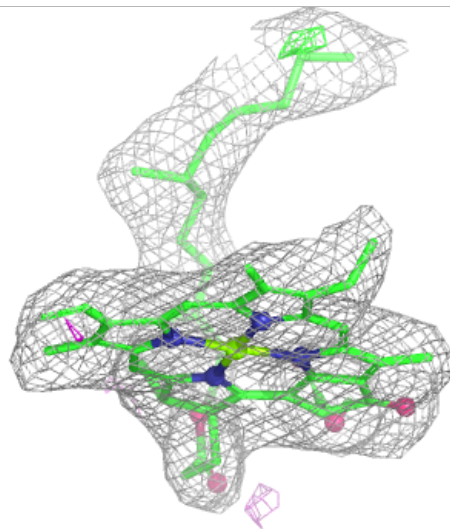
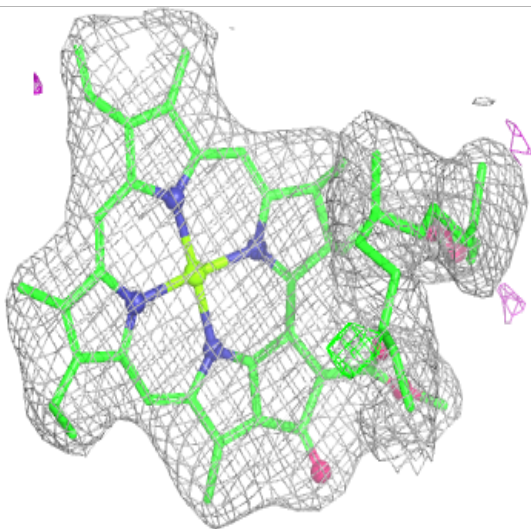
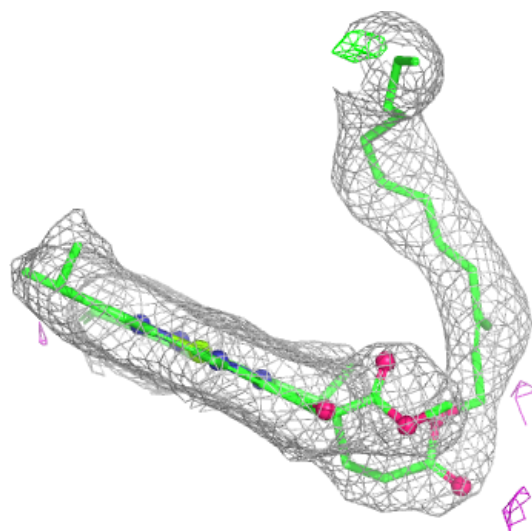
**Electron density around PHO A2 407:**

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



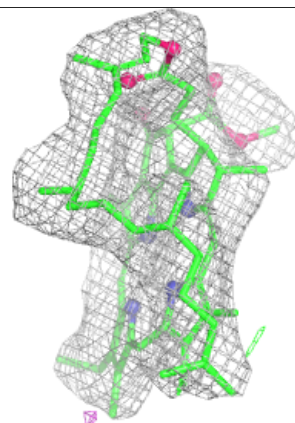
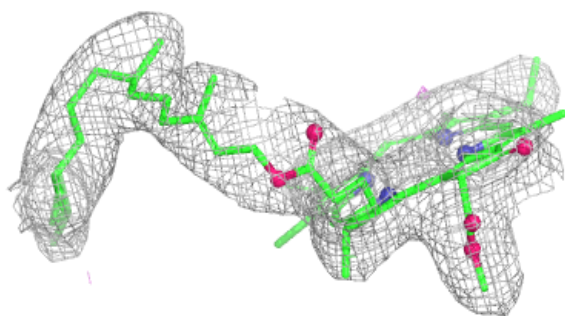
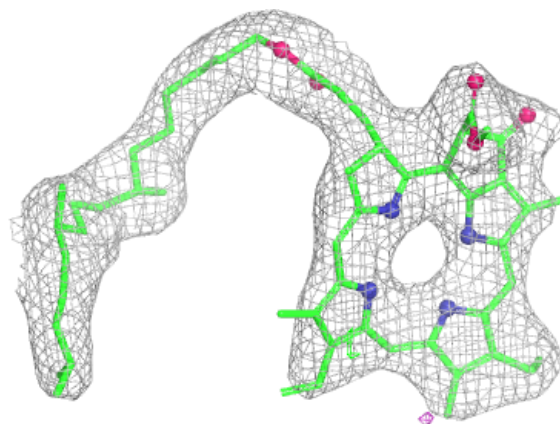
**Electron density around CLA b1 615:**

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



**Electron density around PHO d2 408:**

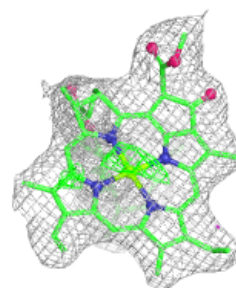
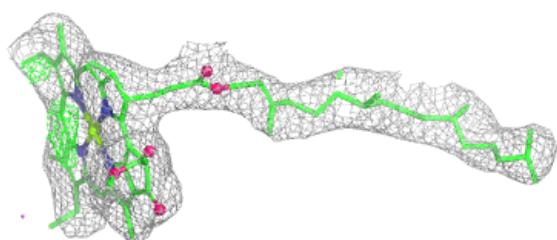
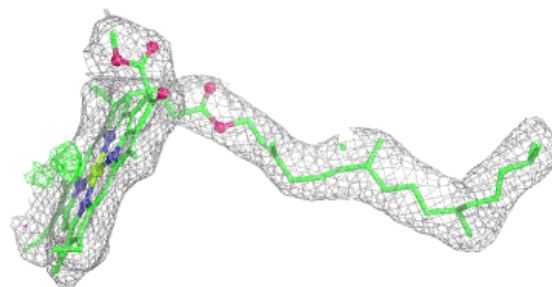
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



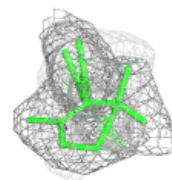
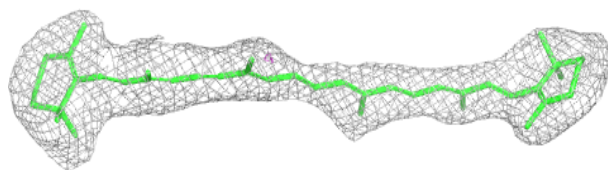
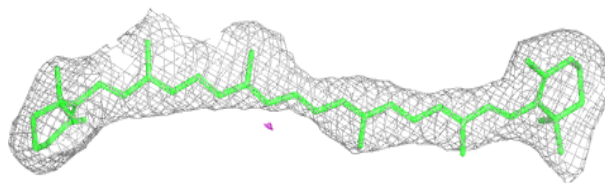


**Electron density around CLA b1 607:**

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

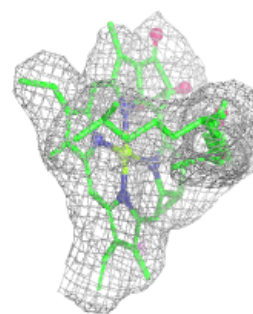
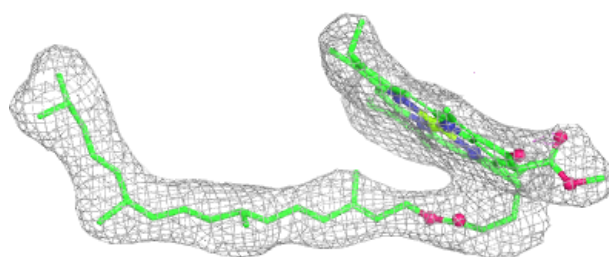
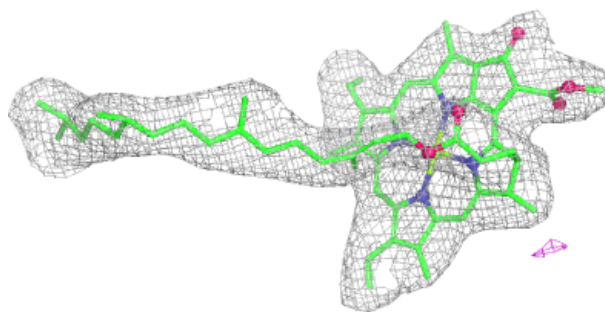
**Electron density around BCR a2 402:**

