



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:41 AM UTC

PDB ID : 4TNI / pdb\_00004tni  
Title : RT XFEL structure of Photosystem II 500 ms after the third illumination at 4.6 Å resolution  
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.  
Deposited on : 2014-06-04  
Resolution : 4.60 Å (reported)

This is a Full wwPDB X-ray Structure Validation 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

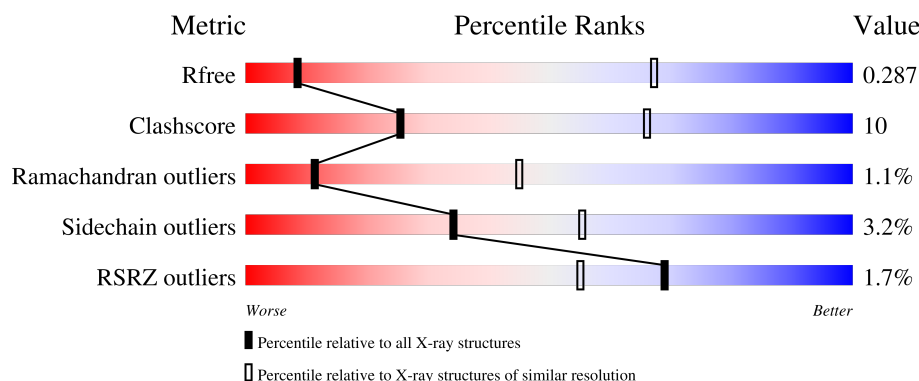
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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                      | 1007 (5.28-3.92)                                      |
| Clashscore            | 190562                      | 1022 (5.26-3.94)                                      |
| Ramachandran outliers | 187476                      | 1069 (5.30-3.90)                                      |
| Sidechain outliers    | 187428                      | 1051 (5.30-3.90)                                      |
| RSRZ outliers         | 180081                      | 1002 (5.28-3.92)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 344    |                  |

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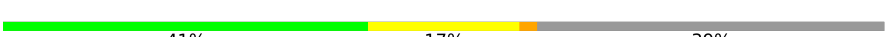
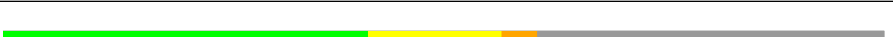
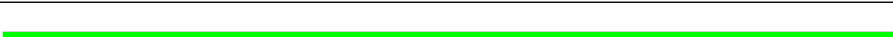
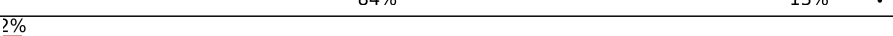
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
 CCP4 : 9.0.010 (Gargrove)  
 Density-Fitness : 1.0.12  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | a     | 344    |                  |
| 2   | B     | 510    |                  |
| 2   | b     | 510    |                  |
| 3   | C     | 461    |                  |
| 3   | c     | 461    |                  |
| 4   | D     | 352    |                  |
| 4   | d     | 352    |                  |
| 5   | E     | 84     |                  |
| 5   | e     | 84     |                  |
| 6   | F     | 45     |                  |
| 6   | f     | 45     |                  |
| 7   | H     | 66     |                  |
| 7   | h     | 66     |                  |
| 8   | I     | 38     |                  |
| 8   | i     | 38     |                  |
| 9   | J     | 40     |                  |
| 9   | j     | 40     |                  |
| 10  | K     | 46     |                  |
| 10  | k     | 46     |                  |
| 11  | L     | 37     |                  |
| 11  | l     | 37     |                  |
| 12  | M     | 36     |                  |
| 12  | m     | 36     |                  |
| 13  | O     | 272    |                  |
| 13  | o     | 272    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 14  | T     | 32     |    |
| 14  | t     | 32     |    |
| 15  | U     | 134    |    |
| 15  | u     | 134    |    |
| 16  | V     | 163    |    |
| 16  | v     | 163    |    |
| 17  | g     | 46     |    |
| 17  | y     | 46     |    |
| 18  | X     | 41     |    |
| 18  | x     | 41     |    |
| 19  | G     | 28     |    |
| 19  | Y     | 28     |    |
| 20  | Z     | 62     |  |
| 20  | z     | 62     |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | A     | 402 | X         | -        | -       | -                |
| 22  | CLA  | A     | 403 | X         | -        | -       | -                |
| 22  | CLA  | A     | 404 | X         | -        | -       | -                |
| 22  | CLA  | A     | 405 | X         | -        | -       | -                |
| 22  | CLA  | B     | 601 | X         | -        | -       | -                |
| 22  | CLA  | B     | 602 | X         | -        | -       | -                |
| 22  | CLA  | B     | 603 | X         | -        | -       | -                |
| 22  | CLA  | B     | 604 | X         | -        | -       | -                |
| 22  | CLA  | B     | 605 | X         | -        | -       | -                |
| 22  | CLA  | B     | 606 | X         | -        | -       | -                |
| 22  | CLA  | B     | 607 | X         | -        | -       | -                |
| 22  | CLA  | B     | 608 | X         | -        | -       | -                |
| 22  | CLA  | B     | 609 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | B     | 610 | X         | -        | -       | -                |
| 22  | CLA  | B     | 611 | X         | -        | -       | -                |
| 22  | CLA  | B     | 612 | X         | -        | -       | -                |
| 22  | CLA  | B     | 613 | X         | -        | -       | -                |
| 22  | CLA  | B     | 614 | X         | -        | -       | -                |
| 22  | CLA  | B     | 615 | X         | -        | -       | -                |
| 22  | CLA  | C     | 501 | X         | -        | -       | -                |
| 22  | CLA  | C     | 502 | X         | -        | -       | -                |
| 22  | CLA  | C     | 503 | X         | -        | -       | -                |
| 22  | CLA  | C     | 504 | X         | -        | -       | -                |
| 22  | CLA  | C     | 505 | X         | -        | -       | -                |
| 22  | CLA  | C     | 506 | X         | -        | -       | -                |
| 22  | CLA  | C     | 507 | X         | -        | -       | -                |
| 22  | CLA  | C     | 508 | X         | -        | -       | -                |
| 22  | CLA  | C     | 509 | X         | -        | -       | -                |
| 22  | CLA  | C     | 510 | X         | -        | -       | -                |
| 22  | CLA  | C     | 511 | X         | -        | -       | -                |
| 22  | CLA  | C     | 512 | X         | -        | -       | -                |
| 22  | CLA  | C     | 520 | X         | -        | -       | -                |
| 22  | CLA  | D     | 405 | X         | -        | -       | -                |
| 22  | CLA  | H     | 101 | X         | -        | -       | -                |
| 22  | CLA  | a     | 404 | X         | -        | -       | -                |
| 22  | CLA  | a     | 405 | X         | -        | -       | -                |
| 22  | CLA  | a     | 406 | X         | -        | -       | -                |
| 22  | CLA  | a     | 407 | X         | -        | -       | -                |
| 22  | CLA  | b     | 605 | X         | -        | -       | -                |
| 22  | CLA  | b     | 606 | X         | -        | -       | -                |
| 22  | CLA  | b     | 607 | X         | -        | -       | -                |
| 22  | CLA  | b     | 608 | X         | -        | -       | -                |
| 22  | CLA  | b     | 609 | X         | -        | -       | -                |
| 22  | CLA  | b     | 610 | X         | -        | -       | -                |
| 22  | CLA  | b     | 611 | X         | -        | -       | -                |
| 22  | CLA  | b     | 612 | X         | -        | -       | -                |
| 22  | CLA  | b     | 613 | X         | -        | -       | -                |
| 22  | CLA  | b     | 614 | X         | -        | -       | -                |
| 22  | CLA  | b     | 615 | X         | -        | -       | -                |
| 22  | CLA  | b     | 616 | X         | -        | -       | -                |
| 22  | CLA  | b     | 617 | X         | -        | -       | -                |
| 22  | CLA  | b     | 618 | X         | -        | -       | -                |
| 22  | CLA  | b     | 619 | X         | -        | -       | -                |
| 22  | CLA  | c     | 501 | X         | -        | -       | -                |
| 22  | CLA  | c     | 502 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | c     | 503 | X         | -        | -       | -                |
| 22  | CLA  | c     | 504 | X         | -        | -       | -                |
| 22  | CLA  | c     | 505 | X         | -        | -       | -                |
| 22  | CLA  | c     | 506 | X         | -        | -       | -                |
| 22  | CLA  | c     | 507 | X         | -        | -       | -                |
| 22  | CLA  | c     | 508 | X         | -        | -       | -                |
| 22  | CLA  | c     | 509 | X         | -        | -       | -                |
| 22  | CLA  | c     | 510 | X         | -        | -       | -                |
| 22  | CLA  | c     | 511 | X         | -        | -       | -                |
| 22  | CLA  | c     | 512 | X         | -        | -       | -                |
| 22  | CLA  | c     | 520 | X         | -        | -       | -                |
| 22  | CLA  | d     | 405 | X         | -        | -       | -                |
| 22  | CLA  | d     | 406 | X         | -        | -       | -                |
| 22  | CLA  | h     | 101 | X         | -        | -       | -                |

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 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 Q(B) protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 335      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2628  | 1720 | 432 | 461 | 15 |         |         |       |
| 1   | a     | 335      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2628  | 1720 | 432 | 461 | 15 |         |         |       |

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 490      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3850  | 2528 | 641 | 668 | 13 |         |         |       |
| 2   | b     | 490      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3850  | 2528 | 641 | 668 | 13 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 447      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3444  | 2256 | 576 | 599 | 13 |         |         |       |
| 3   | c     | 447      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3444  | 2256 | 576 | 599 | 13 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2706  | 1794 | 440 | 460 | 12 |         |         |       |
| 4   | d     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2706  | 1794 | 440 | 460 | 12 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5   | E     | 82       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 666   | 434 | 108 | 124 |         |         |       |
| 5   | e     | 82       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 666   | 434 | 108 | 124 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | F     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 282   | 192 | 46 | 43 | 1 |         |         |       |
| 6   | f     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 282   | 192 | 46 | 43 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | H     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 507   | 338 | 81 | 86 | 2 |         |         |       |
| 7   | h     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 507   | 338 | 81 | 86 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | I     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 286   | 195 | 45 | 45 | 1 |         |         |       |
| 8   | i     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 286   | 195 | 45 | 45 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | J     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 249   | 170 | 38 | 40 | 1 |         |         |       |
| 9   | j     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 249   | 170 | 38 | 40 | 1 |         |         |       |

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

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

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

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11  | L     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 304   | 202 | 48 | 53 | 1 |         |         |       |
| 11  | l     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 304   | 202 | 48 | 53 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | M     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 267   | 178 | 40 | 48 | 1 |         |         |       |
| 12  | m     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 267   | 178 | 40 | 48 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | O     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1845  | 1154 | 308 | 379 | 4 |         |         |       |
| 13  | o     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1845  | 1154 | 308 | 379 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14  | T     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 275   | 192 | 40 | 41 | 2 |         |         |       |
| 14  | t     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 275   | 192 | 40 | 41 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15  | U     | 97       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 774   | 491 | 129 | 154 |         |         |       |
| 15  | u     | 97       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 774   | 491 | 129 | 154 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | V     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1060  | 673 | 177 | 206 | 4 |         |         |       |
| 16  | v     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1060  | 673 | 177 | 206 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 17  | y     | 28       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 201   | 134 | 33 | 31 | 3 |         |         |       |
| 17  | g     | 28       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 201   | 134 | 33 | 31 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 18  | X     | 37       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 270   | 182 | 41 | 47 |  |         |         |       |
| 18  | x     | 37       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 270   | 182 | 41 | 47 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |    |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|--|---------|---------|-------|
| 19  | Y     | 28       | Total | C  | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 140   | 84 | 28 | 28 |  |         |         |       |
| 19  | G     | 28       | Total | C  | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 140   | 84 | 28 | 28 |  |         |         |       |

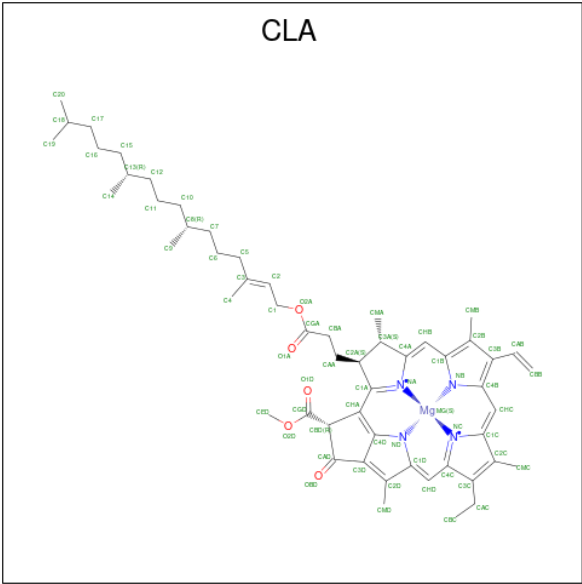
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 20  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 479   | 328 | 72 | 77 | 2 |         |         |       |
| 20  | z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 479   | 328 | 72 | 77 | 2 |         |         |       |

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21  | A     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 21  | a     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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

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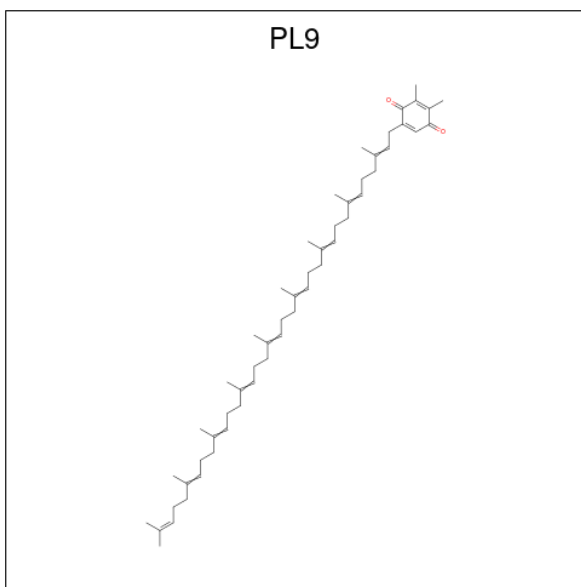
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22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

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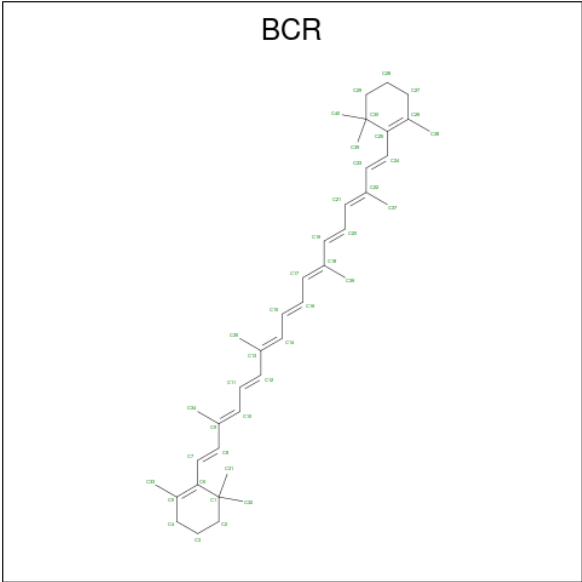
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 22  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | b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

- Molecule 23 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 |
|-----|-------|----------|-------|----|---|---------|---------|
| 23  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 45    | 43 | 2 |         |         |
| 23  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 23  | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 35    | 33 | 2 |         |         |
| 23  | a     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 45    | 43 | 2 |         |         |
| 23  | d     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 23  | j     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 35    | 33 | 2 |         |         |

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



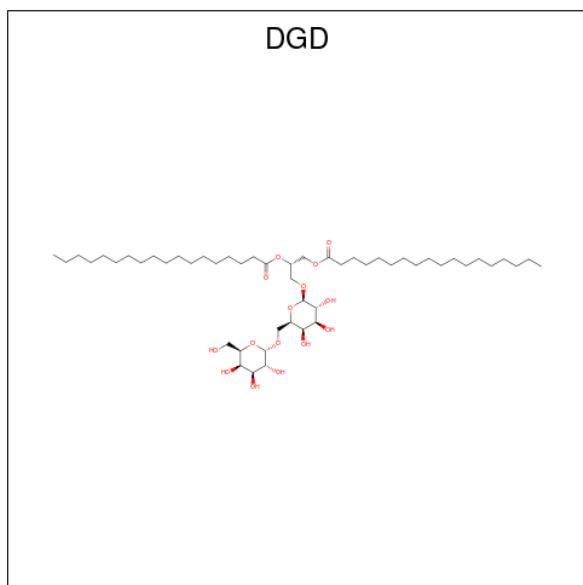
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 24  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | F     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | J     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | y     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | a     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | b     | 1        | Total C<br>40 40 | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 24  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | f     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | j     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | g     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | x     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



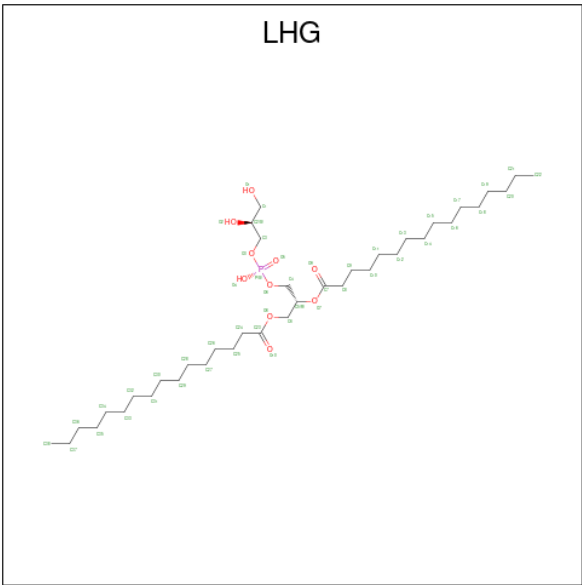
| Mol | Chain | Residues | Atoms                 | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 25  | A     | 1        | Total C O<br>56 41 15 | 0       | 0       |

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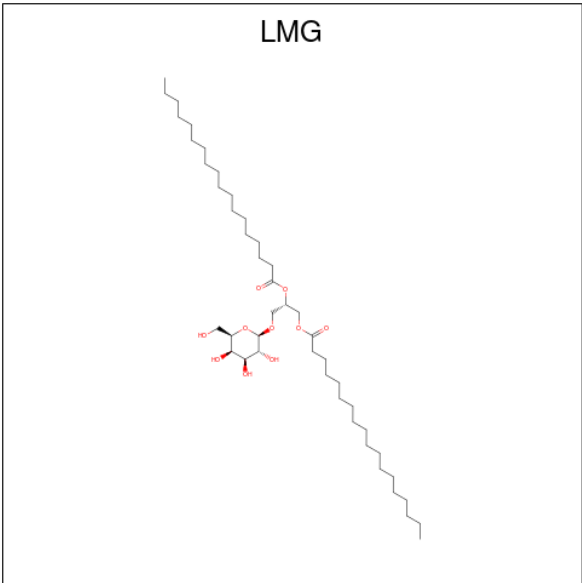
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 25  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 58    | 43 | 15 |         |         |
| 25  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 52    | 37 | 15 |         |         |
| 25  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 53    | 38 | 15 |         |         |
| 25  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 25  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 25  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 63    | 48 | 15 |         |         |
| 25  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 56    | 41 | 15 |         |         |
| 25  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 52    | 37 | 15 |         |         |
| 25  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 58    | 43 | 15 |         |         |
| 25  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 53    | 38 | 15 |         |         |
| 25  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 25  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 25  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 63    | 48 | 15 |         |         |

- Molecule 26 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 |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |         |
| 26  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |         |
| 26  | a     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |         |
| 26  | c     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |         |

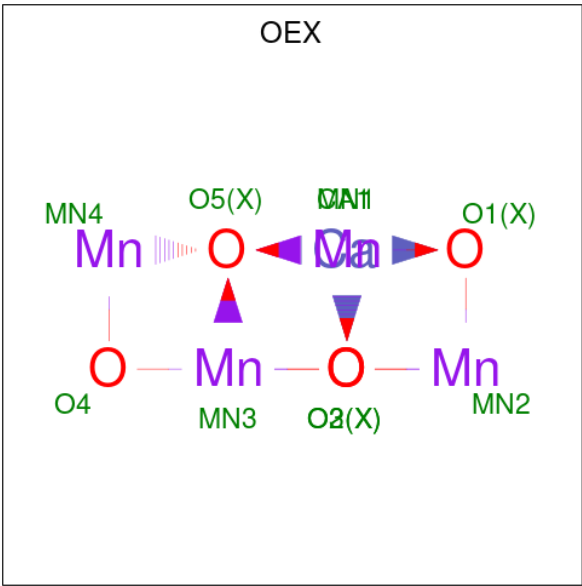
- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 27  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 27  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 42    | 32 | 10 |         |         |
| 27  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 27  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 45    | 35 | 10 |         |         |
| 27  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 27  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 27  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 27  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 46    | 36 | 10 |         |         |
| 27  | E     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 44    | 34 | 10 |         |         |
| 27  | I     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 43    | 33 | 10 |         |         |
| 27  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 42    | 32 | 10 |         |         |
| 27  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 42    | 32 | 10 |         |         |
| 27  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 27  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 27  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 45    | 35 | 10 |         |         |
| 27  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 27  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 27  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 27  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 46    | 36 | 10 |         |         |
| 27  | e     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 44    | 34 | 10 |         |         |
| 27  | i     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 43    | 33 | 10 |         |         |
| 27  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 42    | 32 | 10 |         |         |

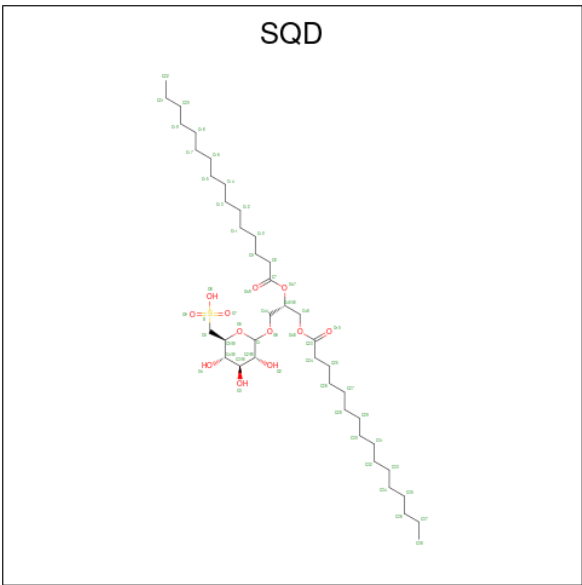


- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



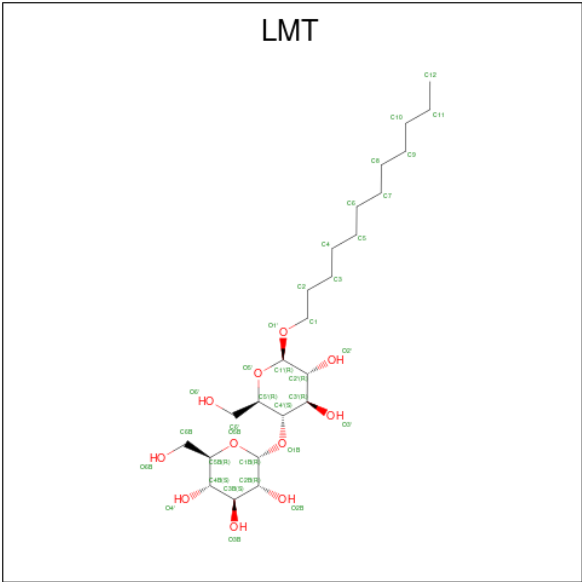
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
|     |       |          | Total | Ca | Mn | O |         |         |
| 28  | A     | 1        | 10    | 1  | 4  | 5 | 0       | 0       |
| 28  | a     | 1        | 10    | 1  | 4  | 5 | 0       | 0       |

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 29  | A     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 51    | 38 | 12 | 1 |         |         |
| 29  | A     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 29  | B     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |
| 29  | B     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 47    | 34 | 12 | 1 |         |         |
| 29  | F     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 45    | 32 | 12 | 1 |         |         |
| 29  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 29  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 51    | 38 | 12 | 1 |         |         |
| 29  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 47    | 34 | 12 | 1 |         |         |
| 29  | d     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |
| 29  | f     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 45    | 32 | 12 | 1 |         |         |

- Molecule 30 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



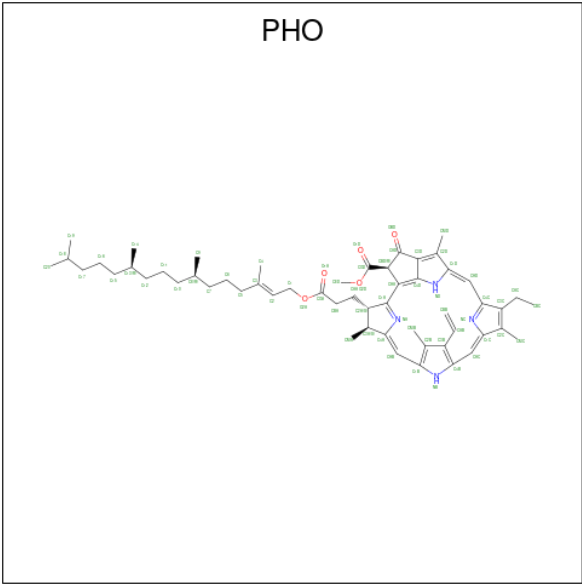
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 30  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

*Continued on next page...*

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 30  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 31    | 20 | 11 |         |         |
| 30  | I     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 30  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 31    | 20 | 11 |         |         |
| 30  | i     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

- Molecule 31 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).

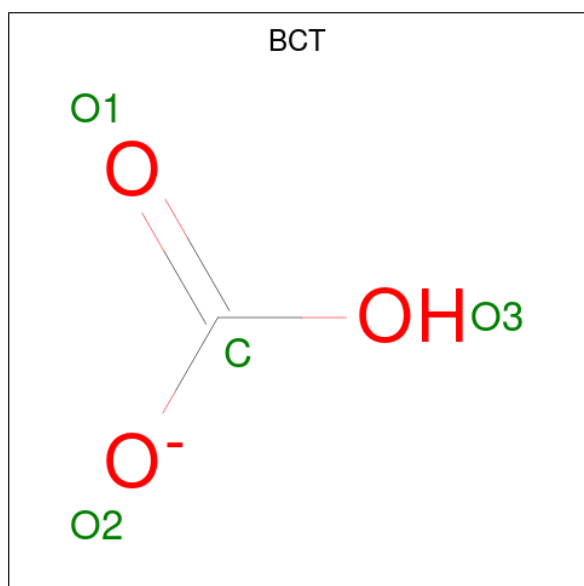


| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 31  | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 31  | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 31  | d     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 31  | d     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |

- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

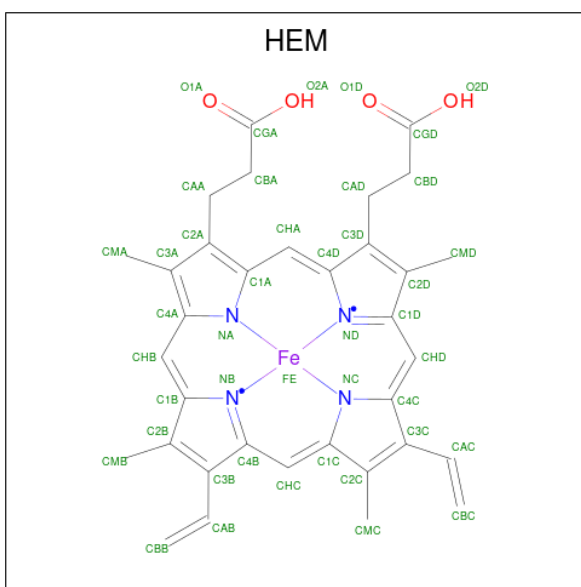
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 32  | D     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 32  | a     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 33  | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 33  | d     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        | ZeroOcc | AltConf |   |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 34  | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 34  | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 34  | f     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 34  | v     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |

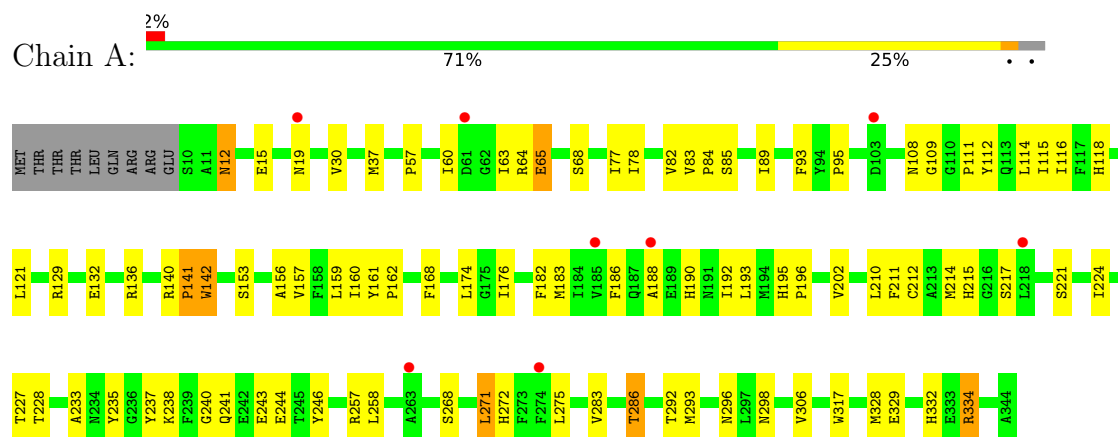
- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 35  | K     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 35  | O     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 35  | k     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 35  | o     | 1        | Total Ca<br>1 1 | 0       | 0       |

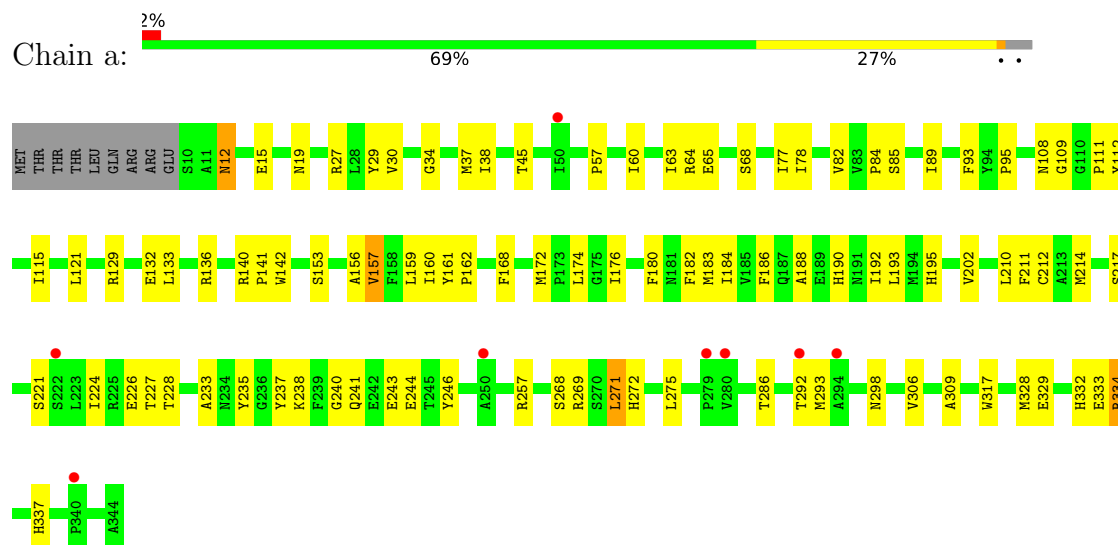
### 3 Residue-property plots [i](#)

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

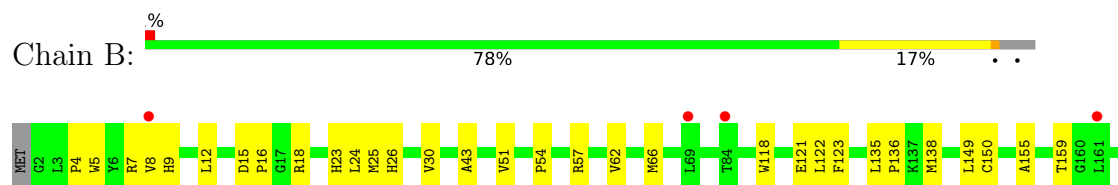
#### • Molecule 1: Photosystem Q(B) protein 1

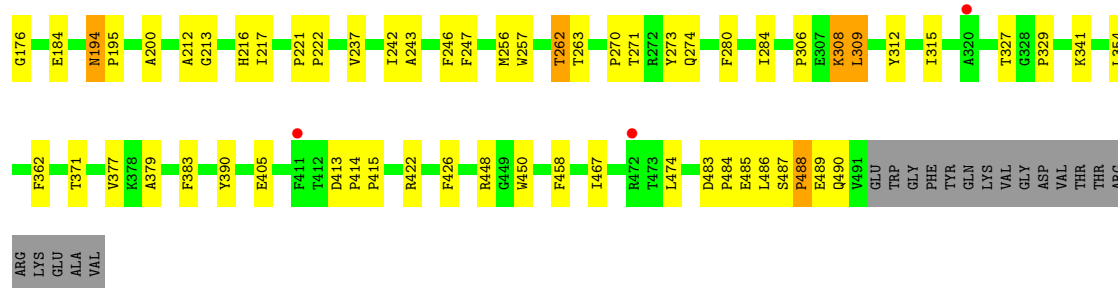


#### • Molecule 1: Photosystem Q(B) protein 1

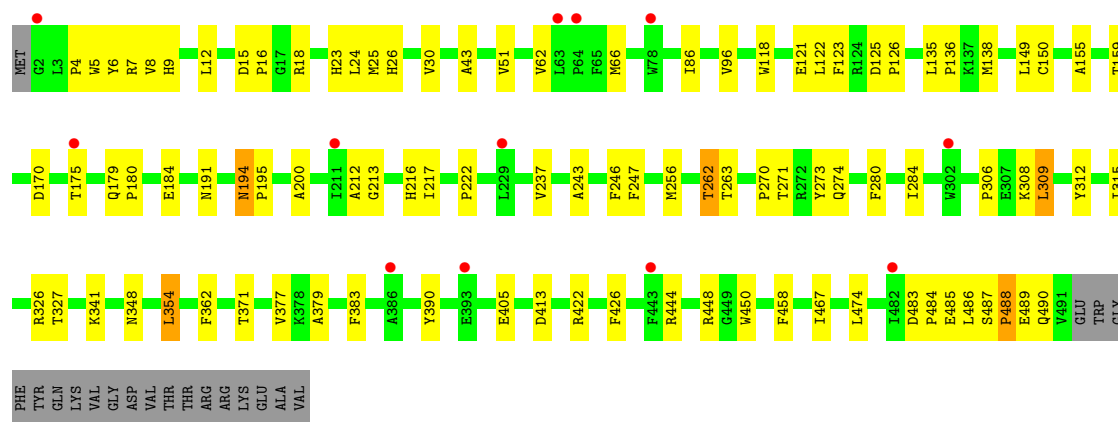
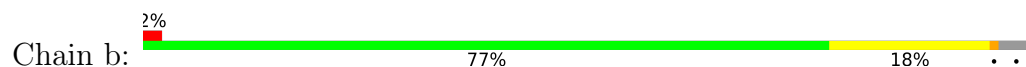


#### • Molecule 2: Photosystem II core light harvesting protein

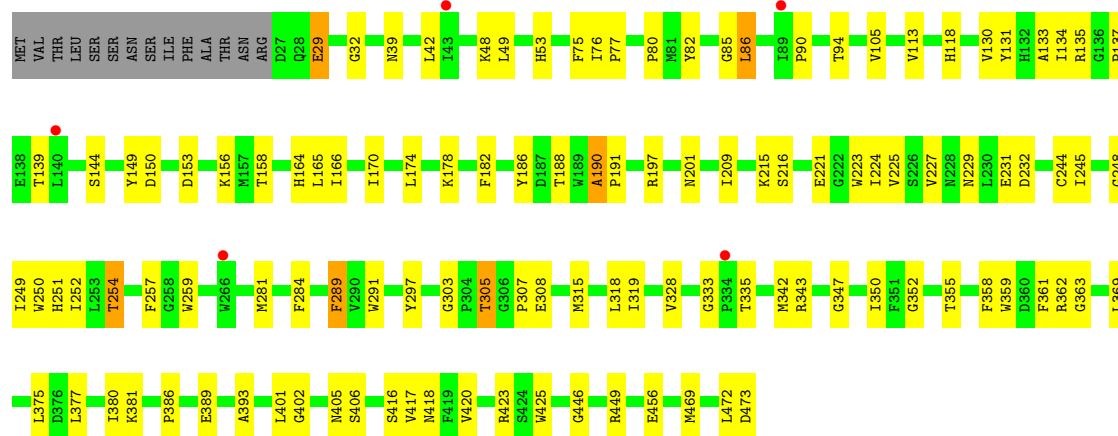
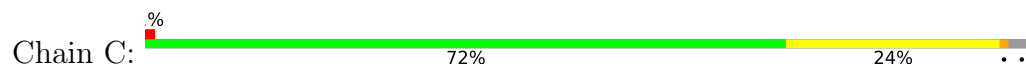




• Molecule 2: Photosystem II core light harvesting protein

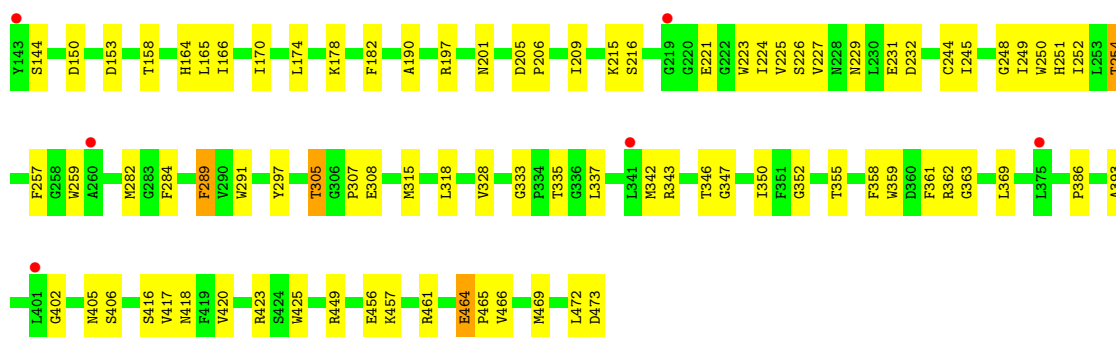


• Molecule 3: Photosystem II CP43 protein

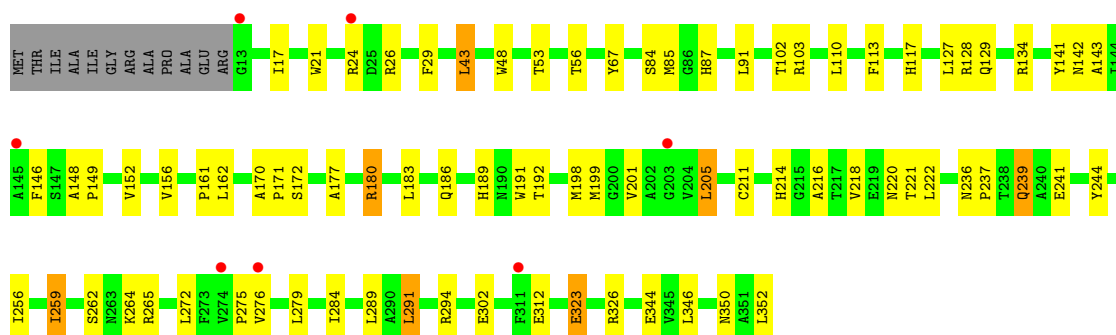
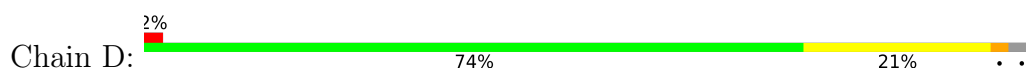


• Molecule 3: Photosystem II CP43 protein

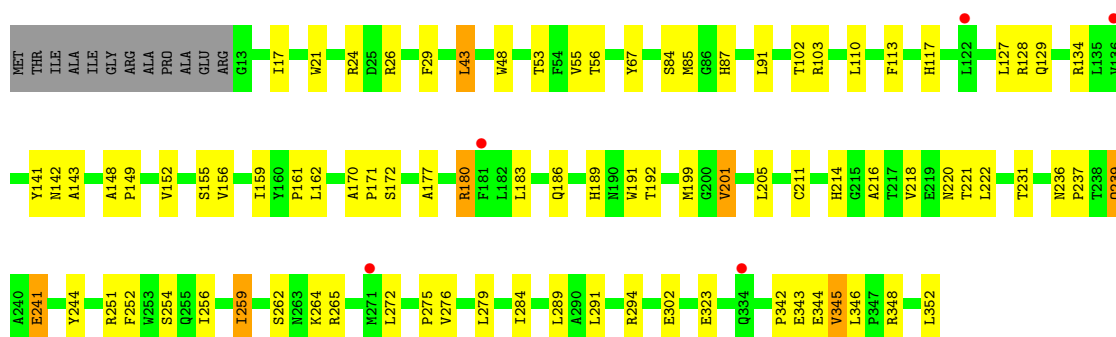
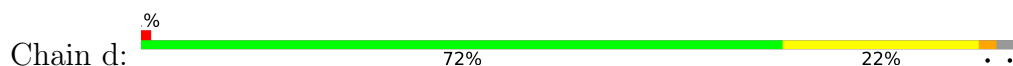




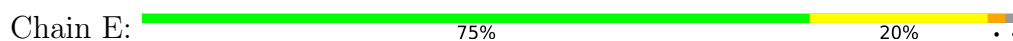
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha







- Molecule 6: Cytochrome b559 subunit beta



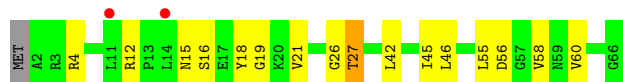
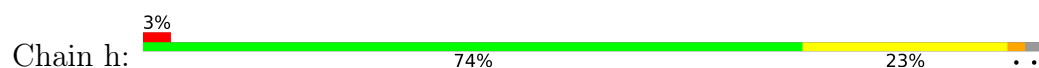
- Molecule 6: Cytochrome b559 subunit beta



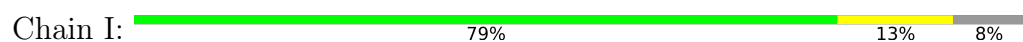
- Molecule 7: Photosystem II reaction center protein H



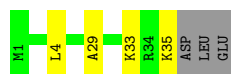
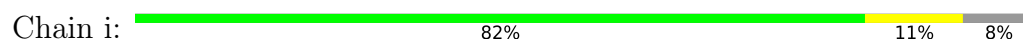
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J





- Molecule 9: Photosystem II reaction center protein J



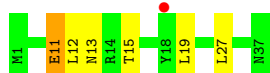
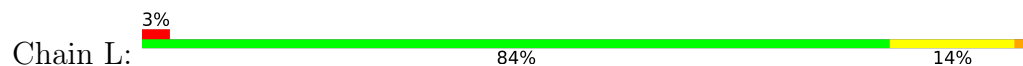
- Molecule 10: Photosystem II reaction center protein K



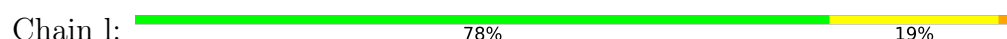
- Molecule 10: Photosystem II reaction center protein K



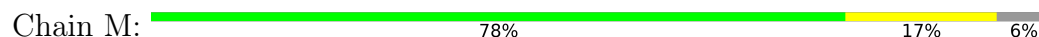
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

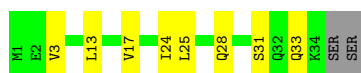


- Molecule 12: Photosystem II reaction center protein M

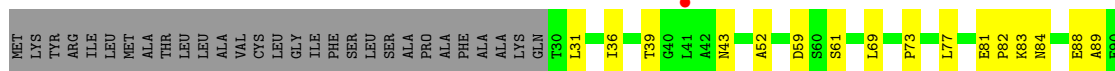


- Molecule 12: Photosystem II reaction center protein M

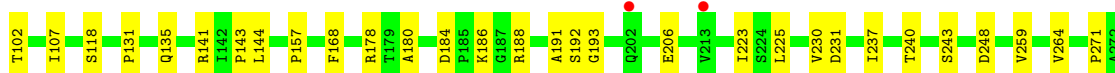




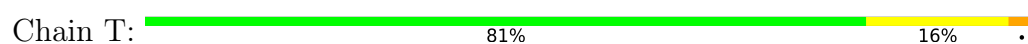
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



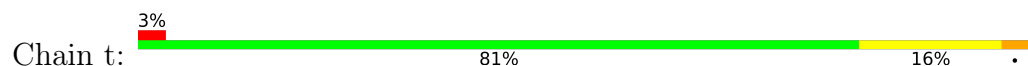
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



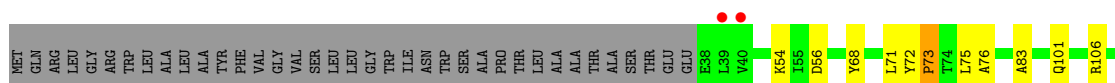
• Molecule 14: Photosystem II reaction center protein T



• Molecule 14: Photosystem II reaction center protein T

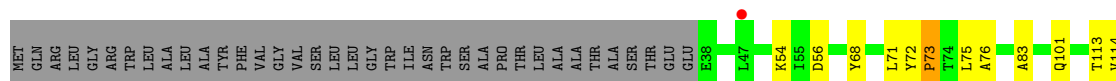


• Molecule 15: Photosystem II 12 kDa extrinsic protein

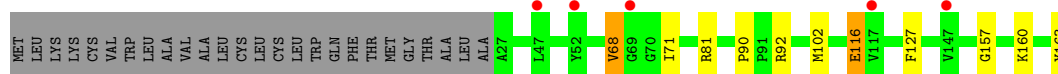
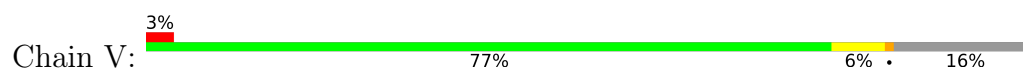




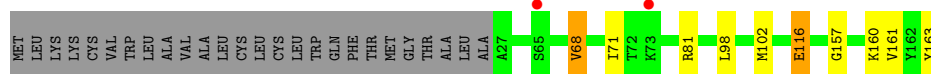
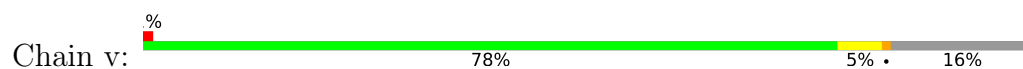
- Molecule 15: Photosystem II 12 kDa extrinsic protein



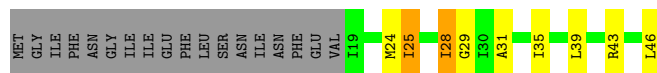
- Molecule 16: Cytochrome c-550



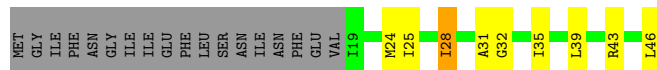
- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

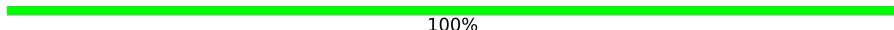


- Molecule 18: Photosystem II reaction center X protein

Chain x:  61% 24% . . 10%

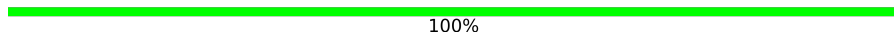


- Molecule 19: Photosystem II reaction center protein Y

Chain Y:  100%

There are no outlier residues recorded for this chain.

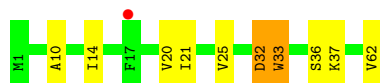
- Molecule 19: Photosystem II reaction center protein Y

Chain G:  100%

There are no outlier residues recorded for this chain.

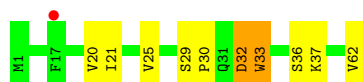
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  2% 84% 13% .



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  2% 84% 13% .



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 132.43Å 228.81Å 307.92Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 72.96 – 4.60<br>72.96 – 4.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.6 (72.96-4.60)<br>97.6 (72.96-4.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.49 (at 4.65Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: dev_1635+SVN)                        | Depositor        |
| R, $R_{free}$                                                           | 0.278 , 0.284<br>0.283 , 0.287                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2522 reflections (4.78%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 159.5                                                       | Xtriage          |
| Anisotropy                                                              | 0.302                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 127.6                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.84                                                        | EDS              |
| Total number of atoms                                                   | 50244                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 179.0                                                       | 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: OEX, LMG, CLA, FE2, BCR, PL9, SQD, LHG, PHO, LMT, CA, DGD, BCT, CL, HEM

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

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | A     | 0.30         | 0/2713  | 0.77        | 2/3700 (0.1%) |
| 1   | a     | 0.30         | 0/2713  | 0.78        | 3/3700 (0.1%) |
| 2   | B     | 0.30         | 0/3986  | 0.80        | 8/5433 (0.1%) |
| 2   | b     | 0.30         | 0/3986  | 0.81        | 8/5433 (0.1%) |
| 3   | C     | 0.30         | 0/3556  | 0.79        | 6/4842 (0.1%) |
| 3   | c     | 0.30         | 0/3556  | 0.80        | 8/4842 (0.2%) |
| 4   | D     | 0.29         | 0/2801  | 0.76        | 0/3818        |
| 4   | d     | 0.29         | 0/2801  | 0.77        | 0/3818        |
| 5   | E     | 0.31         | 0/685   | 0.82        | 0/933         |
| 5   | e     | 0.31         | 0/685   | 0.83        | 0/933         |
| 6   | F     | 0.34         | 0/291   | 0.74        | 0/397         |
| 6   | f     | 0.34         | 0/291   | 0.74        | 0/397         |
| 7   | H     | 0.33         | 0/520   | 0.73        | 0/709         |
| 7   | h     | 0.33         | 0/520   | 0.73        | 0/709         |
| 8   | I     | 0.29         | 0/293   | 0.77        | 0/395         |
| 8   | i     | 0.29         | 0/293   | 0.78        | 0/395         |
| 9   | J     | 0.30         | 0/255   | 0.84        | 0/346         |
| 9   | j     | 0.30         | 0/255   | 0.84        | 0/346         |
| 10  | K     | 0.44         | 0/303   | 0.85        | 0/416         |
| 10  | k     | 0.45         | 0/303   | 0.86        | 0/416         |
| 11  | L     | 0.28         | 0/311   | 0.72        | 0/422         |
| 11  | l     | 0.28         | 0/311   | 0.71        | 0/422         |
| 12  | M     | 0.30         | 0/270   | 0.77        | 0/367         |
| 12  | m     | 0.33         | 0/270   | 0.84        | 1/367 (0.3%)  |
| 13  | O     | 0.27         | 0/1876  | 0.71        | 0/2548        |
| 13  | o     | 0.27         | 0/1876  | 0.70        | 0/2548        |
| 14  | T     | 0.27         | 0/284   | 0.74        | 0/381         |
| 14  | t     | 0.27         | 0/284   | 0.73        | 0/381         |
| 15  | U     | 0.30         | 0/785   | 0.77        | 0/1064        |
| 15  | u     | 0.30         | 0/785   | 0.78        | 0/1064        |
| 16  | V     | 0.29         | 0/1081  | 0.75        | 2/1468 (0.1%) |
| 16  | v     | 0.29         | 0/1081  | 0.75        | 0/1468        |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 17  | g     | 0.32         | 0/202   | 0.78        | 0/272           |
| 17  | y     | 0.32         | 0/202   | 0.76        | 0/272           |
| 18  | X     | 0.38         | 0/273   | 0.79        | 0/370           |
| 18  | x     | 0.37         | 0/273   | 0.79        | 0/370           |
| 20  | Z     | 0.31         | 0/490   | 0.83        | 0/669           |
| 20  | z     | 0.31         | 0/490   | 0.84        | 0/669           |
| All | All   | 0.30         | 0/41950 | 0.78        | 38/57100 (0.1%) |

There are no bond length outliers.

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | b     | 483 | ASP  | CA-C-N | 10.64 | 133.14      | 119.84   |
| 2   | b     | 483 | ASP  | C-N-CA | 10.64 | 133.14      | 119.84   |
| 2   | B     | 483 | ASP  | CA-C-N | 10.56 | 133.04      | 119.84   |
| 2   | B     | 483 | ASP  | C-N-CA | 10.56 | 133.04      | 119.84   |
| 3   | c     | 363 | GLY  | CA-C-N | 6.26  | 125.75      | 119.24   |
| 3   | c     | 363 | GLY  | C-N-CA | 6.26  | 125.75      | 119.24   |
| 3   | c     | 190 | ALA  | CA-C-N | 6.18  | 125.66      | 119.24   |
| 3   | c     | 190 | ALA  | C-N-CA | 6.18  | 125.66      | 119.24   |
| 3   | C     | 363 | GLY  | CA-C-N | 6.09  | 125.58      | 119.24   |
| 3   | C     | 363 | GLY  | C-N-CA | 6.09  | 125.58      | 119.24   |
| 3   | C     | 190 | ALA  | CA-C-N | 6.06  | 125.54      | 119.24   |
| 3   | C     | 190 | ALA  | C-N-CA | 6.06  | 125.54      | 119.24   |
| 2   | b     | 15  | ASP  | CA-C-N | 5.92  | 126.07      | 119.32   |
| 2   | b     | 15  | ASP  | C-N-CA | 5.92  | 126.07      | 119.32   |
| 2   | B     | 413 | ASP  | CA-C-N | 5.73  | 126.29      | 120.38   |
| 2   | B     | 413 | ASP  | C-N-CA | 5.73  | 126.29      | 120.38   |
| 2   | b     | 194 | ASN  | CA-C-N | 5.58  | 125.25      | 119.05   |
| 2   | b     | 194 | ASN  | C-N-CA | 5.58  | 125.25      | 119.05   |
| 2   | b     | 413 | ASP  | CA-C-N | 5.52  | 126.07      | 120.38   |
| 2   | b     | 413 | ASP  | C-N-CA | 5.52  | 126.07      | 120.38   |
| 2   | B     | 15  | ASP  | CA-C-N | 5.45  | 125.54      | 119.32   |
| 2   | B     | 15  | ASP  | C-N-CA | 5.45  | 125.54      | 119.32   |
| 2   | B     | 194 | ASN  | CA-C-N | 5.41  | 125.05      | 119.05   |
| 2   | B     | 194 | ASN  | C-N-CA | 5.41  | 125.05      | 119.05   |
| 3   | C     | 333 | GLY  | CA-C-N | 5.25  | 126.40      | 119.84   |
| 3   | C     | 333 | GLY  | C-N-CA | 5.25  | 126.40      | 119.84   |
| 1   | a     | 195 | HIS  | CA-C-N | 5.22  | 125.28      | 119.32   |
| 1   | a     | 195 | HIS  | C-N-CA | 5.22  | 125.28      | 119.32   |
| 3   | c     | 333 | GLY  | CA-C-N | 5.22  | 126.37      | 119.84   |
| 3   | c     | 333 | GLY  | C-N-CA | 5.22  | 126.37      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 65  | GLU  | CA-C-N  | 5.13  | 125.42      | 119.93   |
| 1   | A     | 65  | GLU  | C-N-CA  | 5.13  | 125.42      | 119.93   |
| 1   | a     | 38  | ILE  | CB-CA-C | -5.11 | 108.85      | 113.70   |
| 3   | c     | 464 | GLU  | CA-C-N  | 5.07  | 126.17      | 119.84   |
| 3   | c     | 464 | GLU  | C-N-CA  | 5.07  | 126.17      | 119.84   |
| 16  | V     | 127 | PHE  | CA-C-N  | 5.03  | 126.13      | 119.84   |
| 16  | V     | 127 | PHE  | C-N-CA  | 5.03  | 126.13      | 119.84   |
| 12  | m     | 17  | VAL  | CB-CA-C | -5.03 | 108.92      | 113.70   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2628  | 0        | 2524     | 71      | 0            |
| 1   | a     | 2628  | 0        | 2524     | 68      | 0            |
| 2   | B     | 3850  | 0        | 3718     | 59      | 0            |
| 2   | b     | 3850  | 0        | 3718     | 62      | 0            |
| 3   | C     | 3444  | 0        | 3365     | 72      | 0            |
| 3   | c     | 3444  | 0        | 3365     | 71      | 0            |
| 4   | D     | 2706  | 0        | 2608     | 63      | 0            |
| 4   | d     | 2706  | 0        | 2608     | 68      | 0            |
| 5   | E     | 666   | 0        | 651      | 13      | 0            |
| 5   | e     | 666   | 0        | 651      | 15      | 0            |
| 6   | F     | 282   | 0        | 291      | 5       | 0            |
| 6   | f     | 282   | 0        | 291      | 5       | 0            |
| 7   | H     | 507   | 0        | 521      | 13      | 0            |
| 7   | h     | 507   | 0        | 521      | 13      | 0            |
| 8   | I     | 286   | 0        | 308      | 3       | 0            |
| 8   | i     | 286   | 0        | 308      | 2       | 0            |
| 9   | J     | 249   | 0        | 262      | 7       | 0            |
| 9   | j     | 249   | 0        | 262      | 7       | 0            |
| 10  | K     | 293   | 0        | 305      | 11      | 0            |
| 10  | k     | 293   | 0        | 305      | 9       | 0            |
| 11  | L     | 304   | 0        | 316      | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | l     | 304   | 0        | 316      | 6       | 0            |
| 12  | M     | 267   | 0        | 289      | 6       | 0            |
| 12  | m     | 267   | 0        | 289      | 7       | 0            |
| 13  | O     | 1845  | 0        | 1801     | 28      | 0            |
| 13  | o     | 1845  | 0        | 1801     | 29      | 0            |
| 14  | T     | 275   | 0        | 288      | 5       | 0            |
| 14  | t     | 275   | 0        | 288      | 5       | 0            |
| 15  | U     | 774   | 0        | 773      | 8       | 0            |
| 15  | u     | 774   | 0        | 773      | 7       | 0            |
| 16  | V     | 1060  | 0        | 1068     | 7       | 0            |
| 16  | v     | 1060  | 0        | 1068     | 8       | 0            |
| 17  | g     | 201   | 0        | 226      | 7       | 0            |
| 17  | y     | 201   | 0        | 226      | 7       | 0            |
| 18  | X     | 270   | 0        | 299      | 10      | 0            |
| 18  | x     | 270   | 0        | 299      | 9       | 0            |
| 19  | G     | 140   | 0        | 31       | 0       | 0            |
| 19  | Y     | 140   | 0        | 31       | 0       | 0            |
| 20  | Z     | 479   | 0        | 516      | 8       | 0            |
| 20  | z     | 479   | 0        | 516      | 9       | 0            |
| 21  | A     | 1     | 0        | 0        | 0       | 0            |
| 21  | a     | 1     | 0        | 0        | 0       | 0            |
| 22  | A     | 260   | 0        | 288      | 27      | 0            |
| 22  | B     | 975   | 0        | 1080     | 52      | 0            |
| 22  | C     | 845   | 0        | 936      | 28      | 0            |
| 22  | D     | 130   | 0        | 144      | 10      | 0            |
| 22  | H     | 65    | 0        | 72       | 8       | 0            |
| 22  | a     | 260   | 0        | 288      | 25      | 0            |
| 22  | b     | 975   | 0        | 1080     | 50      | 0            |
| 22  | c     | 845   | 0        | 936      | 32      | 0            |
| 22  | d     | 130   | 0        | 144      | 11      | 0            |
| 22  | h     | 65    | 0        | 72       | 9       | 0            |
| 23  | A     | 45    | 0        | 61       | 4       | 0            |
| 23  | D     | 55    | 0        | 80       | 8       | 0            |
| 23  | J     | 35    | 0        | 45       | 1       | 0            |
| 23  | a     | 45    | 0        | 61       | 3       | 0            |
| 23  | d     | 55    | 0        | 80       | 6       | 0            |
| 23  | j     | 35    | 0        | 45       | 0       | 0            |
| 24  | A     | 40    | 0        | 56       | 3       | 0            |
| 24  | B     | 160   | 0        | 224      | 11      | 0            |
| 24  | C     | 80    | 0        | 112      | 11      | 0            |
| 24  | F     | 40    | 0        | 56       | 3       | 0            |
| 24  | H     | 40    | 0        | 56       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | J     | 40    | 0        | 56       | 1       | 0            |
| 24  | K     | 40    | 0        | 56       | 3       | 0            |
| 24  | a     | 40    | 0        | 56       | 2       | 0            |
| 24  | b     | 160   | 0        | 224      | 13      | 0            |
| 24  | c     | 120   | 0        | 168      | 15      | 0            |
| 24  | f     | 40    | 0        | 56       | 2       | 0            |
| 24  | g     | 40    | 0        | 56       | 5       | 0            |
| 24  | j     | 40    | 0        | 56       | 1       | 0            |
| 24  | x     | 40    | 0        | 56       | 1       | 0            |
| 24  | y     | 40    | 0        | 56       | 7       | 0            |
| 25  | A     | 56    | 0        | 70       | 1       | 0            |
| 25  | B     | 110   | 0        | 136      | 4       | 0            |
| 25  | C     | 181   | 0        | 245      | 11      | 0            |
| 25  | D     | 63    | 0        | 87       | 1       | 0            |
| 25  | a     | 56    | 0        | 70       | 2       | 0            |
| 25  | b     | 110   | 0        | 136      | 4       | 0            |
| 25  | c     | 181   | 0        | 245      | 10      | 0            |
| 25  | d     | 63    | 0        | 87       | 2       | 0            |
| 26  | A     | 39    | 0        | 51       | 3       | 0            |
| 26  | C     | 37    | 0        | 44       | 2       | 0            |
| 26  | a     | 39    | 0        | 51       | 1       | 0            |
| 26  | c     | 37    | 0        | 44       | 2       | 0            |
| 27  | A     | 93    | 0        | 126      | 3       | 0            |
| 27  | B     | 49    | 0        | 68       | 3       | 0            |
| 27  | C     | 93    | 0        | 126      | 3       | 0            |
| 27  | D     | 143   | 0        | 196      | 9       | 0            |
| 27  | E     | 44    | 0        | 58       | 1       | 0            |
| 27  | I     | 43    | 0        | 56       | 0       | 0            |
| 27  | M     | 42    | 0        | 54       | 2       | 0            |
| 27  | a     | 93    | 0        | 126      | 3       | 0            |
| 27  | b     | 49    | 0        | 68       | 5       | 0            |
| 27  | c     | 93    | 0        | 126      | 3       | 0            |
| 27  | d     | 143   | 0        | 196      | 10      | 0            |
| 27  | e     | 44    | 0        | 58       | 1       | 0            |
| 27  | i     | 43    | 0        | 56       | 1       | 0            |
| 27  | m     | 42    | 0        | 54       | 1       | 0            |
| 28  | A     | 10    | 0        | 0        | 0       | 0            |
| 28  | a     | 10    | 0        | 0        | 0       | 0            |
| 29  | A     | 105   | 0        | 147      | 8       | 0            |
| 29  | B     | 90    | 0        | 111      | 4       | 0            |
| 29  | F     | 45    | 0        | 54       | 2       | 0            |
| 29  | a     | 105   | 0        | 147      | 8       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | b     | 47    | 0        | 61       | 1       | 0            |
| 29  | d     | 43    | 0        | 50       | 4       | 0            |
| 29  | f     | 45    | 0        | 54       | 3       | 0            |
| 30  | B     | 140   | 0        | 184      | 6       | 0            |
| 30  | D     | 31    | 0        | 35       | 0       | 0            |
| 30  | I     | 35    | 0        | 46       | 0       | 0            |
| 30  | M     | 70    | 0        | 91       | 0       | 0            |
| 30  | b     | 140   | 0        | 183      | 5       | 0            |
| 30  | d     | 31    | 0        | 35       | 0       | 0            |
| 30  | i     | 35    | 0        | 46       | 1       | 0            |
| 31  | D     | 128   | 0        | 148      | 12      | 0            |
| 31  | d     | 128   | 0        | 148      | 10      | 0            |
| 32  | D     | 1     | 0        | 0        | 0       | 0            |
| 32  | a     | 1     | 0        | 0        | 0       | 0            |
| 33  | D     | 4     | 0        | 1        | 0       | 0            |
| 33  | d     | 4     | 0        | 1        | 0       | 0            |
| 34  | F     | 43    | 0        | 30       | 4       | 0            |
| 34  | V     | 43    | 0        | 30       | 5       | 0            |
| 34  | f     | 43    | 0        | 30       | 4       | 0            |
| 34  | v     | 43    | 0        | 30       | 5       | 0            |
| 35  | K     | 1     | 0        | 0        | 0       | 0            |
| 35  | O     | 1     | 0        | 0        | 0       | 0            |
| 35  | k     | 1     | 0        | 0        | 0       | 0            |
| 35  | o     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 50244 | 0        | 51372    | 970     | 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 10.