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



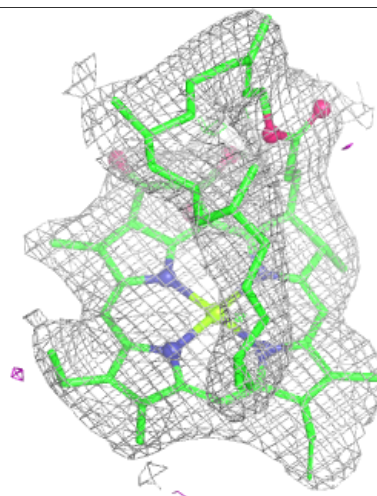
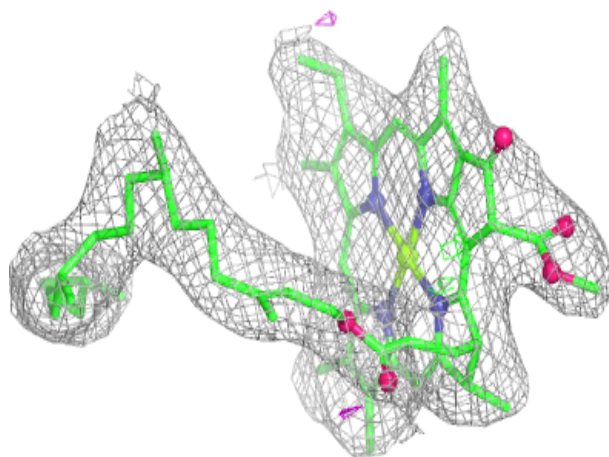
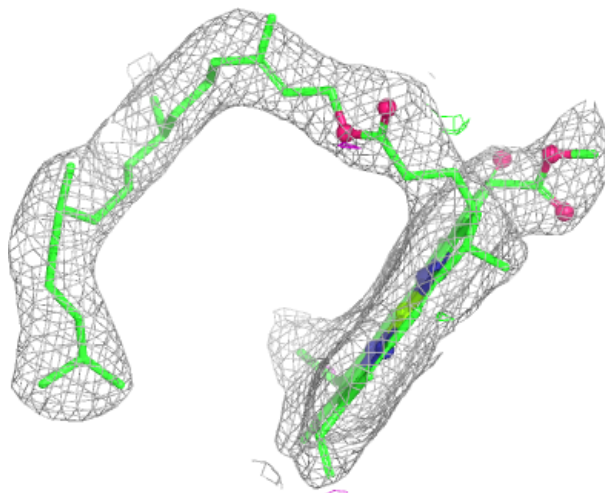
**Electron density around CLA b1 610:**

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



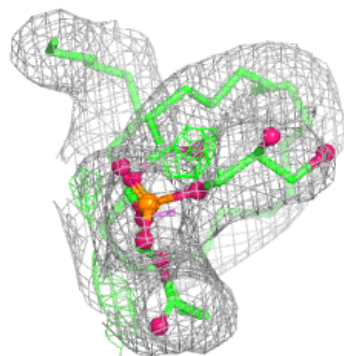
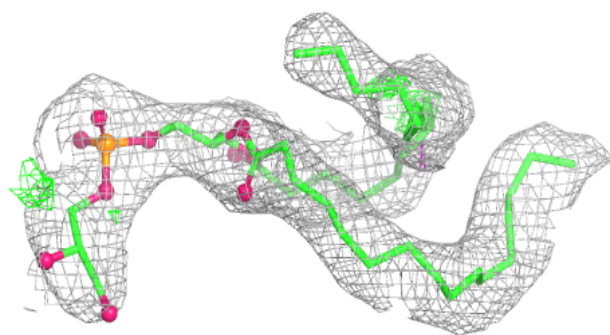
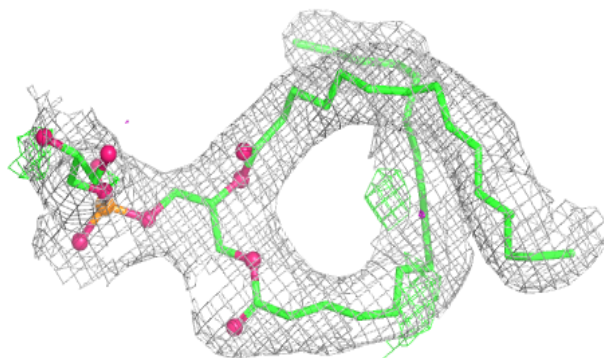
**Electron density around CLA B1 613:**

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



**Electron density around LHG b1 622:**

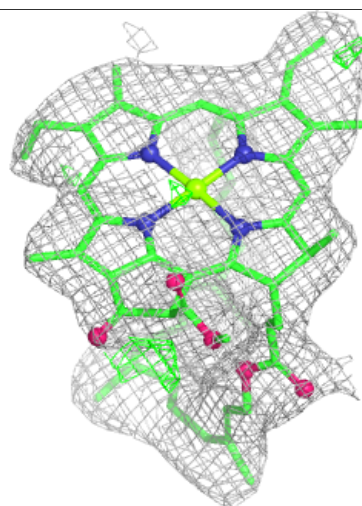
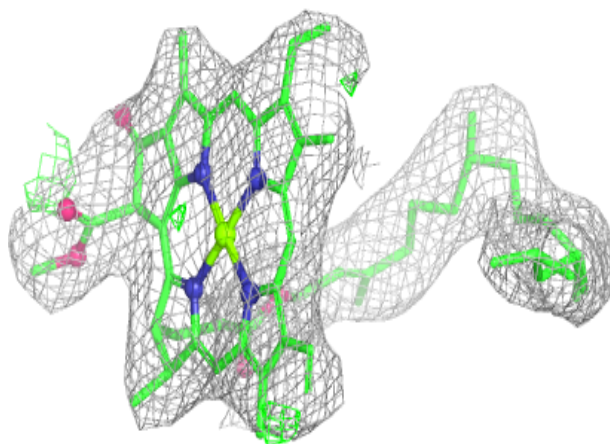
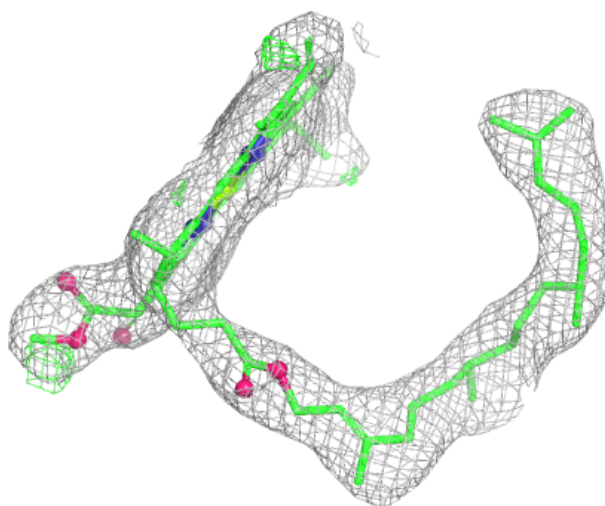
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





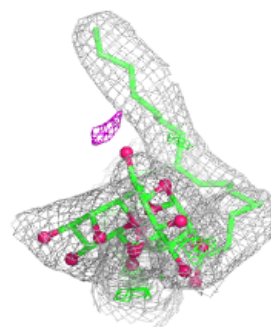
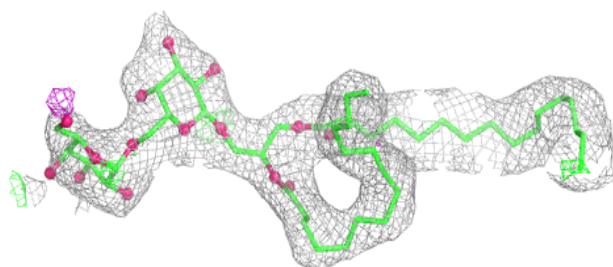
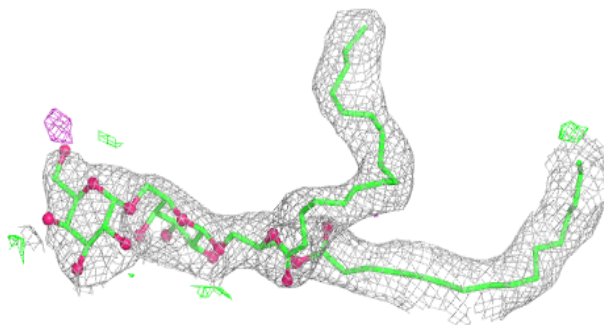
**Electron density around CLA B2 613:**

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



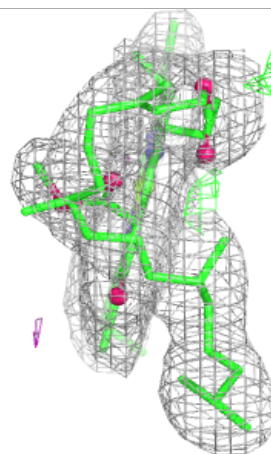
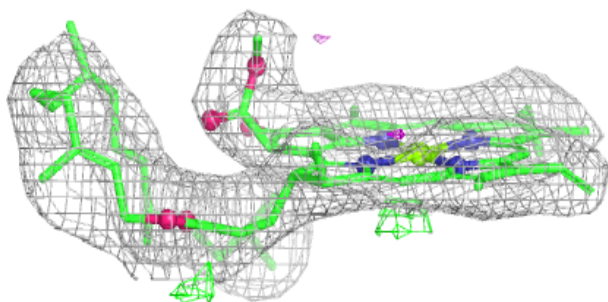
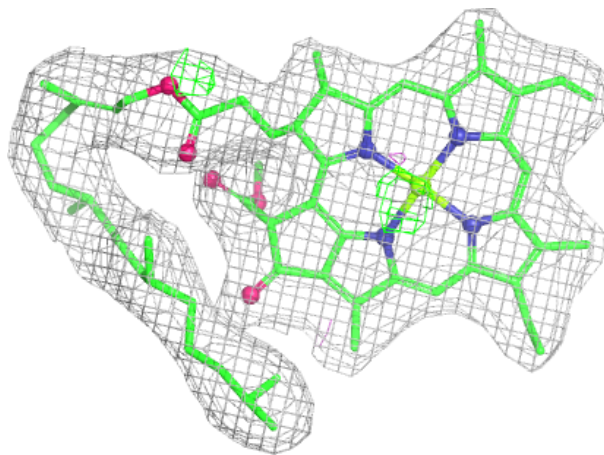
**Electron density around DGD h1 101:**