All (970) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:39:ASN:HB2    | 22:C:507:CLA:HBA1 | 1.55                     | 0.87              |
| 3:c:39:ASN:HB2    | 22:c:507:CLA:HBA1 | 1.58                     | 0.86              |
| 4:D:26:ARG:HD3    | 6:F:18:VAL:HG11   | 1.60                     | 0.81              |
| 3:c:362:ARG:H     | 25:c:515:DGD:HE4  | 1.44                     | 0.81              |
| 12:M:33:GLN:HB3   | 12:m:33:GLN:HB3   | 1.62                     | 0.81              |
| 13:O:82:PRO:HG3   | 13:O:89:ALA:HB2   | 1.61                     | 0.80              |
| 4:d:26:ARG:HD3    | 6:f:18:VAL:HG11   | 1.63                     | 0.79              |
| 34:V:201:HEM:HBC2 | 34:V:201:HEM:HHH  | 1.66                     | 0.77              |
| 13:o:82:PRO:HG3   | 13:o:89:ALA:HB2   | 1.67                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:362:ARG:H     | 25:C:515:DGD:HE4  | 1.51                     | 0.76              |
| 4:D:199:MET:HG2   | 23:D:407:PL9:H322 | 1.69                     | 0.74              |
| 2:b:121:GLU:HG2   | 7:h:4:ARG:HG2     | 1.70                     | 0.74              |
| 34:v:201:HEM:HBC2 | 34:v:201:HEM:HHD  | 1.69                     | 0.73              |
| 22:B:605:CLA:H72  | 24:B:619:BCR:H311 | 1.70                     | 0.73              |
| 4:d:199:MET:HG2   | 23:d:407:PL9:H322 | 1.71                     | 0.72              |
| 1:A:82:VAL:HB     | 1:A:174:LEU:HB2   | 1.70                     | 0.72              |
| 2:B:121:GLU:HG2   | 7:H:4:ARG:HG2     | 1.72                     | 0.72              |
| 2:B:24:LEU:HD21   | 22:B:615:CLA:HAB  | 1.72                     | 0.71              |
| 22:b:609:CLA:H72  | 24:b:623:BCR:H311 | 1.71                     | 0.71              |
| 1:a:192:ILE:HA    | 1:a:293:MET:HE1   | 1.71                     | 0.71              |
| 25:c:517:DGD:HAF2 | 22:c:520:CLA:H202 | 1.73                     | 0.70              |
| 34:F:101:HEM:HHC  | 34:F:101:HEM:HBB2 | 1.73                     | 0.70              |
| 1:a:129:ARG:HH21  | 4:d:256:ILE:HD12  | 1.55                     | 0.70              |
| 2:b:24:LEU:HD21   | 22:b:619:CLA:HAB  | 1.72                     | 0.70              |
| 3:C:165:LEU:HD21  | 22:C:505:CLA:HAB  | 1.74                     | 0.70              |
| 4:D:29:PHE:O      | 4:D:128:ARG:NH2   | 2.25                     | 0.70              |
| 1:A:129:ARG:HH21  | 4:D:256:ILE:HD12  | 1.56                     | 0.70              |
| 13:O:69:LEU:HB3   | 13:O:107:ILE:HB   | 1.74                     | 0.69              |
| 34:f:101:HEM:HHC  | 34:f:101:HEM:HBB2 | 1.73                     | 0.69              |
| 3:C:250:TRP:O     | 3:C:254:THR:OG1   | 2.10                     | 0.69              |
| 10:k:21:LEU:HD13  | 17:g:24:MET:HE2   | 1.75                     | 0.68              |
| 10:K:21:LEU:HD13  | 17:y:24:MET:HE2   | 1.75                     | 0.68              |
| 25:C:517:DGD:HAF2 | 22:C:520:CLA:H202 | 1.74                     | 0.68              |
| 4:D:21:TRP:O      | 4:D:26:ARG:NH2    | 2.26                     | 0.68              |
| 5:e:60:GLN:OE1    | 5:e:84:LYS:NZ     | 2.27                     | 0.68              |
| 1:A:190:HIS:HB3   | 1:A:293:MET:HE2   | 1.75                     | 0.67              |
| 1:A:221:SER:HB3   | 4:D:141:TYR:HB2   | 1.77                     | 0.67              |
| 22:B:607:CLA:H42  | 4:D:127:LEU:HD11  | 1.76                     | 0.67              |
| 4:d:259:ILE:HG12  | 27:d:409:LMG:H292 | 1.76                     | 0.67              |
| 13:o:69:LEU:HB3   | 13:o:107:ILE:HB   | 1.75                     | 0.67              |
| 1:a:63:ILE:HB     | 3:c:335:THR:HG21  | 1.75                     | 0.67              |
| 4:d:152:VAL:HG21  | 4:d:279:LEU:HD12  | 1.76                     | 0.67              |
| 3:c:165:LEU:HD21  | 22:c:505:CLA:HAB  | 1.76                     | 0.67              |
| 1:A:63:ILE:HB     | 3:C:335:THR:HG21  | 1.77                     | 0.67              |
| 17:y:35:ILE:HG22  | 20:Z:21:ILE:HG23  | 1.77                     | 0.67              |
| 22:C:503:CLA:H172 | 22:C:509:CLA:HBB2 | 1.76                     | 0.67              |
| 4:D:152:VAL:HG21  | 4:D:279:LEU:HD12  | 1.76                     | 0.67              |
| 1:A:183:MET:HB3   | 22:A:402:CLA:HBC2 | 1.76                     | 0.66              |
| 22:A:402:CLA:H71  | 22:A:403:CLA:HAB  | 1.77                     | 0.66              |
| 12:m:31:SER:HA    | 27:m:101:LMG:HC1  | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:259:ILE:HG12  | 27:D:409:LMG:H292 | 1.78                     | 0.66              |
| 5:E:60:GLN:OE1    | 5:E:84:LYS:NZ     | 2.28                     | 0.66              |
| 22:b:611:CLA:H42  | 4:d:127:LEU:HD11  | 1.76                     | 0.66              |
| 3:c:250:TRP:O     | 3:c:254:THR:OG1   | 2.13                     | 0.66              |
| 3:C:291:TRP:O     | 3:C:305:THR:OG1   | 2.13                     | 0.66              |
| 22:C:506:CLA:H112 | 24:C:514:BCR:H362 | 1.77                     | 0.66              |
| 4:d:236:ASN:ND2   | 4:d:239:GLN:O     | 2.29                     | 0.66              |
| 1:A:15:GLU:O      | 1:A:19:ASN:ND2    | 2.27                     | 0.66              |
| 1:A:192:ILE:HA    | 1:A:293:MET:HE1   | 1.76                     | 0.65              |
| 4:d:21:TRP:O      | 4:d:26:ARG:NH2    | 2.26                     | 0.65              |
| 3:C:48:LYS:NZ     | 3:C:133:ALA:O     | 2.28                     | 0.65              |
| 29:d:403:SQD:H171 | 29:d:403:SQD:H301 | 1.78                     | 0.65              |
| 4:d:189:HIS:HA    | 4:d:294:ARG:HD2   | 1.77                     | 0.65              |
| 4:D:186:GLN:HB2   | 22:D:405:CLA:HBC1 | 1.79                     | 0.65              |
| 4:D:236:ASN:ND2   | 4:D:239:GLN:O     | 2.30                     | 0.65              |
| 1:a:174:LEU:HD22  | 31:d:401:PHO:H151 | 1.79                     | 0.64              |
| 3:c:216:SER:HB3   | 3:c:221:GLU:HB2   | 1.79                     | 0.64              |
| 22:c:507:CLA:HBC3 | 22:c:509:CLA:H92  | 1.78                     | 0.64              |
| 22:A:404:CLA:H142 | 22:D:405:CLA:H151 | 1.79                     | 0.64              |
| 24:b:621:BCR:H19C | 24:b:622:BCR:H363 | 1.80                     | 0.64              |
| 22:B:607:CLA:HBA2 | 29:B:622:SQD:H101 | 1.80                     | 0.64              |
| 22:C:507:CLA:HBC3 | 22:C:509:CLA:H92  | 1.78                     | 0.64              |
| 16:V:102:MET:HE3  | 34:V:201:HEM:HBB2 | 1.80                     | 0.64              |
| 16:v:102:MET:HE3  | 34:v:201:HEM:HBB2 | 1.80                     | 0.64              |
| 1:a:183:MET:HB3   | 22:a:404:CLA:HBC2 | 1.79                     | 0.63              |
| 2:b:271:THR:HG22  | 2:b:273:TYR:H     | 1.63                     | 0.63              |
| 2:B:271:THR:HG22  | 2:B:273:TYR:H     | 1.63                     | 0.63              |
| 1:a:190:HIS:HB3   | 1:a:293:MET:HE2   | 1.79                     | 0.63              |
| 22:B:606:CLA:HBB1 | 27:B:621:LMG:H341 | 1.80                     | 0.63              |
| 3:C:406:SER:O     | 3:C:418:ASN:ND2   | 2.32                     | 0.63              |
| 3:c:48:LYS:NZ     | 3:c:133:ALA:O     | 2.31                     | 0.63              |
| 31:d:402:PHO:H151 | 22:d:405:CLA:H172 | 1.80                     | 0.63              |
| 2:B:149:LEU:HG    | 22:B:602:CLA:HBC1 | 1.80                     | 0.63              |
| 3:c:291:TRP:O     | 3:c:305:THR:OG1   | 2.17                     | 0.63              |
| 4:d:29:PHE:O      | 4:d:128:ARG:NH2   | 2.32                     | 0.63              |
| 13:o:77:LEU:HB3   | 13:o:91:PHE:HB3   | 1.80                     | 0.63              |
| 6:F:17:THR:HG23   | 6:F:20:TRP:H      | 1.64                     | 0.62              |
| 3:c:150:ASP:HB3   | 3:c:153:ASP:HB2   | 1.81                     | 0.62              |
| 2:B:121:GLU:O     | 7:H:12:ARG:NH2    | 2.32                     | 0.62              |
| 1:a:82:VAL:HB     | 1:a:174:LEU:HB2   | 1.81                     | 0.62              |
| 3:c:406:SER:O     | 3:c:418:ASN:ND2   | 2.33                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:149:LEU:HG    | 22:b:606:CLA:HBC1 | 1.82                     | 0.62              |
| 3:C:49:LEU:O      | 3:C:53:HIS:ND1    | 2.32                     | 0.62              |
| 22:C:508:CLA:HBD  | 22:C:508:CLA:H121 | 1.81                     | 0.62              |
| 1:A:174:LEU:HD22  | 31:D:401:PHO:H151 | 1.82                     | 0.61              |
| 3:C:216:SER:HB3   | 3:C:221:GLU:HB2   | 1.81                     | 0.61              |
| 22:B:602:CLA:H193 | 7:H:42:LEU:HD12   | 1.82                     | 0.61              |
| 1:a:329:GLU:O     | 1:a:332:HIS:ND1   | 2.32                     | 0.61              |
| 22:h:101:CLA:H2   | 22:h:101:CLA:HBD  | 1.83                     | 0.61              |
| 13:O:77:LEU:HB3   | 13:O:91:PHE:HB3   | 1.81                     | 0.61              |
| 3:c:297:TYR:O     | 3:c:423:ARG:NH2   | 2.34                     | 0.61              |
| 22:A:402:CLA:HBB1 | 22:A:402:CLA:HHC  | 1.82                     | 0.61              |
| 3:c:49:LEU:O      | 3:c:53:HIS:ND1    | 2.32                     | 0.61              |
| 22:a:404:CLA:H122 | 31:d:401:PHO:H3A  | 1.81                     | 0.61              |
| 22:c:506:CLA:H112 | 24:c:514:BCR:H362 | 1.83                     | 0.61              |
| 22:a:404:CLA:HHC  | 22:a:404:CLA:HBB1 | 1.82                     | 0.61              |
| 3:c:342:MET:HE3   | 3:c:352:GLY:HA2   | 1.82                     | 0.61              |
| 9:j:15:THR:HG21   | 10:k:38:VAL:HG13  | 1.83                     | 0.61              |
| 1:a:214:MET:HE2   | 1:a:214:MET:HA    | 1.84                     | 0.60              |
| 6:f:17:THR:HG23   | 6:f:20:TRP:H      | 1.66                     | 0.60              |
| 1:A:328:MET:HE1   | 4:D:183:LEU:HD22  | 1.84                     | 0.60              |
| 29:A:412:SQD:H172 | 26:C:519:LHG:H172 | 1.84                     | 0.60              |
| 1:a:15:GLU:O      | 1:a:19:ASN:ND2    | 2.35                     | 0.60              |
| 1:a:89:ILE:HD11   | 1:a:108:ASN:HB3   | 1.84                     | 0.60              |
| 22:b:611:CLA:HBA2 | 29:d:403:SQD:H101 | 1.84                     | 0.60              |
| 4:d:186:GLN:HB2   | 22:d:405:CLA:HBC1 | 1.83                     | 0.60              |
| 3:C:449:ARG:HE    | 22:C:504:CLA:HED1 | 1.67                     | 0.60              |
| 22:a:404:CLA:H71  | 22:a:405:CLA:HAB  | 1.83                     | 0.60              |
| 2:B:62:VAL:HG12   | 2:B:66:MET:HE2    | 1.84                     | 0.60              |
| 1:a:221:SER:HB3   | 4:d:141:TYR:HB2   | 1.83                     | 0.60              |
| 2:B:327:THR:HG21  | 27:B:621:LMG:H111 | 1.83                     | 0.60              |
| 12:M:31:SER:HA    | 27:M:101:LMG:HC1  | 1.83                     | 0.59              |
| 4:D:216:ALA:O     | 4:D:220:ASN:ND2   | 2.34                     | 0.59              |
| 22:c:503:CLA:H172 | 22:c:509:CLA:HBB2 | 1.83                     | 0.59              |
| 2:B:12:LEU:HB2    | 22:B:611:CLA:HMC2 | 1.85                     | 0.59              |
| 3:C:229:ASN:HD22  | 3:C:231:GLU:HB2   | 1.67                     | 0.59              |
| 22:a:406:CLA:H142 | 22:d:405:CLA:H151 | 1.84                     | 0.59              |
| 3:C:297:TYR:O     | 3:C:423:ARG:NH2   | 2.35                     | 0.59              |
| 4:D:24:ARG:NH2    | 18:X:44:ASP:O     | 2.36                     | 0.59              |
| 1:a:328:MET:HE1   | 4:d:183:LEU:HD22  | 1.84                     | 0.59              |
| 2:b:262:THR:OG1   | 22:b:606:CLA:O1D  | 2.20                     | 0.59              |
| 3:C:178:LYS:HA    | 3:C:182:PHE:HB2   | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:b:606:CLA:H193 | 7:h:42:LEU:HD12   | 1.84                     | 0.59              |
| 17:g:35:ILE:HG22  | 20:z:21:ILE:HG23  | 1.84                     | 0.59              |
| 29:A:413:SQD:H61  | 22:b:619:CLA:H2   | 1.85                     | 0.59              |
| 29:a:401:SQD:H311 | 24:a:409:BCR:H342 | 1.85                     | 0.59              |
| 12:M:28:GLN:HA    | 12:m:28:GLN:HA    | 1.85                     | 0.59              |
| 3:C:42:LEU:HD21   | 22:C:510:CLA:H2A  | 1.84                     | 0.58              |
| 4:D:189:HIS:HA    | 4:D:294:ARG:HD2   | 1.84                     | 0.58              |
| 22:B:615:CLA:H2   | 29:a:401:SQD:H61  | 1.85                     | 0.58              |
| 3:c:215:LYS:HB3   | 3:c:223:TRP:HA    | 1.85                     | 0.58              |
| 29:B:622:SQD:H171 | 29:B:622:SQD:H301 | 1.86                     | 0.58              |
| 2:b:121:GLU:O     | 7:h:12:ARG:NH2    | 2.35                     | 0.58              |
| 3:C:342:MET:HE3   | 3:C:352:GLY:HA2   | 1.85                     | 0.58              |
| 20:z:33:TRP:HA    | 20:z:36:SER:HB3   | 1.86                     | 0.58              |
| 29:a:415:SQD:H172 | 26:c:519:LHG:H172 | 1.86                     | 0.58              |
| 2:b:12:LEU:HB2    | 22:b:615:CLA:HMC2 | 1.86                     | 0.58              |
| 3:c:449:ARG:HE    | 22:c:504:CLA:HED1 | 1.69                     | 0.58              |
| 4:d:216:ALA:O     | 4:d:220:ASN:ND2   | 2.34                     | 0.58              |
| 1:A:153:SER:HB3   | 22:A:402:CLA:HED1 | 1.85                     | 0.57              |
| 1:A:329:GLU:O     | 1:A:332:HIS:ND1   | 2.36                     | 0.57              |
| 3:C:118:HIS:CE1   | 27:C:518:LMG:H192 | 2.39                     | 0.57              |
| 3:C:215:LYS:HB3   | 3:C:223:TRP:HA    | 1.86                     | 0.57              |
| 2:b:62:VAL:HG12   | 2:b:66:MET:HE2    | 1.86                     | 0.57              |
| 27:D:409:LMG:O6   | 11:L:15:THR:HG21  | 2.05                     | 0.57              |
| 3:c:75:PHE:HZ     | 3:c:105:VAL:HG21  | 1.69                     | 0.57              |
| 3:C:75:PHE:HZ     | 3:C:105:VAL:HG21  | 1.69                     | 0.57              |
| 13:o:230:VAL:HG13 | 13:o:237:ILE:HG22 | 1.86                     | 0.57              |
| 1:A:214:MET:HA    | 1:A:214:MET:HE2   | 1.85                     | 0.57              |
| 25:c:517:DGD:HA22 | 9:j:29:PHE:HE1    | 1.68                     | 0.57              |
| 9:J:15:THR:HG21   | 10:K:38:VAL:HG13  | 1.85                     | 0.57              |
| 34:v:201:HEM:HBB2 | 34:v:201:HEM:HMB1 | 1.86                     | 0.57              |
| 24:B:617:BCR:H19C | 24:B:618:BCR:H363 | 1.86                     | 0.57              |
| 13:O:83:LYS:HG2   | 13:O:84:ASN:H     | 1.69                     | 0.57              |
| 3:c:164:HIS:ND1   | 22:c:506:CLA:OBD  | 2.33                     | 0.57              |
| 34:V:201:HEM:HBB2 | 34:V:201:HEM:HMB1 | 1.87                     | 0.57              |
| 1:A:89:ILE:HD11   | 1:A:108:ASN:HB3   | 1.86                     | 0.57              |
| 1:A:268:SER:O     | 1:A:272:HIS:ND1   | 2.35                     | 0.57              |
| 1:a:77:ILE:HD11   | 14:t:6:TYR:HB3    | 1.87                     | 0.57              |
| 1:a:64:ARG:O      | 13:o:178:ARG:NH2  | 2.37                     | 0.56              |
| 3:c:42:LEU:HD21   | 22:c:510:CLA:H2A  | 1.87                     | 0.56              |
| 22:A:402:CLA:H122 | 31:D:401:PHO:H3A  | 1.87                     | 0.56              |
| 12:m:25:LEU:O     | 12:m:28:GLN:HG3   | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:404:CLA:H93  | 22:D:405:CLA:H152 | 1.87                     | 0.56              |
| 2:B:262:THR:OG1   | 22:B:602:CLA:O1D  | 2.23                     | 0.56              |
| 22:H:101:CLA:H2   | 22:H:101:CLA:HBD  | 1.87                     | 0.56              |
| 1:a:217:SER:HA    | 4:d:272:LEU:HD12  | 1.87                     | 0.56              |
| 4:d:24:ARG:NH2    | 18:x:44:ASP:O     | 2.39                     | 0.56              |
| 27:d:412:LMG:H171 | 24:f:102:BCR:H383 | 1.88                     | 0.56              |
| 4:D:302:GLU:OE1   | 13:O:186:LYS:NZ   | 2.35                     | 0.56              |
| 1:a:65:GLU:OE2    | 1:a:334:ARG:NH2   | 2.37                     | 0.56              |
| 4:d:192:THR:HG23  | 22:d:405:CLA:HBC2 | 1.88                     | 0.56              |
| 27:d:409:LMG:HO4  | 27:d:409:LMG:HO5  | 1.53                     | 0.56              |
| 2:B:487:SER:N     | 2:B:488:PRO:HD2   | 2.21                     | 0.56              |
| 4:D:192:THR:HG23  | 22:D:405:CLA:HBC2 | 1.88                     | 0.55              |
| 4:d:214:HIS:ND1   | 23:d:407:PL9:O2   | 2.28                     | 0.55              |
| 29:d:403:SQD:H241 | 29:d:403:SQD:H111 | 1.88                     | 0.55              |
| 13:o:83:LYS:HG2   | 13:o:84:ASN:H     | 1.70                     | 0.55              |
| 3:C:150:ASP:HB3   | 3:C:153:ASP:HB2   | 1.87                     | 0.55              |
| 20:Z:33:TRP:HA    | 20:Z:36:SER:HB3   | 1.88                     | 0.55              |
| 22:b:607:CLA:HBD  | 22:b:608:CLA:H43  | 1.88                     | 0.55              |
| 17:g:39:LEU:HD21  | 20:z:25:VAL:HA    | 1.88                     | 0.55              |
| 1:A:227:THR:HG21  | 1:A:233:ALA:HA    | 1.88                     | 0.55              |
| 22:A:403:CLA:H203 | 31:D:401:PHO:H71  | 1.87                     | 0.55              |
| 3:C:197:ARG:NH2   | 3:C:231:GLU:OE2   | 2.40                     | 0.55              |
| 4:D:214:HIS:ND1   | 23:D:407:PL9:O2   | 2.27                     | 0.55              |
| 22:b:606:CLA:C2D  | 22:b:608:CLA:H2   | 2.37                     | 0.55              |
| 27:A:410:LMG:H231 | 23:D:407:PL9:H352 | 1.89                     | 0.55              |
| 22:D:406:CLA:H43  | 18:X:23:LEU:HA    | 1.89                     | 0.55              |
| 22:d:406:CLA:H42  | 18:x:26:GLY:HA3   | 1.89                     | 0.55              |
| 27:d:409:LMG:O6   | 11:l:15:THR:HG21  | 2.06                     | 0.55              |
| 1:A:212:CYS:HB2   | 4:D:211:CYS:HB2   | 1.88                     | 0.55              |
| 5:E:18:ARG:NH1    | 34:F:101:HEM:O1A  | 2.39                     | 0.55              |
| 7:H:45:ILE:HD11   | 22:H:101:CLA:H42  | 1.88                     | 0.55              |
| 1:a:85:SER:HA     | 1:a:109:GLY:HA3   | 1.88                     | 0.55              |
| 3:c:229:ASN:ND2   | 3:c:232:ASP:OD1   | 2.33                     | 0.55              |
| 1:A:84:PRO:HA     | 1:A:112:TYR:CG    | 2.41                     | 0.55              |
| 1:a:29:TYR:O      | 1:a:129:ARG:NH1   | 2.40                     | 0.55              |
| 2:b:184:GLU:H     | 2:b:200:ALA:HB2   | 1.72                     | 0.55              |
| 2:b:379:ALA:HA    | 2:b:390:TYR:HB3   | 1.88                     | 0.55              |
| 15:u:56:ASP:OD2   | 15:u:115:THR:OG1  | 2.21                     | 0.55              |
| 22:A:403:CLA:HMA2 | 23:D:407:PL9:H411 | 1.89                     | 0.55              |
| 27:a:412:LMG:H231 | 23:d:407:PL9:H352 | 1.89                     | 0.55              |
| 2:B:256:MET:O     | 2:B:448:ARG:NH1   | 2.35                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:25:LEU:O     | 12:M:28:GLN:HG3   | 2.07                     | 0.55              |
| 22:b:611:CLA:H151 | 22:b:612:CLA:H203 | 1.89                     | 0.55              |
| 7:H:55:LEU:HB2    | 7:H:58:VAL:HG12   | 1.90                     | 0.54              |
| 2:b:487:SER:N     | 2:b:488:PRO:HD2   | 2.22                     | 0.54              |
| 1:A:140:ARG:NH2   | 26:A:409:LHG:O5   | 2.35                     | 0.54              |
| 22:C:501:CLA:C2D  | 22:C:503:CLA:H2   | 2.37                     | 0.54              |
| 20:Z:33:TRP:O     | 20:Z:37:LYS:HB2   | 2.07                     | 0.54              |
| 2:b:458:PHE:HB3   | 22:b:607:CLA:HBC2 | 1.89                     | 0.54              |
| 22:c:508:CLA:HBD  | 22:c:508:CLA:H121 | 1.88                     | 0.54              |
| 34:f:101:HEM:HBC2 | 34:f:101:HEM:HMC2 | 1.90                     | 0.54              |
| 1:A:64:ARG:O      | 13:O:178:ARG:NH2  | 2.41                     | 0.54              |
| 2:B:25:MET:HE3    | 24:B:616:BCR:H23C | 1.89                     | 0.54              |
| 13:O:230:VAL:HG13 | 13:O:237:ILE:HG22 | 1.88                     | 0.54              |
| 1:a:84:PRO:HA     | 1:a:112:TYR:CG    | 2.42                     | 0.54              |
| 4:d:222:LEU:HD23  | 4:d:244:TYR:HB3   | 1.89                     | 0.54              |
| 2:B:262:THR:HG22  | 2:B:263:THR:HG23  | 1.89                     | 0.54              |
| 22:B:602:CLA:C2D  | 22:B:604:CLA:H2   | 2.38                     | 0.54              |
| 27:D:409:LMG:HO4  | 27:D:409:LMG:HO5  | 1.52                     | 0.54              |
| 22:b:612:CLA:HMD1 | 7:h:27:THR:HB     | 1.90                     | 0.54              |
| 2:B:4:PRO:HD2     | 2:B:7:ARG:HD2     | 1.90                     | 0.54              |
| 2:B:458:PHE:HB3   | 22:B:603:CLA:HBC2 | 1.90                     | 0.54              |
| 22:B:603:CLA:HBD  | 22:B:604:CLA:H43  | 1.90                     | 0.54              |
| 22:a:405:CLA:HED1 | 23:d:407:PL9:H372 | 1.87                     | 0.54              |
| 31:D:402:PHO:H151 | 22:D:405:CLA:H172 | 1.89                     | 0.54              |
| 3:c:229:ASN:HD22  | 3:c:231:GLU:HB2   | 1.73                     | 0.54              |
| 24:A:407:BCR:H342 | 29:A:413:SQD:H311 | 1.90                     | 0.54              |
| 2:b:270:PRO:HG3   | 2:b:312:TYR:HD2   | 1.73                     | 0.54              |
| 25:B:625:DGD:O1B  | 25:B:625:DGD:O2D  | 2.25                     | 0.54              |
| 5:E:10:PHE:N      | 27:E:101:LMG:O3   | 2.40                     | 0.54              |
| 13:O:73:PRO:HG2   | 13:O:102:THR:HB   | 1.90                     | 0.54              |
| 26:c:519:LHG:H101 | 26:c:519:LHG:H271 | 1.90                     | 0.54              |
| 22:b:614:CLA:H41  | 22:b:617:CLA:HBC3 | 1.89                     | 0.54              |
| 22:c:501:CLA:C2D  | 22:c:503:CLA:H2   | 2.37                     | 0.54              |
| 22:A:403:CLA:HED1 | 23:D:407:PL9:H372 | 1.90                     | 0.53              |
| 2:b:327:THR:HG21  | 27:b:625:LMG:H111 | 1.90                     | 0.53              |
| 22:a:405:CLA:H203 | 31:d:401:PHO:H71  | 1.90                     | 0.53              |
| 20:z:33:TRP:O     | 20:z:37:LYS:HB2   | 2.08                     | 0.53              |
| 4:D:222:LEU:HD23  | 4:D:244:TYR:HB3   | 1.89                     | 0.53              |
| 2:b:155:ALA:O     | 2:b:159:THR:OG1   | 2.21                     | 0.53              |
| 29:f:103:SQD:H131 | 18:x:36:VAL:HG11  | 1.89                     | 0.53              |
| 22:c:507:CLA:H172 | 25:c:516:DGD:HBW2 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:57:PRO:HG3    | 1:A:68:SER:HB3    | 1.90                     | 0.53              |
| 1:A:217:SER:HA    | 4:D:272:LEU:HD12  | 1.91                     | 0.53              |
| 29:B:626:SQD:H1   | 29:B:626:SQD:H462 | 1.90                     | 0.53              |
| 1:a:121:LEU:HD13  | 25:a:410:DGD:HB92 | 1.91                     | 0.53              |
| 2:b:474:LEU:O     | 4:d:134:ARG:NH1   | 2.42                     | 0.53              |
| 2:B:184:GLU:H     | 2:B:200:ALA:HB2   | 1.74                     | 0.53              |
| 22:B:607:CLA:H151 | 22:B:608:CLA:H203 | 1.90                     | 0.53              |
| 13:O:180:ALA:HB1  | 13:O:191:ALA:HB2  | 1.91                     | 0.53              |
| 29:a:415:SQD:H311 | 22:c:507:CLA:H71  | 1.91                     | 0.53              |
| 4:d:87:HIS:CD2    | 4:d:162:LEU:HA    | 2.44                     | 0.53              |
| 3:C:305:THR:HG23  | 3:C:307:PRO:HD2   | 1.91                     | 0.53              |
| 4:D:43:LEU:HD23   | 4:D:117:HIS:CE1   | 2.44                     | 0.53              |
| 3:c:284:PHE:HB3   | 25:c:515:DGD:HA51 | 1.91                     | 0.53              |
| 22:B:610:CLA:H41  | 22:B:613:CLA:HBC3 | 1.91                     | 0.53              |
| 1:a:268:SER:O     | 1:a:272:HIS:ND1   | 2.37                     | 0.53              |
| 22:B:605:CLA:OBD  | 30:B:623:LMT:O6'  | 2.20                     | 0.52              |
| 34:F:101:HEM:HBC2 | 34:F:101:HEM:HMC2 | 1.91                     | 0.52              |
| 13:o:180:ALA:HB1  | 13:o:191:ALA:HB2  | 1.92                     | 0.52              |
| 24:A:407:BCR:H321 | 29:A:413:SQD:H321 | 1.91                     | 0.52              |
| 2:B:271:THR:HB    | 2:B:274:GLN:HG3   | 1.91                     | 0.52              |
| 25:b:601:DGD:O1B  | 25:b:601:DGD:O2D  | 2.26                     | 0.52              |
| 1:A:162:PRO:HB3   | 1:A:168:PHE:HA    | 1.91                     | 0.52              |
| 5:e:10:PHE:N      | 27:e:101:LMG:O3   | 2.41                     | 0.52              |
| 10:K:12:PRO:HB2   | 10:K:15:TYR:HD2   | 1.75                     | 0.52              |
| 3:c:305:THR:HG22  | 3:c:308:GLU:HB2   | 1.91                     | 0.52              |
| 1:a:244:GLU:HG3   | 1:a:246:TYR:H     | 1.74                     | 0.52              |
| 22:b:606:CLA:C3D  | 22:b:608:CLA:H2   | 2.39                     | 0.52              |
| 22:B:608:CLA:HMD1 | 7:H:27:THR:HB     | 1.91                     | 0.52              |
| 3:C:164:HIS:ND1   | 22:C:506:CLA:OBD  | 2.34                     | 0.52              |
| 22:a:405:CLA:HMA2 | 23:d:407:PL9:H411 | 1.92                     | 0.52              |
| 2:b:262:THR:HG22  | 2:b:263:THR:HG23  | 1.90                     | 0.52              |
| 3:c:29:GLU:HB3    | 10:k:46:ARG:HH11  | 1.74                     | 0.52              |
| 18:x:11:THR:HG23  | 18:x:12:ILE:HG22  | 1.92                     | 0.52              |
| 1:A:211:PHE:HA    | 1:A:214:MET:HB2   | 1.91                     | 0.52              |
| 22:b:618:CLA:H111 | 22:b:618:CLA:H172 | 1.92                     | 0.52              |
| 3:c:305:THR:HG23  | 3:c:307:PRO:HD2   | 1.90                     | 0.52              |
| 2:B:379:ALA:HA    | 2:B:390:TYR:HB3   | 1.92                     | 0.52              |
| 26:C:519:LHG:H271 | 26:C:519:LHG:H101 | 1.90                     | 0.52              |
| 7:h:45:ILE:HD11   | 22:h:101:CLA:H42  | 1.92                     | 0.52              |
| 2:B:122:LEU:O     | 7:H:15:ASN:ND2    | 2.40                     | 0.51              |
| 5:E:57:ALA:HB3    | 5:E:60:GLN:HB3    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:U:68:TYR:HB2   | 15:U:71:LEU:HD12  | 1.91                     | 0.51              |
| 1:a:153:SER:HB3   | 22:a:404:CLA:HED1 | 1.91                     | 0.51              |
| 25:b:601:DGD:HD1  | 30:b:603:LMT:H32  | 1.91                     | 0.51              |
| 2:B:341:LYS:HA    | 2:B:405:GLU:HB2   | 1.91                     | 0.51              |
| 22:D:406:CLA:H42  | 18:X:26:GLY:HA3   | 1.92                     | 0.51              |
| 1:a:212:CYS:HB2   | 4:d:211:CYS:HB2   | 1.92                     | 0.51              |
| 2:b:25:MET:HE3    | 24:b:620:BCR:H23C | 1.91                     | 0.51              |
| 4:d:275:PRO:O     | 4:d:279:LEU:HD23  | 2.10                     | 0.51              |
| 15:u:72:TYR:HB3   | 15:u:73:PRO:HD3   | 1.92                     | 0.51              |
| 22:a:405:CLA:H42  | 23:d:407:PL9:H162 | 1.93                     | 0.51              |
| 3:c:197:ARG:NH2   | 3:c:231:GLU:OE2   | 2.44                     | 0.51              |
| 29:A:412:SQD:H311 | 22:C:507:CLA:H71  | 1.93                     | 0.51              |
| 4:D:172:SER:HB2   | 4:D:177:ALA:HB1   | 1.92                     | 0.51              |
| 29:b:602:SQD:H1   | 29:b:602:SQD:H462 | 1.91                     | 0.51              |
| 3:C:284:PHE:HB3   | 25:C:515:DGD:HA51 | 1.93                     | 0.51              |
| 7:h:55:LEU:HB2    | 7:h:58:VAL:HG12   | 1.92                     | 0.51              |
| 13:o:240:THR:HG22 | 13:o:264:VAL:HG12 | 1.93                     | 0.51              |
| 3:C:29:GLU:HB3    | 10:K:46:ARG:HH11  | 1.74                     | 0.51              |
| 17:y:39:LEU:HD21  | 20:Z:25:VAL:HA    | 1.92                     | 0.51              |
| 3:c:85:GLY:N      | 25:c:516:DGD:HE4  | 2.25                     | 0.51              |
| 22:c:504:CLA:HBA1 | 22:c:504:CLA:HBD  | 1.93                     | 0.51              |
| 25:c:517:DGD:HA22 | 9:j:29:PHE:CE1    | 2.46                     | 0.51              |
| 3:c:178:LYS:HA    | 3:c:182:PHE:HB2   | 1.93                     | 0.51              |
| 1:a:57:PRO:HG3    | 1:a:68:SER:HB3    | 1.93                     | 0.51              |
| 1:a:183:MET:HE1   | 22:a:405:CLA:HMD2 | 1.93                     | 0.51              |
| 1:A:132:GLU:O     | 1:A:136:ARG:HG2   | 2.11                     | 0.51              |
| 15:U:72:TYR:HB3   | 15:U:73:PRO:HD3   | 1.93                     | 0.51              |
| 4:d:172:SER:HB2   | 4:d:177:ALA:HB1   | 1.92                     | 0.51              |
| 2:b:135:LEU:HA    | 2:b:138:MET:HE3   | 1.93                     | 0.51              |
| 22:b:609:CLA:OBD  | 30:b:626:LMT:O6'  | 2.21                     | 0.51              |
| 7:h:45:ILE:HD12   | 22:h:101:CLA:HAA2 | 1.93                     | 0.50              |
| 4:D:103:ARG:HG3   | 5:E:73:LYS:HG3    | 1.94                     | 0.50              |
| 3:c:131:TYR:HE1   | 3:c:135:ARG:HD2   | 1.75                     | 0.50              |
| 3:C:85:GLY:N      | 25:C:516:DGD:HE4  | 2.26                     | 0.50              |
| 22:b:608:CLA:H202 | 22:b:612:CLA:HBB2 | 1.93                     | 0.50              |
| 2:B:135:LEU:HA    | 2:B:138:MET:HE3   | 1.94                     | 0.50              |
| 8:I:4:LEU:HD22    | 30:b:603:LMT:H62  | 1.93                     | 0.50              |
| 18:X:11:THR:HG23  | 18:X:12:ILE:HG22  | 1.93                     | 0.50              |
| 3:c:405:ASN:HB2   | 25:c:517:DGD:HG31 | 1.93                     | 0.50              |
| 17:g:24:MET:O     | 17:g:28:ILE:HG23  | 2.12                     | 0.50              |
| 10:k:26:PRO:O     | 10:k:29:PRO:HD2   | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:403:CLA:CHA  | 22:A:403:CLA:HBA1 | 2.42                     | 0.50              |
| 22:C:507:CLA:H172 | 25:C:516:DGD:HBW2 | 1.94                     | 0.50              |
| 2:b:150:CYS:HA    | 22:b:606:CLA:HBC2 | 1.92                     | 0.50              |
| 4:d:85:MET:HA     | 5:e:69:ARG:HB3    | 1.92                     | 0.50              |
| 1:A:244:GLU:HG3   | 1:A:246:TYR:H     | 1.76                     | 0.50              |
| 16:v:81:ARG:CZ    | 16:v:157:GLY:HA3  | 2.42                     | 0.50              |
| 29:A:412:SQD:H223 | 25:C:517:DGD:HAE1 | 1.93                     | 0.50              |
| 22:C:504:CLA:HBA1 | 22:C:504:CLA:HBD  | 1.94                     | 0.50              |
| 1:a:188:ALA:HB2   | 1:a:328:MET:HB2   | 1.94                     | 0.50              |
| 2:b:4:PRO:HD2     | 2:b:7:ARG:HD2     | 1.93                     | 0.50              |
| 2:b:341:LYS:HA    | 2:b:405:GLU:HB2   | 1.94                     | 0.50              |
| 4:d:103:ARG:HG3   | 5:e:73:LYS:HG3    | 1.93                     | 0.50              |
| 4:d:279:LEU:HG    | 31:d:402:PHO:HBC3 | 1.94                     | 0.50              |
| 25:d:410:DGD:O5E  | 25:d:410:DGD:O4E  | 2.25                     | 0.50              |
| 2:b:271:THR:HB    | 2:b:274:GLN:HG3   | 1.94                     | 0.50              |
| 3:c:361:PHE:HD1   | 25:c:515:DGD:HE61 | 1.77                     | 0.50              |
| 2:B:450:TRP:NE1   | 22:B:606:CLA:HBA1 | 2.27                     | 0.49              |
| 3:C:209:ILE:HG23  | 24:C:514:BCR:H382 | 1.93                     | 0.49              |
| 13:o:168:PHE:HB2  | 13:o:225:LEU:HB2  | 1.92                     | 0.49              |
| 4:D:191:TRP:CE3   | 4:D:289:LEU:HD11  | 2.47                     | 0.49              |
| 1:A:65:GLU:OE2    | 1:A:334:ARG:NH2   | 2.45                     | 0.49              |
| 1:a:132:GLU:O     | 1:a:136:ARG:HG2   | 2.12                     | 0.49              |
| 2:b:383:PHE:CZ    | 13:o:193:GLY:HA2  | 2.47                     | 0.49              |
| 4:d:191:TRP:CE3   | 4:d:289:LEU:HD11  | 2.47                     | 0.49              |
| 4:d:348:ARG:NH2   | 4:d:352:LEU:O     | 2.33                     | 0.49              |
| 12:m:3:VAL:HG11   | 14:t:2:GLU:HG2    | 1.95                     | 0.49              |
| 2:B:327:THR:HG22  | 22:B:606:CLA:H12  | 1.94                     | 0.49              |
| 2:B:5:TRP:HZ3     | 22:B:610:CLA:H51  | 1.77                     | 0.49              |
| 18:x:12:ILE:HG12  | 18:x:16:LEU:HD12  | 1.95                     | 0.49              |
| 2:B:155:ALA:O     | 2:B:159:THR:OG1   | 2.20                     | 0.49              |
| 3:C:75:PHE:HD1    | 3:C:86:LEU:HD21   | 1.75                     | 0.49              |
| 22:a:406:CLA:HAB  | 22:d:405:CLA:H72  | 1.94                     | 0.49              |
| 13:o:73:PRO:HG2   | 13:o:102:THR:HB   | 1.94                     | 0.49              |
| 22:B:602:CLA:C3D  | 22:B:604:CLA:H2   | 2.42                     | 0.49              |
| 1:a:190:HIS:O     | 1:a:298:ASN:HB3   | 2.13                     | 0.49              |
| 2:b:122:LEU:O     | 7:h:15:ASN:ND2    | 2.43                     | 0.49              |
| 27:d:409:LMG:H111 | 11:l:19:LEU:HD21  | 1.94                     | 0.49              |
| 25:C:517:DGD:HA22 | 9:J:29:PHE:HE1    | 1.78                     | 0.49              |
| 13:O:240:THR:HG22 | 13:O:264:VAL:HG12 | 1.94                     | 0.49              |
| 5:e:57:ALA:HB3    | 5:e:60:GLN:HB3    | 1.95                     | 0.49              |
| 1:A:210:LEU:HG    | 31:D:402:PHO:NC   | 2.28                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:U:75:LEU:HD21  | 15:U:101:GLN:HB3  | 1.94                     | 0.49              |
| 17:y:24:MET:O     | 17:y:28:ILE:HG23  | 2.13                     | 0.49              |
| 29:f:103:SQD:H162 | 18:x:33:THR:HA    | 1.95                     | 0.49              |
| 1:A:85:SER:HA     | 1:A:109:GLY:HA3   | 1.94                     | 0.49              |
| 4:D:87:HIS:CD2    | 4:D:162:LEU:HA    | 2.47                     | 0.49              |
| 22:b:610:CLA:HBB1 | 27:b:625:LMG:H341 | 1.95                     | 0.49              |
| 22:b:611:CLA:H51  | 22:b:612:CLA:H101 | 1.95                     | 0.49              |
| 5:e:15:THR:HG23   | 9:j:8:ILE:O       | 2.12                     | 0.49              |
| 2:B:222:PRO:HG3   | 7:H:27:THR:H      | 1.78                     | 0.48              |
| 22:B:612:CLA:H51  | 27:D:408:LMG:H231 | 1.95                     | 0.48              |
| 29:B:622:SQD:H241 | 29:B:622:SQD:H111 | 1.96                     | 0.48              |
| 30:B:627:LMT:H62  | 8:i:4:LEU:HD22    | 1.94                     | 0.48              |
| 29:F:103:SQD:H162 | 18:X:33:THR:HA    | 1.94                     | 0.48              |
| 15:U:54:LYS:HD2   | 15:U:113:THR:HG23 | 1.95                     | 0.48              |
| 15:U:56:ASP:OD2   | 15:U:115:THR:OG1  | 2.25                     | 0.48              |
| 1:A:78:ILE:O      | 1:A:176:ILE:HB    | 2.13                     | 0.48              |
| 1:A:317:TRP:CZ3   | 4:D:180:ARG:HD3   | 2.48                     | 0.48              |
| 29:a:415:SQD:H223 | 25:c:517:DGD:HAE1 | 1.95                     | 0.48              |
| 3:c:166:ILE:O     | 3:c:170:ILE:HG13  | 2.13                     | 0.48              |
| 22:d:406:CLA:H43  | 18:x:23:LEU:HA    | 1.95                     | 0.48              |
| 1:A:12:ASN:HB3    | 1:A:15:GLU:HB3    | 1.94                     | 0.48              |
| 1:A:77:ILE:HD11   | 14:T:6:TYR:HB3    | 1.94                     | 0.48              |
| 2:b:327:THR:HG22  | 22:b:610:CLA:H12  | 1.95                     | 0.48              |
| 4:d:43:LEU:HD23   | 4:d:117:HIS:CE1   | 2.47                     | 0.48              |
| 22:B:606:CLA:H193 | 11:L:27:LEU:HD11  | 1.94                     | 0.48              |
| 25:B:625:DGD:HD1  | 30:B:627:LMT:H32  | 1.95                     | 0.48              |
| 27:A:414:LMG:H112 | 2:b:43:ALA:HA     | 1.95                     | 0.48              |
| 3:C:305:THR:HG22  | 3:C:308:GLU:HB2   | 1.94                     | 0.48              |
| 1:a:211:PHE:HA    | 1:a:214:MET:HB2   | 1.95                     | 0.48              |
| 4:d:102:THR:OG1   | 25:d:410:DGD:HD62 | 2.12                     | 0.48              |
| 1:A:183:MET:HE1   | 22:A:403:CLA:HMD2 | 1.95                     | 0.48              |
| 1:A:271:LEU:HD11  | 23:A:406:PL9:C4   | 2.44                     | 0.48              |
| 10:K:26:PRO:O     | 10:K:29:PRO:HD2   | 2.13                     | 0.48              |
| 13:O:144:LEU:HD13 | 13:O:259:VAL:HG11 | 1.95                     | 0.48              |
| 29:a:401:SQD:H321 | 24:a:409:BCR:H321 | 1.96                     | 0.48              |
| 9:j:14:ALA:O      | 9:j:18:GLY:N      | 2.44                     | 0.48              |
| 13:o:118:SER:HB3  | 13:o:157:PRO:HA   | 1.96                     | 0.48              |
| 2:B:51:VAL:HG13   | 2:B:308:LYS:HB2   | 1.96                     | 0.48              |
| 22:a:405:CLA:CHA  | 22:a:405:CLA:HBA1 | 2.42                     | 0.48              |
| 22:b:617:CLA:H51  | 24:b:620:BCR:H372 | 1.94                     | 0.48              |
| 3:C:473:ASP:HB2   | 14:T:26:PRO:HB3   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:140:ARG:NH2   | 26:a:411:LHG:O5   | 2.34                     | 0.48              |
| 5:e:18:ARG:NH1    | 34:f:101:HEM:O1A  | 2.46                     | 0.48              |
| 13:o:144:LEU:HD13 | 13:o:259:VAL:HG11 | 1.95                     | 0.48              |
| 27:C:518:LMG:H292 | 27:C:518:LMG:H111 | 1.95                     | 0.48              |
| 29:F:103:SQD:H131 | 18:X:36:VAL:HG11  | 1.96                     | 0.48              |
| 2:B:256:MET:HA    | 2:B:263:THR:HG21  | 1.96                     | 0.47              |
| 3:C:131:TYR:HE1   | 3:C:135:ARG:HD2   | 1.79                     | 0.47              |
| 25:b:624:DGD:HAW2 | 22:h:101:CLA:H152 | 1.95                     | 0.47              |
| 3:c:209:ILE:HG23  | 24:c:514:BCR:H382 | 1.95                     | 0.47              |
| 2:B:150:CYS:HA    | 22:B:602:CLA:HBC2 | 1.96                     | 0.47              |
| 4:D:279:LEU:HG    | 31:D:402:PHO:HBC3 | 1.96                     | 0.47              |
| 27:D:412:LMG:H171 | 24:F:102:BCR:H383 | 1.95                     | 0.47              |
| 5:E:15:THR:HG23   | 9:J:8:ILE:O       | 2.13                     | 0.47              |
| 4:d:302:GLU:OE1   | 13:o:186:LYS:NZ   | 2.40                     | 0.47              |
| 16:V:81:ARG:CZ    | 16:V:157:GLY:HA3  | 2.44                     | 0.47              |
| 10:k:12:PRO:HB2   | 10:k:15:TYR:HD2   | 1.79                     | 0.47              |
| 1:A:190:HIS:O     | 1:A:298:ASN:HB3   | 2.14                     | 0.47              |
| 13:O:154:SER:N    | 13:O:169:LYS:O    | 2.46                     | 0.47              |
| 13:O:168:PHE:HB2  | 13:O:225:LEU:HB2  | 1.94                     | 0.47              |
| 1:a:162:PRO:HB3   | 1:a:168:PHE:HA    | 1.95                     | 0.47              |
| 2:b:8:VAL:HG23    | 2:b:9:HIS:CD2     | 2.50                     | 0.47              |
| 3:C:158:THR:O     | 3:C:251:HIS:HB3   | 2.14                     | 0.47              |
| 1:a:156:ALA:HA    | 1:a:160:ILE:HB    | 1.97                     | 0.47              |
| 3:c:225:VAL:HG13  | 3:c:289:PHE:HA    | 1.97                     | 0.47              |
| 3:c:461:ARG:NH1   | 4:d:241:GLU:OE1   | 2.45                     | 0.47              |
| 2:b:247:PHE:HE1   | 22:h:101:CLA:H101 | 1.78                     | 0.47              |
| 22:B:615:CLA:H12  | 22:B:615:CLA:H72  | 1.97                     | 0.47              |
| 3:C:223:TRP:CG    | 3:C:224:ILE:H     | 2.32                     | 0.47              |
| 3:C:318:LEU:HG    | 3:C:328:VAL:HG11  | 1.97                     | 0.47              |
| 3:C:405:ASN:HB2   | 25:C:517:DGD:HG31 | 1.97                     | 0.47              |
| 22:b:616:CLA:H51  | 27:d:408:LMG:H231 | 1.97                     | 0.47              |
| 3:c:158:THR:O     | 3:c:251:HIS:HB3   | 2.15                     | 0.47              |
| 13:o:223:ILE:HG13 | 13:o:243:SER:HB3  | 1.97                     | 0.47              |
| 1:a:210:LEU:HG    | 31:d:402:PHO:NC   | 2.30                     | 0.47              |
| 3:c:130:VAL:O     | 3:c:134:ILE:HG12  | 2.15                     | 0.47              |
| 15:u:75:LEU:HD21  | 15:u:101:GLN:HB3  | 1.96                     | 0.47              |
| 3:C:402:GLY:HA3   | 3:C:420:VAL:HG22  | 1.97                     | 0.47              |
| 2:b:450:TRP:NE1   | 22:b:610:CLA:HBA1 | 2.29                     | 0.47              |
| 22:c:501:CLA:H193 | 22:c:506:CLA:H111 | 1.97                     | 0.47              |
| 24:c:513:BCR:H391 | 10:k:36:ALA:HB2   | 1.96                     | 0.47              |
| 4:d:262:SER:N     | 27:d:409:LMG:O3   | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:A:410:LMG:O5   | 11:L:13:ASN:ND2   | 2.47                     | 0.47              |
| 22:C:510:CLA:HMB1 | 24:C:513:BCR:H382 | 1.97                     | 0.47              |
| 1:a:227:THR:HG21  | 1:a:233:ALA:HA    | 1.97                     | 0.47              |
| 1:a:317:TRP:CZ3   | 4:d:180:ARG:HD3   | 2.49                     | 0.47              |
| 22:A:405:CLA:H141 | 22:A:405:CLA:H162 | 1.71                     | 0.46              |
| 22:B:607:CLA:H18  | 22:B:608:CLA:H192 | 1.97                     | 0.46              |
| 27:i:101:LMG:H181 | 30:i:102:LMT:H42  | 1.96                     | 0.46              |
| 10:k:40:GLN:HA    | 10:k:43:VAL:HG12  | 1.97                     | 0.46              |
| 3:C:386:PRO:HB3   | 16:V:116:GLU:HG2  | 1.98                     | 0.46              |
| 4:D:275:PRO:O     | 4:D:279:LEU:HD23  | 2.14                     | 0.46              |
| 1:a:78:ILE:O      | 1:a:176:ILE:HB    | 2.15                     | 0.46              |
| 1:a:193:LEU:HD11  | 22:a:404:CLA:HMC2 | 1.97                     | 0.46              |
| 22:b:619:CLA:H72  | 22:b:619:CLA:H12  | 1.97                     | 0.46              |
| 8:i:29:ALA:HA     | 8:i:35:LYS:HB2    | 1.97                     | 0.46              |
| 17:g:32:GLY:O     | 17:g:35:ILE:HG12  | 2.16                     | 0.46              |
| 2:B:315:ILE:HG22  | 2:B:426:PHE:HB3   | 1.98                     | 0.46              |
| 4:D:48:TRP:CE2    | 31:D:402:PHO:H161 | 2.50                     | 0.46              |
| 4:d:17:ILE:HG21   | 18:x:42:GLN:HG3   | 1.98                     | 0.46              |
| 22:B:605:CLA:H18  | 22:B:615:CLA:H121 | 1.98                     | 0.46              |
| 22:H:101:CLA:H41  | 22:H:101:CLA:H62  | 1.56                     | 0.46              |
| 2:b:315:ILE:HG22  | 2:b:426:PHE:HB3   | 1.98                     | 0.46              |
| 2:b:326:ARG:HB3   | 2:b:444:ARG:HG2   | 1.97                     | 0.46              |
| 22:h:101:CLA:H41  | 22:h:101:CLA:H62  | 1.55                     | 0.46              |
| 13:O:230:VAL:HG12 | 13:O:231:ASP:H    | 1.79                     | 0.46              |
| 24:y:101:BCR:H20C | 24:y:101:BCR:H361 | 1.80                     | 0.46              |
| 2:b:51:VAL:HG13   | 2:b:308:LYS:HB2   | 1.97                     | 0.46              |
| 3:c:75:PHE:HD1    | 3:c:86:LEU:HD21   | 1.79                     | 0.46              |
| 3:c:343:ARG:NH1   | 3:c:347:GLY:O     | 2.49                     | 0.46              |
| 22:h:101:CLA:H162 | 22:h:101:CLA:H122 | 1.53                     | 0.46              |
| 24:x:101:BCR:H20C | 24:x:101:BCR:H361 | 1.78                     | 0.46              |
| 22:A:404:CLA:H161 | 23:A:406:PL9:H253 | 1.96                     | 0.46              |
| 3:C:86:LEU:HB3    | 3:C:90:PRO:HD3    | 1.96                     | 0.46              |
| 1:A:188:ALA:HB2   | 1:A:328:MET:HB2   | 1.97                     | 0.46              |
| 3:C:223:TRP:CD2   | 3:C:224:ILE:HG13  | 2.51                     | 0.46              |
| 3:C:425:TRP:CE2   | 22:C:520:CLA:HBA1 | 2.51                     | 0.46              |
| 4:D:148:ALA:HB3   | 4:D:149:PRO:HD3   | 1.97                     | 0.46              |
| 31:D:401:PHO:H41  | 31:D:401:PHO:H62  | 1.47                     | 0.46              |
| 2:b:170:ASP:OD1   | 2:b:175:THR:N     | 2.45                     | 0.46              |
| 3:c:223:TRP:CG    | 3:c:224:ILE:H     | 2.31                     | 0.46              |
| 3:c:386:PRO:HB3   | 16:v:116:GLU:HG2  | 1.97                     | 0.46              |
| 4:d:244:TYR:OH    | 4:d:264:LYS:HE3   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:u:54:LYS:HD2   | 15:u:113:THR:HG23 | 1.98                     | 0.46              |
| 2:B:16:PRO:HB2    | 2:B:123:PHE:CG    | 2.51                     | 0.46              |
| 2:B:371:THR:HG22  | 2:B:377:VAL:HA    | 1.98                     | 0.46              |
| 24:B:616:BCR:H20C | 24:B:616:BCR:H361 | 1.76                     | 0.46              |
| 22:C:510:CLA:H93  | 22:C:510:CLA:H61  | 1.81                     | 0.46              |
| 4:D:43:LEU:HD23   | 4:D:117:HIS:HE1   | 1.79                     | 0.46              |
| 2:b:306:PRO:HG2   | 2:b:309:LEU:HB2   | 1.97                     | 0.46              |
| 3:c:223:TRP:CD2   | 3:c:224:ILE:HG13  | 2.50                     | 0.46              |
| 13:o:230:VAL:HG12 | 13:o:231:ASP:H    | 1.80                     | 0.46              |
| 2:B:383:PHE:N     | 4:D:344:GLU:O     | 2.36                     | 0.46              |
| 24:C:513:BCR:H11C | 24:y:101:BCR:H322 | 1.98                     | 0.46              |
| 4:d:84:SER:HB2    | 4:d:85:MET:HE2    | 1.98                     | 0.46              |
| 4:d:148:ALA:HB3   | 4:d:149:PRO:HD3   | 1.97                     | 0.46              |
| 15:u:68:TYR:HB2   | 15:u:71:LEU:HD12  | 1.97                     | 0.46              |
| 2:b:222:PRO:HG3   | 7:h:27:THR:H      | 1.81                     | 0.45              |
| 3:c:318:LEU:HG    | 3:c:328:VAL:HG11  | 1.98                     | 0.45              |
| 27:d:409:LMG:HC1  | 27:d:409:LMG:O9   | 2.16                     | 0.45              |
| 20:z:32:ASP:CG    | 20:z:33:TRP:H     | 2.24                     | 0.45              |
| 3:C:80:PRO:HB3    | 3:C:82:TYR:CE1    | 2.52                     | 0.45              |
| 3:C:350:ILE:HG21  | 3:C:359:TRP:HB2   | 1.98                     | 0.45              |
| 24:g:101:BCR:HC31 | 24:g:101:BCR:H323 | 1.69                     | 0.45              |
| 1:A:121:LEU:HD13  | 25:A:408:DGD:HB92 | 1.99                     | 0.45              |
| 3:C:130:VAL:O     | 3:C:134:ILE:HG12  | 2.17                     | 0.45              |
| 22:C:509:CLA:H2   | 22:C:509:CLA:H61  | 1.72                     | 0.45              |
| 4:D:102:THR:OG1   | 25:D:410:DGD:HD62 | 2.16                     | 0.45              |
| 4:D:146:PHE:C     | 4:D:149:PRO:HD2   | 2.41                     | 0.45              |
| 5:e:60:GLN:HG2    | 5:e:62:SER:H      | 1.81                     | 0.45              |
| 27:M:101:LMG:H322 | 12:m:24:ILE:HG21  | 1.97                     | 0.45              |
| 1:a:159:LEU:C     | 1:a:162:PRO:HD2   | 2.41                     | 0.45              |
| 22:c:506:CLA:H92  | 22:c:506:CLA:H62  | 1.76                     | 0.45              |
| 4:d:148:ALA:HB2   | 4:d:276:VAL:HG13  | 1.98                     | 0.45              |
| 2:B:8:VAL:HG23    | 2:B:9:HIS:CD2     | 2.52                     | 0.45              |
| 2:B:383:PHE:CZ    | 13:O:193:GLY:HA2  | 2.51                     | 0.45              |
| 22:B:607:CLA:H51  | 22:B:608:CLA:H101 | 1.98                     | 0.45              |
| 9:J:38:SER:OG     | 9:J:39:SER:N      | 2.48                     | 0.45              |
| 1:a:12:ASN:HB3    | 1:a:15:GLU:HB3    | 1.97                     | 0.45              |
| 3:c:86:LEU:HB3    | 3:c:90:PRO:HD3    | 1.98                     | 0.45              |
| 31:d:401:PHO:H41  | 31:d:401:PHO:H62  | 1.47                     | 0.45              |
| 1:A:176:ILE:HD12  | 22:A:403:CLA:HED3 | 1.99                     | 0.45              |
| 24:B:618:BCR:H20C | 24:B:618:BCR:H361 | 1.82                     | 0.45              |
| 27:D:409:LMG:H111 | 11:L:19:LEU:HD21  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:b:610:CLA:H193 | 11:l:27:LEU:HD11  | 1.99                     | 0.45              |
| 3:c:337:LEU:HA    | 13:o:131:PRO:HG3  | 1.99                     | 0.45              |
| 4:d:43:LEU:HD23   | 4:d:117:HIS:HE1   | 1.82                     | 0.45              |
| 5:e:27:ILE:HB     | 5:e:28:PRO:HD3    | 1.99                     | 0.45              |
| 7:h:46:LEU:HD13   | 22:h:101:CLA:H72  | 1.97                     | 0.45              |
| 16:v:160:LYS:HA   | 16:v:163:TYR:CD2  | 2.52                     | 0.45              |
| 1:A:114:LEU:O     | 1:A:118:HIS:ND1   | 2.46                     | 0.45              |
| 22:A:402:CLA:H3A  | 22:A:402:CLA:HBA1 | 1.53                     | 0.45              |
| 2:B:247:PHE:HB2   | 22:B:607:CLA:HBC1 | 1.99                     | 0.45              |
| 2:b:212:ALA:O     | 2:b:216:HIS:ND1   | 2.44                     | 0.45              |
| 13:o:184:ASP:OD2  | 13:o:188:ARG:HB2  | 2.16                     | 0.45              |
| 22:B:604:CLA:H62  | 22:B:604:CLA:H41  | 1.79                     | 0.45              |
| 22:B:614:CLA:H172 | 22:B:614:CLA:H111 | 1.99                     | 0.45              |
| 24:C:514:BCR:H20C | 24:C:514:BCR:H361 | 1.83                     | 0.45              |
| 13:O:118:SER:HB3  | 13:O:157:PRO:HA   | 1.99                     | 0.45              |
| 13:O:143:PRO:HG2  | 13:O:248:ASP:HB3  | 1.98                     | 0.45              |
| 3:c:80:PRO:HB3    | 3:c:82:TYR:CE1    | 2.51                     | 0.45              |
| 22:A:402:CLA:H51  | 31:D:401:PHO:C3B  | 2.47                     | 0.45              |
| 22:B:611:CLA:H122 | 22:B:611:CLA:H162 | 1.76                     | 0.45              |
| 30:B:628:LMT:H122 | 14:t:7:VAL:HG12   | 1.97                     | 0.45              |
| 3:C:113:VAL:HG11  | 27:C:518:LMG:H132 | 1.99                     | 0.45              |
| 3:c:137:PRO:HB2   | 3:c:139:THR:O     | 2.17                     | 0.45              |
| 3:c:402:GLY:HA3   | 3:c:420:VAL:HG22  | 1.98                     | 0.45              |
| 22:c:512:CLA:HAB  | 24:c:521:BCR:H24C | 1.99                     | 0.45              |
| 16:v:98:LEU:O     | 16:v:102:MET:HG3  | 2.17                     | 0.45              |
| 1:A:224:ILE:O     | 4:D:265:ARG:NH2   | 2.49                     | 0.45              |
| 2:B:247:PHE:HE1   | 22:H:101:CLA:H101 | 1.80                     | 0.45              |
| 3:C:190:ALA:HA    | 3:C:191:PRO:HD3   | 1.88                     | 0.45              |
| 4:D:323:GLU:HG3   | 4:D:326:ARG:NH2   | 2.31                     | 0.45              |
| 9:J:14:ALA:O      | 9:J:18:GLY:N      | 2.48                     | 0.45              |
| 14:T:7:VAL:HG12   | 30:b:604:LMT:H122 | 1.99                     | 0.45              |
| 22:a:405:CLA:H202 | 22:a:405:CLA:H162 | 1.76                     | 0.45              |
| 2:b:18:ARG:HD3    | 2:b:118:TRP:HB3   | 1.98                     | 0.45              |
| 2:b:30:VAL:HG12   | 22:b:608:CLA:HHD  | 1.99                     | 0.45              |
| 3:c:347:GLY:HA3   | 13:o:43:ASN:HB2   | 1.99                     | 0.45              |
| 22:c:510:CLA:H121 | 24:c:513:BCR:H21C | 1.98                     | 0.45              |
| 1:A:159:LEU:C     | 1:A:162:PRO:HD2   | 2.42                     | 0.44              |
| 13:O:81:GLU:HA    | 13:O:82:PRO:HD3   | 1.79                     | 0.44              |
| 3:c:131:TYR:CE1   | 3:c:135:ARG:HD2   | 2.53                     | 0.44              |
| 1:A:136:ARG:NH2   | 8:I:27:ASP:OD1    | 2.42                     | 0.44              |
| 22:B:605:CLA:H3A  | 22:B:605:CLA:HBA2 | 1.26                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:B:620:DGD:HA71 | 22:H:101:CLA:H193 | 2.00                     | 0.44              |
| 4:D:17:ILE:HG21   | 18:X:42:GLN:HG3   | 1.99                     | 0.44              |
| 1:a:214:MET:HE1   | 4:d:142:ASN:HD21  | 1.82                     | 0.44              |
| 22:a:404:CLA:H3A  | 22:a:404:CLA:HBA1 | 1.52                     | 0.44              |
| 22:c:508:CLA:H11  | 22:c:508:CLA:H51  | 1.82                     | 0.44              |
| 24:c:521:BCR:H20C | 24:c:521:BCR:H361 | 1.80                     | 0.44              |
| 2:B:18:ARG:HD3    | 2:B:118:TRP:HB3   | 1.99                     | 0.44              |
| 4:D:221:THR:HG23  | 4:D:244:TYR:HB2   | 2.00                     | 0.44              |
| 7:H:46:LEU:HD13   | 22:H:101:CLA:H72  | 2.00                     | 0.44              |
| 22:c:504:CLA:H11  | 24:c:514:BCR:H312 | 2.00                     | 0.44              |
| 22:B:613:CLA:H51  | 24:B:616:BCR:H372 | 1.98                     | 0.44              |
| 5:E:27:ILE:HB     | 5:E:28:PRO:HD3    | 1.99                     | 0.44              |
| 24:H:102:BCR:H20C | 24:H:102:BCR:H361 | 1.78                     | 0.44              |
| 1:a:93:PHE:CD2    | 1:a:95:PRO:HD3    | 2.52                     | 0.44              |
| 1:a:317:TRP:HZ3   | 4:d:180:ARG:HD3   | 1.82                     | 0.44              |
| 23:a:408:PL9:H371 | 23:a:408:PL9:H351 | 1.81                     | 0.44              |
| 4:d:221:THR:HG23  | 4:d:244:TYR:HB2   | 1.99                     | 0.44              |
| 9:j:38:SER:OG     | 9:j:39:SER:N      | 2.49                     | 0.44              |
| 1:A:240:GLY:HA3   | 14:T:29:ILE:HG22  | 1.99                     | 0.44              |
| 3:C:76:ILE:HA     | 3:C:77:PRO:HD2    | 1.86                     | 0.44              |
| 3:C:229:ASN:ND2   | 3:C:232:ASP:OD1   | 2.41                     | 0.44              |
| 22:C:506:CLA:H62  | 22:C:506:CLA:H92  | 1.73                     | 0.44              |
| 5:E:60:GLN:HG2    | 5:E:62:SER:H      | 1.82                     | 0.44              |
| 10:K:37:PHE:HB3   | 24:y:101:BCR:C40  | 2.47                     | 0.44              |
| 2:b:213:GLY:O     | 2:b:217:ILE:HG13  | 2.17                     | 0.44              |
| 20:z:29:SER:HA    | 20:z:30:PRO:HD3   | 1.83                     | 0.44              |
| 3:C:149:TYR:HA    | 3:C:156:LYS:HD3   | 1.99                     | 0.44              |
| 3:C:361:PHE:HD1   | 25:C:515:DGD:HE61 | 1.83                     | 0.44              |
| 13:O:223:ILE:HG13 | 13:O:243:SER:HB3  | 1.98                     | 0.44              |
| 20:Z:32:ASP:CG    | 20:Z:33:TRP:H     | 2.26                     | 0.44              |
| 20:Z:33:TRP:O     | 20:Z:33:TRP:CD1   | 2.71                     | 0.44              |
| 22:a:406:CLA:H93  | 22:d:405:CLA:H152 | 1.98                     | 0.44              |
| 3:c:113:VAL:HG11  | 27:c:518:LMG:H132 | 1.98                     | 0.44              |
| 22:c:501:CLA:H162 | 22:c:501:CLA:H141 | 1.78                     | 0.44              |
| 4:d:56:THR:HG21   | 5:e:50:PRO:HD3    | 2.00                     | 0.44              |
| 2:B:474:LEU:O     | 4:D:134:ARG:NH1   | 2.50                     | 0.44              |
| 1:a:45:THR:HG21   | 29:a:401:SQD:H201 | 1.99                     | 0.44              |
| 2:B:26:HIS:CE1    | 22:B:611:CLA:HMA2 | 2.52                     | 0.44              |
| 3:C:137:PRO:HB2   | 3:C:139:THR:O     | 2.18                     | 0.44              |
| 3:C:224:ILE:O     | 3:C:227:VAL:HG23  | 2.18                     | 0.44              |
| 4:D:161:PRO:HB3   | 4:D:170:ALA:HB2   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:K:40:GLN:HA    | 10:K:43:VAL:HG12  | 2.00                     | 0.44              |
| 1:a:271:LEU:HD11  | 23:a:408:PL9:C4   | 2.48                     | 0.44              |
| 2:b:26:HIS:CE1    | 22:b:615:CLA:HMA2 | 2.53                     | 0.44              |
| 2:b:135:LEU:HD22  | 2:b:237:VAL:HG21  | 1.99                     | 0.44              |
| 2:b:371:THR:HG22  | 2:b:377:VAL:HA    | 1.99                     | 0.44              |
| 13:o:240:THR:HA   | 13:o:264:VAL:HA   | 1.99                     | 0.44              |
| 15:u:117:VAL:HG13 | 15:u:122:VAL:HG21 | 1.99                     | 0.44              |
| 1:A:111:PRO:O     | 1:A:115:ILE:HG13  | 2.18                     | 0.44              |
| 2:B:213:GLY:O     | 2:B:217:ILE:HG13  | 2.18                     | 0.44              |
| 3:C:166:ILE:O     | 3:C:170:ILE:HG13  | 2.17                     | 0.44              |
| 4:D:262:SER:N     | 27:D:409:LMG:O3   | 2.46                     | 0.44              |
| 13:O:77:LEU:HB2   | 13:O:260:LYS:HB3  | 2.00                     | 0.44              |
| 16:V:102:MET:HE3  | 34:V:201:HEM:HMB1 | 1.99                     | 0.44              |
| 22:a:406:CLA:H161 | 23:a:408:PL9:H253 | 2.00                     | 0.44              |
| 22:b:610:CLA:H102 | 27:b:625:LMG:H392 | 2.00                     | 0.44              |
| 3:c:223:TRP:O     | 3:c:226:SER:OG    | 2.31                     | 0.44              |
| 5:e:49:THR:HA     | 5:e:50:PRO:HD3    | 1.90                     | 0.44              |
| 13:o:143:PRO:HG2  | 13:o:248:ASP:HB3  | 1.98                     | 0.44              |
| 1:A:156:ALA:HA    | 1:A:160:ILE:HB    | 1.99                     | 0.43              |
| 22:C:512:CLA:H3A  | 22:C:512:CLA:HBA2 | 1.72                     | 0.43              |
| 24:J:102:BCR:H351 | 24:J:102:BCR:H15C | 1.77                     | 0.43              |
| 24:K:102:BCR:H24C | 24:K:102:BCR:H371 | 1.81                     | 0.43              |
| 24:b:623:BCR:H24C | 24:b:623:BCR:H371 | 1.88                     | 0.43              |
| 3:c:346:THR:HG21  | 13:o:38:GLY:HA2   | 1.99                     | 0.43              |
| 13:o:81:GLU:HA    | 13:o:82:PRO:HD3   | 1.78                     | 0.43              |
| 1:A:93:PHE:CD2    | 1:A:95:PRO:HD3    | 2.53                     | 0.43              |
| 3:C:245:ILE:O     | 3:C:249:ILE:HG12  | 2.17                     | 0.43              |
| 15:U:106:ARG:HA   | 15:U:109:LEU:HG   | 1.99                     | 0.43              |
| 2:b:256:MET:HA    | 2:b:263:THR:HG21  | 2.00                     | 0.43              |
| 25:b:624:DGD:HA71 | 22:h:101:CLA:H193 | 1.99                     | 0.43              |
| 4:d:201:VAL:HB    | 22:d:405:CLA:HMB2 | 1.99                     | 0.43              |
| 1:A:141:PRO:HB2   | 1:A:142:TRP:H     | 1.66                     | 0.43              |
| 1:A:214:MET:HE1   | 4:D:142:ASN:HD21  | 1.83                     | 0.43              |
| 22:A:403:CLA:H51  | 22:A:403:CLA:H11  | 1.81                     | 0.43              |
| 22:B:605:CLA:C3D  | 30:B:623:LMT:H11  | 2.49                     | 0.43              |
| 4:D:244:TYR:OH    | 4:D:264:LYS:HE3   | 2.18                     | 0.43              |
| 5:E:81:GLU:C      | 5:E:83:LEU:H      | 2.26                     | 0.43              |
| 6:F:22:ALA:O      | 6:F:25:THR:OG1    | 2.33                     | 0.43              |
| 4:d:53:THR:HG22   | 4:d:67:TYR:CD2    | 2.52                     | 0.43              |
| 1:A:271:LEU:HD21  | 23:A:406:PL9:HC71 | 1.99                     | 0.43              |
| 24:B:616:BCR:H333 | 12:M:13:LEU:HD12  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:D:401:PHO:H13  | 31:D:401:PHO:H102 | 1.82                     | 0.43              |
| 22:D:405:CLA:H92  | 22:D:405:CLA:H62  | 1.79                     | 0.43              |
| 13:O:240:THR:HA   | 13:O:264:VAL:HA   | 1.99                     | 0.43              |
| 22:b:619:CLA:H111 | 22:b:619:CLA:H143 | 1.74                     | 0.43              |
| 4:d:161:PRO:HB3   | 4:d:170:ALA:HB2   | 2.00                     | 0.43              |
| 24:j:102:BCR:H15C | 24:j:102:BCR:H351 | 1.77                     | 0.43              |
| 1:A:195:HIS:HA    | 1:A:196:PRO:HD3   | 1.93                     | 0.43              |
| 1:A:334:ARG:NH2   | 4:D:312:GLU:OE2   | 2.51                     | 0.43              |
| 22:B:608:CLA:H11  | 7:H:35:MET:HE1    | 1.99                     | 0.43              |
| 4:D:129:GLN:OE1   | 4:D:143:ALA:HA    | 2.18                     | 0.43              |
| 2:b:247:PHE:HB2   | 22:b:611:CLA:HBC1 | 1.99                     | 0.43              |
| 3:c:315:MET:HE1   | 3:c:369:LEU:HD12  | 1.99                     | 0.43              |
| 20:z:33:TRP:O     | 20:z:33:TRP:CD1   | 2.71                     | 0.43              |
| 1:A:272:HIS:CD2   | 4:D:218:VAL:HG21  | 2.54                     | 0.43              |
| 2:B:306:PRO:HG2   | 2:B:309:LEU:HB2   | 2.01                     | 0.43              |
| 27:D:409:LMG:HC1  | 27:D:409:LMG:O9   | 2.18                     | 0.43              |
| 22:b:606:CLA:H2   | 22:b:608:CLA:H93  | 2.01                     | 0.43              |
| 22:b:616:CLA:H171 | 27:d:408:LMG:H401 | 1.99                     | 0.43              |
| 24:b:623:BCR:H15C | 24:b:623:BCR:H351 | 1.88                     | 0.43              |
| 24:c:513:BCR:H371 | 24:c:513:BCR:H24C | 1.81                     | 0.43              |
| 6:f:28:VAL:HB     | 6:f:29:PRO:HD3    | 2.01                     | 0.43              |
| 16:v:68:VAL:O     | 16:v:71:ILE:HG12  | 2.19                     | 0.43              |
| 1:A:141:PRO:HG3   | 3:C:446:GLY:C     | 2.43                     | 0.43              |
| 22:A:404:CLA:H161 | 22:A:404:CLA:H143 | 1.86                     | 0.43              |
| 30:B:628:LMT:H1B  | 30:B:628:LMT:H3'  | 1.53                     | 0.43              |
| 3:C:225:VAL:HG13  | 3:C:289:PHE:HA    | 2.01                     | 0.43              |
| 2:b:5:TRP:HZ3     | 22:b:614:CLA:H51  | 1.84                     | 0.43              |
| 4:d:87:HIS:CD2    | 4:d:162:LEU:HD23  | 2.54                     | 0.43              |
| 11:l:4:ASN:OD1    | 11:l:6:ASN:ND2    | 2.41                     | 0.43              |
| 1:A:235:TYR:C     | 1:A:237:TYR:H     | 2.26                     | 0.43              |
| 10:K:12:PRO:HB2   | 10:K:15:TYR:CD2   | 2.52                     | 0.43              |
| 12:M:3:VAL:HG11   | 14:T:2:GLU:HG2    | 1.99                     | 0.43              |
| 1:a:309:ALA:HA    | 6:f:45:ARG:HB2    | 2.01                     | 0.43              |
| 22:b:615:CLA:H162 | 22:b:615:CLA:H122 | 1.73                     | 0.43              |
| 3:c:29:GLU:HB2    | 3:c:30:SER:H      | 1.64                     | 0.43              |
| 3:c:224:ILE:O     | 3:c:227:VAL:HG23  | 2.19                     | 0.43              |
| 3:c:245:ILE:O     | 3:c:249:ILE:HG12  | 2.19                     | 0.43              |
| 3:c:473:ASP:HB2   | 14:t:26:PRO:HB3   | 2.00                     | 0.43              |
| 4:d:48:TRP:CE2    | 31:d:402:PHO:H161 | 2.54                     | 0.43              |
| 6:f:16:PHE:HB3    | 29:f:103:SQD:H241 | 2.01                     | 0.43              |
| 16:v:102:MET:HE3  | 34:v:201:HEM:HMB1 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:g:101:BCR:H20C | 24:g:101:BCR:H361 | 1.80                     | 0.43              |
| 2:B:43:ALA:HA     | 27:a:402:LMG:H112 | 2.00                     | 0.43              |
| 22:B:611:CLA:H171 | 22:B:612:CLA:HBB2 | 2.00                     | 0.43              |
| 22:B:613:CLA:H91  | 22:B:613:CLA:H112 | 1.84                     | 0.43              |
| 24:C:513:BCR:H20C | 24:C:513:BCR:H361 | 1.78                     | 0.43              |
| 4:D:84:SER:HB2    | 4:D:85:MET:HE2    | 2.01                     | 0.43              |
| 1:a:157:VAL:HG13  | 1:a:172:MET:HB3   | 2.01                     | 0.43              |
| 3:c:90:PRO:O      | 3:c:94:THR:HG23   | 2.18                     | 0.43              |
| 4:d:156:VAL:HG12  | 4:d:171:PRO:HG3   | 2.00                     | 0.43              |
| 26:A:409:LHG:H382 | 22:C:509:CLA:H93  | 2.01                     | 0.43              |
| 3:C:281:MET:HE3   | 22:C:504:CLA:HAC2 | 2.01                     | 0.43              |
| 3:C:319:ILE:HG21  | 3:C:389:GLU:HG3   | 2.01                     | 0.43              |
| 25:C:516:DGD:HA91 | 25:C:516:DGD:HAW2 | 1.76                     | 0.43              |
| 4:D:156:VAL:HG12  | 4:D:171:PRO:HG3   | 2.01                     | 0.43              |
| 22:D:405:CLA:H3A  | 22:D:405:CLA:HBA1 | 1.82                     | 0.43              |
| 1:a:224:ILE:O     | 4:d:265:ARG:NH2   | 2.44                     | 0.43              |
| 5:e:23:HIS:NE2    | 34:f:101:HEM:ND   | 2.67                     | 0.43              |
| 13:o:135:GLN:HG2  | 13:o:141:ARG:HG3  | 2.01                     | 0.43              |
| 1:A:193:LEU:HD11  | 22:A:402:CLA:HMC2 | 2.01                     | 0.42              |
| 2:B:280:PHE:O     | 2:B:284:ILE:HG13  | 2.18                     | 0.42              |
| 22:C:510:CLA:H141 | 20:Z:20:VAL:HG13  | 2.00                     | 0.42              |
| 24:C:513:BCR:H353 | 24:y:101:BCR:H321 | 2.01                     | 0.42              |
| 7:H:12:ARG:O      | 7:H:12:ARG:HD3    | 2.19                     | 0.42              |
| 15:U:117:VAL:HG13 | 15:U:122:VAL:HG21 | 2.01                     | 0.42              |
| 25:a:410:DGD:HD2  | 25:a:410:DGD:HG32 | 1.75                     | 0.42              |
| 2:b:383:PHE:N     | 4:d:344:GLU:O     | 2.37                     | 0.42              |
| 22:b:606:CLA:H61  | 22:b:606:CLA:H41  | 1.64                     | 0.42              |
| 22:b:611:CLA:CHA  | 22:b:611:CLA:HBA1 | 2.49                     | 0.42              |
| 3:c:248:GLY:O     | 3:c:252:ILE:HG12  | 2.18                     | 0.42              |
| 4:d:129:GLN:OE1   | 4:d:143:ALA:HA    | 2.19                     | 0.42              |
| 1:A:37:MET:HE1    | 1:A:129:ARG:CZ    | 2.49                     | 0.42              |
| 27:B:621:LMG:H421 | 4:D:284:ILE:HD13  | 2.01                     | 0.42              |
| 3:C:343:ARG:NH1   | 3:C:347:GLY:O     | 2.52                     | 0.42              |
| 4:D:53:THR:HG22   | 4:D:67:TYR:CD2    | 2.54                     | 0.42              |
| 4:D:56:THR:HG21   | 5:E:50:PRO:HD3    | 2.01                     | 0.42              |
| 23:D:407:PL9:H401 | 23:D:407:PL9:H421 | 1.86                     | 0.42              |
| 8:I:29:ALA:HA     | 8:I:35:LYS:HB2    | 2.01                     | 0.42              |
| 3:c:456:GLU:HG2   | 3:c:457:LYS:HG3   | 2.02                     | 0.42              |
| 24:f:102:BCR:H15C | 24:f:102:BCR:H351 | 1.91                     | 0.42              |
| 15:u:72:TYR:O     | 15:u:76:ALA:HB3   | 2.19                     | 0.42              |
| 2:B:30:VAL:HG12   | 22:B:604:CLA:HHD  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:B:620:DGD:HAW2 | 22:H:101:CLA:H152 | 2.02                     | 0.42              |
| 22:C:504:CLA:H11  | 24:C:514:BCR:H312 | 2.01                     | 0.42              |
| 2:b:86:ILE:H      | 2:b:86:ILE:HG13   | 1.73                     | 0.42              |
| 24:c:513:BCR:H15C | 24:c:513:BCR:H351 | 1.89                     | 0.42              |
| 1:A:183:MET:HA    | 22:A:402:CLA:HMD2 | 2.01                     | 0.42              |
| 3:C:90:PRO:O      | 3:C:94:THR:HG23   | 2.18                     | 0.42              |
| 3:C:318:LEU:HD21  | 3:C:380:ILE:HG23  | 2.01                     | 0.42              |
| 1:a:27:ARG:NH1    | 4:d:254:SER:O     | 2.48                     | 0.42              |
| 1:a:111:PRO:O     | 1:a:115:ILE:HG13  | 2.18                     | 0.42              |
| 1:a:129:ARG:NH2   | 4:d:256:ILE:HD12  | 2.30                     | 0.42              |
| 22:c:511:CLA:H13  | 22:c:511:CLA:H61  | 2.02                     | 0.42              |
| 1:A:140:ARG:HH22  | 26:A:409:LHG:P    | 2.41                     | 0.42              |
| 2:B:194:ASN:HA    | 2:B:195:PRO:HD3   | 1.91                     | 0.42              |
| 22:B:605:CLA:H203 | 29:a:401:SQD:H332 | 2.02                     | 0.42              |
| 24:B:616:BCR:H15C | 24:B:616:BCR:H351 | 1.86                     | 0.42              |
| 3:C:307:PRO:HB3   | 3:C:358:PHE:HB3   | 2.02                     | 0.42              |
| 3:C:377:LEU:O     | 3:C:381:LYS:HB2   | 2.20                     | 0.42              |
| 1:a:161:TYR:HB3   | 1:a:162:PRO:HD3   | 2.01                     | 0.42              |
| 22:a:404:CLA:H51  | 31:d:401:PHO:C3B  | 2.50                     | 0.42              |
| 22:a:406:CLA:H161 | 22:a:406:CLA:H143 | 1.87                     | 0.42              |
| 22:c:512:CLA:HBA2 | 22:c:512:CLA:H3A  | 1.72                     | 0.42              |
| 7:h:12:ARG:O      | 7:h:12:ARG:HD3    | 2.19                     | 0.42              |
| 13:o:41:LEU:HD12  | 13:o:41:LEU:HA    | 1.92                     | 0.42              |
| 1:A:317:TRP:HZ3   | 4:D:180:ARG:HD3   | 1.85                     | 0.42              |
| 22:B:612:CLA:H171 | 27:D:408:LMG:H401 | 2.01                     | 0.42              |
| 22:C:511:CLA:H143 | 22:C:512:CLA:H162 | 2.02                     | 0.42              |
| 5:E:23:HIS:NE2    | 34:F:101:HEM:ND   | 2.67                     | 0.42              |
| 18:X:12:ILE:HG12  | 18:X:16:LEU:HD12  | 2.00                     | 0.42              |
| 27:a:412:LMG:O5   | 11:l:13:ASN:ND2   | 2.52                     | 0.42              |
| 22:A:403:CLA:H42  | 23:D:407:PL9:H162 | 2.01                     | 0.42              |
| 24:C:514:BCR:H15C | 24:C:514:BCR:H351 | 1.84                     | 0.42              |
| 4:D:148:ALA:HB2   | 4:D:276:VAL:HG13  | 2.01                     | 0.42              |
| 1:a:60:ILE:HD12   | 1:a:84:PRO:HD2    | 2.01                     | 0.42              |
| 22:b:613:CLA:H12  | 22:b:613:CLA:H51  | 1.89                     | 0.42              |
| 24:b:623:BCR:H20C | 24:b:623:BCR:H361 | 1.76                     | 0.42              |
| 4:d:113:PHE:O     | 4:d:117:HIS:HB2   | 2.19                     | 0.42              |
| 13:o:135:GLN:HE21 | 13:o:135:GLN:HB3  | 1.72                     | 0.42              |
| 29:A:412:SQD:H171 | 23:J:101:PL9:H522 | 2.01                     | 0.42              |
| 3:C:456:GLU:OE1   | 3:C:456:GLU:N     | 2.52                     | 0.42              |
| 24:C:513:BCR:H391 | 10:K:36:ALA:HB2   | 2.02                     | 0.42              |
| 4:D:236:ASN:HA    | 4:D:237:PRO:HD2   | 1.96                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:9:PRO:HB2     | 9:J:12:ILE:HG13   | 2.02                     | 0.42              |
| 2:b:25:MET:HG2    | 24:b:620:BCR:H23C | 2.02                     | 0.42              |
| 24:b:620:BCR:H333 | 12:m:13:LEU:HD12  | 2.01                     | 0.42              |
| 3:c:425:TRP:CE2   | 22:c:520:CLA:HBA1 | 2.54                     | 0.42              |
| 22:c:520:CLA:H142 | 22:c:520:CLA:H112 | 1.78                     | 0.42              |
| 3:C:315:MET:HE1   | 3:C:369:LEU:HD12  | 2.01                     | 0.42              |
| 3:C:393:ALA:HB1   | 34:V:201:HEM:HBC1 | 2.01                     | 0.42              |
| 31:D:401:PHO:H202 | 31:D:401:PHO:H162 | 1.87                     | 0.42              |
| 13:O:192:SER:OG   | 13:O:193:GLY:N    | 2.52                     | 0.42              |
| 15:U:72:TYR:O     | 15:U:76:ALA:HB3   | 2.19                     | 0.42              |
| 22:a:405:CLA:H51  | 22:a:405:CLA:H11  | 1.83                     | 0.42              |
| 22:c:509:CLA:H2   | 22:c:509:CLA:H61  | 1.72                     | 0.42              |
| 22:c:520:CLA:H141 | 22:c:520:CLA:H161 | 1.83                     | 0.42              |
| 5:e:81:GLU:C      | 5:e:83:LEU:H      | 2.28                     | 0.42              |
| 10:k:31:LEU:HB3   | 24:g:101:BCR:C15  | 2.50                     | 0.42              |
| 18:x:17:LYS:O     | 18:x:21:ILE:HG13  | 2.19                     | 0.42              |
| 2:B:135:LEU:HB2   | 2:B:136:PRO:HD3   | 2.00                     | 0.42              |
| 2:B:329:PRO:HB3   | 22:B:606:CLA:HED1 | 2.02                     | 0.42              |
| 24:C:514:BCR:H11C | 24:C:514:BCR:H341 | 1.89                     | 0.42              |
| 1:a:182:PHE:O     | 1:a:186:PHE:HB2   | 2.20                     | 0.42              |
| 1:a:257:ARG:HH22  | 2:b:488:PRO:C     | 2.28                     | 0.42              |
| 22:c:510:CLA:H141 | 20:z:20:VAL:HG13  | 2.02                     | 0.42              |
| 4:d:155:SER:HA    | 4:d:159:ILE:HB    | 2.01                     | 0.42              |
| 4:d:236:ASN:HA    | 4:d:237:PRO:HD2   | 1.94                     | 0.42              |
| 5:e:42:LEU:O      | 5:e:46:VAL:HG23   | 2.20                     | 0.42              |
| 13:O:184:ASP:OD2  | 13:O:188:ARG:HB2  | 2.19                     | 0.41              |
| 16:V:68:VAL:O     | 16:V:71:ILE:HG12  | 2.19                     | 0.41              |
| 22:b:609:CLA:H3A  | 22:b:609:CLA:HBA2 | 1.25                     | 0.41              |
| 3:c:456:GLU:OE1   | 3:c:456:GLU:N     | 2.50                     | 0.41              |
| 22:c:508:CLA:H141 | 22:c:511:CLA:HMD3 | 2.01                     | 0.41              |
| 22:d:406:CLA:H61  | 22:d:406:CLA:H41  | 1.85                     | 0.41              |
| 9:j:9:PRO:HB2     | 9:j:12:ILE:HG13   | 2.01                     | 0.41              |
| 17:g:28:ILE:O     | 24:g:101:BCR:H14C | 2.20                     | 0.41              |
| 2:B:270:PRO:HG3   | 2:B:312:TYR:HD2   | 1.85                     | 0.41              |
| 24:B:618:BCR:H24C | 24:B:618:BCR:H371 | 1.83                     | 0.41              |
| 22:C:501:CLA:C1D  | 22:C:503:CLA:H2   | 2.50                     | 0.41              |
| 22:C:512:CLA:HAB  | 24:K:102:BCR:H371 | 2.02                     | 0.41              |
| 4:D:350:ASN:O     | 4:D:352:LEU:N     | 2.48                     | 0.41              |
| 6:F:28:VAL:HB     | 6:F:29:PRO:HD3    | 2.02                     | 0.41              |
| 16:V:90:PRO:O     | 16:V:92:ARG:HD3   | 2.19                     | 0.41              |
| 22:a:406:CLA:HAB  | 22:d:405:CLA:H42  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:16:PRO:HB2    | 2:b:123:PHE:CG    | 2.55                     | 0.41              |
| 4:d:252:PHE:O     | 4:d:256:ILE:HG22  | 2.20                     | 0.41              |
| 13:o:206:GLU:H    | 13:o:206:GLU:CD   | 2.28                     | 0.41              |
| 17:g:31:ALA:O     | 17:g:35:ILE:HG23  | 2.19                     | 0.41              |
| 22:A:403:CLA:H162 | 22:A:403:CLA:H202 | 1.76                     | 0.41              |
| 22:C:510:CLA:H122 | 10:K:32:PHE:HE1   | 1.85                     | 0.41              |
| 4:D:85:MET:HA     | 5:E:69:ARG:HB3    | 2.03                     | 0.41              |
| 22:a:407:CLA:H141 | 22:a:407:CLA:H162 | 1.69                     | 0.41              |
| 2:b:135:LEU:HB2   | 2:b:136:PRO:HD3   | 2.02                     | 0.41              |
| 2:b:348:ASN:HB3   | 2:b:354:LEU:HD21  | 2.01                     | 0.41              |
| 22:b:608:CLA:H41  | 22:b:608:CLA:H62  | 1.78                     | 0.41              |
| 22:b:611:CLA:H18  | 22:b:612:CLA:H192 | 2.01                     | 0.41              |
| 3:c:205:ASP:HA    | 3:c:206:PRO:HD2   | 1.93                     | 0.41              |
| 1:A:238:LYS:O     | 1:A:241:GLN:HG3   | 2.21                     | 0.41              |
| 22:A:403:CLA:H62  | 22:A:403:CLA:H41  | 1.76                     | 0.41              |
| 22:A:403:CLA:HED2 | 4:D:198:MET:SD    | 2.60                     | 0.41              |
| 22:B:602:CLA:HBB2 | 22:B:602:CLA:H92  | 2.03                     | 0.41              |
| 4:D:113:PHE:O     | 4:D:117:HIS:HB2   | 2.20                     | 0.41              |
| 4:D:205:LEU:HA    | 4:D:205:LEU:HD12  | 1.84                     | 0.41              |
| 24:F:102:BCR:H11C | 24:F:102:BCR:H341 | 1.94                     | 0.41              |
| 13:O:206:GLU:CD   | 13:O:206:GLU:H    | 2.27                     | 0.41              |
| 27:b:625:LMG:H421 | 4:d:284:ILE:HD13  | 2.01                     | 0.41              |
| 3:c:350:ILE:HG21  | 3:c:359:TRP:HB2   | 2.02                     | 0.41              |
| 3:c:464:GLU:HA    | 3:c:465:PRO:HD2   | 1.78                     | 0.41              |
| 27:c:522:LMG:H322 | 10:k:27:VAL:HG23  | 2.02                     | 0.41              |
| 1:A:283:VAL:O     | 1:A:286:THR:HG22  | 2.20                     | 0.41              |
| 2:B:135:LEU:HD22  | 2:B:237:VAL:HG21  | 2.01                     | 0.41              |
| 22:B:601:CLA:HMB2 | 24:H:102:BCR:H393 | 2.02                     | 0.41              |
| 3:C:248:GLY:O     | 3:C:252:ILE:HG12  | 2.21                     | 0.41              |
| 3:C:259:TRP:H     | 3:C:259:TRP:CD1   | 2.38                     | 0.41              |
| 24:F:102:BCR:H361 | 24:F:102:BCR:H20C | 1.81                     | 0.41              |
| 22:H:101:CLA:H162 | 22:H:101:CLA:H122 | 1.50                     | 0.41              |
| 10:K:31:LEU:HB3   | 24:y:101:BCR:C15  | 2.50                     | 0.41              |
| 17:y:25:ILE:O     | 17:y:29:GLY:N     | 2.53                     | 0.41              |
| 18:X:34:PHE:O     | 18:X:38:ILE:HG12  | 2.20                     | 0.41              |
| 22:b:618:CLA:H12  | 22:b:618:CLA:H52  | 1.84                     | 0.41              |
| 3:c:282:MET:HG2   | 22:c:501:CLA:H61  | 2.01                     | 0.41              |
| 24:c:521:BCR:H15C | 24:c:521:BCR:H351 | 1.84                     | 0.41              |
| 1:A:257:ARG:HH22  | 2:B:488:PRO:C     | 2.29                     | 0.41              |
| 2:B:257:TRP:CE2   | 4:D:291:LEU:HD12  | 2.56                     | 0.41              |
| 6:F:17:THR:OG1    | 6:F:18:VAL:N      | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:y:31:ALA:O     | 17:y:35:ILE:HG23  | 2.21                     | 0.41              |
| 1:a:235:TYR:C     | 1:a:237:TYR:H     | 2.29                     | 0.41              |
| 1:a:240:GLY:HA3   | 14:t:29:ILE:HG22  | 2.02                     | 0.41              |
| 3:c:466:VAL:HG13  | 4:d:251:ARG:HD2   | 2.01                     | 0.41              |
| 1:A:215:HIS:ND1   | 23:A:406:PL9:O1   | 2.54                     | 0.41              |
| 2:B:242:ILE:HG12  | 22:B:610:CLA:HBB1 | 2.03                     | 0.41              |
| 13:O:36:ILE:O     | 13:O:39:THR:OG1   | 2.34                     | 0.41              |
| 1:a:89:ILE:HG12   | 13:o:99:ARG:NH2   | 2.36                     | 0.41              |
| 1:a:269:ARG:NH1   | 4:d:231:THR:HB    | 2.36                     | 0.41              |
| 2:b:243:ALA:HA    | 2:b:246:PHE:CE2   | 2.56                     | 0.41              |
| 2:b:280:PHE:O     | 2:b:284:ILE:HG13  | 2.20                     | 0.41              |
| 4:d:55:VAL:HG21   | 4:d:110:LEU:HD12  | 2.03                     | 0.41              |
| 5:e:7:GLU:H       | 5:e:7:GLU:CD      | 2.28                     | 0.41              |
| 1:A:83:VAL:HA     | 1:A:84:PRO:HD3    | 1.97                     | 0.41              |
| 1:A:182:PHE:O     | 1:A:186:PHE:HB2   | 2.21                     | 0.41              |
| 24:B:618:BCR:H11C | 24:B:618:BCR:H341 | 1.88                     | 0.41              |
| 31:D:402:PHO:CHB  | 22:D:405:CLA:H101 | 2.51                     | 0.41              |
| 13:O:178:ARG:HD2  | 13:O:182:PHE:CD1  | 2.56                     | 0.41              |
| 1:a:153:SER:HB2   | 22:a:404:CLA:H43  | 2.03                     | 0.41              |
| 22:b:610:CLA:H122 | 27:b:625:LMG:H412 | 2.03                     | 0.41              |
| 24:c:513:BCR:H11C | 24:g:101:BCR:H322 | 2.03                     | 0.41              |
| 24:c:513:BCR:H361 | 24:c:513:BCR:H20C | 1.80                     | 0.41              |
| 13:o:192:SER:OG   | 13:o:193:GLY:N    | 2.53                     | 0.41              |
| 1:A:258:LEU:O     | 4:D:128:ARG:NH1   | 2.54                     | 0.41              |
| 22:A:403:CLA:HAA1 | 23:D:407:PL9:H362 | 2.02                     | 0.41              |
| 24:A:407:BCR:H11C | 24:A:407:BCR:H341 | 1.94                     | 0.41              |
| 22:B:602:CLA:H192 | 22:B:602:CLA:H162 | 1.77                     | 0.41              |
| 3:C:303:GLY:O     | 3:C:423:ARG:NE    | 2.41                     | 0.41              |
| 25:C:517:DGD:HA22 | 9:J:29:PHE:CE1    | 2.54                     | 0.41              |
| 7:H:19:GLY:O      | 7:H:21:VAL:HG13   | 2.21                     | 0.41              |
| 20:Z:10:ALA:O     | 20:Z:14:ILE:HG13  | 2.21                     | 0.41              |
| 1:a:34:GLY:HA2    | 1:a:37:MET:HB3    | 2.03                     | 0.41              |
| 1:a:333:GLU:HB2   | 1:a:337:HIS:HE1   | 1.85                     | 0.41              |
| 22:b:611:CLA:H143 | 22:b:611:CLA:H161 | 1.91                     | 0.41              |
| 3:c:119:LEU:HG    | 24:c:513:BCR:H10C | 2.02                     | 0.41              |
| 3:c:259:TRP:CD1   | 3:c:259:TRP:H     | 2.39                     | 0.41              |
| 3:c:393:ALA:HB1   | 34:v:201:HEM:HBC1 | 2.03                     | 0.41              |
| 4:d:342:PRO:O     | 4:d:345:VAL:HG12  | 2.20                     | 0.41              |
| 4:d:343:GLU:HG2   | 16:v:161:VAL:HG11 | 2.02                     | 0.41              |
| 31:d:401:PHO:H13  | 31:d:401:PHO:H102 | 1.89                     | 0.41              |
| 7:h:19:GLY:O      | 7:h:21:VAL:HG13   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:161:TYR:HB3   | 1:A:162:PRO:HD3   | 2.02                     | 0.41              |
| 2:B:221:PRO:HA    | 2:B:222:PRO:HD3   | 1.94                     | 0.41              |
| 24:H:102:BCR:HC31 | 24:H:102:BCR:H323 | 1.89                     | 0.41              |
| 24:y:101:BCR:H15C | 24:y:101:BCR:H351 | 1.91                     | 0.41              |
| 22:a:404:CLA:H102 | 22:a:404:CLA:H62  | 1.85                     | 0.41              |
| 2:b:96:VAL:HG22   | 22:b:609:CLA:HBA1 | 2.03                     | 0.41              |
| 2:b:191:ASN:HB2   | 7:h:58:VAL:HG23   | 2.03                     | 0.41              |
| 30:b:604:LMT:H3'  | 30:b:604:LMT:H1B  | 1.55                     | 0.41              |
| 22:c:512:CLA:HAB  | 24:c:521:BCR:H371 | 2.02                     | 0.41              |
| 2:B:16:PRO:HG2    | 2:B:123:PHE:HB3   | 2.03                     | 0.40              |
| 22:B:605:CLA:H62  | 22:B:605:CLA:H41  | 1.86                     | 0.40              |
| 3:C:347:GLY:HA3   | 13:O:43:ASN:HB2   | 2.03                     | 0.40              |
| 13:O:59:ASP:C     | 13:O:61:SER:H     | 2.30                     | 0.40              |
| 16:V:160:LYS:HA   | 16:V:163:TYR:CD2  | 2.57                     | 0.40              |
| 17:y:28:ILE:O     | 24:y:101:BCR:H14C | 2.21                     | 0.40              |
| 1:a:238:LYS:O     | 1:a:241:GLN:HG3   | 2.21                     | 0.40              |
| 2:b:125:ASP:HA    | 2:b:126:PRO:HD3   | 1.98                     | 0.40              |
| 2:B:212:ALA:O     | 2:B:216:HIS:ND1   | 2.52                     | 0.40              |
| 2:B:414:PRO:HB2   | 2:B:415:PRO:HD3   | 2.04                     | 0.40              |
| 3:C:375:LEU:HB3   | 3:C:380:ILE:HD11  | 2.04                     | 0.40              |
| 7:H:12:ARG:N      | 7:H:13:PRO:HD2    | 2.37                     | 0.40              |
| 24:K:102:BCR:H361 | 24:K:102:BCR:H20C | 1.81                     | 0.40              |
| 2:b:179:GLN:HA    | 2:b:180:PRO:HD3   | 1.96                     | 0.40              |
| 2:b:256:MET:O     | 2:b:448:ARG:NH1   | 2.39                     | 0.40              |
| 24:b:622:BCR:H11C | 24:b:622:BCR:H341 | 1.89                     | 0.40              |
| 1:A:112:TYR:O     | 1:A:116:ILE:HG12  | 2.21                     | 0.40              |
| 1:A:296:ASN:HB3   | 3:C:401:LEU:HD13  | 2.04                     | 0.40              |
| 22:B:602:CLA:H61  | 22:B:602:CLA:H41  | 1.67                     | 0.40              |
| 22:B:606:CLA:H62  | 22:B:606:CLA:H41  | 1.90                     | 0.40              |
| 1:a:317:TRP:CD1   | 4:d:177:ALA:HB2   | 2.55                     | 0.40              |
| 24:b:620:BCR:H361 | 24:b:620:BCR:H20C | 1.76                     | 0.40              |
| 3:c:307:PRO:HB3   | 3:c:358:PHE:HB3   | 2.03                     | 0.40              |
| 22:c:510:CLA:H171 | 20:z:20:VAL:HA    | 2.02                     | 0.40              |
| 27:c:518:LMG:H292 | 27:c:518:LMG:H111 | 2.03                     | 0.40              |
| 22:A:402:CLA:H202 | 22:A:403:CLA:H93  | 2.03                     | 0.40              |
| 2:B:54:PRO:HD2    | 2:B:57:ARG:HG3    | 2.02                     | 0.40              |
| 2:B:243:ALA:HA    | 2:B:246:PHE:CE2   | 2.56                     | 0.40              |
| 22:B:602:CLA:CBB  | 22:B:604:CLA:H152 | 2.52                     | 0.40              |
| 22:B:607:CLA:CHA  | 22:B:607:CLA:HBA1 | 2.51                     | 0.40              |
| 3:C:186:TYR:HE2   | 3:C:188:THR:HG22  | 1.86                     | 0.40              |
| 4:D:110:LEU:HD23  | 4:D:110:LEU:HA    | 1.96                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:11:GLU:HG2   | 11:L:12:LEU:N     | 2.35                     | 0.40              |
| 1:a:180:PHE:O     | 1:a:184:ILE:HG13  | 2.22                     | 0.40              |
| 1:a:272:HIS:CD2   | 4:d:218:VAL:HG21  | 2.57                     | 0.40              |
| 22:b:606:CLA:H161 | 22:b:606:CLA:H141 | 1.85                     | 0.40              |
| 24:b:620:BCR:H24C | 24:b:620:BCR:H371 | 1.90                     | 0.40              |
| 24:b:622:BCR:H15C | 24:b:622:BCR:H351 | 1.85                     | 0.40              |
| 24:c:514:BCR:H15C | 24:c:514:BCR:H351 | 1.84                     | 0.40              |
| 29:d:403:SQD:H45  | 29:d:403:SQD:H81  | 1.87                     | 0.40              |
| 1:A:60:ILE:HD12   | 1:A:84:PRO:HD2    | 2.04                     | 0.40              |
| 29:A:413:SQD:H332 | 22:b:609:CLA:H203 | 2.04                     | 0.40              |
| 24:B:617:BCR:H15C | 24:B:617:BCR:H351 | 1.89                     | 0.40              |
| 5:E:7:GLU:CD      | 5:E:7:GLU:H       | 2.30                     | 0.40              |
| 18:X:17:LYS:O     | 18:X:21:ILE:HG13  | 2.22                     | 0.40              |
| 1:a:29:TYR:CG     | 1:a:133:LEU:HD13  | 2.55                     | 0.40              |
| 2:b:6:TYR:OH      | 27:d:408:LMG:HC5  | 2.22                     | 0.40              |
| 2:b:194:ASN:HA    | 2:b:195:PRO:HD3   | 1.92                     | 0.40              |
| 22:b:615:CLA:H171 | 22:b:616:CLA:HBB2 | 2.04                     | 0.40              |
| 11:l:11:GLU:HG2   | 11:l:12:LEU:N     | 2.35                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 333/344 (97%) | 311 (93%) | 18 (5%) | 4 (1%)   | 10          | 42 |
| 1   | a     | 333/344 (97%) | 309 (93%) | 20 (6%) | 4 (1%)   | 10          | 42 |
| 2   | B     | 488/510 (96%) | 451 (92%) | 33 (7%) | 4 (1%)   | 16          | 53 |
| 2   | b     | 488/510 (96%) | 449 (92%) | 36 (7%) | 3 (1%)   | 21          | 58 |
| 3   | C     | 445/461 (96%) | 406 (91%) | 35 (8%) | 4 (1%)   | 14          | 49 |
| 3   | c     | 445/461 (96%) | 405 (91%) | 36 (8%) | 4 (1%)   | 14          | 49 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4   | D     | 338/352 (96%) | 314 (93%) | 23 (7%)  | 1 (0%)   | 36          | 71  |
| 4   | d     | 338/352 (96%) | 314 (93%) | 23 (7%)  | 1 (0%)   | 36          | 71  |
| 5   | E     | 80/84 (95%)   | 77 (96%)  | 2 (2%)   | 1 (1%)   | 9           | 41  |
| 5   | e     | 80/84 (95%)   | 76 (95%)  | 3 (4%)   | 1 (1%)   | 9           | 41  |
| 6   | F     | 33/45 (73%)   | 29 (88%)  | 4 (12%)  | 0        | 100         | 100 |
| 6   | f     | 33/45 (73%)   | 29 (88%)  | 4 (12%)  | 0        | 100         | 100 |
| 7   | H     | 63/66 (96%)   | 54 (86%)  | 6 (10%)  | 3 (5%)   | 2           | 16  |
| 7   | h     | 63/66 (96%)   | 54 (86%)  | 6 (10%)  | 3 (5%)   | 2           | 16  |
| 8   | I     | 33/38 (87%)   | 27 (82%)  | 6 (18%)  | 0        | 100         | 100 |
| 8   | i     | 33/38 (87%)   | 26 (79%)  | 7 (21%)  | 0        | 100         | 100 |
| 9   | J     | 32/40 (80%)   | 28 (88%)  | 3 (9%)   | 1 (3%)   | 3           | 22  |
| 9   | j     | 32/40 (80%)   | 28 (88%)  | 3 (9%)   | 1 (3%)   | 3           | 22  |
| 10  | K     | 35/46 (76%)   | 32 (91%)  | 3 (9%)   | 0        | 100         | 100 |
| 10  | k     | 35/46 (76%)   | 32 (91%)  | 3 (9%)   | 0        | 100         | 100 |
| 11  | L     | 35/37 (95%)   | 33 (94%)  | 2 (6%)   | 0        | 100         | 100 |
| 11  | l     | 35/37 (95%)   | 33 (94%)  | 2 (6%)   | 0        | 100         | 100 |
| 12  | M     | 32/36 (89%)   | 29 (91%)  | 3 (9%)   | 0        | 100         | 100 |
| 12  | m     | 32/36 (89%)   | 29 (91%)  | 3 (9%)   | 0        | 100         | 100 |
| 13  | O     | 241/272 (89%) | 208 (86%) | 30 (12%) | 3 (1%)   | 10          | 42  |
| 13  | o     | 241/272 (89%) | 208 (86%) | 30 (12%) | 3 (1%)   | 10          | 42  |
| 14  | T     | 30/32 (94%)   | 27 (90%)  | 2 (7%)   | 1 (3%)   | 3           | 21  |
| 14  | t     | 30/32 (94%)   | 27 (90%)  | 2 (7%)   | 1 (3%)   | 3           | 21  |
| 15  | U     | 95/134 (71%)  | 87 (92%)  | 6 (6%)   | 2 (2%)   | 5           | 30  |
| 15  | u     | 95/134 (71%)  | 87 (92%)  | 6 (6%)   | 2 (2%)   | 5           | 30  |
| 16  | V     | 135/163 (83%) | 123 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 16  | v     | 135/163 (83%) | 124 (92%) | 11 (8%)  | 0        | 100         | 100 |
| 17  | g     | 26/46 (56%)   | 20 (77%)  | 5 (19%)  | 1 (4%)   | 2           | 19  |
| 17  | y     | 26/46 (56%)   | 19 (73%)  | 6 (23%)  | 1 (4%)   | 2           | 19  |
| 18  | X     | 35/41 (85%)   | 31 (89%)  | 2 (6%)   | 2 (6%)   | 1           | 14  |
| 18  | x     | 35/41 (85%)   | 31 (89%)  | 2 (6%)   | 2 (6%)   | 1           | 14  |
| 20  | Z     | 60/62 (97%)   | 54 (90%)  | 5 (8%)   | 1 (2%)   | 7           | 35  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 20  | z     | 60/62 (97%)     | 54 (90%)   | 5 (8%)   | 1 (2%)   | 7           | 35 |
| All | All   | 5138/5618 (92%) | 4675 (91%) | 408 (8%) | 55 (1%)  | 11          | 45 |

All (55) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ASN  |
| 2   | B     | 484 | PRO  |
| 2   | B     | 488 | PRO  |
| 7   | H     | 18  | TYR  |
| 1   | a     | 12  | ASN  |
| 2   | b     | 484 | PRO  |
| 2   | b     | 488 | PRO  |
| 7   | h     | 18  | TYR  |
| 1   | A     | 141 | PRO  |
| 3   | C     | 257 | PHE  |
| 3   | C     | 416 | SER  |
| 7   | H     | 26  | GLY  |
| 9   | J     | 38  | SER  |
| 13  | O     | 52  | ALA  |
| 14  | T     | 30  | THR  |
| 17  | y     | 43  | ARG  |
| 18  | X     | 45  | LYS  |
| 20  | Z     | 32  | ASP  |
| 1   | a     | 141 | PRO  |
| 3   | c     | 257 | PHE  |
| 3   | c     | 416 | SER  |
| 13  | o     | 52  | ALA  |
| 14  | t     | 30  | THR  |
| 17  | g     | 43  | ARG  |
| 18  | x     | 12  | ILE  |
| 18  | x     | 45  | LYS  |
| 20  | z     | 32  | ASP  |
| 2   | B     | 489 | GLU  |
| 4   | D     | 239 | GLN  |
| 13  | O     | 88  | GLU  |
| 13  | O     | 271 | PRO  |
| 18  | X     | 12  | ILE  |
| 2   | b     | 489 | GLU  |
| 3   | c     | 32  | GLY  |
| 4   | d     | 239 | GLN  |
| 7   | h     | 26  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | j     | 38  | SER  |
| 13  | o     | 88  | GLU  |
| 1   | A     | 142 | TRP  |
| 3   | C     | 32  | GLY  |
| 5   | E     | 82  | GLN  |
| 1   | a     | 142 | TRP  |
| 1   | a     | 334 | ARG  |
| 5   | e     | 82  | GLN  |
| 13  | o     | 271 | PRO  |
| 1   | A     | 334 | ARG  |
| 7   | H     | 16  | SER  |
| 15  | U     | 73  | PRO  |
| 3   | c     | 144 | SER  |
| 7   | h     | 16  | SER  |
| 15  | u     | 73  | PRO  |
| 3   | C     | 144 | SER  |
| 15  | U     | 83  | ALA  |
| 15  | u     | 83  | ALA  |
| 2   | B     | 176 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 271/280 (97%) | 261 (96%) | 10 (4%)  | 30          | 51 |
| 1   | a     | 271/280 (97%) | 260 (96%) | 11 (4%)  | 27          | 49 |
| 2   | B     | 390/407 (96%) | 379 (97%) | 11 (3%)  | 38          | 59 |
| 2   | b     | 390/407 (96%) | 380 (97%) | 10 (3%)  | 40          | 60 |
| 3   | C     | 347/362 (96%) | 335 (96%) | 12 (4%)  | 32          | 53 |
| 3   | c     | 347/362 (96%) | 335 (96%) | 12 (4%)  | 32          | 53 |
| 4   | D     | 275/283 (97%) | 265 (96%) | 10 (4%)  | 31          | 52 |
| 4   | d     | 275/283 (97%) | 264 (96%) | 11 (4%)  | 28          | 49 |
| 5   | E     | 72/73 (99%)   | 68 (94%)  | 4 (6%)   | 19          | 41 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 5   | e     | 72/73 (99%)     | 68 (94%)   | 4 (6%)   | 19          | 41  |
| 6   | F     | 29/39 (74%)     | 29 (100%)  | 0        | 100         | 100 |
| 6   | f     | 29/39 (74%)     | 29 (100%)  | 0        | 100         | 100 |
| 7   | H     | 53/55 (96%)     | 50 (94%)   | 3 (6%)   | 18          | 40  |
| 7   | h     | 53/55 (96%)     | 50 (94%)   | 3 (6%)   | 18          | 40  |
| 8   | I     | 32/35 (91%)     | 31 (97%)   | 1 (3%)   | 35          | 56  |
| 8   | i     | 32/35 (91%)     | 31 (97%)   | 1 (3%)   | 35          | 56  |
| 9   | J     | 24/28 (86%)     | 23 (96%)   | 1 (4%)   | 26          | 48  |
| 9   | j     | 24/28 (86%)     | 23 (96%)   | 1 (4%)   | 26          | 48  |
| 10  | K     | 30/37 (81%)     | 30 (100%)  | 0        | 100         | 100 |
| 10  | k     | 30/37 (81%)     | 30 (100%)  | 0        | 100         | 100 |
| 11  | L     | 35/35 (100%)    | 34 (97%)   | 1 (3%)   | 37          | 57  |
| 11  | l     | 35/35 (100%)    | 34 (97%)   | 1 (3%)   | 37          | 57  |
| 12  | M     | 31/33 (94%)     | 31 (100%)  | 0        | 100         | 100 |
| 12  | m     | 31/33 (94%)     | 31 (100%)  | 0        | 100         | 100 |
| 13  | O     | 202/228 (89%)   | 200 (99%)  | 2 (1%)   | 68          | 76  |
| 13  | o     | 202/228 (89%)   | 200 (99%)  | 2 (1%)   | 68          | 76  |
| 14  | T     | 29/29 (100%)    | 28 (97%)   | 1 (3%)   | 32          | 54  |
| 14  | t     | 29/29 (100%)    | 28 (97%)   | 1 (3%)   | 32          | 54  |
| 15  | U     | 84/112 (75%)    | 82 (98%)   | 2 (2%)   | 43          | 63  |
| 15  | u     | 84/112 (75%)    | 82 (98%)   | 2 (2%)   | 43          | 63  |
| 16  | V     | 116/138 (84%)   | 114 (98%)  | 2 (2%)   | 53          | 67  |
| 16  | v     | 116/138 (84%)   | 114 (98%)  | 2 (2%)   | 53          | 67  |
| 17  | g     | 20/37 (54%)     | 17 (85%)   | 3 (15%)  | 3           | 13  |
| 17  | y     | 20/37 (54%)     | 17 (85%)   | 3 (15%)  | 3           | 13  |
| 18  | X     | 30/34 (88%)     | 28 (93%)   | 2 (7%)   | 15          | 36  |
| 18  | x     | 30/34 (88%)     | 28 (93%)   | 2 (7%)   | 15          | 36  |
| 20  | Z     | 52/52 (100%)    | 50 (96%)   | 2 (4%)   | 29          | 51  |
| 20  | z     | 52/52 (100%)    | 50 (96%)   | 2 (4%)   | 29          | 51  |
| All | All   | 4244/4594 (92%) | 4109 (97%) | 135 (3%) | 34          | 55  |

All (135) residues with a non-rotameric sidechain are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 30  | VAL  |
| 1   | A     | 157 | VAL  |
| 1   | A     | 202 | VAL  |
| 1   | A     | 228 | THR  |
| 1   | A     | 243 | GLU  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 275 | LEU  |
| 1   | A     | 286 | THR  |
| 1   | A     | 292 | THR  |
| 1   | A     | 306 | VAL  |
| 2   | B     | 23  | HIS  |
| 2   | B     | 262 | THR  |
| 2   | B     | 308 | LYS  |
| 2   | B     | 309 | LEU  |
| 2   | B     | 354 | LEU  |
| 2   | B     | 362 | PHE  |
| 2   | B     | 422 | ARG  |
| 2   | B     | 467 | ILE  |
| 2   | B     | 485 | GLU  |
| 2   | B     | 486 | LEU  |
| 2   | B     | 490 | GLN  |
| 3   | C     | 29  | GLU  |
| 3   | C     | 86  | LEU  |
| 3   | C     | 174 | LEU  |
| 3   | C     | 201 | ASN  |
| 3   | C     | 244 | CYS  |
| 3   | C     | 254 | THR  |
| 3   | C     | 289 | PHE  |
| 3   | C     | 305 | THR  |
| 3   | C     | 355 | THR  |
| 3   | C     | 417 | VAL  |
| 3   | C     | 469 | MET  |
| 3   | C     | 472 | LEU  |
| 4   | D     | 43  | LEU  |
| 4   | D     | 91  | LEU  |
| 4   | D     | 180 | ARG  |
| 4   | D     | 201 | VAL  |
| 4   | D     | 205 | LEU  |
| 4   | D     | 241 | GLU  |
| 4   | D     | 259 | ILE  |
| 4   | D     | 291 | LEU  |
| 4   | D     | 323 | GLU  |
| 4   | D     | 346 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 18  | ARG  |
| 5   | E     | 77  | GLU  |
| 5   | E     | 80  | LEU  |
| 5   | E     | 84  | LYS  |
| 7   | H     | 27  | THR  |
| 7   | H     | 56  | ASP  |
| 7   | H     | 60  | VAL  |
| 8   | I     | 33  | LYS  |
| 9   | J     | 7   | ARG  |
| 11  | L     | 11  | GLU  |
| 13  | O     | 31  | LEU  |
| 13  | O     | 97  | VAL  |
| 14  | T     | 29  | ILE  |
| 15  | U     | 114 | VAL  |
| 15  | U     | 132 | LEU  |
| 16  | V     | 68  | VAL  |
| 16  | V     | 116 | GLU  |
| 17  | y     | 25  | ILE  |
| 17  | y     | 28  | ILE  |
| 17  | y     | 46  | LEU  |
| 18  | X     | 12  | ILE  |
| 18  | X     | 42  | GLN  |
| 20  | Z     | 33  | TRP  |
| 20  | Z     | 62  | VAL  |
| 1   | a     | 30  | VAL  |
| 1   | a     | 157 | VAL  |
| 1   | a     | 202 | VAL  |
| 1   | a     | 226 | GLU  |
| 1   | a     | 228 | THR  |
| 1   | a     | 243 | GLU  |
| 1   | a     | 271 | LEU  |
| 1   | a     | 275 | LEU  |
| 1   | a     | 286 | THR  |
| 1   | a     | 292 | THR  |
| 1   | a     | 306 | VAL  |
| 2   | b     | 23  | HIS  |
| 2   | b     | 262 | THR  |
| 2   | b     | 309 | LEU  |
| 2   | b     | 354 | LEU  |
| 2   | b     | 362 | PHE  |
| 2   | b     | 422 | ARG  |
| 2   | b     | 467 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 485 | GLU  |
| 2   | b     | 486 | LEU  |
| 2   | b     | 490 | GLN  |
| 3   | c     | 29  | GLU  |
| 3   | c     | 86  | LEU  |
| 3   | c     | 174 | LEU  |
| 3   | c     | 201 | ASN  |
| 3   | c     | 244 | CYS  |
| 3   | c     | 254 | THR  |
| 3   | c     | 289 | PHE  |
| 3   | c     | 305 | THR  |
| 3   | c     | 355 | THR  |
| 3   | c     | 417 | VAL  |
| 3   | c     | 469 | MET  |
| 3   | c     | 472 | LEU  |
| 4   | d     | 43  | LEU  |
| 4   | d     | 91  | LEU  |
| 4   | d     | 180 | ARG  |
| 4   | d     | 201 | VAL  |
| 4   | d     | 205 | LEU  |
| 4   | d     | 241 | GLU  |
| 4   | d     | 259 | ILE  |
| 4   | d     | 291 | LEU  |
| 4   | d     | 323 | GLU  |
| 4   | d     | 345 | VAL  |
| 4   | d     | 346 | LEU  |
| 5   | e     | 18  | ARG  |
| 5   | e     | 77  | GLU  |
| 5   | e     | 80  | LEU  |
| 5   | e     | 84  | LYS  |
| 7   | h     | 27  | THR  |
| 7   | h     | 56  | ASP  |
| 7   | h     | 60  | VAL  |
| 8   | i     | 33  | LYS  |
| 9   | j     | 7   | ARG  |
| 11  | l     | 11  | GLU  |
| 13  | o     | 31  | LEU  |
| 13  | o     | 97  | VAL  |
| 14  | t     | 29  | ILE  |
| 15  | u     | 114 | VAL  |
| 15  | u     | 132 | LEU  |
| 16  | v     | 68  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | v     | 116 | GLU  |
| 17  | g     | 25  | ILE  |
| 17  | g     | 28  | ILE  |
| 17  | g     | 46  | LEU  |
| 18  | x     | 12  | ILE  |
| 18  | x     | 42  | GLN  |
| 20  | z     | 33  | TRP  |
| 20  | z     | 62  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 165 | GLN  |
| 1   | A     | 241 | GLN  |
| 1   | A     | 303 | ASN  |
| 1   | A     | 337 | HIS  |
| 2   | B     | 9   | HIS  |
| 2   | B     | 26  | HIS  |
| 2   | B     | 223 | GLN  |
| 2   | B     | 374 | ASN  |
| 3   | C     | 44  | ASN  |
| 3   | C     | 56  | HIS  |
| 3   | C     | 118 | HIS  |
| 3   | C     | 229 | ASN  |
| 3   | C     | 441 | HIS  |
| 4   | D     | 117 | HIS  |
| 4   | D     | 186 | GLN  |
| 4   | D     | 250 | ASN  |
| 4   | D     | 301 | GLN  |
| 4   | D     | 322 | ASN  |
| 12  | M     | 33  | GLN  |
| 13  | O     | 150 | ASN  |
| 13  | O     | 173 | ASN  |
| 15  | U     | 93  | ASN  |
| 1   | a     | 241 | GLN  |
| 1   | a     | 337 | HIS  |
| 2   | b     | 26  | HIS  |
| 2   | b     | 223 | GLN  |
| 2   | b     | 282 | GLN  |
| 2   | b     | 331 | ASN  |
| 2   | b     | 374 | ASN  |
| 3   | c     | 44  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | c     | 56  | HIS  |
| 3   | c     | 229 | ASN  |
| 3   | c     | 441 | HIS  |
| 4   | d     | 117 | HIS  |
| 4   | d     | 250 | ASN  |
| 4   | d     | 301 | GLN  |
| 12  | m     | 33  | GLN  |
| 13  | o     | 130 | GLN  |
| 13  | o     | 150 | ASN  |
| 13  | o     | 173 | ASN  |
| 15  | u     | 93  | ASN  |

### 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 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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 | $\# Z  > 2$ |
| 27  | LMG  | e     | 101 | -    | 44,44,55     | 0.75 | 0           | 52,52,63    | 1.29 | 5 (9%)      |
| 24  | BCR  | c     | 513 | -    | 41,41,41     | 1.11 | 2 (4%)      | 56,56,56    | 1.37 | 9 (16%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | LMG  | D     | 409 | -    | 48,48,55     | 0.76 | 0        | 56,56,63    | 1.37 | 4 (7%)   |
| 22  | CLA  | c     | 506 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.28 | 5 (6%)   |
| 33  | BCT  | D     | 404 | 21   | 3,3,3        | 1.11 | 0        | 2,3,3       | 4.29 | 2 (100%) |
| 23  | PL9  | j     | 101 | -    | 35,35,55     | 0.98 | 2 (5%)   | 44,45,69    | 1.58 | 9 (20%)  |
| 31  | PHO  | D     | 401 | -    | 58,69,69     | 2.15 | 9 (15%)  | 55,99,99    | 1.42 | 6 (10%)  |
| 24  | BCR  | H     | 102 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 22  | CLA  | c     | 510 | 3    | 69,73,73     | 1.20 | 5 (7%)   | 82,113,113  | 1.28 | 5 (6%)   |
| 22  | CLA  | c     | 520 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 24  | BCR  | F     | 102 | -    | 41,41,41     | 1.16 | 3 (7%)   | 56,56,56    | 1.26 | 6 (10%)  |
| 24  | BCR  | g     | 101 | -    | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 24  | BCR  | x     | 101 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.20 | 4 (7%)   |
| 30  | LMT  | d     | 411 | -    | 32,32,36     | 1.16 | 4 (12%)  | 43,43,47    | 1.00 | 2 (4%)   |
| 34  | HEM  | v     | 201 | 16   | 50,50,50     | 2.00 | 10 (20%) | 67,82,82    | 1.25 | 4 (5%)   |
| 25  | DGD  | B     | 620 | -    | 59,59,67     | 0.90 | 1 (1%)   | 73,73,81    | 1.34 | 9 (12%)  |
| 24  | BCR  | c     | 514 | -    | 41,41,41     | 1.13 | 3 (7%)   | 56,56,56    | 1.29 | 9 (16%)  |
| 29  | SQD  | A     | 412 | -    | 49,51,54     | 0.96 | 2 (4%)   | 59,62,65    | 1.67 | 10 (16%) |
| 22  | CLA  | b     | 611 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.24 | 4 (4%)   |
| 22  | CLA  | B     | 608 | -    | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 22  | CLA  | b     | 618 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.27 | 5 (6%)   |
| 25  | DGD  | c     | 517 | -    | 67,67,67     | 0.87 | 0        | 81,81,81    | 1.39 | 9 (11%)  |
| 25  | DGD  | b     | 601 | -    | 53,53,67     | 1.04 | 4 (7%)   | 67,67,81    | 1.32 | 7 (10%)  |
| 31  | PHO  | d     | 401 | -    | 58,69,69     | 2.15 | 9 (15%)  | 55,99,99    | 1.42 | 7 (12%)  |
| 22  | CLA  | b     | 607 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.33 | 7 (8%)   |
| 31  | PHO  | d     | 402 | -    | 58,69,69     | 2.18 | 9 (15%)  | 55,99,99    | 1.39 | 5 (9%)   |
| 29  | SQD  | B     | 622 | -    | 41,43,54     | 1.05 | 2 (4%)   | 51,54,65    | 1.68 | 11 (21%) |
| 28  | OEX  | a     | 414 | 3,1  | 0,15,15      | -    | -        | -           | -    | -        |
| 22  | CLA  | b     | 608 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 4 (4%)   |
| 24  | BCR  | B     | 619 | -    | 41,41,41     | 1.11 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 25  | DGD  | c     | 515 | -    | 54,54,67     | 0.95 | 1 (1%)   | 68,68,81    | 1.26 | 6 (8%)   |
| 27  | LMG  | a     | 402 | -    | 42,42,55     | 0.82 | 2 (4%)   | 50,50,63    | 1.26 | 5 (10%)  |
| 25  | DGD  | D     | 410 | -    | 64,64,67     | 0.91 | 0        | 78,78,81    | 1.32 | 9 (11%)  |
| 23  | PL9  | a     | 408 | -    | 45,45,55     | 1.05 | 4 (8%)   | 56,57,69    | 1.54 | 10 (17%) |
| 24  | BCR  | K     | 102 | -    | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.26 | 8 (14%)  |
| 22  | CLA  | D     | 405 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.20 | 5 (6%)   |
| 22  | CLA  | C     | 508 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.23 | 5 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 29  | SQD  | d     | 403 | -    | 41,43,54     | 1.05 | 2 (4%)   | 51,54,65    | 1.70 | 11 (21%) |
| 22  | CLA  | B     | 607 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 22  | CLA  | B     | 601 | -    | 69,73,73     | 1.21 | 7 (10%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 22  | CLA  | a     | 404 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.25 | 7 (8%)   |
| 24  | BCR  | J     | 102 | -    | 41,41,41     | 1.11 | 3 (7%)   | 56,56,56    | 1.62 | 12 (21%) |
| 22  | CLA  | C     | 511 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 27  | LMG  | I     | 101 | -    | 43,43,55     | 0.79 | 0        | 51,51,63    | 1.27 | 4 (7%)   |
| 23  | PL9  | D     | 407 | -    | 55,55,55     | 1.06 | 4 (7%)   | 68,69,69    | 1.50 | 13 (19%) |
| 27  | LMG  | D     | 408 | -    | 49,49,55     | 0.76 | 1 (2%)   | 57,57,63    | 1.31 | 5 (8%)   |
| 22  | CLA  | B     | 613 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 22  | CLA  | B     | 604 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.25 | 4 (4%)   |
| 26  | LHG  | a     | 411 | -    | 38,38,48     | 0.69 | 1 (2%)   | 41,44,54    | 1.23 | 3 (7%)   |
| 30  | LMT  | M     | 102 | -    | 36,36,36     | 1.12 | 5 (13%)  | 47,47,47    | 1.01 | 2 (4%)   |
| 30  | LMT  | b     | 626 | -    | 36,36,36     | 1.11 | 4 (11%)  | 47,47,47    | 0.96 | 1 (2%)   |
| 22  | CLA  | b     | 613 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 24  | BCR  | C     | 513 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.35 | 9 (16%)  |
| 22  | CLA  | h     | 101 | -    | 69,73,73     | 1.20 | 8 (11%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 24  | BCR  | f     | 102 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 29  | SQD  | b     | 602 | -    | 45,47,54     | 1.02 | 3 (6%)   | 55,58,65    | 1.72 | 10 (18%) |
| 22  | CLA  | c     | 508 | -    | 69,73,73     | 1.20 | 7 (10%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 22  | CLA  | C     | 502 | -    | 69,73,73     | 1.19 | 9 (13%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 22  | CLA  | c     | 509 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 22  | CLA  | B     | 610 | -    | 69,73,73     | 1.24 | 6 (8%)   | 82,113,113  | 1.34 | 6 (7%)   |
| 27  | LMG  | A     | 410 | -    | 51,51,55     | 0.74 | 0        | 59,59,63    | 1.36 | 7 (11%)  |
| 27  | LMG  | d     | 409 | -    | 48,48,55     | 0.76 | 0        | 56,56,63    | 1.37 | 4 (7%)   |
| 29  | SQD  | F     | 103 | -    | 43,45,54     | 1.03 | 2 (4%)   | 53,56,65    | 1.57 | 10 (18%) |
| 22  | CLA  | B     | 605 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 27  | LMG  | A     | 414 | -    | 42,42,55     | 0.83 | 2 (4%)   | 50,50,63    | 1.25 | 4 (8%)   |
| 29  | SQD  | f     | 103 | -    | 43,45,54     | 1.03 | 2 (4%)   | 53,56,65    | 1.57 | 10 (18%) |
| 30  | LMT  | D     | 411 | -    | 32,32,36     | 1.16 | 4 (12%)  | 43,43,47    | 1.03 | 2 (4%)   |
| 22  | CLA  | C     | 501 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.27 | 5 (6%)   |
| 22  | CLA  | C     | 520 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 22  | CLA  | C     | 507 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 22  | CLA  | A     | 405 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.24 | 4 (4%)   |
| 25  | DGD  | C     | 517 | -    | 67,67,67     | 0.86 | 0        | 81,81,81    | 1.40 | 9 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | BCR  | C     | 514 | -    | 41,41,41     | 1.14 | 3 (7%)   | 56,56,56    | 1.31 | 9 (16%)  |
| 27  | LMG  | d     | 412 | -    | 46,46,55     | 0.77 | 1 (2%)   | 54,54,63    | 1.30 | 6 (11%)  |
| 22  | CLA  | d     | 405 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.19 | 6 (7%)   |
| 22  | CLA  | B     | 612 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.26 | 7 (8%)   |
| 27  | LMG  | B     | 621 | -    | 49,49,55     | 0.77 | 1 (2%)   | 57,57,63    | 1.32 | 7 (12%)  |
| 24  | BCR  | y     | 101 | -    | 41,41,41     | 1.18 | 3 (7%)   | 56,56,56    | 1.27 | 8 (14%)  |
| 24  | BCR  | b     | 623 | -    | 41,41,41     | 1.11 | 2 (4%)   | 56,56,56    | 1.31 | 9 (16%)  |
| 22  | CLA  | B     | 603 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.35 | 7 (8%)   |
| 22  | CLA  | B     | 606 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 22  | CLA  | b     | 605 | -    | 69,73,73     | 1.21 | 7 (10%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 27  | LMG  | d     | 408 | -    | 49,49,55     | 0.76 | 1 (2%)   | 57,57,63    | 1.31 | 5 (8%)   |
| 22  | CLA  | b     | 617 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 4 (4%)   |
| 22  | CLA  | c     | 504 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.30 | 5 (6%)   |
| 31  | PHO  | D     | 402 | -    | 58,69,69     | 2.20 | 9 (15%)  | 55,99,99    | 1.42 | 5 (9%)   |
| 22  | CLA  | c     | 503 | -    | 69,73,73     | 1.20 | 8 (11%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 29  | SQD  | A     | 413 | -    | 52,54,54     | 0.95 | 3 (5%)   | 62,65,65    | 1.48 | 9 (14%)  |
| 22  | CLA  | C     | 505 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.28 | 4 (4%)   |
| 27  | LMG  | c     | 522 | -    | 48,48,55     | 0.76 | 0        | 56,56,63    | 1.30 | 5 (8%)   |
| 22  | CLA  | c     | 502 | -    | 69,73,73     | 1.19 | 9 (13%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 27  | LMG  | b     | 625 | -    | 49,49,55     | 0.77 | 1 (2%)   | 57,57,63    | 1.32 | 7 (12%)  |
| 22  | CLA  | b     | 616 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.28 | 7 (8%)   |
| 22  | CLA  | C     | 504 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.31 | 5 (6%)   |
| 22  | CLA  | C     | 503 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.26 | 4 (4%)   |
| 22  | CLA  | b     | 612 | -    | 69,73,73     | 1.20 | 6 (8%)   | 82,113,113  | 1.22 | 5 (6%)   |
| 22  | CLA  | C     | 506 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.28 | 5 (6%)   |
| 25  | DGD  | c     | 516 | -    | 63,63,67     | 0.90 | 1 (1%)   | 77,77,81    | 1.42 | 11 (14%) |
| 22  | CLA  | c     | 505 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 27  | LMG  | c     | 518 | -    | 45,45,55     | 0.76 | 0        | 53,53,63    | 1.28 | 5 (9%)   |
| 30  | LMT  | b     | 604 | -    | 36,36,36     | 1.11 | 4 (11%)  | 47,47,47    | 1.05 | 1 (2%)   |
| 22  | CLA  | c     | 507 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 30  | LMT  | B     | 624 | -    | 36,36,36     | 1.08 | 3 (8%)   | 47,47,47    | 1.02 | 2 (4%)   |
| 25  | DGD  | C     | 516 | -    | 63,63,67     | 0.90 | 1 (1%)   | 77,77,81    | 1.42 | 12 (15%) |
| 22  | CLA  | B     | 602 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 22  | CLA  | A     | 404 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 22  | CLA  | a     | 407 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.24 | 5 (6%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | BCR  | B     | 616 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 22  | CLA  | C     | 509 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 27  | LMG  | C     | 518 | -    | 45,45,55     | 0.76 | 0        | 53,53,63    | 1.28 | 5 (9%)   |
| 30  | LMT  | M     | 103 | -    | 36,36,36     | 1.13 | 5 (13%)  | 47,47,47    | 1.00 | 2 (4%)   |
| 25  | DGD  | a     | 410 | -    | 57,57,67     | 0.92 | 1 (1%)   | 71,71,81    | 1.40 | 9 (12%)  |
| 24  | BCR  | B     | 617 | -    | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.34 | 7 (12%)  |
| 30  | LMT  | I     | 102 | -    | 36,36,36     | 1.09 | 4 (11%)  | 47,47,47    | 1.02 | 2 (4%)   |
| 22  | CLA  | B     | 614 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.26 | 5 (6%)   |
| 30  | LMT  | B     | 623 | -    | 36,36,36     | 1.10 | 4 (11%)  | 47,47,47    | 0.97 | 1 (2%)   |
| 22  | CLA  | c     | 512 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.26 | 5 (6%)   |
| 33  | BCT  | d     | 404 | 21   | 3,3,3        | 1.11 | 0        | 2,3,3       | 4.26 | 2 (100%) |
| 30  | LMT  | i     | 102 | -    | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 1.00 | 2 (4%)   |
| 34  | HEM  | V     | 201 | 16   | 50,50,50     | 1.98 | 9 (18%)  | 67,82,82    | 1.22 | 4 (5%)   |
| 23  | PL9  | A     | 406 | -    | 45,45,55     | 1.01 | 4 (8%)   | 56,57,69    | 1.55 | 10 (17%) |
| 22  | CLA  | d     | 406 | -    | 69,73,73     | 1.19 | 5 (7%)   | 82,113,113  | 1.27 | 5 (6%)   |
| 22  | CLA  | b     | 610 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 30  | LMT  | B     | 627 | -    | 36,36,36     | 1.10 | 4 (11%)  | 47,47,47    | 0.96 | 1 (2%)   |
| 24  | BCR  | j     | 102 | -    | 41,41,41     | 1.10 | 3 (7%)   | 56,56,56    | 1.60 | 12 (21%) |
| 22  | CLA  | C     | 510 | 3    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.30 | 6 (7%)   |
| 22  | CLA  | B     | 609 | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 27  | LMG  | C     | 521 | -    | 48,48,55     | 0.77 | 1 (2%)   | 56,56,63    | 1.30 | 5 (8%)   |
| 29  | SQD  | a     | 401 | -    | 52,54,54     | 0.95 | 2 (3%)   | 62,65,65    | 1.48 | 9 (14%)  |
| 22  | CLA  | a     | 406 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 25  | DGD  | A     | 408 | -    | 57,57,67     | 0.92 | 0        | 71,71,81    | 1.41 | 9 (12%)  |
| 34  | HEM  | f     | 101 | 5,6  | 50,50,50     | 1.97 | 8 (16%)  | 67,82,82    | 1.33 | 4 (5%)   |
| 27  | LMG  | E     | 101 | -    | 44,44,55     | 0.75 | 0        | 52,52,63    | 1.29 | 4 (7%)   |
| 25  | DGD  | B     | 625 | -    | 53,53,67     | 1.06 | 3 (5%)   | 67,67,81    | 1.32 | 7 (10%)  |
| 24  | BCR  | c     | 521 | -    | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.26 | 8 (14%)  |
| 25  | DGD  | b     | 624 | -    | 59,59,67     | 0.90 | 1 (1%)   | 73,73,81    | 1.33 | 7 (9%)   |
| 28  | OEX  | A     | 411 | 3,1  | 0,15,15      | -    | -        | -           | -    | -        |
| 27  | LMG  | a     | 412 | -    | 51,51,55     | 0.75 | 0        | 59,59,63    | 1.34 | 6 (10%)  |
| 24  | BCR  | B     | 618 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.38 | 9 (16%)  |
| 22  | CLA  | A     | 403 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.30 | 5 (6%)   |
| 22  | CLA  | b     | 606 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.22 | 5 (6%)   |
| 34  | HEM  | F     | 101 | 5,6  | 50,50,50     | 1.97 | 9 (18%)  | 67,82,82    | 1.32 | 4 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | B     | 615 | -    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 29  | SQD  | B     | 626 | -    | 45,47,54     | 1.01 | 3 (6%)   | 55,58,65    | 1.70 | 10 (18%) |
| 24  | BCR  | A     | 407 | -    | 41,41,41     | 1.11 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 22  | CLA  | b     | 619 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.23 | 4 (4%)   |
| 30  | LMT  | B     | 628 | -    | 36,36,36     | 1.12 | 4 (11%)  | 47,47,47    | 1.05 | 1 (2%)   |
| 30  | LMT  | b     | 627 | -    | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 1.00 | 2 (4%)   |
| 27  | LMG  | M     | 101 | -    | 42,42,55     | 0.84 | 1 (2%)   | 50,50,63    | 1.23 | 4 (8%)   |
| 23  | PL9  | d     | 407 | -    | 55,55,55     | 1.05 | 3 (5%)   | 68,69,69    | 1.51 | 12 (17%) |
| 27  | LMG  | m     | 101 | -    | 42,42,55     | 0.84 | 0        | 50,50,63    | 1.23 | 4 (8%)   |
| 22  | CLA  | b     | 614 | -    | 69,73,73     | 1.24 | 7 (10%)  | 82,113,113  | 1.34 | 6 (7%)   |
| 23  | PL9  | J     | 101 | -    | 35,35,55     | 1.00 | 2 (5%)   | 44,45,69    | 1.58 | 8 (18%)  |
| 22  | CLA  | b     | 609 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.29 | 5 (6%)   |
| 26  | LHG  | A     | 409 | -    | 38,38,48     | 0.70 | 1 (2%)   | 41,44,54    | 1.22 | 3 (7%)   |
| 26  | LHG  | c     | 519 | -    | 36,36,48     | 0.73 | 2 (5%)   | 39,42,54    | 1.30 | 4 (10%)  |
| 22  | CLA  | c     | 501 | -    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.26 | 5 (6%)   |
| 22  | CLA  | b     | 615 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 22  | CLA  | H     | 101 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 27  | LMG  | i     | 101 | -    | 43,43,55     | 0.80 | 0        | 51,51,63    | 1.27 | 6 (11%)  |
| 22  | CLA  | B     | 611 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 30  | LMT  | b     | 603 | -    | 36,36,36     | 1.10 | 4 (11%)  | 47,47,47    | 0.96 | 1 (2%)   |
| 22  | CLA  | D     | 406 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 22  | CLA  | a     | 405 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.29 | 5 (6%)   |
| 22  | CLA  | A     | 402 | -    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 24  | BCR  | a     | 409 | -    | 41,41,41     | 1.11 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 24  | BCR  | b     | 620 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 25  | DGD  | C     | 515 | -    | 54,54,67     | 0.97 | 2 (3%)   | 68,68,81    | 1.25 | 5 (7%)   |
| 26  | LHG  | C     | 519 | -    | 36,36,48     | 0.72 | 1 (2%)   | 39,42,54    | 1.30 | 4 (10%)  |
| 25  | DGD  | d     | 410 | -    | 64,64,67     | 0.92 | 2 (3%)   | 78,78,81    | 1.34 | 9 (11%)  |
| 22  | CLA  | C     | 512 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.27 | 5 (6%)   |
| 22  | CLA  | c     | 511 | -    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.25 | 5 (6%)   |
| 27  | LMG  | D     | 412 | -    | 46,46,55     | 0.76 | 1 (2%)   | 54,54,63    | 1.31 | 6 (11%)  |
| 24  | BCR  | b     | 622 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.39 | 11 (19%) |
| 29  | SQD  | a     | 415 | -    | 49,51,54     | 0.97 | 2 (4%)   | 59,62,65    | 1.69 | 10 (16%) |
| 24  | BCR  | b     | 621 | -    | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.35 | 9 (16%)  |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | LMG  | e     | 101 | -    | -         | 19/39/59/70   | 0/1/1/1 |
| 24  | BCR  | c     | 513 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 27  | LMG  | D     | 409 | -    | -         | 21/43/63/70   | 0/1/1/1 |
| 22  | CLA  | c     | 506 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 23  | PL9  | j     | 101 | -    | -         | 8/29/49/73    | 0/1/1/1 |
| 31  | PHO  | D     | 401 | -    | -         | 10/37/103/103 | 0/5/6/6 |
| 24  | BCR  | H     | 102 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 22  | CLA  | c     | 510 | 3    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | c     | 520 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 24  | BCR  | F     | 102 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 24  | BCR  | g     | 101 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 24  | BCR  | x     | 101 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 30  | LMT  | d     | 411 | -    | -         | 0/17/57/61    | 0/2/2/2 |
| 34  | HEM  | v     | 201 | 16   | -         | 5/14/54/54    | -       |
| 25  | DGD  | B     | 620 | -    | -         | 19/47/87/95   | 0/2/2/2 |
| 24  | BCR  | c     | 514 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 29  | SQD  | A     | 412 | -    | -         | 18/46/66/69   | 0/1/1/1 |
| 22  | CLA  | b     | 611 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | B     | 608 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 22  | CLA  | b     | 618 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | DGD  | c     | 517 | -    | -         | 20/55/95/95   | 0/2/2/2 |
| 25  | DGD  | b     | 601 | -    | -         | 19/41/81/95   | 0/2/2/2 |
| 31  | PHO  | d     | 401 | -    | -         | 10/37/103/103 | 0/5/6/6 |
| 22  | CLA  | b     | 607 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 31  | PHO  | d     | 402 | -    | -         | 11/37/103/103 | 0/5/6/6 |
| 29  | SQD  | B     | 622 | -    | -         | 14/38/58/69   | 0/1/1/1 |
| 22  | CLA  | b     | 608 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 24  | BCR  | B     | 619 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 25  | DGD  | c     | 515 | -    | -         | 19/42/82/95   | 0/2/2/2 |
| 27  | LMG  | a     | 402 | -    | -         | 16/37/57/70   | 0/1/1/1 |
| 25  | DGD  | D     | 410 | -    | -         | 34/52/92/95   | 0/2/2/2 |
| 23  | PL9  | a     | 408 | -    | -         | 18/41/61/73   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24  | BCR  | K     | 102 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | D     | 405 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | C     | 508 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 29  | SQD  | d     | 403 | -    | -         | 14/38/58/69   | 0/1/1/1 |
| 22  | CLA  | B     | 607 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | B     | 601 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | a     | 404 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 24  | BCR  | J     | 102 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 22  | CLA  | C     | 511 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 27  | LMG  | I     | 101 | -    | -         | 18/38/58/70   | 0/1/1/1 |
| 23  | PL9  | D     | 407 | -    | -         | 12/53/73/73   | 0/1/1/1 |
| 27  | LMG  | D     | 408 | -    | -         | 25/44/64/70   | 0/1/1/1 |
| 22  | CLA  | B     | 613 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | B     | 604 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 26  | LHG  | a     | 411 | -    | -         | 11/43/43/53   | -       |
| 30  | LMT  | M     | 102 | -    | -         | 0/21/61/61    | 0/2/2/2 |
| 30  | LMT  | b     | 626 | -    | -         | 2/21/61/61    | 0/2/2/2 |
| 22  | CLA  | b     | 613 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 24  | BCR  | C     | 513 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 22  | CLA  | h     | 101 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 24  | BCR  | f     | 102 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 29  | SQD  | b     | 602 | -    | -         | 13/42/62/69   | 0/1/1/1 |
| 22  | CLA  | c     | 508 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | C     | 502 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 22  | CLA  | c     | 509 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | B     | 610 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 27  | LMG  | A     | 410 | -    | -         | 26/46/66/70   | 0/1/1/1 |
| 27  | LMG  | d     | 409 | -    | -         | 20/43/63/70   | 0/1/1/1 |
| 29  | SQD  | F     | 103 | -    | -         | 11/40/60/69   | 0/1/1/1 |
| 22  | CLA  | B     | 605 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 27  | LMG  | A     | 414 | -    | -         | 15/37/57/70   | 0/1/1/1 |
| 29  | SQD  | f     | 103 | -    | -         | 12/40/60/69   | 0/1/1/1 |
| 30  | LMT  | D     | 411 | -    | -         | 0/17/57/61    | 0/2/2/2 |
| 22  | CLA  | C     | 501 | -    | 1/1/15/20 | 16/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | C     | 520 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | C     | 507 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | A     | 405 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | DGD  | C     | 517 | -    | -         | 21/55/95/95   | 0/2/2/2 |
| 24  | BCR  | C     | 514 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 27  | LMG  | d     | 412 | -    | -         | 16/41/61/70   | 0/1/1/1 |
| 22  | CLA  | d     | 405 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | B     | 612 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 27  | LMG  | B     | 621 | -    | -         | 15/44/64/70   | 0/1/1/1 |
| 24  | BCR  | y     | 101 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 24  | BCR  | b     | 623 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 603 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 22  | CLA  | B     | 606 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 22  | CLA  | b     | 605 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 27  | LMG  | d     | 408 | -    | -         | 23/44/64/70   | 0/1/1/1 |
| 22  | CLA  | b     | 617 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | c     | 504 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 31  | PHO  | D     | 402 | -    | -         | 11/37/103/103 | 0/5/6/6 |
| 22  | CLA  | c     | 503 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 29  | SQD  | A     | 413 | -    | -         | 12/49/69/69   | 0/1/1/1 |
| 22  | CLA  | C     | 505 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 27  | LMG  | c     | 522 | -    | -         | 20/43/63/70   | 0/1/1/1 |
| 22  | CLA  | c     | 502 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 27  | LMG  | b     | 625 | -    | -         | 14/44/64/70   | 0/1/1/1 |
| 22  | CLA  | b     | 616 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | C     | 504 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | C     | 503 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | b     | 612 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 22  | CLA  | C     | 506 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 25  | DGD  | c     | 516 | -    | -         | 19/51/91/95   | 0/2/2/2 |
| 22  | CLA  | c     | 505 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 27  | LMG  | c     | 518 | -    | -         | 22/40/60/70   | 0/1/1/1 |
| 30  | LMT  | b     | 604 | -    | -         | 5/21/61/61    | 0/2/2/2 |
| 22  | CLA  | c     | 507 | -    | 1/1/15/20 | 13/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 30  | LMT  | B     | 624 | -    | -         | 4/21/61/61    | 0/2/2/2 |
| 25  | DGD  | C     | 516 | -    | -         | 19/51/91/95   | 0/2/2/2 |
| 22  | CLA  | B     | 602 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | A     | 404 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | a     | 407 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 24  | BCR  | B     | 616 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 22  | CLA  | C     | 509 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 27  | LMG  | C     | 518 | -    | -         | 22/40/60/70   | 0/1/1/1 |
| 30  | LMT  | M     | 103 | -    | -         | 0/21/61/61    | 0/2/2/2 |
| 25  | DGD  | a     | 410 | -    | -         | 15/45/85/95   | 0/2/2/2 |
| 24  | BCR  | B     | 617 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 30  | LMT  | I     | 102 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 22  | CLA  | B     | 614 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 30  | LMT  | B     | 623 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 22  | CLA  | c     | 512 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 34  | HEM  | V     | 201 | 16   | -         | 5/14/54/54    | -       |
| 30  | LMT  | i     | 102 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 23  | PL9  | A     | 406 | -    | -         | 19/41/61/73   | 0/1/1/1 |
| 22  | CLA  | d     | 406 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 22  | CLA  | b     | 610 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 30  | LMT  | B     | 627 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 24  | BCR  | j     | 102 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 22  | CLA  | C     | 510 | 3    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | B     | 609 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 27  | LMG  | C     | 521 | -    | -         | 20/43/63/70   | 0/1/1/1 |
| 29  | SQD  | a     | 401 | -    | -         | 14/49/69/69   | 0/1/1/1 |
| 22  | CLA  | a     | 406 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | DGD  | A     | 408 | -    | -         | 13/45/85/95   | 0/2/2/2 |
| 34  | HEM  | f     | 101 | 5,6  | -         | 2/14/54/54    | -       |
| 27  | LMG  | E     | 101 | -    | -         | 19/39/59/70   | 0/1/1/1 |
| 25  | DGD  | B     | 625 | -    | -         | 17/41/81/95   | 0/2/2/2 |
| 24  | BCR  | c     | 521 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 25  | DGD  | b     | 624 | -    | -         | 18/47/87/95   | 0/2/2/2 |
| 27  | LMG  | a     | 412 | -    | -         | 26/46/66/70   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24  | BCR  | B     | 618 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 22  | CLA  | A     | 403 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | b     | 606 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 34  | HEM  | F     | 101 | 5,6  | -         | 2/14/54/54    | -       |
| 22  | CLA  | B     | 615 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 29  | SQD  | B     | 626 | -    | -         | 14/42/62/69   | 0/1/1/1 |
| 24  | BCR  | A     | 407 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 22  | CLA  | b     | 619 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 30  | LMT  | B     | 628 | -    | -         | 5/21/61/61    | 0/2/2/2 |
| 30  | LMT  | b     | 627 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 27  | LMG  | M     | 101 | -    | -         | 18/37/57/70   | 0/1/1/1 |
| 23  | PL9  | d     | 407 | -    | -         | 12/53/73/73   | 0/1/1/1 |
| 27  | LMG  | m     | 101 | -    | -         | 17/37/57/70   | 0/1/1/1 |
| 22  | CLA  | b     | 614 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 23  | PL9  | J     | 101 | -    | -         | 8/29/49/73    | 0/1/1/1 |
| 22  | CLA  | b     | 609 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 26  | LHG  | A     | 409 | -    | -         | 12/43/43/53   | -       |
| 26  | LHG  | c     | 519 | -    | -         | 17/41/41/53   | -       |
| 22  | CLA  | c     | 501 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | b     | 615 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | H     | 101 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 27  | LMG  | i     | 101 | -    | -         | 18/38/58/70   | 0/1/1/1 |
| 22  | CLA  | B     | 611 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 30  | LMT  | b     | 603 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 22  | CLA  | D     | 406 | -    | -         | 8/39/115/115  | -       |
| 22  | CLA  | a     | 405 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | A     | 402 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 24  | BCR  | a     | 409 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 24  | BCR  | b     | 620 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 25  | DGD  | C     | 515 | -    | -         | 19/42/82/95   | 0/2/2/2 |
| 26  | LHG  | C     | 519 | -    | -         | 17/41/41/53   | -       |
| 25  | DGD  | d     | 410 | -    | -         | 35/52/92/95   | 0/2/2/2 |
| 22  | CLA  | C     | 512 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | c     | 511 | -    | 1/1/15/20 | 17/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 27  | LMG  | D     | 412 | -    | -       | 14/41/61/70 | 0/1/1/1 |
| 24  | BCR  | b     | 622 | -    | -       | 0/29/63/63  | 0/2/2/2 |
| 29  | SQD  | a     | 415 | -    | -       | 18/46/66/69 | 0/1/1/1 |
| 24  | BCR  | b     | 621 | -    | -       | 7/29/63/63  | 0/2/2/2 |

All (752) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | D     | 402 | PHO  | C1B-C2B | 9.76  | 1.50        | 1.39     |
| 31  | d     | 401 | PHO  | C1B-C2B | 9.67  | 1.50        | 1.39     |
| 31  | d     | 402 | PHO  | C1B-C2B | 9.57  | 1.50        | 1.39     |
| 31  | D     | 401 | PHO  | C1B-C2B | 9.55  | 1.50        | 1.39     |
| 31  | D     | 402 | PHO  | C3B-C4B | 8.71  | 1.50        | 1.41     |
| 31  | d     | 402 | PHO  | C3B-C4B | 8.68  | 1.50        | 1.41     |
| 31  | D     | 401 | PHO  | C3B-C4B | 8.47  | 1.50        | 1.41     |
| 31  | d     | 401 | PHO  | C3B-C4B | 8.29  | 1.49        | 1.41     |
| 34  | V     | 201 | HEM  | C3D-C2D | 8.18  | 1.54        | 1.36     |
| 34  | v     | 201 | HEM  | C3D-C2D | 8.17  | 1.54        | 1.36     |
| 34  | F     | 101 | HEM  | C3D-C2D | 7.91  | 1.53        | 1.36     |
| 34  | f     | 101 | HEM  | C3D-C2D | 7.88  | 1.53        | 1.36     |
| 34  | F     | 101 | HEM  | FE-ND   | 5.66  | 2.12        | 1.94     |
| 34  | f     | 101 | HEM  | FE-ND   | 5.30  | 2.11        | 1.94     |
| 34  | v     | 201 | HEM  | FE-ND   | 5.08  | 2.10        | 1.94     |
| 34  | V     | 201 | HEM  | FE-ND   | 5.05  | 2.10        | 1.94     |
| 34  | v     | 201 | HEM  | FE-NB   | 4.64  | 2.09        | 1.94     |
| 34  | f     | 101 | HEM  | FE-NB   | 4.57  | 2.09        | 1.94     |
| 31  | d     | 402 | PHO  | C1D-C2D | 4.41  | 1.44        | 1.39     |
| 31  | D     | 402 | PHO  | C1D-C2D | 4.34  | 1.44        | 1.39     |
| 34  | V     | 201 | HEM  | FE-NB   | 4.32  | 2.08        | 1.94     |
| 31  | d     | 401 | PHO  | C1D-C2D | 4.12  | 1.44        | 1.39     |
| 31  | D     | 401 | PHO  | C1D-C2D | 4.07  | 1.44        | 1.39     |
| 24  | y     | 101 | BCR  | C1-C6   | -4.02 | 1.48        | 1.53     |
| 34  | F     | 101 | HEM  | FE-NB   | 4.01  | 2.07        | 1.94     |
| 24  | H     | 102 | BCR  | C1-C6   | -3.95 | 1.48        | 1.53     |
| 24  | g     | 101 | BCR  | C1-C6   | -3.92 | 1.48        | 1.53     |
| 24  | F     | 102 | BCR  | C1-C6   | -3.90 | 1.48        | 1.53     |
| 34  | V     | 201 | HEM  | FE-NA   | 3.88  | 2.08        | 1.95     |
| 34  | f     | 101 | HEM  | FE-NA   | 3.87  | 2.07        | 1.95     |
| 24  | x     | 101 | BCR  | C1-C6   | -3.85 | 1.48        | 1.53     |
| 24  | f     | 102 | BCR  | C1-C6   | -3.84 | 1.48        | 1.53     |
| 31  | D     | 402 | PHO  | C4D-CHA | 3.84  | 1.45        | 1.39     |
| 31  | D     | 401 | PHO  | C4D-CHA | 3.81  | 1.45        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | C     | 501 | CLA  | C1D-ND  | 3.78 | 1.42        | 1.37     |
| 31  | d     | 401 | PHO  | C4D-CHA | 3.78 | 1.45        | 1.39     |
| 22  | B     | 601 | CLA  | C1D-ND  | 3.77 | 1.42        | 1.37     |
| 22  | c     | 503 | CLA  | C1D-ND  | 3.77 | 1.42        | 1.37     |
| 22  | b     | 605 | CLA  | C1D-ND  | 3.77 | 1.42        | 1.37     |
| 34  | F     | 101 | HEM  | FE-NA   | 3.76 | 2.07        | 1.95     |
| 34  | v     | 201 | HEM  | FE-NA   | 3.75 | 2.07        | 1.95     |
| 31  | d     | 402 | PHO  | C4D-CHA | 3.75 | 1.45        | 1.39     |
| 22  | C     | 512 | CLA  | C1D-ND  | 3.74 | 1.42        | 1.37     |
| 22  | B     | 608 | CLA  | C1D-ND  | 3.74 | 1.42        | 1.37     |
| 22  | c     | 510 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 22  | c     | 512 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 22  | h     | 101 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 22  | d     | 406 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 22  | b     | 618 | CLA  | C1D-ND  | 3.71 | 1.42        | 1.37     |
| 22  | c     | 501 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 22  | a     | 407 | CLA  | C1D-ND  | 3.68 | 1.42        | 1.37     |
| 22  | A     | 403 | CLA  | C1D-ND  | 3.68 | 1.42        | 1.37     |
| 22  | C     | 505 | CLA  | C1D-ND  | 3.68 | 1.42        | 1.37     |
| 22  | c     | 505 | CLA  | C1D-ND  | 3.68 | 1.42        | 1.37     |
| 22  | C     | 510 | CLA  | C1D-ND  | 3.68 | 1.42        | 1.37     |
| 22  | H     | 101 | CLA  | C1D-ND  | 3.68 | 1.42        | 1.37     |
| 22  | c     | 506 | CLA  | C1D-ND  | 3.67 | 1.42        | 1.37     |
| 22  | b     | 608 | CLA  | C1D-ND  | 3.67 | 1.42        | 1.37     |
| 22  | A     | 405 | CLA  | C1D-ND  | 3.67 | 1.42        | 1.37     |
| 22  | b     | 612 | CLA  | C1D-ND  | 3.67 | 1.42        | 1.37     |
| 22  | b     | 616 | CLA  | C1D-ND  | 3.66 | 1.42        | 1.37     |
| 22  | B     | 604 | CLA  | C1D-ND  | 3.65 | 1.42        | 1.37     |
| 22  | C     | 506 | CLA  | C1D-ND  | 3.65 | 1.42        | 1.37     |
| 22  | D     | 406 | CLA  | C1D-ND  | 3.65 | 1.42        | 1.37     |
| 22  | b     | 613 | CLA  | C1D-ND  | 3.65 | 1.42        | 1.37     |
| 22  | B     | 614 | CLA  | C1D-ND  | 3.64 | 1.42        | 1.37     |
| 22  | C     | 503 | CLA  | C1D-ND  | 3.64 | 1.42        | 1.37     |
| 22  | b     | 607 | CLA  | C1D-ND  | 3.64 | 1.42        | 1.37     |
| 22  | C     | 511 | CLA  | C1D-ND  | 3.64 | 1.42        | 1.37     |
| 22  | c     | 508 | CLA  | C1D-ND  | 3.63 | 1.42        | 1.37     |
| 22  | d     | 405 | CLA  | C1D-ND  | 3.63 | 1.42        | 1.37     |
| 22  | b     | 609 | CLA  | C1D-ND  | 3.63 | 1.42        | 1.37     |
| 22  | C     | 502 | CLA  | C1D-ND  | 3.62 | 1.42        | 1.37     |
| 22  | b     | 606 | CLA  | C1D-ND  | 3.62 | 1.42        | 1.37     |
| 22  | B     | 603 | CLA  | C1D-ND  | 3.62 | 1.42        | 1.37     |
| 22  | c     | 502 | CLA  | C1D-ND  | 3.62 | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 612 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 22  | c     | 504 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 22  | C     | 520 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 24  | B     | 616 | BCR  | C1-C6   | -3.61 | 1.49        | 1.53     |
| 24  | C     | 514 | BCR  | C1-C6   | -3.61 | 1.49        | 1.53     |
| 22  | C     | 504 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 22  | B     | 605 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 22  | a     | 405 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 22  | B     | 607 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 22  | B     | 606 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 22  | b     | 611 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 24  | c     | 514 | BCR  | C1-C6   | -3.59 | 1.49        | 1.53     |
| 22  | B     | 613 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 22  | a     | 406 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 22  | b     | 610 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 22  | c     | 520 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 22  | B     | 602 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 22  | c     | 511 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 24  | b     | 620 | BCR  | C1-C6   | -3.56 | 1.49        | 1.53     |
| 34  | v     | 201 | HEM  | FE-NC   | 3.54  | 2.06        | 1.95     |
| 22  | B     | 609 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 22  | A     | 404 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 22  | a     | 404 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 24  | b     | 621 | BCR  | C1-C6   | -3.53 | 1.49        | 1.53     |
| 22  | c     | 507 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 22  | b     | 617 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 24  | y     | 101 | BCR  | C30-C25 | -3.51 | 1.49        | 1.53     |
| 22  | B     | 615 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 24  | b     | 622 | BCR  | C30-C25 | -3.50 | 1.49        | 1.53     |
| 22  | C     | 509 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 22  | C     | 507 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 22  | b     | 619 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 22  | C     | 508 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 22  | c     | 509 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 22  | A     | 402 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 22  | B     | 610 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 22  | D     | 405 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 24  | B     | 617 | BCR  | C1-C6   | -3.45 | 1.49        | 1.53     |
| 24  | J     | 102 | BCR  | C30-C25 | -3.45 | 1.49        | 1.53     |
| 24  | C     | 513 | BCR  | C1-C6   | -3.45 | 1.49        | 1.53     |
| 24  | g     | 101 | BCR  | C30-C25 | -3.45 | 1.49        | 1.53     |
| 22  | b     | 614 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | j     | 102 | BCR  | C30-C25 | -3.43 | 1.49        | 1.53     |
| 24  | c     | 513 | BCR  | C1-C6   | -3.40 | 1.49        | 1.53     |
| 24  | B     | 618 | BCR  | C30-C25 | -3.39 | 1.49        | 1.53     |
| 24  | K     | 102 | BCR  | C30-C25 | -3.38 | 1.49        | 1.53     |
| 24  | F     | 102 | BCR  | C30-C25 | -3.36 | 1.49        | 1.53     |
| 24  | c     | 521 | BCR  | C30-C25 | -3.33 | 1.49        | 1.53     |
| 24  | A     | 407 | BCR  | C30-C25 | -3.32 | 1.49        | 1.53     |
| 22  | A     | 402 | CLA  | C4B-NB  | 3.31  | 1.42        | 1.37     |
| 24  | B     | 618 | BCR  | C1-C6   | -3.31 | 1.49        | 1.53     |
| 22  | c     | 508 | CLA  | C4B-NB  | 3.31  | 1.42        | 1.37     |
| 24  | a     | 409 | BCR  | C30-C25 | -3.30 | 1.49        | 1.53     |
| 24  | f     | 102 | BCR  | C30-C25 | -3.30 | 1.49        | 1.53     |
| 24  | b     | 623 | BCR  | C1-C6   | -3.29 | 1.49        | 1.53     |
| 22  | b     | 614 | CLA  | CMB-C2B | -3.29 | 1.44        | 1.50     |
| 24  | B     | 619 | BCR  | C30-C25 | -3.29 | 1.49        | 1.53     |
| 24  | B     | 616 | BCR  | C30-C25 | -3.29 | 1.49        | 1.53     |
| 24  | b     | 620 | BCR  | C30-C25 | -3.28 | 1.49        | 1.53     |
| 22  | C     | 509 | CLA  | C4B-NB  | 3.27  | 1.42        | 1.37     |
| 24  | b     | 623 | BCR  | C30-C25 | -3.26 | 1.49        | 1.53     |
| 22  | b     | 615 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 22  | B     | 601 | CLA  | C4B-NB  | 3.26  | 1.42        | 1.37     |
| 24  | B     | 619 | BCR  | C1-C6   | -3.26 | 1.49        | 1.53     |
| 24  | b     | 622 | BCR  | C1-C6   | -3.26 | 1.49        | 1.53     |
| 22  | a     | 404 | CLA  | C4B-NB  | 3.26  | 1.42        | 1.37     |
| 22  | b     | 605 | CLA  | C4B-NB  | 3.26  | 1.42        | 1.37     |
| 24  | A     | 407 | BCR  | C1-C6   | -3.26 | 1.49        | 1.53     |
| 24  | a     | 409 | BCR  | C1-C6   | -3.25 | 1.49        | 1.53     |
| 22  | C     | 508 | CLA  | C4B-NB  | 3.25  | 1.42        | 1.37     |
| 22  | B     | 611 | CLA  | C1D-ND  | 3.22  | 1.42        | 1.37     |
| 22  | b     | 619 | CLA  | C4B-NB  | 3.22  | 1.42        | 1.37     |
| 22  | C     | 505 | CLA  | C4B-NB  | 3.22  | 1.42        | 1.37     |
| 22  | c     | 509 | CLA  | C4B-NB  | 3.22  | 1.42        | 1.37     |
| 22  | b     | 614 | CLA  | C4B-NB  | 3.21  | 1.42        | 1.37     |
| 24  | C     | 514 | BCR  | C30-C25 | -3.21 | 1.49        | 1.53     |
| 24  | K     | 102 | BCR  | C1-C6   | -3.20 | 1.49        | 1.53     |
| 22  | B     | 610 | CLA  | CMB-C2B | -3.20 | 1.44        | 1.50     |
| 29  | a     | 401 | SQD  | O48-C23 | 3.19  | 1.42        | 1.33     |
| 22  | B     | 610 | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 22  | c     | 505 | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 22  | B     | 615 | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 22  | c     | 511 | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 24  | C     | 513 | BCR  | C30-C25 | -3.17 | 1.49        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | c     | 514 | BCR  | C30-C25 | -3.17 | 1.49        | 1.53     |
| 22  | C     | 507 | CLA  | C4B-NB  | 3.17  | 1.42        | 1.37     |
| 29  | b     | 602 | SQD  | O48-C23 | 3.17  | 1.42        | 1.33     |
| 22  | c     | 504 | CLA  | C4B-NB  | 3.16  | 1.42        | 1.37     |
| 29  | d     | 403 | SQD  | O48-C23 | 3.16  | 1.42        | 1.33     |
| 29  | f     | 103 | SQD  | O48-C23 | 3.15  | 1.42        | 1.33     |
| 22  | b     | 612 | CLA  | C4B-NB  | 3.15  | 1.42        | 1.37     |
| 22  | b     | 615 | CLA  | C4B-NB  | 3.15  | 1.42        | 1.37     |
| 22  | c     | 520 | CLA  | C4B-NB  | 3.15  | 1.42        | 1.37     |
| 22  | B     | 614 | CLA  | C4B-NB  | 3.14  | 1.42        | 1.37     |
| 29  | F     | 103 | SQD  | O48-C23 | 3.14  | 1.42        | 1.33     |
| 22  | c     | 503 | CLA  | C4B-NB  | 3.14  | 1.42        | 1.37     |
| 22  | D     | 405 | CLA  | C4B-NB  | 3.14  | 1.42        | 1.37     |
| 22  | b     | 610 | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 22  | d     | 406 | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 34  | V     | 201 | HEM  | CAB-C3B | 3.13  | 1.55        | 1.47     |
| 22  | a     | 405 | CLA  | C4B-NB  | 3.12  | 1.42        | 1.37     |
| 29  | A     | 413 | SQD  | O48-C23 | 3.12  | 1.42        | 1.33     |
| 22  | b     | 618 | CLA  | C4B-NB  | 3.12  | 1.42        | 1.37     |
| 22  | B     | 611 | CLA  | C4B-NB  | 3.12  | 1.42        | 1.37     |
| 22  | B     | 606 | CLA  | C4B-NB  | 3.12  | 1.42        | 1.37     |
| 29  | B     | 622 | SQD  | O48-C23 | 3.12  | 1.42        | 1.33     |
| 24  | x     | 101 | BCR  | C30-C25 | -3.12 | 1.49        | 1.53     |
| 29  | B     | 626 | SQD  | O48-C23 | 3.11  | 1.42        | 1.33     |
| 34  | v     | 201 | HEM  | CAB-C3B | 3.11  | 1.55        | 1.47     |
| 22  | B     | 608 | CLA  | C4B-NB  | 3.11  | 1.41        | 1.37     |
| 34  | f     | 101 | HEM  | CAC-C3C | 3.11  | 1.55        | 1.47     |
| 22  | c     | 510 | CLA  | C4B-NB  | 3.11  | 1.41        | 1.37     |
| 22  | B     | 609 | CLA  | C4B-NB  | 3.11  | 1.41        | 1.37     |
| 24  | c     | 521 | BCR  | C1-C6   | -3.10 | 1.49        | 1.53     |
| 22  | a     | 406 | CLA  | C4B-NB  | 3.10  | 1.41        | 1.37     |
| 29  | a     | 415 | SQD  | O48-C23 | 3.09  | 1.42        | 1.33     |
| 22  | d     | 405 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 22  | c     | 512 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 22  | C     | 511 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 22  | A     | 403 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 22  | H     | 101 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 22  | c     | 507 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 22  | B     | 604 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 22  | b     | 608 | CLA  | C4B-NB  | 3.07  | 1.41        | 1.37     |
| 34  | F     | 101 | HEM  | CAC-C3C | 3.07  | 1.55        | 1.47     |
| 22  | A     | 405 | CLA  | C4B-NB  | 3.07  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | H     | 102 | BCR  | C30-C25 | -3.07 | 1.49        | 1.53     |
| 22  | C     | 512 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 22  | D     | 406 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 29  | A     | 412 | SQD  | O48-C23 | 3.05  | 1.42        | 1.33     |
| 22  | h     | 101 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 22  | C     | 510 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 34  | F     | 101 | HEM  | FE-NC   | 3.05  | 2.05        | 1.95     |
| 34  | V     | 201 | HEM  | FE-NC   | 3.05  | 2.05        | 1.95     |
| 22  | a     | 407 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 22  | b     | 611 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 22  | b     | 609 | CLA  | C4B-NB  | 3.04  | 1.41        | 1.37     |
| 22  | C     | 502 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 34  | v     | 201 | HEM  | CAC-C3C | 3.03  | 1.55        | 1.47     |
| 34  | f     | 101 | HEM  | FE-NC   | 3.02  | 2.05        | 1.95     |
| 22  | B     | 607 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 34  | V     | 201 | HEM  | CAC-C3C | 3.02  | 1.55        | 1.47     |
| 22  | A     | 404 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 22  | C     | 503 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 22  | b     | 616 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 22  | B     | 605 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 22  | B     | 613 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 22  | C     | 504 | CLA  | C4B-NB  | 3.01  | 1.41        | 1.37     |
| 22  | C     | 520 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 22  | c     | 501 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 22  | b     | 617 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 24  | J     | 102 | BCR  | C1-C6   | -2.99 | 1.50        | 1.53     |
| 22  | C     | 501 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 22  | b     | 613 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 24  | j     | 102 | BCR  | C1-C6   | -2.98 | 1.50        | 1.53     |
| 22  | b     | 607 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |
| 24  | c     | 513 | BCR  | C30-C25 | -2.98 | 1.50        | 1.53     |
| 22  | c     | 506 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |
| 22  | c     | 502 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 22  | B     | 612 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 22  | b     | 606 | CLA  | C4B-NB  | 2.96  | 1.41        | 1.37     |
| 22  | C     | 506 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 29  | d     | 403 | SQD  | O47-C7  | 2.94  | 1.42        | 1.34     |
| 22  | B     | 603 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 34  | F     | 101 | HEM  | CAB-C3B | 2.93  | 1.55        | 1.47     |
| 22  | B     | 602 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 23  | d     | 407 | PL9  | C7-C3   | -2.92 | 1.47        | 1.51     |
| 24  | b     | 621 | BCR  | C30-C25 | -2.92 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29  | B     | 622 | SQD  | O47-C7  | 2.92  | 1.42        | 1.34     |
| 22  | c     | 504 | CLA  | C1B-C2B | 2.91  | 1.50        | 1.43     |
| 24  | B     | 617 | BCR  | C30-C25 | -2.91 | 1.50        | 1.53     |
| 29  | a     | 415 | SQD  | O47-C7  | 2.90  | 1.42        | 1.34     |
| 34  | f     | 101 | HEM  | CAB-C3B | 2.90  | 1.55        | 1.47     |
| 29  | a     | 401 | SQD  | O47-C7  | 2.90  | 1.42        | 1.34     |
| 29  | A     | 413 | SQD  | O47-C7  | 2.89  | 1.42        | 1.34     |
| 29  | A     | 412 | SQD  | O47-C7  | 2.89  | 1.42        | 1.34     |
| 22  | D     | 405 | CLA  | C1B-C2B | 2.89  | 1.49        | 1.43     |
| 25  | b     | 601 | DGD  | C1E-C2E | 2.89  | 1.61        | 1.52     |
| 23  | a     | 408 | PL9  | C3-C4   | -2.88 | 1.45        | 1.49     |
| 22  | C     | 501 | CLA  | C1B-C2B | 2.88  | 1.49        | 1.43     |
| 29  | F     | 103 | SQD  | O47-C7  | 2.87  | 1.42        | 1.34     |
| 22  | b     | 619 | CLA  | C1B-C2B | 2.86  | 1.49        | 1.43     |
| 22  | d     | 405 | CLA  | C1B-C2B | 2.85  | 1.49        | 1.43     |
| 22  | B     | 611 | CLA  | C1B-C2B | 2.85  | 1.49        | 1.43     |
| 22  | c     | 501 | CLA  | C1B-C2B | 2.85  | 1.49        | 1.43     |
| 22  | C     | 504 | CLA  | C1B-C2B | 2.84  | 1.49        | 1.43     |
| 29  | b     | 602 | SQD  | O47-C7  | 2.83  | 1.42        | 1.34     |
| 23  | D     | 407 | PL9  | C3-C4   | -2.83 | 1.45        | 1.49     |
| 29  | B     | 626 | SQD  | O47-C7  | 2.82  | 1.42        | 1.34     |
| 22  | B     | 615 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 22  | h     | 101 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 29  | f     | 103 | SQD  | O47-C7  | 2.82  | 1.42        | 1.34     |
| 22  | B     | 603 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 22  | B     | 613 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 22  | H     | 101 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 22  | c     | 503 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 22  | b     | 615 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 22  | B     | 601 | CLA  | C1B-C2B | 2.81  | 1.49        | 1.43     |
| 25  | B     | 625 | DGD  | C1E-C2E | 2.81  | 1.60        | 1.52     |
| 22  | c     | 511 | CLA  | C1B-C2B | 2.81  | 1.49        | 1.43     |
| 22  | b     | 607 | CLA  | C1B-C2B | 2.81  | 1.49        | 1.43     |
| 22  | b     | 618 | CLA  | C1B-C2B | 2.81  | 1.49        | 1.43     |
| 22  | B     | 614 | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 22  | b     | 609 | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 22  | b     | 617 | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 22  | C     | 511 | CLA  | C1B-C2B | 2.79  | 1.49        | 1.43     |
| 22  | c     | 510 | CLA  | C1B-C2B | 2.79  | 1.49        | 1.43     |
| 22  | b     | 616 | CLA  | C1B-C2B | 2.79  | 1.49        | 1.43     |
| 23  | d     | 407 | PL9  | C3-C4   | -2.79 | 1.45        | 1.49     |
| 22  | b     | 612 | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | a     | 406 | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 22  | C     | 502 | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 22  | c     | 502 | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 22  | b     | 605 | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 22  | C     | 503 | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 22  | B     | 608 | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 22  | B     | 606 | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 22  | C     | 510 | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 22  | b     | 608 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 22  | B     | 612 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 22  | B     | 604 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 22  | B     | 605 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 22  | d     | 406 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 22  | c     | 520 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 22  | C     | 512 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 22  | A     | 404 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 22  | b     | 606 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 22  | b     | 610 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 22  | c     | 512 | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 22  | c     | 506 | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 22  | c     | 508 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 22  | B     | 602 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 22  | D     | 406 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 22  | C     | 509 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | C     | 505 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | A     | 405 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | c     | 505 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | C     | 506 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | C     | 508 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | c     | 509 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 22  | B     | 607 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 22  | b     | 613 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 23  | A     | 406 | PL9  | C3-C4   | -2.69 | 1.45        | 1.49     |
| 23  | D     | 407 | PL9  | C7-C3   | -2.69 | 1.47        | 1.51     |
| 22  | B     | 609 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 22  | a     | 405 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 22  | C     | 520 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 22  | C     | 507 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 22  | a     | 407 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 25  | C     | 515 | DGD  | O2G-C2G | -2.67 | 1.40        | 1.46     |
| 22  | b     | 611 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 22  | A     | 402 | CLA  | C3B-C4B | 2.65  | 1.50        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | A     | 403 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 23  | a     | 408 | PL9  | C7-C3   | -2.64 | 1.47        | 1.51     |
| 22  | a     | 404 | CLA  | C3B-C4B | 2.64  | 1.50        | 1.42     |
| 31  | D     | 402 | PHO  | CMC-C2C | -2.62 | 1.46        | 1.50     |
| 22  | A     | 402 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 22  | c     | 507 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 31  | d     | 402 | PHO  | C3D-C4D | 2.57  | 1.44        | 1.41     |
| 31  | d     | 402 | PHO  | CMC-C2C | -2.57 | 1.46        | 1.50     |
| 22  | B     | 610 | CLA  | MG-NB   | -2.56 | 2.00        | 2.05     |
| 22  | a     | 404 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 31  | d     | 401 | PHO  | CMC-C2C | -2.54 | 1.46        | 1.50     |
| 31  | d     | 401 | PHO  | C3D-C4D | 2.54  | 1.44        | 1.41     |
| 22  | b     | 614 | CLA  | MG-NB   | -2.53 | 2.00        | 2.05     |
| 31  | D     | 401 | PHO  | CMC-C2C | -2.53 | 1.46        | 1.50     |
| 31  | D     | 402 | PHO  | C3D-C4D | 2.53  | 1.44        | 1.41     |
| 31  | D     | 401 | PHO  | C3D-C4D | 2.52  | 1.44        | 1.41     |
| 30  | d     | 411 | LMT  | O3'-C3' | -2.49 | 1.36        | 1.43     |
| 30  | b     | 627 | LMT  | O3'-C3' | -2.49 | 1.36        | 1.43     |
| 31  | d     | 401 | PHO  | CMD-C2D | -2.47 | 1.46        | 1.51     |
| 30  | D     | 411 | LMT  | O3'-C3' | -2.47 | 1.36        | 1.43     |
| 30  | M     | 102 | LMT  | O3'-C3' | -2.47 | 1.36        | 1.43     |
| 30  | I     | 102 | LMT  | O3'-C3' | -2.47 | 1.36        | 1.43     |
| 31  | D     | 402 | PHO  | CMD-C2D | -2.46 | 1.46        | 1.51     |
| 30  | M     | 103 | LMT  | O3'-C3' | -2.46 | 1.36        | 1.43     |
| 22  | c     | 508 | CLA  | C3B-C4B | 2.46  | 1.49        | 1.42     |
| 31  | D     | 401 | PHO  | CMD-C2D | -2.46 | 1.46        | 1.51     |
| 22  | a     | 405 | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 31  | d     | 401 | PHO  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 31  | d     | 402 | PHO  | CMD-C2D | -2.45 | 1.46        | 1.51     |
| 30  | b     | 626 | LMT  | O3'-C3' | -2.45 | 1.36        | 1.43     |
| 22  | B     | 608 | CLA  | CHC-C1C | 2.45  | 1.43        | 1.38     |
| 31  | D     | 401 | PHO  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 22  | B     | 613 | CLA  | CHC-C1C | 2.44  | 1.43        | 1.38     |
| 31  | D     | 402 | PHO  | CAC-C3C | -2.44 | 1.47        | 1.51     |
| 22  | C     | 508 | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 30  | b     | 603 | LMT  | O3'-C3' | -2.43 | 1.36        | 1.43     |
| 30  | b     | 604 | LMT  | O3'-C3' | -2.43 | 1.36        | 1.43     |
| 22  | A     | 403 | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 30  | B     | 627 | LMT  | O3'-C3' | -2.42 | 1.37        | 1.43     |
| 30  | B     | 624 | LMT  | O3'-C3' | -2.42 | 1.37        | 1.43     |
| 25  | B     | 625 | DGD  | C4D-C5D | 2.41  | 1.58        | 1.53     |
| 31  | d     | 401 | PHO  | CAC-C3C | -2.41 | 1.47        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | i     | 102 | LMT  | O3'-C3' | -2.40 | 1.37        | 1.43     |
| 22  | h     | 101 | CLA  | CHC-C1C | 2.40  | 1.43        | 1.38     |
| 31  | d     | 402 | PHO  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 22  | b     | 605 | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 30  | B     | 623 | LMT  | O3'-C3' | -2.40 | 1.37        | 1.43     |
| 22  | C     | 505 | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 31  | D     | 402 | PHO  | CMB-C2B | -2.39 | 1.46        | 1.51     |
| 22  | c     | 520 | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 22  | b     | 612 | CLA  | CHC-C1C | 2.38  | 1.43        | 1.38     |
| 22  | H     | 101 | CLA  | CHC-C1C | 2.38  | 1.43        | 1.38     |
| 22  | C     | 520 | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 22  | B     | 613 | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 22  | c     | 505 | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 22  | b     | 611 | CLA  | CHC-C1C | 2.37  | 1.43        | 1.38     |
| 22  | B     | 601 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 22  | c     | 511 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 23  | J     | 101 | PL9  | C7-C3   | -2.36 | 1.48        | 1.51     |
| 22  | b     | 606 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 22  | b     | 611 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 22  | b     | 612 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 22  | c     | 510 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 22  | c     | 509 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 22  | d     | 406 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 25  | c     | 515 | DGD  | O2G-C2G | -2.35 | 1.41        | 1.46     |
| 23  | A     | 406 | PL9  | C7-C3   | -2.35 | 1.48        | 1.51     |
| 22  | h     | 101 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 22  | b     | 606 | CLA  | CHC-C1C | 2.35  | 1.43        | 1.38     |
| 30  | B     | 628 | LMT  | O3'-C3' | -2.35 | 1.37        | 1.43     |
| 22  | C     | 511 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 31  | d     | 402 | PHO  | CAC-C3C | -2.35 | 1.47        | 1.51     |
| 22  | B     | 608 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 22  | b     | 615 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 22  | b     | 617 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 22  | B     | 611 | CLA  | CMD-C2D | -2.34 | 1.46        | 1.50     |
| 22  | H     | 101 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 22  | C     | 507 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 22  | b     | 618 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 22  | a     | 406 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 22  | D     | 405 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 22  | B     | 614 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 31  | D     | 401 | PHO  | CAC-C3C | -2.33 | 1.47        | 1.51     |
| 22  | C     | 509 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | c     | 507 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 22  | B     | 607 | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 22  | a     | 404 | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 22  | B     | 612 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 22  | d     | 406 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 22  | c     | 512 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 22  | c     | 502 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 22  | b     | 619 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 22  | B     | 607 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 22  | C     | 510 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 22  | B     | 615 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 22  | B     | 611 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 23  | D     | 407 | PL9  | C6-C1   | -2.31 | 1.44        | 1.48     |
| 22  | C     | 505 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 22  | D     | 406 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 23  | a     | 408 | PL9  | C53-C6  | -2.31 | 1.46        | 1.50     |
| 22  | A     | 404 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 22  | C     | 512 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 22  | c     | 511 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 22  | b     | 617 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 22  | c     | 512 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 22  | c     | 507 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 22  | a     | 407 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 22  | b     | 616 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 22  | B     | 609 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 25  | c     | 516 | DGD  | O2G-C2G | -2.30 | 1.41        | 1.46     |
| 22  | C     | 511 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 22  | d     | 405 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 22  | c     | 509 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 22  | C     | 512 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 22  | B     | 602 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 22  | B     | 604 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 22  | a     | 406 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 22  | c     | 505 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 22  | C     | 502 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 22  | C     | 502 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 22  | c     | 504 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 22  | c     | 503 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 22  | B     | 606 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 22  | C     | 509 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 22  | D     | 405 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 22  | b     | 613 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | a     | 411 | LHG  | O7-C5   | -2.28 | 1.41        | 1.46     |
| 22  | b     | 615 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 22  | b     | 608 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 22  | a     | 407 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 22  | B     | 609 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 22  | B     | 603 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 22  | b     | 616 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 23  | j     | 101 | PL9  | C7-C3   | -2.28 | 1.48        | 1.51     |
| 22  | C     | 504 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 22  | B     | 604 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 22  | b     | 607 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 22  | c     | 502 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 22  | B     | 605 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 25  | C     | 516 | DGD  | O2G-C2G | -2.27 | 1.41        | 1.46     |
| 22  | B     | 614 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 22  | b     | 618 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 22  | C     | 506 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 22  | b     | 610 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 22  | d     | 405 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 22  | B     | 602 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 22  | c     | 508 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 22  | C     | 508 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 22  | c     | 506 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 23  | A     | 406 | PL9  | C53-C6  | -2.26 | 1.46        | 1.50     |
| 22  | c     | 510 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 22  | A     | 405 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 22  | A     | 404 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 22  | c     | 504 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 22  | C     | 503 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 22  | b     | 609 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 27  | D     | 412 | LMG  | O7-C8   | -2.24 | 1.41        | 1.46     |
| 22  | C     | 520 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 24  | g     | 101 | BCR  | C33-C5  | -2.24 | 1.47        | 1.50     |
| 25  | B     | 620 | DGD  | O2G-C2G | -2.24 | 1.41        | 1.46     |
| 22  | b     | 613 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 22  | B     | 603 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 22  | A     | 403 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 23  | J     | 101 | PL9  | C3-C4   | -2.23 | 1.46        | 1.49     |
| 30  | I     | 102 | LMT  | O2'-C2' | -2.23 | 1.37        | 1.43     |
| 22  | B     | 605 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 22  | B     | 606 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 22  | b     | 608 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | C     | 515 | DGD  | O1G-C1G | -2.23 | 1.40        | 1.45     |
| 22  | C     | 510 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 22  | c     | 503 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 22  | C     | 504 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 22  | A     | 402 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 22  | B     | 612 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 22  | b     | 610 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 27  | B     | 621 | LMG  | C4-C5   | 2.22  | 1.57        | 1.53     |
| 22  | b     | 607 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 27  | d     | 412 | LMG  | O7-C8   | -2.22 | 1.41        | 1.46     |
| 22  | c     | 504 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 30  | I     | 102 | LMT  | O2B-C2B | -2.22 | 1.37        | 1.43     |
| 22  | C     | 501 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 22  | c     | 520 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 22  | C     | 506 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 22  | C     | 507 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 22  | B     | 610 | CLA  | C1B-NB  | -2.20 | 1.35        | 1.37     |
| 30  | i     | 102 | LMT  | O2'-C2' | -2.20 | 1.37        | 1.43     |
| 22  | B     | 601 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 30  | b     | 626 | LMT  | O2'-C2' | -2.20 | 1.37        | 1.43     |
| 30  | i     | 102 | LMT  | O2B-C2B | -2.20 | 1.37        | 1.43     |
| 22  | b     | 605 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 22  | c     | 507 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 22  | b     | 609 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 22  | C     | 504 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 23  | j     | 101 | PL9  | C3-C4   | -2.20 | 1.46        | 1.49     |
| 22  | C     | 507 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 23  | A     | 406 | PL9  | C6-C1   | -2.19 | 1.44        | 1.48     |
| 27  | D     | 408 | LMG  | O7-C8   | -2.19 | 1.41        | 1.46     |
| 22  | c     | 506 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 22  | b     | 615 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 22  | c     | 509 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 22  | C     | 501 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 22  | C     | 503 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 22  | c     | 501 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 22  | D     | 406 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 22  | D     | 405 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 25  | b     | 624 | DGD  | O2G-C2G | -2.17 | 1.41        | 1.46     |
| 22  | b     | 619 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 22  | A     | 405 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 22  | B     | 611 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 24  | y     | 101 | BCR  | C33-C5  | -2.16 | 1.47        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | M     | 103 | LMT  | O2'-C2' | -2.16 | 1.37        | 1.43     |
| 30  | M     | 102 | LMT  | O1'-C1' | -2.15 | 1.36        | 1.40     |
| 22  | B     | 615 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 30  | B     | 623 | LMT  | O2'-C2' | -2.15 | 1.37        | 1.43     |
| 22  | b     | 614 | CLA  | C1B-C2B | 2.15  | 1.48        | 1.43     |
| 26  | C     | 519 | LHG  | O7-C5   | -2.15 | 1.41        | 1.46     |
| 30  | M     | 103 | LMT  | O3B-C3B | -2.15 | 1.37        | 1.43     |
| 22  | b     | 613 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 30  | b     | 627 | LMT  | O2'-C2' | -2.15 | 1.37        | 1.43     |
| 27  | b     | 625 | LMG  | C4-C5   | 2.15  | 1.57        | 1.53     |
| 30  | B     | 628 | LMT  | O3B-C3B | -2.14 | 1.37        | 1.43     |
| 30  | B     | 627 | LMT  | O2'-C2' | -2.14 | 1.37        | 1.43     |
| 34  | f     | 101 | HEM  | CMC-C2C | 2.14  | 1.55        | 1.50     |
| 22  | B     | 610 | CLA  | C1B-C2B | 2.14  | 1.48        | 1.43     |
| 22  | c     | 501 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 22  | C     | 509 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 30  | M     | 102 | LMT  | O3B-C3B | -2.14 | 1.37        | 1.43     |
| 22  | B     | 602 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 30  | b     | 627 | LMT  | O3B-C3B | -2.13 | 1.37        | 1.43     |
| 26  | A     | 409 | LHG  | O7-C5   | -2.13 | 1.41        | 1.46     |
| 22  | b     | 611 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 30  | M     | 103 | LMT  | O2B-C2B | -2.13 | 1.37        | 1.43     |
| 22  | a     | 405 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 23  | a     | 408 | PL9  | C6-C1   | -2.13 | 1.45        | 1.48     |
| 30  | M     | 102 | LMT  | O2'-C2' | -2.13 | 1.37        | 1.43     |
| 22  | b     | 614 | CLA  | C1B-NB  | -2.13 | 1.35        | 1.37     |
| 30  | D     | 411 | LMT  | O3B-C3B | -2.13 | 1.37        | 1.43     |
| 30  | b     | 603 | LMT  | O2B-C2B | -2.13 | 1.37        | 1.43     |
| 22  | B     | 603 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 22  | C     | 503 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 26  | c     | 519 | LHG  | O7-C5   | -2.12 | 1.41        | 1.46     |
| 30  | b     | 603 | LMT  | O3B-C3B | -2.12 | 1.37        | 1.43     |
| 30  | B     | 623 | LMT  | O3B-C3B | -2.12 | 1.37        | 1.43     |
| 30  | M     | 102 | LMT  | O2B-C2B | -2.12 | 1.37        | 1.43     |
| 30  | b     | 626 | LMT  | O2B-C2B | -2.12 | 1.37        | 1.43     |
| 22  | c     | 507 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 30  | b     | 604 | LMT  | O3B-C3B | -2.11 | 1.37        | 1.43     |
| 34  | F     | 101 | HEM  | CMC-C2C | 2.11  | 1.55        | 1.50     |
| 30  | I     | 102 | LMT  | O3B-C3B | -2.11 | 1.37        | 1.43     |
| 30  | B     | 624 | LMT  | O3B-C3B | -2.11 | 1.37        | 1.43     |
| 25  | a     | 410 | DGD  | O1G-C1G | -2.11 | 1.40        | 1.45     |
| 22  | A     | 402 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 607 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 22  | a     | 404 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 22  | b     | 606 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 34  | V     | 201 | HEM  | CMB-C2B | 2.10  | 1.55        | 1.50     |
| 30  | B     | 627 | LMT  | O2B-C2B | -2.10 | 1.37        | 1.43     |
| 30  | D     | 411 | LMT  | O2'-C2' | -2.10 | 1.37        | 1.43     |
| 30  | d     | 411 | LMT  | O3B-C3B | -2.10 | 1.37        | 1.43     |
| 29  | b     | 602 | SQD  | O2-C2   | -2.10 | 1.37        | 1.43     |
| 25  | b     | 601 | DGD  | C4D-C5D | 2.10  | 1.57        | 1.53     |
| 22  | B     | 605 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 30  | b     | 603 | LMT  | O2'-C2' | -2.09 | 1.37        | 1.43     |
| 22  | A     | 404 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | C     | 509 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 22  | a     | 404 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | a     | 406 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | c     | 509 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 30  | b     | 604 | LMT  | O2B-C2B | -2.09 | 1.37        | 1.43     |
| 30  | d     | 411 | LMT  | O2'-C2' | -2.09 | 1.37        | 1.43     |
| 24  | C     | 514 | BCR  | C38-C26 | -2.08 | 1.47        | 1.50     |
| 30  | D     | 411 | LMT  | O2B-C2B | -2.08 | 1.37        | 1.43     |
| 30  | b     | 626 | LMT  | O3B-C3B | -2.08 | 1.37        | 1.43     |
| 30  | i     | 102 | LMT  | O3B-C3B | -2.08 | 1.37        | 1.43     |
| 34  | v     | 201 | HEM  | CMD-C2D | 2.08  | 1.55        | 1.50     |
| 30  | B     | 624 | LMT  | O2'-C2' | -2.08 | 1.37        | 1.43     |
| 22  | b     | 619 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 22  | C     | 506 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 22  | C     | 520 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 22  | B     | 607 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 22  | b     | 611 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 25  | B     | 625 | DGD  | C3G-C2G | 2.08  | 1.57        | 1.50     |
| 26  | c     | 519 | LHG  | P-O6    | 2.08  | 1.67        | 1.59     |
| 30  | B     | 627 | LMT  | O3B-C3B | -2.08 | 1.37        | 1.43     |
| 30  | B     | 628 | LMT  | O2'-C2' | -2.08 | 1.37        | 1.43     |
| 22  | A     | 403 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 30  | B     | 628 | LMT  | O2B-C2B | -2.08 | 1.37        | 1.43     |
| 22  | b     | 607 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 34  | v     | 201 | HEM  | CMB-C2B | 2.07  | 1.55        | 1.50     |
| 22  | b     | 611 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 25  | d     | 410 | DGD  | C1D-C2D | 2.07  | 1.58        | 1.52     |
| 22  | B     | 607 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 22  | c     | 506 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 29  | B     | 626 | SQD  | O2-C2   | -2.07 | 1.37        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 609 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 22  | B     | 603 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 22  | b     | 619 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | b     | 607 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 34  | V     | 201 | HEM  | CMD-C2D | 2.07  | 1.55        | 1.50     |
| 22  | B     | 615 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 22  | B     | 615 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 30  | B     | 623 | LMT  | O2B-C2B | -2.06 | 1.37        | 1.43     |
| 22  | B     | 603 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 22  | A     | 404 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 22  | D     | 406 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 30  | d     | 411 | LMT  | O2B-C2B | -2.06 | 1.37        | 1.43     |
| 23  | d     | 407 | PL9  | C6-C1   | -2.06 | 1.45        | 1.48     |
| 22  | D     | 405 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 22  | C     | 501 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 22  | d     | 405 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | c     | 502 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 22  | a     | 405 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | A     | 404 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 22  | C     | 502 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 22  | A     | 405 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 22  | A     | 402 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 22  | A     | 403 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | B     | 612 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 22  | B     | 602 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | B     | 609 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 22  | b     | 617 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 22  | c     | 501 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 22  | a     | 407 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 22  | C     | 505 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 24  | J     | 102 | BCR  | C38-C26 | -2.05 | 1.47        | 1.50     |
| 27  | A     | 414 | LMG  | O7-C8   | -2.05 | 1.41        | 1.46     |
| 24  | c     | 514 | BCR  | C38-C26 | -2.05 | 1.47        | 1.50     |
| 22  | a     | 405 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 22  | C     | 508 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | a     | 406 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 25  | b     | 601 | DGD  | C3G-C2G | 2.04  | 1.57        | 1.50     |
| 23  | D     | 407 | PL9  | C53-C6  | -2.04 | 1.46        | 1.50     |
| 30  | b     | 604 | LMT  | O2'-C2' | -2.04 | 1.37        | 1.43     |
| 22  | d     | 405 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 27  | a     | 402 | LMG  | O7-C8   | -2.04 | 1.41        | 1.46     |
| 22  | b     | 607 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27  | C     | 521 | LMG  | O7-C8   | -2.04 | 1.41        | 1.46     |
| 22  | B     | 604 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | b     | 608 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | C     | 508 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 22  | H     | 101 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | C     | 502 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 22  | c     | 505 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 22  | B     | 606 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 22  | A     | 405 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 22  | B     | 605 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 34  | v     | 201 | HEM  | CMA-C3A | 2.03  | 1.54        | 1.50     |
| 22  | B     | 601 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | b     | 610 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | C     | 505 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 24  | j     | 102 | BCR  | C38-C26 | -2.03 | 1.47        | 1.50     |
| 22  | C     | 502 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | b     | 605 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | C     | 512 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | C     | 520 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | c     | 508 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | C     | 502 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | b     | 613 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | c     | 502 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | h     | 101 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 30  | M     | 103 | LMT  | O1'-C1' | -2.02 | 1.36        | 1.40     |
| 22  | B     | 608 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | b     | 615 | CLA  | MG-NB   | -2.02 | 2.01        | 2.05     |
| 25  | d     | 410 | DGD  | O1G-C1G | -2.02 | 1.40        | 1.45     |
| 22  | c     | 508 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | H     | 101 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | b     | 609 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | b     | 612 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | A     | 405 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | B     | 604 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | b     | 605 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | B     | 611 | CLA  | MG-NB   | -2.02 | 2.01        | 2.05     |
| 22  | C     | 504 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | C     | 507 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | c     | 503 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | B     | 615 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | b     | 615 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | B     | 614 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 610 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | c     | 512 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | c     | 520 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | c     | 502 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | b     | 608 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | c     | 520 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | b     | 614 | CLA  | MG-ND   | -2.01 | 2.01        | 2.05     |
| 22  | C     | 510 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | b     | 606 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | b     | 609 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | h     | 101 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | b     | 617 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | b     | 610 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | C     | 511 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | B     | 609 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | C     | 503 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | c     | 503 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | h     | 101 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | c     | 507 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | C     | 507 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | c     | 509 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | B     | 606 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | b     | 616 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 29  | A     | 413 | SQD  | O3-C3   | -2.01 | 1.38        | 1.43     |
| 27  | M     | 101 | LMG  | C4-C5   | 2.01  | 1.57        | 1.53     |
| 22  | b     | 609 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 27  | A     | 414 | LMG  | C4-C5   | 2.01  | 1.57        | 1.53     |
| 22  | D     | 406 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | c     | 503 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 25  | b     | 601 | DGD  | C1G-C2G | 2.01  | 1.57        | 1.50     |
| 27  | d     | 408 | LMG  | O7-C8   | -2.01 | 1.41        | 1.46     |
| 22  | B     | 615 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | B     | 608 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 22  | B     | 613 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 22  | C     | 503 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 34  | F     | 101 | HEM  | CMA-C3A | 2.00  | 1.54        | 1.50     |
| 22  | c     | 502 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 22  | b     | 618 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 22  | c     | 511 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 22  | B     | 601 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 22  | c     | 505 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 24  | F     | 102 | BCR  | C33-C5  | -2.00 | 1.47        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | C     | 511 | CLA  | MG-NB   | -2.00 | 2.01        | 2.05     |
| 27  | a     | 402 | LMG  | C4-C5   | 2.00  | 1.57        | 1.53     |
| 30  | b     | 627 | LMT  | O2B-C2B | -2.00 | 1.38        | 1.43     |
| 22  | B     | 613 | CLA  | MG-NB   | -2.00 | 2.01        | 2.05     |