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



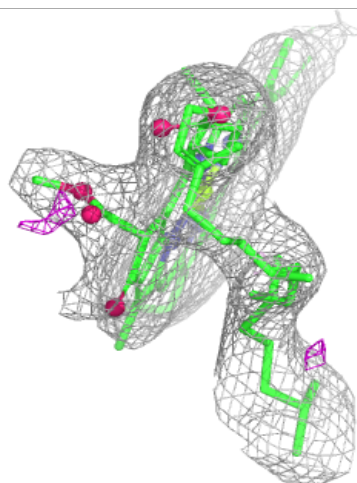
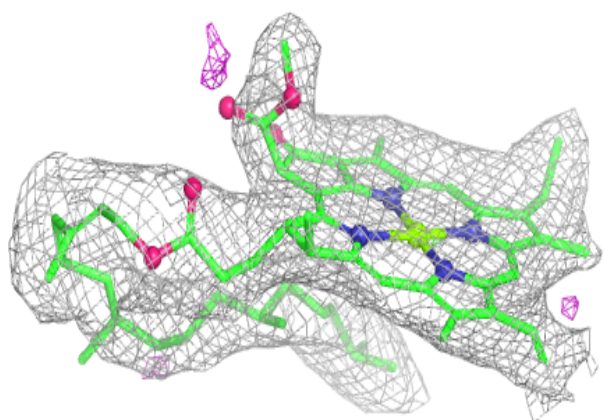
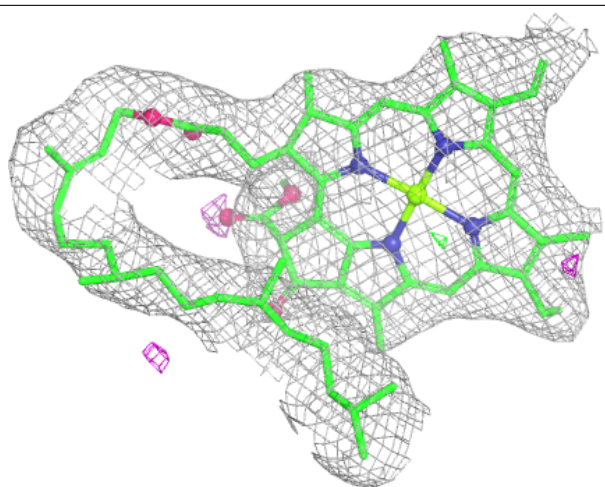
**Electron density around CLA b1 612:**

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



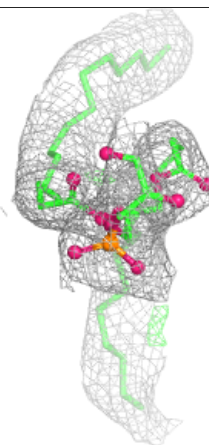
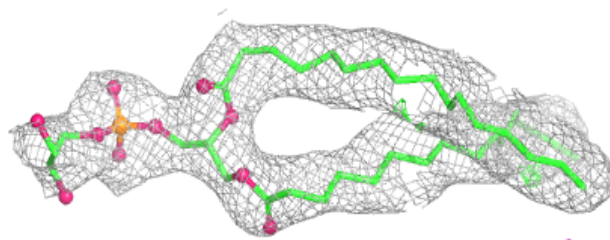
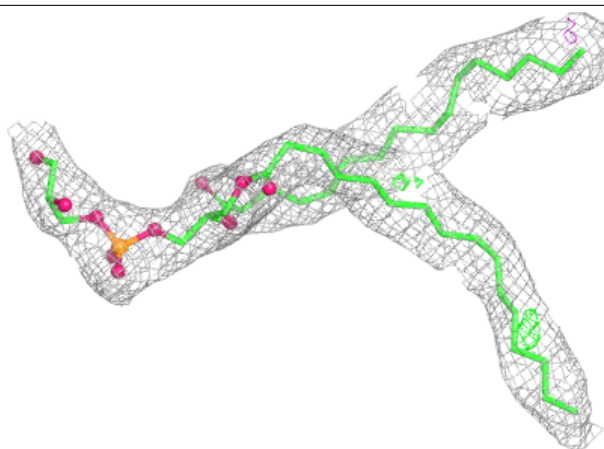
**Electron density around CLA c1 511:**

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



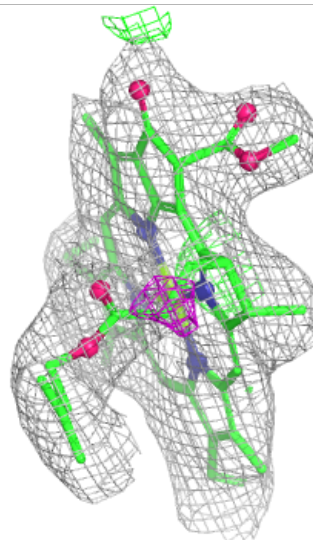
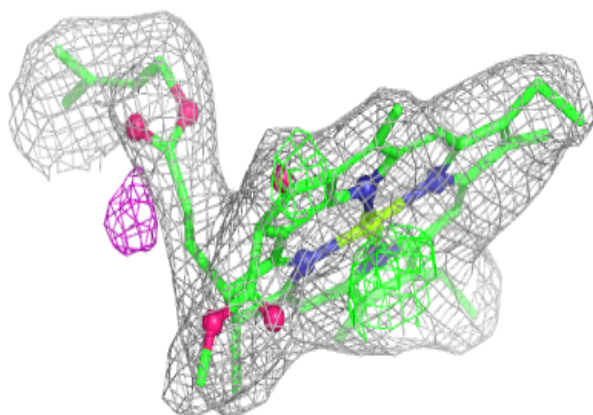
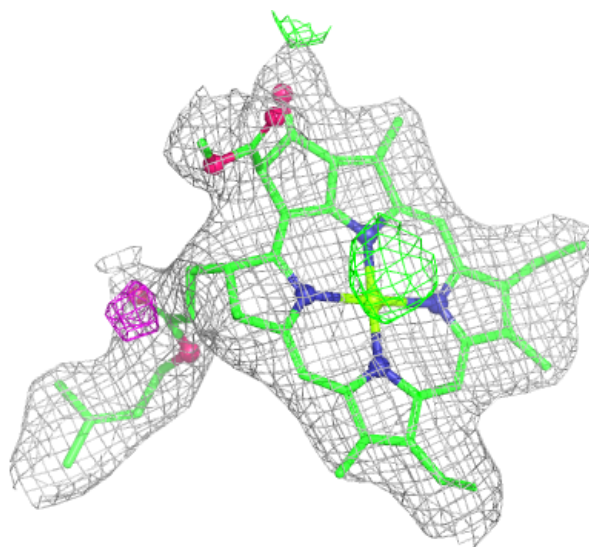
**Electron density around LHG d1 407:**

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



**Electron density around CLA a1 405:**

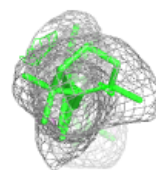
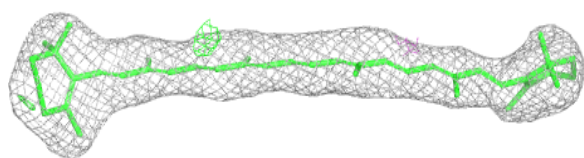
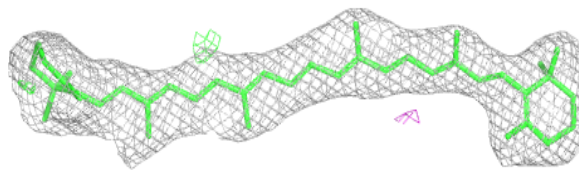
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





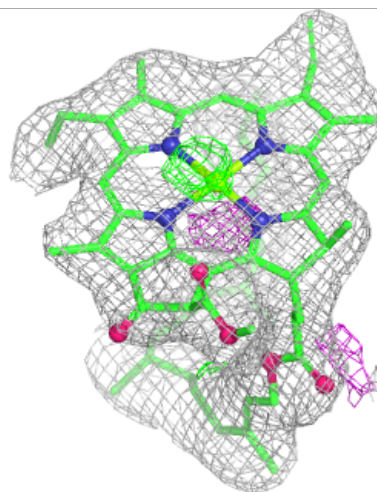
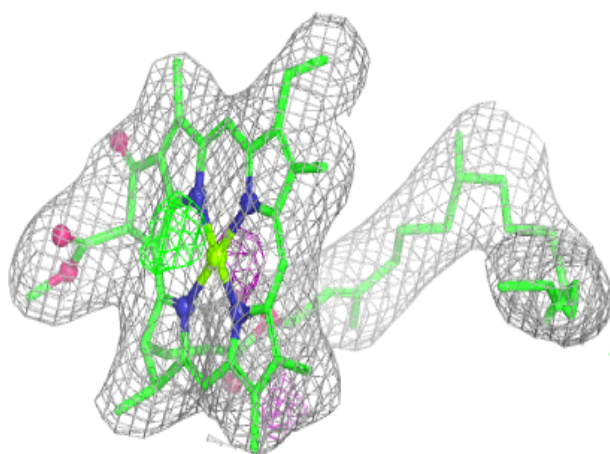
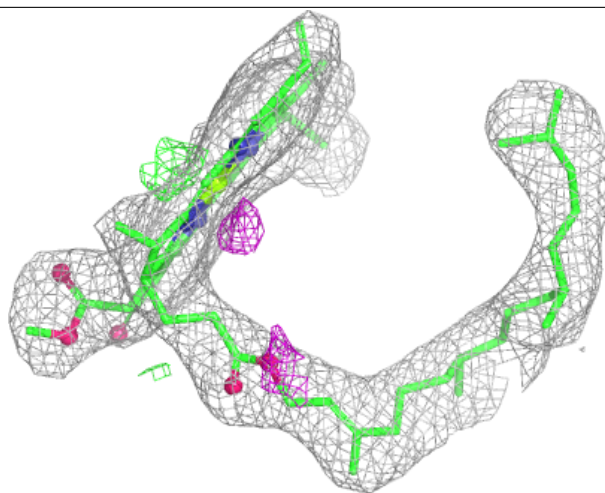
**Electron density around BCR b1 601:**

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



**Electron density around CLA b1 613:**

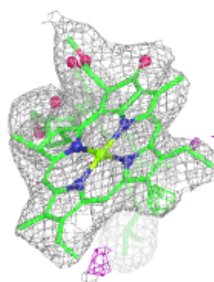
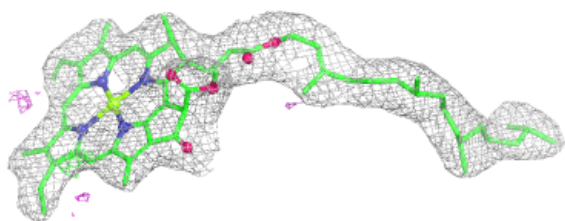
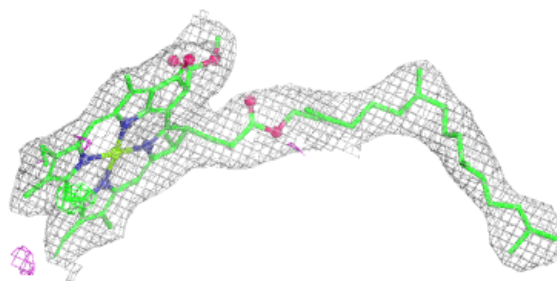
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





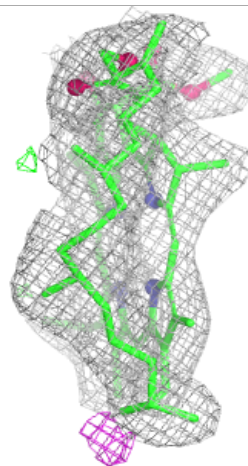
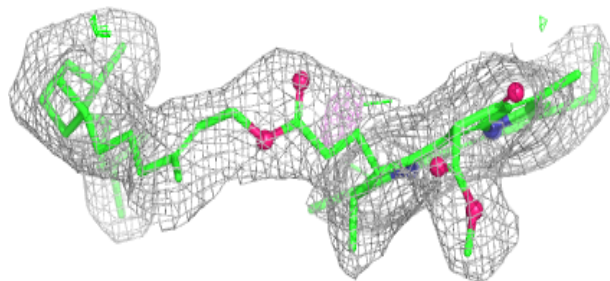
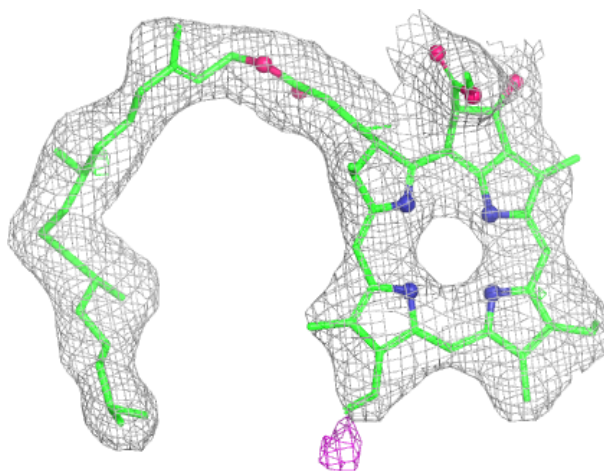
**Electron density around CLA a2 404:**

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



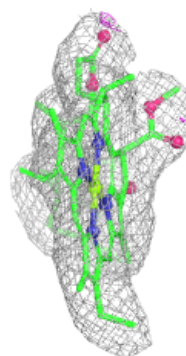
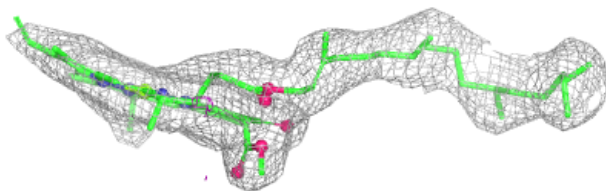
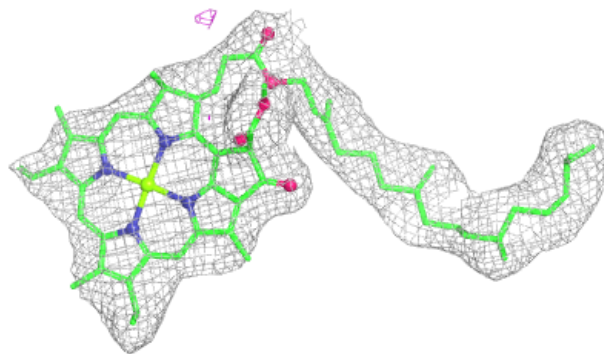
**Electron density around PHO a2 416:**

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



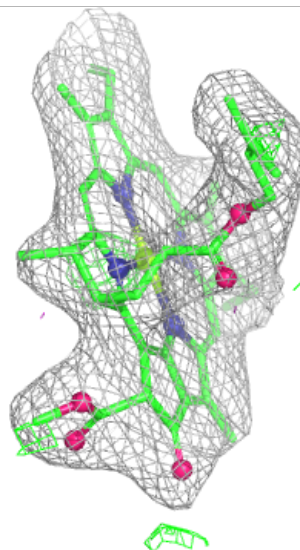
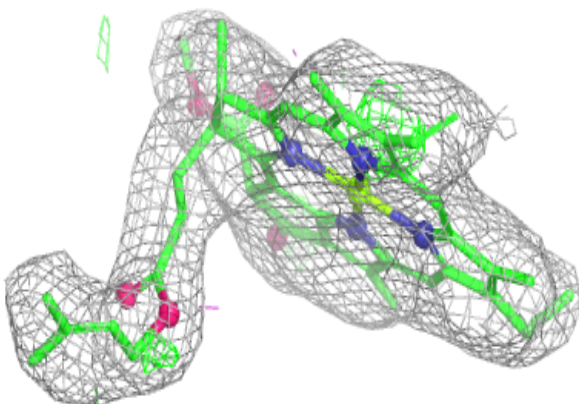
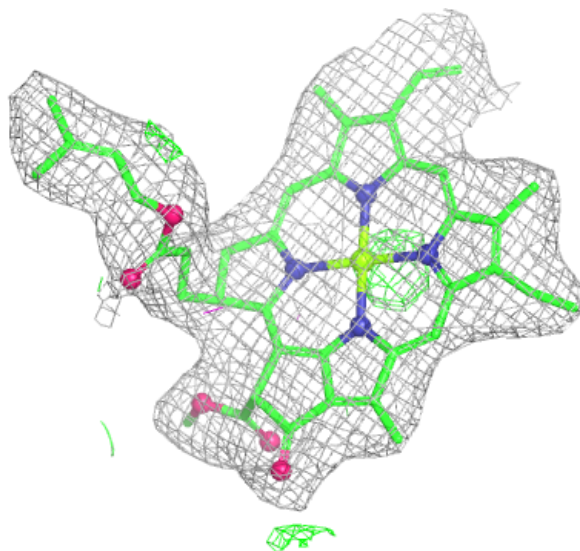
**Electron density around CLA b1 605:**