All (1031) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 22  | C     | 504 | CLA  | C4A-NA-C1A | 7.27 | 110.00      | 106.68   |
| 22  | B     | 611 | CLA  | C4A-NA-C1A | 7.25 | 109.99      | 106.68   |
| 22  | c     | 504 | CLA  | C4A-NA-C1A | 7.17 | 109.95      | 106.68   |
| 22  | B     | 603 | CLA  | C4A-NA-C1A | 7.15 | 109.94      | 106.68   |
| 22  | b     | 615 | CLA  | C4A-NA-C1A | 7.01 | 109.88      | 106.68   |
| 22  | b     | 609 | CLA  | C4A-NA-C1A | 6.99 | 109.87      | 106.68   |
| 22  | C     | 510 | CLA  | C4A-NA-C1A | 6.97 | 109.86      | 106.68   |
| 22  | b     | 607 | CLA  | C4A-NA-C1A | 6.95 | 109.85      | 106.68   |
| 22  | C     | 501 | CLA  | C4A-NA-C1A | 6.89 | 109.82      | 106.68   |
| 22  | A     | 403 | CLA  | C4A-NA-C1A | 6.85 | 109.80      | 106.68   |
| 22  | c     | 503 | CLA  | C4A-NA-C1A | 6.84 | 109.80      | 106.68   |
| 22  | a     | 405 | CLA  | C4A-NA-C1A | 6.79 | 109.78      | 106.68   |
| 22  | b     | 616 | CLA  | C4A-NA-C1A | 6.79 | 109.78      | 106.68   |
| 22  | C     | 520 | CLA  | C4A-NA-C1A | 6.78 | 109.77      | 106.68   |
| 22  | c     | 501 | CLA  | C4A-NA-C1A | 6.78 | 109.77      | 106.68   |
| 22  | B     | 605 | CLA  | C4A-NA-C1A | 6.76 | 109.76      | 106.68   |
| 22  | b     | 618 | CLA  | C4A-NA-C1A | 6.73 | 109.75      | 106.68   |
| 22  | C     | 511 | CLA  | C4A-NA-C1A | 6.72 | 109.75      | 106.68   |
| 22  | b     | 608 | CLA  | C4A-NA-C1A | 6.69 | 109.73      | 106.68   |
| 22  | B     | 606 | CLA  | C4A-NA-C1A | 6.69 | 109.73      | 106.68   |
| 22  | c     | 520 | CLA  | C4A-NA-C1A | 6.67 | 109.72      | 106.68   |
| 22  | A     | 405 | CLA  | C4A-NA-C1A | 6.66 | 109.72      | 106.68   |
| 22  | c     | 511 | CLA  | C4A-NA-C1A | 6.66 | 109.72      | 106.68   |
| 22  | C     | 512 | CLA  | C4A-NA-C1A | 6.63 | 109.70      | 106.68   |
| 22  | B     | 614 | CLA  | C4A-NA-C1A | 6.62 | 109.70      | 106.68   |
| 22  | B     | 615 | CLA  | C4A-NA-C1A | 6.61 | 109.70      | 106.68   |
| 22  | C     | 506 | CLA  | C4A-NA-C1A | 6.60 | 109.69      | 106.68   |
| 22  | B     | 612 | CLA  | C4A-NA-C1A | 6.60 | 109.69      | 106.68   |
| 22  | c     | 506 | CLA  | C4A-NA-C1A | 6.57 | 109.67      | 106.68   |
| 22  | b     | 617 | CLA  | C4A-NA-C1A | 6.55 | 109.67      | 106.68   |
| 22  | C     | 505 | CLA  | C4A-NA-C1A | 6.55 | 109.67      | 106.68   |
| 22  | a     | 406 | CLA  | C4A-NA-C1A | 6.55 | 109.67      | 106.68   |
| 22  | c     | 510 | CLA  | C4A-NA-C1A | 6.54 | 109.66      | 106.68   |
| 22  | C     | 507 | CLA  | C4A-NA-C1A | 6.53 | 109.66      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 604 | CLA  | C4A-NA-C1A  | 6.52  | 109.65      | 106.68   |
| 22  | C     | 503 | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 22  | a     | 407 | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 22  | c     | 505 | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 22  | b     | 619 | CLA  | C4A-NA-C1A  | 6.46  | 109.62      | 106.68   |
| 22  | h     | 101 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 22  | B     | 607 | CLA  | C4A-NA-C1A  | 6.44  | 109.62      | 106.68   |
| 22  | B     | 613 | CLA  | C4A-NA-C1A  | 6.44  | 109.61      | 106.68   |
| 22  | H     | 101 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 22  | B     | 608 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 22  | B     | 609 | CLA  | C4A-NA-C1A  | 6.41  | 109.60      | 106.68   |
| 22  | b     | 610 | CLA  | C4A-NA-C1A  | 6.41  | 109.60      | 106.68   |
| 22  | A     | 404 | CLA  | C4A-NA-C1A  | 6.39  | 109.59      | 106.68   |
| 22  | c     | 508 | CLA  | C4A-NA-C1A  | 6.38  | 109.59      | 106.68   |
| 22  | c     | 502 | CLA  | C4A-NA-C1A  | 6.37  | 109.58      | 106.68   |
| 22  | c     | 512 | CLA  | C4A-NA-C1A  | 6.37  | 109.58      | 106.68   |
| 22  | c     | 507 | CLA  | C4A-NA-C1A  | 6.37  | 109.58      | 106.68   |
| 22  | B     | 602 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 22  | D     | 405 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 22  | d     | 406 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 22  | b     | 611 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 22  | C     | 508 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 22  | C     | 502 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 22  | A     | 402 | CLA  | C4A-NA-C1A  | 6.18  | 109.50      | 106.68   |
| 22  | C     | 509 | CLA  | C4A-NA-C1A  | 6.17  | 109.49      | 106.68   |
| 22  | c     | 509 | CLA  | C4A-NA-C1A  | 6.16  | 109.49      | 106.68   |
| 22  | D     | 406 | CLA  | C4A-NA-C1A  | 6.14  | 109.48      | 106.68   |
| 22  | b     | 613 | CLA  | C4A-NA-C1A  | 6.13  | 109.47      | 106.68   |
| 22  | d     | 405 | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 22  | B     | 601 | CLA  | C4A-NA-C1A  | 6.11  | 109.47      | 106.68   |
| 22  | b     | 605 | CLA  | C4A-NA-C1A  | 6.09  | 109.46      | 106.68   |
| 22  | b     | 612 | CLA  | C4A-NA-C1A  | 6.07  | 109.45      | 106.68   |
| 22  | a     | 404 | CLA  | C4A-NA-C1A  | 6.01  | 109.42      | 106.68   |
| 22  | b     | 606 | CLA  | C4A-NA-C1A  | 6.01  | 109.42      | 106.68   |
| 31  | D     | 402 | PHO  | C4D-CHA-CBD | -5.87 | 105.64      | 108.45   |
| 31  | D     | 401 | PHO  | C4D-CHA-CBD | -5.86 | 105.64      | 108.45   |
| 31  | d     | 401 | PHO  | C4D-CHA-CBD | -5.85 | 105.65      | 108.45   |
| 29  | a     | 415 | SQD  | O6-C1-C2    | 5.83  | 117.13      | 108.27   |
| 31  | d     | 402 | PHO  | C4D-CHA-CBD | -5.80 | 105.67      | 108.45   |
| 29  | A     | 412 | SQD  | O6-C1-C2    | 5.68  | 116.91      | 108.27   |
| 33  | D     | 404 | BCT  | O2-C-O1     | 5.67  | 134.18      | 119.68   |
| 33  | d     | 404 | BCT  | O2-C-O1     | 5.63  | 134.08      | 119.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | b     | 602 | SQD  | O6-C1-C2    | 5.57  | 116.74      | 108.27   |
| 23  | j     | 101 | PL9  | C7-C3-C4    | 5.57  | 121.50      | 116.91   |
| 22  | b     | 614 | CLA  | C4A-NA-C1A  | 5.50  | 109.19      | 106.68   |
| 23  | J     | 101 | PL9  | C7-C3-C4    | 5.48  | 121.42      | 116.91   |
| 34  | v     | 201 | HEM  | C4D-ND-C1D  | 5.45  | 111.66      | 105.21   |
| 29  | B     | 626 | SQD  | O6-C1-C2    | 5.44  | 116.53      | 108.27   |
| 22  | B     | 610 | CLA  | C4A-NA-C1A  | 5.40  | 109.14      | 106.68   |
| 23  | A     | 406 | PL9  | C7-C3-C4    | 5.33  | 121.30      | 116.91   |
| 34  | V     | 201 | HEM  | C4D-ND-C1D  | 5.28  | 111.46      | 105.21   |
| 34  | f     | 101 | HEM  | C4D-ND-C1D  | 5.19  | 111.36      | 105.21   |
| 23  | d     | 407 | PL9  | C7-C3-C4    | 5.16  | 121.16      | 116.91   |
| 23  | D     | 407 | PL9  | C7-C3-C4    | 5.11  | 121.12      | 116.91   |
| 34  | F     | 101 | HEM  | C4D-ND-C1D  | 5.10  | 111.24      | 105.21   |
| 23  | a     | 408 | PL9  | C7-C3-C4    | 5.07  | 121.08      | 116.91   |
| 25  | A     | 408 | DGD  | O3G-C3G-C2G | -4.77 | 99.22       | 110.82   |
| 25  | a     | 410 | DGD  | O3G-C3G-C2G | -4.67 | 99.45       | 110.82   |
| 29  | d     | 403 | SQD  | O5-C5-C4    | 4.57  | 117.94      | 109.70   |
| 29  | B     | 622 | SQD  | O5-C5-C4    | 4.49  | 117.79      | 109.70   |
| 26  | c     | 519 | LHG  | O4-P-O5     | 4.43  | 133.05      | 112.44   |
| 26  | C     | 519 | LHG  | O4-P-O5     | 4.43  | 133.04      | 112.44   |
| 26  | a     | 411 | LHG  | O4-P-O5     | 4.42  | 133.03      | 112.44   |
| 26  | A     | 409 | LHG  | O4-P-O5     | 4.39  | 132.89      | 112.44   |
| 25  | C     | 517 | DGD  | O3G-C3G-C2G | -4.39 | 100.13      | 110.82   |
| 29  | d     | 403 | SQD  | O6-C1-C2    | 4.30  | 114.81      | 108.27   |
| 29  | B     | 622 | SQD  | O6-C1-C2    | 4.29  | 114.79      | 108.27   |
| 23  | j     | 101 | PL9  | C7-C3-C2    | -4.27 | 118.36      | 123.39   |
| 23  | J     | 101 | PL9  | C7-C3-C2    | -4.22 | 118.41      | 123.39   |
| 25  | c     | 517 | DGD  | O3G-C3G-C2G | -4.19 | 100.62      | 110.82   |
| 29  | A     | 412 | SQD  | O9-S-C6     | 4.13  | 112.92      | 106.76   |
| 23  | d     | 407 | PL9  | C7-C3-C2    | -4.11 | 118.55      | 123.39   |
| 29  | a     | 415 | SQD  | O9-S-C6     | 4.05  | 112.80      | 106.76   |
| 24  | C     | 513 | BCR  | C2-C1-C6    | 4.03  | 116.29      | 110.44   |
| 29  | F     | 103 | SQD  | O9-S-O7     | -4.02 | 100.74      | 113.82   |
| 23  | D     | 407 | PL9  | C7-C3-C2    | -4.01 | 118.66      | 123.39   |
| 29  | f     | 103 | SQD  | O9-S-O7     | -4.01 | 100.78      | 113.82   |
| 23  | A     | 406 | PL9  | C7-C3-C2    | -4.01 | 118.66      | 123.39   |
| 24  | c     | 513 | BCR  | C2-C1-C6    | 4.00  | 116.25      | 110.44   |
| 29  | A     | 412 | SQD  | O9-S-O7     | -3.97 | 100.90      | 113.82   |
| 24  | J     | 102 | BCR  | C11-C10-C9  | -3.97 | 121.71      | 127.28   |
| 29  | a     | 415 | SQD  | O9-S-O7     | -3.96 | 100.93      | 113.82   |
| 29  | d     | 403 | SQD  | O9-S-O7     | -3.95 | 100.97      | 113.82   |
| 29  | A     | 413 | SQD  | O5-C5-C4    | 3.95  | 116.81      | 109.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | B     | 622 | SQD  | O9-S-O7     | -3.92 | 101.06      | 113.82   |
| 29  | a     | 401 | SQD  | O9-S-O7     | -3.92 | 101.07      | 113.82   |
| 29  | B     | 626 | SQD  | O9-S-O7     | -3.92 | 101.08      | 113.82   |
| 24  | J     | 102 | BCR  | C2-C1-C6    | 3.92  | 116.13      | 110.44   |
| 24  | j     | 102 | BCR  | C2-C1-C6    | 3.91  | 116.12      | 110.44   |
| 23  | a     | 408 | PL9  | C7-C3-C2    | -3.91 | 118.78      | 123.39   |
| 29  | b     | 602 | SQD  | O9-S-O7     | -3.90 | 101.12      | 113.82   |
| 29  | A     | 413 | SQD  | O9-S-O7     | -3.90 | 101.13      | 113.82   |
| 29  | B     | 626 | SQD  | O5-C5-C4    | 3.90  | 116.72      | 109.70   |
| 29  | a     | 401 | SQD  | O5-C5-C4    | 3.88  | 116.70      | 109.70   |
| 29  | b     | 602 | SQD  | O5-C5-C4    | 3.84  | 116.61      | 109.70   |
| 27  | D     | 409 | LMG  | C1-C2-C3    | -3.83 | 101.95      | 110.01   |
| 27  | d     | 409 | LMG  | C1-C2-C3    | -3.80 | 102.01      | 110.01   |
| 24  | j     | 102 | BCR  | C11-C10-C9  | -3.79 | 121.97      | 127.28   |
| 31  | d     | 401 | PHO  | C2B-C1B-NB  | -3.78 | 106.70      | 109.43   |
| 29  | a     | 415 | SQD  | O5-C5-C4    | 3.72  | 116.41      | 109.70   |
| 29  | a     | 415 | SQD  | O47-C7-C8   | 3.72  | 119.53      | 111.48   |
| 29  | f     | 103 | SQD  | O5-C5-C4    | 3.68  | 116.33      | 109.70   |
| 31  | D     | 402 | PHO  | C2B-C1B-NB  | -3.68 | 106.77      | 109.43   |
| 31  | D     | 401 | PHO  | C2B-C1B-NB  | -3.66 | 106.79      | 109.43   |
| 29  | F     | 103 | SQD  | O5-C5-C4    | 3.64  | 116.27      | 109.70   |
| 25  | d     | 410 | DGD  | O6D-C1D-O3G | -3.63 | 101.46      | 110.04   |
| 29  | A     | 412 | SQD  | O47-C7-C8   | 3.63  | 119.33      | 111.48   |
| 29  | A     | 412 | SQD  | O5-C5-C4    | 3.62  | 116.23      | 109.70   |
| 25  | D     | 410 | DGD  | O6D-C1D-O3G | -3.61 | 101.51      | 110.04   |
| 29  | b     | 602 | SQD  | O47-C7-C8   | 3.59  | 119.24      | 111.48   |
| 29  | B     | 626 | SQD  | O47-C7-C8   | 3.59  | 119.24      | 111.48   |
| 29  | f     | 103 | SQD  | O7-S-C6     | 3.51  | 111.99      | 106.76   |
| 24  | A     | 407 | BCR  | C2-C1-C6    | 3.50  | 115.53      | 110.44   |
| 29  | F     | 103 | SQD  | O7-S-C6     | 3.48  | 111.95      | 106.76   |
| 25  | C     | 516 | DGD  | O3G-C3G-C2G | -3.47 | 102.37      | 110.82   |
| 25  | c     | 516 | DGD  | O3G-C3G-C2G | -3.47 | 102.39      | 110.82   |
| 31  | d     | 402 | PHO  | C2B-C1B-NB  | -3.46 | 106.93      | 109.43   |
| 29  | d     | 403 | SQD  | O47-C7-C8   | 3.46  | 118.97      | 111.48   |
| 29  | B     | 622 | SQD  | O47-C7-C8   | 3.46  | 118.96      | 111.48   |
| 29  | F     | 103 | SQD  | O6-C1-C2    | 3.43  | 113.49      | 108.27   |
| 29  | F     | 103 | SQD  | O47-C7-C8   | 3.42  | 118.88      | 111.48   |
| 29  | a     | 401 | SQD  | O7-S-C6     | 3.38  | 111.81      | 106.76   |
| 24  | a     | 409 | BCR  | C2-C1-C6    | 3.38  | 115.34      | 110.44   |
| 29  | A     | 413 | SQD  | O7-S-C6     | 3.36  | 111.78      | 106.76   |
| 29  | b     | 602 | SQD  | O9-S-C6     | 3.35  | 111.76      | 106.76   |
| 29  | B     | 626 | SQD  | O9-S-C6     | 3.34  | 111.75      | 106.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | f     | 103 | SQD  | O47-C7-C8   | 3.34  | 118.71      | 111.48   |
| 29  | A     | 413 | SQD  | O47-C7-C8   | 3.34  | 118.70      | 111.48   |
| 24  | B     | 618 | BCR  | C2-C1-C6    | 3.33  | 115.28      | 110.44   |
| 25  | B     | 620 | DGD  | O3G-C3G-C2G | -3.30 | 102.78      | 110.82   |
| 24  | b     | 622 | BCR  | C24-C23-C22 | -3.29 | 121.37      | 126.23   |
| 24  | j     | 102 | BCR  | C24-C23-C22 | -3.28 | 121.38      | 126.23   |
| 24  | b     | 622 | BCR  | C2-C1-C6    | 3.27  | 115.20      | 110.44   |
| 25  | C     | 515 | DGD  | O3G-C3G-C2G | -3.26 | 102.89      | 110.82   |
| 25  | c     | 516 | DGD  | O5D-C6D-C5D | -3.24 | 102.11      | 109.42   |
| 25  | c     | 515 | DGD  | O3G-C3G-C2G | -3.24 | 102.93      | 110.82   |
| 22  | B     | 605 | CLA  | O2D-CGD-O1D | -3.24 | 117.54      | 123.85   |
| 24  | J     | 102 | BCR  | C24-C23-C22 | -3.24 | 121.44      | 126.23   |
| 29  | f     | 103 | SQD  | O6-C1-C2    | 3.23  | 113.17      | 108.27   |
| 25  | b     | 624 | DGD  | O3G-C3G-C2G | -3.22 | 102.98      | 110.82   |
| 29  | b     | 602 | SQD  | O7-S-C6     | 3.22  | 111.56      | 106.76   |
| 22  | a     | 404 | CLA  | C3B-C4B-NB  | -3.22 | 107.66      | 110.53   |
| 22  | B     | 603 | CLA  | O2D-CGD-O1D | -3.21 | 117.60      | 123.85   |
| 22  | b     | 609 | CLA  | O2D-CGD-O1D | -3.21 | 117.60      | 123.85   |
| 22  | B     | 610 | CLA  | CMB-C2B-C1B | -3.21 | 120.54      | 125.42   |
| 29  | a     | 401 | SQD  | O47-C7-C8   | 3.21  | 118.42      | 111.48   |
| 22  | B     | 613 | CLA  | O2D-CGD-O1D | -3.19 | 117.64      | 123.85   |
| 25  | b     | 624 | DGD  | O6D-C1D-O3G | -3.17 | 102.54      | 110.04   |
| 24  | J     | 102 | BCR  | C27-C26-C25 | 3.17  | 126.98      | 122.70   |
| 29  | a     | 401 | SQD  | C44-O6-C1   | 3.16  | 120.57      | 113.80   |
| 25  | B     | 620 | DGD  | O6D-C1D-O3G | -3.16 | 102.58      | 110.04   |
| 22  | c     | 503 | CLA  | O2D-CGD-O1D | -3.16 | 117.70      | 123.85   |
| 31  | d     | 402 | PHO  | O1D-CGD-CBD | 3.15  | 129.50      | 124.72   |
| 24  | B     | 617 | BCR  | C15-C16-C17 | -3.15 | 117.08      | 123.52   |
| 31  | D     | 402 | PHO  | O1D-CGD-CBD | 3.14  | 129.49      | 124.72   |
| 30  | B     | 628 | LMT  | C1'-O5'-C5' | -3.14 | 107.59      | 113.72   |
| 25  | c     | 516 | DGD  | O6D-C1D-O3G | -3.14 | 102.62      | 110.04   |
| 22  | b     | 617 | CLA  | O2D-CGD-O1D | -3.14 | 117.74      | 123.85   |
| 22  | b     | 606 | CLA  | O2D-CGD-O1D | -3.14 | 117.74      | 123.85   |
| 29  | A     | 412 | SQD  | O7-S-C6     | 3.14  | 111.44      | 106.76   |
| 24  | c     | 521 | BCR  | C2-C1-C6    | 3.13  | 114.99      | 110.44   |
| 29  | B     | 622 | SQD  | O7-S-C6     | 3.13  | 111.42      | 106.76   |
| 22  | b     | 614 | CLA  | CMB-C2B-C1B | -3.12 | 120.67      | 125.42   |
| 25  | C     | 516 | DGD  | O5D-C6D-C5D | -3.11 | 102.40      | 109.42   |
| 24  | j     | 102 | BCR  | C7-C8-C9    | -3.11 | 121.63      | 126.23   |
| 29  | B     | 626 | SQD  | O7-S-C6     | 3.11  | 111.39      | 106.76   |
| 22  | A     | 402 | CLA  | C3B-C4B-NB  | -3.10 | 107.76      | 110.53   |
| 25  | d     | 410 | DGD  | O3G-C3G-C2G | -3.10 | 103.28      | 110.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 507 | CLA  | O2D-CGD-O1D | -3.10 | 117.81      | 123.85   |
| 24  | J     | 102 | BCR  | C3-C4-C5    | -3.10 | 108.53      | 114.06   |
| 29  | B     | 626 | SQD  | C3-C4-C5    | 3.10  | 115.84      | 110.23   |
| 24  | J     | 102 | BCR  | C7-C8-C9    | -3.09 | 121.66      | 126.23   |
| 22  | b     | 607 | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 25  | A     | 408 | DGD  | O6D-C1D-O3G | -3.09 | 102.75      | 110.04   |
| 24  | j     | 102 | BCR  | C27-C26-C25 | 3.09  | 126.88      | 122.70   |
| 31  | d     | 401 | PHO  | O1D-CGD-CBD | 3.09  | 129.41      | 124.72   |
| 22  | C     | 505 | CLA  | O2D-CGD-O1D | -3.09 | 117.84      | 123.85   |
| 24  | b     | 621 | BCR  | C15-C16-C17 | -3.08 | 117.21      | 123.52   |
| 29  | d     | 403 | SQD  | O9-S-C6     | 3.08  | 111.36      | 106.76   |
| 22  | C     | 503 | CLA  | O2D-CGD-O1D | -3.08 | 117.85      | 123.85   |
| 29  | a     | 415 | SQD  | O7-S-C6     | 3.08  | 111.35      | 106.76   |
| 22  | B     | 608 | CLA  | O2D-CGD-O1D | -3.07 | 117.87      | 123.85   |
| 25  | C     | 516 | DGD  | O6D-C1D-O3G | -3.07 | 102.79      | 110.04   |
| 22  | b     | 610 | CLA  | O2D-CGD-O1D | -3.07 | 117.87      | 123.85   |
| 22  | c     | 504 | CLA  | O2D-CGD-O1D | -3.07 | 117.87      | 123.85   |
| 22  | C     | 502 | CLA  | O2D-CGD-O1D | -3.07 | 117.88      | 123.85   |
| 24  | B     | 617 | BCR  | C33-C5-C6   | -3.07 | 121.14      | 124.48   |
| 30  | b     | 604 | LMT  | C1'-O5'-C5' | -3.07 | 107.73      | 113.72   |
| 29  | b     | 602 | SQD  | C3-C4-C5    | 3.06  | 115.78      | 110.23   |
| 24  | b     | 621 | BCR  | C33-C5-C6   | -3.06 | 121.15      | 124.48   |
| 31  | D     | 401 | PHO  | O1D-CGD-CBD | 3.06  | 129.36      | 124.72   |
| 22  | B     | 606 | CLA  | O2D-CGD-O1D | -3.05 | 117.90      | 123.85   |
| 22  | C     | 504 | CLA  | O2D-CGD-O1D | -3.05 | 117.91      | 123.85   |
| 22  | b     | 605 | CLA  | O2D-CGD-O1D | -3.05 | 117.92      | 123.85   |
| 25  | B     | 625 | DGD  | O5D-C1E-C2E | 3.05  | 112.90      | 108.27   |
| 24  | b     | 623 | BCR  | C2-C1-C6    | 3.04  | 114.86      | 110.44   |
| 24  | B     | 619 | BCR  | C2-C1-C6    | 3.04  | 114.86      | 110.44   |
| 24  | j     | 102 | BCR  | C3-C4-C5    | -3.04 | 108.63      | 114.06   |
| 25  | D     | 410 | DGD  | O3G-C3G-C2G | -3.03 | 103.44      | 110.82   |
| 24  | f     | 102 | BCR  | C29-C30-C25 | 3.00  | 114.80      | 110.44   |
| 22  | b     | 611 | CLA  | O2D-CGD-O1D | -3.00 | 118.00      | 123.85   |
| 22  | b     | 608 | CLA  | O2D-CGD-O1D | -2.99 | 118.02      | 123.85   |
| 24  | y     | 101 | BCR  | C27-C26-C25 | 2.99  | 126.75      | 122.70   |
| 24  | F     | 102 | BCR  | C33-C5-C6   | -2.99 | 121.22      | 124.48   |
| 30  | B     | 624 | LMT  | C3'-C4'-C5' | -2.99 | 104.31      | 110.93   |
| 24  | H     | 102 | BCR  | C33-C5-C6   | -2.98 | 121.23      | 124.48   |
| 27  | d     | 408 | LMG  | O6-C1-O1    | -2.98 | 103.00      | 110.04   |
| 22  | B     | 602 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 22  | B     | 604 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 29  | B     | 622 | SQD  | O9-S-C6     | 2.97  | 111.19      | 106.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 612 | CLA  | O2D-CGD-O1D | -2.97 | 118.08      | 123.85   |
| 25  | c     | 515 | DGD  | O6D-C1D-O3G | -2.97 | 103.04      | 110.04   |
| 22  | a     | 406 | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 24  | K     | 102 | BCR  | C2-C1-C6    | 2.96  | 114.74      | 110.44   |
| 22  | C     | 507 | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 22  | c     | 505 | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 22  | b     | 613 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 22  | C     | 506 | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 29  | d     | 403 | SQD  | O7-S-C6     | 2.96  | 111.17      | 106.76   |
| 25  | a     | 410 | DGD  | O6D-C1D-O3G | -2.95 | 103.06      | 110.04   |
| 30  | I     | 102 | LMT  | O1'-C1'-C2' | 2.95  | 112.76      | 108.27   |
| 22  | a     | 404 | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 24  | g     | 101 | BCR  | C27-C26-C25 | 2.95  | 126.69      | 122.70   |
| 24  | f     | 102 | BCR  | C33-C5-C6   | -2.95 | 121.27      | 124.48   |
| 24  | x     | 101 | BCR  | C33-C5-C6   | -2.95 | 121.27      | 124.48   |
| 34  | F     | 101 | HEM  | C3B-C4B-NB  | -2.94 | 107.35      | 109.47   |
| 22  | C     | 508 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 22  | B     | 609 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 22  | B     | 607 | CLA  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 22  | c     | 520 | CLA  | O2D-CGD-O1D | -2.94 | 118.14      | 123.85   |
| 22  | c     | 511 | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 22  | C     | 501 | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 22  | C     | 510 | CLA  | O2D-CGD-O1D | -2.93 | 118.15      | 123.85   |
| 22  | b     | 616 | CLA  | O2D-CGD-O1D | -2.93 | 118.15      | 123.85   |
| 22  | c     | 501 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 22  | c     | 506 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 22  | d     | 406 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 22  | A     | 402 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 22  | b     | 611 | CLA  | C3B-C4B-NB  | -2.92 | 107.92      | 110.53   |
| 22  | c     | 512 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 22  | A     | 403 | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 22  | c     | 510 | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 22  | b     | 613 | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 22  | c     | 512 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 22  | B     | 605 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 25  | C     | 515 | DGD  | O6D-C1D-O3G | -2.91 | 103.17      | 110.04   |
| 29  | d     | 403 | SQD  | C3-C4-C5    | 2.91  | 115.51      | 110.23   |
| 34  | f     | 101 | HEM  | C3B-C4B-NB  | -2.90 | 107.38      | 109.47   |
| 30  | i     | 102 | LMT  | O1'-C1'-C2' | 2.90  | 112.68      | 108.27   |
| 22  | B     | 601 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 25  | c     | 517 | DGD  | CDB-CCB-CBB | -2.90 | 99.70       | 114.37   |
| 22  | H     | 101 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | C     | 517 | DGD  | CDB-CCB-CBB | -2.90 | 99.70       | 114.37   |
| 30  | b     | 627 | LMT  | C3'-C4'-C5' | -2.90 | 104.50      | 110.93   |
| 22  | b     | 612 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 25  | b     | 601 | DGD  | O5D-C1E-C2E | 2.90  | 112.67      | 108.27   |
| 24  | B     | 618 | BCR  | C29-C30-C25 | 2.89  | 114.64      | 110.44   |
| 24  | F     | 102 | BCR  | C29-C30-C25 | 2.89  | 114.64      | 110.44   |
| 22  | C     | 520 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 22  | B     | 609 | CLA  | O2D-CGD-O1D | -2.89 | 118.23      | 123.85   |
| 22  | B     | 613 | CLA  | C3B-C4B-NB  | -2.88 | 107.95      | 110.53   |
| 22  | B     | 612 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 22  | b     | 618 | CLA  | O2D-CGD-O1D | -2.88 | 118.25      | 123.85   |
| 34  | F     | 101 | HEM  | C3B-C2B-C1B | 2.87  | 108.57      | 106.41   |
| 22  | c     | 502 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 22  | c     | 508 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 22  | C     | 502 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 26  | A     | 409 | LHG  | O8-C23-C24  | 2.87  | 120.58      | 111.83   |
| 22  | B     | 614 | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 22  | C     | 512 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 29  | A     | 413 | SQD  | C44-O6-C1   | 2.87  | 119.94      | 113.80   |
| 22  | c     | 509 | CLA  | C3B-C4B-NB  | -2.86 | 107.97      | 110.53   |
| 23  | A     | 406 | PL9  | C22-C23-C24 | -2.86 | 121.08      | 127.62   |
| 22  | C     | 520 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 22  | B     | 607 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 29  | f     | 103 | SQD  | O9-S-C6     | 2.86  | 111.02      | 106.76   |
| 22  | C     | 509 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 25  | c     | 517 | DGD  | C1D-C2D-C3D | -2.85 | 104.01      | 110.01   |
| 22  | D     | 406 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 25  | c     | 516 | DGD  | CDB-CCB-CBB | -2.85 | 99.97       | 114.37   |
| 27  | D     | 408 | LMG  | O6-C1-O1    | -2.84 | 103.32      | 110.04   |
| 22  | d     | 405 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 23  | a     | 408 | PL9  | C22-C23-C24 | -2.84 | 121.13      | 127.62   |
| 29  | A     | 412 | SQD  | C3-C4-C5    | 2.84  | 115.38      | 110.23   |
| 22  | C     | 509 | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 22  | c     | 502 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 22  | A     | 404 | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 26  | a     | 411 | LHG  | O8-C23-C24  | 2.83  | 120.46      | 111.83   |
| 31  | D     | 402 | PHO  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 22  | b     | 607 | CLA  | C1-C2-C3    | -2.83 | 121.56      | 126.20   |
| 22  | B     | 603 | CLA  | C1-C2-C3    | -2.83 | 121.56      | 126.20   |
| 29  | a     | 401 | SQD  | O9-S-C6     | 2.83  | 110.98      | 106.76   |
| 25  | C     | 516 | DGD  | CDB-CCB-CBB | -2.82 | 100.10      | 114.37   |
| 24  | c     | 521 | BCR  | C15-C16-C17 | -2.82 | 117.76      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | K     | 102 | BCR  | C15-C16-C17 | -2.81 | 117.76      | 123.52   |
| 22  | b     | 617 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 29  | A     | 413 | SQD  | O9-S-C6     | 2.81  | 110.96      | 106.76   |
| 22  | b     | 609 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 22  | C     | 511 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 22  | b     | 614 | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 22  | h     | 101 | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 22  | b     | 606 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 25  | B     | 625 | DGD  | C1D-C2D-C3D | -2.80 | 104.12      | 110.01   |
| 34  | f     | 101 | HEM  | C3B-C2B-C1B | 2.80  | 108.51      | 106.41   |
| 24  | b     | 621 | BCR  | C15-C14-C13 | -2.80 | 123.36      | 127.28   |
| 23  | d     | 407 | PL9  | C40-C39-C41 | 2.80  | 120.08      | 115.23   |
| 22  | c     | 511 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 29  | a     | 415 | SQD  | C3-C4-C5    | 2.79  | 115.30      | 110.23   |
| 25  | b     | 601 | DGD  | C3G-C2G-C1G | -2.79 | 105.27      | 111.78   |
| 24  | C     | 514 | BCR  | C15-C16-C17 | -2.79 | 117.81      | 123.52   |
| 24  | b     | 622 | BCR  | C29-C30-C25 | 2.79  | 114.49      | 110.44   |
| 29  | B     | 622 | SQD  | C3-C4-C5    | 2.79  | 115.29      | 110.23   |
| 25  | C     | 517 | DGD  | C1D-C2D-C3D | -2.79 | 104.14      | 110.01   |
| 22  | C     | 512 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 22  | B     | 608 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 25  | D     | 410 | DGD  | CDB-CCB-CBB | -2.78 | 100.31      | 114.37   |
| 22  | c     | 507 | CLA  | C3B-C4B-NB  | -2.78 | 108.05      | 110.53   |
| 23  | D     | 407 | PL9  | C22-C23-C24 | -2.78 | 121.27      | 127.62   |
| 22  | B     | 610 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 22  | c     | 520 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 22  | C     | 511 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 22  | B     | 602 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 29  | F     | 103 | SQD  | O9-S-C6     | 2.77  | 110.89      | 106.76   |
| 22  | c     | 509 | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |
| 24  | B     | 618 | BCR  | C24-C23-C22 | -2.77 | 122.14      | 126.23   |
| 24  | j     | 102 | BCR  | C15-C14-C13 | -2.77 | 123.40      | 127.28   |
| 25  | d     | 410 | DGD  | CDB-CCB-CBB | -2.77 | 100.39      | 114.37   |
| 22  | a     | 405 | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 22  | c     | 503 | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 31  | D     | 401 | PHO  | O2D-CGD-O1D | -2.75 | 118.49      | 123.85   |
| 22  | A     | 404 | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 22  | D     | 406 | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 22  | C     | 503 | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 22  | C     | 506 | CLA  | C3B-C4B-NB  | -2.74 | 108.08      | 110.53   |
| 25  | B     | 625 | DGD  | C3G-C2G-C1G | -2.74 | 105.39      | 111.78   |
| 29  | F     | 103 | SQD  | O8-S-C6     | 2.74  | 111.27      | 105.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 506 | CLA  | C3B-C4B-NB  | -2.74 | 108.08      | 110.53   |
| 24  | y     | 101 | BCR  | C7-C8-C9    | -2.74 | 122.18      | 126.23   |
| 24  | c     | 513 | BCR  | C11-C10-C9  | -2.74 | 123.44      | 127.28   |
| 31  | d     | 401 | PHO  | O2D-CGD-O1D | -2.73 | 118.53      | 123.85   |
| 24  | B     | 619 | BCR  | C3-C4-C5    | -2.73 | 109.18      | 114.06   |
| 25  | b     | 601 | DGD  | C1D-C2D-C3D | -2.73 | 104.26      | 110.01   |
| 23  | D     | 407 | PL9  | C40-C39-C41 | 2.73  | 119.97      | 115.23   |
| 22  | a     | 407 | CLA  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 27  | C     | 518 | LMG  | O6-C1-O1    | -2.72 | 103.61      | 110.04   |
| 25  | b     | 601 | DGD  | O3G-C3G-C2G | -2.72 | 104.20      | 110.82   |
| 24  | y     | 101 | BCR  | C38-C26-C25 | -2.72 | 121.52      | 124.48   |
| 22  | A     | 403 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 24  | b     | 623 | BCR  | C3-C4-C5    | -2.72 | 109.21      | 114.06   |
| 24  | J     | 102 | BCR  | C15-C14-C13 | -2.72 | 123.47      | 127.28   |
| 22  | b     | 607 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | b     | 619 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 27  | i     | 101 | LMG  | O6-C1-O1    | -2.71 | 103.65      | 110.04   |
| 24  | B     | 617 | BCR  | C28-C27-C26 | -2.71 | 109.23      | 114.06   |
| 22  | B     | 603 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 22  | b     | 619 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 24  | g     | 101 | BCR  | C38-C26-C25 | -2.70 | 121.54      | 124.48   |
| 22  | b     | 608 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 22  | A     | 405 | CLA  | O2D-CGD-O1D | -2.70 | 118.60      | 123.85   |
| 23  | J     | 101 | PL9  | C22-C23-C24 | -2.70 | 121.45      | 127.62   |
| 26  | C     | 519 | LHG  | O8-C23-C24  | 2.69  | 120.04      | 111.83   |
| 22  | b     | 615 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 26  | c     | 519 | LHG  | O8-C23-C24  | 2.69  | 120.03      | 111.83   |
| 22  | c     | 510 | CLA  | C3B-C4B-NB  | -2.68 | 108.13      | 110.53   |
| 24  | c     | 514 | BCR  | C11-C10-C9  | -2.68 | 123.51      | 127.28   |
| 24  | b     | 621 | BCR  | C28-C27-C26 | -2.68 | 109.27      | 114.06   |
| 24  | C     | 514 | BCR  | C29-C30-C25 | 2.68  | 114.34      | 110.44   |
| 27  | I     | 101 | LMG  | O6-C1-O1    | -2.68 | 103.71      | 110.04   |
| 23  | d     | 407 | PL9  | C22-C23-C24 | -2.68 | 121.49      | 127.62   |
| 31  | d     | 402 | PHO  | CMB-C2B-C3B | 2.68  | 130.03      | 124.68   |
| 23  | d     | 407 | PL9  | C7-C8-C9    | -2.67 | 122.22      | 126.83   |
| 22  | d     | 406 | CLA  | C3B-C4B-NB  | -2.67 | 108.14      | 110.53   |
| 22  | c     | 508 | CLA  | O2D-CGD-O1D | -2.67 | 118.65      | 123.85   |
| 24  | g     | 101 | BCR  | C7-C8-C9    | -2.67 | 122.29      | 126.23   |
| 22  | D     | 405 | CLA  | O2D-CGD-O1D | -2.66 | 118.66      | 123.85   |
| 31  | D     | 402 | PHO  | CMB-C2B-C3B | 2.66  | 130.01      | 124.68   |
| 23  | J     | 101 | PL9  | C7-C8-C9    | -2.66 | 122.24      | 126.83   |
| 22  | a     | 406 | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 403 | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 24  | c     | 514 | BCR  | C29-C30-C25 | 2.66  | 114.30      | 110.44   |
| 24  | c     | 521 | BCR  | C27-C26-C25 | 2.66  | 126.30      | 122.70   |
| 24  | C     | 513 | BCR  | C15-C16-C17 | -2.66 | 118.08      | 123.52   |
| 24  | B     | 618 | BCR  | C11-C10-C9  | -2.66 | 123.55      | 127.28   |
| 22  | b     | 618 | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 24  | b     | 620 | BCR  | C33-C5-C6   | -2.66 | 121.58      | 124.48   |
| 31  | d     | 402 | PHO  | O2D-CGD-O1D | -2.66 | 118.68      | 123.85   |
| 22  | B     | 614 | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 23  | j     | 101 | PL9  | C22-C23-C24 | -2.65 | 121.55      | 127.62   |
| 24  | B     | 616 | BCR  | C33-C5-C6   | -2.65 | 121.59      | 124.48   |
| 22  | B     | 603 | CLA  | CHB-C4A-NA  | 2.65  | 128.23      | 124.40   |
| 25  | B     | 625 | DGD  | O3G-C3G-C2G | -2.65 | 104.37      | 110.82   |
| 22  | B     | 615 | CLA  | C3B-C4B-NB  | -2.65 | 108.17      | 110.53   |
| 27  | c     | 518 | LMG  | O6-C1-O1    | -2.65 | 103.79      | 110.04   |
| 22  | a     | 405 | CLA  | C3B-C4B-NB  | -2.65 | 108.17      | 110.53   |
| 29  | b     | 602 | SQD  | C4-C3-C2    | 2.65  | 115.47      | 110.83   |
| 24  | K     | 102 | BCR  | C27-C26-C25 | 2.64  | 126.28      | 122.70   |
| 29  | f     | 103 | SQD  | O8-S-C6     | 2.64  | 111.08      | 105.97   |
| 23  | j     | 101 | PL9  | C7-C8-C9    | -2.64 | 122.28      | 126.83   |
| 24  | C     | 513 | BCR  | C24-C23-C22 | -2.63 | 122.34      | 126.23   |
| 22  | d     | 406 | CLA  | C1-C2-C3    | -2.63 | 121.89      | 126.20   |
| 22  | a     | 405 | CLA  | CHB-C4A-NA  | 2.63  | 128.19      | 124.40   |
| 22  | B     | 611 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 30  | M     | 102 | LMT  | C1'-O5'-C5' | -2.62 | 108.60      | 113.72   |
| 22  | b     | 607 | CLA  | CHB-C4A-NA  | 2.62  | 128.18      | 124.40   |
| 22  | B     | 615 | CLA  | O2D-CGD-O1D | -2.62 | 118.75      | 123.85   |
| 22  | b     | 610 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 25  | C     | 517 | DGD  | C1D-O6D-C5D | -2.62 | 108.61      | 113.72   |
| 24  | c     | 514 | BCR  | C15-C16-C17 | -2.61 | 118.17      | 123.52   |
| 25  | c     | 517 | DGD  | C1D-O6D-C5D | -2.61 | 108.62      | 113.72   |
| 24  | B     | 618 | BCR  | C15-C16-C17 | -2.61 | 118.17      | 123.52   |
| 27  | a     | 402 | LMG  | O6-C1-O1    | -2.61 | 103.88      | 110.04   |
| 24  | B     | 618 | BCR  | C15-C14-C13 | -2.61 | 123.62      | 127.28   |
| 23  | D     | 407 | PL9  | C7-C8-C9    | -2.61 | 122.34      | 126.83   |
| 24  | c     | 514 | BCR  | C28-C27-C26 | -2.61 | 109.41      | 114.06   |
| 24  | g     | 101 | BCR  | C33-C5-C6   | -2.61 | 121.64      | 124.48   |
| 22  | B     | 604 | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 22  | b     | 608 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |
| 30  | B     | 623 | LMT  | C1'-O5'-C5' | -2.59 | 108.65      | 113.72   |
| 24  | A     | 407 | BCR  | C27-C26-C25 | 2.59  | 126.21      | 122.70   |
| 22  | C     | 510 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 506 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |
| 22  | a     | 407 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 22  | C     | 505 | CLA  | CHB-C4A-NA  | 2.59  | 128.13      | 124.40   |
| 24  | J     | 102 | BCR  | C38-C26-C25 | -2.59 | 121.66      | 124.48   |
| 22  | b     | 615 | CLA  | O2D-CGD-O1D | -2.58 | 118.82      | 123.85   |
| 24  | b     | 620 | BCR  | C2-C1-C6    | 2.58  | 114.19      | 110.44   |
| 29  | d     | 403 | SQD  | O8-S-C6     | 2.58  | 110.96      | 105.97   |
| 22  | C     | 510 | CLA  | C3B-C4B-NB  | -2.58 | 108.22      | 110.53   |
| 22  | C     | 520 | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 22  | b     | 614 | CLA  | C1-C2-C3    | -2.58 | 121.97      | 126.20   |
| 22  | c     | 506 | CLA  | CHB-C4A-NA  | 2.58  | 128.12      | 124.40   |
| 24  | C     | 514 | BCR  | C11-C10-C9  | -2.58 | 123.66      | 127.28   |
| 24  | C     | 514 | BCR  | C28-C27-C26 | -2.58 | 109.46      | 114.06   |
| 31  | D     | 401 | PHO  | CMB-C2B-C3B | 2.58  | 129.83      | 124.68   |
| 24  | B     | 619 | BCR  | C7-C8-C9    | -2.58 | 122.42      | 126.23   |
| 22  | C     | 504 | CLA  | CHB-C4A-NA  | 2.57  | 128.12      | 124.40   |
| 22  | b     | 609 | CLA  | CHB-C4A-NA  | 2.57  | 128.12      | 124.40   |
| 22  | H     | 101 | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 24  | a     | 409 | BCR  | C27-C26-C25 | 2.57  | 126.18      | 122.70   |
| 24  | b     | 623 | BCR  | C27-C26-C25 | 2.57  | 126.18      | 122.70   |
| 22  | c     | 501 | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 22  | C     | 501 | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 23  | a     | 408 | PL9  | C7-C8-C9    | -2.57 | 122.41      | 126.83   |
| 24  | B     | 619 | BCR  | C27-C26-C25 | 2.57  | 126.17      | 122.70   |
| 22  | c     | 505 | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 24  | b     | 621 | BCR  | C29-C30-C25 | 2.56  | 114.16      | 110.44   |
| 24  | B     | 617 | BCR  | C29-C30-C25 | 2.56  | 114.15      | 110.44   |
| 24  | c     | 521 | BCR  | C15-C14-C13 | -2.56 | 123.69      | 127.28   |
| 22  | C     | 504 | CLA  | C3B-C4B-NB  | -2.56 | 108.25      | 110.53   |
| 24  | B     | 617 | BCR  | C15-C14-C13 | -2.55 | 123.70      | 127.28   |
| 24  | b     | 622 | BCR  | C11-C10-C9  | -2.55 | 123.70      | 127.28   |
| 22  | B     | 610 | CLA  | C1-C2-C3    | -2.55 | 122.01      | 126.20   |
| 22  | h     | 101 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 24  | C     | 514 | BCR  | C15-C14-C13 | -2.55 | 123.70      | 127.28   |
| 22  | c     | 504 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 24  | b     | 622 | BCR  | C15-C16-C17 | -2.55 | 118.31      | 123.52   |
| 29  | B     | 626 | SQD  | C4-C3-C2    | 2.55  | 115.30      | 110.83   |
| 30  | M     | 102 | LMT  | C3'-C4'-C5' | -2.55 | 105.28      | 110.93   |
| 24  | C     | 513 | BCR  | C15-C14-C13 | -2.55 | 123.71      | 127.28   |
| 22  | c     | 511 | CLA  | CHB-C4A-NA  | 2.55  | 128.07      | 124.40   |
| 25  | D     | 410 | DGD  | CFB-CEB-CDB | -2.55 | 101.50      | 114.37   |
| 24  | j     | 102 | BCR  | C15-C16-C17 | -2.54 | 118.31      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | y     | 101 | BCR  | C1-C6-C5    | -2.54 | 119.16      | 122.64   |
| 22  | a     | 406 | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 24  | b     | 623 | BCR  | C7-C8-C9    | -2.54 | 122.47      | 126.23   |
| 22  | c     | 520 | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 27  | M     | 101 | LMG  | C1-C2-C3    | -2.54 | 104.67      | 110.01   |
| 24  | j     | 102 | BCR  | C38-C26-C25 | -2.54 | 121.72      | 124.48   |
| 24  | y     | 101 | BCR  | C33-C5-C6   | -2.54 | 121.72      | 124.48   |
| 27  | A     | 414 | LMG  | O6-C1-O1    | -2.54 | 104.05      | 110.04   |
| 34  | F     | 101 | HEM  | C1B-NB-C4B  | 2.54  | 108.21      | 105.21   |
| 22  | B     | 608 | CLA  | C1-C2-C3    | -2.53 | 122.05      | 126.20   |
| 22  | C     | 507 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 22  | B     | 605 | CLA  | CHB-C4A-NA  | 2.53  | 128.06      | 124.40   |
| 22  | C     | 508 | CLA  | O2D-CGD-O1D | -2.53 | 118.92      | 123.85   |
| 22  | b     | 605 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 24  | c     | 513 | BCR  | C15-C16-C17 | -2.53 | 118.34      | 123.52   |
| 22  | C     | 512 | CLA  | CHB-C4A-NA  | 2.53  | 128.04      | 124.40   |
| 22  | c     | 508 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 22  | c     | 505 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 22  | C     | 501 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 22  | B     | 608 | CLA  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |
| 22  | C     | 511 | CLA  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |
| 30  | M     | 103 | LMT  | C3'-C4'-C5' | -2.52 | 105.35      | 110.93   |
| 22  | C     | 505 | CLA  | C3B-C4B-NB  | -2.51 | 108.28      | 110.53   |
| 30  | b     | 626 | LMT  | C1'-O5'-C5' | -2.51 | 108.82      | 113.72   |
| 24  | C     | 514 | BCR  | C33-C5-C6   | -2.51 | 121.74      | 124.48   |
| 24  | K     | 102 | BCR  | C24-C23-C22 | -2.51 | 122.52      | 126.23   |
| 22  | B     | 610 | CLA  | C3B-C4B-NB  | -2.51 | 108.29      | 110.53   |
| 22  | B     | 611 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 22  | b     | 615 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 22  | B     | 611 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 22  | b     | 618 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 25  | d     | 410 | DGD  | CFB-CEB-CDB | -2.50 | 101.72      | 114.37   |
| 22  | c     | 504 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 30  | M     | 103 | LMT  | C1'-O5'-C5' | -2.50 | 108.84      | 113.72   |
| 29  | d     | 403 | SQD  | C44-O6-C1   | 2.50  | 119.15      | 113.80   |
| 22  | a     | 407 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 34  | f     | 101 | HEM  | C1B-NB-C4B  | 2.50  | 108.16      | 105.21   |
| 29  | A     | 412 | SQD  | O48-C23-C24 | 2.50  | 119.44      | 111.83   |
| 23  | a     | 408 | PL9  | C41-C39-C40 | 2.49  | 120.33      | 114.59   |
| 27  | d     | 412 | LMG  | C38-C37-C36 | -2.49 | 101.77      | 114.37   |
| 22  | B     | 604 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 24  | c     | 514 | BCR  | C33-C5-C6   | -2.49 | 121.77      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 510 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 22  | D     | 405 | CLA  | C3B-C4B-NB  | -2.49 | 108.31      | 110.53   |
| 25  | d     | 410 | DGD  | C3G-C2G-C1G | -2.49 | 105.99      | 111.78   |
| 24  | B     | 616 | BCR  | C2-C1-C6    | 2.49  | 114.05      | 110.44   |
| 27  | d     | 409 | LMG  | C38-C37-C36 | -2.49 | 101.81      | 114.37   |
| 25  | C     | 517 | DGD  | O5D-C6D-C5D | -2.48 | 103.82      | 109.42   |
| 27  | D     | 412 | LMG  | C38-C37-C36 | -2.48 | 101.83      | 114.37   |
| 25  | a     | 410 | DGD  | CBB-CAB-C9B | -2.48 | 101.83      | 114.37   |
| 22  | c     | 501 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 27  | B     | 621 | LMG  | C1-C2-C3    | -2.48 | 104.79      | 110.01   |
| 23  | D     | 407 | PL9  | C27-C28-C29 | -2.48 | 121.95      | 127.62   |
| 25  | c     | 517 | DGD  | O5D-C6D-C5D | -2.48 | 103.83      | 109.42   |
| 22  | A     | 404 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 27  | A     | 410 | LMG  | C40-C39-C38 | -2.47 | 101.86      | 114.37   |
| 24  | j     | 102 | BCR  | C29-C30-C25 | 2.47  | 114.03      | 110.44   |
| 22  | c     | 512 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 22  | B     | 606 | CLA  | C3B-C4B-NB  | -2.47 | 108.32      | 110.53   |
| 22  | B     | 614 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 22  | B     | 609 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 22  | B     | 612 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 22  | c     | 503 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 29  | B     | 622 | SQD  | O8-S-C6     | 2.47  | 110.74      | 105.97   |
| 24  | c     | 513 | BCR  | C15-C14-C13 | -2.47 | 123.82      | 127.28   |
| 25  | A     | 408 | DGD  | CBB-CAB-C9B | -2.47 | 101.89      | 114.37   |
| 23  | A     | 406 | PL9  | C7-C8-C9    | -2.47 | 122.58      | 126.83   |
| 22  | B     | 606 | CLA  | CHB-C4A-NA  | 2.46  | 127.96      | 124.40   |
| 22  | C     | 508 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 22  | b     | 614 | CLA  | C3B-C4B-NB  | -2.46 | 108.33      | 110.53   |
| 22  | b     | 610 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 24  | g     | 101 | BCR  | C1-C6-C5    | -2.46 | 119.27      | 122.64   |
| 29  | f     | 103 | SQD  | C44-O6-C1   | 2.46  | 119.07      | 113.80   |
| 30  | D     | 411 | LMT  | C1'-O5'-C5' | -2.46 | 108.92      | 113.72   |
| 22  | B     | 607 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 29  | B     | 622 | SQD  | O48-C23-C24 | 2.46  | 119.33      | 111.83   |
| 22  | b     | 616 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 31  | d     | 401 | PHO  | CMB-C2B-C3B | 2.46  | 129.59      | 124.68   |
| 24  | b     | 623 | BCR  | C11-C10-C9  | -2.45 | 123.84      | 127.28   |
| 24  | b     | 622 | BCR  | C15-C14-C13 | -2.45 | 123.84      | 127.28   |
| 26  | c     | 519 | LHG  | C11-C10-C9  | -2.45 | 101.99      | 114.37   |
| 22  | d     | 406 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 24  | K     | 102 | BCR  | C15-C14-C13 | -2.45 | 123.84      | 127.28   |
| 29  | a     | 401 | SQD  | O48-C23-C24 | 2.45  | 119.30      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | a     | 404 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 25  | c     | 516 | DGD  | O6E-C1E-O5D | -2.45 | 104.27      | 110.04   |
| 24  | c     | 513 | BCR  | C7-C8-C9    | -2.44 | 122.62      | 126.23   |
| 22  | B     | 610 | CLA  | CHB-C1B-NB  | 2.44  | 127.71      | 124.05   |
| 22  | B     | 601 | CLA  | C3B-C4B-NB  | -2.44 | 108.35      | 110.53   |
| 23  | a     | 408 | PL9  | C27-C28-C29 | -2.44 | 122.05      | 127.62   |
| 25  | C     | 516 | DGD  | O6E-C1E-O5D | -2.44 | 104.29      | 110.04   |
| 24  | J     | 102 | BCR  | C35-C13-C14 | -2.44 | 118.87      | 122.82   |
| 22  | C     | 507 | CLA  | C1-C2-C3    | -2.43 | 122.21      | 126.20   |
| 24  | b     | 620 | BCR  | C11-C10-C9  | -2.43 | 123.86      | 127.28   |
| 24  | B     | 616 | BCR  | C27-C26-C25 | 2.43  | 125.99      | 122.70   |
| 23  | A     | 406 | PL9  | C27-C28-C29 | -2.43 | 122.06      | 127.62   |
| 22  | C     | 511 | CLA  | O2A-CGA-O1A | -2.43 | 117.55      | 123.63   |
| 30  | d     | 411 | LMT  | C3'-C4'-C5' | -2.43 | 105.54      | 110.93   |
| 24  | J     | 102 | BCR  | C29-C30-C25 | 2.43  | 113.97      | 110.44   |
| 27  | D     | 409 | LMG  | C38-C37-C36 | -2.43 | 102.10      | 114.37   |
| 27  | d     | 408 | LMG  | C38-C37-C36 | -2.43 | 102.10      | 114.37   |
| 25  | B     | 620 | DGD  | CBB-CAB-C9B | -2.43 | 102.10      | 114.37   |
| 27  | E     | 101 | LMG  | O6-C1-O1    | -2.43 | 104.31      | 110.04   |
| 22  | c     | 502 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 23  | d     | 407 | PL9  | C27-C28-C29 | -2.43 | 122.07      | 127.62   |
| 22  | A     | 402 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 22  | D     | 406 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 22  | b     | 614 | CLA  | CHB-C1B-NB  | 2.42  | 127.68      | 124.05   |
| 22  | d     | 405 | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |
| 22  | b     | 617 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 22  | C     | 503 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 25  | b     | 624 | DGD  | CBB-CAB-C9B | -2.42 | 102.13      | 114.37   |
| 22  | B     | 613 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 22  | A     | 405 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 26  | C     | 519 | LHG  | C11-C10-C9  | -2.42 | 102.14      | 114.37   |
| 23  | a     | 408 | PL9  | C20-C19-C21 | 2.42  | 119.42      | 115.23   |
| 27  | c     | 522 | LMG  | O6-C1-O1    | -2.42 | 104.33      | 110.04   |
| 27  | a     | 412 | LMG  | C40-C39-C38 | -2.42 | 102.15      | 114.37   |
| 29  | B     | 622 | SQD  | C44-O6-C1   | 2.42  | 118.98      | 113.80   |
| 22  | B     | 603 | CLA  | O1D-CGD-CBD | 2.41  | 129.28      | 124.52   |
| 23  | j     | 101 | PL9  | O2-C1-C6    | 2.41  | 124.32      | 120.48   |
| 23  | A     | 406 | PL9  | C41-C39-C40 | 2.41  | 120.14      | 114.59   |
| 24  | b     | 620 | BCR  | C27-C26-C25 | 2.41  | 125.96      | 122.70   |
| 24  | B     | 616 | BCR  | C11-C10-C9  | -2.41 | 123.90      | 127.28   |
| 27  | C     | 521 | LMG  | C40-C39-C38 | -2.41 | 102.19      | 114.37   |
| 25  | C     | 517 | DGD  | CFB-CEB-CDB | -2.41 | 102.19      | 114.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | h     | 101 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 23  | a     | 408 | PL9  | O2-C1-C6    | 2.41  | 124.31      | 120.48   |
| 29  | a     | 415 | SQD  | O48-C23-C24 | 2.41  | 119.17      | 111.83   |
| 25  | c     | 517 | DGD  | CFB-CEB-CDB | -2.40 | 102.21      | 114.37   |
| 22  | b     | 611 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 22  | B     | 612 | CLA  | C3B-C4B-NB  | -2.40 | 108.39      | 110.53   |
| 22  | B     | 602 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 27  | B     | 621 | LMG  | O6-C1-O1    | -2.40 | 104.37      | 110.04   |
| 24  | c     | 513 | BCR  | C27-C26-C25 | 2.40  | 125.95      | 122.70   |
| 24  | C     | 513 | BCR  | C27-C26-C25 | 2.40  | 125.94      | 122.70   |
| 30  | b     | 603 | LMT  | C1'-O5'-C5' | -2.40 | 109.04      | 113.72   |
| 24  | c     | 514 | BCR  | C15-C14-C13 | -2.40 | 123.92      | 127.28   |
| 22  | c     | 507 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 27  | c     | 522 | LMG  | C40-C39-C38 | -2.39 | 102.28      | 114.37   |
| 23  | J     | 101 | PL9  | O2-C1-C6    | 2.39  | 124.28      | 120.48   |
| 22  | H     | 101 | CLA  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |
| 25  | c     | 515 | DGD  | C3G-C2G-C1G | -2.39 | 106.22      | 111.78   |
| 23  | D     | 407 | PL9  | C37-C38-C39 | -2.38 | 122.17      | 127.62   |
| 25  | c     | 516 | DGD  | CFB-CEB-CDB | -2.38 | 102.31      | 114.37   |
| 25  | c     | 516 | DGD  | C3G-C2G-C1G | -2.38 | 106.23      | 111.78   |
| 27  | D     | 408 | LMG  | C38-C37-C36 | -2.38 | 102.34      | 114.37   |
| 22  | C     | 502 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 22  | b     | 612 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 23  | D     | 407 | PL9  | C20-C19-C21 | 2.38  | 119.36      | 115.23   |
| 22  | c     | 509 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 23  | d     | 407 | PL9  | O2-C1-C6    | 2.37  | 124.26      | 120.48   |
| 25  | C     | 515 | DGD  | C3G-C2G-C1G | -2.37 | 106.25      | 111.78   |
| 27  | E     | 101 | LMG  | C1-C2-C3    | -2.37 | 105.02      | 110.01   |
| 23  | A     | 406 | PL9  | O2-C1-C6    | 2.37  | 124.25      | 120.48   |
| 24  | a     | 409 | BCR  | C15-C16-C17 | -2.37 | 118.66      | 123.52   |
| 23  | J     | 101 | PL9  | C20-C19-C21 | 2.37  | 119.35      | 115.23   |
| 27  | C     | 521 | LMG  | O6-C1-O1    | -2.37 | 104.44      | 110.04   |
| 30  | B     | 627 | LMT  | C1'-O5'-C5' | -2.37 | 109.09      | 113.72   |
| 22  | b     | 606 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 27  | e     | 101 | LMG  | O6-C1-O1    | -2.37 | 104.45      | 110.04   |
| 27  | D     | 409 | LMG  | O6-C1-C2    | -2.37 | 105.50      | 110.37   |
| 29  | d     | 403 | SQD  | O48-C23-C24 | 2.37  | 119.05      | 111.83   |
| 27  | b     | 625 | LMG  | C1-C2-C3    | -2.37 | 105.03      | 110.01   |
| 25  | C     | 516 | DGD  | C3G-C2G-C1G | -2.36 | 106.27      | 111.78   |
| 27  | A     | 410 | LMG  | C38-C37-C36 | -2.36 | 102.42      | 114.37   |
| 30  | D     | 411 | LMT  | C3'-C4'-C5' | -2.36 | 105.69      | 110.93   |
| 24  | f     | 102 | BCR  | C27-C26-C25 | 2.36  | 125.90      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 509 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 23  | d     | 407 | PL9  | C37-C38-C39 | -2.36 | 122.22      | 127.62   |
| 24  | c     | 513 | BCR  | C24-C23-C22 | -2.36 | 122.74      | 126.23   |
| 22  | C     | 507 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 29  | a     | 415 | SQD  | C4-C3-C2    | 2.36  | 114.97      | 110.83   |
| 23  | d     | 407 | PL9  | C20-C19-C21 | 2.36  | 119.32      | 115.23   |
| 22  | b     | 613 | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 24  | B     | 619 | BCR  | C11-C10-C9  | -2.35 | 123.98      | 127.28   |
| 24  | F     | 102 | BCR  | C27-C26-C25 | 2.35  | 125.88      | 122.70   |
| 27  | C     | 518 | LMG  | C38-C37-C36 | -2.35 | 102.49      | 114.37   |
| 25  | A     | 408 | DGD  | O5D-C6D-C5D | -2.35 | 104.12      | 109.42   |
| 29  | B     | 626 | SQD  | O48-C23-C24 | 2.35  | 119.00      | 111.83   |
| 25  | D     | 410 | DGD  | C3G-C2G-C1G | -2.35 | 106.31      | 111.78   |
| 22  | A     | 405 | CLA  | C3B-C4B-NB  | -2.35 | 108.44      | 110.53   |
| 24  | j     | 102 | BCR  | C35-C13-C14 | -2.34 | 119.02      | 122.82   |
| 30  | i     | 102 | LMT  | C1'-O5'-C5' | -2.34 | 109.14      | 113.72   |
| 24  | F     | 102 | BCR  | C11-C10-C9  | -2.34 | 123.99      | 127.28   |
| 22  | c     | 511 | CLA  | O2A-CGA-O1A | -2.34 | 117.78      | 123.63   |
| 29  | A     | 413 | SQD  | O48-C23-C24 | 2.34  | 118.96      | 111.83   |
| 22  | B     | 615 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 22  | B     | 606 | CLA  | C1-C2-C3    | -2.34 | 122.37      | 126.20   |
| 24  | J     | 102 | BCR  | C15-C16-C17 | -2.33 | 118.74      | 123.52   |
| 22  | c     | 507 | CLA  | C1-C2-C3    | -2.33 | 122.37      | 126.20   |
| 27  | B     | 621 | LMG  | C40-C39-C38 | -2.33 | 102.58      | 114.37   |
| 27  | c     | 518 | LMG  | C38-C37-C36 | -2.33 | 102.58      | 114.37   |
| 25  | C     | 516 | DGD  | CFB-CEB-CDB | -2.33 | 102.58      | 114.37   |
| 24  | x     | 101 | BCR  | C29-C30-C25 | 2.33  | 113.83      | 110.44   |
| 24  | C     | 513 | BCR  | C11-C10-C9  | -2.33 | 124.01      | 127.28   |
| 27  | d     | 412 | LMG  | O6-C1-O1    | -2.33 | 104.55      | 110.04   |
| 24  | K     | 102 | BCR  | C11-C10-C9  | -2.33 | 124.02      | 127.28   |
| 23  | D     | 407 | PL9  | C32-C33-C34 | -2.33 | 122.30      | 127.62   |
| 24  | J     | 102 | BCR  | C20-C21-C22 | -2.32 | 124.02      | 127.28   |
| 22  | C     | 502 | CLA  | C1-C2-C3    | -2.32 | 122.39      | 126.20   |
| 27  | b     | 625 | LMG  | O6-C1-O1    | -2.32 | 104.56      | 110.04   |
| 29  | a     | 401 | SQD  | C1-O5-C5    | 2.32  | 118.25      | 113.72   |
| 27  | A     | 410 | LMG  | O3-C3-C2    | -2.32 | 104.91      | 110.38   |
| 22  | D     | 406 | CLA  | C1-C2-C3    | -2.32 | 122.40      | 126.20   |
| 24  | j     | 102 | BCR  | C20-C21-C22 | -2.32 | 124.03      | 127.28   |
| 25  | b     | 601 | DGD  | O6D-C1D-O3G | -2.31 | 104.58      | 110.04   |
| 27  | a     | 412 | LMG  | C38-C37-C36 | -2.31 | 102.68      | 114.37   |
| 24  | A     | 407 | BCR  | C15-C16-C17 | -2.31 | 118.79      | 123.52   |
| 27  | b     | 625 | LMG  | C40-C39-C38 | -2.31 | 102.70      | 114.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | a     | 401 | SQD  | O8-S-C6     | 2.31  | 110.43      | 105.97   |
| 24  | B     | 616 | BCR  | C15-C16-C17 | -2.31 | 118.80      | 123.52   |
| 23  | D     | 407 | PL9  | O2-C1-C6    | 2.31  | 124.15      | 120.48   |
| 29  | B     | 626 | SQD  | O8-S-C6     | 2.30  | 110.42      | 105.97   |
| 30  | d     | 411 | LMT  | C1'-O5'-C5' | -2.30 | 109.22      | 113.72   |
| 24  | f     | 102 | BCR  | C11-C10-C9  | -2.30 | 124.05      | 127.28   |
| 22  | b     | 607 | CLA  | O1D-CGD-CBD | 2.30  | 129.06      | 124.52   |
| 22  | b     | 619 | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 27  | e     | 101 | LMG  | C1-C2-C3    | -2.29 | 105.19      | 110.01   |
| 24  | C     | 513 | BCR  | C3-C4-C5    | -2.29 | 109.97      | 114.06   |
| 24  | B     | 616 | BCR  | C15-C14-C13 | -2.29 | 124.07      | 127.28   |
| 22  | b     | 616 | CLA  | C3B-C4B-NB  | -2.29 | 108.49      | 110.53   |
| 29  | b     | 602 | SQD  | O48-C23-C24 | 2.28  | 118.80      | 111.83   |
| 24  | b     | 620 | BCR  | C15-C14-C13 | -2.28 | 124.07      | 127.28   |
| 27  | C     | 521 | LMG  | C38-C37-C36 | -2.28 | 102.82      | 114.37   |
| 24  | F     | 102 | BCR  | C15-C16-C17 | -2.28 | 118.85      | 123.52   |
| 24  | c     | 521 | BCR  | C11-C10-C9  | -2.28 | 124.08      | 127.28   |
| 22  | b     | 605 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 23  | d     | 407 | PL9  | O1-C4-C3    | -2.28 | 118.33      | 120.73   |
| 25  | d     | 410 | DGD  | C3D-C4D-C5D | -2.28 | 106.10      | 110.23   |
| 27  | D     | 412 | LMG  | O6-C1-O1    | -2.28 | 104.66      | 110.04   |
| 23  | j     | 101 | PL9  | C20-C19-C21 | 2.27  | 119.17      | 115.23   |
| 24  | a     | 409 | BCR  | C33-C5-C6   | -2.27 | 122.01      | 124.48   |
| 22  | c     | 507 | CLA  | CMB-C2B-C1B | -2.27 | 121.97      | 125.42   |
| 27  | b     | 625 | LMG  | C38-C37-C36 | -2.27 | 102.91      | 114.37   |
| 22  | B     | 601 | CLA  | CHB-C4A-NA  | 2.26  | 127.67      | 124.40   |
| 27  | a     | 412 | LMG  | O3-C3-C2    | -2.26 | 105.05      | 110.38   |
| 29  | F     | 103 | SQD  | C44-O6-C1   | 2.26  | 118.64      | 113.80   |
| 27  | m     | 101 | LMG  | O2-C2-C1    | -2.26 | 104.70      | 110.08   |
| 29  | F     | 103 | SQD  | O48-C23-C24 | 2.26  | 118.71      | 111.83   |
| 24  | B     | 617 | BCR  | C11-C10-C9  | -2.25 | 124.12      | 127.28   |
| 24  | H     | 102 | BCR  | C29-C30-C25 | 2.25  | 113.71      | 110.44   |
| 29  | A     | 412 | SQD  | C4-C3-C2    | 2.25  | 114.78      | 110.83   |
| 24  | b     | 622 | BCR  | C27-C26-C25 | 2.25  | 125.75      | 122.70   |
| 24  | c     | 513 | BCR  | C3-C4-C5    | -2.25 | 110.04      | 114.06   |
| 24  | K     | 102 | BCR  | C33-C5-C6   | -2.25 | 122.03      | 124.48   |
| 27  | A     | 410 | LMG  | C1-C2-C3    | -2.25 | 105.28      | 110.01   |
| 24  | A     | 407 | BCR  | C15-C14-C13 | -2.25 | 124.12      | 127.28   |
| 30  | I     | 102 | LMT  | C1'-O5'-C5' | -2.25 | 109.33      | 113.72   |
| 29  | A     | 413 | SQD  | O8-S-C6     | 2.25  | 110.31      | 105.97   |
| 23  | D     | 407 | PL9  | O1-C4-C3    | -2.25 | 118.36      | 120.73   |
| 27  | c     | 518 | LMG  | O7-C10-O9   | -2.25 | 118.45      | 123.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | A     | 408 | DGD  | C3G-C2G-C1G | -2.25 | 106.55      | 111.78   |
| 23  | d     | 407 | PL9  | C32-C33-C34 | -2.25 | 122.48      | 127.62   |
| 24  | f     | 102 | BCR  | C15-C16-C17 | -2.24 | 118.93      | 123.52   |
| 27  | c     | 522 | LMG  | C38-C37-C36 | -2.24 | 103.04      | 114.37   |
| 25  | B     | 620 | DGD  | C1D-C2D-C3D | -2.24 | 105.30      | 110.01   |
| 22  | b     | 610 | CLA  | C1-C2-C3    | -2.24 | 122.53      | 126.20   |
| 27  | D     | 412 | LMG  | O3-C3-C2    | -2.24 | 105.11      | 110.38   |
| 22  | b     | 612 | CLA  | C1-C2-C3    | -2.23 | 122.54      | 126.20   |
| 24  | a     | 409 | BCR  | C15-C14-C13 | -2.23 | 124.14      | 127.28   |
| 27  | I     | 101 | LMG  | O7-C10-O9   | -2.23 | 118.48      | 123.70   |
| 27  | B     | 621 | LMG  | C38-C37-C36 | -2.23 | 103.08      | 114.37   |
| 29  | b     | 602 | SQD  | O8-S-C6     | 2.23  | 110.28      | 105.97   |
| 24  | A     | 407 | BCR  | C33-C5-C6   | -2.23 | 122.05      | 124.48   |
| 24  | c     | 521 | BCR  | C24-C23-C22 | -2.23 | 122.94      | 126.23   |
| 22  | c     | 506 | CLA  | O2A-CGA-O1A | -2.23 | 118.06      | 123.63   |
| 25  | a     | 410 | DGD  | C3G-C2G-C1G | -2.23 | 106.59      | 111.78   |
| 24  | b     | 622 | BCR  | C7-C8-C9    | -2.23 | 122.94      | 126.23   |
| 27  | m     | 101 | LMG  | C1-C2-C3    | -2.22 | 105.33      | 110.01   |
| 22  | b     | 605 | CLA  | C1-C2-C3    | -2.22 | 122.56      | 126.20   |
| 25  | a     | 410 | DGD  | O5D-C6D-C5D | -2.22 | 104.41      | 109.42   |
| 27  | D     | 408 | LMG  | O2-C2-C1    | -2.22 | 104.79      | 110.08   |
| 24  | H     | 102 | BCR  | C16-C15-C14 | -2.22 | 118.98      | 123.52   |
| 22  | b     | 618 | CLA  | O2A-CGA-O1A | -2.22 | 118.09      | 123.63   |
| 25  | B     | 625 | DGD  | O6D-C1D-O3G | -2.21 | 104.81      | 110.04   |
| 24  | g     | 101 | BCR  | C15-C16-C17 | -2.21 | 118.99      | 123.52   |
| 27  | D     | 412 | LMG  | C1-C2-C3    | -2.21 | 105.36      | 110.01   |
| 27  | d     | 409 | LMG  | O6-C1-O1    | -2.21 | 104.82      | 110.04   |
| 25  | b     | 624 | DGD  | C1D-C2D-C3D | -2.21 | 105.36      | 110.01   |
| 27  | C     | 521 | LMG  | O2-C2-C1    | -2.21 | 104.81      | 110.08   |
| 25  | B     | 620 | DGD  | C3G-C2G-C1G | -2.21 | 106.64      | 111.78   |
| 27  | C     | 518 | LMG  | O7-C10-O9   | -2.21 | 118.55      | 123.70   |
| 27  | D     | 409 | LMG  | O6-C1-O1    | -2.21 | 104.83      | 110.04   |
| 24  | b     | 623 | BCR  | C24-C23-C22 | -2.21 | 122.97      | 126.23   |
| 25  | a     | 410 | DGD  | CAB-C9B-C8B | -2.20 | 103.22      | 114.37   |
| 24  | b     | 621 | BCR  | C7-C8-C9    | -2.20 | 122.97      | 126.23   |
| 23  | A     | 406 | PL9  | C20-C19-C21 | 2.20  | 119.05      | 115.23   |
| 22  | B     | 605 | CLA  | O1D-CGD-CBD | 2.20  | 128.86      | 124.52   |
| 22  | H     | 101 | CLA  | C1-C2-C3    | -2.20 | 122.59      | 126.20   |
| 22  | c     | 502 | CLA  | C1-C2-C3    | -2.20 | 122.59      | 126.20   |
| 27  | i     | 101 | LMG  | O2-C2-C1    | -2.20 | 104.83      | 110.08   |
| 24  | C     | 513 | BCR  | C7-C8-C9    | -2.20 | 122.99      | 126.23   |
| 27  | A     | 410 | LMG  | O7-C10-O9   | -2.19 | 118.57      | 123.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | a     | 412 | LMG  | O7-C10-O9   | -2.19 | 118.58      | 123.70   |
| 25  | c     | 516 | DGD  | CBB-CAB-C9B | -2.19 | 103.28      | 114.37   |
| 26  | a     | 411 | LHG  | C27-C26-C25 | -2.19 | 103.29      | 114.37   |
| 30  | B     | 624 | LMT  | C1'-O5'-C5' | -2.19 | 109.44      | 113.72   |
| 25  | C     | 516 | DGD  | O3D-C3D-C4D | -2.19 | 105.21      | 110.38   |
| 22  | d     | 405 | CLA  | O1D-CGD-CBD | 2.19  | 128.84      | 124.52   |
| 27  | m     | 101 | LMG  | C1-O6-C5    | -2.19 | 109.44      | 113.72   |
| 25  | c     | 516 | DGD  | O3D-C3D-C4D | -2.19 | 105.21      | 110.38   |
| 24  | F     | 102 | BCR  | C7-C8-C9    | -2.19 | 123.00      | 126.23   |
| 34  | v     | 201 | HEM  | C2A-C1A-NA  | -2.19 | 107.72      | 110.15   |
| 22  | c     | 507 | CLA  | O2D-CGD-CBD | 2.19  | 115.05      | 111.23   |
| 27  | I     | 101 | LMG  | O2-C2-C1    | -2.19 | 104.87      | 110.08   |
| 22  | B     | 601 | CLA  | O2A-CGA-O1A | -2.19 | 118.16      | 123.63   |
| 25  | A     | 408 | DGD  | CAB-C9B-C8B | -2.18 | 103.33      | 114.37   |
| 22  | B     | 603 | CLA  | O2A-CGA-O1A | -2.18 | 118.17      | 123.63   |
| 25  | C     | 516 | DGD  | CBB-CAB-C9B | -2.18 | 103.33      | 114.37   |
| 24  | b     | 621 | BCR  | C11-C10-C9  | -2.18 | 124.22      | 127.28   |
| 22  | B     | 611 | CLA  | C1-C2-C3    | -2.18 | 122.62      | 126.20   |
| 24  | c     | 521 | BCR  | C33-C5-C6   | -2.18 | 122.11      | 124.48   |
| 27  | d     | 412 | LMG  | C1-C2-C3    | -2.18 | 105.42      | 110.01   |
| 25  | C     | 517 | DGD  | CBB-CAB-C9B | -2.18 | 103.35      | 114.37   |
| 23  | d     | 407 | PL9  | O2-C1-C2    | -2.18 | 116.87      | 121.83   |
| 27  | d     | 408 | LMG  | O3-C3-C2    | -2.18 | 105.25      | 110.38   |
| 27  | d     | 408 | LMG  | O2-C2-C1    | -2.17 | 104.89      | 110.08   |
| 27  | A     | 414 | LMG  | O7-C10-O9   | -2.17 | 118.62      | 123.70   |
| 24  | B     | 617 | BCR  | C7-C8-C9    | -2.17 | 123.02      | 126.23   |
| 23  | j     | 101 | PL9  | O2-C1-C2    | -2.17 | 116.89      | 121.83   |
| 24  | b     | 623 | BCR  | C38-C26-C25 | -2.17 | 122.11      | 124.48   |
| 25  | b     | 601 | DGD  | CBB-CAB-C9B | -2.17 | 103.39      | 114.37   |
| 22  | C     | 507 | CLA  | CMB-C2B-C1B | -2.17 | 122.11      | 125.42   |
| 24  | y     | 101 | BCR  | C15-C16-C17 | -2.17 | 119.08      | 123.52   |
| 27  | a     | 412 | LMG  | C1-C2-C3    | -2.17 | 105.44      | 110.01   |
| 24  | C     | 514 | BCR  | C38-C26-C25 | -2.17 | 122.11      | 124.48   |
| 24  | B     | 618 | BCR  | C7-C8-C9    | -2.17 | 123.02      | 126.23   |
| 25  | b     | 624 | DGD  | C3G-C2G-C1G | -2.17 | 106.73      | 111.78   |
| 27  | i     | 101 | LMG  | O1-C7-C8    | -2.17 | 105.55      | 110.82   |
| 25  | C     | 515 | DGD  | C1D-C2D-C3D | -2.17 | 105.45      | 110.01   |
| 25  | a     | 410 | DGD  | C1D-C2D-C3D | -2.17 | 105.45      | 110.01   |
| 24  | C     | 514 | BCR  | C24-C23-C22 | -2.17 | 123.03      | 126.23   |
| 29  | F     | 103 | SQD  | C3-C4-C5    | 2.16  | 114.15      | 110.23   |
| 29  | f     | 103 | SQD  | C3-C4-C5    | 2.16  | 114.15      | 110.23   |
| 25  | C     | 516 | DGD  | CAB-C9B-C8B | -2.16 | 103.45      | 114.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | B     | 622 | SQD  | C4-C3-C2    | 2.16  | 114.62      | 110.83   |
| 24  | B     | 619 | BCR  | C38-C26-C25 | -2.16 | 122.13      | 124.48   |
| 25  | C     | 516 | DGD  | C3D-C4D-C5D | -2.16 | 106.32      | 110.23   |
| 33  | D     | 404 | BCT  | O3-C-O1     | -2.16 | 114.16      | 119.68   |
| 27  | d     | 409 | LMG  | O6-C1-C2    | -2.16 | 105.94      | 110.37   |
| 24  | b     | 623 | BCR  | C33-C5-C6   | -2.16 | 122.13      | 124.48   |
| 24  | B     | 619 | BCR  | C24-C23-C22 | -2.16 | 123.05      | 126.23   |
| 22  | c     | 509 | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 22  | b     | 616 | CLA  | CMB-C2B-C1B | -2.15 | 122.14      | 125.42   |
| 27  | D     | 408 | LMG  | O3-C3-C2    | -2.15 | 105.31      | 110.38   |
| 23  | J     | 101 | PL9  | O2-C1-C2    | -2.15 | 116.94      | 121.83   |
| 25  | D     | 410 | DGD  | C3D-C4D-C5D | -2.15 | 106.33      | 110.23   |
| 24  | g     | 101 | BCR  | C3-C2-C1    | -2.15 | 106.82      | 114.43   |
| 22  | D     | 405 | CLA  | O2A-CGA-O1A | -2.15 | 118.25      | 123.63   |
| 22  | B     | 602 | CLA  | O2A-CGA-O1A | -2.15 | 118.25      | 123.63   |
| 29  | a     | 415 | SQD  | O8-S-C6     | 2.15  | 110.12      | 105.97   |
| 24  | c     | 514 | BCR  | C24-C23-C22 | -2.15 | 123.06      | 126.23   |
| 25  | B     | 625 | DGD  | CBB-CAB-C9B | -2.15 | 103.51      | 114.37   |
| 27  | a     | 402 | LMG  | O3-C3-C2    | -2.15 | 105.31      | 110.38   |
| 27  | b     | 625 | LMG  | O3-C3-C2    | -2.15 | 105.31      | 110.38   |
| 22  | b     | 607 | CLA  | O2A-CGA-O1A | -2.15 | 118.26      | 123.63   |
| 27  | B     | 621 | LMG  | O3-C3-C2    | -2.15 | 105.32      | 110.38   |
| 27  | i     | 101 | LMG  | O7-C10-O9   | -2.15 | 118.69      | 123.70   |
| 25  | c     | 517 | DGD  | CBB-CAB-C9B | -2.15 | 103.52      | 114.37   |
| 27  | I     | 101 | LMG  | O3-C3-C2    | -2.14 | 105.32      | 110.38   |
| 30  | b     | 627 | LMT  | C1'-O5'-C5' | -2.14 | 109.53      | 113.72   |
| 33  | d     | 404 | BCT  | O3-C-O1     | -2.14 | 114.19      | 119.68   |
| 24  | B     | 618 | BCR  | C27-C26-C25 | 2.14  | 125.60      | 122.70   |
| 29  | f     | 103 | SQD  | O48-C23-C24 | 2.14  | 118.37      | 111.83   |
| 26  | A     | 409 | LHG  | C27-C26-C25 | -2.14 | 103.54      | 114.37   |
| 22  | c     | 504 | CLA  | O1D-CGD-CBD | 2.14  | 128.74      | 124.52   |
| 29  | d     | 403 | SQD  | C4-C3-C2    | 2.14  | 114.59      | 110.83   |
| 22  | b     | 615 | CLA  | C1-C2-C3    | -2.14 | 122.69      | 126.20   |
| 27  | c     | 522 | LMG  | O2-C2-C1    | -2.14 | 104.98      | 110.08   |
| 22  | b     | 615 | CLA  | O2A-CGA-O1A | -2.14 | 118.28      | 123.63   |
| 23  | a     | 408 | PL9  | O1-C4-C3    | -2.14 | 118.48      | 120.73   |
| 27  | d     | 412 | LMG  | O3-C3-C2    | -2.14 | 105.34      | 110.38   |
| 31  | d     | 401 | PHO  | C1-C2-C3    | -2.14 | 122.70      | 126.20   |
| 25  | b     | 601 | DGD  | CAB-C9B-C8B | -2.13 | 103.58      | 114.37   |
| 25  | B     | 620 | DGD  | C4E-C3E-C2E | -2.13 | 107.08      | 110.83   |
| 22  | B     | 612 | CLA  | CMB-C2B-C1B | -2.13 | 122.17      | 125.42   |
| 22  | C     | 506 | CLA  | O2A-CGA-O1A | -2.13 | 118.29      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | D     | 407 | PL9  | O2-C1-C2    | -2.13 | 116.99      | 121.83   |
| 22  | B     | 611 | CLA  | O2A-CGA-O1A | -2.13 | 118.30      | 123.63   |
| 24  | H     | 102 | BCR  | C27-C26-C25 | 2.13  | 125.58      | 122.70   |
| 23  | A     | 406 | PL9  | O2-C1-C2    | -2.12 | 117.00      | 121.83   |
| 22  | c     | 510 | CLA  | C1-C2-C3    | -2.12 | 122.72      | 126.20   |
| 23  | a     | 408 | PL9  | O2-C1-C2    | -2.12 | 117.00      | 121.83   |
| 25  | d     | 410 | DGD  | C5B-C4B-C3B | -2.12 | 103.64      | 114.37   |
| 22  | B     | 612 | CLA  | O2A-CGA-O1A | -2.12 | 118.32      | 123.63   |
| 22  | C     | 501 | CLA  | O2A-CGA-O1A | -2.12 | 118.32      | 123.63   |
| 27  | b     | 625 | LMG  | O2-C2-C1    | -2.12 | 105.03      | 110.08   |
| 25  | c     | 517 | DGD  | CAB-C9B-C8B | -2.12 | 103.66      | 114.37   |
| 34  | V     | 201 | HEM  | C3B-C2B-C1B | 2.12  | 108.00      | 106.41   |
| 22  | b     | 609 | CLA  | O1D-CGD-CBD | 2.12  | 128.69      | 124.52   |
| 22  | c     | 503 | CLA  | O2D-CGD-CBD | 2.12  | 114.93      | 111.23   |
| 24  | b     | 622 | BCR  | C33-C5-C6   | -2.12 | 122.17      | 124.48   |
| 27  | D     | 412 | LMG  | O7-C10-O9   | -2.12 | 118.76      | 123.70   |
| 25  | B     | 625 | DGD  | CAB-C9B-C8B | -2.11 | 103.68      | 114.37   |
| 29  | A     | 412 | SQD  | O8-S-C6     | 2.11  | 110.06      | 105.97   |
| 24  | a     | 409 | BCR  | C24-C23-C22 | -2.11 | 123.11      | 126.23   |
| 22  | b     | 616 | CLA  | O2A-CGA-O1A | -2.11 | 118.35      | 123.63   |
| 25  | c     | 515 | DGD  | C1D-C2D-C3D | -2.11 | 105.57      | 110.01   |
| 22  | d     | 405 | CLA  | CHB-C4A-NA  | 2.11  | 127.44      | 124.40   |
| 24  | B     | 619 | BCR  | C33-C5-C6   | -2.11 | 122.18      | 124.48   |
| 27  | M     | 101 | LMG  | O2-C2-C1    | -2.11 | 105.05      | 110.08   |
| 24  | c     | 514 | BCR  | C38-C26-C25 | -2.11 | 122.19      | 124.48   |
| 27  | a     | 402 | LMG  | O1-C7-C8    | -2.11 | 105.69      | 110.82   |
| 27  | c     | 522 | LMG  | O3-C3-C2    | -2.11 | 105.41      | 110.38   |
| 22  | B     | 606 | CLA  | O2A-CGA-O1A | -2.11 | 118.36      | 123.63   |
| 22  | B     | 614 | CLA  | O2A-CGA-O1A | -2.10 | 118.36      | 123.63   |
| 22  | b     | 610 | CLA  | O2A-CGA-O1A | -2.10 | 118.36      | 123.63   |
| 26  | C     | 519 | LHG  | C27-C26-C25 | -2.10 | 103.73      | 114.37   |
| 34  | v     | 201 | HEM  | C1B-NB-C4B  | 2.10  | 107.70      | 105.21   |
| 22  | c     | 508 | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 22  | b     | 616 | CLA  | C1-C2-C3    | -2.10 | 122.75      | 126.20   |
| 23  | D     | 407 | PL9  | C12-C13-C14 | -2.10 | 122.81      | 127.62   |
| 27  | C     | 521 | LMG  | O3-C3-C2    | -2.10 | 105.42      | 110.38   |
| 27  | i     | 101 | LMG  | O3-C3-C2    | -2.10 | 105.42      | 110.38   |
| 25  | D     | 410 | DGD  | C5B-C4B-C3B | -2.10 | 103.75      | 114.37   |
| 27  | d     | 412 | LMG  | O7-C10-O9   | -2.10 | 118.80      | 123.70   |
| 22  | C     | 520 | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 22  | c     | 520 | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 24  | y     | 101 | BCR  | C3-C2-C1    | -2.10 | 107.01      | 114.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | i     | 101 | LMG  | O1-C1-C2    | -2.10 | 105.09      | 108.27   |
| 22  | h     | 101 | CLA  | C1-C2-C3    | -2.09 | 122.77      | 126.20   |
| 22  | C     | 508 | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 25  | C     | 517 | DGD  | CAB-C9B-C8B | -2.09 | 103.80      | 114.37   |
| 27  | B     | 621 | LMG  | O7-C10-O9   | -2.09 | 118.81      | 123.70   |
| 24  | C     | 514 | BCR  | C7-C8-C9    | -2.09 | 123.14      | 126.23   |
| 27  | e     | 101 | LMG  | O3-C3-C2    | -2.09 | 105.45      | 110.38   |
| 22  | C     | 512 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 22  | B     | 601 | CLA  | C1-C2-C3    | -2.09 | 122.77      | 126.20   |
| 25  | c     | 516 | DGD  | CAB-C9B-C8B | -2.09 | 103.81      | 114.37   |
| 22  | D     | 405 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.40   |
| 27  | A     | 414 | LMG  | O3-C3-C2    | -2.09 | 105.45      | 110.38   |
| 22  | a     | 405 | CLA  | O2A-CGA-O1A | -2.09 | 118.41      | 123.63   |
| 24  | K     | 102 | BCR  | C7-C8-C9    | -2.09 | 123.15      | 126.23   |
| 22  | C     | 504 | CLA  | O1D-CGD-CBD | 2.09  | 128.63      | 124.52   |
| 22  | c     | 501 | CLA  | O2A-CGA-O1A | -2.08 | 118.41      | 123.63   |
| 27  | c     | 518 | LMG  | O3-C3-C2    | -2.08 | 105.46      | 110.38   |
| 25  | A     | 408 | DGD  | CDB-CCB-CBB | -2.08 | 99.30       | 113.36   |
| 26  | c     | 519 | LHG  | C27-C26-C25 | -2.08 | 103.84      | 114.37   |
| 25  | C     | 515 | DGD  | C5B-C4B-C3B | -2.08 | 103.85      | 114.37   |
| 25  | a     | 410 | DGD  | CDB-CCB-CBB | -2.08 | 99.32       | 113.36   |
| 22  | b     | 606 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 25  | c     | 515 | DGD  | C5B-C4B-C3B | -2.08 | 103.87      | 114.37   |
| 24  | A     | 407 | BCR  | C38-C26-C25 | -2.08 | 122.22      | 124.48   |
| 27  | b     | 625 | LMG  | O7-C10-O9   | -2.08 | 118.85      | 123.70   |
| 22  | B     | 612 | CLA  | C1-C2-C3    | -2.08 | 122.80      | 126.20   |
| 27  | C     | 518 | LMG  | O2-C2-C1    | -2.08 | 105.13      | 110.08   |
| 27  | e     | 101 | LMG  | O1-C7-C8    | -2.08 | 105.77      | 110.82   |
| 27  | c     | 518 | LMG  | O2-C2-C1    | -2.07 | 105.13      | 110.08   |
| 24  | b     | 621 | BCR  | C24-C23-C22 | -2.07 | 123.17      | 126.23   |
| 22  | a     | 404 | CLA  | C1-C2-C3    | -2.07 | 122.81      | 126.20   |
| 24  | x     | 101 | BCR  | C27-C26-C25 | 2.07  | 125.50      | 122.70   |
| 22  | c     | 512 | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 25  | A     | 408 | DGD  | C1D-C2D-C3D | -2.06 | 105.67      | 110.01   |
| 22  | C     | 510 | CLA  | C1-C2-C3    | -2.06 | 122.82      | 126.20   |
| 24  | b     | 620 | BCR  | C15-C16-C17 | -2.06 | 119.30      | 123.52   |
| 22  | B     | 609 | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 24  | H     | 102 | BCR  | C7-C8-C9    | -2.06 | 123.19      | 126.23   |
| 27  | M     | 101 | LMG  | C1-O6-C5    | -2.06 | 109.70      | 113.72   |
| 24  | a     | 409 | BCR  | C38-C26-C25 | -2.06 | 122.24      | 124.48   |
| 22  | d     | 405 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 25  | D     | 410 | DGD  | CAB-C9B-C8B | -2.06 | 103.96      | 114.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | A     | 406 | PL9  | O1-C4-C3    | -2.06 | 118.56      | 120.73   |
| 27  | C     | 518 | LMG  | O3-C3-C2    | -2.06 | 105.53      | 110.38   |
| 22  | a     | 406 | CLA  | C1-C2-C3    | -2.06 | 122.83      | 126.20   |
| 24  | x     | 101 | BCR  | C16-C15-C14 | -2.06 | 119.31      | 123.52   |
| 25  | c     | 516 | DGD  | C3D-C4D-C5D | -2.05 | 106.51      | 110.23   |
| 25  | D     | 410 | DGD  | CBB-CAB-C9B | -2.05 | 103.98      | 114.37   |
| 27  | a     | 412 | LMG  | O2-C2-C1    | -2.05 | 105.18      | 110.08   |
| 24  | c     | 513 | BCR  | C8-C7-C6    | -2.05 | 121.52      | 127.00   |
| 22  | B     | 607 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 27  | E     | 101 | LMG  | O1-C7-C8    | -2.05 | 105.83      | 110.82   |
| 27  | A     | 410 | LMG  | O2-C2-C1    | -2.05 | 105.19      | 110.08   |
| 25  | d     | 410 | DGD  | CAB-C9B-C8B | -2.05 | 104.00      | 114.37   |
| 27  | d     | 412 | LMG  | O2-C2-C1    | -2.05 | 105.19      | 110.08   |
| 24  | B     | 618 | BCR  | C33-C5-C6   | -2.05 | 122.25      | 124.48   |
| 29  | A     | 413 | SQD  | C1-O5-C5    | 2.05  | 117.72      | 113.72   |
| 34  | V     | 201 | HEM  | C2A-C1A-NA  | -2.05 | 107.88      | 110.15   |
| 24  | B     | 616 | BCR  | C7-C8-C9    | -2.05 | 123.21      | 126.23   |
| 24  | b     | 622 | BCR  | C20-C21-C22 | -2.05 | 124.41      | 127.28   |
| 25  | b     | 624 | DGD  | CAB-C9B-C8B | -2.05 | 104.02      | 114.37   |
| 25  | d     | 410 | DGD  | CBB-CAB-C9B | -2.05 | 104.03      | 114.37   |
| 27  | E     | 101 | LMG  | O3-C3-C2    | -2.05 | 105.56      | 110.38   |
| 27  | B     | 621 | LMG  | O2-C2-C1    | -2.04 | 105.20      | 110.08   |
| 27  | a     | 402 | LMG  | O2-C2-C1    | -2.04 | 105.21      | 110.08   |
| 31  | d     | 401 | PHO  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 24  | b     | 623 | BCR  | C15-C16-C17 | -2.04 | 119.34      | 123.52   |
| 31  | D     | 401 | PHO  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 24  | C     | 513 | BCR  | C8-C7-C6    | -2.04 | 121.55      | 127.00   |
| 22  | A     | 403 | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 27  | M     | 101 | LMG  | O3-C3-C2    | -2.04 | 105.57      | 110.38   |
| 27  | A     | 414 | LMG  | O1-C7-C8    | -2.04 | 105.86      | 110.82   |
| 25  | c     | 517 | DGD  | C5B-C4B-C3B | -2.04 | 104.08      | 114.37   |
| 25  | C     | 517 | DGD  | C5B-C4B-C3B | -2.03 | 104.08      | 114.37   |
| 25  | B     | 620 | DGD  | C5B-C4B-C3B | -2.03 | 104.09      | 114.37   |
| 22  | b     | 613 | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 23  | j     | 101 | PL9  | C12-C13-C14 | -2.03 | 122.97      | 127.62   |
| 24  | f     | 102 | BCR  | C7-C8-C9    | -2.03 | 123.23      | 126.23   |
| 27  | e     | 101 | LMG  | O7-C10-O9   | -2.03 | 118.96      | 123.70   |
| 25  | C     | 516 | DGD  | C5B-C4B-C3B | -2.03 | 104.12      | 114.37   |
| 25  | c     | 515 | DGD  | O5D-C6D-C5D | -2.03 | 104.85      | 109.42   |
| 24  | A     | 407 | BCR  | C11-C10-C9  | -2.03 | 124.44      | 127.28   |
| 24  | b     | 622 | BCR  | C29-C28-C27 | 2.02  | 115.73      | 111.28   |
| 25  | A     | 408 | DGD  | C5B-C4B-C3B | -2.02 | 104.14      | 114.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | D     | 408 | LMG  | O7-C10-O9   | -2.02 | 118.98      | 123.70   |
| 24  | b     | 621 | BCR  | C35-C13-C14 | -2.02 | 119.54      | 122.82   |
| 22  | C     | 510 | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 22  | b     | 605 | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 22  | c     | 505 | CLA  | C1-C2-C3    | -2.02 | 122.89      | 126.20   |
| 25  | a     | 410 | DGD  | C5B-C4B-C3B | -2.02 | 104.15      | 114.37   |
| 22  | A     | 402 | CLA  | C1-C2-C3    | -2.02 | 122.89      | 126.20   |
| 25  | B     | 620 | DGD  | CAB-C9B-C8B | -2.02 | 104.16      | 114.37   |
| 22  | B     | 615 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 24  | g     | 101 | BCR  | C24-C23-C22 | -2.02 | 123.25      | 126.23   |
| 22  | C     | 509 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 27  | m     | 101 | LMG  | O3-C3-C2    | -2.02 | 105.62      | 110.38   |
| 24  | c     | 521 | BCR  | C7-C8-C9    | -2.02 | 123.25      | 126.23   |
| 23  | J     | 101 | PL9  | C12-C13-C14 | -2.02 | 123.01      | 127.62   |
| 27  | D     | 412 | LMG  | O2-C2-C1    | -2.01 | 105.28      | 110.08   |
| 22  | a     | 407 | CLA  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 24  | H     | 102 | BCR  | C15-C16-C17 | -2.01 | 119.40      | 123.52   |
| 24  | y     | 101 | BCR  | C24-C23-C22 | -2.01 | 123.26      | 126.23   |
| 22  | A     | 404 | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 34  | v     | 201 | HEM  | C3B-C2B-C1B | 2.01  | 107.92      | 106.41   |
| 22  | a     | 404 | CLA  | O1D-CGD-CBD | 2.01  | 128.48      | 124.52   |
| 22  | a     | 404 | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 23  | j     | 101 | PL9  | O1-C4-C3    | -2.01 | 118.61      | 120.73   |
| 27  | a     | 402 | LMG  | O7-C10-O9   | -2.01 | 119.01      | 123.70   |
| 25  | b     | 624 | DGD  | C5B-C4B-C3B | -2.01 | 104.22      | 114.37   |
| 34  | V     | 201 | HEM  | C1B-NB-C4B  | 2.01  | 107.58      | 105.21   |
| 27  | A     | 410 | LMG  | O1-C1-C2    | -2.01 | 105.23      | 108.27   |
| 27  | d     | 408 | LMG  | O7-C10-O9   | -2.00 | 119.02      | 123.70   |
| 25  | B     | 620 | DGD  | CDB-CCB-CBB | -2.00 | 99.84       | 113.36   |
| 24  | c     | 514 | BCR  | C7-C8-C9    | -2.00 | 123.27      | 126.23   |
| 22  | B     | 613 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |