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



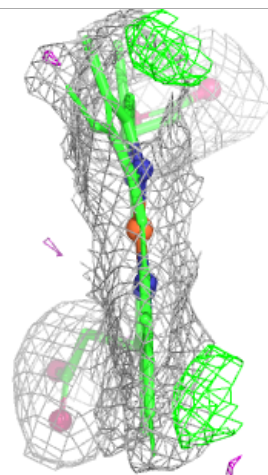
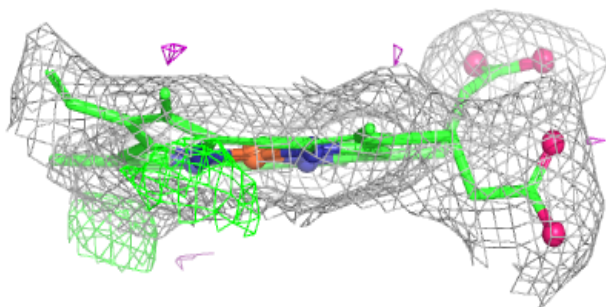
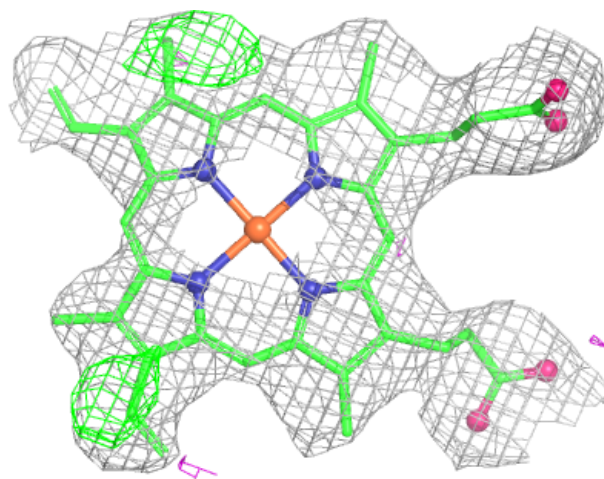
**Electron density around CLA a2 413:**

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



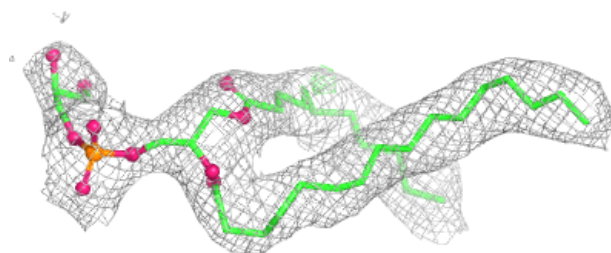
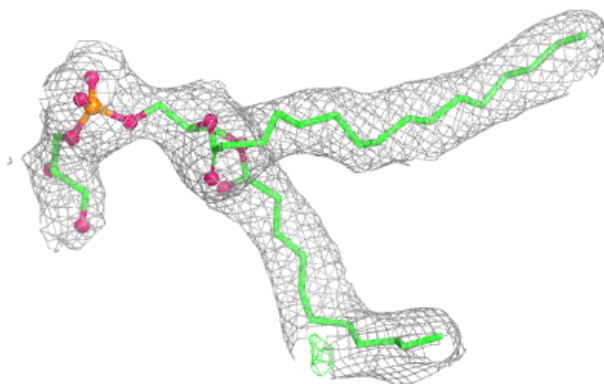
**Electron density around HEM V1 201:**

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

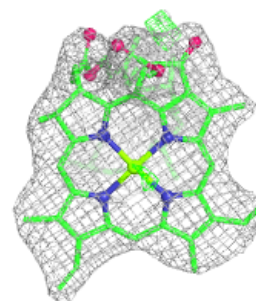
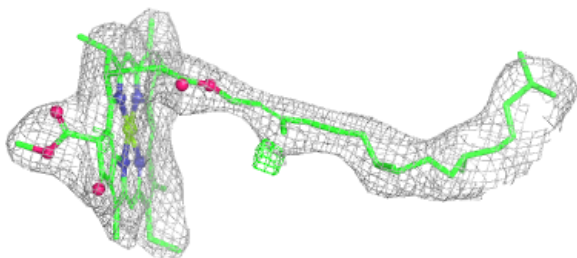
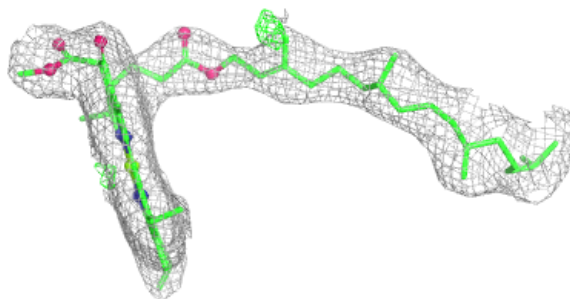


**Electron density around LHG 12 101:**

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

**Electron density around CLA B2 608:**

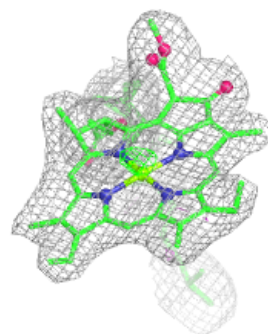
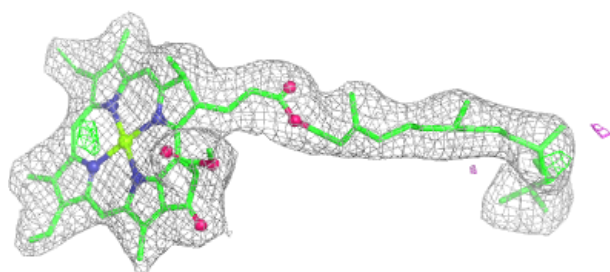
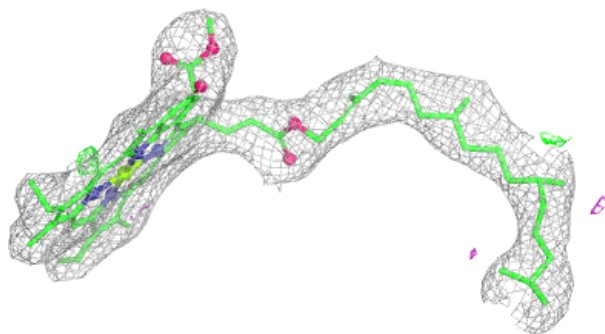
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



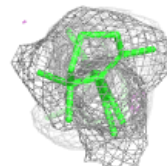
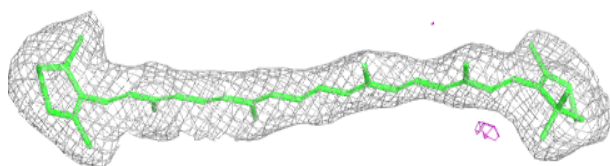
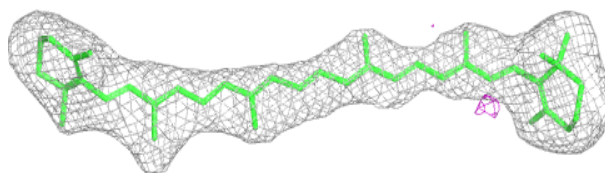


**Electron density around CLA D1 402:**

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

**Electron density around BCR A1 401:**

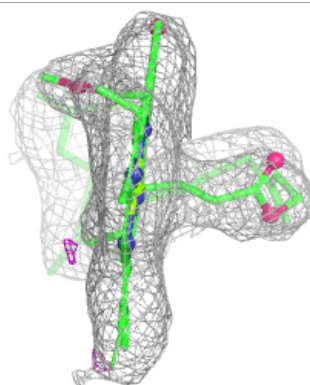
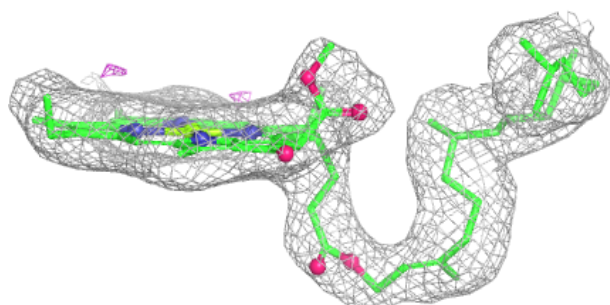
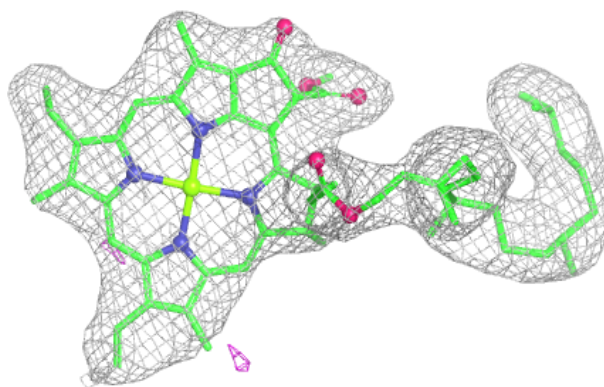
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



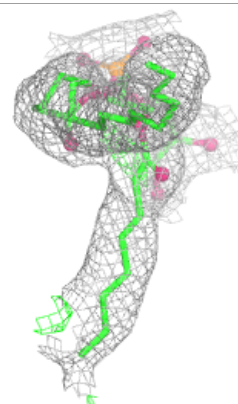
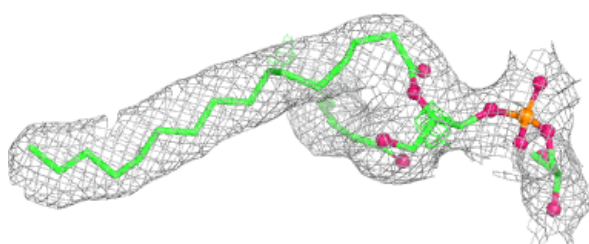
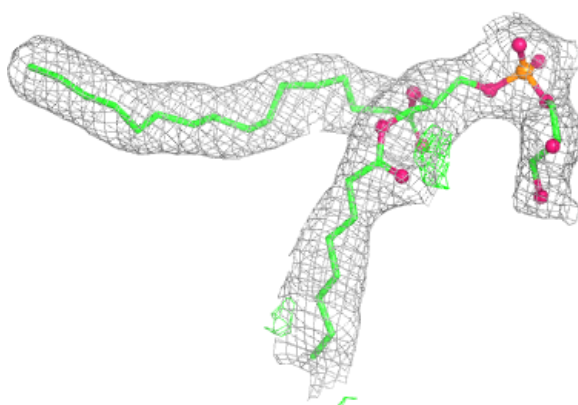


**Electron density around CLA B1 614:**

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

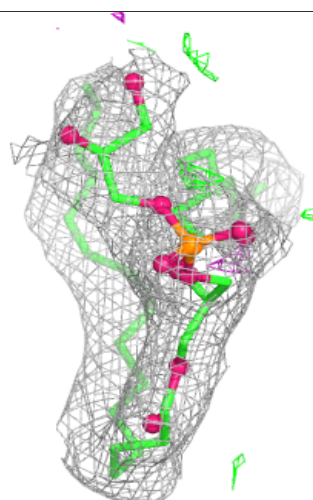
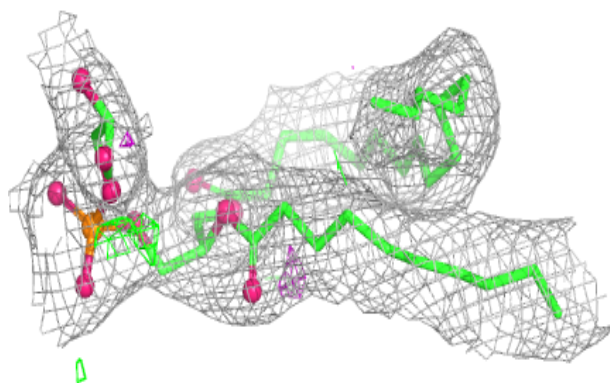
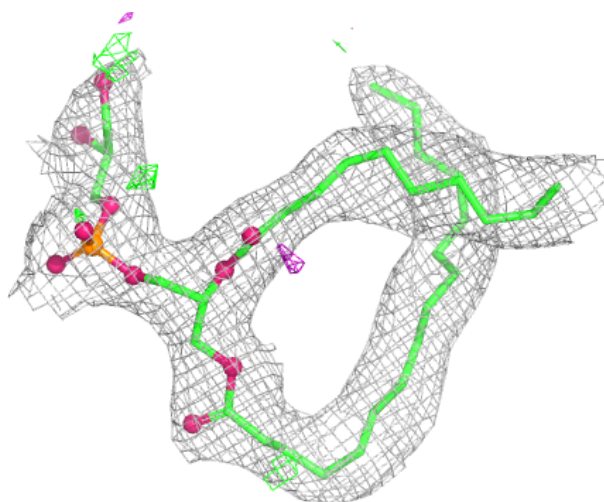
**Electron density around LHG L1 101:**

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



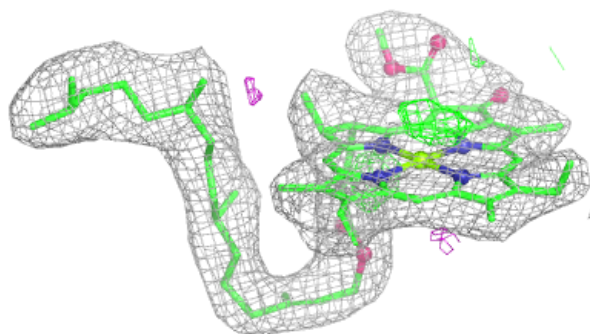
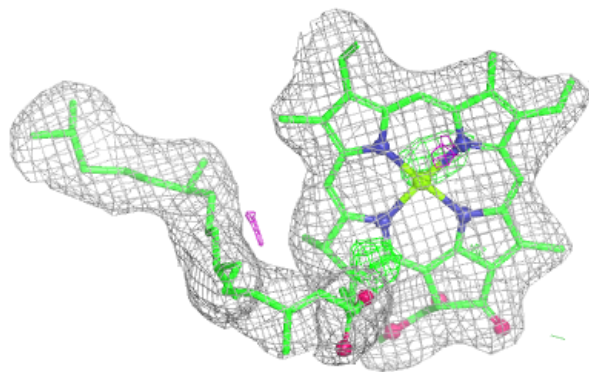
**Electron density around LHG a1 407:**

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



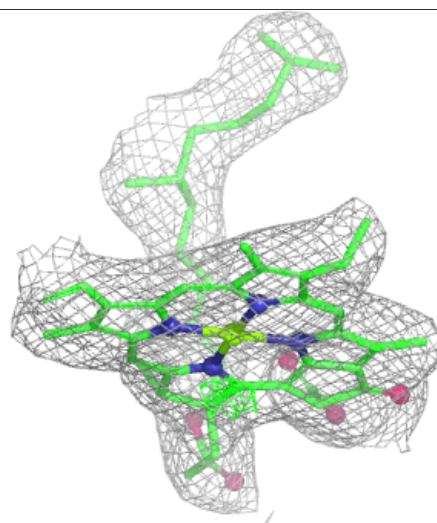
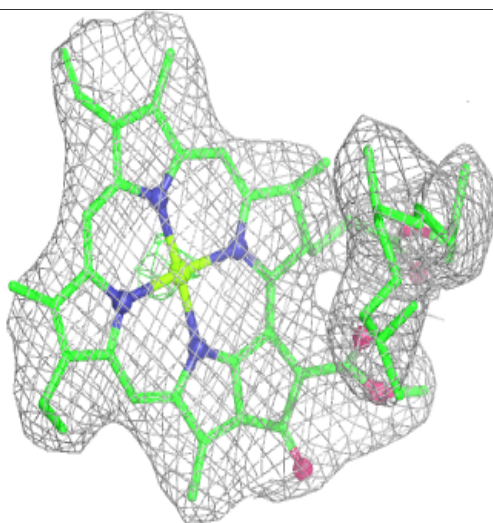
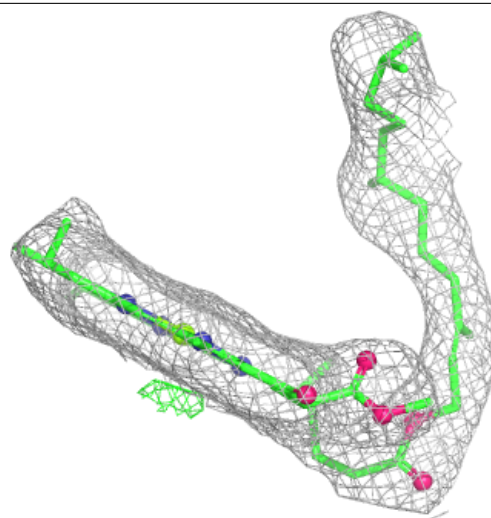
**Electron density around CLA d2 402:**