All (69) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | A     | 402 | CLA  | ND   |
| 22  | A     | 403 | CLA  | ND   |
| 22  | A     | 404 | CLA  | ND   |
| 22  | A     | 405 | CLA  | ND   |
| 22  | B     | 601 | CLA  | ND   |
| 22  | B     | 602 | CLA  | ND   |
| 22  | B     | 603 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | B     | 604 | CLA  | ND   |
| 22  | B     | 605 | CLA  | ND   |
| 22  | B     | 606 | CLA  | ND   |
| 22  | B     | 607 | CLA  | ND   |
| 22  | B     | 608 | CLA  | ND   |
| 22  | B     | 609 | CLA  | ND   |
| 22  | B     | 610 | CLA  | ND   |
| 22  | B     | 611 | CLA  | ND   |
| 22  | B     | 612 | CLA  | ND   |
| 22  | B     | 613 | CLA  | ND   |
| 22  | B     | 614 | CLA  | ND   |
| 22  | B     | 615 | CLA  | ND   |
| 22  | C     | 501 | CLA  | ND   |
| 22  | C     | 502 | CLA  | ND   |
| 22  | C     | 503 | CLA  | ND   |
| 22  | C     | 504 | CLA  | ND   |
| 22  | C     | 505 | CLA  | ND   |
| 22  | C     | 506 | CLA  | ND   |
| 22  | C     | 507 | CLA  | ND   |
| 22  | C     | 508 | CLA  | ND   |
| 22  | C     | 509 | CLA  | ND   |
| 22  | C     | 510 | CLA  | ND   |
| 22  | C     | 511 | CLA  | ND   |
| 22  | C     | 512 | CLA  | ND   |
| 22  | C     | 520 | CLA  | ND   |
| 22  | D     | 405 | CLA  | ND   |
| 22  | H     | 101 | CLA  | ND   |
| 22  | a     | 404 | CLA  | ND   |
| 22  | a     | 405 | CLA  | ND   |
| 22  | a     | 406 | CLA  | ND   |
| 22  | a     | 407 | CLA  | ND   |
| 22  | b     | 605 | CLA  | ND   |
| 22  | b     | 606 | CLA  | ND   |
| 22  | b     | 607 | CLA  | ND   |
| 22  | b     | 608 | CLA  | ND   |
| 22  | b     | 609 | CLA  | ND   |
| 22  | b     | 610 | CLA  | ND   |
| 22  | b     | 611 | CLA  | ND   |
| 22  | b     | 612 | CLA  | ND   |
| 22  | b     | 613 | CLA  | ND   |
| 22  | b     | 614 | CLA  | ND   |
| 22  | b     | 615 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | b     | 616 | CLA  | ND   |
| 22  | b     | 617 | CLA  | ND   |
| 22  | b     | 618 | CLA  | ND   |
| 22  | b     | 619 | CLA  | ND   |
| 22  | c     | 501 | CLA  | ND   |
| 22  | c     | 502 | CLA  | ND   |
| 22  | c     | 503 | CLA  | ND   |
| 22  | c     | 504 | CLA  | ND   |
| 22  | c     | 505 | CLA  | ND   |
| 22  | c     | 506 | CLA  | ND   |
| 22  | c     | 507 | CLA  | ND   |
| 22  | c     | 508 | CLA  | ND   |
| 22  | c     | 509 | CLA  | ND   |
| 22  | c     | 510 | CLA  | ND   |
| 22  | c     | 511 | CLA  | ND   |
| 22  | c     | 512 | CLA  | ND   |
| 22  | c     | 520 | CLA  | ND   |
| 22  | d     | 405 | CLA  | ND   |
| 22  | d     | 406 | CLA  | ND   |
| 22  | h     | 101 | CLA  | ND   |

All (2091) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 402 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 403 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 404 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 601 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 604 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 605 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 605 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 606 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 606 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 607 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 608 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 608 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 609 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 609 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 609 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 610 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 610 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 613 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 613 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 615 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 615 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 615 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 504 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 504 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 504 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 508 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 509 | CLA  | C2B-C3B-CAB-CBB |
| 22  | C     | 509 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 511 | CLA  | C1A-C2A-CAA-CBA |
| 22  | D     | 405 | CLA  | C1A-C2A-CAA-CBA |
| 22  | H     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 22  | H     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 22  | H     | 101 | CLA  | C6-C7-C8-C9     |
| 22  | a     | 404 | CLA  | CBD-CGD-O2D-CED |
| 22  | a     | 405 | CLA  | C1A-C2A-CAA-CBA |
| 22  | a     | 406 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 605 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 606 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 607 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 608 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 610 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 610 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 611 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 612 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 612 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 613 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 613 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 614 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 614 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 617 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 617 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 619 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 619 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 619 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 504 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 504 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 504 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 508 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 508 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 509 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 509 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 510 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 511 | CLA  | C1A-C2A-CAA-CBA |
| 22  | d     | 405 | CLA  | C2-C3-C5-C6     |
| 22  | d     | 405 | CLA  | C4-C3-C5-C6     |
| 22  | h     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 22  | h     | 101 | CLA  | C6-C7-C8-C9     |
| 23  | A     | 406 | PL9  | C7-C8-C9-C10    |
| 23  | A     | 406 | PL9  | C7-C8-C9-C11    |
| 23  | A     | 406 | PL9  | C12-C13-C14-C15 |
| 23  | A     | 406 | PL9  | C12-C13-C14-C16 |
| 23  | A     | 406 | PL9  | C17-C18-C19-C21 |
| 23  | A     | 406 | PL9  | C22-C23-C24-C25 |
| 23  | A     | 406 | PL9  | C27-C28-C29-C30 |
| 23  | A     | 406 | PL9  | C27-C28-C29-C31 |
| 23  | A     | 406 | PL9  | C37-C38-C39-C40 |
| 23  | A     | 406 | PL9  | C37-C38-C39-C41 |
| 23  | D     | 407 | PL9  | C27-C28-C29-C31 |
| 23  | D     | 407 | PL9  | C34-C36-C37-C38 |
| 23  | J     | 101 | PL9  | C12-C13-C14-C16 |
| 23  | J     | 101 | PL9  | C22-C23-C24-C25 |
| 23  | J     | 101 | PL9  | C22-C23-C24-C26 |
| 23  | a     | 408 | PL9  | C7-C8-C9-C11    |
| 23  | a     | 408 | PL9  | C12-C13-C14-C15 |
| 23  | a     | 408 | PL9  | C12-C13-C14-C16 |
| 23  | a     | 408 | PL9  | C17-C18-C19-C21 |
| 23  | a     | 408 | PL9  | C22-C23-C24-C25 |
| 23  | a     | 408 | PL9  | C27-C28-C29-C30 |
| 23  | a     | 408 | PL9  | C27-C28-C29-C31 |
| 23  | a     | 408 | PL9  | C37-C38-C39-C41 |
| 23  | d     | 407 | PL9  | C27-C28-C29-C31 |
| 23  | d     | 407 | PL9  | C34-C36-C37-C38 |
| 23  | j     | 101 | PL9  | C12-C13-C14-C16 |
| 23  | j     | 101 | PL9  | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | j     | 101 | PL9  | C22-C23-C24-C26 |
| 24  | B     | 617 | BCR  | C21-C22-C23-C24 |
| 24  | B     | 617 | BCR  | C23-C24-C25-C26 |
| 24  | C     | 513 | BCR  | C6-C7-C8-C9     |
| 24  | F     | 102 | BCR  | C7-C8-C9-C10    |
| 24  | H     | 102 | BCR  | C21-C22-C23-C24 |
| 24  | J     | 102 | BCR  | C21-C22-C23-C24 |
| 24  | K     | 102 | BCR  | C7-C8-C9-C10    |
| 24  | K     | 102 | BCR  | C7-C8-C9-C34    |
| 24  | y     | 101 | BCR  | C7-C8-C9-C10    |
| 24  | b     | 621 | BCR  | C21-C22-C23-C24 |
| 24  | b     | 621 | BCR  | C23-C24-C25-C26 |
| 24  | c     | 513 | BCR  | C6-C7-C8-C9     |
| 24  | c     | 521 | BCR  | C7-C8-C9-C10    |
| 24  | c     | 521 | BCR  | C7-C8-C9-C34    |
| 24  | f     | 102 | BCR  | C7-C8-C9-C10    |
| 24  | j     | 102 | BCR  | C21-C22-C23-C24 |
| 24  | g     | 101 | BCR  | C7-C8-C9-C10    |
| 24  | x     | 101 | BCR  | C21-C22-C23-C24 |
| 25  | A     | 408 | DGD  | C2D-C1D-O3G-C3G |
| 25  | B     | 620 | DGD  | C2E-C1E-O5D-C6D |
| 25  | B     | 625 | DGD  | O1B-C1B-O2G-C2G |
| 25  | B     | 625 | DGD  | O2G-C2G-C3G-O3G |
| 25  | B     | 625 | DGD  | C2E-C1E-O5D-C6D |
| 25  | B     | 625 | DGD  | O6E-C1E-O5D-C6D |
| 25  | C     | 515 | DGD  | C2B-C1B-O2G-C2G |
| 25  | C     | 515 | DGD  | O1B-C1B-O2G-C2G |
| 25  | C     | 515 | DGD  | C2E-C1E-O5D-C6D |
| 25  | C     | 516 | DGD  | C2B-C1B-O2G-C2G |
| 25  | C     | 516 | DGD  | O1B-C1B-O2G-C2G |
| 25  | C     | 516 | DGD  | C2D-C1D-O3G-C3G |
| 25  | C     | 517 | DGD  | C2D-C1D-O3G-C3G |
| 25  | C     | 517 | DGD  | O6D-C1D-O3G-C3G |
| 25  | D     | 410 | DGD  | O6D-C1D-O3G-C3G |
| 25  | a     | 410 | DGD  | C2D-C1D-O3G-C3G |
| 25  | b     | 601 | DGD  | O1B-C1B-O2G-C2G |
| 25  | b     | 601 | DGD  | O2G-C2G-C3G-O3G |
| 25  | b     | 601 | DGD  | C2E-C1E-O5D-C6D |
| 25  | b     | 601 | DGD  | O6E-C1E-O5D-C6D |
| 25  | b     | 624 | DGD  | C2E-C1E-O5D-C6D |
| 25  | c     | 515 | DGD  | C2B-C1B-O2G-C2G |
| 25  | c     | 515 | DGD  | O1B-C1B-O2G-C2G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | c     | 515 | DGD  | C2E-C1E-O5D-C6D |
| 25  | c     | 516 | DGD  | O1B-C1B-O2G-C2G |
| 25  | c     | 516 | DGD  | C2D-C1D-O3G-C3G |
| 25  | c     | 517 | DGD  | C2D-C1D-O3G-C3G |
| 25  | c     | 517 | DGD  | O6D-C1D-O3G-C3G |
| 25  | d     | 410 | DGD  | O6D-C1D-O3G-C3G |
| 26  | A     | 409 | LHG  | C1-C2-C3-O3     |
| 26  | C     | 519 | LHG  | C3-O3-P-O6      |
| 26  | C     | 519 | LHG  | C4-O6-P-O3      |
| 26  | C     | 519 | LHG  | C4-O6-P-O4      |
| 26  | a     | 411 | LHG  | C1-C2-C3-O3     |
| 26  | c     | 519 | LHG  | C3-O3-P-O6      |
| 26  | c     | 519 | LHG  | C4-O6-P-O3      |
| 26  | c     | 519 | LHG  | C4-O6-P-O4      |
| 27  | B     | 621 | LMG  | C11-C10-O7-C8   |
| 27  | C     | 518 | LMG  | O9-C10-O7-C8    |
| 27  | C     | 518 | LMG  | C11-C10-O7-C8   |
| 27  | C     | 521 | LMG  | C2-C1-O1-C7     |
| 27  | D     | 408 | LMG  | O1-C7-C8-O7     |
| 27  | D     | 408 | LMG  | C11-C10-O7-C8   |
| 27  | D     | 408 | LMG  | O10-C28-O8-C9   |
| 27  | D     | 409 | LMG  | O6-C1-O1-C7     |
| 27  | D     | 412 | LMG  | O9-C10-O7-C8    |
| 27  | D     | 412 | LMG  | C11-C10-O7-C8   |
| 27  | M     | 101 | LMG  | O9-C10-O7-C8    |
| 27  | b     | 625 | LMG  | C11-C10-O7-C8   |
| 27  | c     | 518 | LMG  | O9-C10-O7-C8    |
| 27  | c     | 518 | LMG  | C11-C10-O7-C8   |
| 27  | d     | 408 | LMG  | O1-C7-C8-O7     |
| 27  | d     | 408 | LMG  | C11-C10-O7-C8   |
| 27  | d     | 409 | LMG  | O6-C1-O1-C7     |
| 27  | d     | 412 | LMG  | O9-C10-O7-C8    |
| 27  | d     | 412 | LMG  | C11-C10-O7-C8   |
| 27  | e     | 101 | LMG  | C7-C8-O7-C10    |
| 27  | m     | 101 | LMG  | O9-C10-O7-C8    |
| 29  | A     | 412 | SQD  | C5-C6-S-O7      |
| 29  | A     | 412 | SQD  | C5-C6-S-O8      |
| 29  | A     | 412 | SQD  | C5-C6-S-O9      |
| 29  | A     | 413 | SQD  | C24-C23-O48-C46 |
| 29  | B     | 622 | SQD  | C2-C1-O6-C44    |
| 29  | B     | 622 | SQD  | O5-C1-O6-C44    |
| 29  | B     | 622 | SQD  | O49-C7-O47-C45  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | B     | 622 | SQD  | C8-C7-O47-C45   |
| 29  | B     | 626 | SQD  | O5-C5-C6-S      |
| 29  | a     | 401 | SQD  | C24-C23-O48-C46 |
| 29  | a     | 415 | SQD  | C5-C6-S-O7      |
| 29  | a     | 415 | SQD  | C5-C6-S-O8      |
| 29  | a     | 415 | SQD  | C5-C6-S-O9      |
| 29  | b     | 602 | SQD  | O5-C5-C6-S      |
| 29  | d     | 403 | SQD  | C2-C1-O6-C44    |
| 29  | d     | 403 | SQD  | O5-C1-O6-C44    |
| 29  | d     | 403 | SQD  | O49-C7-O47-C45  |
| 29  | d     | 403 | SQD  | C8-C7-O47-C45   |
| 22  | C     | 503 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 504 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 619 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 503 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 504 | CLA  | O1D-CGD-O2D-CED |
| 30  | B     | 628 | LMT  | C3'-C4'-O1B-C1B |
| 30  | b     | 604 | LMT  | C3'-C4'-O1B-C1B |
| 22  | A     | 402 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 603 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 615 | CLA  | O1D-CGD-O2D-CED |
| 22  | a     | 404 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 607 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 608 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 501 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 503 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 505 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 507 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 508 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 510 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 520 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 614 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 616 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 617 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 501 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 503 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 505 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 507 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 508 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 520 | CLA  | CBD-CGD-O2D-CED |
| 27  | E     | 101 | LMG  | O10-C28-O8-C9   |
| 29  | A     | 413 | SQD  | O10-C23-O48-C46 |
| 29  | a     | 401 | SQD  | O10-C23-O48-C46 |
| 23  | a     | 408 | PL9  | C37-C38-C39-C40 |
| 27  | C     | 518 | LMG  | C8-C9-O8-C28    |
| 22  | C     | 510 | CLA  | O1D-CGD-O2D-CED |
| 27  | a     | 412 | LMG  | C29-C28-O8-C9   |
| 27  | d     | 409 | LMG  | C29-C28-O8-C9   |
| 29  | F     | 103 | SQD  | C24-C23-O48-C46 |
| 29  | f     | 103 | SQD  | C24-C23-O48-C46 |
| 27  | A     | 410 | LMG  | O10-C28-O8-C9   |
| 27  | C     | 518 | LMG  | O10-C28-O8-C9   |
| 27  | D     | 409 | LMG  | O10-C28-O8-C9   |
| 27  | a     | 412 | LMG  | O10-C28-O8-C9   |
| 27  | c     | 518 | LMG  | O10-C28-O8-C9   |
| 27  | d     | 408 | LMG  | O10-C28-O8-C9   |
| 27  | d     | 409 | LMG  | O10-C28-O8-C9   |
| 27  | e     | 101 | LMG  | O10-C28-O8-C9   |
| 29  | F     | 103 | SQD  | O10-C23-O48-C46 |
| 29  | f     | 103 | SQD  | O10-C23-O48-C46 |
| 22  | B     | 601 | CLA  | O1D-CGD-O2D-CED |
| 30  | B     | 627 | LMT  | C3'-C4'-O1B-C1B |
| 30  | b     | 603 | LMT  | C3'-C4'-O1B-C1B |
| 22  | B     | 604 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 609 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 605 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 608 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 510 | CLA  | O1D-CGD-O2D-CED |
| 25  | D     | 410 | DGD  | O1B-C1B-O2G-C2G |
| 25  | d     | 410 | DGD  | O1B-C1B-O2G-C2G |
| 27  | A     | 414 | LMG  | O9-C10-O7-C8    |
| 27  | B     | 621 | LMG  | O9-C10-O7-C8    |
| 27  | D     | 408 | LMG  | O9-C10-O7-C8    |
| 27  | I     | 101 | LMG  | O9-C10-O7-C8    |
| 27  | a     | 402 | LMG  | O9-C10-O7-C8    |
| 27  | b     | 625 | LMG  | O9-C10-O7-C8    |
| 27  | d     | 408 | LMG  | O9-C10-O7-C8    |
| 27  | i     | 101 | LMG  | O9-C10-O7-C8    |
| 22  | A     | 404 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 607 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 613 | CLA  | C3-C5-C6-C7     |
| 22  | a     | 406 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 611 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 617 | CLA  | C3-C5-C6-C7     |
| 27  | c     | 518 | LMG  | C8-C9-O8-C28    |
| 22  | b     | 613 | CLA  | O1D-CGD-O2D-CED |
| 27  | A     | 410 | LMG  | C29-C28-O8-C9   |
| 27  | C     | 518 | LMG  | C29-C28-O8-C9   |
| 27  | D     | 409 | LMG  | C29-C28-O8-C9   |
| 27  | c     | 518 | LMG  | C29-C28-O8-C9   |
| 27  | I     | 101 | LMG  | O6-C5-C6-O5     |
| 27  | i     | 101 | LMG  | O6-C5-C6-O5     |
| 22  | B     | 605 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 606 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 511 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 609 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 511 | CLA  | CBD-CGD-O2D-CED |
| 31  | D     | 402 | PHO  | CBD-CGD-O2D-CED |
| 31  | d     | 402 | PHO  | CBD-CGD-O2D-CED |
| 25  | B     | 625 | DGD  | C2B-C1B-O2G-C2G |
| 25  | b     | 601 | DGD  | C2B-C1B-O2G-C2G |
| 25  | c     | 516 | DGD  | C2B-C1B-O2G-C2G |
| 27  | M     | 101 | LMG  | C11-C10-O7-C8   |
| 27  | m     | 101 | LMG  | C11-C10-O7-C8   |
| 22  | B     | 612 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 520 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 606 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 616 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 602 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 602 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 604 | CLA  | C4-C3-C5-C6     |
| 22  | D     | 405 | CLA  | C4-C3-C5-C6     |
| 22  | H     | 101 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 606 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 608 | CLA  | C4-C3-C5-C6     |
| 22  | h     | 101 | CLA  | C4-C3-C5-C6     |
| 23  | A     | 406 | PL9  | C30-C29-C31-C32 |
| 23  | a     | 408 | PL9  | C30-C29-C31-C32 |
| 22  | B     | 602 | CLA  | C2-C3-C5-C6     |
| 22  | D     | 405 | CLA  | C2-C3-C5-C6     |
| 22  | H     | 101 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 606 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | h     | 101 | CLA  | C2-C3-C5-C6     |
| 30  | I     | 102 | LMT  | C3'-C4'-O1B-C1B |
| 30  | i     | 102 | LMT  | C3'-C4'-O1B-C1B |
| 22  | c     | 505 | CLA  | O1D-CGD-O2D-CED |
| 25  | A     | 408 | DGD  | O6E-C5E-C6E-O5E |
| 22  | b     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 31  | d     | 401 | PHO  | C3-C5-C6-C7     |
| 25  | D     | 410 | DGD  | C2A-C1A-O1G-C1G |
| 25  | d     | 410 | DGD  | C2A-C1A-O1G-C1G |
| 27  | C     | 521 | LMG  | C29-C28-O8-C9   |
| 27  | D     | 408 | LMG  | C29-C28-O8-C9   |
| 27  | c     | 522 | LMG  | C29-C28-O8-C9   |
| 27  | d     | 408 | LMG  | C29-C28-O8-C9   |
| 23  | A     | 406 | PL9  | C17-C18-C19-C20 |
| 23  | J     | 101 | PL9  | C7-C8-C9-C10    |
| 23  | a     | 408 | PL9  | C7-C8-C9-C10    |
| 23  | a     | 408 | PL9  | C17-C18-C19-C20 |
| 23  | j     | 101 | PL9  | C7-C8-C9-C10    |
| 25  | B     | 620 | DGD  | C4D-C5D-C6D-O5D |
| 25  | b     | 624 | DGD  | C4D-C5D-C6D-O5D |
| 23  | A     | 406 | PL9  | C22-C23-C24-C26 |
| 23  | J     | 101 | PL9  | C7-C8-C9-C11    |
| 23  | a     | 408 | PL9  | C22-C23-C24-C26 |
| 23  | j     | 101 | PL9  | C7-C8-C9-C11    |
| 25  | B     | 620 | DGD  | O6E-C5E-C6E-O5E |
| 25  | a     | 410 | DGD  | O6E-C5E-C6E-O5E |
| 25  | b     | 624 | DGD  | O6E-C5E-C6E-O5E |
| 25  | D     | 410 | DGD  | O1A-C1A-O1G-C1G |
| 25  | d     | 410 | DGD  | O1A-C1A-O1G-C1G |
| 25  | C     | 516 | DGD  | C4E-C5E-C6E-O5E |
| 25  | c     | 516 | DGD  | C4E-C5E-C6E-O5E |
| 22  | C     | 507 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 508 | CLA  | O1D-CGD-O2D-CED |
| 23  | J     | 101 | PL9  | C27-C28-C29-C31 |
| 22  | C     | 508 | CLA  | C3-C5-C6-C7     |
| 31  | D     | 401 | PHO  | C3-C5-C6-C7     |
| 22  | B     | 607 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 512 | CLA  | CBD-CGD-O2D-CED |
| 26  | A     | 409 | LHG  | O2-C2-C3-O3     |
| 26  | a     | 411 | LHG  | O2-C2-C3-O3     |
| 22  | C     | 505 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 508 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 612 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 615 | CLA  | CBA-CGA-O2A-C1  |
| 27  | E     | 101 | LMG  | C29-C28-O8-C9   |
| 27  | e     | 101 | LMG  | C29-C28-O8-C9   |
| 27  | D     | 408 | LMG  | O6-C5-C6-O5     |
| 27  | d     | 408 | LMG  | O6-C5-C6-O5     |
| 27  | C     | 521 | LMG  | O10-C28-O8-C9   |
| 27  | c     | 522 | LMG  | O10-C28-O8-C9   |
| 22  | b     | 610 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 507 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 520 | CLA  | O1D-CGD-O2D-CED |
| 25  | b     | 624 | DGD  | C4E-C5E-C6E-O5E |
| 27  | i     | 101 | LMG  | C4-C5-C6-O5     |
| 25  | D     | 410 | DGD  | C2B-C1B-O2G-C2G |
| 27  | A     | 414 | LMG  | C11-C10-O7-C8   |
| 27  | D     | 409 | LMG  | C11-C10-O7-C8   |
| 27  | a     | 402 | LMG  | C11-C10-O7-C8   |
| 27  | d     | 409 | LMG  | C11-C10-O7-C8   |
| 29  | F     | 103 | SQD  | C8-C7-O47-C45   |
| 29  | f     | 103 | SQD  | C8-C7-O47-C45   |
| 22  | b     | 614 | CLA  | O1D-CGD-O2D-CED |
| 25  | C     | 515 | DGD  | O6E-C5E-C6E-O5E |
| 27  | I     | 101 | LMG  | C4-C5-C6-O5     |
| 23  | j     | 101 | PL9  | C27-C28-C29-C31 |
| 22  | B     | 613 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 501 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 508 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 512 | CLA  | CBD-CGD-O2D-CED |
| 25  | c     | 515 | DGD  | O6E-C5E-C6E-O5E |
| 22  | B     | 608 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 610 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 501 | CLA  | O1D-CGD-O2D-CED |
| 31  | D     | 401 | PHO  | C4-C3-C5-C6     |
| 31  | d     | 401 | PHO  | C4-C3-C5-C6     |
| 31  | D     | 401 | PHO  | C2-C3-C5-C6     |
| 31  | d     | 401 | PHO  | C2-C3-C5-C6     |
| 27  | e     | 101 | LMG  | O9-C10-O7-C8    |
| 23  | A     | 406 | PL9  | C24-C26-C27-C28 |
| 23  | a     | 408 | PL9  | C24-C26-C27-C28 |
| 25  | A     | 408 | DGD  | C4E-C5E-C6E-O5E |
| 22  | B     | 606 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 609 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 617 | CLA  | O1D-CGD-O2D-CED |
| 25  | B     | 620 | DGD  | O6E-C1E-O5D-C6D |
| 25  | C     | 516 | DGD  | O6D-C1D-O3G-C3G |
| 25  | b     | 624 | DGD  | O6E-C1E-O5D-C6D |
| 25  | c     | 515 | DGD  | O6E-C1E-O5D-C6D |
| 25  | c     | 516 | DGD  | O6D-C1D-O3G-C3G |
| 27  | C     | 518 | LMG  | O6-C1-O1-C7     |
| 27  | C     | 521 | LMG  | O6-C1-O1-C7     |
| 27  | E     | 101 | LMG  | O6-C1-O1-C7     |
| 27  | a     | 402 | LMG  | O6-C1-O1-C7     |
| 27  | c     | 518 | LMG  | O6-C1-O1-C7     |
| 27  | c     | 522 | LMG  | O6-C1-O1-C7     |
| 27  | e     | 101 | LMG  | O6-C1-O1-C7     |
| 25  | B     | 620 | DGD  | C4E-C5E-C6E-O5E |
| 22  | c     | 512 | CLA  | CBA-CGA-O2A-C1  |
| 31  | d     | 401 | PHO  | CBA-CGA-O2A-C1  |
| 22  | B     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 615 | CLA  | CBD-CGD-O2D-CED |
| 25  | C     | 516 | DGD  | O6E-C5E-C6E-O5E |
| 27  | C     | 518 | LMG  | O6-C5-C6-O5     |
| 22  | B     | 615 | CLA  | O1A-CGA-O2A-C1  |
| 25  | c     | 516 | DGD  | O6E-C5E-C6E-O5E |
| 27  | c     | 518 | LMG  | O6-C5-C6-O5     |
| 25  | d     | 410 | DGD  | C2B-C1B-O2G-C2G |
| 27  | i     | 101 | LMG  | C11-C10-O7-C8   |
| 25  | a     | 410 | DGD  | C4E-C5E-C6E-O5E |
| 27  | C     | 518 | LMG  | C4-C5-C6-O5     |
| 31  | d     | 401 | PHO  | O1A-CGA-O2A-C1  |
| 22  | C     | 512 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 619 | CLA  | CBA-CGA-O2A-C1  |
| 31  | D     | 401 | PHO  | CBA-CGA-O2A-C1  |
| 22  | C     | 509 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 606 | CLA  | O1D-CGD-O2D-CED |
| 27  | c     | 522 | LMG  | O6-C5-C6-O5     |
| 25  | C     | 515 | DGD  | C4E-C5E-C6E-O5E |
| 22  | B     | 604 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 608 | CLA  | C2-C3-C5-C6     |
| 22  | h     | 101 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 607 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 609 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 508 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 510 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 611 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 613 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 508 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 510 | CLA  | C6-C7-C8-C9     |
| 27  | c     | 518 | LMG  | C4-C5-C6-O5     |
| 27  | c     | 522 | LMG  | C4-C5-C6-O5     |
| 27  | C     | 518 | LMG  | C2-C1-O1-C7     |
| 27  | D     | 409 | LMG  | C2-C1-O1-C7     |
| 27  | E     | 101 | LMG  | C2-C1-O1-C7     |
| 27  | c     | 518 | LMG  | C2-C1-O1-C7     |
| 27  | c     | 522 | LMG  | C2-C1-O1-C7     |
| 27  | d     | 409 | LMG  | C2-C1-O1-C7     |
| 27  | e     | 101 | LMG  | C2-C1-O1-C7     |
| 29  | A     | 412 | SQD  | C2-C1-O6-C44    |
| 29  | a     | 415 | SQD  | C2-C1-O6-C44    |
| 27  | C     | 518 | LMG  | C10-C11-C12-C13 |
| 31  | D     | 401 | PHO  | O1A-CGA-O2A-C1  |
| 31  | d     | 402 | PHO  | O1D-CGD-O2D-CED |
| 24  | H     | 102 | BCR  | C7-C8-C9-C34    |
| 24  | H     | 102 | BCR  | C37-C22-C23-C24 |
| 24  | y     | 101 | BCR  | C7-C8-C9-C34    |
| 24  | g     | 101 | BCR  | C7-C8-C9-C34    |
| 24  | x     | 101 | BCR  | C7-C8-C9-C34    |
| 24  | x     | 101 | BCR  | C37-C22-C23-C24 |
| 24  | B     | 617 | BCR  | C7-C8-C9-C10    |
| 24  | b     | 621 | BCR  | C7-C8-C9-C10    |
| 34  | V     | 201 | HEM  | C2D-C3D-CAD-CBD |
| 25  | c     | 515 | DGD  | C4E-C5E-C6E-O5E |
| 22  | b     | 619 | CLA  | O1A-CGA-O2A-C1  |
| 29  | b     | 602 | SQD  | O10-C23-O48-C46 |
| 22  | H     | 101 | CLA  | C3-C5-C6-C7     |
| 27  | E     | 101 | LMG  | O9-C10-O7-C8    |
| 27  | I     | 101 | LMG  | C11-C10-O7-C8   |
| 27  | c     | 522 | LMG  | C11-C10-O7-C8   |
| 25  | C     | 516 | DGD  | O2G-C2G-C3G-O3G |
| 25  | c     | 516 | DGD  | O2G-C2G-C3G-O3G |
| 27  | m     | 101 | LMG  | O1-C7-C8-O7     |
| 27  | d     | 408 | LMG  | C4-C5-C6-O5     |
| 22  | c     | 511 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 605 | CLA  | O1D-CGD-O2D-CED |
| 23  | D     | 407 | PL9  | C27-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 404 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 608 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 611 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 615 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 508 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 612 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 615 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 609 | CLA  | O1D-CGD-O2D-CED |
| 22  | c     | 511 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 615 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 619 | CLA  | C5-C6-C7-C8     |
| 25  | d     | 410 | DGD  | C1B-C2B-C3B-C4B |
| 27  | C     | 521 | LMG  | C10-C11-C12-C13 |
| 27  | c     | 522 | LMG  | C10-C11-C12-C13 |
| 25  | C     | 517 | DGD  | O1B-C1B-O2G-C2G |
| 23  | D     | 407 | PL9  | C29-C31-C32-C33 |
| 23  | d     | 407 | PL9  | C29-C31-C32-C33 |
| 22  | A     | 402 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 611 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 610 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 508 | CLA  | C5-C6-C7-C8     |
| 31  | d     | 402 | PHO  | C15-C16-C17-C18 |
| 25  | D     | 410 | DGD  | C1B-C2B-C3B-C4B |
| 25  | c     | 515 | DGD  | C1B-C2B-C3B-C4B |
| 27  | A     | 414 | LMG  | C28-C29-C30-C31 |
| 27  | D     | 412 | LMG  | C10-C11-C12-C13 |
| 27  | c     | 518 | LMG  | C10-C11-C12-C13 |
| 27  | d     | 412 | LMG  | C10-C11-C12-C13 |
| 29  | B     | 626 | SQD  | O10-C23-O48-C46 |
| 22  | c     | 509 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 606 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 520 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 520 | CLA  | C15-C16-C17-C18 |
| 22  | D     | 405 | CLA  | C15-C16-C17-C18 |
| 22  | a     | 406 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 613 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 619 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 507 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 511 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 507 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 511 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 501 | CLA  | C8-C10-C11-C12  |
| 22  | D     | 405 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 505 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 507 | CLA  | C15-C16-C17-C18 |
| 25  | C     | 515 | DGD  | C1B-C2B-C3B-C4B |
| 27  | C     | 518 | LMG  | C28-C29-C30-C31 |
| 27  | c     | 518 | LMG  | C28-C29-C30-C31 |
| 22  | C     | 511 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 22  | a     | 404 | CLA  | C3-C5-C6-C7     |
| 25  | C     | 515 | DGD  | O6E-C1E-O5D-C6D |
| 27  | A     | 414 | LMG  | O6-C1-O1-C7     |
| 27  | I     | 101 | LMG  | O6-C1-O1-C7     |
| 27  | i     | 101 | LMG  | O6-C1-O1-C7     |
| 29  | A     | 412 | SQD  | O5-C1-O6-C44    |
| 29  | a     | 415 | SQD  | O5-C1-O6-C44    |
| 31  | D     | 402 | PHO  | O1D-CGD-O2D-CED |
| 22  | B     | 603 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 606 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 609 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 615 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 503 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 505 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 507 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 509 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 607 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 501 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 503 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 505 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 509 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 520 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 520 | CLA  | C15-C16-C17-C18 |
| 22  | d     | 405 | CLA  | C13-C15-C16-C17 |
| 22  | d     | 405 | CLA  | C15-C16-C17-C18 |
| 31  | D     | 402 | PHO  | C15-C16-C17-C18 |
| 22  | b     | 608 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 27  | B     | 621 | LMG  | C10-C11-C12-C13 |
| 22  | B     | 601 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 501 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 605 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 610 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 506 | CLA  | C5-C6-C7-C8     |
| 25  | c     | 517 | DGD  | O1B-C1B-O2G-C2G |
| 27  | d     | 409 | LMG  | O9-C10-O7-C8    |
| 27  | D     | 408 | LMG  | C4-C5-C6-O5     |
| 22  | A     | 403 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 404 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 505 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 507 | CLA  | C10-C11-C12-C13 |
| 27  | b     | 625 | LMG  | C10-C11-C12-C13 |
| 22  | C     | 512 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 512 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 614 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 501 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 504 | CLA  | C10-C11-C12-C13 |
| 22  | C     | 511 | CLA  | CBA-CGA-O2A-C1  |
| 27  | i     | 101 | LMG  | C29-C28-O8-C9   |
| 27  | C     | 521 | LMG  | C11-C10-O7-C8   |
| 22  | c     | 511 | CLA  | O1A-CGA-O2A-C1  |
| 25  | b     | 624 | DGD  | C1B-C2B-C3B-C4B |
| 22  | B     | 607 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 505 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 607 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 610 | CLA  | C15-C16-C17-C18 |
| 27  | D     | 409 | LMG  | O9-C10-O7-C8    |
| 27  | c     | 522 | LMG  | O9-C10-O7-C8    |
| 22  | B     | 601 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 605 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 29  | b     | 602 | SQD  | C24-C23-O48-C46 |
| 22  | B     | 615 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 506 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 507 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 510 | CLA  | C5-C6-C7-C8     |
| 22  | a     | 405 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 611 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 618 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 619 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 501 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 510 | CLA  | C5-C6-C7-C8     |
| 27  | a     | 402 | LMG  | C28-C29-C30-C31 |
| 22  | C     | 504 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 611 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 512 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 607 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 612 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 614 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 505 | CLA  | C5-C6-C7-C8     |
| 22  | a     | 406 | CLA  | C15-C16-C17-C18 |
| 27  | I     | 101 | LMG  | C29-C28-O8-C9   |
| 23  | A     | 406 | PL9  | C33-C34-C36-C37 |
| 22  | b     | 619 | CLA  | C3-C5-C6-C7     |
| 27  | d     | 412 | LMG  | O6-C5-C6-O5     |
| 27  | C     | 521 | LMG  | O9-C10-O7-C8    |
| 29  | F     | 103 | SQD  | O49-C7-O47-C45  |
| 25  | D     | 410 | DGD  | C2D-C1D-O3G-C3G |
| 25  | D     | 410 | DGD  | C2E-C1E-O5D-C6D |
| 25  | d     | 410 | DGD  | C2D-C1D-O3G-C3G |
| 25  | d     | 410 | DGD  | C2E-C1E-O5D-C6D |
| 27  | I     | 101 | LMG  | C2-C1-O1-C7     |
| 27  | i     | 101 | LMG  | C2-C1-O1-C7     |
| 30  | b     | 604 | LMT  | O1'-C1-C2-C3    |
| 29  | a     | 415 | SQD  | C7-C8-C9-C10    |
| 24  | B     | 617 | BCR  | C7-C8-C9-C34    |
| 24  | B     | 617 | BCR  | C37-C22-C23-C24 |
| 24  | J     | 102 | BCR  | C37-C22-C23-C24 |
| 24  | b     | 621 | BCR  | C7-C8-C9-C34    |
| 24  | b     | 621 | BCR  | C37-C22-C23-C24 |
| 24  | j     | 102 | BCR  | C37-C22-C23-C24 |
| 22  | B     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 520 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 520 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 520 | CLA  | C10-C11-C12-C13 |
| 27  | C     | 518 | LMG  | C9-C8-O7-C10    |
| 22  | b     | 608 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 615 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 509 | CLA  | C3-C5-C6-C7     |
| 34  | V     | 201 | HEM  | C4D-C3D-CAD-CBD |
| 24  | H     | 102 | BCR  | C11-C10-C9-C8   |
| 24  | j     | 102 | BCR  | C20-C21-C22-C23 |
| 24  | x     | 101 | BCR  | C11-C10-C9-C8   |
| 25  | D     | 410 | DGD  | O6E-C1E-O5D-C6D |
| 27  | D     | 408 | LMG  | O6-C1-O1-C7     |
| 27  | d     | 408 | LMG  | O6-C1-O1-C7     |
| 22  | b     | 611 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 512 | CLA  | O1D-CGD-O2D-CED |
| 27  | a     | 402 | LMG  | O6-C5-C6-O5     |
| 22  | c     | 520 | CLA  | CBA-CGA-O2A-C1  |
| 29  | B     | 626 | SQD  | C24-C23-O48-C46 |
| 22  | c     | 508 | CLA  | C2-C1-O2A-CGA   |
| 22  | C     | 511 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 501 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 616 | CLA  | C5-C6-C7-C8     |
| 29  | F     | 103 | SQD  | C12-C13-C14-C15 |
| 30  | I     | 102 | LMT  | C6-C7-C8-C9     |
| 30  | B     | 623 | LMT  | C1-C2-C3-C4     |
| 25  | C     | 516 | DGD  | C2A-C3A-C4A-C5A |
| 25  | a     | 410 | DGD  | C8B-C9B-CAB-CBB |
| 25  | b     | 601 | DGD  | C9B-CAB-CBB-CCB |
| 25  | c     | 515 | DGD  | C3B-C4B-C5B-C6B |
| 27  | C     | 518 | LMG  | C29-C30-C31-C32 |
| 27  | b     | 625 | LMG  | C31-C32-C33-C34 |
| 25  | B     | 620 | DGD  | C1B-C2B-C3B-C4B |
| 25  | C     | 515 | DGD  | C3B-C4B-C5B-C6B |
| 25  | b     | 601 | DGD  | C5B-C6B-C7B-C8B |
| 25  | b     | 624 | DGD  | C3B-C4B-C5B-C6B |
| 27  | c     | 522 | LMG  | C12-C13-C14-C15 |
| 30  | i     | 102 | LMT  | C6-C7-C8-C9     |
| 30  | b     | 626 | LMT  | C1-C2-C3-C4     |
| 25  | B     | 620 | DGD  | C6B-C7B-C8B-C9B |
| 25  | B     | 625 | DGD  | C5B-C6B-C7B-C8B |
| 25  | B     | 625 | DGD  | C9B-CAB-CBB-CCB |
| 25  | D     | 410 | DGD  | C4B-C5B-C6B-C7B |
| 25  | D     | 410 | DGD  | CCB-CDB-CEB-CFB |
| 25  | c     | 516 | DGD  | C2A-C3A-C4A-C5A |
| 25  | c     | 516 | DGD  | C4A-C5A-C6A-C7A |
| 27  | A     | 410 | LMG  | C33-C34-C35-C36 |
| 27  | A     | 410 | LMG  | C34-C35-C36-C37 |
| 27  | A     | 414 | LMG  | C30-C31-C32-C33 |
| 27  | B     | 621 | LMG  | C31-C32-C33-C34 |
| 27  | I     | 101 | LMG  | C12-C13-C14-C15 |
| 27  | I     | 101 | LMG  | C14-C15-C16-C17 |
| 27  | a     | 402 | LMG  | C30-C31-C32-C33 |
| 27  | c     | 518 | LMG  | C29-C30-C31-C32 |
| 29  | b     | 602 | SQD  | C11-C10-C9-C8   |
| 29  | f     | 103 | SQD  | C12-C13-C14-C15 |
| 29  | f     | 103 | SQD  | O49-C7-O47-C45  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | D     | 410 | DGD  | C5B-C6B-C7B-C8B |
| 25  | d     | 410 | DGD  | C5B-C6B-C7B-C8B |
| 25  | d     | 410 | DGD  | CCB-CDB-CEB-CFB |
| 27  | i     | 101 | LMG  | C12-C13-C14-C15 |
| 22  | B     | 605 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 501 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 504 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 609 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 501 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 504 | CLA  | C4B-C3B-CAB-CBB |
| 25  | D     | 410 | DGD  | CEB-CFB-CGB-CHB |
| 25  | d     | 410 | DGD  | CEB-CFB-CGB-CHB |
| 27  | a     | 412 | LMG  | C34-C35-C36-C37 |
| 22  | b     | 615 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 605 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 609 | CLA  | C2A-CAA-CBA-CGA |
| 25  | A     | 408 | DGD  | C8B-C9B-CAB-CBB |
| 25  | C     | 515 | DGD  | C3A-C4A-C5A-C6A |
| 27  | D     | 408 | LMG  | C18-C19-C20-C21 |
| 29  | B     | 626 | SQD  | C9-C10-C11-C12  |
| 29  | B     | 626 | SQD  | C8-C7-O47-C45   |
| 29  | b     | 602 | SQD  | C8-C7-O47-C45   |
| 25  | c     | 515 | DGD  | C3A-C4A-C5A-C6A |
| 22  | C     | 503 | CLA  | C11-C12-C13-C15 |
| 22  | D     | 405 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 503 | CLA  | C11-C12-C13-C15 |
| 25  | C     | 515 | DGD  | C2B-C3B-C4B-C5B |
| 25  | b     | 624 | DGD  | C6B-C7B-C8B-C9B |
| 25  | d     | 410 | DGD  | C4B-C5B-C6B-C7B |
| 27  | a     | 412 | LMG  | C33-C34-C35-C36 |
| 25  | C     | 515 | DGD  | C1A-C2A-C3A-C4A |
| 27  | m     | 101 | LMG  | C29-C28-O8-C9   |
| 22  | C     | 503 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 503 | CLA  | C5-C6-C7-C8     |
| 25  | B     | 620 | DGD  | C3B-C4B-C5B-C6B |
| 27  | C     | 521 | LMG  | C12-C13-C14-C15 |
| 27  | i     | 101 | LMG  | C16-C17-C18-C19 |
| 22  | B     | 606 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 607 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 615 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 506 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 511 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | a     | 405 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 611 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 619 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 506 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 511 | CLA  | C3A-C2A-CAA-CBA |
| 22  | h     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 25  | C     | 517 | DGD  | CBA-CCA-CDA-CEA |
| 29  | B     | 626 | SQD  | C11-C10-C9-C8   |
| 23  | a     | 408 | PL9  | C33-C34-C36-C37 |
| 25  | b     | 624 | DGD  | C7A-C8A-C9A-CAA |
| 22  | H     | 101 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 611 | CLA  | O1D-CGD-O2D-CED |
| 25  | c     | 517 | DGD  | C1A-C2A-C3A-C4A |
| 27  | d     | 408 | LMG  | C18-C19-C20-C21 |
| 27  | M     | 101 | LMG  | O6-C5-C6-O5     |
| 27  | a     | 402 | LMG  | C32-C33-C34-C35 |
| 25  | c     | 515 | DGD  | C2B-C3B-C4B-C5B |
| 27  | A     | 414 | LMG  | C15-C16-C17-C18 |
| 27  | D     | 409 | LMG  | C14-C15-C16-C17 |
| 22  | C     | 520 | CLA  | CBA-CGA-O2A-C1  |
| 26  | C     | 519 | LHG  | C24-C23-O8-C6   |
| 25  | d     | 410 | DGD  | C7B-C8B-C9B-CAB |
| 29  | b     | 602 | SQD  | C9-C10-C11-C12  |
| 27  | D     | 408 | LMG  | C28-C29-C30-C31 |
| 25  | B     | 620 | DGD  | C7A-C8A-C9A-CAA |
| 25  | D     | 410 | DGD  | C7B-C8B-C9B-CAB |
| 27  | A     | 414 | LMG  | C18-C19-C20-C21 |
| 27  | D     | 409 | LMG  | C19-C20-C21-C22 |
| 27  | d     | 409 | LMG  | C14-C15-C16-C17 |
| 27  | i     | 101 | LMG  | C14-C15-C16-C17 |
| 29  | A     | 412 | SQD  | C14-C15-C16-C17 |
| 29  | a     | 415 | SQD  | C14-C15-C16-C17 |
| 30  | B     | 628 | LMT  | O1'-C1-C2-C3    |
| 27  | C     | 521 | LMG  | C4-C5-C6-O5     |
| 27  | A     | 410 | LMG  | C30-C31-C32-C33 |
| 27  | D     | 408 | LMG  | C31-C32-C33-C34 |
| 29  | a     | 415 | SQD  | C27-C28-C29-C30 |
| 25  | B     | 620 | DGD  | O6D-C5D-C6D-O5D |
| 25  | b     | 624 | DGD  | O6D-C5D-C6D-O5D |
| 27  | a     | 402 | LMG  | C18-C19-C20-C21 |
| 25  | C     | 516 | DGD  | C4A-C5A-C6A-C7A |
| 25  | c     | 517 | DGD  | CBA-CCA-CDA-CEA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | a     | 402 | LMG  | C15-C16-C17-C18 |
| 25  | B     | 625 | DGD  | C1A-C2A-C3A-C4A |
| 27  | d     | 408 | LMG  | C28-C29-C30-C31 |
| 22  | A     | 404 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 606 | CLA  | C2B-C3B-CAB-CBB |
| 22  | a     | 406 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 610 | CLA  | C2B-C3B-CAB-CBB |
| 24  | B     | 617 | BCR  | C23-C24-C25-C30 |
| 24  | C     | 514 | BCR  | C23-C24-C25-C26 |
| 24  | C     | 514 | BCR  | C23-C24-C25-C30 |
| 24  | H     | 102 | BCR  | C1-C6-C7-C8     |
| 24  | H     | 102 | BCR  | C5-C6-C7-C8     |
| 24  | y     | 101 | BCR  | C23-C24-C25-C26 |
| 24  | y     | 101 | BCR  | C23-C24-C25-C30 |
| 24  | b     | 621 | BCR  | C23-C24-C25-C30 |
| 24  | c     | 513 | BCR  | C1-C6-C7-C8     |
| 24  | c     | 514 | BCR  | C23-C24-C25-C26 |
| 24  | c     | 514 | BCR  | C23-C24-C25-C30 |
| 24  | g     | 101 | BCR  | C23-C24-C25-C26 |
| 24  | g     | 101 | BCR  | C23-C24-C25-C30 |
| 24  | x     | 101 | BCR  | C1-C6-C7-C8     |
| 24  | x     | 101 | BCR  | C5-C6-C7-C8     |
| 27  | a     | 412 | LMG  | C30-C31-C32-C33 |
| 25  | c     | 517 | DGD  | C2B-C1B-O2G-C2G |
| 22  | a     | 407 | CLA  | C10-C11-C12-C13 |
| 25  | C     | 517 | DGD  | C9B-CAB-CBB-CCB |
| 27  | I     | 101 | LMG  | C16-C17-C18-C19 |
| 27  | a     | 412 | LMG  | C31-C32-C33-C34 |
| 29  | F     | 103 | SQD  | C11-C12-C13-C14 |
| 29  | A     | 412 | SQD  | C27-C28-C29-C30 |
| 22  | A     | 402 | CLA  | C2A-CAA-CBA-CGA |
| 22  | a     | 404 | CLA  | C2A-CAA-CBA-CGA |
| 27  | E     | 101 | LMG  | C28-C29-C30-C31 |
| 27  | A     | 410 | LMG  | C31-C32-C33-C34 |
| 27  | A     | 414 | LMG  | C32-C33-C34-C35 |
| 22  | c     | 520 | CLA  | O1A-CGA-O2A-C1  |
| 27  | d     | 408 | LMG  | C31-C32-C33-C34 |
| 29  | f     | 103 | SQD  | C11-C12-C13-C14 |
| 26  | A     | 409 | LHG  | O9-C7-O7-C5     |
| 25  | a     | 410 | DGD  | C5B-C6B-C7B-C8B |
| 25  | b     | 624 | DGD  | C4B-C5B-C6B-C7B |
| 25  | c     | 517 | DGD  | CAB-CBB-CCB-CDB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 612 | CLA  | C16-C17-C18-C19 |
| 25  | B     | 625 | DGD  | C2B-C3B-C4B-C5B |
| 25  | c     | 517 | DGD  | C9B-CAB-CBB-CCB |
| 27  | d     | 409 | LMG  | C19-C20-C21-C22 |
| 25  | c     | 515 | DGD  | C1A-C2A-C3A-C4A |
| 29  | A     | 412 | SQD  | C7-C8-C9-C10    |
| 22  | b     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 508 | CLA  | CBA-CGA-O2A-C1  |
| 27  | M     | 101 | LMG  | C29-C28-O8-C9   |
| 22  | a     | 405 | CLA  | C3-C5-C6-C7     |
| 27  | D     | 412 | LMG  | C17-C18-C19-C20 |
| 25  | A     | 408 | DGD  | C5B-C6B-C7B-C8B |
| 25  | C     | 515 | DGD  | C4A-C5A-C6A-C7A |
| 25  | d     | 410 | DGD  | O6E-C1E-O5D-C6D |
| 22  | B     | 603 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 511 | CLA  | C13-C15-C16-C17 |
| 22  | h     | 101 | CLA  | C5-C6-C7-C8     |
| 27  | D     | 412 | LMG  | O6-C5-C6-O5     |
| 25  | b     | 601 | DGD  | C4A-C5A-C6A-C7A |
| 25  | c     | 515 | DGD  | C4A-C5A-C6A-C7A |
| 27  | c     | 518 | LMG  | C12-C13-C14-C15 |
| 25  | C     | 517 | DGD  | CAB-CBB-CCB-CDB |
| 27  | I     | 101 | LMG  | C13-C14-C15-C16 |
| 27  | d     | 409 | LMG  | C15-C16-C17-C18 |
| 26  | c     | 519 | LHG  | C24-C23-O8-C6   |
| 22  | b     | 605 | CLA  | C16-C17-C18-C20 |
| 25  | C     | 517 | DGD  | C2B-C1B-O2G-C2G |
| 26  | A     | 409 | LHG  | C8-C7-O7-C5     |
| 26  | a     | 411 | LHG  | C8-C7-O7-C5     |
| 27  | E     | 101 | LMG  | C11-C10-O7-C8   |
| 27  | e     | 101 | LMG  | C11-C10-O7-C8   |
| 25  | C     | 517 | DGD  | C1A-C2A-C3A-C4A |
| 25  | a     | 410 | DGD  | C1B-C2B-C3B-C4B |
| 27  | C     | 518 | LMG  | C34-C35-C36-C37 |
| 22  | H     | 101 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 607 | CLA  | C8-C10-C11-C12  |
| 27  | C     | 521 | LMG  | O6-C5-C6-O5     |
| 26  | a     | 411 | LHG  | O9-C7-O7-C5     |
| 25  | b     | 601 | DGD  | C2B-C3B-C4B-C5B |
| 27  | c     | 518 | LMG  | C34-C35-C36-C37 |
| 24  | f     | 102 | BCR  | C37-C22-C23-C24 |
| 25  | B     | 625 | DGD  | C4A-C5A-C6A-C7A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 502 | CLA  | C3-C5-C6-C7     |
| 27  | m     | 101 | LMG  | O6-C5-C6-O5     |
| 27  | D     | 409 | LMG  | C8-C7-O1-C1     |
| 27  | d     | 409 | LMG  | C8-C7-O1-C1     |
| 30  | B     | 628 | LMT  | C7-C8-C9-C10    |
| 22  | C     | 520 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 612 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 605 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 616 | CLA  | C16-C17-C18-C19 |
| 26  | a     | 411 | LHG  | C25-C26-C27-C28 |
| 27  | a     | 412 | LMG  | C14-C15-C16-C17 |
| 27  | m     | 101 | LMG  | C29-C30-C31-C32 |
| 23  | j     | 101 | PL9  | C15-C14-C16-C17 |
| 27  | i     | 101 | LMG  | C13-C14-C15-C16 |
| 29  | F     | 103 | SQD  | C10-C11-C12-C13 |
| 22  | A     | 405 | CLA  | C10-C11-C12-C13 |
| 22  | h     | 101 | CLA  | C13-C15-C16-C17 |
| 25  | D     | 410 | DGD  | C6B-C7B-C8B-C9B |
| 29  | b     | 602 | SQD  | C11-C12-C13-C14 |
| 25  | A     | 408 | DGD  | C1B-C2B-C3B-C4B |
| 27  | e     | 101 | LMG  | C28-C29-C30-C31 |
| 25  | B     | 620 | DGD  | C4B-C5B-C6B-C7B |
| 25  | d     | 410 | DGD  | C5A-C6A-C7A-C8A |
| 22  | c     | 512 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 616 | CLA  | C16-C17-C18-C20 |
| 25  | b     | 624 | DGD  | C5B-C6B-C7B-C8B |
| 26  | a     | 411 | LHG  | C30-C31-C32-C33 |
| 27  | D     | 409 | LMG  | C32-C33-C34-C35 |
| 27  | d     | 409 | LMG  | C32-C33-C34-C35 |
| 22  | C     | 520 | CLA  | O1A-CGA-O2A-C1  |
| 25  | D     | 410 | DGD  | C5A-C6A-C7A-C8A |
| 30  | b     | 604 | LMT  | C7-C8-C9-C10    |
| 25  | c     | 516 | DGD  | C1A-C2A-C3A-C4A |
| 22  | C     | 505 | CLA  | C10-C11-C12-C13 |
| 26  | A     | 409 | LHG  | C30-C31-C32-C33 |
| 27  | d     | 412 | LMG  | C34-C35-C36-C37 |
| 27  | e     | 101 | LMG  | O6-C5-C6-O5     |
| 27  | A     | 410 | LMG  | O1-C7-C8-O7     |
| 27  | I     | 101 | LMG  | O1-C7-C8-O7     |
| 27  | M     | 101 | LMG  | O1-C7-C8-O7     |
| 27  | i     | 101 | LMG  | O1-C7-C8-O7     |
| 29  | A     | 412 | SQD  | O47-C45-C46-O48 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | A     | 413 | SQD  | O6-C44-C45-O47  |
| 29  | a     | 401 | SQD  | O6-C44-C45-O47  |
| 29  | a     | 415 | SQD  | O47-C45-C46-O48 |
| 27  | A     | 410 | LMG  | C14-C15-C16-C17 |
| 27  | D     | 408 | LMG  | C30-C31-C32-C33 |
| 27  | D     | 409 | LMG  | C15-C16-C17-C18 |
| 29  | f     | 103 | SQD  | C10-C11-C12-C13 |
| 30  | B     | 623 | LMT  | O1'-C1-C2-C3    |
| 27  | C     | 518 | LMG  | C12-C13-C14-C15 |
| 22  | C     | 512 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 505 | CLA  | C10-C11-C12-C13 |
| 22  | d     | 406 | CLA  | C15-C16-C17-C18 |
| 27  | A     | 414 | LMG  | O6-C5-C6-O5     |
| 25  | B     | 620 | DGD  | C5B-C6B-C7B-C8B |
| 25  | c     | 516 | DGD  | CAB-CBB-CCB-CDB |
| 26  | A     | 409 | LHG  | C25-C26-C27-C28 |
| 27  | c     | 518 | LMG  | C36-C37-C38-C39 |
| 27  | d     | 408 | LMG  | C36-C37-C38-C39 |
| 27  | E     | 101 | LMG  | C15-C16-C17-C18 |
| 27  | d     | 408 | LMG  | C30-C31-C32-C33 |
| 27  | e     | 101 | LMG  | C15-C16-C17-C18 |
| 29  | B     | 622 | SQD  | C9-C10-C11-C12  |
| 29  | B     | 626 | SQD  | C11-C12-C13-C14 |
| 22  | c     | 509 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 509 | CLA  | C3-C5-C6-C7     |
| 25  | C     | 516 | DGD  | CAB-CBB-CCB-CDB |
| 27  | D     | 412 | LMG  | C34-C35-C36-C37 |
| 29  | d     | 403 | SQD  | C9-C10-C11-C12  |
| 22  | c     | 501 | CLA  | C2A-CAA-CBA-CGA |
| 27  | M     | 101 | LMG  | C29-C30-C31-C32 |
| 22  | D     | 406 | CLA  | C15-C16-C17-C18 |
| 23  | D     | 407 | PL9  | C47-C48-C49-C51 |
| 23  | d     | 407 | PL9  | C47-C48-C49-C51 |
| 22  | c     | 506 | CLA  | CBD-CGD-O2D-CED |
| 25  | D     | 410 | DGD  | C3A-C4A-C5A-C6A |
| 25  | d     | 410 | DGD  | C6B-C7B-C8B-C9B |
| 27  | A     | 414 | LMG  | C31-C32-C33-C34 |
| 27  | B     | 621 | LMG  | C34-C35-C36-C37 |
| 27  | C     | 518 | LMG  | C36-C37-C38-C39 |
| 22  | c     | 508 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 502 | CLA  | C3-C5-C6-C7     |
| 26  | c     | 519 | LHG  | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | d     | 412 | LMG  | C17-C18-C19-C20 |
| 27  | D     | 409 | LMG  | C13-C14-C15-C16 |
| 22  | B     | 615 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 501 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 506 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 619 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 501 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 506 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 605 | CLA  | C10-C11-C12-C13 |
| 25  | C     | 515 | DGD  | C2A-C3A-C4A-C5A |
| 30  | I     | 102 | LMT  | C5'-C4'-O1B-C1B |
| 30  | i     | 102 | LMT  | C5'-C4'-O1B-C1B |
| 22  | B     | 603 | CLA  | C15-C16-C17-C18 |
| 27  | E     | 101 | LMG  | O6-C5-C6-O5     |
| 25  | D     | 410 | DGD  | C2A-C3A-C4A-C5A |
| 25  | d     | 410 | DGD  | CAB-CBB-CCB-CDB |
| 25  | b     | 601 | DGD  | C1A-C2A-C3A-C4A |
| 22  | A     | 403 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 605 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 614 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 502 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 503 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 504 | CLA  | C6-C7-C8-C10    |
| 22  | H     | 101 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 618 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 618 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 502 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 503 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 504 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 510 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 510 | CLA  | C12-C13-C15-C16 |
| 22  | d     | 405 | CLA  | C12-C13-C15-C16 |
| 22  | h     | 101 | CLA  | C6-C7-C8-C10    |
| 31  | D     | 402 | PHO  | C12-C13-C15-C16 |
| 31  | d     | 402 | PHO  | C12-C13-C15-C16 |
| 25  | d     | 410 | DGD  | C2A-C3A-C4A-C5A |
| 26  | C     | 519 | LHG  | C24-C25-C26-C27 |
| 22  | B     | 609 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 511 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 509 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 504 | CLA  | CBA-CGA-O2A-C1  |
| 25  | B     | 625 | DGD  | O6D-C5D-C6D-O5D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | C     | 516 | DGD  | C1A-C2A-C3A-C4A |
| 26  | a     | 411 | LHG  | C23-C24-C25-C26 |
| 25  | D     | 410 | DGD  | CAB-CBB-CCB-CDB |
| 25  | d     | 410 | DGD  | C3A-C4A-C5A-C6A |
| 27  | D     | 412 | LMG  | C31-C32-C33-C34 |
| 22  | C     | 509 | CLA  | C4-C3-C5-C6     |
| 22  | c     | 512 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 512 | CLA  | C2-C3-C5-C6     |
| 27  | A     | 410 | LMG  | C15-C16-C17-C18 |
| 22  | b     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 511 | CLA  | C13-C15-C16-C17 |
| 30  | b     | 626 | LMT  | O1'-C1-C2-C3    |
| 22  | C     | 501 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 512 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 402 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 602 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 614 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 502 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 503 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 503 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 504 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 510 | CLA  | C14-C13-C15-C16 |
| 22  | a     | 405 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 606 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 612 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 618 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 502 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 503 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 503 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 505 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 507 | CLA  | C11-C10-C8-C9   |
| 22  | d     | 405 | CLA  | C14-C13-C15-C16 |
| 27  | D     | 408 | LMG  | C17-C18-C19-C20 |
| 29  | B     | 626 | SQD  | C12-C13-C14-C15 |
| 27  | d     | 409 | LMG  | C13-C14-C15-C16 |
| 22  | B     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 504 | CLA  | CBA-CGA-O2A-C1  |
| 22  | d     | 406 | CLA  | CBA-CGA-O2A-C1  |
| 25  | D     | 410 | DGD  | CAA-CBA-CCA-CDA |
| 27  | d     | 408 | LMG  | C17-C18-C19-C20 |
| 30  | b     | 627 | LMT  | C2B-C1B-O1B-C4' |
| 34  | v     | 201 | HEM  | C4D-C3D-CAD-CBD |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | D     | 408 | LMG  | C2-C1-O1-C7     |
| 30  | B     | 624 | LMT  | C2B-C1B-O1B-C4' |
| 25  | C     | 515 | DGD  | C4B-C5B-C6B-C7B |
| 25  | c     | 515 | DGD  | C2A-C3A-C4A-C5A |
| 27  | D     | 408 | LMG  | C36-C37-C38-C39 |
| 27  | d     | 412 | LMG  | C31-C32-C33-C34 |
| 25  | A     | 408 | DGD  | C1G-C2G-C3G-O3G |
| 25  | C     | 517 | DGD  | O1G-C1G-C2G-C3G |
| 25  | c     | 516 | DGD  | C1G-C2G-C3G-O3G |
| 25  | c     | 517 | DGD  | O1G-C1G-C2G-C3G |
| 27  | B     | 621 | LMG  | C7-C8-C9-O8     |
| 27  | C     | 521 | LMG  | C7-C8-C9-O8     |
| 27  | D     | 408 | LMG  | O1-C7-C8-C9     |
| 27  | D     | 409 | LMG  | O1-C7-C8-C9     |
| 27  | I     | 101 | LMG  | O1-C7-C8-C9     |
| 27  | M     | 101 | LMG  | C7-C8-C9-O8     |
| 27  | b     | 625 | LMG  | C7-C8-C9-O8     |
| 27  | c     | 522 | LMG  | C7-C8-C9-O8     |
| 27  | d     | 408 | LMG  | O1-C7-C8-C9     |
| 27  | d     | 409 | LMG  | O1-C7-C8-C9     |
| 27  | i     | 101 | LMG  | O1-C7-C8-C9     |
| 27  | m     | 101 | LMG  | C7-C8-C9-O8     |
| 29  | b     | 602 | SQD  | C44-C45-C46-O48 |
| 25  | d     | 410 | DGD  | C8B-C9B-CAB-CBB |
| 27  | A     | 414 | LMG  | C17-C18-C19-C20 |
| 22  | B     | 601 | CLA  | C10-C11-C12-C13 |
| 26  | c     | 519 | LHG  | C25-C26-C27-C28 |
| 22  | C     | 510 | CLA  | CBA-CGA-O2A-C1  |
| 22  | D     | 406 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 601 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 613 | CLA  | C16-C17-C18-C20 |
| 27  | b     | 625 | LMG  | C34-C35-C36-C37 |
| 29  | b     | 602 | SQD  | C12-C13-C14-C15 |
| 25  | A     | 408 | DGD  | C3B-C4B-C5B-C6B |
| 27  | i     | 101 | LMG  | O10-C28-O8-C9   |
| 27  | a     | 402 | LMG  | C31-C32-C33-C34 |
| 27  | a     | 412 | LMG  | C15-C16-C17-C18 |
| 22  | C     | 509 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 509 | CLA  | C2-C3-C5-C6     |
| 27  | D     | 408 | LMG  | C15-C16-C17-C18 |
| 34  | v     | 201 | HEM  | C2D-C3D-CAD-CBD |
| 22  | A     | 405 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 502 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 503 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 607 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 608 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 503 | CLA  | C8-C10-C11-C12  |
| 27  | C     | 521 | LMG  | C16-C17-C18-C19 |
| 27  | c     | 522 | LMG  | C16-C17-C18-C19 |
| 25  | D     | 410 | DGD  | C8B-C9B-CAB-CBB |
| 25  | C     | 517 | DGD  | C3B-C4B-C5B-C6B |
| 22  | C     | 508 | CLA  | CBA-CGA-O2A-C1  |
| 25  | D     | 410 | DGD  | C1G-C2G-O2G-C1B |
| 25  | d     | 410 | DGD  | C1G-C2G-O2G-C1B |
| 27  | E     | 101 | LMG  | C7-C8-O7-C10    |
| 27  | c     | 518 | LMG  | C9-C8-O7-C10    |
| 22  | a     | 407 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 502 | CLA  | C13-C15-C16-C17 |
| 25  | A     | 408 | DGD  | C4B-C5B-C6B-C7B |
| 25  | a     | 410 | DGD  | C3B-C4B-C5B-C6B |
| 22  | B     | 609 | CLA  | C16-C17-C18-C19 |
| 25  | c     | 515 | DGD  | C4B-C5B-C6B-C7B |
| 27  | B     | 621 | LMG  | C13-C14-C15-C16 |
| 22  | C     | 506 | CLA  | CBD-CGD-O2D-CED |
| 27  | A     | 410 | LMG  | C11-C10-O7-C8   |
| 27  | b     | 625 | LMG  | C13-C14-C15-C16 |
| 25  | B     | 625 | DGD  | C5A-C6A-C7A-C8A |
| 25  | a     | 410 | DGD  | C4B-C5B-C6B-C7B |
| 22  | C     | 512 | CLA  | C4-C3-C5-C6     |
| 23  | d     | 407 | PL9  | C35-C34-C36-C37 |
| 22  | c     | 512 | CLA  | C2-C3-C5-C6     |
| 25  | c     | 517 | DGD  | C3B-C4B-C5B-C6B |
| 27  | i     | 101 | LMG  | C18-C19-C20-C21 |
| 22  | C     | 511 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 613 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 511 | CLA  | C16-C17-C18-C19 |
| 27  | I     | 101 | LMG  | C18-C19-C20-C21 |
| 27  | e     | 101 | LMG  | C18-C19-C20-C21 |
| 25  | C     | 516 | DGD  | O6D-C5D-C6D-O5D |
| 25  | c     | 516 | DGD  | O6D-C5D-C6D-O5D |
| 27  | d     | 408 | LMG  | C32-C33-C34-C35 |
| 29  | A     | 412 | SQD  | C17-C18-C19-C20 |
| 25  | C     | 515 | DGD  | O2G-C2G-C3G-O3G |
| 25  | C     | 517 | DGD  | O1G-C1G-C2G-O2G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | c     | 517 | DGD  | O1G-C1G-C2G-O2G |
| 27  | a     | 412 | LMG  | O1-C7-C8-O7     |
| 29  | a     | 401 | SQD  | C10-C11-C12-C13 |
| 29  | a     | 415 | SQD  | C17-C18-C19-C20 |
| 22  | C     | 504 | CLA  | O1A-CGA-O2A-C1  |
| 27  | a     | 402 | LMG  | C17-C18-C19-C20 |
| 22  | C     | 511 | CLA  | C3-C5-C6-C7     |
| 25  | d     | 410 | DGD  | CDB-CEB-CFB-CGB |
| 26  | c     | 519 | LHG  | C11-C10-C9-C8   |
| 27  | D     | 408 | LMG  | C32-C33-C34-C35 |
| 22  | c     | 509 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 510 | CLA  | CBA-CGA-O2A-C1  |
| 29  | A     | 412 | SQD  | C10-C11-C12-C13 |
| 23  | d     | 407 | PL9  | C27-C28-C29-C30 |
| 25  | b     | 601 | DGD  | O6D-C5D-C6D-O5D |
| 22  | d     | 406 | CLA  | O1A-CGA-O2A-C1  |
| 26  | A     | 409 | LHG  | C23-C24-C25-C26 |
| 22  | C     | 504 | CLA  | C15-C16-C17-C18 |
| 22  | a     | 407 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 617 | CLA  | C5-C6-C7-C8     |
| 25  | C     | 516 | DGD  | C4D-C5D-C6D-O5D |
| 25  | c     | 516 | DGD  | C4D-C5D-C6D-O5D |
| 22  | B     | 613 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 617 | CLA  | C16-C17-C18-C20 |
| 23  | D     | 407 | PL9  | C35-C34-C36-C37 |
| 25  | d     | 410 | DGD  | C4E-C5E-C6E-O5E |
| 25  | D     | 410 | DGD  | CDB-CEB-CFB-CGB |
| 22  | A     | 403 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 605 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 608 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 614 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 502 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 504 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 505 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 507 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 511 | CLA  | C11-C12-C13-C14 |
| 22  | D     | 405 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 609 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 618 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 502 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 504 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 504 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 510 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 511 | CLA  | C11-C12-C13-C14 |
| 31  | D     | 402 | PHO  | C14-C13-C15-C16 |
| 31  | d     | 402 | PHO  | C14-C13-C15-C16 |
| 22  | B     | 615 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 610 | CLA  | O1A-CGA-O2A-C1  |
| 29  | A     | 413 | SQD  | C10-C11-C12-C13 |
| 27  | A     | 410 | LMG  | C8-C9-O8-C28    |
| 22  | B     | 601 | CLA  | C16-C17-C18-C19 |
| 23  | D     | 407 | PL9  | C32-C33-C34-C36 |
| 25  | D     | 410 | DGD  | CBA-CCA-CDA-CEA |
| 27  | d     | 408 | LMG  | C2-C1-O1-C7     |
| 26  | C     | 519 | LHG  | C11-C10-C9-C8   |
| 26  | C     | 519 | LHG  | C25-C26-C27-C28 |
| 27  | d     | 408 | LMG  | C19-C20-C21-C22 |
| 27  | i     | 101 | LMG  | C17-C18-C19-C20 |
| 27  | d     | 409 | LMG  | C28-C29-C30-C31 |
| 27  | a     | 412 | LMG  | C11-C10-O7-C8   |
| 22  | B     | 602 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 607 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 609 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 614 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 615 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 501 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 502 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 504 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 505 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 505 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 507 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 508 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 510 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 510 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 511 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 606 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 609 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 612 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 619 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 502 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 504 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 505 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 507 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 511 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 613 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 615 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 508 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 504 | CLA  | C15-C16-C17-C18 |
| 25  | c     | 517 | DGD  | CFA-CGA-CHA-CIA |
| 25  | d     | 410 | DGD  | CBA-CCA-CDA-CEA |
| 22  | b     | 608 | CLA  | C10-C11-C12-C13 |
| 27  | c     | 522 | LMG  | C17-C18-C19-C20 |
| 27  | d     | 408 | LMG  | C15-C16-C17-C18 |
| 22  | D     | 406 | CLA  | O1A-CGA-O2A-C1  |
| 27  | C     | 521 | LMG  | C17-C18-C19-C20 |
| 22  | A     | 402 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 504 | CLA  | C4-C3-C5-C6     |
| 22  | a     | 404 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 504 | CLA  | C4-C3-C5-C6     |
| 23  | D     | 407 | PL9  | C15-C14-C16-C17 |
| 23  | d     | 407 | PL9  | C15-C14-C16-C17 |
| 27  | d     | 409 | LMG  | C29-C30-C31-C32 |
| 27  | E     | 101 | LMG  | O7-C10-C11-C12  |
| 23  | J     | 101 | PL9  | C27-C28-C29-C30 |
| 22  | c     | 504 | CLA  | O1A-CGA-O2A-C1  |
| 27  | a     | 412 | LMG  | C4-C5-C6-O5     |
| 27  | E     | 101 | LMG  | C17-C18-C19-C20 |
| 27  | C     | 521 | LMG  | C34-C35-C36-C37 |
| 22  | C     | 511 | CLA  | C16-C17-C18-C19 |
| 27  | D     | 412 | LMG  | C38-C39-C40-C41 |
| 27  | E     | 101 | LMG  | C19-C20-C21-C22 |
| 22  | C     | 508 | CLA  | O1A-CGA-O2A-C1  |
| 22  | C     | 510 | CLA  | O1A-CGA-O2A-C1  |
| 27  | d     | 412 | LMG  | C38-C39-C40-C41 |
| 27  | A     | 414 | LMG  | C11-C12-C13-C14 |
| 27  | e     | 101 | LMG  | C19-C20-C21-C22 |
| 27  | I     | 101 | LMG  | C31-C32-C33-C34 |
| 22  | b     | 619 | CLA  | C8-C10-C11-C12  |
| 25  | B     | 625 | DGD  | C1G-C2G-C3G-O3G |
| 25  | C     | 516 | DGD  | C1G-C2G-C3G-O3G |
| 25  | a     | 410 | DGD  | C1G-C2G-C3G-O3G |
| 25  | d     | 410 | DGD  | C1G-C2G-C3G-O3G |
| 27  | A     | 410 | LMG  | O1-C7-C8-C9     |
| 27  | C     | 518 | LMG  | O1-C7-C8-C9     |
| 27  | a     | 412 | LMG  | O1-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | c     | 518 | LMG  | O1-C7-C8-C9     |
| 27  | m     | 101 | LMG  | O1-C7-C8-C9     |
| 29  | A     | 412 | SQD  | C44-C45-C46-O48 |
| 29  | A     | 413 | SQD  | O6-C44-C45-C46  |
| 29  | B     | 626 | SQD  | C44-C45-C46-O48 |
| 29  | a     | 401 | SQD  | O6-C44-C45-C46  |
| 27  | D     | 412 | LMG  | C19-C20-C21-C22 |
| 27  | d     | 408 | LMG  | C13-C14-C15-C16 |
| 22  | b     | 613 | CLA  | C16-C17-C18-C19 |
| 27  | I     | 101 | LMG  | C17-C18-C19-C20 |
| 29  | a     | 415 | SQD  | C31-C32-C33-C34 |
| 27  | E     | 101 | LMG  | C18-C19-C20-C21 |
| 26  | C     | 519 | LHG  | O10-C23-O8-C6   |
| 27  | c     | 522 | LMG  | C34-C35-C36-C37 |
| 27  | D     | 408 | LMG  | C19-C20-C21-C22 |
| 27  | D     | 409 | LMG  | C29-C30-C31-C32 |
| 25  | C     | 517 | DGD  | CDB-CEB-CFB-CGB |
| 27  | b     | 625 | LMG  | C17-C18-C19-C20 |
| 27  | i     | 101 | LMG  | C31-C32-C33-C34 |
| 24  | B     | 616 | BCR  | C1-C6-C7-C8     |
| 24  | C     | 513 | BCR  | C1-C6-C7-C8     |
| 24  | F     | 102 | BCR  | C1-C6-C7-C8     |
| 24  | J     | 102 | BCR  | C1-C6-C7-C8     |
| 24  | b     | 620 | BCR  | C1-C6-C7-C8     |
| 24  | f     | 102 | BCR  | C1-C6-C7-C8     |
| 24  | j     | 102 | BCR  | C1-C6-C7-C8     |
| 27  | a     | 402 | LMG  | C11-C12-C13-C14 |
| 22  | c     | 511 | CLA  | C3-C5-C6-C7     |
| 27  | B     | 621 | LMG  | C17-C18-C19-C20 |
| 30  | B     | 628 | LMT  | C2-C3-C4-C5     |
| 22  | b     | 617 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 619 | CLA  | C15-C16-C17-C18 |
| 29  | a     | 415 | SQD  | C10-C11-C12-C13 |
| 30  | B     | 624 | LMT  | O5B-C1B-O1B-C4' |
| 27  | A     | 410 | LMG  | C4-C5-C6-O5     |
| 23  | j     | 101 | PL9  | C27-C28-C29-C30 |
| 27  | e     | 101 | LMG  | C17-C18-C19-C20 |
| 22  | c     | 512 | CLA  | C2A-CAA-CBA-CGA |
| 25  | c     | 515 | DGD  | O2G-C2G-C3G-O3G |
| 27  | B     | 621 | LMG  | O7-C8-C9-O8     |
| 27  | C     | 518 | LMG  | O1-C7-C8-O7     |
| 27  | C     | 521 | LMG  | O7-C8-C9-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | M     | 101 | LMG  | O7-C8-C9-O8     |
| 27  | c     | 518 | LMG  | O1-C7-C8-O7     |
| 27  | c     | 522 | LMG  | O7-C8-C9-O8     |
| 27  | m     | 101 | LMG  | O7-C8-C9-O8     |
| 29  | b     | 602 | SQD  | O47-C45-C46-O48 |
| 29  | d     | 403 | SQD  | O6-C44-C45-O47  |
| 27  | d     | 412 | LMG  | C19-C20-C21-C22 |
| 25  | D     | 410 | DGD  | C3B-C4B-C5B-C6B |
| 23  | A     | 406 | PL9  | C4-C3-C7-C8     |
| 23  | a     | 408 | PL9  | C4-C3-C7-C8     |
| 25  | C     | 516 | DGD  | C3A-C4A-C5A-C6A |
| 22  | c     | 504 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 617 | CLA  | C16-C17-C18-C19 |
| 25  | d     | 410 | DGD  | C3B-C4B-C5B-C6B |
| 25  | C     | 517 | DGD  | CFA-CGA-CHA-CIA |
| 27  | D     | 409 | LMG  | C28-C29-C30-C31 |
| 31  | D     | 401 | PHO  | CBD-CGD-O2D-CED |
| 22  | B     | 608 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 507 | CLA  | C14-C13-C15-C16 |
| 22  | a     | 404 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 612 | CLA  | C14-C13-C15-C16 |
| 31  | d     | 401 | PHO  | C6-C7-C8-C9     |
| 22  | B     | 604 | CLA  | C5-C6-C7-C8     |
| 29  | A     | 412 | SQD  | C31-C32-C33-C34 |
| 30  | B     | 627 | LMT  | C5'-C4'-O1B-C1B |
| 30  | b     | 603 | LMT  | C5'-C4'-O1B-C1B |
| 22  | B     | 613 | CLA  | C15-C16-C17-C18 |
| 22  | a     | 405 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 501 | CLA  | C13-C15-C16-C17 |
| 25  | D     | 410 | DGD  | C1A-C2A-C3A-C4A |
| 30  | b     | 627 | LMT  | O5B-C1B-O1B-C4' |
| 22  | B     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 22  | C     | 504 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 604 | CLA  | C10-C11-C12-C13 |
| 25  | c     | 516 | DGD  | C3A-C4A-C5A-C6A |
| 29  | b     | 602 | SQD  | C10-C11-C12-C13 |
| 24  | b     | 621 | BCR  | C20-C21-C22-C37 |
| 27  | I     | 101 | LMG  | O10-C28-O8-C9   |
| 22  | A     | 405 | CLA  | C13-C15-C16-C17 |
| 24  | F     | 102 | BCR  | C37-C22-C23-C24 |
| 29  | f     | 103 | SQD  | C29-C30-C31-C32 |
| 22  | A     | 403 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 604 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 608 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 610 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 612 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 615 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 507 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 511 | CLA  | C12-C13-C15-C16 |
| 22  | a     | 405 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 606 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 608 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 614 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 616 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 619 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 501 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 507 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 511 | CLA  | C12-C13-C15-C16 |
| 27  | m     | 101 | LMG  | C30-C31-C32-C33 |
| 24  | H     | 102 | BCR  | C7-C8-C9-C10    |
| 24  | J     | 102 | BCR  | C7-C8-C9-C10    |
| 24  | c     | 514 | BCR  | C7-C8-C9-C10    |
| 26  | c     | 519 | LHG  | O10-C23-O8-C6   |
| 27  | A     | 410 | LMG  | C8-C7-O1-C1     |
| 27  | a     | 412 | LMG  | C8-C7-O1-C1     |
| 29  | B     | 622 | SQD  | C45-C44-O6-C1   |
| 29  | B     | 622 | SQD  | C5-C6-S-O8      |
| 29  | d     | 403 | SQD  | C45-C44-O6-C1   |
| 29  | d     | 403 | SQD  | C5-C6-S-O8      |
| 22  | c     | 508 | CLA  | C15-C16-C17-C18 |
| 31  | D     | 401 | PHO  | C5-C6-C7-C8     |
| 29  | b     | 602 | SQD  | C17-C18-C19-C20 |
| 23  | A     | 406 | PL9  | C35-C34-C36-C37 |
| 27  | e     | 101 | LMG  | O7-C10-C11-C12  |
| 22  | b     | 613 | CLA  | O1A-CGA-O2A-C1  |
| 22  | c     | 510 | CLA  | O1A-CGA-O2A-C1  |
| 25  | b     | 601 | DGD  | C5A-C6A-C7A-C8A |
| 25  | c     | 516 | DGD  | C4B-C5B-C6B-C7B |
| 22  | B     | 609 | CLA  | C10-C11-C12-C13 |
| 29  | a     | 415 | SQD  | C15-C16-C17-C18 |
| 31  | D     | 402 | PHO  | C10-C11-C12-C13 |
| 29  | A     | 412 | SQD  | C15-C16-C17-C18 |
| 26  | C     | 519 | LHG  | O2-C2-C3-O3     |
| 22  | C     | 511 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | J     | 102 | BCR  | C20-C21-C22-C23 |
| 26  | c     | 519 | LHG  | O6-C4-C5-O7     |
| 23  | D     | 407 | PL9  | C24-C26-C27-C28 |
| 25  | D     | 410 | DGD  | C1G-C2G-C3G-O3G |
| 25  | b     | 601 | DGD  | C1G-C2G-C3G-O3G |
| 27  | M     | 101 | LMG  | O1-C7-C8-C9     |
| 29  | a     | 415 | SQD  | C44-C45-C46-O48 |
| 22  | b     | 613 | CLA  | C5-C6-C7-C8     |
| 34  | F     | 101 | HEM  | C4B-C3B-CAB-CBB |
| 34  | V     | 201 | HEM  | C4C-C3C-CAC-CBC |
| 34  | f     | 101 | HEM  | C4B-C3B-CAB-CBB |
| 34  | v     | 201 | HEM  | C4C-C3C-CAC-CBC |
| 22  | c     | 506 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 29  | B     | 626 | SQD  | C10-C11-C12-C13 |
| 25  | a     | 410 | DGD  | O2G-C2G-C3G-O3G |
| 29  | B     | 622 | SQD  | O6-C44-C45-O47  |
| 31  | d     | 401 | PHO  | C5-C6-C7-C8     |
| 22  | A     | 403 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 612 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 612 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 501 | CLA  | C11-C12-C13-C14 |
| 22  | D     | 405 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 616 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 511 | CLA  | C14-C13-C15-C16 |
| 25  | C     | 516 | DGD  | C4B-C5B-C6B-C7B |
| 27  | C     | 518 | LMG  | C13-C14-C15-C16 |
| 22  | b     | 607 | CLA  | CBA-CGA-O2A-C1  |
| 25  | D     | 410 | DGD  | C2B-C3B-C4B-C5B |
| 27  | c     | 518 | LMG  | C13-C14-C15-C16 |
| 25  | c     | 517 | DGD  | CDB-CEB-CFB-CGB |
| 27  | A     | 410 | LMG  | C20-C21-C22-C23 |
| 27  | d     | 408 | LMG  | C20-C21-C22-C23 |
| 22  | B     | 604 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 611 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 608 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 511 | CLA  | C5-C6-C7-C8     |
| 27  | d     | 409 | LMG  | C31-C32-C33-C34 |
| 25  | d     | 410 | DGD  | CAA-CBA-CCA-CDA |
| 27  | D     | 408 | LMG  | C16-C17-C18-C19 |
| 22  | C     | 508 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 405 | CLA  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | d     | 410 | DGD  | C2B-C3B-C4B-C5B |
| 23  | a     | 408 | PL9  | C35-C34-C36-C37 |
| 23  | d     | 407 | PL9  | C20-C19-C21-C22 |
| 22  | b     | 615 | CLA  | C10-C11-C12-C13 |
| 22  | a     | 407 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 613 | CLA  | C10-C11-C12-C13 |
| 27  | d     | 409 | LMG  | C36-C37-C38-C39 |
| 22  | B     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 25  | D     | 410 | DGD  | C4A-C5A-C6A-C7A |
| 27  | b     | 625 | LMG  | C28-C29-C30-C31 |
| 22  | C     | 506 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 402 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 601 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 508 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 520 | CLA  | C4B-C3B-CAB-CBB |
| 22  | a     | 404 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 605 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 520 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 29  | B     | 626 | SQD  | C17-C18-C19-C20 |
| 22  | A     | 403 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 611 | CLA  | C4-C3-C5-C6     |
| 24  | j     | 102 | BCR  | C7-C8-C9-C10    |
| 29  | A     | 413 | SQD  | C9-C10-C11-C12  |
| 26  | C     | 519 | LHG  | O6-C4-C5-C6     |
| 26  | c     | 519 | LHG  | O6-C4-C5-C6     |
| 31  | d     | 401 | PHO  | CBD-CGD-O2D-CED |
| 29  | B     | 626 | SQD  | O49-C7-O47-C45  |
| 29  | b     | 602 | SQD  | O49-C7-O47-C45  |
| 25  | d     | 410 | DGD  | C1A-C2A-C3A-C4A |
| 22  | B     | 609 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 506 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 405 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 607 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 609 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 612 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 508 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 509 | CLA  | C6-C7-C8-C10    |
| 22  | D     | 406 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 611 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 611 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 613 | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 613 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 616 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 505 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 508 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 509 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 520 | CLA  | C6-C7-C8-C10    |
| 22  | d     | 406 | CLA  | C11-C10-C8-C7   |
| 22  | h     | 101 | CLA  | C11-C10-C8-C7   |
| 31  | d     | 402 | PHO  | C6-C7-C8-C10    |
| 25  | b     | 624 | DGD  | C5A-C6A-C7A-C8A |
| 29  | F     | 103 | SQD  | C29-C30-C31-C32 |
| 27  | C     | 521 | LMG  | C35-C36-C37-C38 |
| 27  | D     | 409 | LMG  | C31-C32-C33-C34 |
| 27  | a     | 412 | LMG  | C20-C21-C22-C23 |
| 29  | A     | 413 | SQD  | C32-C33-C34-C35 |
| 26  | A     | 409 | LHG  | C2-C3-O3-P      |
| 22  | b     | 615 | CLA  | C4-C3-C5-C6     |
| 26  | C     | 519 | LHG  | O6-C4-C5-O7     |
| 29  | a     | 401 | SQD  | C9-C10-C11-C12  |
| 22  | C     | 508 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 508 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 604 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 610 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 615 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 509 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 511 | CLA  | C14-C13-C15-C16 |
| 22  | a     | 405 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 606 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 608 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 614 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 619 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 501 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 507 | CLA  | C14-C13-C15-C16 |
| 27  | c     | 522 | LMG  | C35-C36-C37-C38 |
| 31  | d     | 402 | PHO  | C10-C11-C12-C13 |
| 25  | c     | 515 | DGD  | C5A-C6A-C7A-C8A |
| 22  | A     | 403 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 616 | CLA  | C13-C15-C16-C17 |
| 29  | B     | 622 | SQD  | O5-C5-C6-S      |
| 22  | c     | 506 | CLA  | C3-C5-C6-C7     |
| 29  | f     | 103 | SQD  | C24-C25-C26-C27 |
| 22  | b     | 607 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | A     | 408 | DGD  | O2G-C2G-C3G-O3G |
| 25  | D     | 410 | DGD  | O2G-C2G-C3G-O3G |
| 25  | d     | 410 | DGD  | O2G-C2G-C3G-O3G |
| 27  | D     | 409 | LMG  | O1-C7-C8-O7     |
| 27  | b     | 625 | LMG  | O7-C8-C9-O8     |
| 29  | B     | 626 | SQD  | O47-C45-C46-O48 |
| 25  | B     | 620 | DGD  | C5A-C6A-C7A-C8A |
| 22  | A     | 404 | CLA  | C5-C6-C7-C8     |
| 27  | D     | 408 | LMG  | C20-C21-C22-C23 |
| 29  | d     | 403 | SQD  | O6-C44-C45-C46  |
| 27  | A     | 410 | LMG  | C29-C30-C31-C32 |
| 29  | B     | 622 | SQD  | C10-C11-C12-C13 |
| 31  | d     | 402 | PHO  | C13-C15-C16-C17 |
| 27  | A     | 410 | LMG  | O6-C5-C6-O5     |
| 22  | C     | 503 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 505 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 503 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 505 | CLA  | CAD-CBD-CGD-O2D |
| 27  | a     | 412 | LMG  | C16-C17-C18-C19 |
| 25  | d     | 410 | DGD  | C4A-C5A-C6A-C7A |
| 31  | D     | 401 | PHO  | O1D-CGD-O2D-CED |
| 29  | d     | 403 | SQD  | C10-C11-C12-C13 |
| 22  | B     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 25  | B     | 620 | DGD  | O1A-C1A-O1G-C1G |
| 27  | a     | 412 | LMG  | O6-C5-C6-O5     |
| 22  | C     | 503 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 505 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 508 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 503 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 505 | CLA  | CAD-CBD-CGD-O1D |
| 26  | A     | 409 | LHG  | C3-O3-P-O5      |
| 26  | C     | 519 | LHG  | C3-O3-P-O5      |
| 26  | C     | 519 | LHG  | C4-O6-P-O5      |
| 26  | a     | 411 | LHG  | C3-O3-P-O5      |
| 26  | c     | 519 | LHG  | C3-O3-P-O5      |
| 26  | c     | 519 | LHG  | C4-O6-P-O5      |
| 29  | a     | 401 | SQD  | C32-C33-C34-C35 |
| 22  | B     | 612 | CLA  | C10-C11-C12-C13 |
| 23  | J     | 101 | PL9  | C15-C14-C16-C17 |
| 22  | B     | 601 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 605 | CLA  | C2B-C3B-CAB-CBB |
| 22  | C     | 501 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 504 | CLA  | C2B-C3B-CAB-CBB |
| 22  | C     | 520 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 605 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 609 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 501 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 504 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 520 | CLA  | C2B-C3B-CAB-CBB |
| 24  | b     | 623 | BCR  | C23-C24-C25-C30 |
| 23  | D     | 407 | PL9  | C13-C14-C16-C17 |
| 23  | d     | 407 | PL9  | C13-C14-C16-C17 |
| 26  | a     | 411 | LHG  | C2-C3-O3-P      |
| 30  | b     | 604 | LMT  | C2-C3-C4-C5     |
| 27  | E     | 101 | LMG  | C31-C32-C33-C34 |
| 30  | b     | 603 | LMT  | C4'-C5'-C6'-O6' |
| 22  | A     | 405 | CLA  | C16-C17-C18-C20 |
| 22  | a     | 407 | CLA  | C16-C17-C18-C20 |
| 27  | a     | 412 | LMG  | C10-C11-C12-C13 |
| 22  | C     | 507 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 609 | CLA  | C13-C15-C16-C17 |
| 25  | C     | 515 | DGD  | C5A-C6A-C7A-C8A |
| 27  | B     | 621 | LMG  | C12-C13-C14-C15 |
| 25  | C     | 517 | DGD  | C3G-C2G-O2G-C1B |
| 25  | c     | 517 | DGD  | C3G-C2G-O2G-C1B |
| 26  | A     | 409 | LHG  | C6-C5-O7-C7     |
| 26  | a     | 411 | LHG  | C6-C5-O7-C7     |
| 25  | b     | 624 | DGD  | CCA-CDA-CEA-CFA |
| 22  | c     | 507 | CLA  | C5-C6-C7-C8     |
| 27  | A     | 410 | LMG  | C10-C11-C12-C13 |
| 29  | a     | 415 | SQD  | C11-C10-C9-C8   |
| 27  | A     | 410 | LMG  | C16-C17-C18-C19 |
| 25  | d     | 410 | DGD  | O6E-C5E-C6E-O5E |
| 22  | A     | 404 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 601 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 602 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 609 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 505 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 508 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 510 | CLA  | C11-C10-C8-C9   |
| 22  | a     | 406 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 616 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 618 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 619 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 619 | CLA  | C14-C13-C15-C16 |
| 22  | d     | 405 | CLA  | C6-C7-C8-C9     |
| 31  | D     | 401 | PHO  | C6-C7-C8-C9     |
| 22  | A     | 404 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 601 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 602 | CLA  | C11-C12-C13-C15 |
| 22  | H     | 101 | CLA  | C11-C10-C8-C7   |
| 22  | H     | 101 | CLA  | C12-C13-C15-C16 |
| 22  | a     | 406 | CLA  | C6-C7-C8-C10    |
| 31  | D     | 402 | PHO  | C6-C7-C8-C10    |
| 22  | b     | 617 | CLA  | C2C-C3C-CAC-CBC |
| 26  | c     | 519 | LHG  | C7-C8-C9-C10    |
| 27  | c     | 518 | LMG  | C32-C33-C34-C35 |
| 29  | A     | 412 | SQD  | C11-C10-C9-C8   |
| 27  | A     | 410 | LMG  | O6-C1-O1-C7     |
| 22  | b     | 616 | CLA  | C8-C10-C11-C12  |
| 27  | A     | 414 | LMG  | C16-C17-C18-C19 |
| 25  | c     | 516 | DGD  | C6A-C7A-C8A-C9A |
| 22  | B     | 610 | CLA  | C4-C3-C5-C6     |
| 27  | c     | 522 | LMG  | C30-C31-C32-C33 |
| 22  | c     | 510 | CLA  | C3-C5-C6-C7     |
| 27  | A     | 410 | LMG  | C38-C39-C40-C41 |
| 25  | c     | 516 | DGD  | C7B-C8B-C9B-CAB |
| 27  | B     | 621 | LMG  | C28-C29-C30-C31 |
| 22  | C     | 504 | CLA  | C8-C10-C11-C12  |
| 27  | d     | 409 | LMG  | O1-C7-C8-O7     |
| 25  | B     | 620 | DGD  | CAB-CBB-CCB-CDB |
| 27  | C     | 518 | LMG  | C32-C33-C34-C35 |
| 27  | D     | 408 | LMG  | C13-C14-C15-C16 |
| 34  | F     | 101 | HEM  | C3D-CAD-CBD-CGD |
| 27  | a     | 402 | LMG  | C16-C17-C18-C19 |
| 22  | a     | 406 | CLA  | C5-C6-C7-C8     |
| 22  | a     | 405 | CLA  | C4-C3-C5-C6     |
| 23  | d     | 407 | PL9  | C24-C26-C27-C28 |
| 27  | e     | 101 | LMG  | O1-C7-C8-C9     |
| 29  | B     | 622 | SQD  | O6-C44-C45-C46  |
| 25  | d     | 410 | DGD  | CBB-CCB-CDB-CEB |
| 22  | C     | 511 | CLA  | CAA-CBA-CGA-O2A |
| 24  | f     | 102 | BCR  | C7-C8-C9-C34    |
| 25  | D     | 410 | DGD  | CBB-CCB-CDB-CEB |
| 23  | d     | 407 | PL9  | C32-C33-C34-C36 |
| 24  | C     | 514 | BCR  | C7-C8-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 609 | CLA  | CBA-CGA-O2A-C1  |
| 25  | B     | 625 | DGD  | C2G-C3G-O3G-C1D |
| 25  | b     | 601 | DGD  | C2G-C3G-O3G-C1D |
| 27  | d     | 412 | LMG  | C8-C7-O1-C1     |
| 22  | b     | 616 | CLA  | C10-C11-C12-C13 |
| 31  | D     | 402 | PHO  | C13-C15-C16-C17 |
| 22  | b     | 617 | CLA  | C2A-CAA-CBA-CGA |
| 31  | d     | 401 | PHO  | O1D-CGD-O2D-CED |
| 27  | a     | 412 | LMG  | C11-C12-C13-C14 |
| 26  | c     | 519 | LHG  | O2-C2-C3-O3     |
| 23  | D     | 407 | PL9  | C20-C19-C21-C22 |
| 27  | b     | 625 | LMG  | C15-C16-C17-C18 |
| 25  | C     | 516 | DGD  | C7B-C8B-C9B-CAB |
| 27  | A     | 414 | LMG  | C12-C13-C14-C15 |
| 22  | B     | 607 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 615 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 605 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 611 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 613 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 505 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 508 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 510 | CLA  | C11-C10-C8-C9   |
| 31  | D     | 402 | PHO  | C11-C10-C8-C9   |
| 31  | d     | 402 | PHO  | C11-C10-C8-C9   |
| 22  | B     | 609 | CLA  | CBA-CGA-O2A-C1  |
| 22  | b     | 608 | CLA  | C4B-C3B-CAB-CBB |
| 27  | b     | 625 | LMG  | C12-C13-C14-C15 |
| 29  | a     | 401 | SQD  | C12-C13-C14-C15 |
| 34  | f     | 101 | HEM  | C3D-CAD-CBD-CGD |
| 22  | B     | 605 | CLA  | CBA-CGA-O2A-C1  |
| 22  | h     | 101 | CLA  | CBA-CGA-O2A-C1  |
| 25  | C     | 515 | DGD  | C5B-C6B-C7B-C8B |
| 25  | b     | 624 | DGD  | O1A-C1A-O1G-C1G |
| 22  | b     | 614 | CLA  | C4-C3-C5-C6     |
| 22  | c     | 511 | CLA  | CAA-CBA-CGA-O2A |
| 29  | A     | 413 | SQD  | C12-C13-C14-C15 |
| 27  | C     | 521 | LMG  | C32-C33-C34-C35 |
| 27  | d     | 412 | LMG  | C16-C17-C18-C19 |
| 22  | C     | 506 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 520 | CLA  | C6-C7-C8-C10    |
| 22  | D     | 405 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 505 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 510 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 609 | CLA  | O1A-CGA-O2A-C1  |
| 27  | m     | 101 | LMG  | O10-C28-O8-C9   |
| 25  | b     | 624 | DGD  | C4A-C5A-C6A-C7A |
| 27  | a     | 412 | LMG  | C35-C36-C37-C38 |
| 27  | e     | 101 | LMG  | C31-C32-C33-C34 |
| 25  | c     | 517 | DGD  | C8B-C9B-CAB-CBB |
| 22  | B     | 605 | CLA  | C13-C15-C16-C17 |
| 29  | a     | 401 | SQD  | C26-C27-C28-C29 |
| 22  | C     | 512 | CLA  | C3A-C2A-CAA-CBA |
| 22  | D     | 405 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 512 | CLA  | C3A-C2A-CAA-CBA |
| 22  | c     | 504 | CLA  | C8-C10-C11-C12  |
| 27  | D     | 409 | LMG  | C36-C37-C38-C39 |
| 22  | B     | 610 | CLA  | C2-C3-C5-C6     |
| 27  | a     | 412 | LMG  | C8-C9-O8-C28    |
| 25  | c     | 515 | DGD  | C5B-C6B-C7B-C8B |
| 27  | c     | 522 | LMG  | C32-C33-C34-C35 |
| 22  | a     | 405 | CLA  | C2-C1-O2A-CGA   |
| 31  | D     | 401 | PHO  | C2-C1-O2A-CGA   |
| 22  | B     | 612 | CLA  | C8-C10-C11-C12  |
| 27  | a     | 412 | LMG  | C29-C30-C31-C32 |
| 24  | x     | 101 | BCR  | C7-C8-C9-C10    |
| 22  | B     | 611 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 615 | CLA  | C2-C3-C5-C6     |
| 26  | C     | 519 | LHG  | C1-C2-C3-O3     |
| 22  | h     | 101 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 618 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 605 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 609 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 614 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 506 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 505 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 509 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 512 | CLA  | C11-C10-C8-C9   |
| 22  | d     | 406 | CLA  | C11-C10-C8-C9   |
| 31  | d     | 402 | PHO  | C6-C7-C8-C9     |
| 22  | B     | 602 | CLA  | C16-C17-C18-C19 |
| 25  | C     | 517 | DGD  | C8B-C9B-CAB-CBB |
| 27  | M     | 101 | LMG  | C16-C17-C18-C19 |
| 30  | B     | 624 | LMT  | C6-C7-C8-C9     |
| 25  | B     | 620 | DGD  | CCA-CDA-CEA-CFA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | A     | 409 | LHG  | C4-C5-O7-C7     |
| 27  | M     | 101 | LMG  | C9-C8-O7-C10    |
| 27  | m     | 101 | LMG  | C9-C8-O7-C10    |
| 27  | a     | 402 | LMG  | C12-C13-C14-C15 |
| 22  | B     | 602 | CLA  | C15-C16-C17-C18 |
| 29  | F     | 103 | SQD  | C24-C25-C26-C27 |
| 23  | D     | 407 | PL9  | C40-C39-C41-C42 |
| 26  | C     | 519 | LHG  | C7-C8-C9-C10    |
| 22  | b     | 606 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 617 | CLA  | C4C-C3C-CAC-CBC |
| 27  | M     | 101 | LMG  | C31-C32-C33-C34 |
| 22  | d     | 406 | CLA  | C2A-CAA-CBA-CGA |
| 27  | D     | 408 | LMG  | C29-C30-C31-C32 |
| 22  | C     | 512 | CLA  | C1A-C2A-CAA-CBA |
| 22  | d     | 405 | CLA  | C1A-C2A-CAA-CBA |
| 25  | d     | 410 | DGD  | C8A-C9A-CAA-CBA |
| 25  | b     | 624 | DGD  | CAB-CBB-CCB-CDB |
| 27  | A     | 410 | LMG  | C17-C18-C19-C20 |
| 29  | f     | 103 | SQD  | C14-C15-C16-C17 |
| 22  | B     | 604 | CLA  | C2B-C3B-CAB-CBB |
| 22  | C     | 508 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 608 | CLA  | C2B-C3B-CAB-CBB |
| 22  | d     | 406 | CLA  | C2B-C3B-CAB-CBB |
| 24  | A     | 407 | BCR  | C1-C6-C7-C8     |
| 24  | A     | 407 | BCR  | C23-C24-C25-C30 |
| 24  | B     | 616 | BCR  | C5-C6-C7-C8     |
| 24  | B     | 619 | BCR  | C1-C6-C7-C8     |
| 24  | B     | 619 | BCR  | C23-C24-C25-C30 |
| 24  | C     | 513 | BCR  | C5-C6-C7-C8     |
| 24  | C     | 513 | BCR  | C23-C24-C25-C30 |
| 24  | F     | 102 | BCR  | C5-C6-C7-C8     |
| 24  | J     | 102 | BCR  | C5-C6-C7-C8     |
| 24  | K     | 102 | BCR  | C23-C24-C25-C30 |
| 24  | a     | 409 | BCR  | C1-C6-C7-C8     |
| 24  | a     | 409 | BCR  | C23-C24-C25-C30 |
| 24  | b     | 620 | BCR  | C5-C6-C7-C8     |
| 24  | b     | 623 | BCR  | C1-C6-C7-C8     |
| 24  | c     | 513 | BCR  | C5-C6-C7-C8     |
| 24  | c     | 513 | BCR  | C23-C24-C25-C30 |
| 24  | f     | 102 | BCR  | C5-C6-C7-C8     |
| 24  | j     | 102 | BCR  | C5-C6-C7-C8     |
| 27  | B     | 621 | LMG  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | e     | 101 | LMG  | C30-C31-C32-C33 |
| 25  | B     | 625 | DGD  | C2A-C3A-C4A-C5A |
| 22  | b     | 614 | CLA  | C2-C3-C5-C6     |
| 27  | A     | 410 | LMG  | C35-C36-C37-C38 |
| 27  | D     | 409 | LMG  | C18-C19-C20-C21 |
| 27  | a     | 412 | LMG  | C38-C39-C40-C41 |
| 22  | B     | 601 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 505 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 507 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 510 | CLA  | C11-C10-C8-C7   |
| 22  | a     | 407 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 605 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 605 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 505 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 508 | CLA  | C6-C7-C8-C10    |
| 22  | d     | 405 | CLA  | C11-C10-C8-C7   |
| 31  | D     | 402 | PHO  | C11-C10-C8-C7   |
| 31  | d     | 402 | PHO  | C11-C10-C8-C7   |
| 22  | c     | 509 | CLA  | C16-C17-C18-C19 |
| 27  | d     | 408 | LMG  | C16-C17-C18-C19 |
| 29  | F     | 103 | SQD  | C9-C10-C11-C12  |
| 25  | b     | 601 | DGD  | C2A-C3A-C4A-C5A |
| 27  | m     | 101 | LMG  | C31-C32-C33-C34 |
| 26  | c     | 519 | LHG  | C1-C2-C3-O3     |
| 22  | C     | 510 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 612 | CLA  | C13-C15-C16-C17 |
| 27  | C     | 521 | LMG  | C30-C31-C32-C33 |
| 22  | C     | 507 | CLA  | C2-C1-O2A-CGA   |
| 22  | b     | 608 | CLA  | C8-C10-C11-C12  |
| 24  | F     | 102 | BCR  | C21-C22-C23-C24 |
| 22  | b     | 609 | CLA  | C16-C17-C18-C20 |
| 27  | A     | 410 | LMG  | C11-C12-C13-C14 |
| 25  | a     | 410 | DGD  | C2A-C3A-C4A-C5A |
| 29  | f     | 103 | SQD  | C9-C10-C11-C12  |
| 22  | B     | 601 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 505 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 512 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 506 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 512 | CLA  | C14-C13-C15-C16 |
| 27  | D     | 412 | LMG  | C16-C17-C18-C19 |
| 22  | B     | 604 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 607 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 606 | CLA  | C15-C16-C17-C18 |
| 29  | a     | 415 | SQD  | C12-C13-C14-C15 |
| 22  | c     | 510 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 403 | CLA  | C2-C3-C5-C6     |
| 30  | B     | 624 | LMT  | O5'-C5'-C6'-O6' |
| 22  | c     | 509 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 618 | CLA  | O1A-CGA-O2A-C1  |
| 27  | d     | 408 | LMG  | C29-C30-C31-C32 |
| 25  | B     | 620 | DGD  | C7B-C8B-C9B-CAB |
| 25  | C     | 517 | DGD  | C4A-C5A-C6A-C7A |
| 25  | C     | 515 | DGD  | C1G-C2G-C3G-O3G |
| 27  | d     | 412 | LMG  | O1-C7-C8-C9     |
| 30  | b     | 604 | LMT  | C6-C7-C8-C9     |
| 22  | c     | 510 | CLA  | C2A-CAA-CBA-CGA |
| 25  | c     | 517 | DGD  | CBB-CCB-CDB-CEB |
| 22  | B     | 605 | CLA  | C16-C17-C18-C20 |
| 23  | d     | 407 | PL9  | C40-C39-C41-C42 |
| 22  | B     | 604 | CLA  | C4B-C3B-CAB-CBB |
| 22  | d     | 406 | CLA  | C4B-C3B-CAB-CBB |
| 27  | D     | 412 | LMG  | C32-C33-C34-C35 |
| 27  | D     | 408 | LMG  | C10-C11-C12-C13 |
| 25  | A     | 408 | DGD  | C2A-C3A-C4A-C5A |
| 27  | D     | 412 | LMG  | C36-C37-C38-C39 |
| 22  | c     | 510 | CLA  | C2-C3-C5-C6     |
| 25  | c     | 515 | DGD  | O6D-C1D-O3G-C3G |
| 22  | C     | 512 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 608 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 506 | CLA  | C11-C10-C8-C7   |
| 25  | C     | 516 | DGD  | C6A-C7A-C8A-C9A |
| 22  | A     | 403 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 512 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 605 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 509 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 520 | CLA  | C6-C7-C8-C9     |
| 27  | D     | 412 | LMG  | C8-C7-O1-C1     |
| 22  | B     | 612 | CLA  | C2-C1-O2A-CGA   |
| 22  | b     | 613 | CLA  | C2-C1-O2A-CGA   |
| 22  | b     | 616 | CLA  | C2-C1-O2A-CGA   |
| 31  | d     | 401 | PHO  | C2-C1-O2A-CGA   |
| 22  | b     | 606 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 509 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 502 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 405 | CLA  | C4-C3-C5-C6     |
| 22  | C     | 520 | CLA  | C3A-C2A-CAA-CBA |
| 22  | a     | 407 | CLA  | C4-C3-C5-C6     |
| 22  | c     | 520 | CLA  | C3A-C2A-CAA-CBA |
| 22  | C     | 502 | CLA  | O1A-CGA-O2A-C1  |
| 25  | b     | 601 | DGD  | C4E-C5E-C6E-O5E |
| 26  | a     | 411 | LHG  | C4-C5-O7-C7     |
| 24  | j     | 102 | BCR  | C18-C19-C20-C21 |
| 27  | B     | 621 | LMG  | C35-C36-C37-C38 |
| 27  | M     | 101 | LMG  | C30-C31-C32-C33 |
| 25  | B     | 625 | DGD  | CAB-CBB-CCB-CDB |
| 22  | C     | 509 | CLA  | C13-C15-C16-C17 |
| 25  | D     | 410 | DGD  | C4E-C5E-C6E-O5E |
| 27  | M     | 101 | LMG  | O10-C28-O8-C9   |
| 22  | C     | 502 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 611 | CLA  | C13-C15-C16-C17 |
| 27  | M     | 101 | LMG  | O6-C1-O1-C7     |
| 27  | a     | 412 | LMG  | O6-C1-O1-C7     |
| 29  | A     | 412 | SQD  | C16-C17-C18-C19 |
| 22  | H     | 101 | CLA  | CBA-CGA-O2A-C1  |
| 25  | c     | 515 | DGD  | C1G-C2G-C3G-O3G |
| 27  | C     | 518 | LMG  | C7-C8-C9-O8     |
| 27  | I     | 101 | LMG  | C7-C8-C9-O8     |
| 27  | c     | 518 | LMG  | C7-C8-C9-O8     |
| 22  | H     | 101 | CLA  | O1A-CGA-O2A-C1  |
| 27  | E     | 101 | LMG  | C30-C31-C32-C33 |
| 27  | m     | 101 | LMG  | C16-C17-C18-C19 |
| 29  | a     | 415 | SQD  | C16-C17-C18-C19 |
| 22  | D     | 406 | CLA  | C2A-CAA-CBA-CGA |
| 22  | a     | 405 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 602 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 609 | CLA  | C16-C17-C18-C19 |
| 25  | d     | 410 | DGD  | C9B-CAB-CBB-CCB |
| 27  | b     | 625 | LMG  | O1-C7-C8-O7     |
| 27  | e     | 101 | LMG  | O1-C7-C8-O7     |
| 22  | A     | 405 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 615 | CLA  | C11-C12-C13-C14 |
| 22  | H     | 101 | CLA  | C11-C12-C13-C14 |
| 22  | a     | 405 | CLA  | C11-C10-C8-C9   |
| 22  | h     | 101 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 501 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 509 | CLA  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | F     | 103 | SQD  | C14-C15-C16-C17 |
| 22  | B     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 27  | A     | 410 | LMG  | O7-C10-C11-C12  |
| 27  | a     | 412 | LMG  | O7-C10-C11-C12  |
| 30  | B     | 627 | LMT  | C4'-C5'-C6'-O6' |
| 22  | C     | 501 | CLA  | C13-C15-C16-C17 |
| 27  | E     | 101 | LMG  | C33-C34-C35-C36 |
| 27  | d     | 412 | LMG  | C11-C12-C13-C14 |
| 22  | B     | 601 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 505 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 512 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 605 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 609 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 506 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 507 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 509 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 512 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 512 | CLA  | C12-C13-C15-C16 |
| 22  | h     | 101 | CLA  | C12-C13-C15-C16 |
| 24  | A     | 407 | BCR  | C5-C6-C7-C8     |
| 24  | A     | 407 | BCR  | C23-C24-C25-C26 |
| 24  | B     | 619 | BCR  | C5-C6-C7-C8     |
| 24  | B     | 619 | BCR  | C23-C24-C25-C26 |
| 24  | C     | 514 | BCR  | C1-C6-C7-C8     |
| 24  | K     | 102 | BCR  | C1-C6-C7-C8     |
| 24  | K     | 102 | BCR  | C23-C24-C25-C26 |
| 24  | a     | 409 | BCR  | C5-C6-C7-C8     |
| 24  | a     | 409 | BCR  | C23-C24-C25-C26 |
| 24  | b     | 623 | BCR  | C5-C6-C7-C8     |
| 24  | b     | 623 | BCR  | C23-C24-C25-C26 |
| 24  | c     | 514 | BCR  | C1-C6-C7-C8     |
| 24  | c     | 514 | BCR  | C5-C6-C7-C8     |
| 24  | c     | 521 | BCR  | C23-C24-C25-C30 |
| 22  | b     | 616 | CLA  | CAA-CBA-CGA-O2A |
| 26  | C     | 519 | LHG  | O7-C7-C8-C9     |
| 26  | c     | 519 | LHG  | O7-C7-C8-C9     |
| 22  | A     | 402 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 403 | CLA  | C2-C1-O2A-CGA   |
| 22  | a     | 404 | CLA  | C2-C1-O2A-CGA   |
| 29  | A     | 412 | SQD  | C12-C13-C14-C15 |
| 22  | B     | 611 | CLA  | CAA-CBA-CGA-O2A |
| 22  | d     | 405 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | B     | 625 | DGD  | O6D-C1D-O3G-C3G |
| 25  | a     | 410 | DGD  | O6E-C1E-O5D-C6D |
| 30  | B     | 623 | LMT  | C4-C5-C6-C7     |
| 22  | C     | 506 | CLA  | CAA-CBA-CGA-O2A |
| 25  | b     | 601 | DGD  | CAB-CBB-CCB-CDB |
| 22  | b     | 606 | CLA  | C2A-CAA-CBA-CGA |
| 27  | b     | 625 | LMG  | C29-C28-O8-C9   |
| 22  | B     | 605 | CLA  | C16-C17-C18-C19 |
| 27  | c     | 518 | LMG  | C17-C18-C19-C20 |
| 22  | b     | 609 | CLA  | C15-C16-C17-C18 |
| 27  | A     | 414 | LMG  | O7-C10-C11-C12  |
| 27  | d     | 412 | LMG  | C36-C37-C38-C39 |
| 34  | V     | 201 | HEM  | CAA-CBA-CGA-O2A |
| 22  | C     | 501 | CLA  | CAA-CBA-CGA-O2A |
| 25  | C     | 517 | DGD  | O1G-C1A-C2A-C3A |
| 23  | A     | 406 | PL9  | C28-C29-C31-C32 |
| 25  | a     | 410 | DGD  | O1A-C1A-O1G-C1G |
| 22  | C     | 510 | CLA  | C2A-CAA-CBA-CGA |
| 29  | a     | 401 | SQD  | C17-C18-C19-C20 |
| 22  | c     | 506 | CLA  | CAA-CBA-CGA-O2A |
| 27  | c     | 522 | LMG  | O8-C28-C29-C30  |
| 29  | a     | 401 | SQD  | O47-C7-C8-C9    |
| 22  | A     | 404 | CLA  | O1A-CGA-O2A-C1  |
| 34  | v     | 201 | HEM  | CAA-CBA-CGA-O2A |
| 22  | C     | 505 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 507 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 520 | CLA  | C6-C7-C8-C9     |
| 22  | D     | 405 | CLA  | C11-C10-C8-C9   |
| 22  | D     | 406 | CLA  | C11-C10-C8-C9   |
| 22  | H     | 101 | CLA  | C11-C10-C8-C9   |
| 22  | a     | 407 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 605 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 505 | CLA  | C6-C7-C8-C9     |
| 22  | d     | 405 | CLA  | C11-C10-C8-C9   |
| 24  | b     | 623 | BCR  | C7-C8-C9-C34    |
| 22  | C     | 509 | CLA  | CAA-CBA-CGA-O2A |
| 25  | c     | 517 | DGD  | O1G-C1A-C2A-C3A |
| 29  | A     | 413 | SQD  | O47-C7-C8-C9    |
| 26  | A     | 409 | LHG  | C24-C25-C26-C27 |
| 26  | c     | 519 | LHG  | C11-C12-C13-C14 |
| 27  | E     | 101 | LMG  | O1-C7-C8-C9     |
| 22  | A     | 403 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 614 | CLA  | C4B-C3B-CAB-CBB |
| 22  | D     | 406 | CLA  | C4B-C3B-CAB-CBB |
| 22  | a     | 405 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 618 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 508 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 512 | CLA  | C1A-C2A-CAA-CBA |
| 25  | C     | 515 | DGD  | O6D-C1D-O3G-C3G |
| 25  | C     | 516 | DGD  | O6E-C1E-O5D-C6D |
| 25  | b     | 601 | DGD  | O6D-C1D-O3G-C3G |
| 25  | c     | 516 | DGD  | O6E-C1E-O5D-C6D |
| 27  | m     | 101 | LMG  | O6-C1-O1-C7     |
| 22  | b     | 615 | CLA  | CAA-CBA-CGA-O2A |
| 27  | a     | 402 | LMG  | O7-C10-C11-C12  |
| 27  | B     | 621 | LMG  | O1-C7-C8-O7     |
| 24  | f     | 102 | BCR  | C21-C22-C23-C24 |
| 22  | c     | 501 | CLA  | CAA-CBA-CGA-O2A |
| 27  | C     | 521 | LMG  | O8-C28-C29-C30  |
| 29  | B     | 622 | SQD  | O47-C7-C8-C9    |
| 27  | e     | 101 | LMG  | C14-C15-C16-C17 |
| 29  | A     | 413 | SQD  | C26-C27-C28-C29 |
| 22  | B     | 610 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 509 | CLA  | CAA-CBA-CGA-O2A |
| 29  | B     | 622 | SQD  | C5-C6-S-O9      |
| 29  | a     | 401 | SQD  | C5-C6-S-O9      |
| 29  | d     | 403 | SQD  | C5-C6-S-O9      |
| 22  | B     | 613 | CLA  | C2C-C3C-CAC-CBC |
| 29  | d     | 403 | SQD  | O47-C7-C8-C9    |
| 22  | B     | 602 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 604 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 506 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 606 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 512 | CLA  | C11-C12-C13-C15 |
| 25  | a     | 410 | DGD  | C4A-C5A-C6A-C7A |
| 22  | C     | 501 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 509 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 502 | CLA  | C16-C17-C18-C20 |
| 27  | M     | 101 | LMG  | C7-C8-O7-C10    |
| 22  | D     | 405 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 606 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 404 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 602 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | c     | 517 | DGD  | C5B-C6B-C7B-C8B |
| 34  | V     | 201 | HEM  | CAA-CBA-CGA-O1A |
| 22  | B     | 603 | CLA  | C4C-C3C-CAC-CBC |
| 25  | B     | 620 | DGD  | C4A-C5A-C6A-C7A |
| 29  | A     | 413 | SQD  | C17-C18-C19-C20 |
| 25  | c     | 517 | DGD  | C4A-C5A-C6A-C7A |
| 25  | C     | 517 | DGD  | O2G-C1B-C2B-C3B |
| 22  | B     | 601 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 602 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 504 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 504 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 506 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 507 | CLA  | C11-C12-C13-C14 |
| 31  | D     | 402 | PHO  | C6-C7-C8-C9     |
| 22  | b     | 616 | CLA  | CAA-CBA-CGA-O1A |
| 29  | B     | 622 | SQD  | O49-C7-C8-C9    |
| 22  | B     | 601 | CLA  | C5-C6-C7-C8     |
| 25  | C     | 517 | DGD  | C4B-C5B-C6B-C7B |
| 27  | C     | 521 | LMG  | O10-C28-C29-C30 |
| 29  | d     | 403 | SQD  | O49-C7-C8-C9    |
| 27  | D     | 409 | LMG  | C34-C35-C36-C37 |
| 27  | D     | 409 | LMG  | O7-C10-C11-C12  |
| 29  | d     | 403 | SQD  | O5-C5-C6-S      |
| 22  | B     | 613 | CLA  | C4C-C3C-CAC-CBC |
| 30  | B     | 628 | LMT  | C6-C7-C8-C9     |
| 27  | d     | 412 | LMG  | O9-C10-C11-C12  |
| 22  | D     | 405 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 615 | CLA  | C3-C5-C6-C7     |
| 34  | v     | 201 | HEM  | CAA-CBA-CGA-O1A |
| 27  | B     | 621 | LMG  | C29-C28-O8-C9   |
| 22  | c     | 509 | CLA  | CAA-CBA-CGA-O1A |
| 27  | D     | 412 | LMG  | O9-C10-C11-C12  |
| 25  | A     | 408 | DGD  | C5D-C6D-O5D-C1E |
| 25  | a     | 410 | DGD  | C5D-C6D-O5D-C1E |
| 27  | i     | 101 | LMG  | C8-C7-O1-C1     |
| 27  | C     | 518 | LMG  | O7-C8-C9-O8     |
| 22  | B     | 611 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 22  | C     | 506 | CLA  | CAA-CBA-CGA-O1A |
| 22  | C     | 509 | CLA  | CAA-CBA-CGA-O1A |
| 22  | b     | 615 | CLA  | CAA-CBA-CGA-O1A |
| 22  | c     | 506 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | D     | 408 | LMG  | C7-C8-C9-O8     |
| 25  | A     | 408 | DGD  | O6D-C5D-C6D-O5D |
| 25  | D     | 410 | DGD  | C8A-C9A-CAA-CBA |
| 29  | A     | 412 | SQD  | C9-C10-C11-C12  |
| 22  | c     | 501 | CLA  | CAA-CBA-CGA-O1A |
| 22  | d     | 405 | CLA  | CAA-CBA-CGA-O1A |
| 30  | b     | 627 | LMT  | O5'-C5'-C6'-O6' |
| 25  | C     | 517 | DGD  | CBB-CCB-CDB-CEB |
| 25  | b     | 601 | DGD  | C8B-C9B-CAB-CBB |
| 22  | D     | 406 | CLA  | C8-C10-C11-C12  |
| 25  | B     | 620 | DGD  | O2G-C1B-C2B-C3B |
| 25  | c     | 517 | DGD  | O2G-C1B-C2B-C3B |
| 27  | M     | 101 | LMG  | O8-C28-C29-C30  |
| 22  | C     | 510 | CLA  | C2-C3-C5-C6     |
| 23  | a     | 408 | PL9  | C28-C29-C31-C32 |
| 29  | A     | 413 | SQD  | O49-C7-C8-C9    |
| 22  | c     | 512 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 506 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 612 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 602 | CLA  | C8-C10-C11-C12  |
| 29  | a     | 401 | SQD  | O49-C7-C8-C9    |
| 27  | m     | 101 | LMG  | C17-C18-C19-C20 |
| 22  | B     | 609 | CLA  | C2-C1-O2A-CGA   |
| 22  | c     | 507 | CLA  | C2-C1-O2A-CGA   |
| 26  | C     | 519 | LHG  | C11-C12-C13-C14 |
| 27  | M     | 101 | LMG  | C17-C18-C19-C20 |
| 29  | a     | 415 | SQD  | C32-C33-C34-C35 |
| 27  | a     | 402 | LMG  | O9-C10-C11-C12  |
| 27  | c     | 522 | LMG  | O10-C28-C29-C30 |
| 25  | b     | 624 | DGD  | O2G-C1B-C2B-C3B |
| 27  | d     | 409 | LMG  | O7-C10-C11-C12  |
| 22  | B     | 610 | CLA  | C16-C17-C18-C20 |
| 27  | E     | 101 | LMG  | C14-C15-C16-C17 |
| 22  | C     | 503 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 502 | CLA  | O1A-CGA-O2A-C1  |
| 29  | a     | 401 | SQD  | C23-C24-C25-C26 |
| 27  | d     | 412 | LMG  | C32-C33-C34-C35 |
| 22  | B     | 601 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 609 | CLA  | CAA-CBA-CGA-O2A |
| 22  | C     | 504 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 22  | h     | 101 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | m     | 101 | LMG  | O8-C28-C29-C30  |
| 22  | c     | 502 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 501 | CLA  | CAA-CBA-CGA-O1A |
| 22  | D     | 405 | CLA  | CAA-CBA-CGA-O1A |
| 27  | a     | 412 | LMG  | O9-C10-C11-C12  |
| 23  | A     | 406 | PL9  | C2-C3-C7-C8     |
| 25  | D     | 410 | DGD  | C9B-CAB-CBB-CCB |
| 22  | b     | 617 | CLA  | CAA-CBA-CGA-O2A |
| 27  | a     | 412 | LMG  | C13-C14-C15-C16 |
| 29  | f     | 103 | SQD  | C27-C28-C29-C30 |
| 25  | C     | 517 | DGD  | O1A-C1A-C2A-C3A |
| 27  | A     | 410 | LMG  | O9-C10-C11-C12  |
| 22  | B     | 603 | CLA  | C2C-C3C-CAC-CBC |
| 27  | d     | 409 | LMG  | C34-C35-C36-C37 |
| 29  | B     | 626 | SQD  | C15-C16-C17-C18 |