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



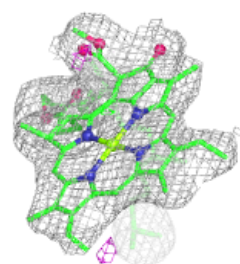
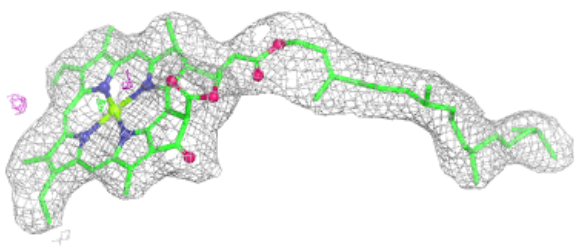
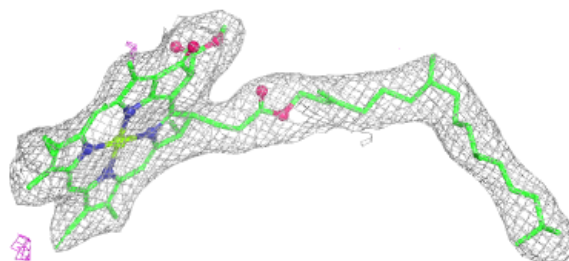
**Electron density around CLA b2 615:**

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

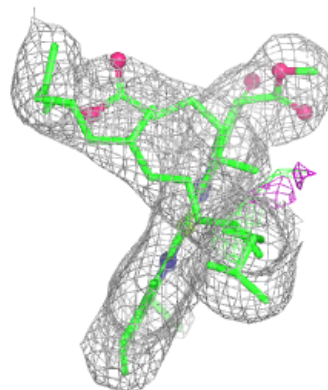
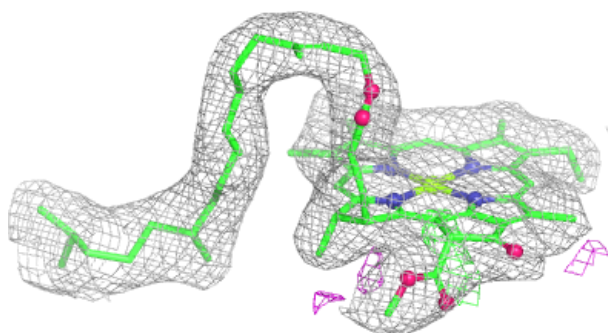
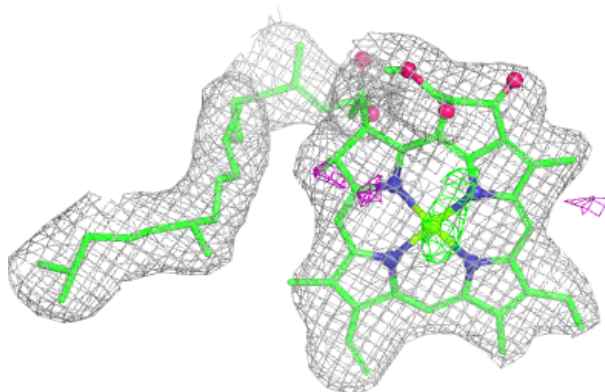


**Electron density around CLA a1 403:**

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

**Electron density around CLA A1 406:**

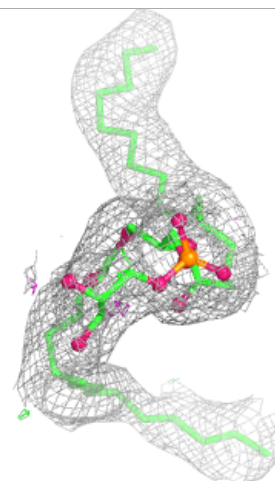
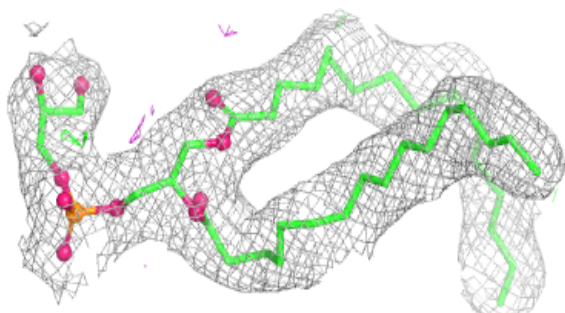
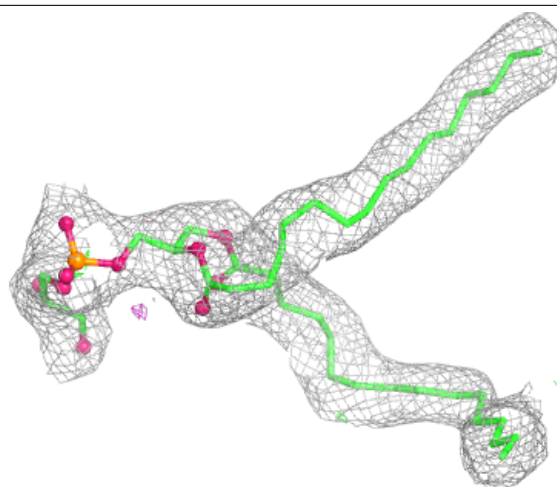
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





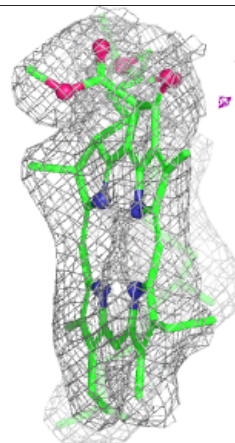
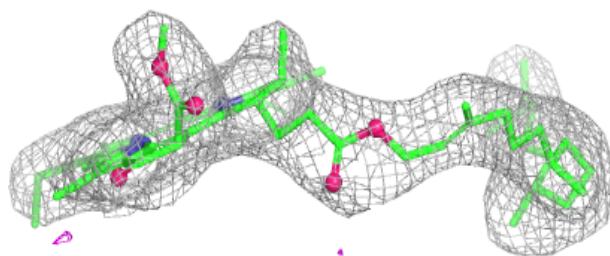
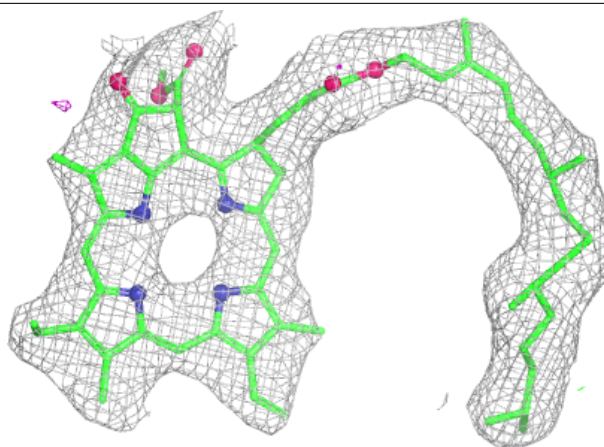
**Electron density around LHG l1 102:**

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



**Electron density around PHO A1 408:**

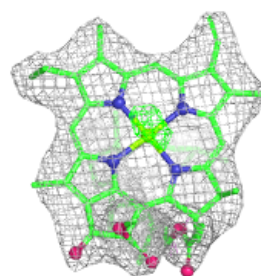
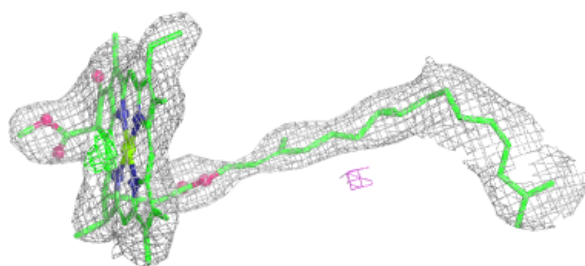
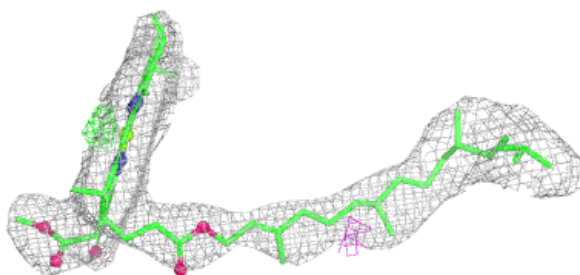
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





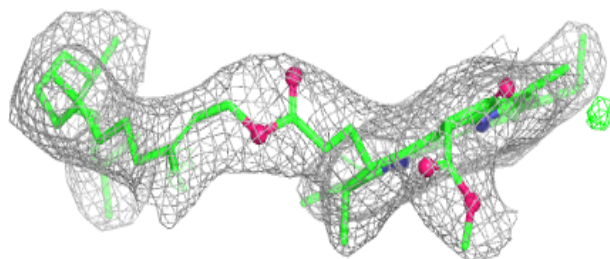
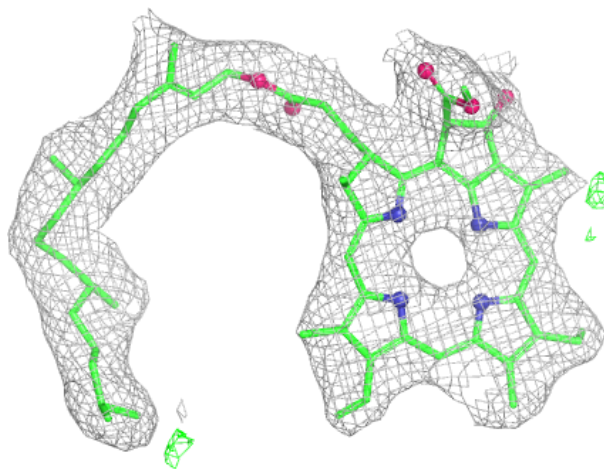
**Electron density around CLA B1 608:**

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



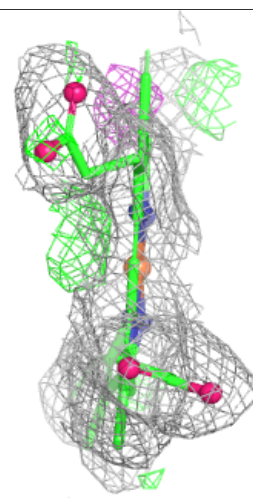
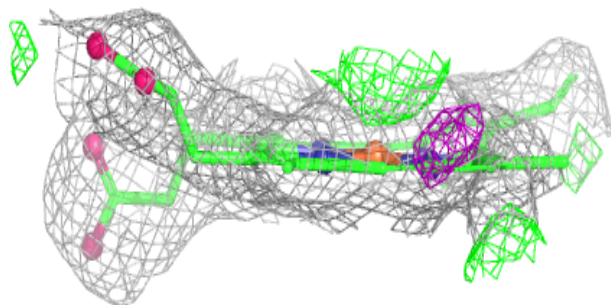
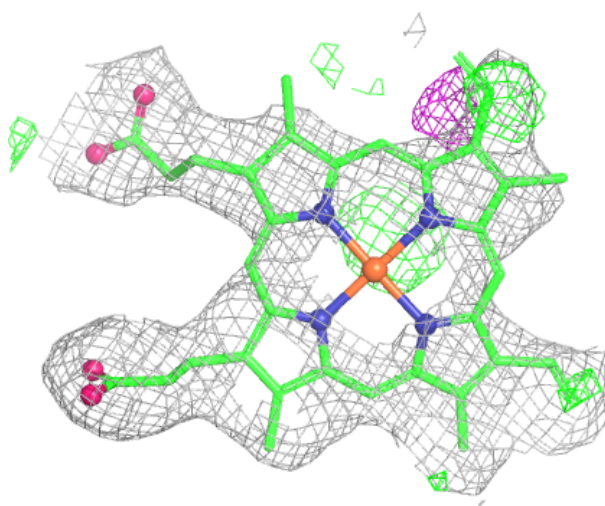
**Electron density around PHO a1 411:**

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



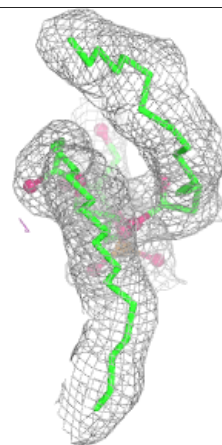
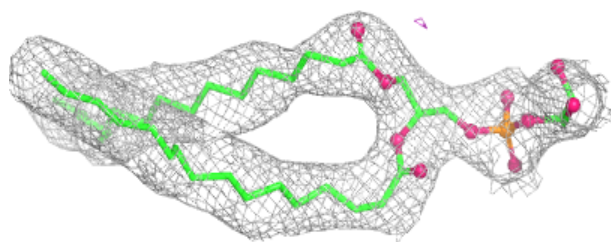
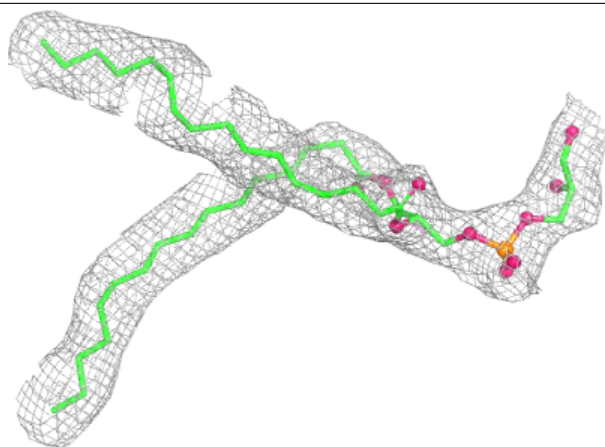
**Electron density around HEM v2 201:**

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

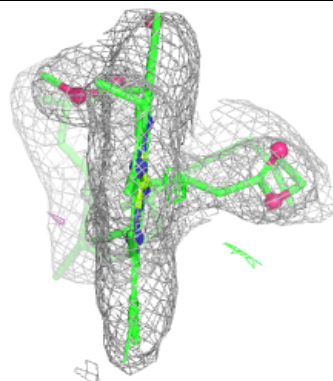
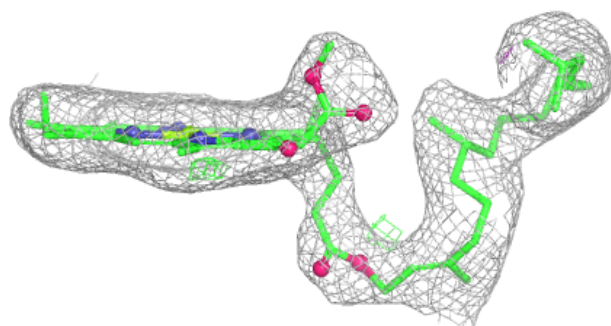
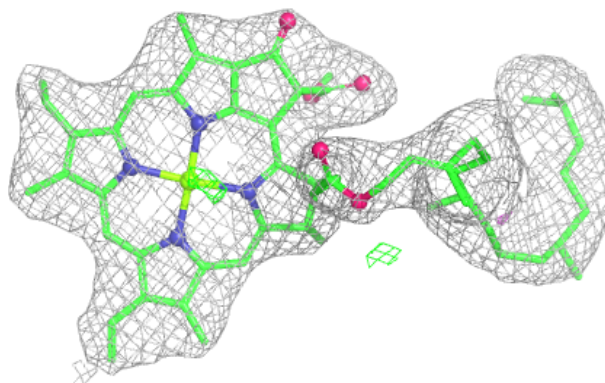


**Electron density around LHG D1 405:**

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

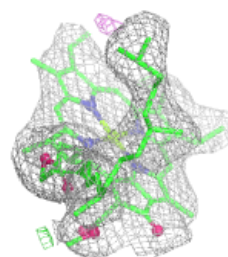
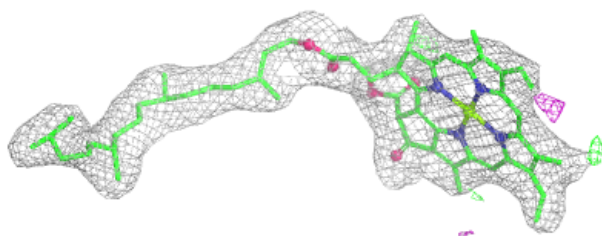
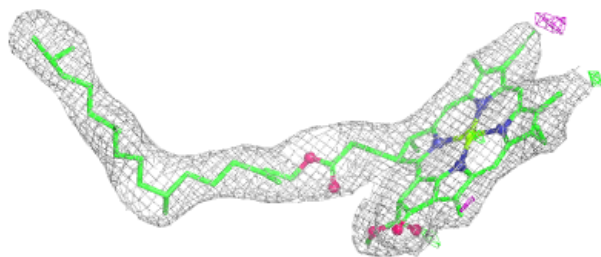
**Electron density around CLA b1 614:**

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

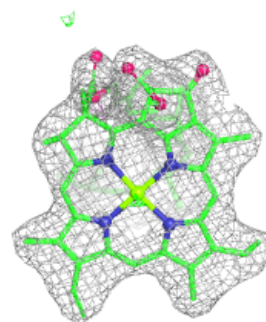
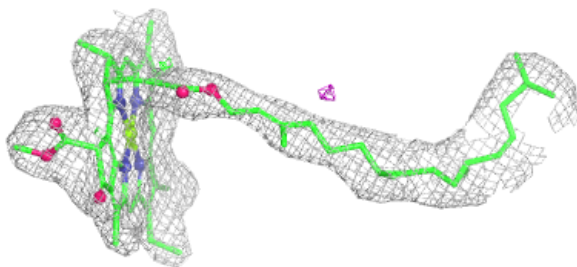
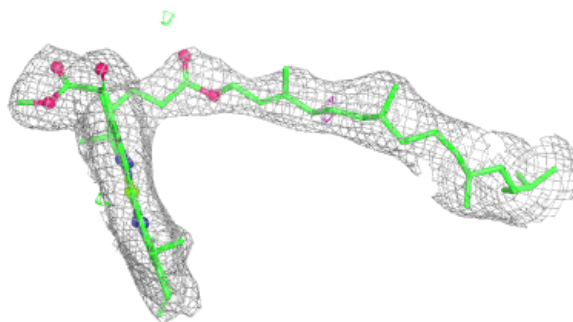


**Electron density around CLA A1 403:**

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

**Electron density around CLA b1 608:**

$2mF_o-DF_c$  (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.