There are no ring outliers.

158 monomers are involved in 440 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 27  | e     | 101 | LMG  | 1       | 0            |
| 24  | c     | 513 | BCR  | 7       | 0            |
| 27  | D     | 409 | LMG  | 6       | 0            |
| 22  | c     | 506 | CLA  | 4       | 0            |
| 31  | D     | 401 | PHO  | 7       | 0            |
| 24  | H     | 102 | BCR  | 3       | 0            |
| 22  | c     | 510 | CLA  | 4       | 0            |
| 22  | c     | 520 | CLA  | 4       | 0            |
| 24  | F     | 102 | BCR  | 3       | 0            |
| 24  | g     | 101 | BCR  | 5       | 0            |
| 24  | x     | 101 | BCR  | 1       | 0            |
| 34  | v     | 201 | HEM  | 5       | 0            |
| 25  | B     | 620 | DGD  | 2       | 0            |
| 24  | c     | 514 | BCR  | 4       | 0            |
| 29  | A     | 412 | SQD  | 4       | 0            |
| 22  | b     | 611 | CLA  | 8       | 0            |
| 22  | B     | 608 | CLA  | 5       | 0            |
| 22  | b     | 618 | CLA  | 2       | 0            |
| 25  | c     | 517 | DGD  | 5       | 0            |
| 25  | b     | 601 | DGD  | 2       | 0            |
| 31  | d     | 401 | PHO  | 6       | 0            |
| 22  | b     | 607 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | d     | 402 | PHO  | 4       | 0            |
| 29  | B     | 622 | SQD  | 3       | 0            |
| 22  | b     | 608 | CLA  | 7       | 0            |
| 24  | B     | 619 | BCR  | 1       | 0            |
| 25  | c     | 515 | DGD  | 3       | 0            |
| 27  | a     | 402 | LMG  | 1       | 0            |
| 25  | D     | 410 | DGD  | 1       | 0            |
| 23  | a     | 408 | PL9  | 3       | 0            |
| 24  | K     | 102 | BCR  | 3       | 0            |
| 22  | D     | 405 | CLA  | 8       | 0            |
| 22  | C     | 508 | CLA  | 1       | 0            |
| 29  | d     | 403 | SQD  | 4       | 0            |
| 22  | B     | 607 | CLA  | 7       | 0            |
| 22  | B     | 601 | CLA  | 1       | 0            |
| 22  | a     | 404 | CLA  | 10      | 0            |
| 24  | J     | 102 | BCR  | 1       | 0            |
| 22  | C     | 511 | CLA  | 1       | 0            |
| 23  | D     | 407 | PL9  | 8       | 0            |
| 27  | D     | 408 | LMG  | 2       | 0            |
| 22  | B     | 613 | CLA  | 3       | 0            |
| 22  | B     | 604 | CLA  | 6       | 0            |
| 26  | a     | 411 | LHG  | 1       | 0            |
| 30  | b     | 626 | LMT  | 1       | 0            |
| 22  | b     | 613 | CLA  | 1       | 0            |
| 24  | C     | 513 | BCR  | 5       | 0            |
| 22  | h     | 101 | CLA  | 9       | 0            |
| 24  | f     | 102 | BCR  | 2       | 0            |
| 29  | b     | 602 | SQD  | 1       | 0            |
| 22  | c     | 508 | CLA  | 3       | 0            |
| 22  | c     | 509 | CLA  | 3       | 0            |
| 22  | B     | 610 | CLA  | 3       | 0            |
| 27  | A     | 410 | LMG  | 2       | 0            |
| 27  | d     | 409 | LMG  | 6       | 0            |
| 29  | F     | 103 | SQD  | 2       | 0            |
| 22  | B     | 605 | CLA  | 7       | 0            |
| 27  | A     | 414 | LMG  | 1       | 0            |
| 29  | f     | 103 | SQD  | 3       | 0            |
| 22  | C     | 501 | CLA  | 2       | 0            |
| 22  | C     | 520 | CLA  | 2       | 0            |
| 22  | C     | 507 | CLA  | 4       | 0            |
| 22  | A     | 405 | CLA  | 1       | 0            |
| 25  | C     | 517 | DGD  | 5       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | C     | 514 | BCR  | 6       | 0            |
| 27  | d     | 412 | LMG  | 1       | 0            |
| 22  | d     | 405 | CLA  | 8       | 0            |
| 22  | B     | 612 | CLA  | 3       | 0            |
| 27  | B     | 621 | LMG  | 3       | 0            |
| 24  | y     | 101 | BCR  | 7       | 0            |
| 24  | b     | 623 | BCR  | 4       | 0            |
| 22  | B     | 603 | CLA  | 2       | 0            |
| 22  | B     | 606 | CLA  | 6       | 0            |
| 27  | d     | 408 | LMG  | 3       | 0            |
| 22  | b     | 617 | CLA  | 2       | 0            |
| 22  | c     | 504 | CLA  | 3       | 0            |
| 31  | D     | 402 | PHO  | 5       | 0            |
| 22  | c     | 503 | CLA  | 2       | 0            |
| 29  | A     | 413 | SQD  | 4       | 0            |
| 22  | C     | 505 | CLA  | 1       | 0            |
| 27  | c     | 522 | LMG  | 1       | 0            |
| 27  | b     | 625 | LMG  | 5       | 0            |
| 22  | b     | 616 | CLA  | 3       | 0            |
| 22  | C     | 504 | CLA  | 4       | 0            |
| 22  | C     | 503 | CLA  | 3       | 0            |
| 22  | b     | 612 | CLA  | 5       | 0            |
| 22  | C     | 506 | CLA  | 3       | 0            |
| 25  | c     | 516 | DGD  | 2       | 0            |
| 22  | c     | 505 | CLA  | 1       | 0            |
| 27  | c     | 518 | LMG  | 2       | 0            |
| 30  | b     | 604 | LMT  | 2       | 0            |
| 22  | c     | 507 | CLA  | 4       | 0            |
| 25  | C     | 516 | DGD  | 3       | 0            |
| 22  | B     | 602 | CLA  | 10      | 0            |
| 22  | A     | 404 | CLA  | 4       | 0            |
| 22  | a     | 407 | CLA  | 1       | 0            |
| 24  | B     | 616 | BCR  | 5       | 0            |
| 22  | C     | 509 | CLA  | 4       | 0            |
| 27  | C     | 518 | LMG  | 3       | 0            |
| 25  | a     | 410 | DGD  | 2       | 0            |
| 24  | B     | 617 | BCR  | 2       | 0            |
| 22  | B     | 614 | CLA  | 1       | 0            |
| 30  | B     | 623 | LMT  | 2       | 0            |
| 22  | c     | 512 | CLA  | 3       | 0            |
| 30  | i     | 102 | LMT  | 1       | 0            |
| 34  | V     | 201 | HEM  | 5       | 0            |

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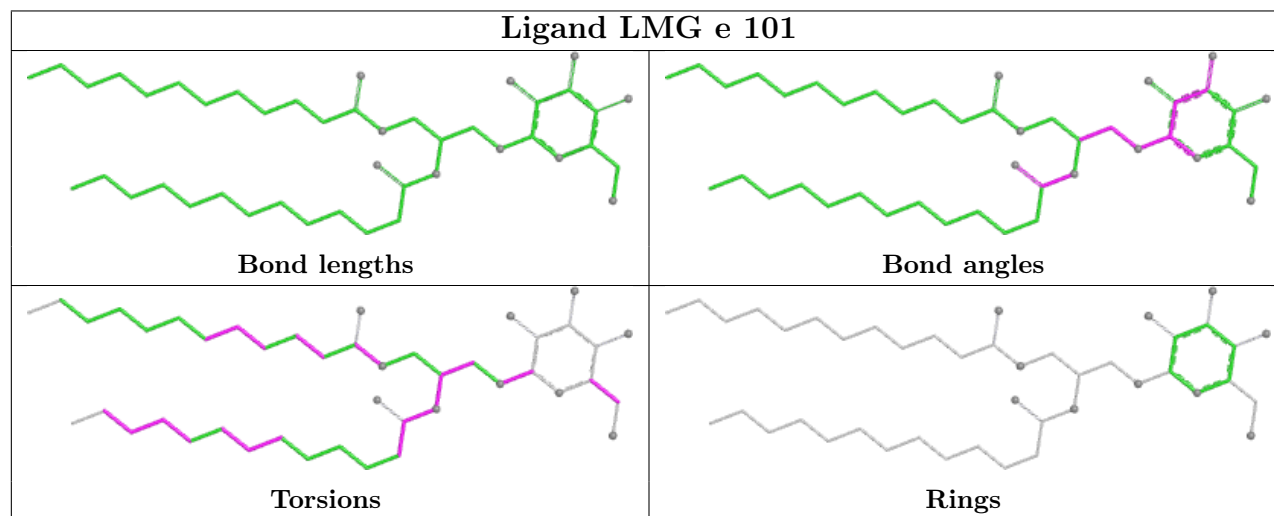
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | A     | 406 | PL9  | 4       | 0            |
| 22  | d     | 406 | CLA  | 3       | 0            |
| 22  | b     | 610 | CLA  | 6       | 0            |
| 30  | B     | 627 | LMT  | 2       | 0            |
| 24  | j     | 102 | BCR  | 1       | 0            |
| 22  | C     | 510 | CLA  | 5       | 0            |
| 29  | a     | 401 | SQD  | 5       | 0            |
| 22  | a     | 406 | CLA  | 6       | 0            |
| 25  | A     | 408 | DGD  | 1       | 0            |
| 34  | f     | 101 | HEM  | 4       | 0            |
| 27  | E     | 101 | LMG  | 1       | 0            |
| 25  | B     | 625 | DGD  | 2       | 0            |
| 24  | c     | 521 | BCR  | 4       | 0            |
| 25  | b     | 624 | DGD  | 2       | 0            |
| 27  | a     | 412 | LMG  | 2       | 0            |
| 24  | B     | 618 | BCR  | 4       | 0            |
| 22  | A     | 403 | CLA  | 14      | 0            |
| 22  | b     | 606 | CLA  | 9       | 0            |
| 34  | F     | 101 | HEM  | 4       | 0            |
| 22  | B     | 615 | CLA  | 4       | 0            |
| 29  | B     | 626 | SQD  | 1       | 0            |
| 24  | A     | 407 | BCR  | 3       | 0            |
| 22  | b     | 619 | CLA  | 4       | 0            |
| 30  | B     | 628 | LMT  | 2       | 0            |
| 27  | M     | 101 | LMG  | 2       | 0            |
| 23  | d     | 407 | PL9  | 6       | 0            |
| 27  | m     | 101 | LMG  | 1       | 0            |
| 22  | b     | 614 | CLA  | 2       | 0            |
| 23  | J     | 101 | PL9  | 1       | 0            |
| 22  | b     | 609 | CLA  | 5       | 0            |
| 26  | A     | 409 | LHG  | 3       | 0            |
| 26  | c     | 519 | LHG  | 2       | 0            |
| 22  | c     | 501 | CLA  | 4       | 0            |
| 22  | b     | 615 | CLA  | 4       | 0            |
| 22  | H     | 101 | CLA  | 8       | 0            |
| 27  | i     | 101 | LMG  | 1       | 0            |
| 22  | B     | 611 | CLA  | 4       | 0            |
| 30  | b     | 603 | LMT  | 2       | 0            |
| 22  | D     | 406 | CLA  | 2       | 0            |
| 22  | a     | 405 | CLA  | 9       | 0            |
| 22  | A     | 402 | CLA  | 10      | 0            |
| 24  | a     | 409 | BCR  | 2       | 0            |

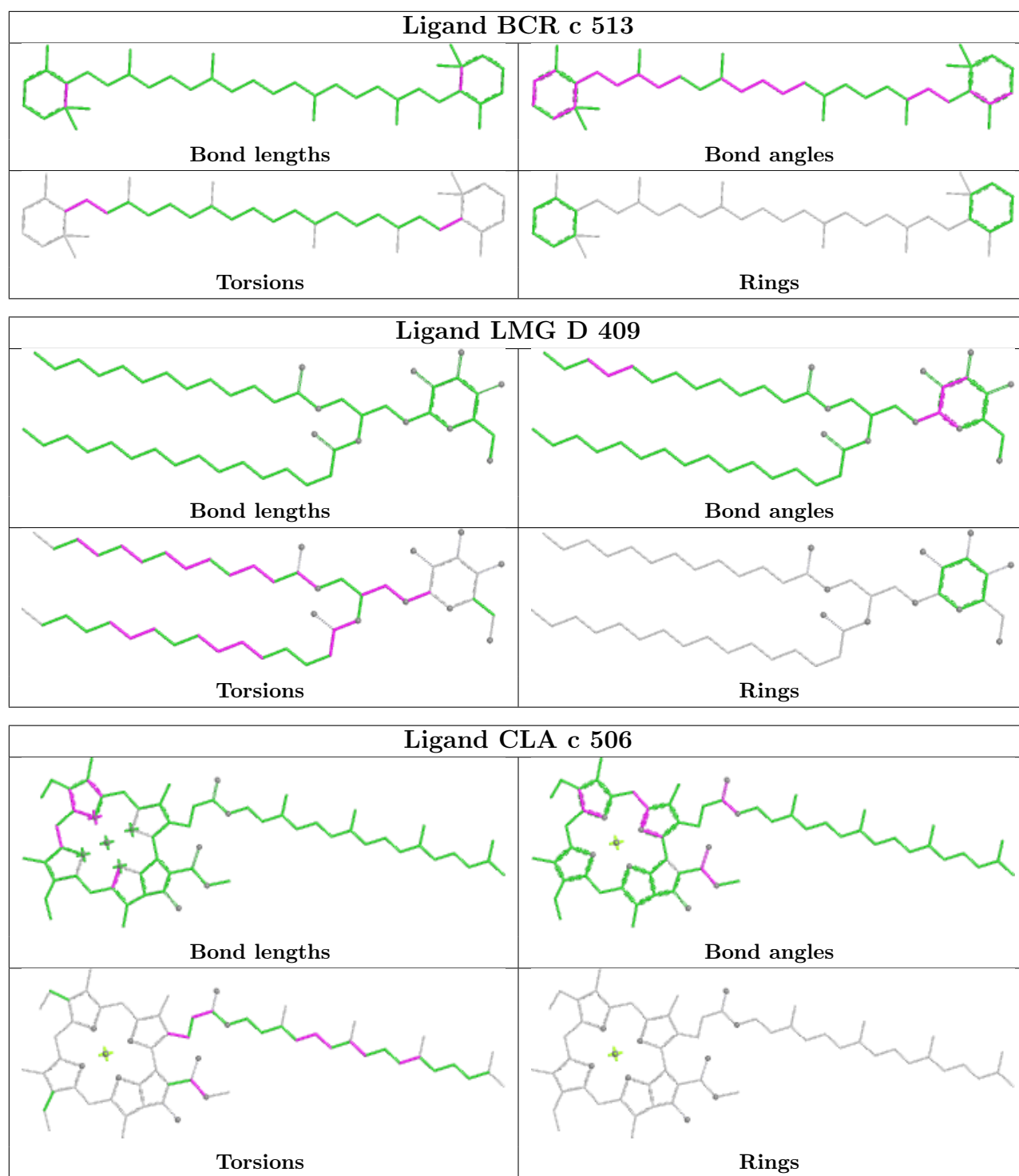
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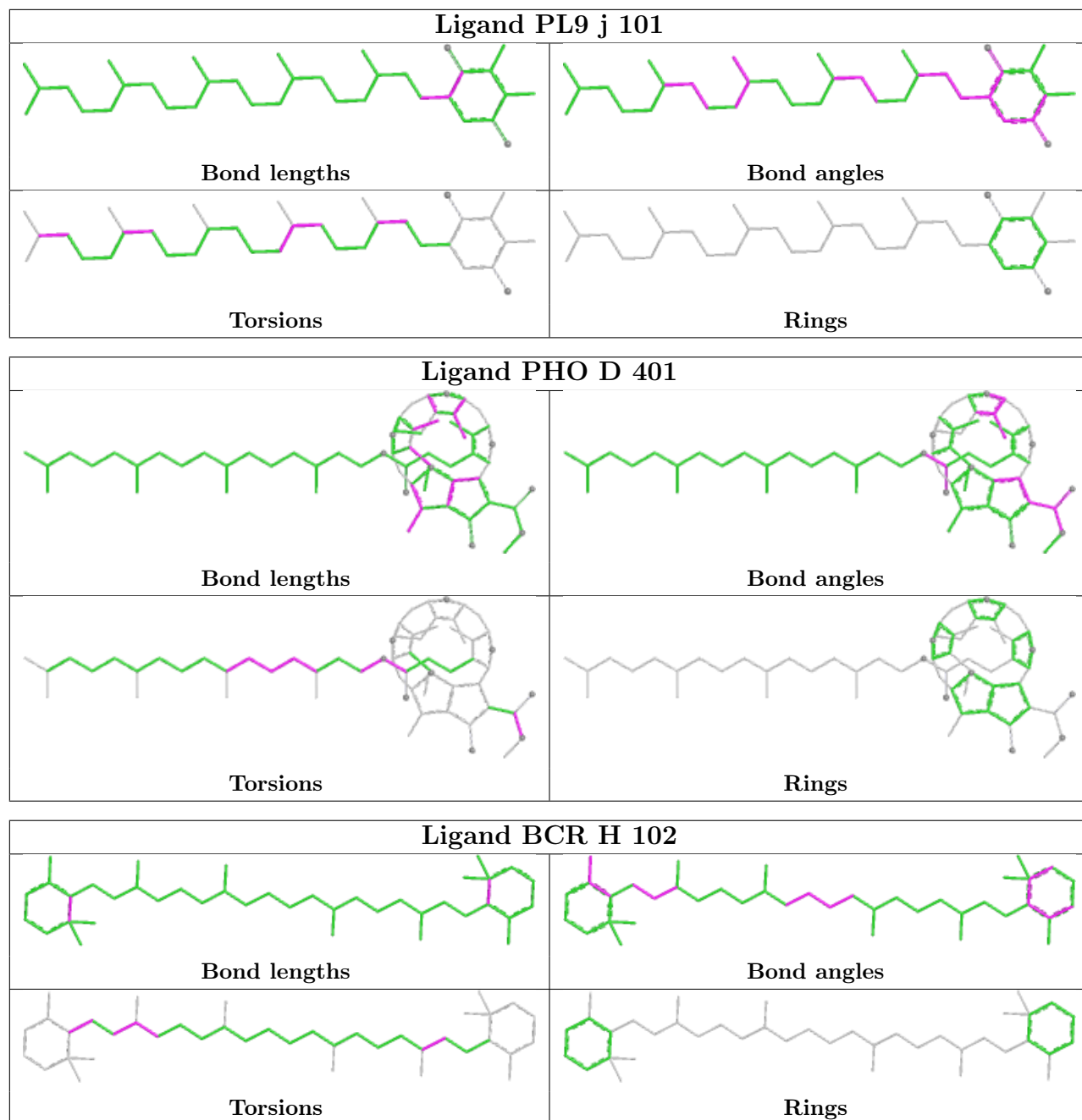
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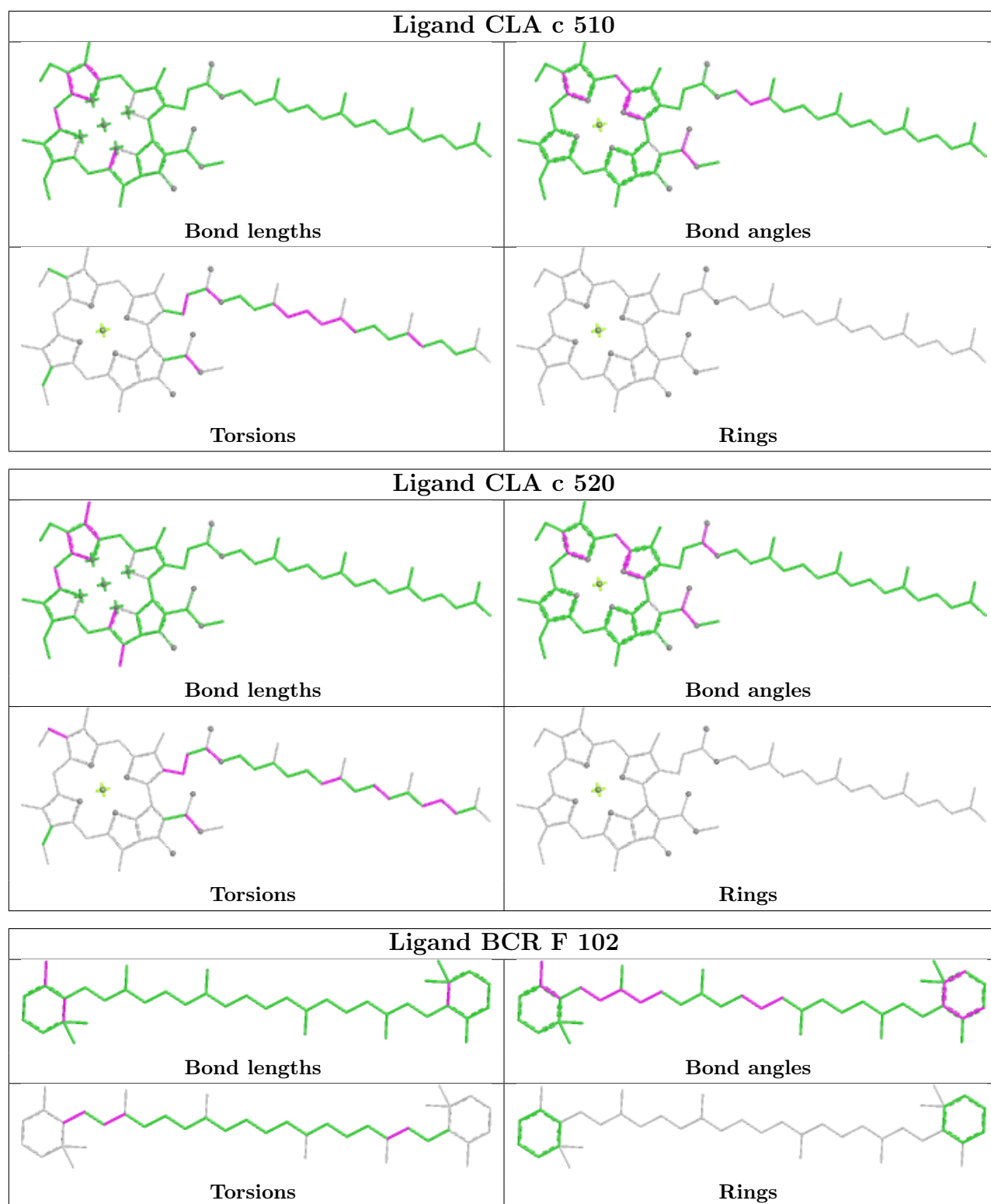
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | b     | 620 | BCR  | 6       | 0            |
| 25  | C     | 515 | DGD  | 3       | 0            |
| 26  | C     | 519 | LHG  | 2       | 0            |
| 25  | d     | 410 | DGD  | 2       | 0            |
| 22  | C     | 512 | CLA  | 3       | 0            |
| 22  | c     | 511 | CLA  | 2       | 0            |
| 27  | D     | 412 | LMG  | 1       | 0            |
| 24  | b     | 622 | BCR  | 3       | 0            |
| 29  | a     | 415 | SQD  | 3       | 0            |
| 24  | b     | 621 | BCR  | 1       | 0            |

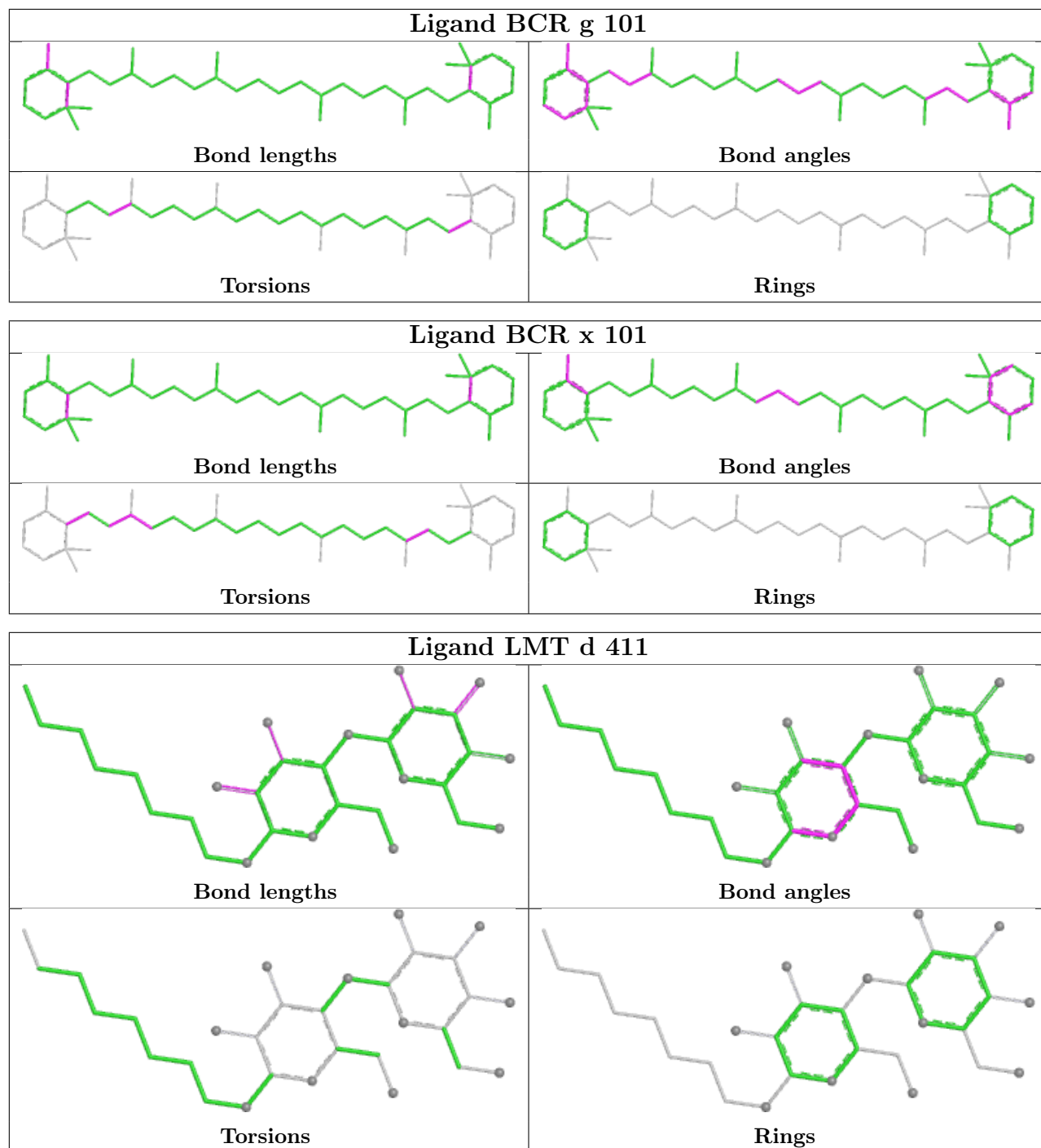
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

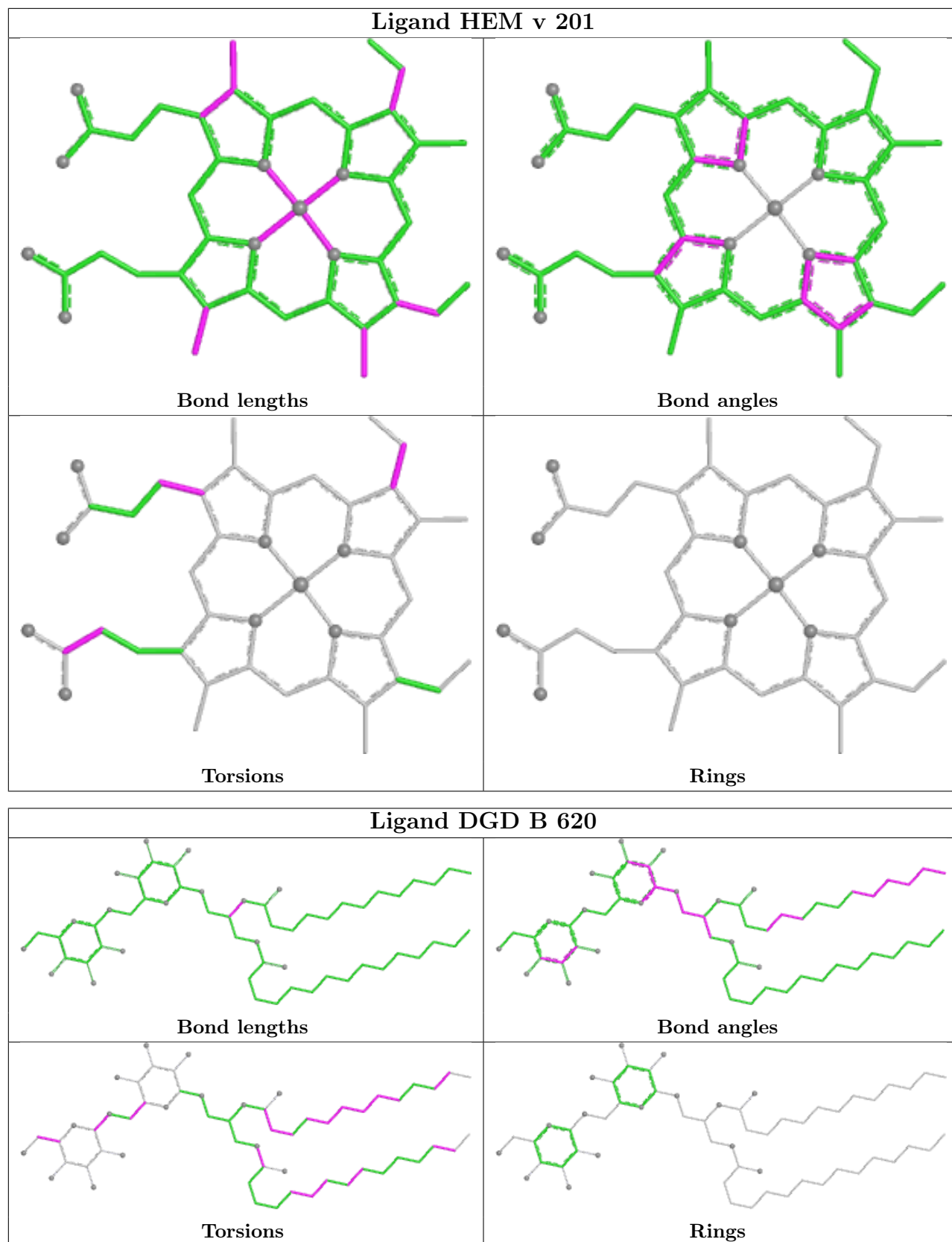


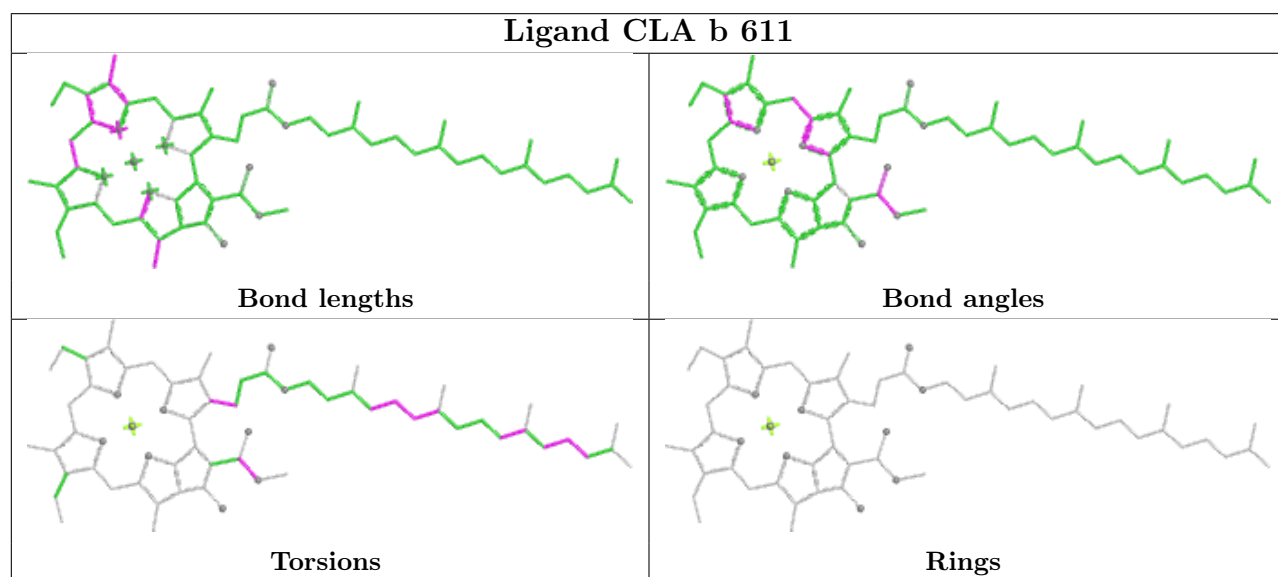
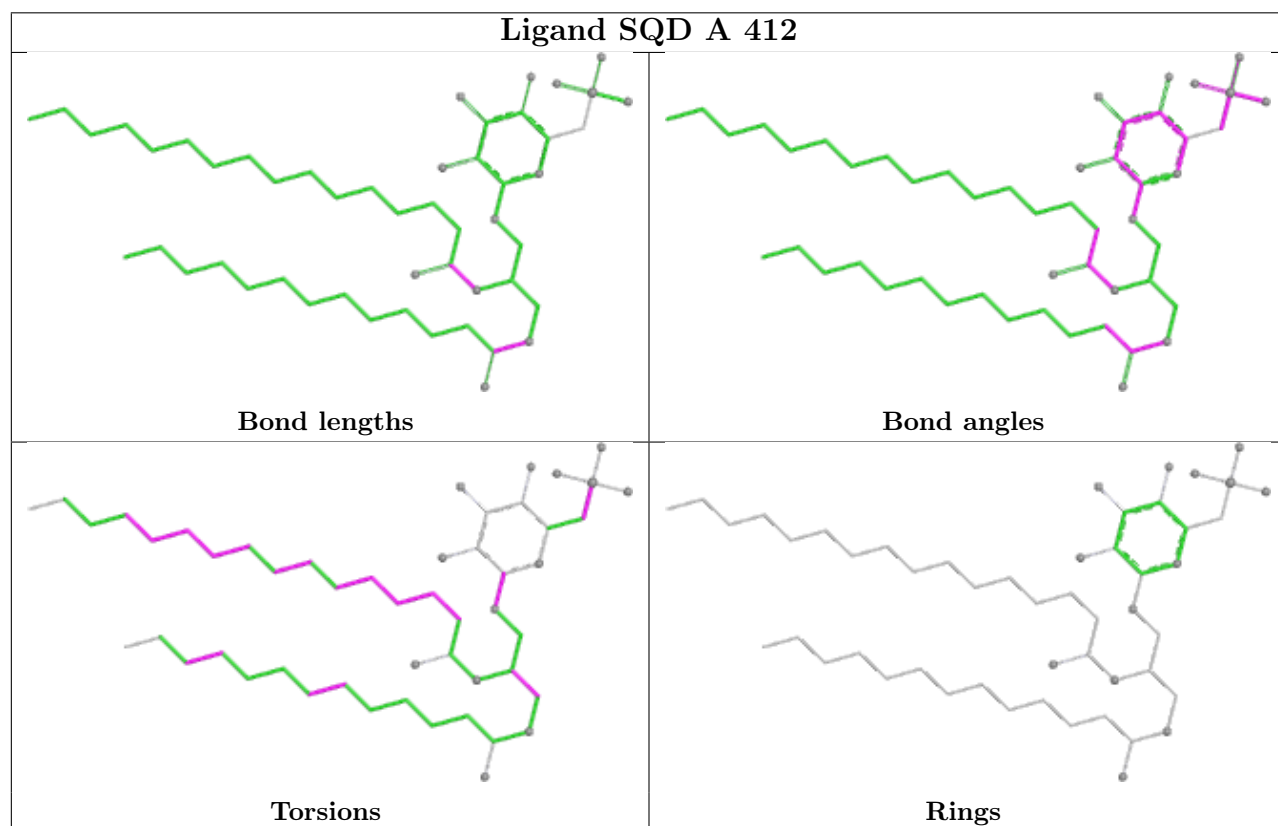
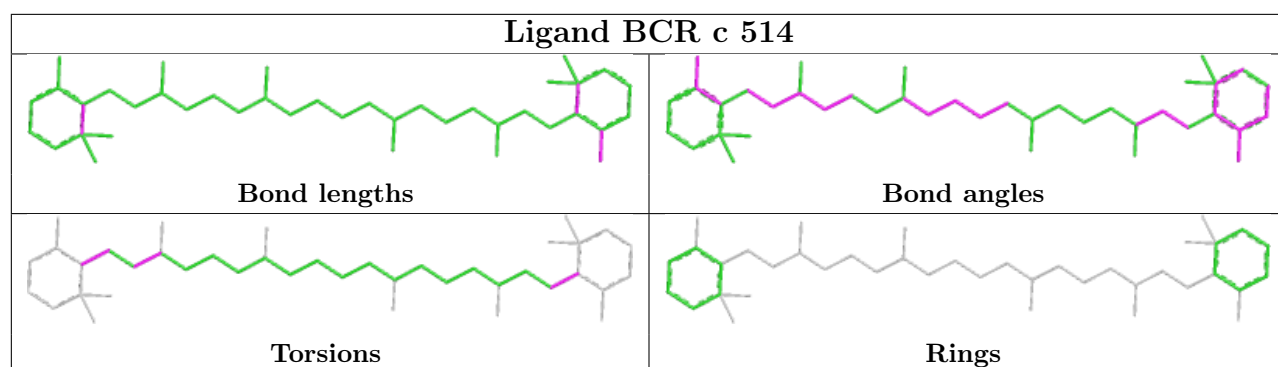




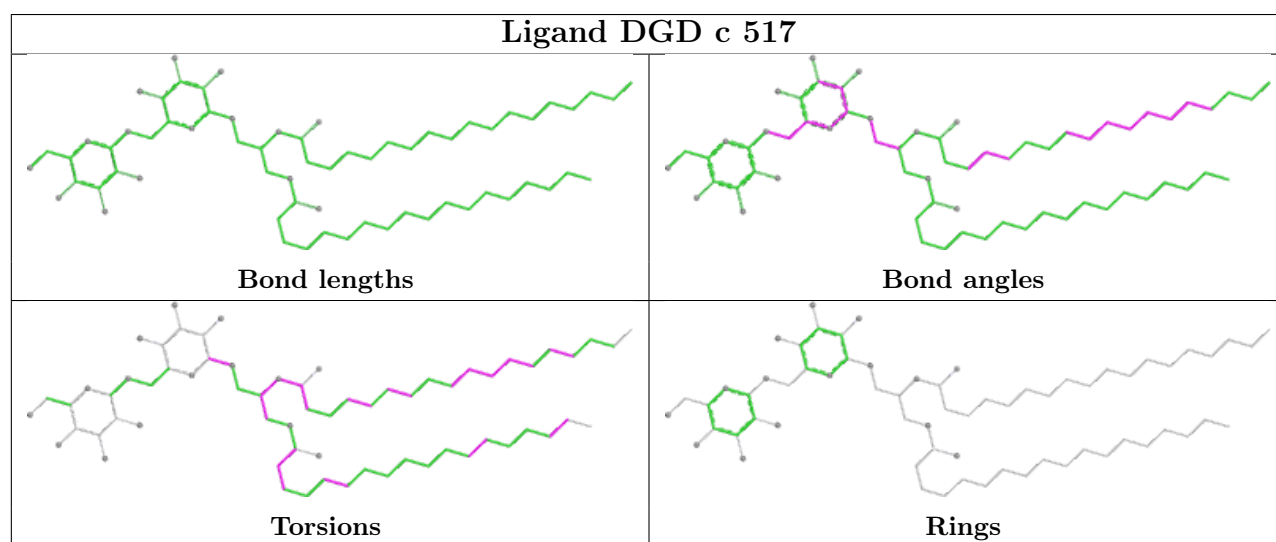
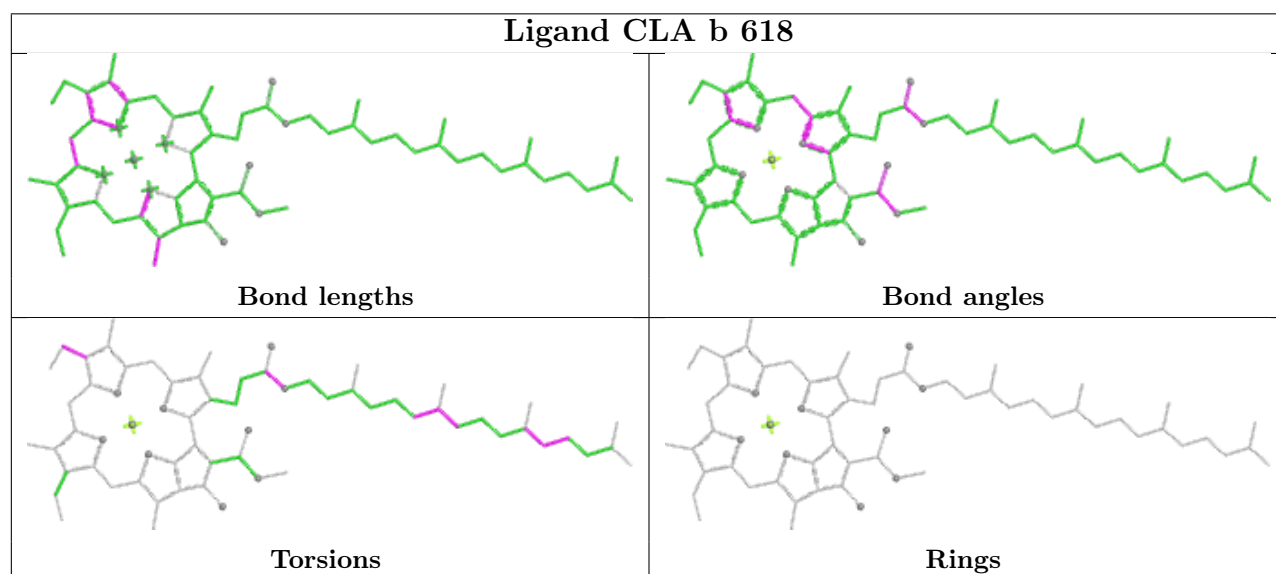
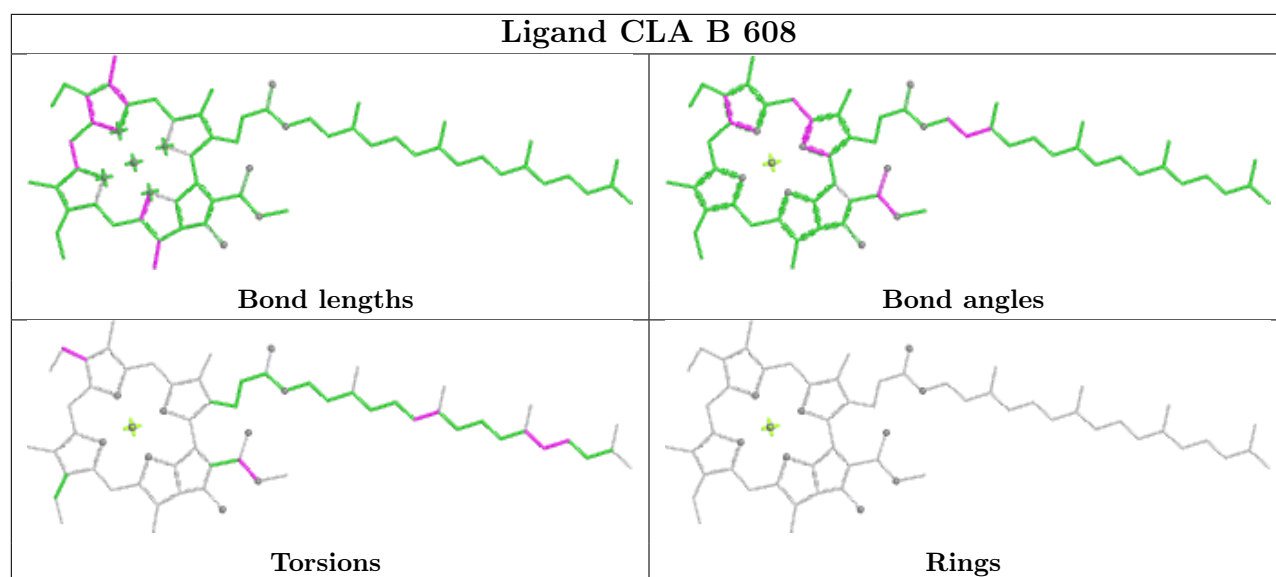


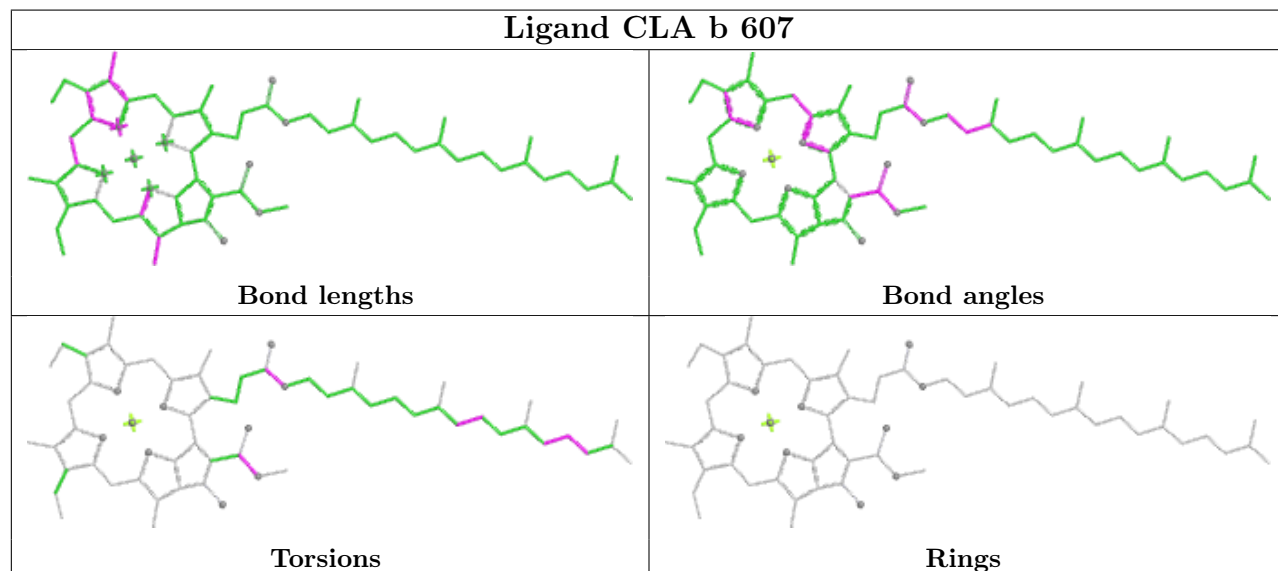
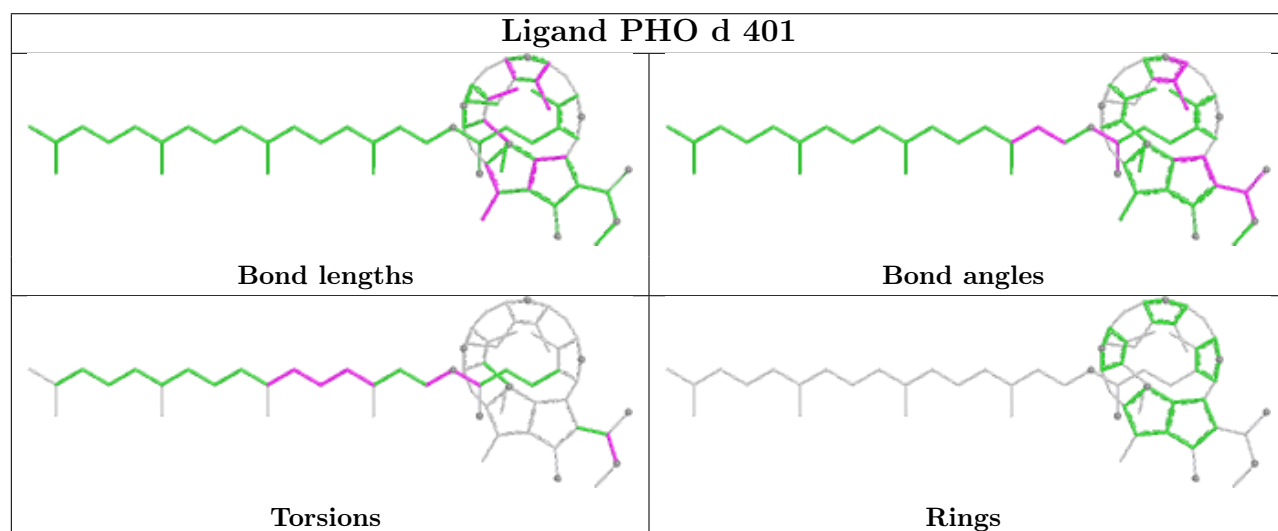
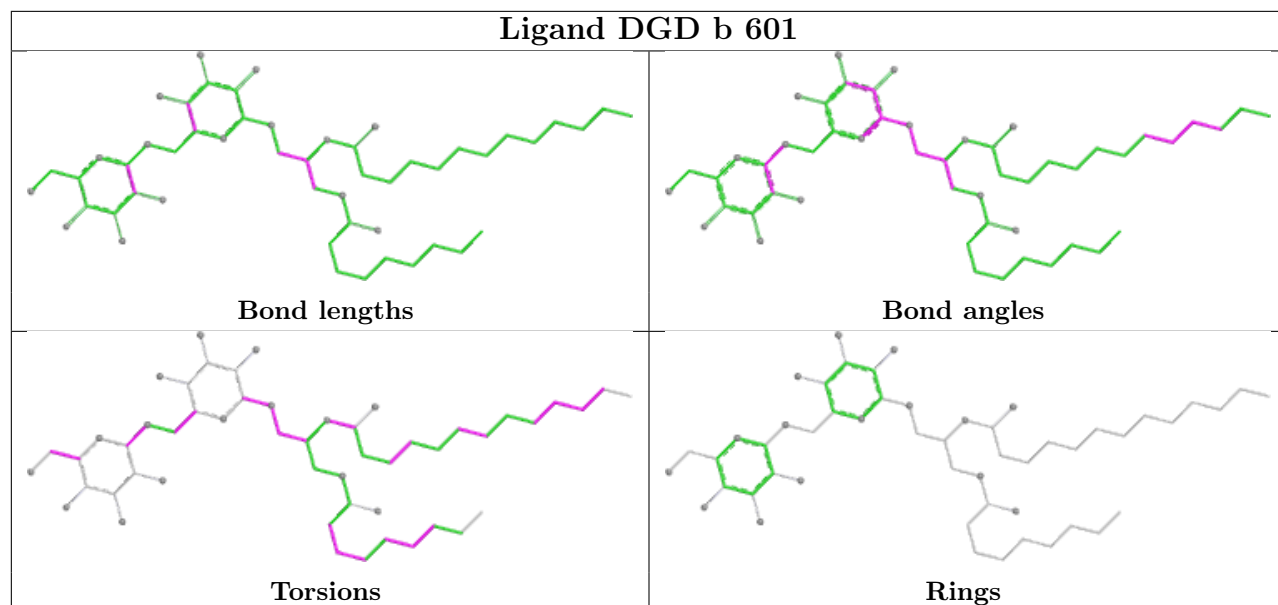


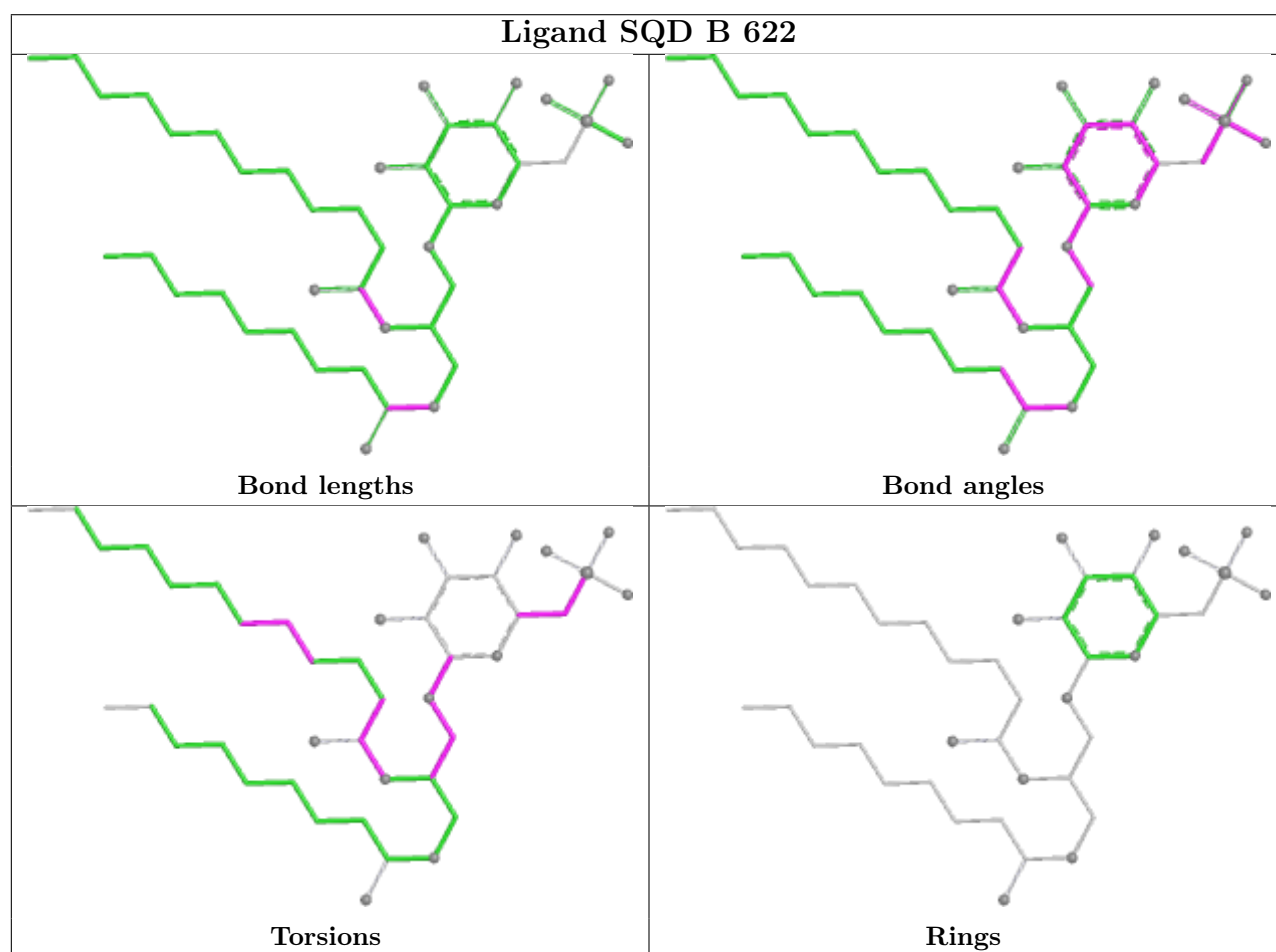
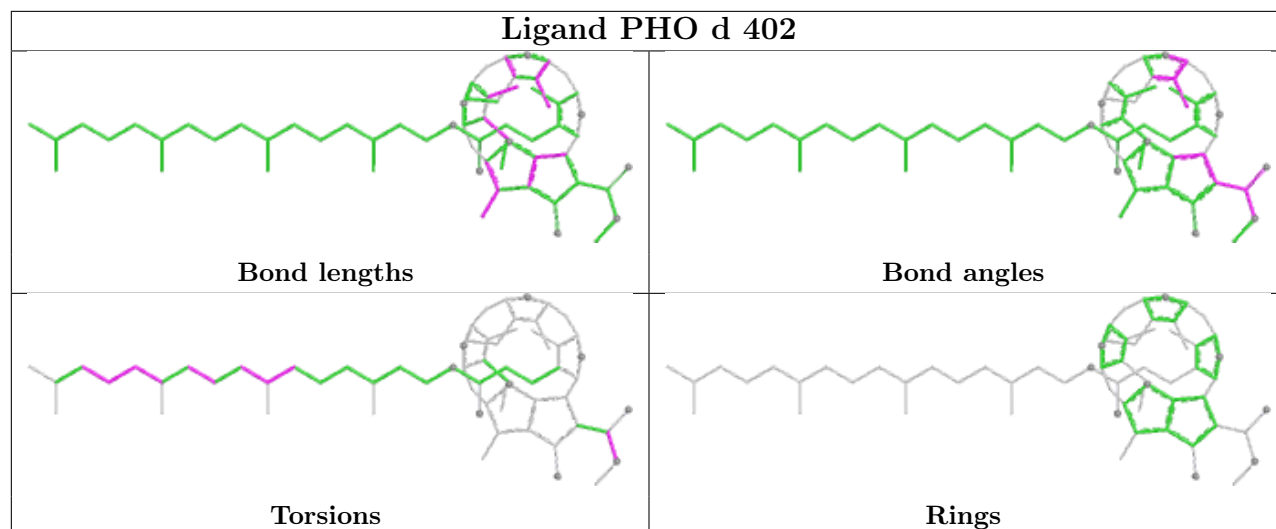


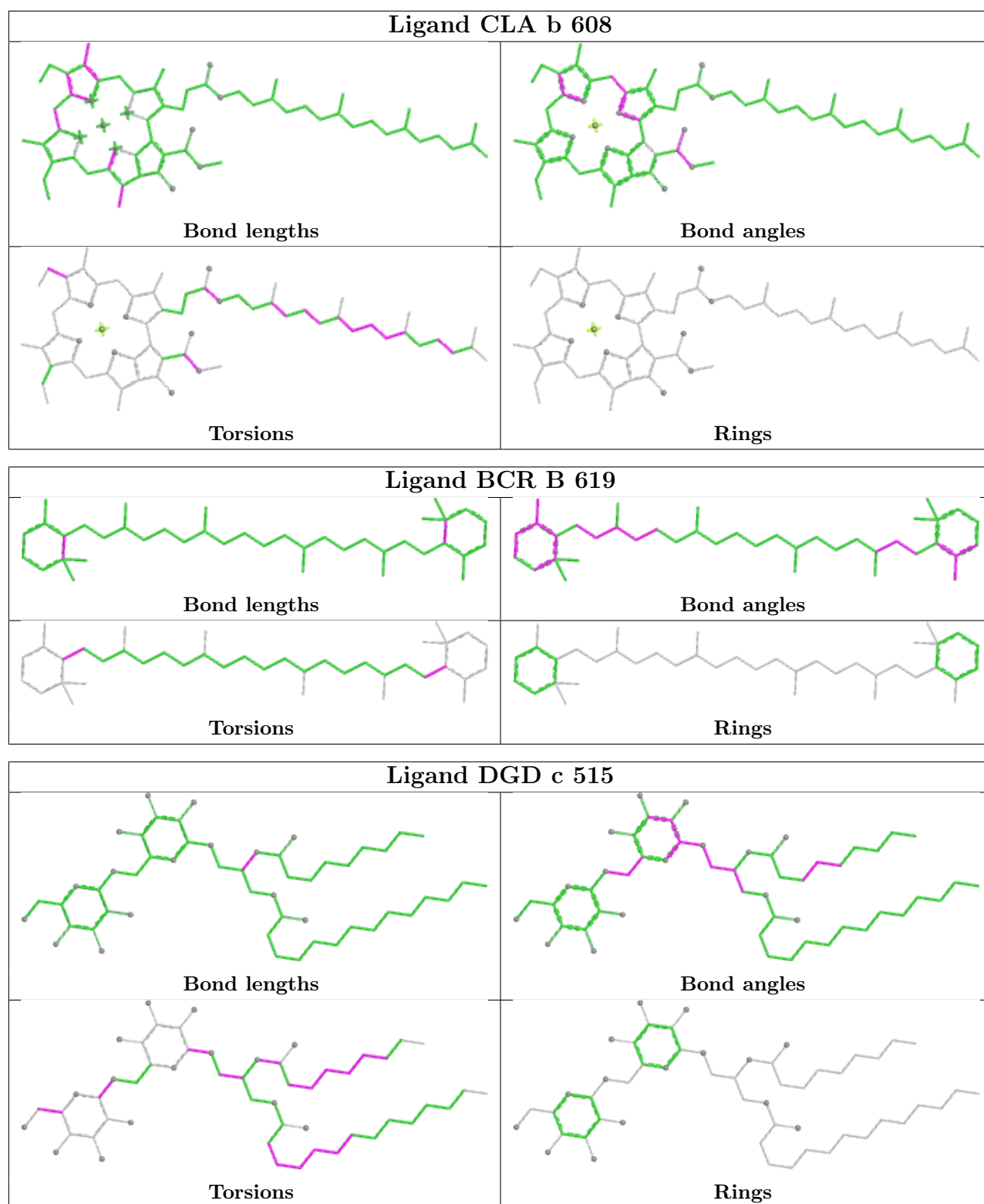


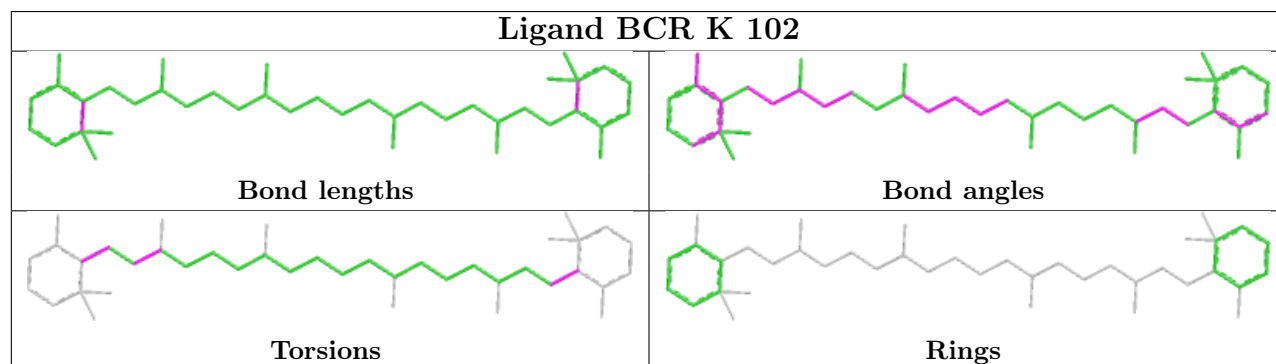
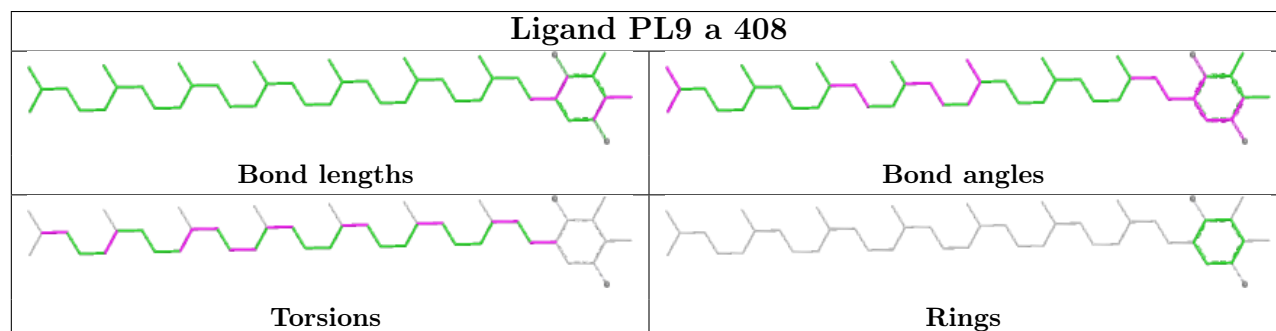
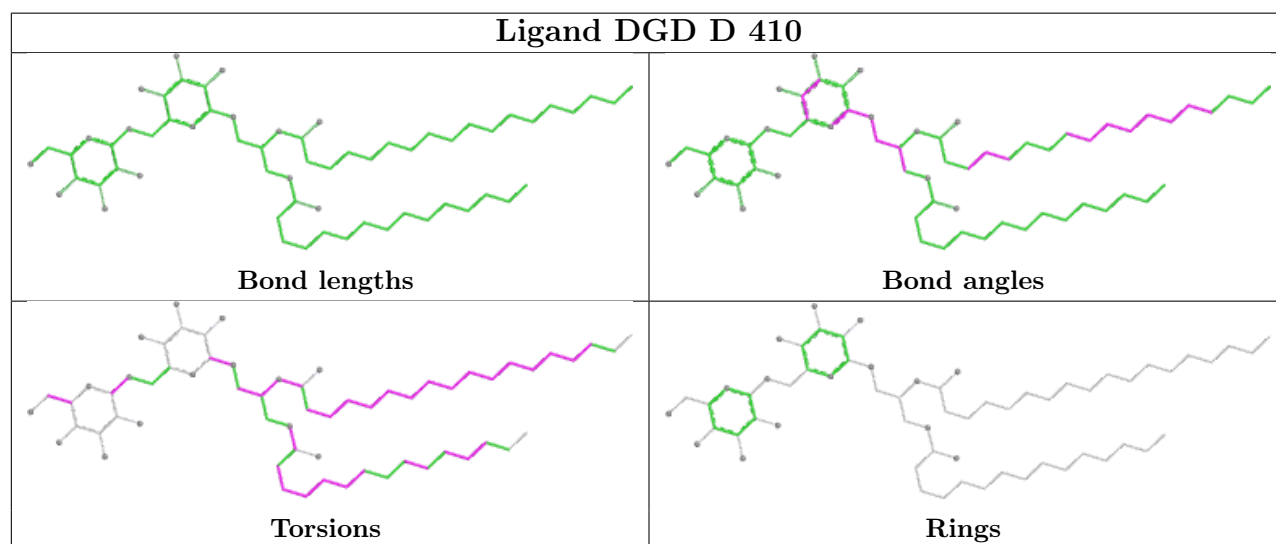
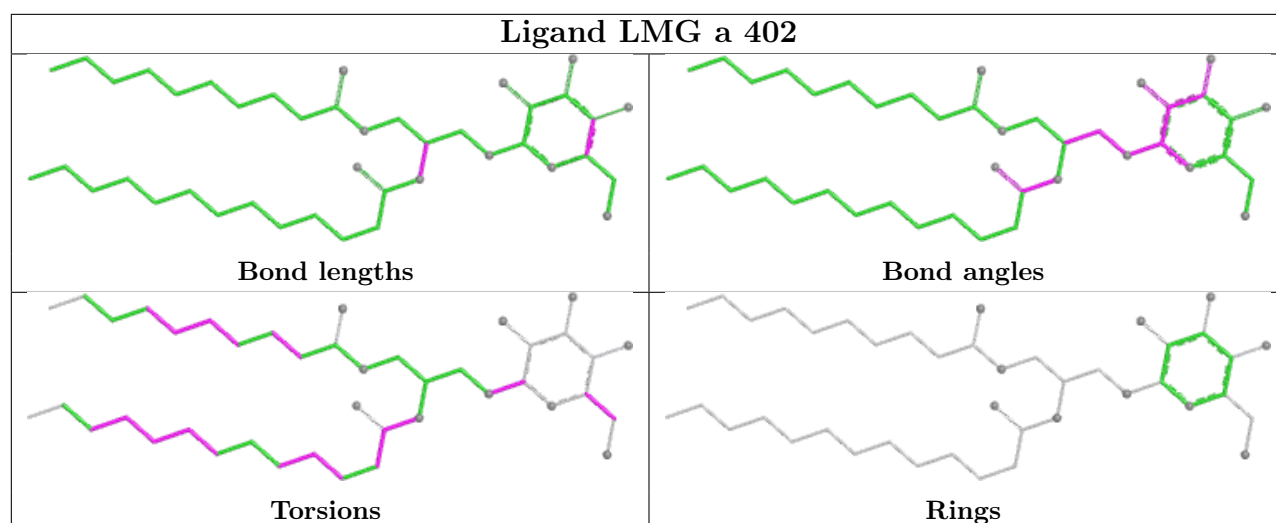




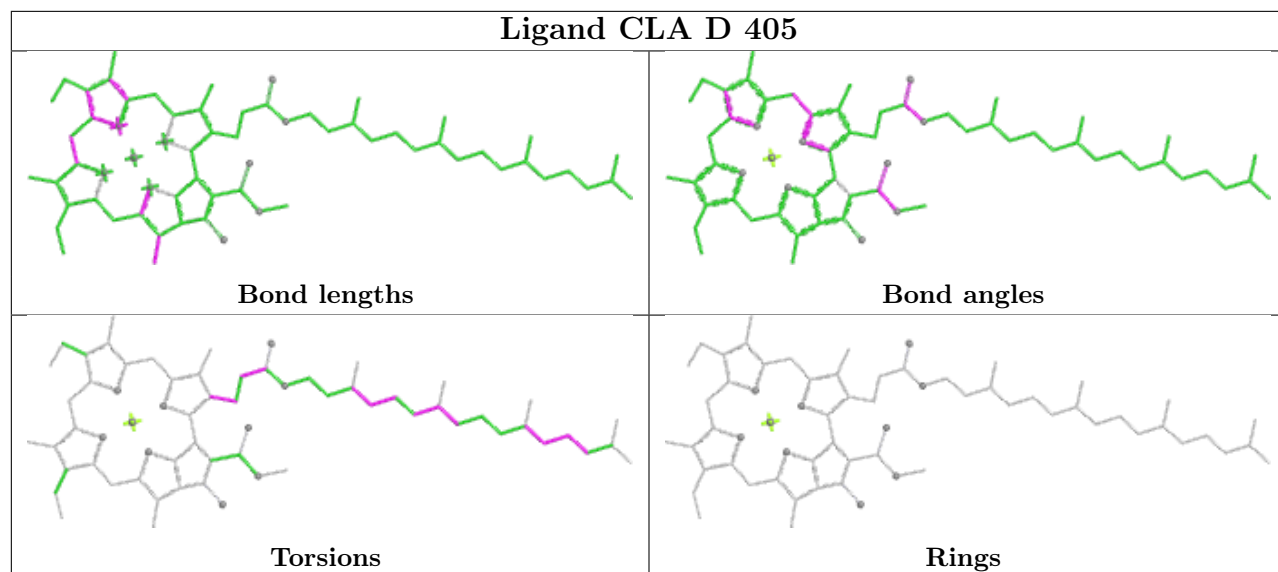




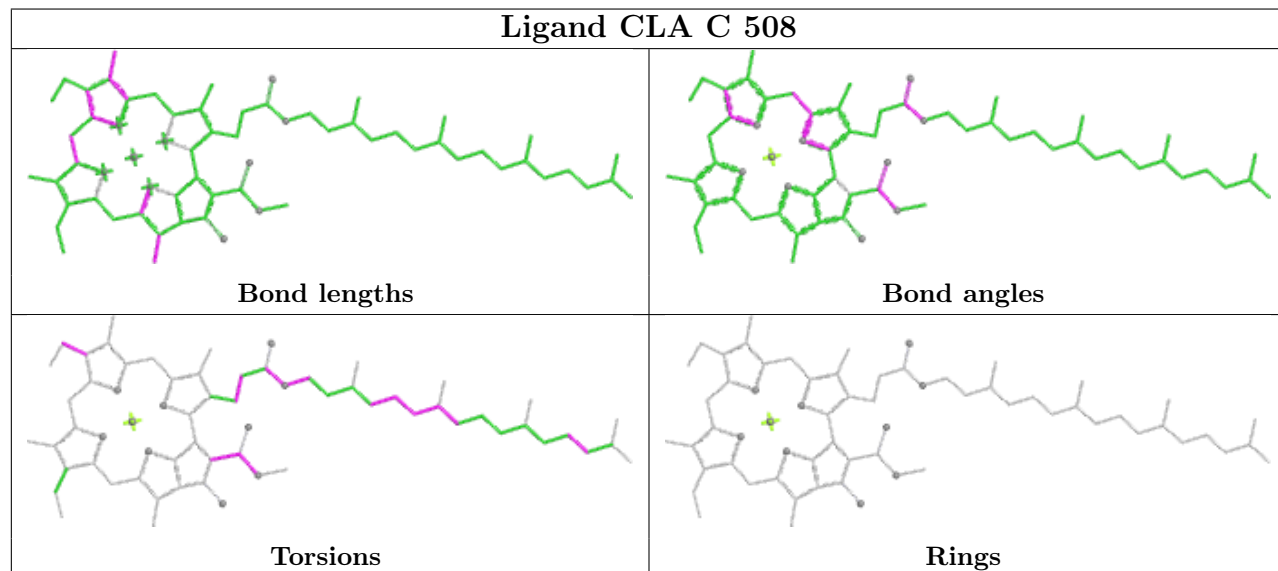




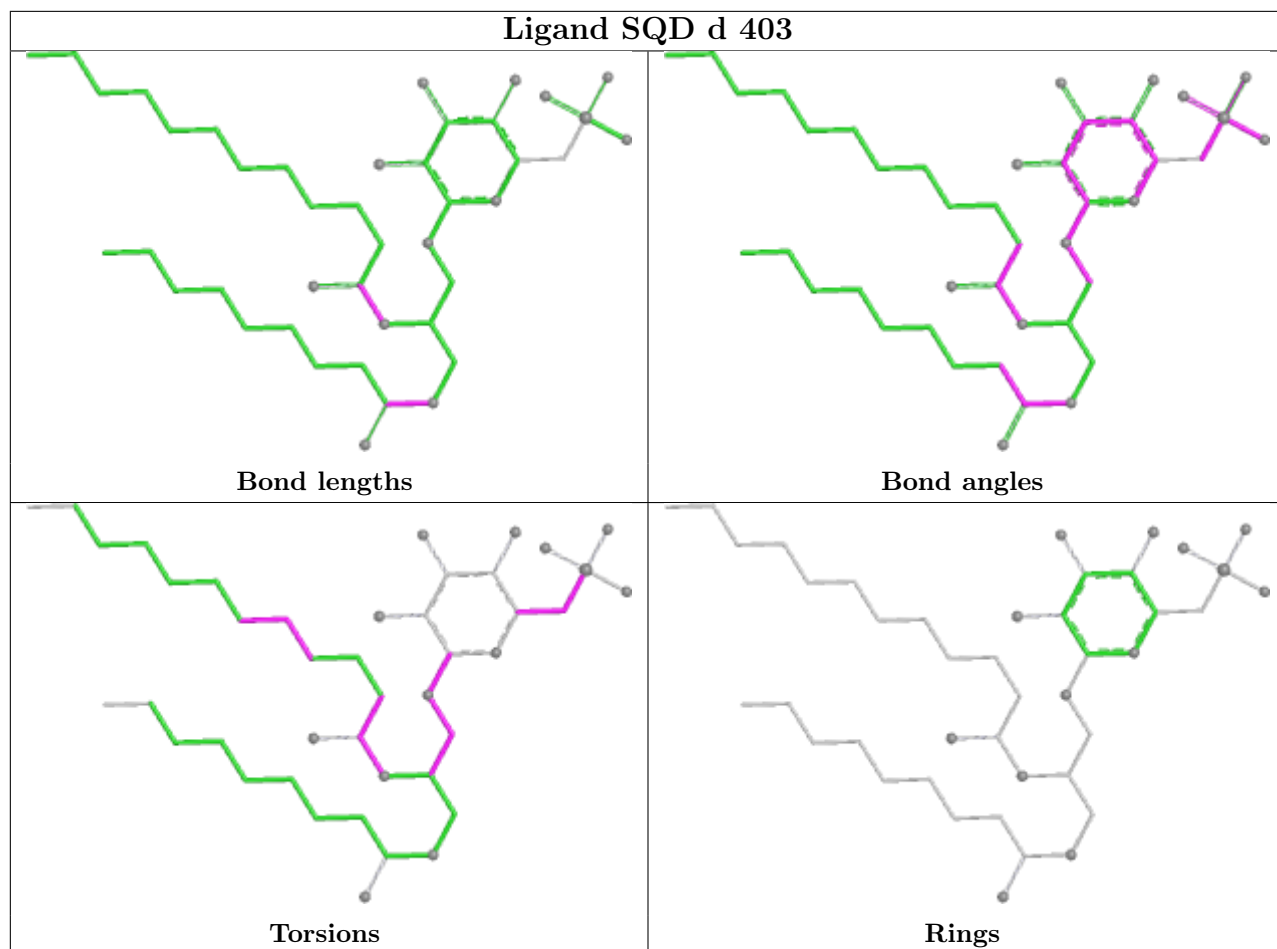
## Ligand CLA D 405



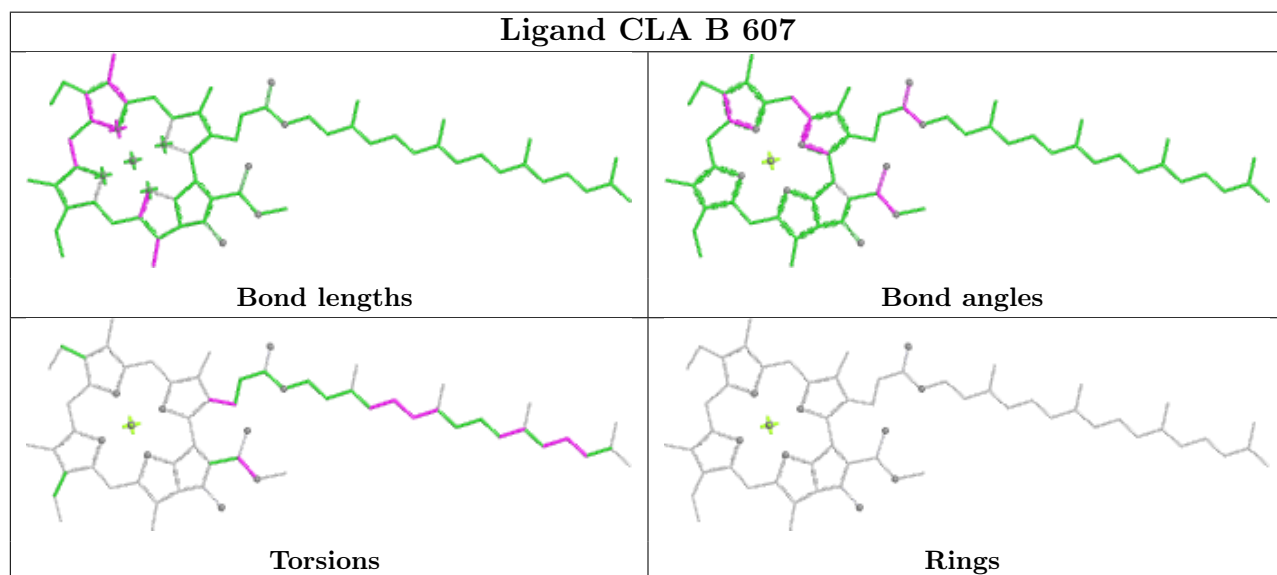
## Ligand CLA C 508



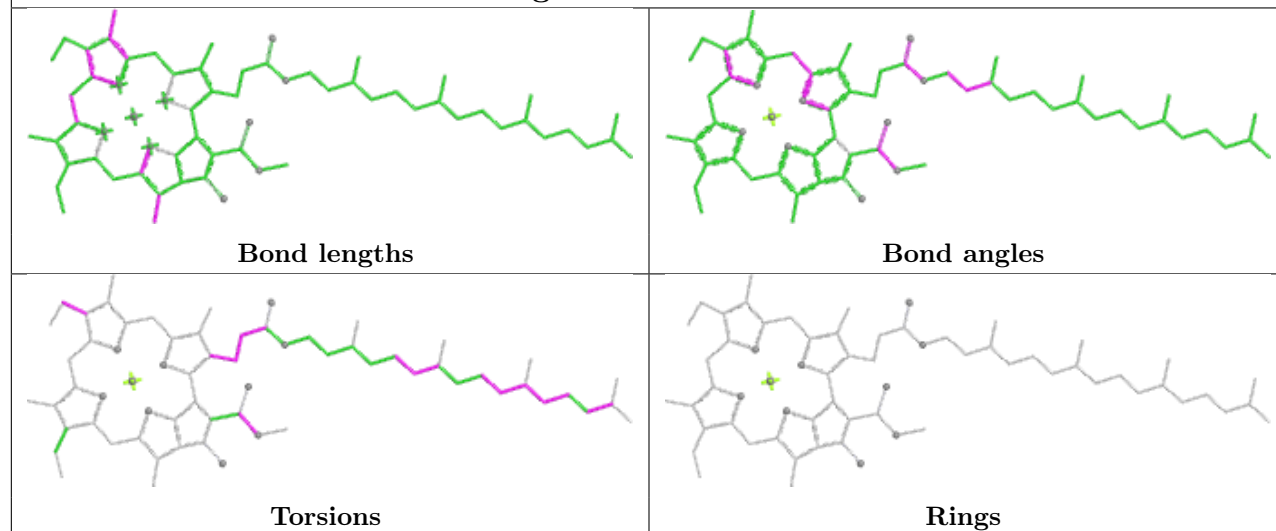
## Ligand SQD d 403



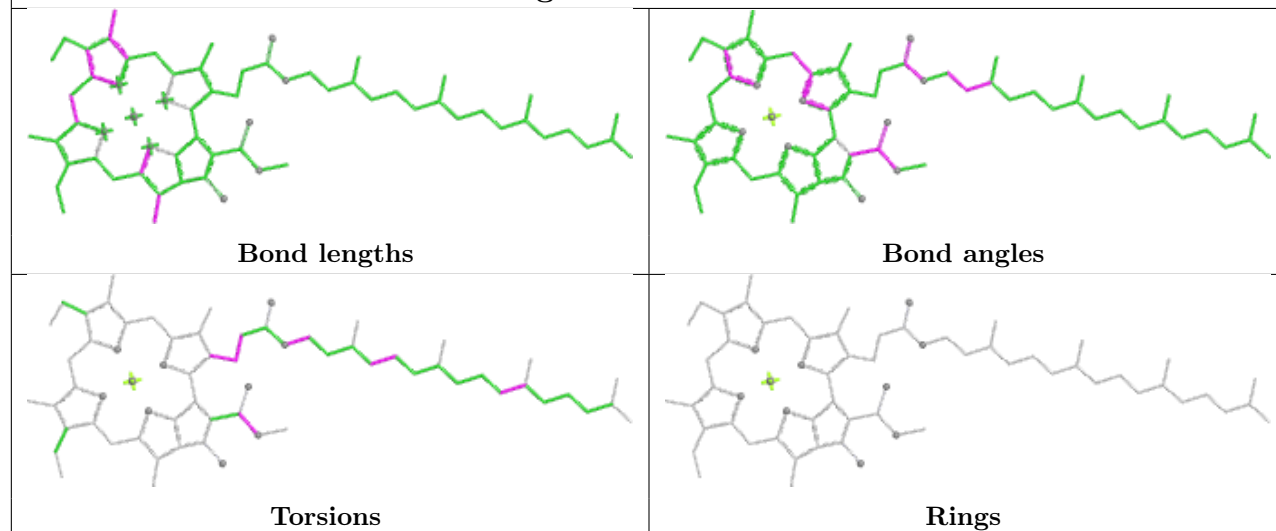
## Ligand CLA B 607



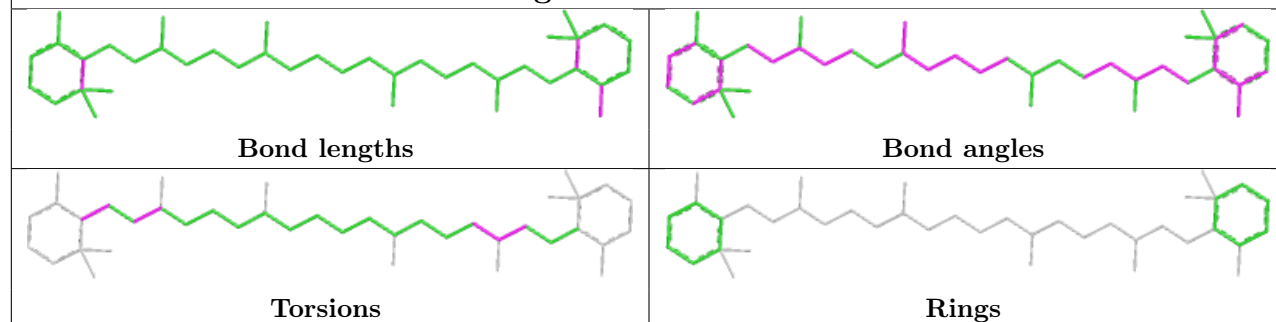
## Ligand CLA B 601



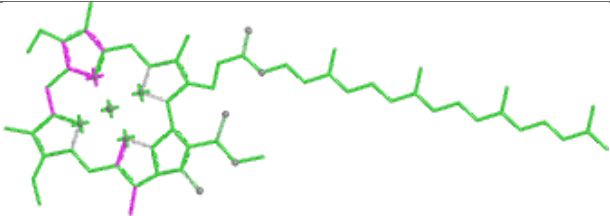
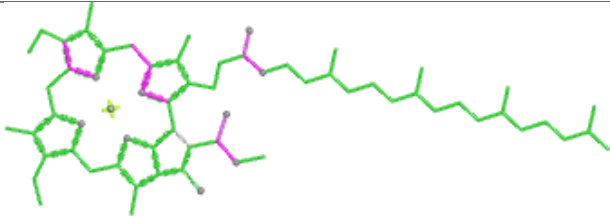
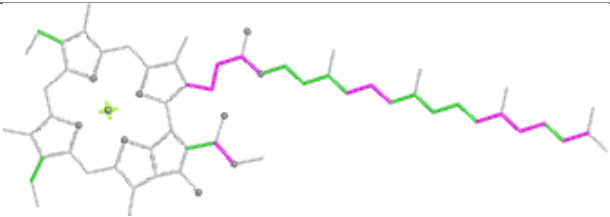
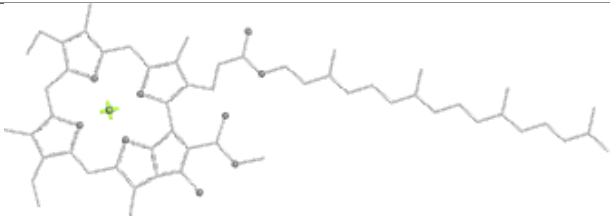
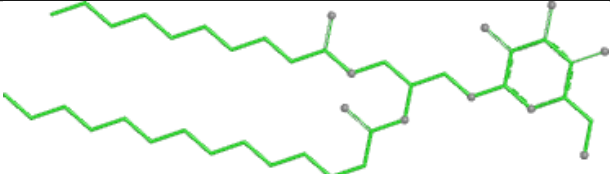
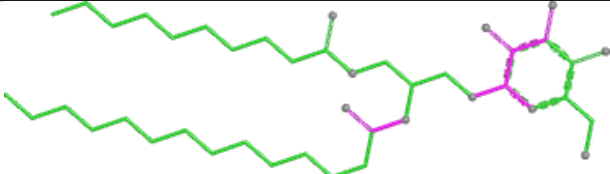
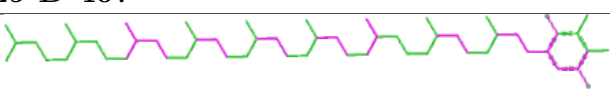
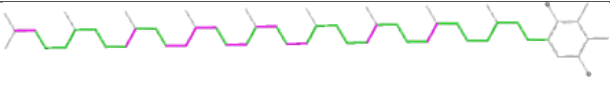
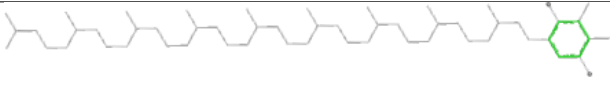
## Ligand CLA a 404

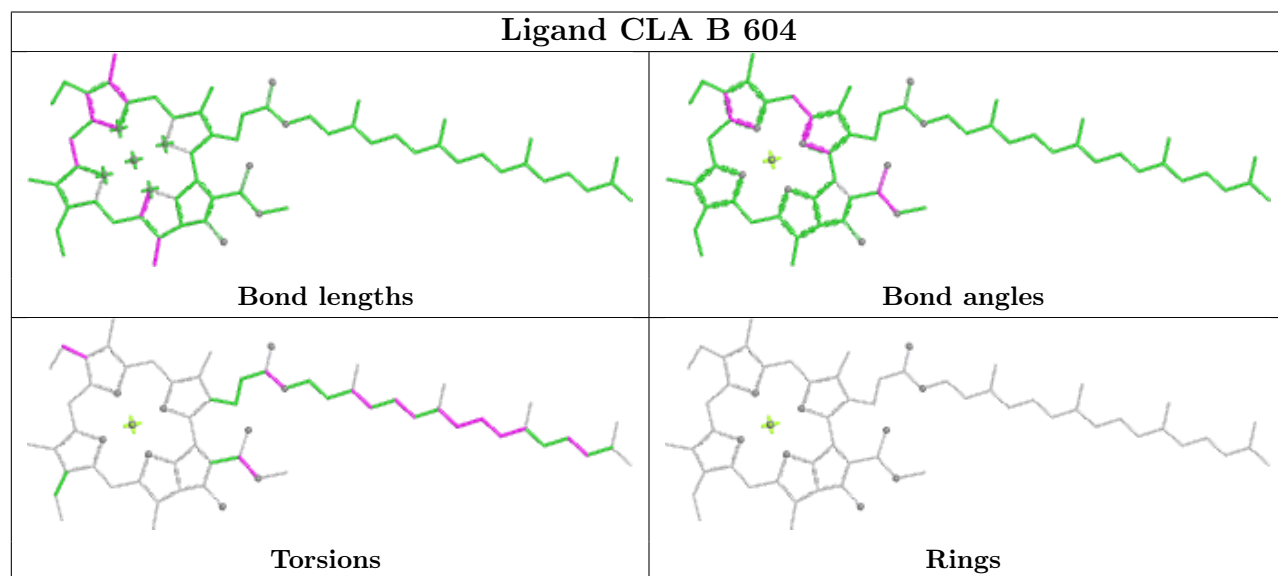
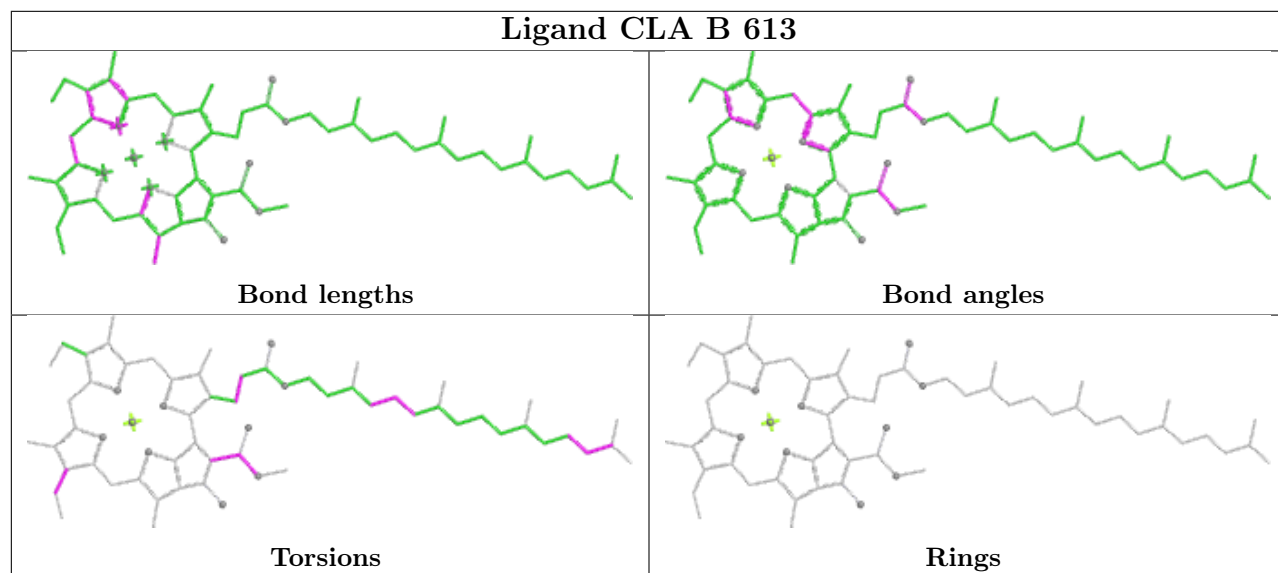
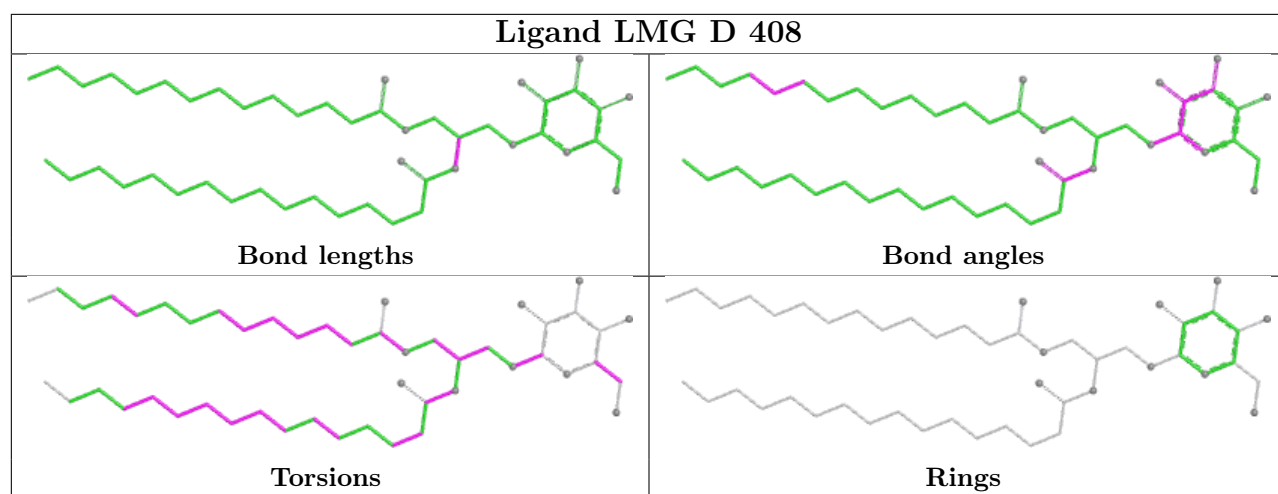


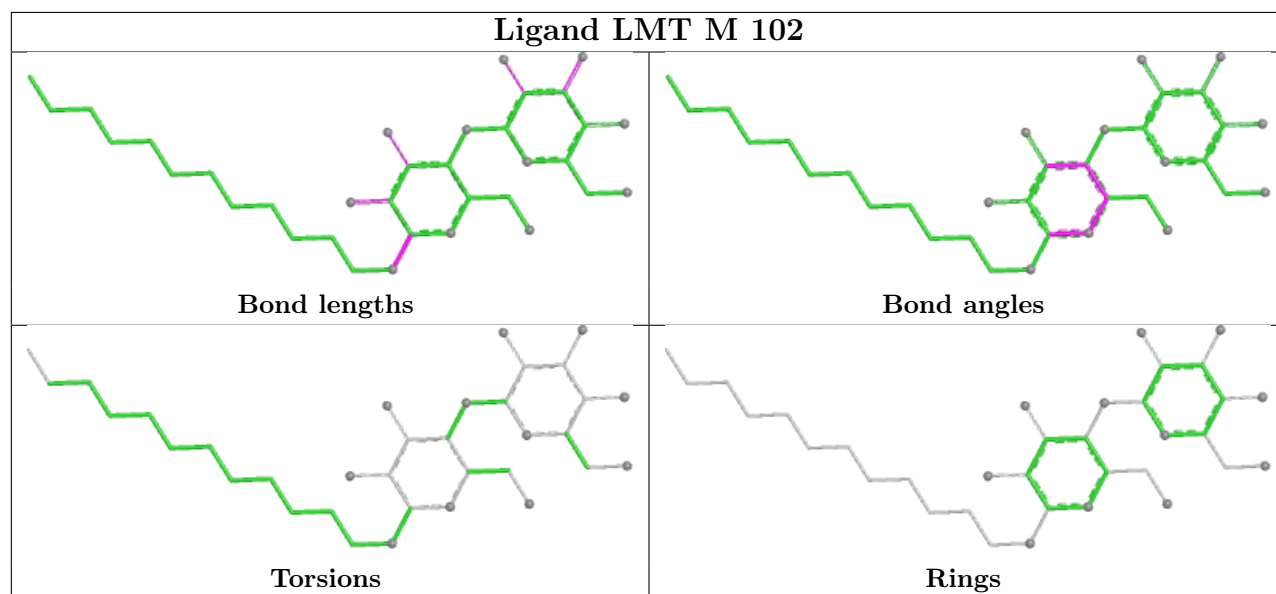
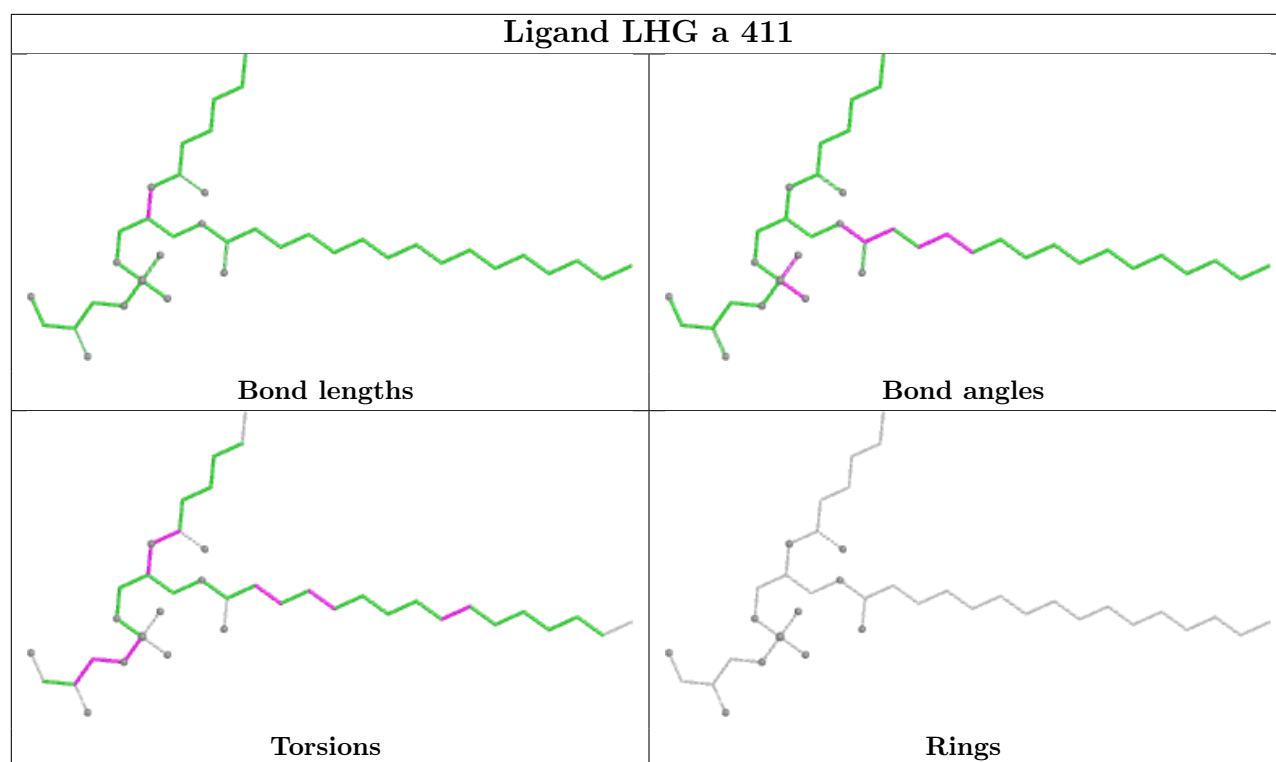
## Ligand BCR J 102

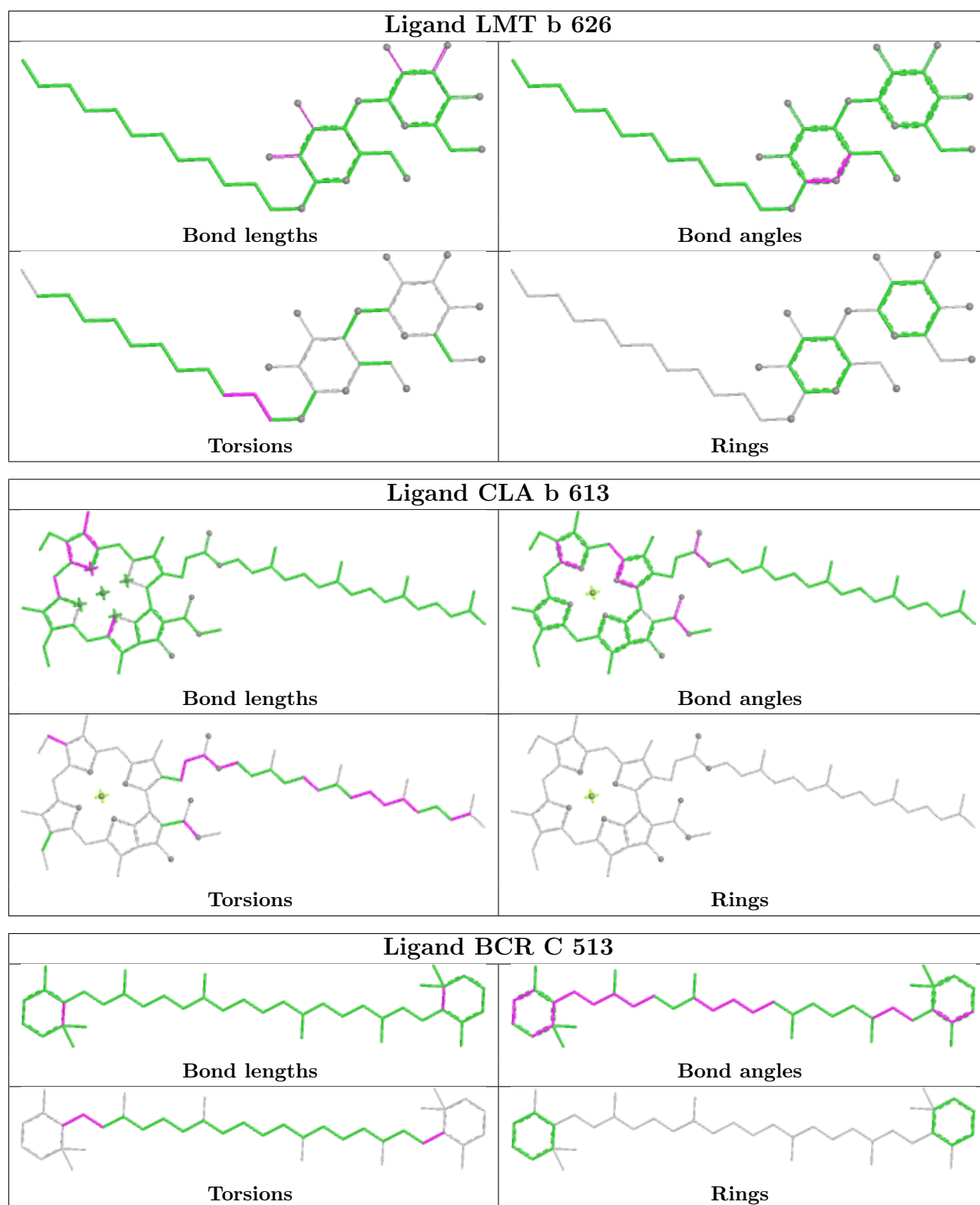




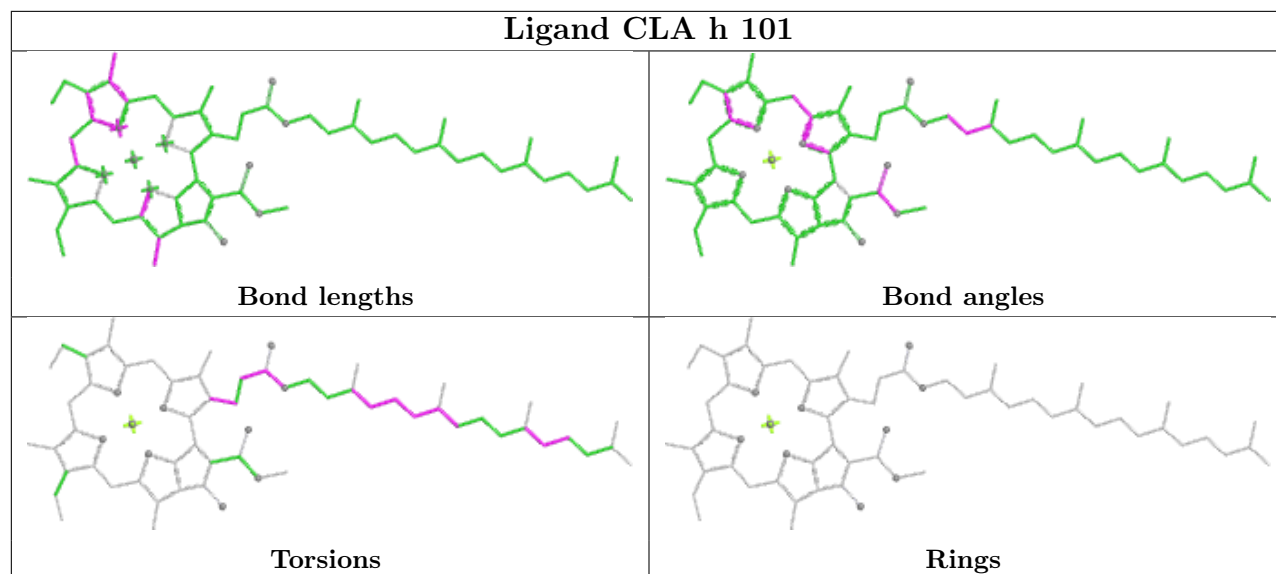
| Ligand CLA C 511                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMG I 101                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand PL9 D 407                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |



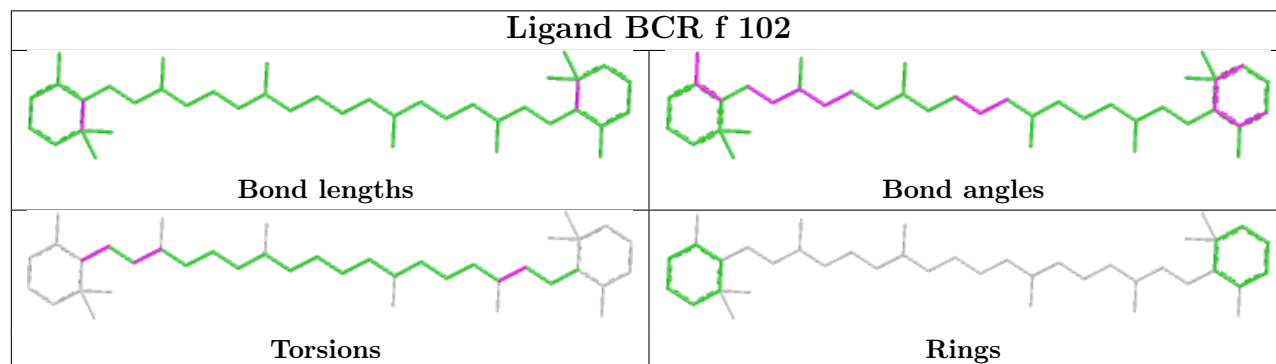




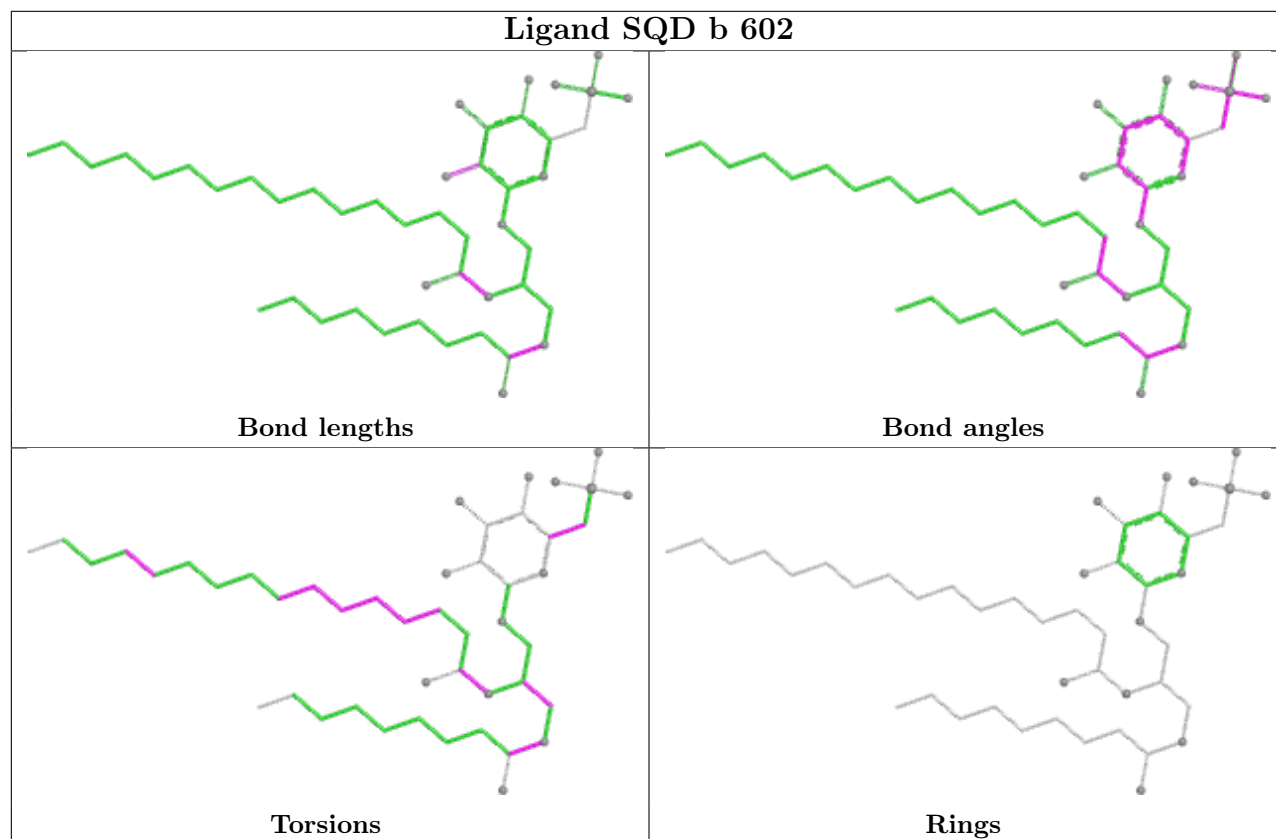
## Ligand CLA h 101

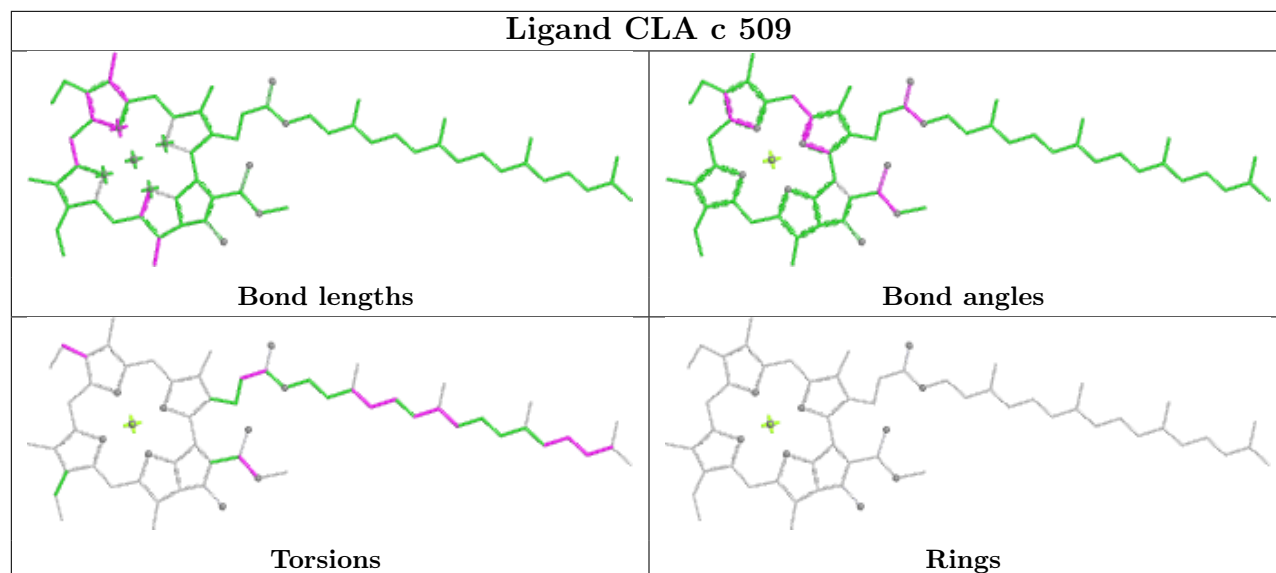
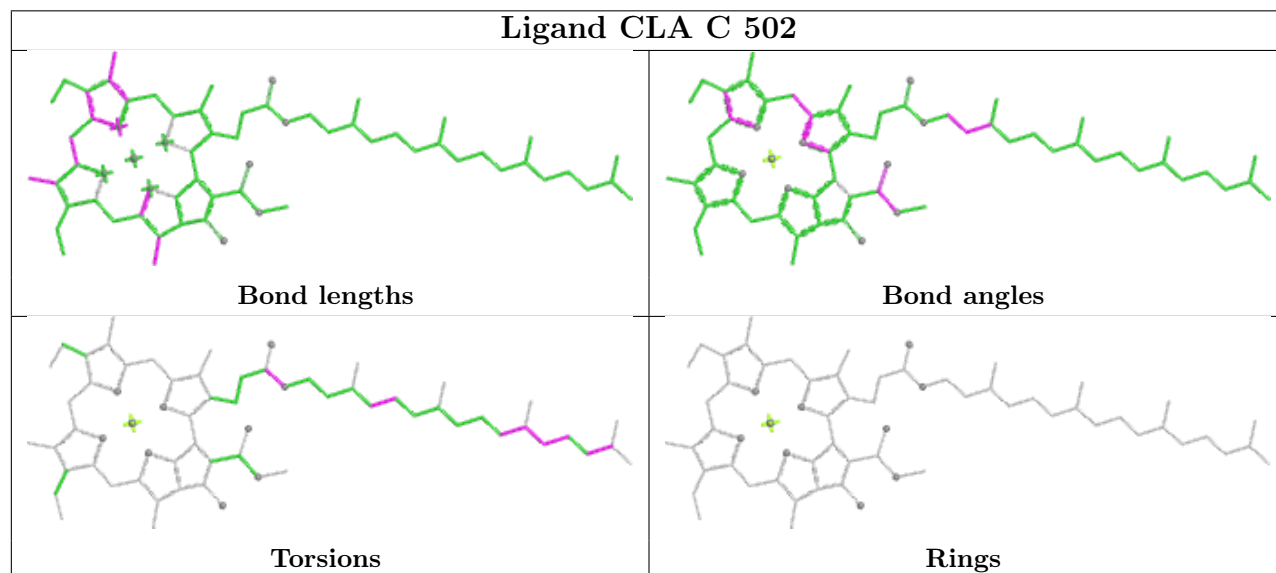
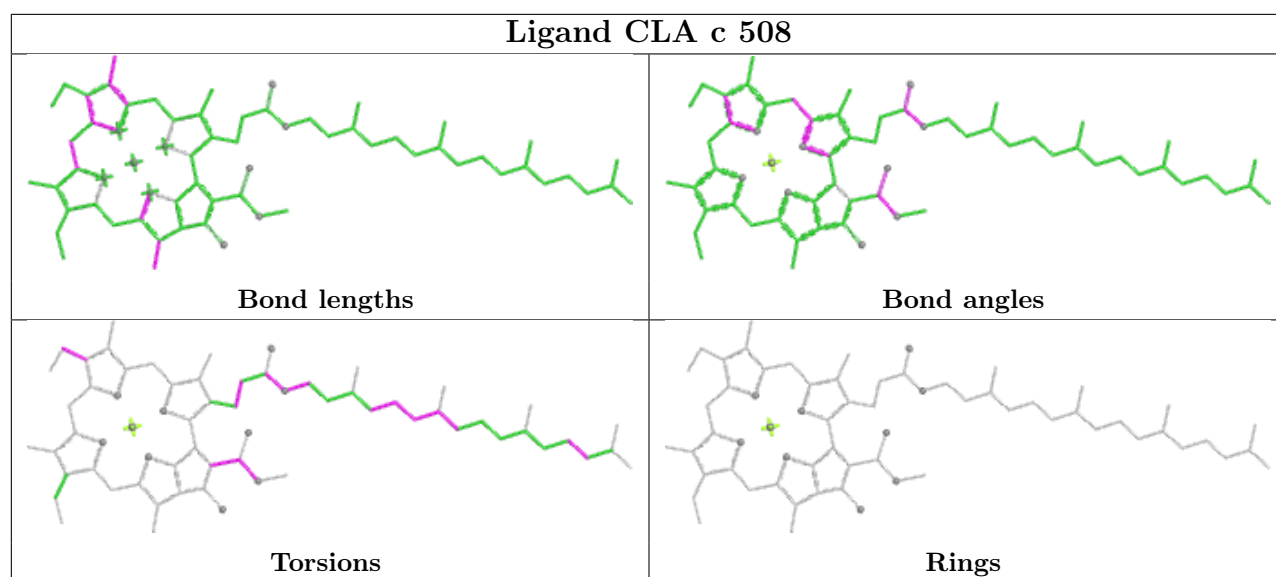


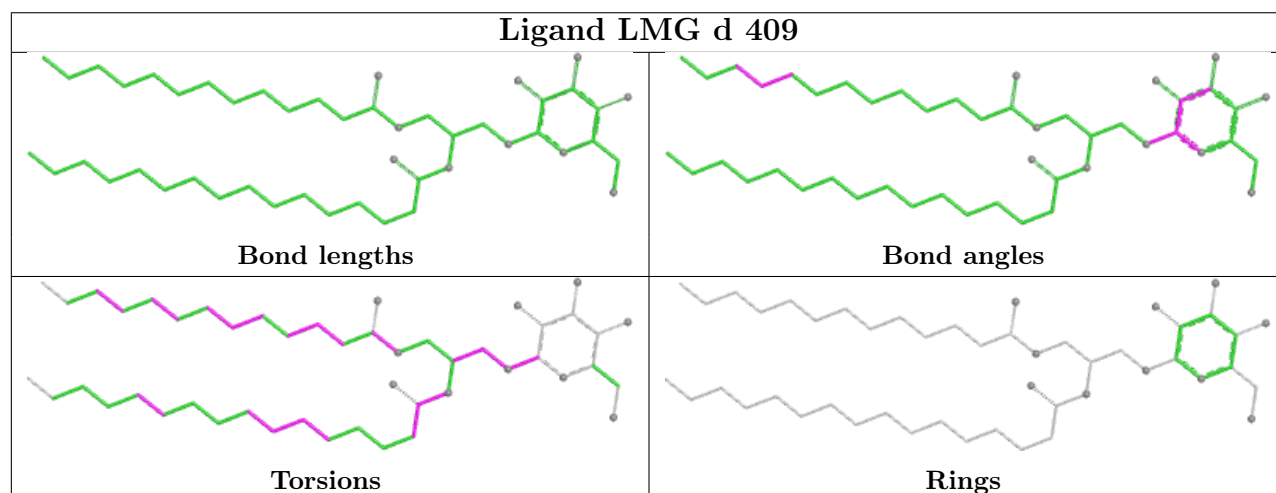
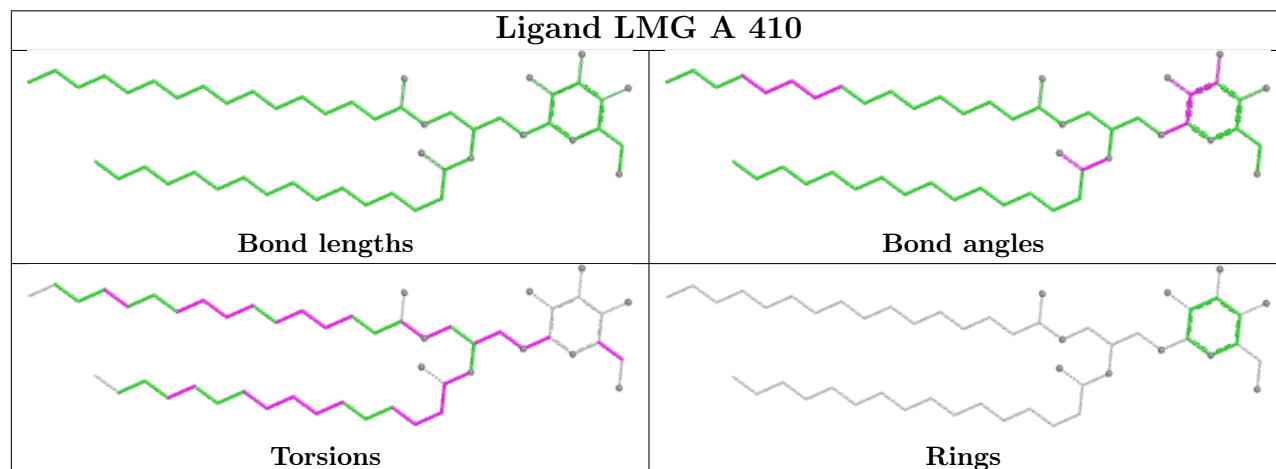
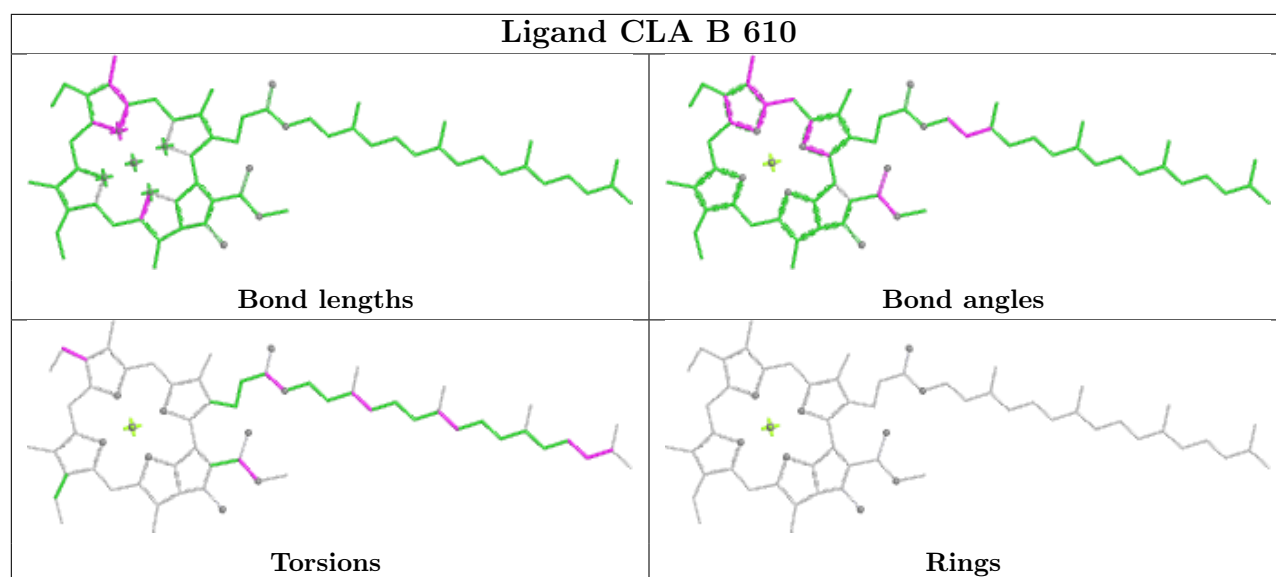
## Ligand BCR f 102

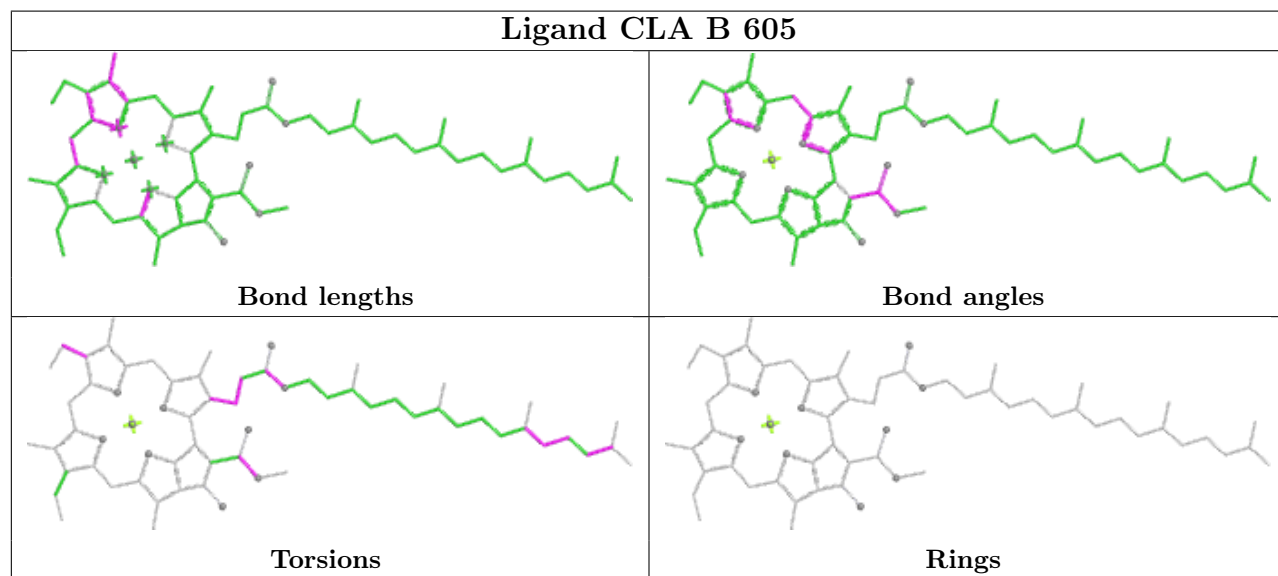
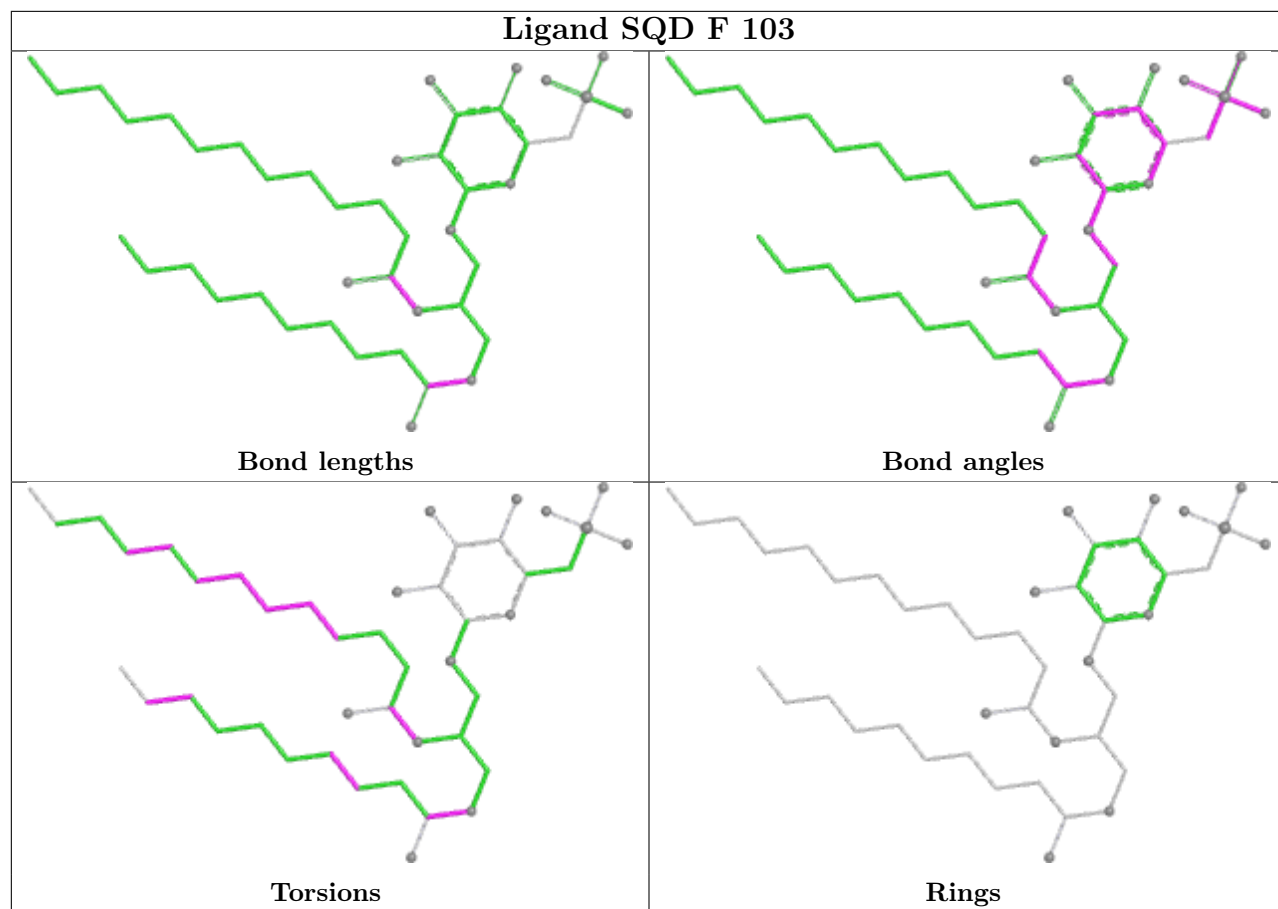


## Ligand SQD b 602

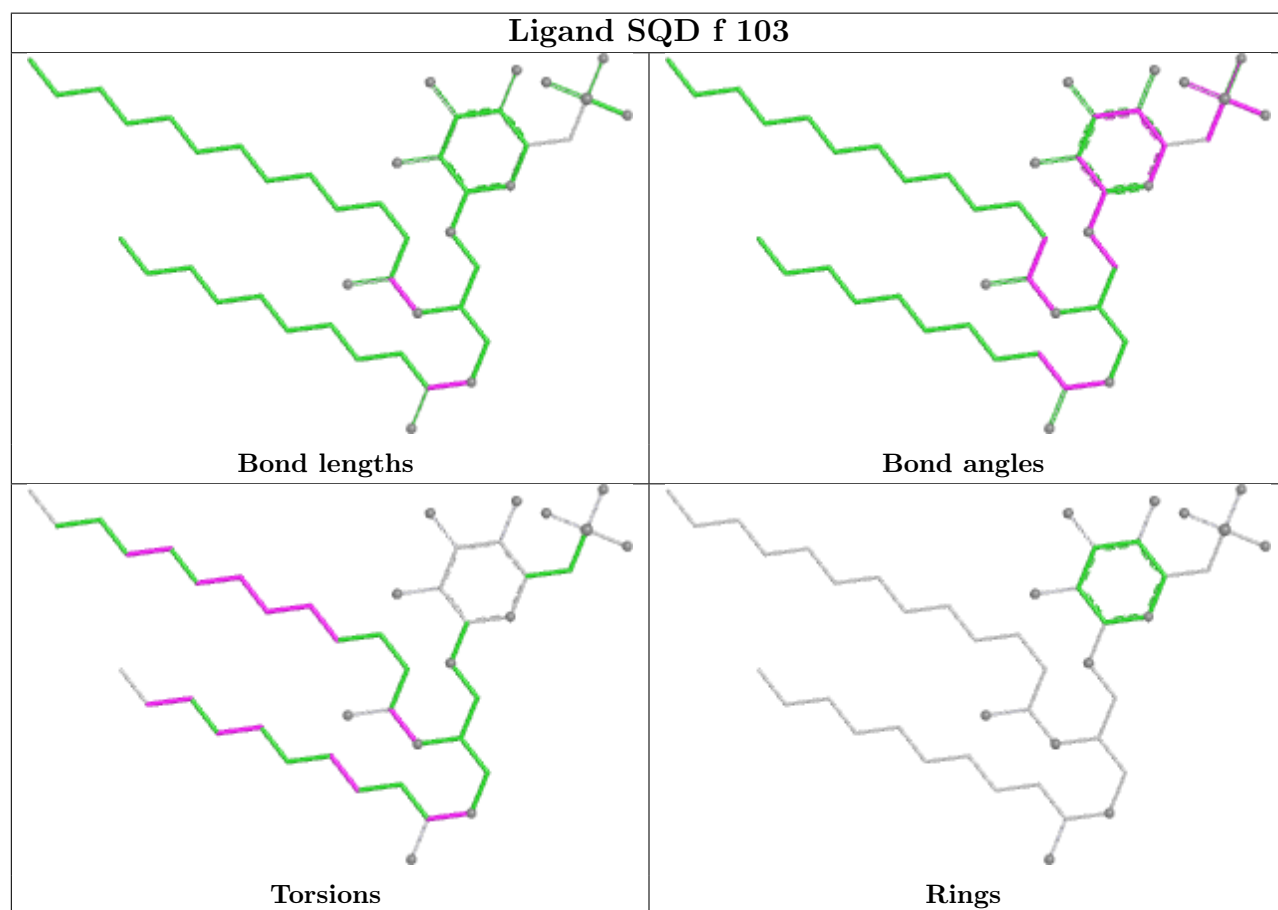
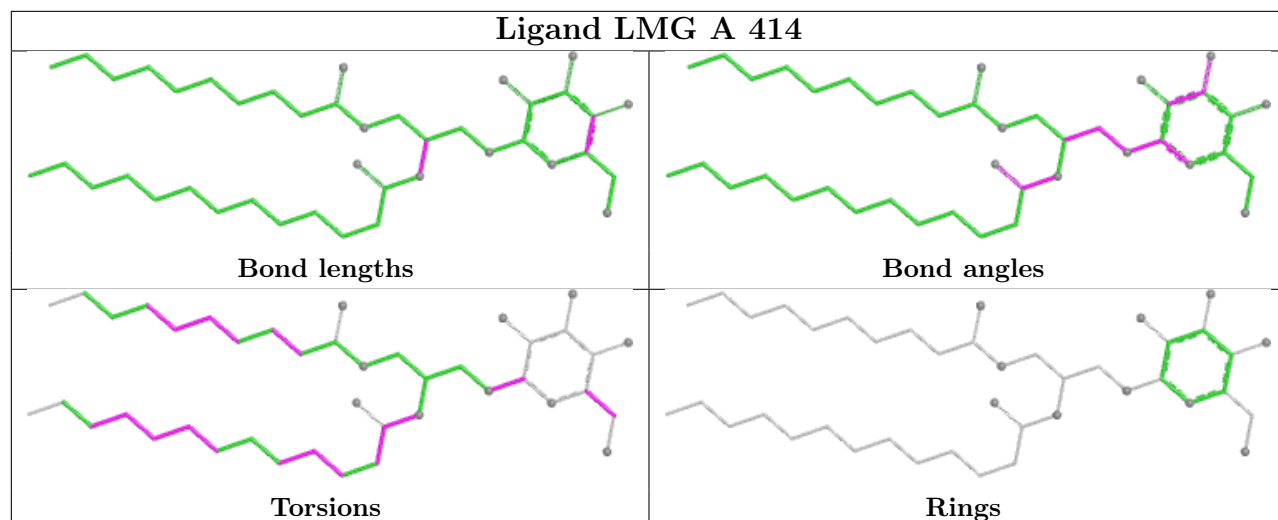


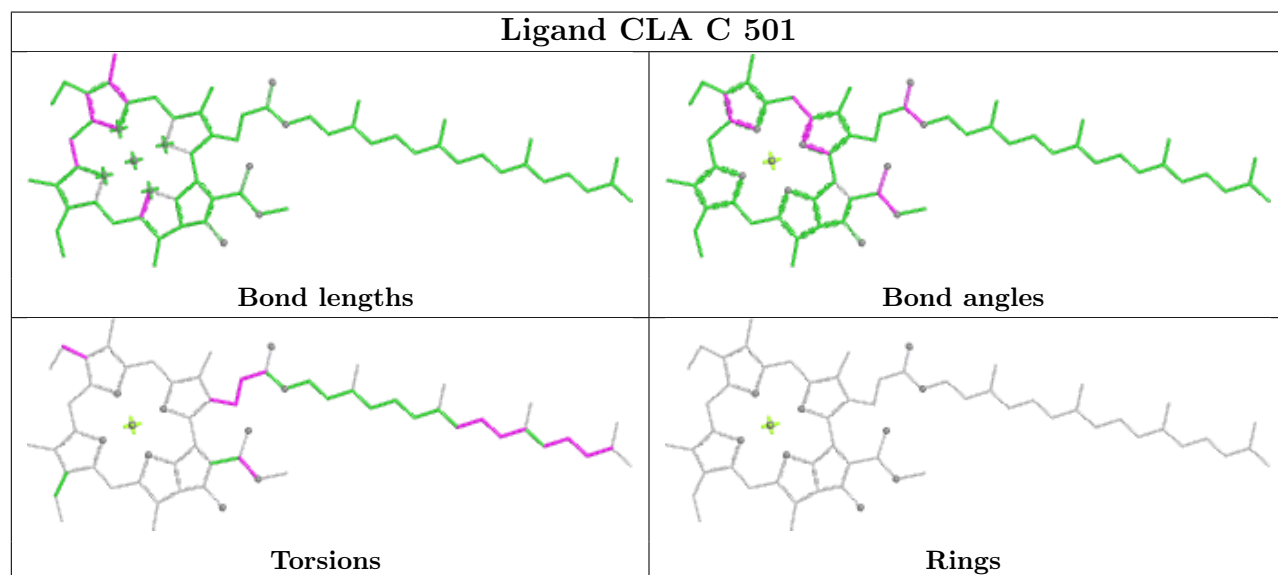
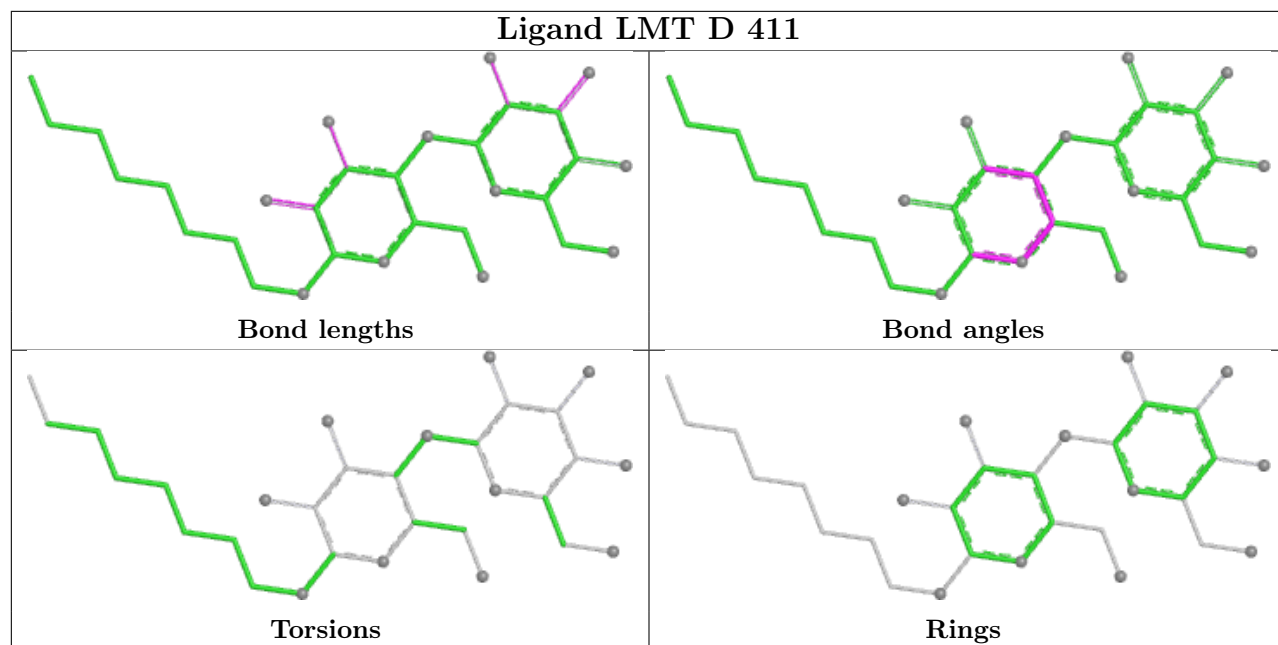




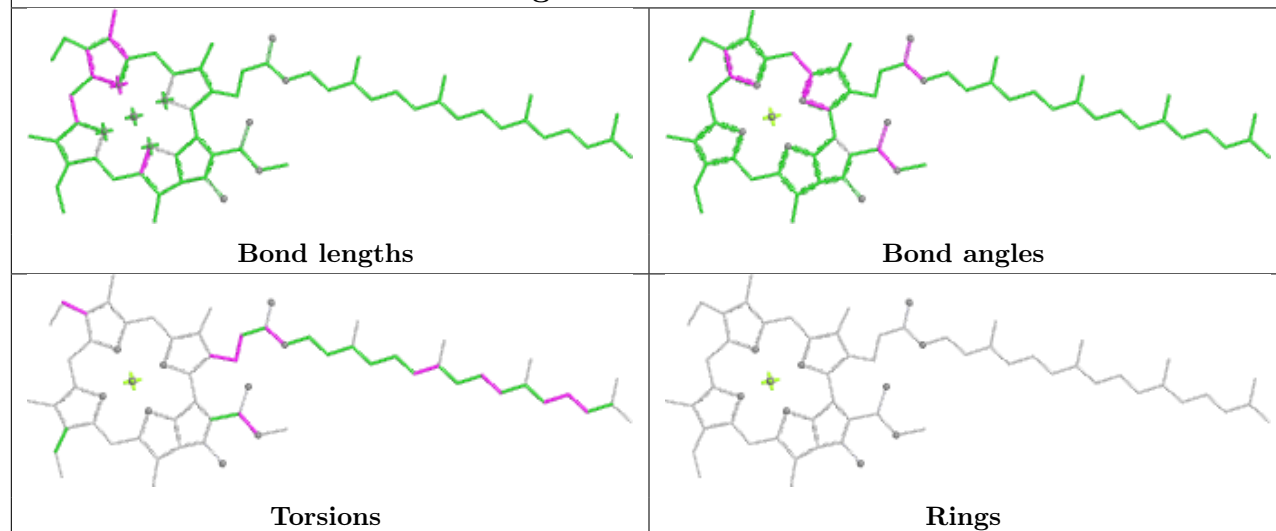




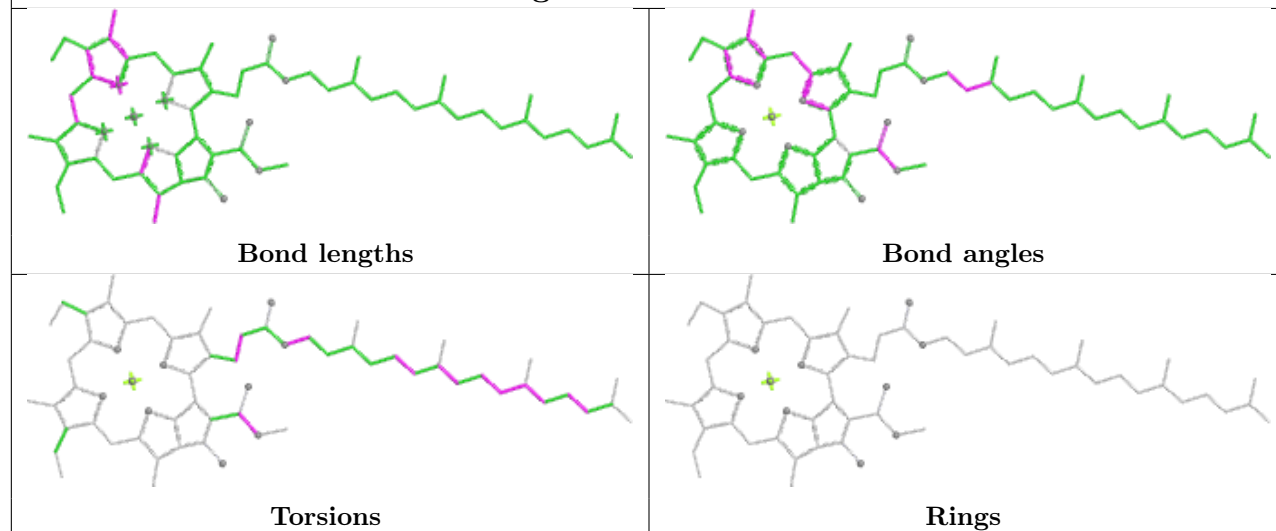




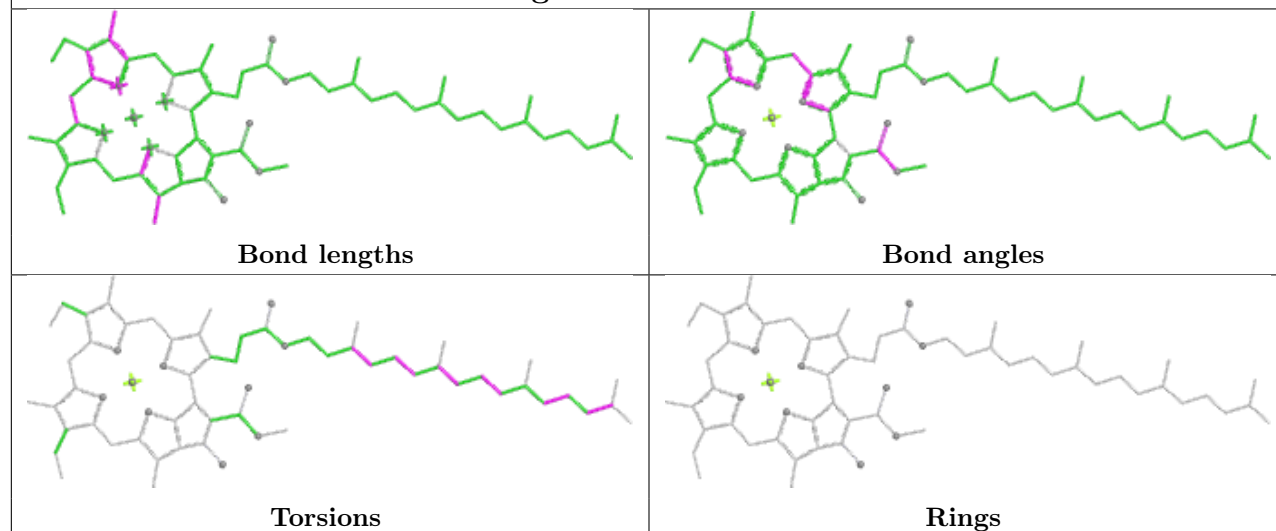
## Ligand CLA C 520

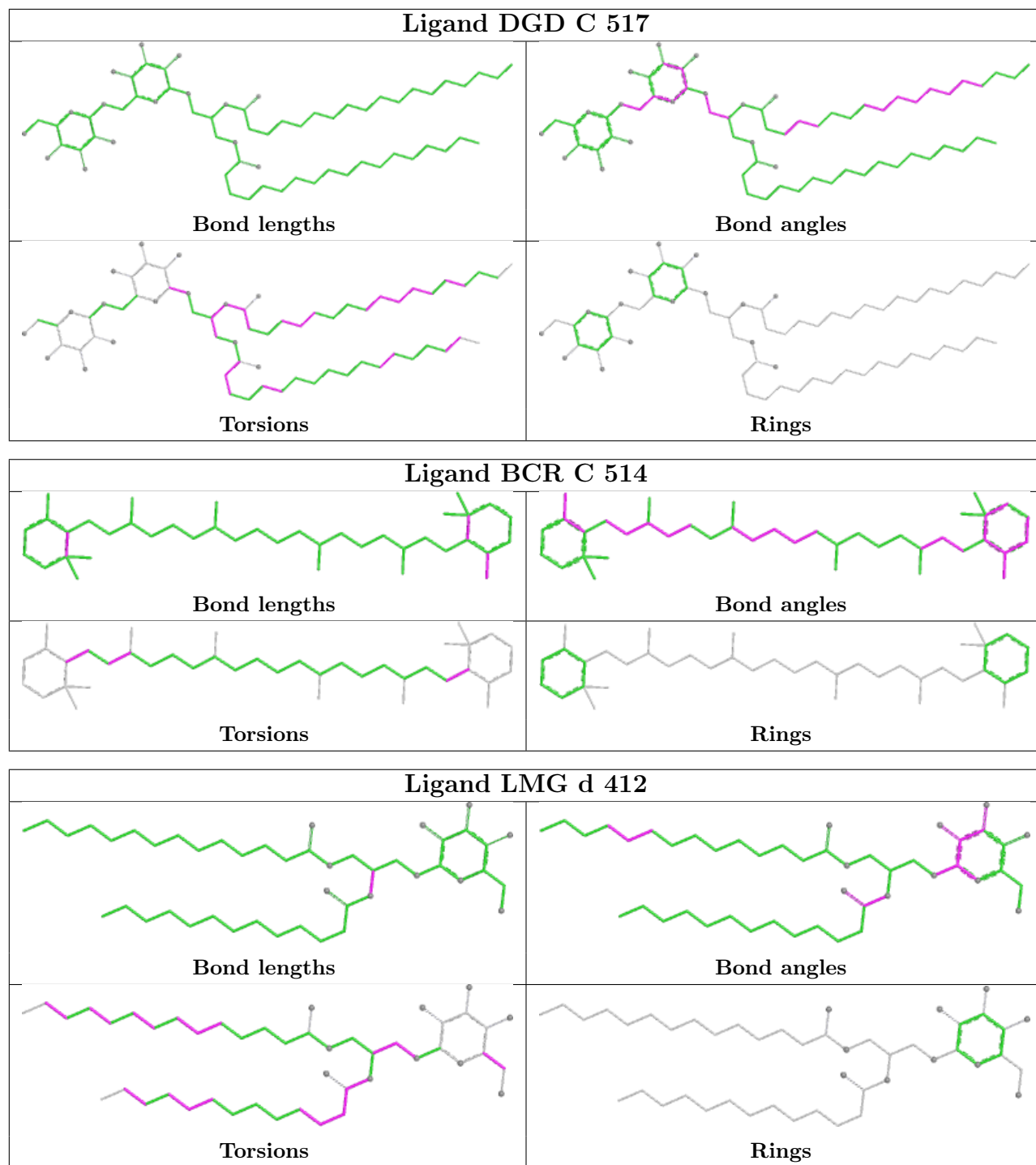


## Ligand CLA C 507

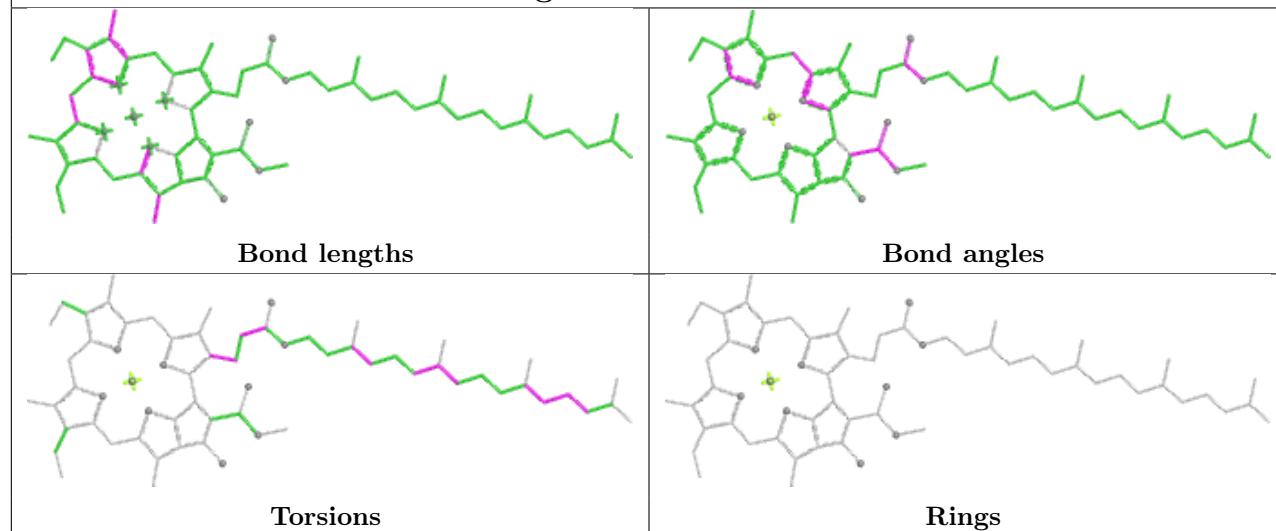


## Ligand CLA A 405

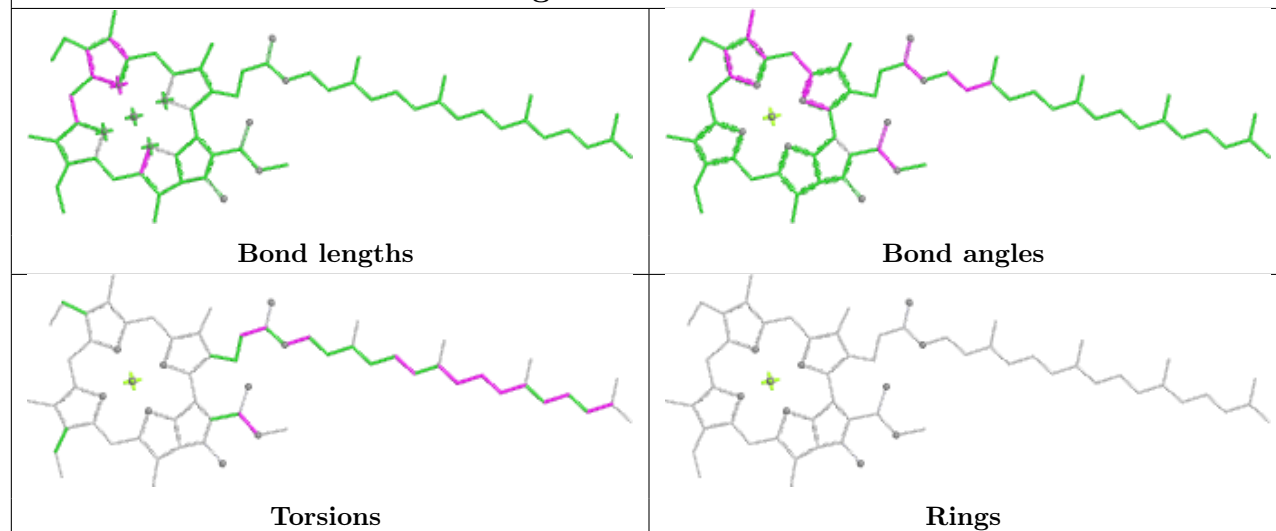




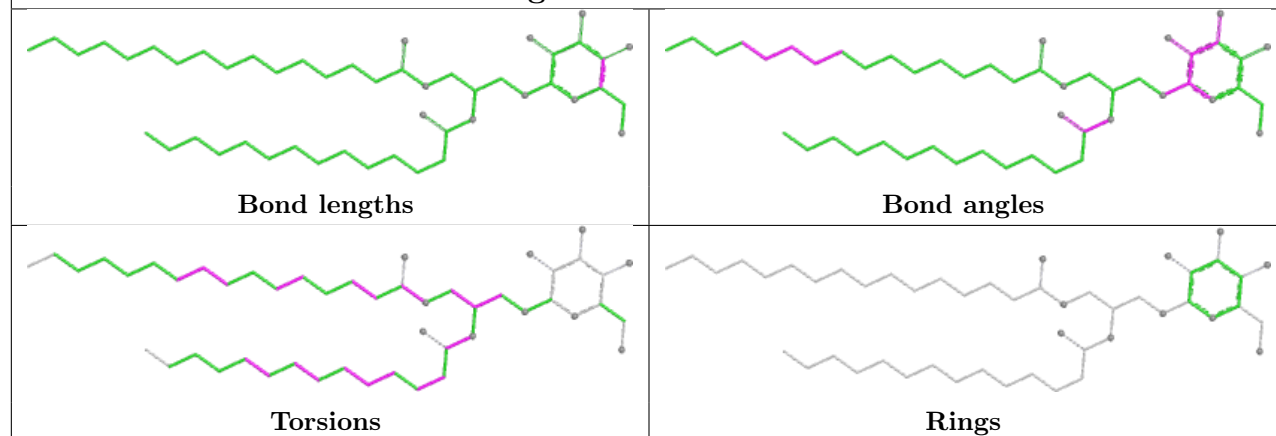
## Ligand CLA d 405

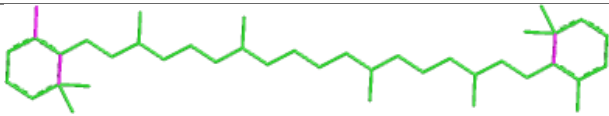
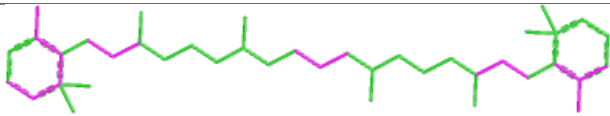
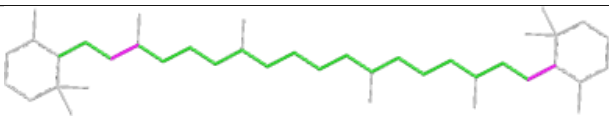
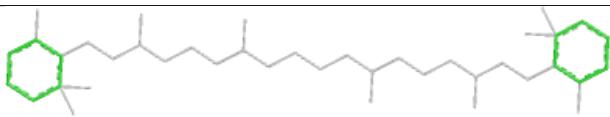


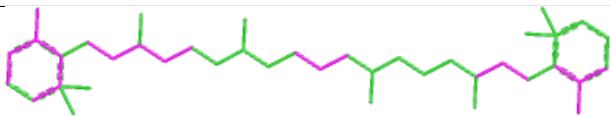
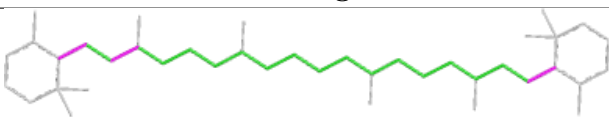
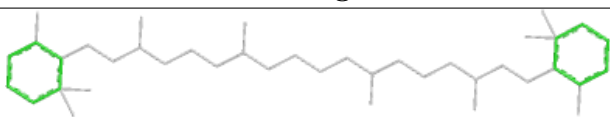
## Ligand CLA B 612

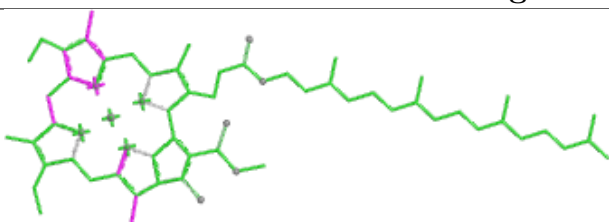
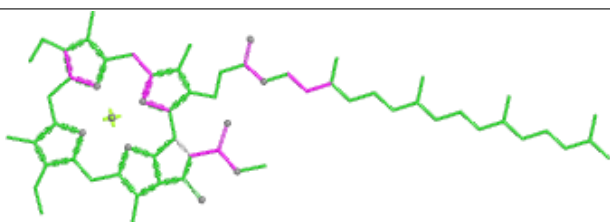
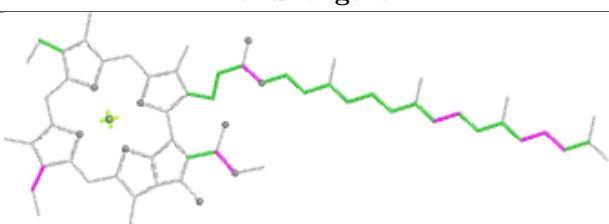
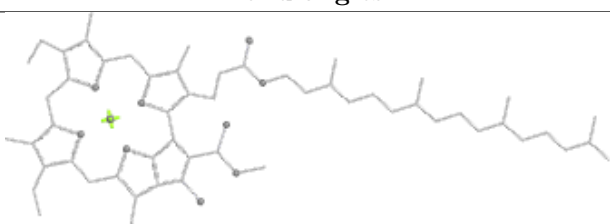


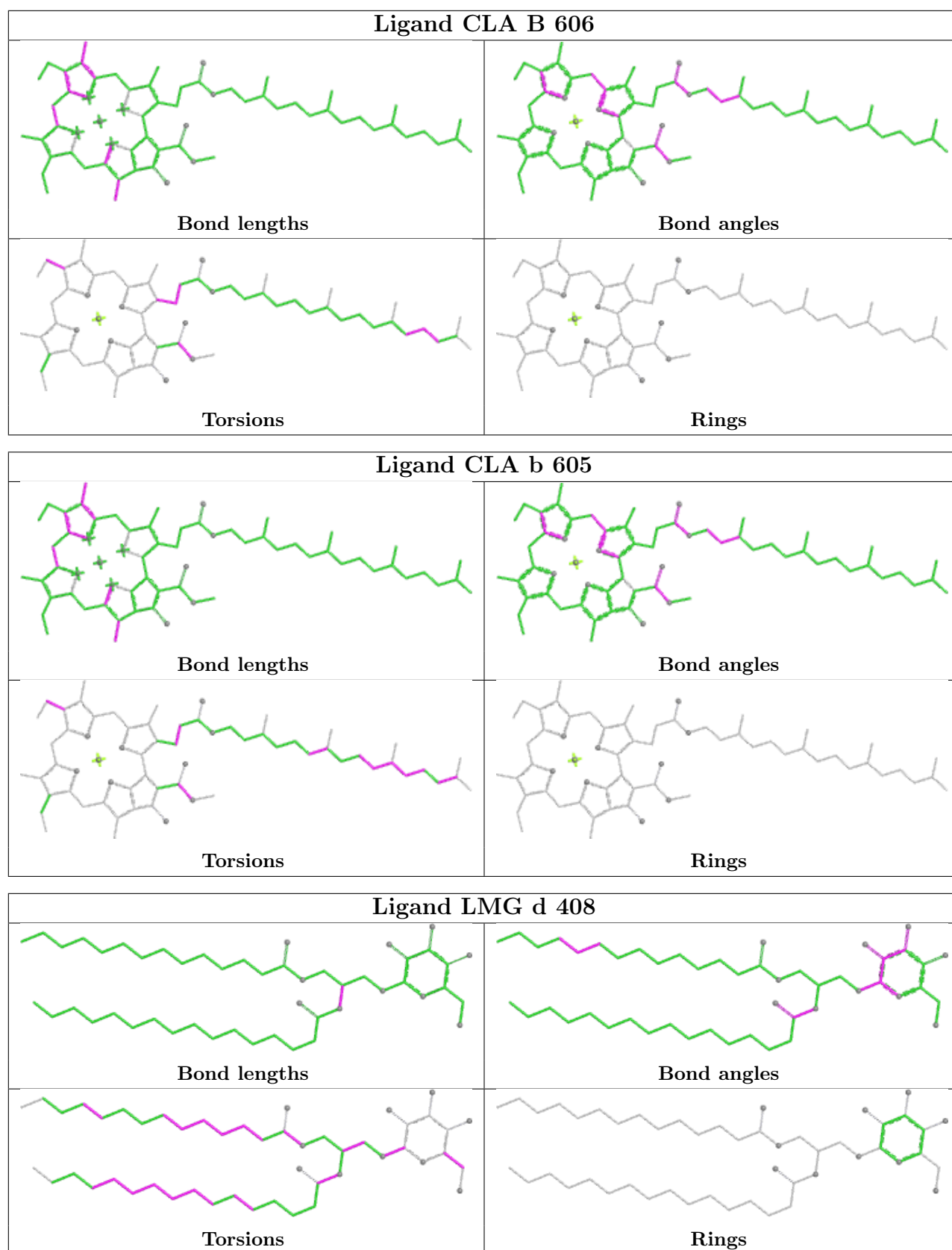
## Ligand LMG B 621



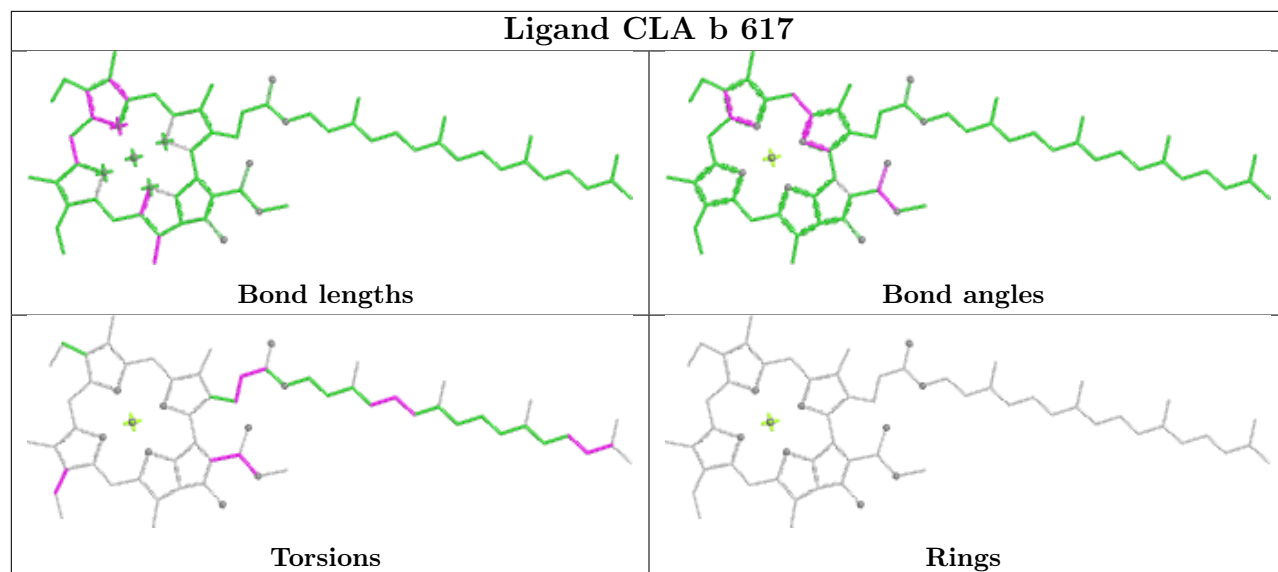
| Ligand BCR y 101                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|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

| Ligand BCR b 623                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

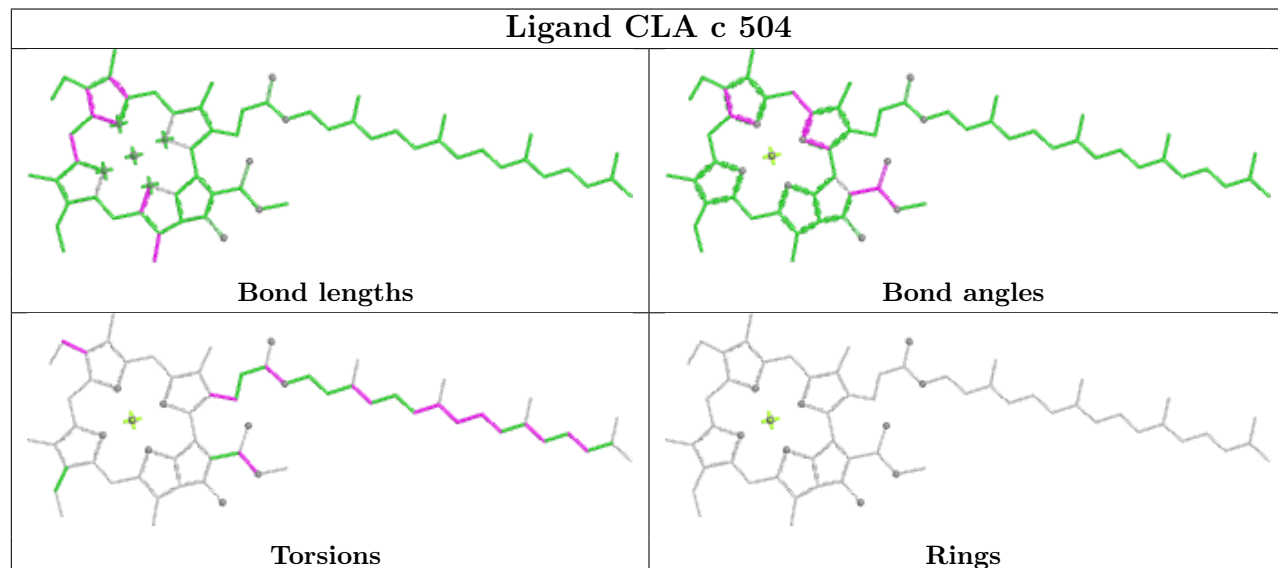
| Ligand CLA B 603                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



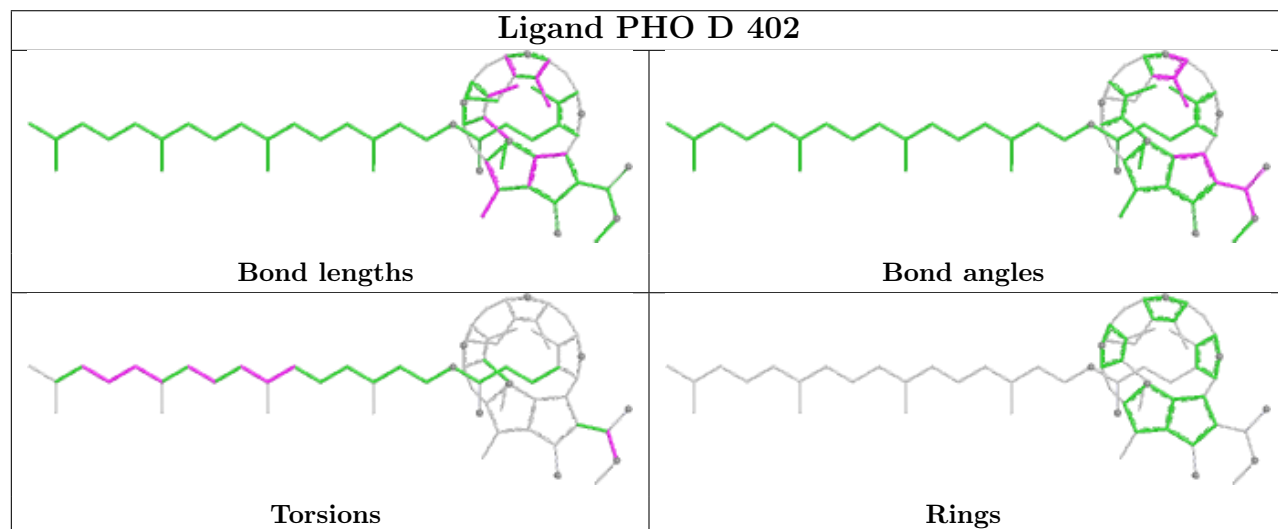
## Ligand CLA b 617



## Ligand CLA c 504

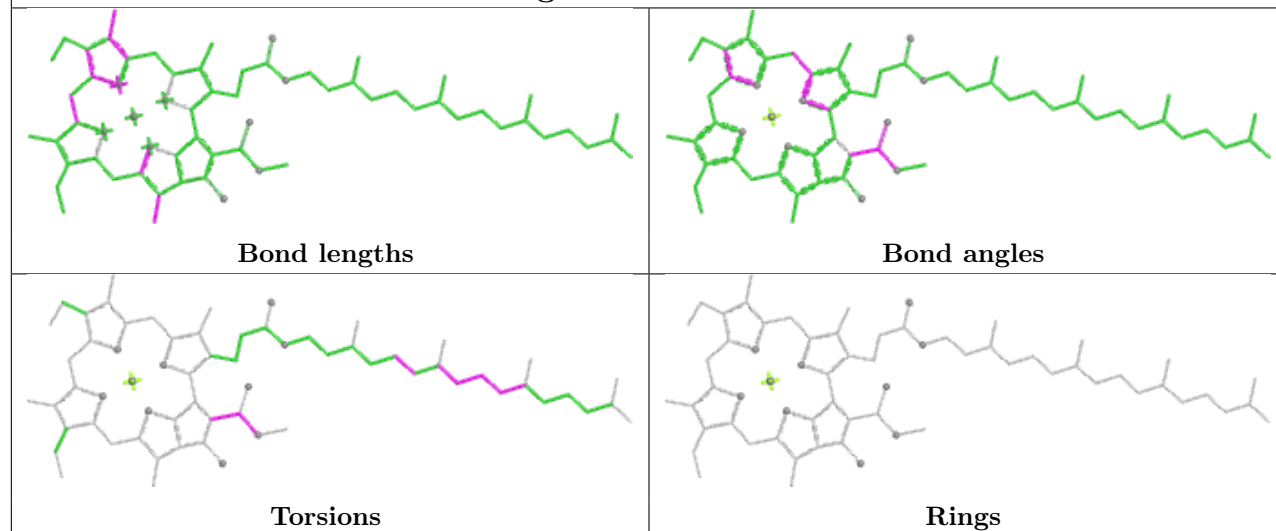


## Ligand PHO D 402

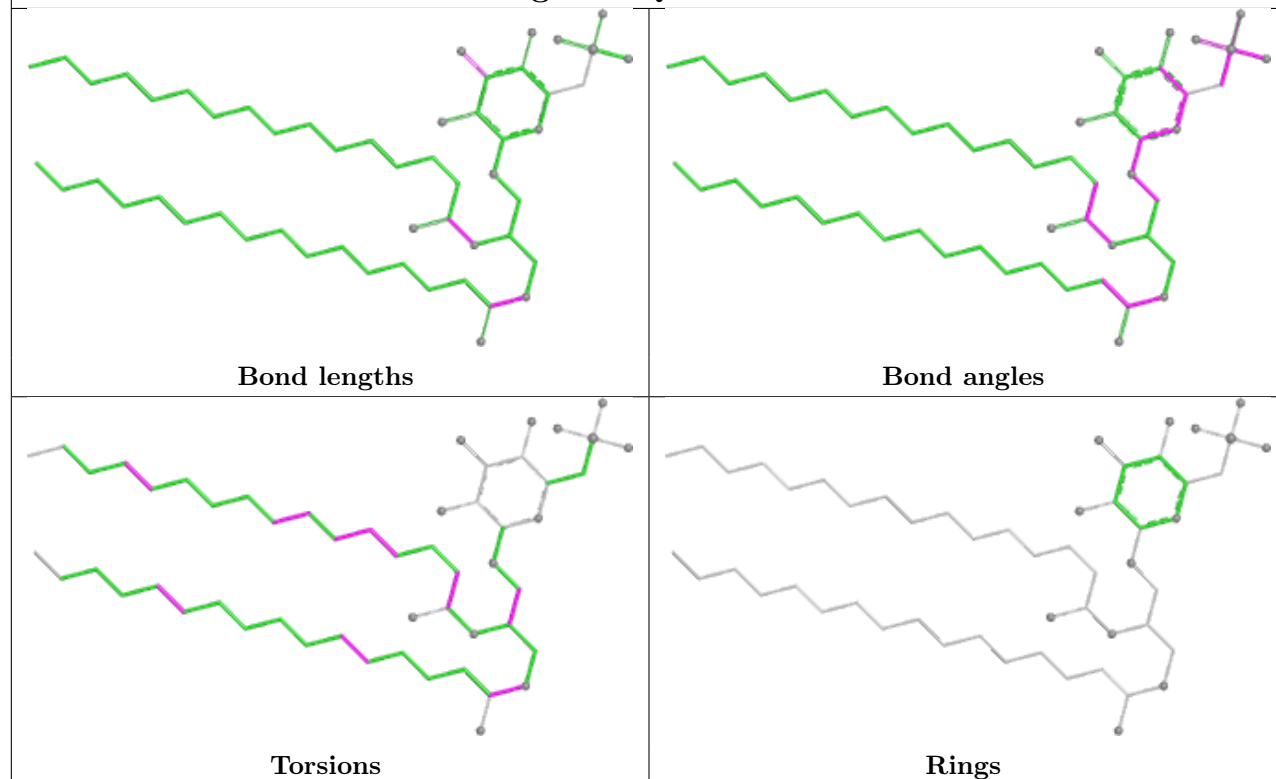




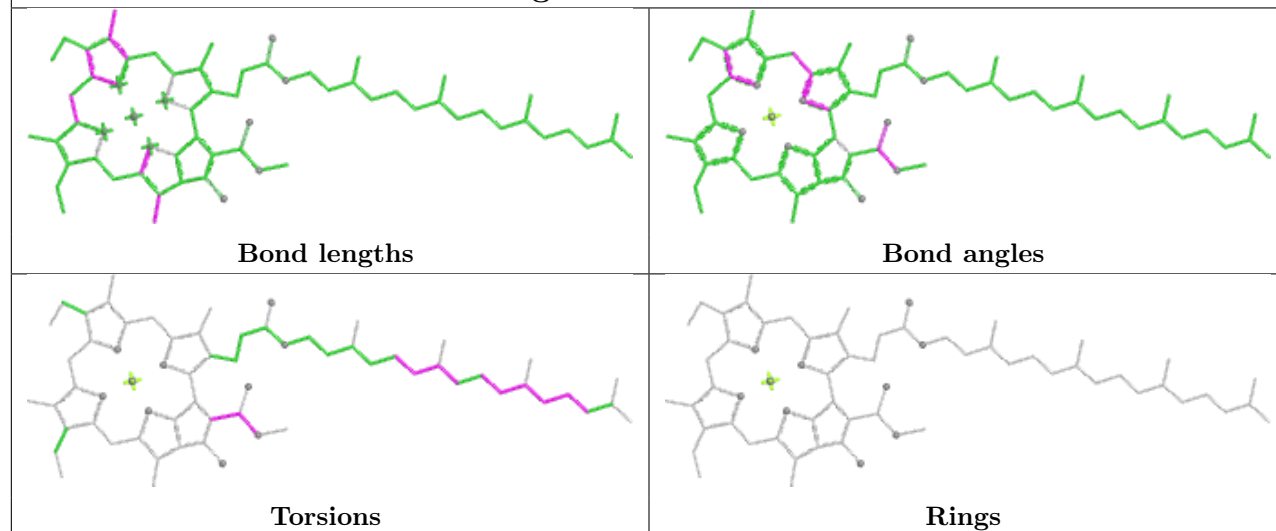
## Ligand CLA c 503



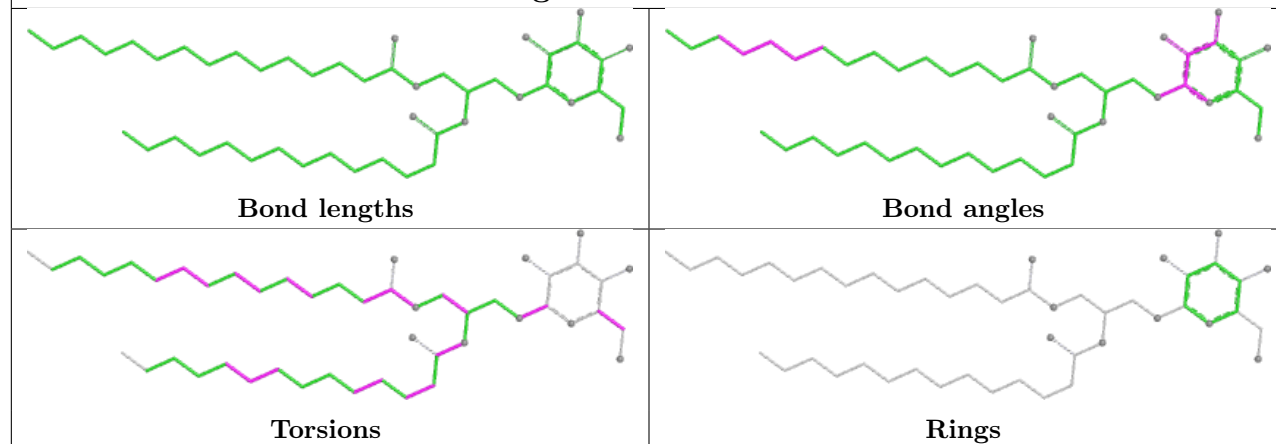
## Ligand SQD A 413



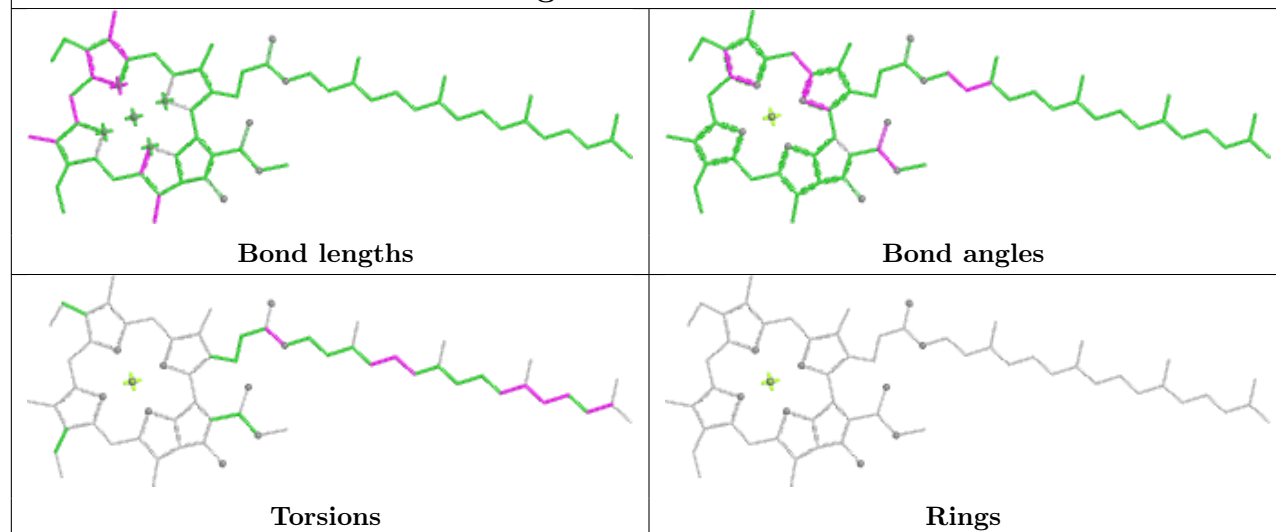
## Ligand CLA C 505

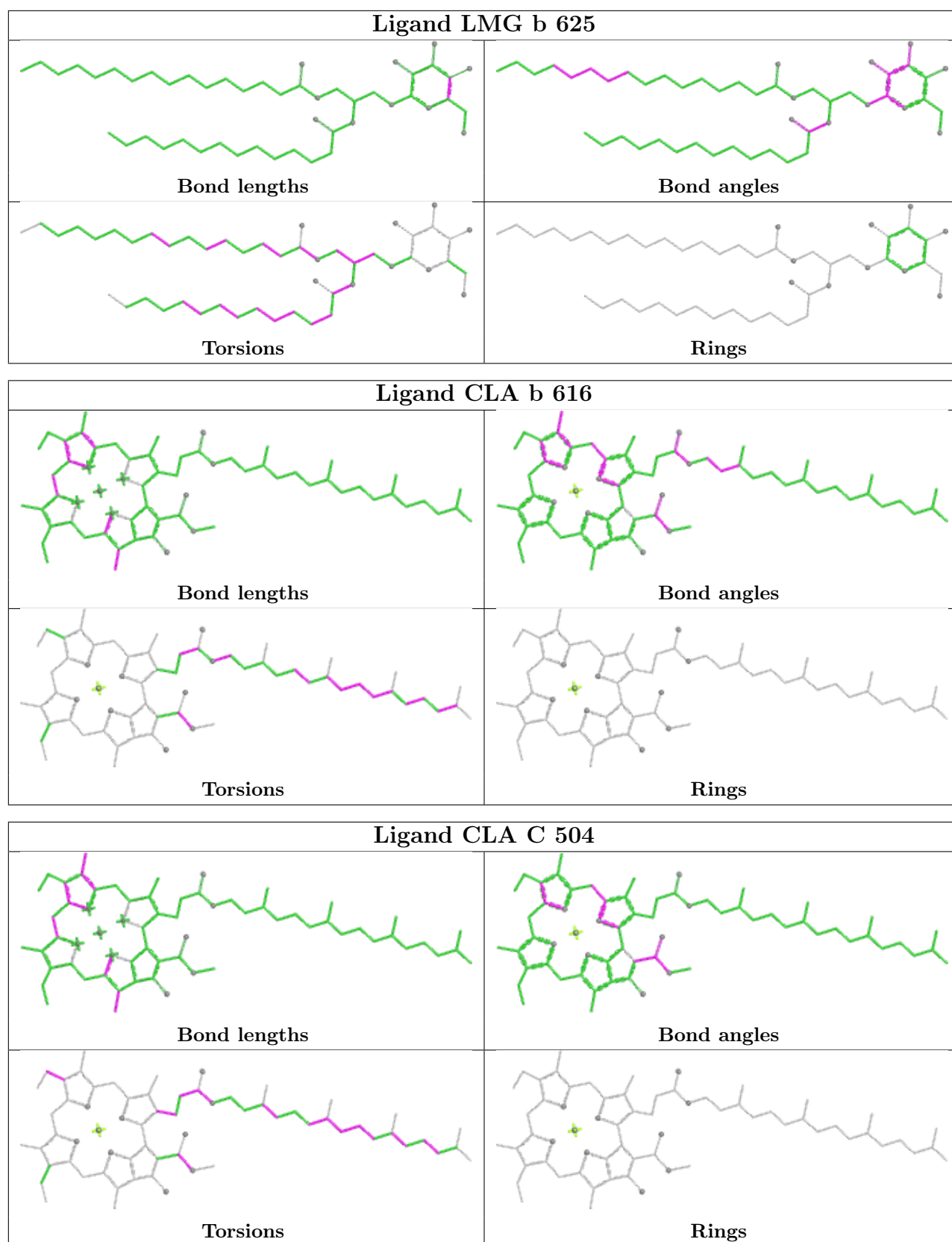


## Ligand LMG c 522

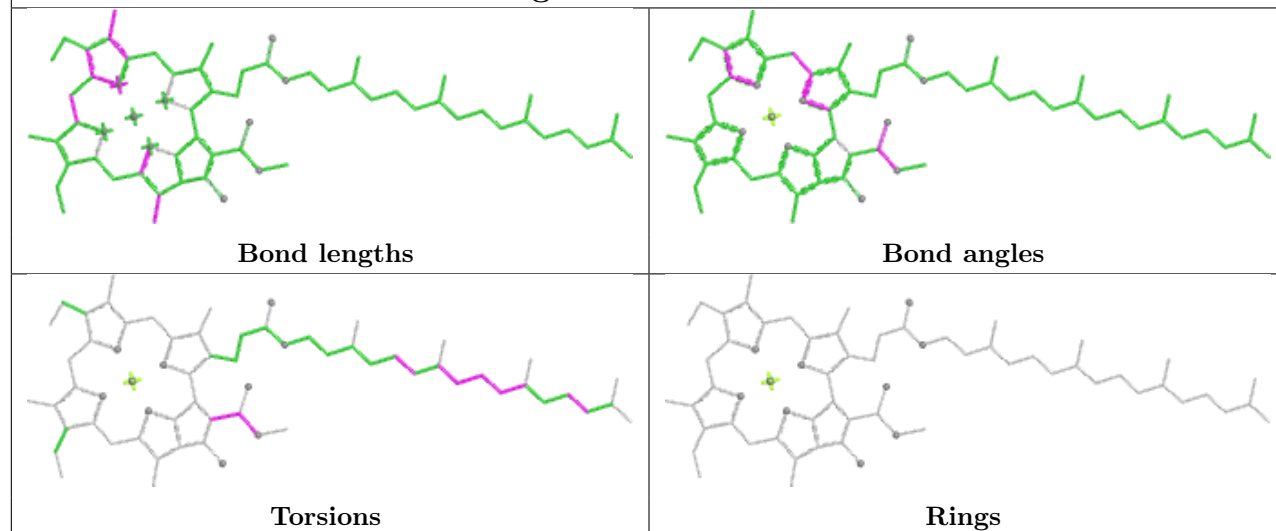


## Ligand CLA c 502

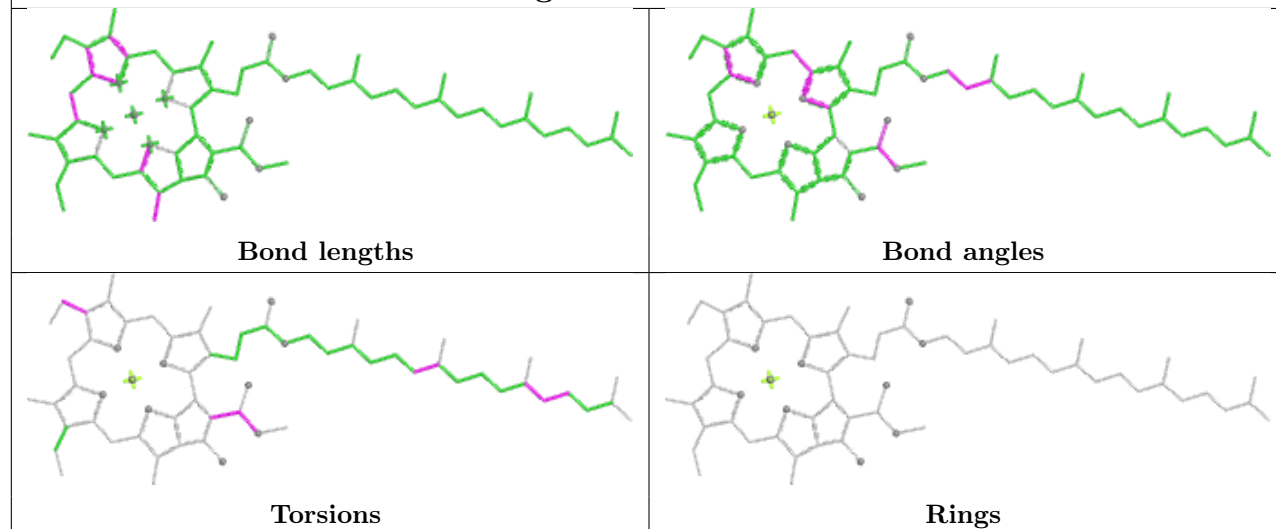




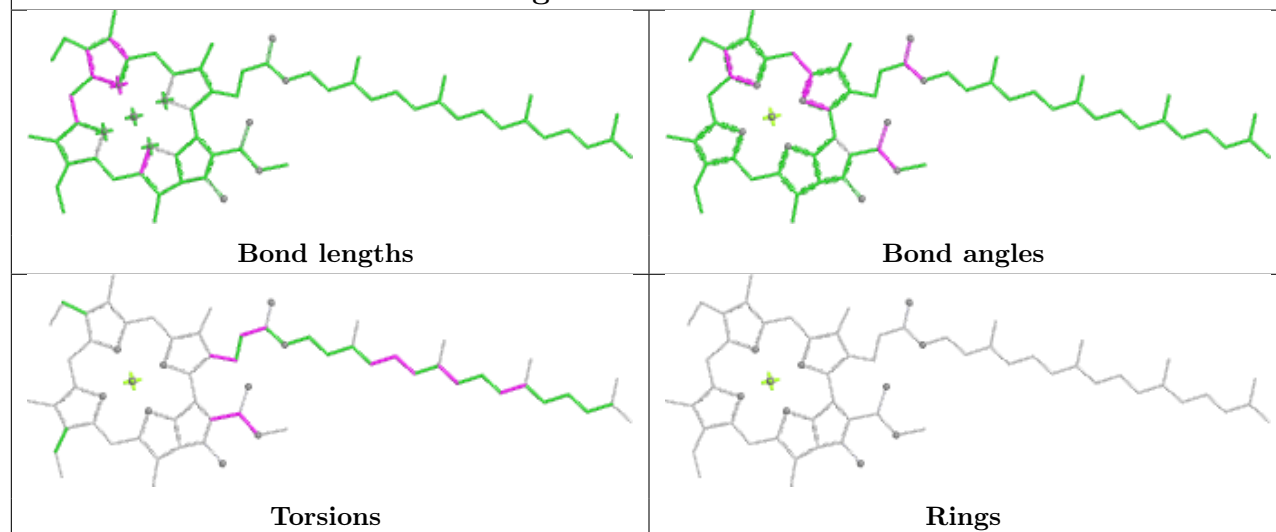
## Ligand CLA C 503

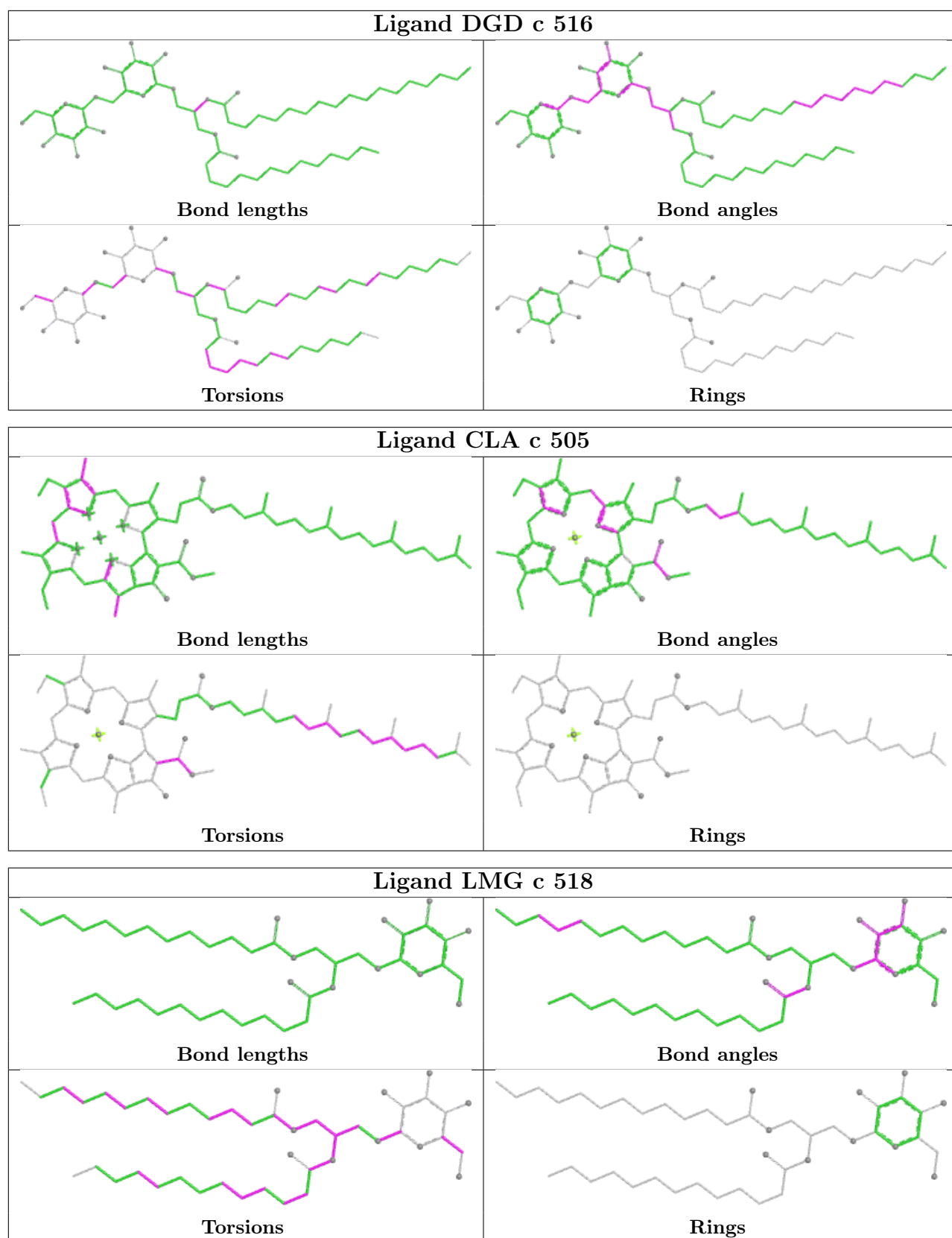


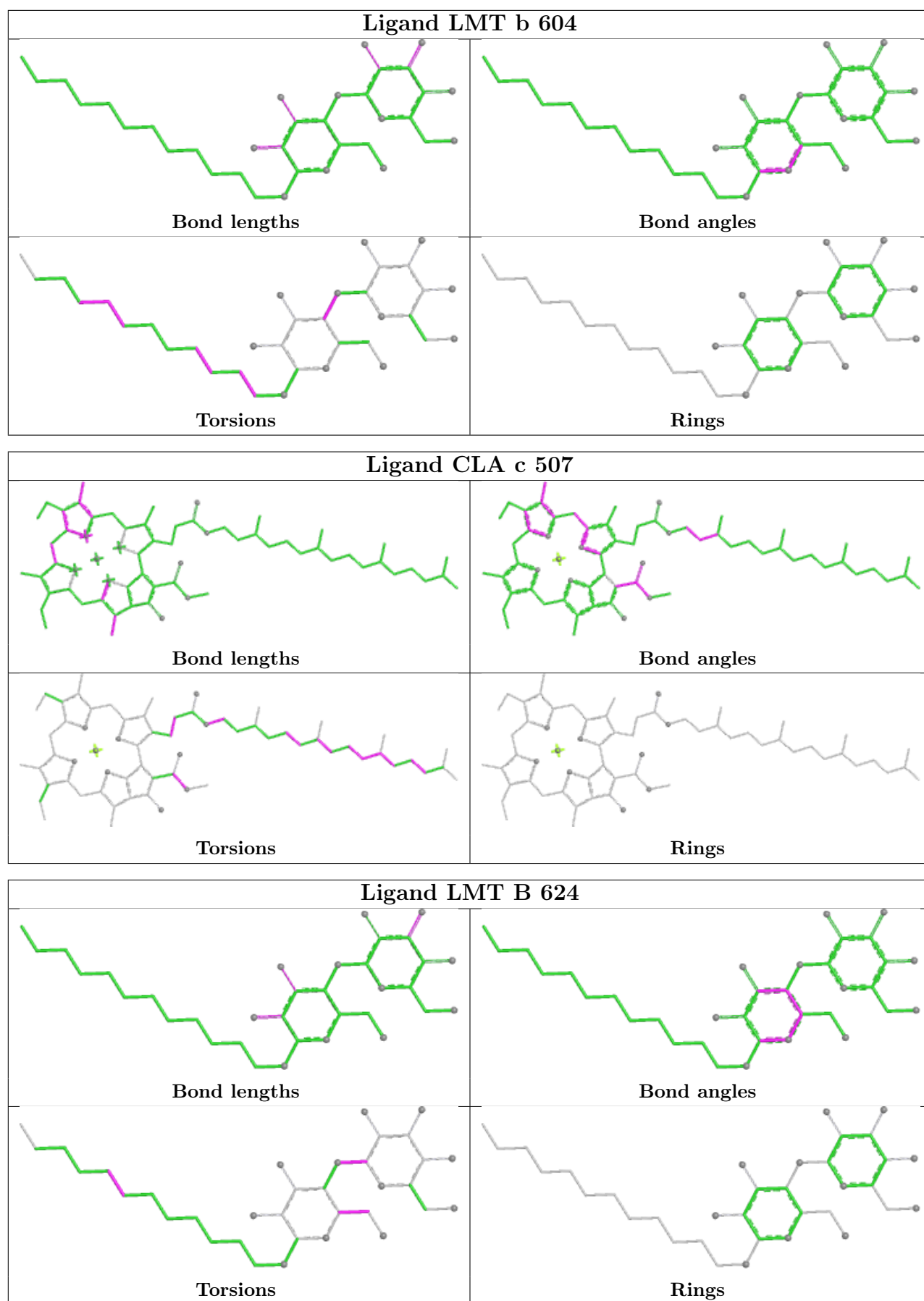
## Ligand CLA b 612

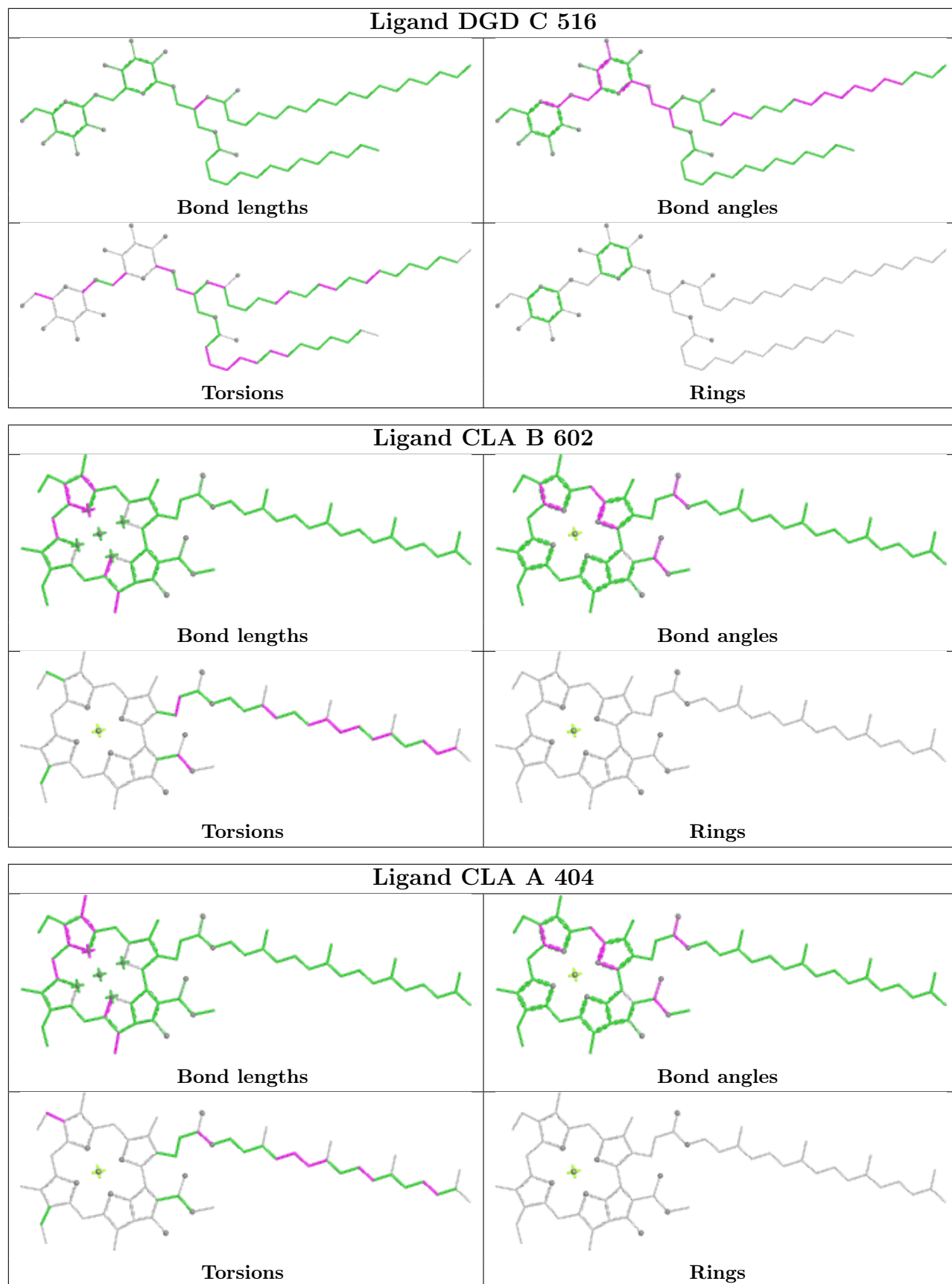


## Ligand CLA C 506

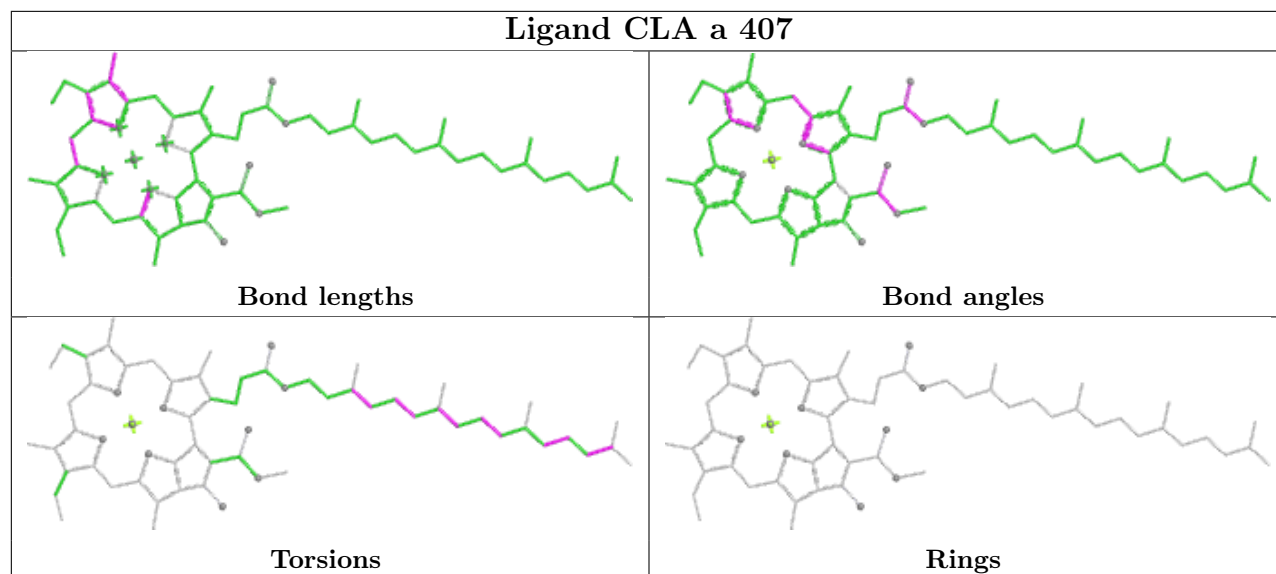




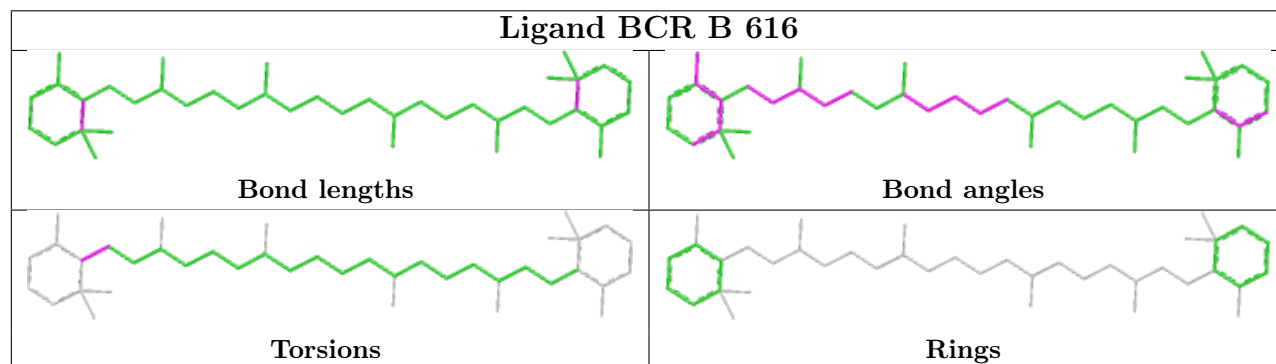




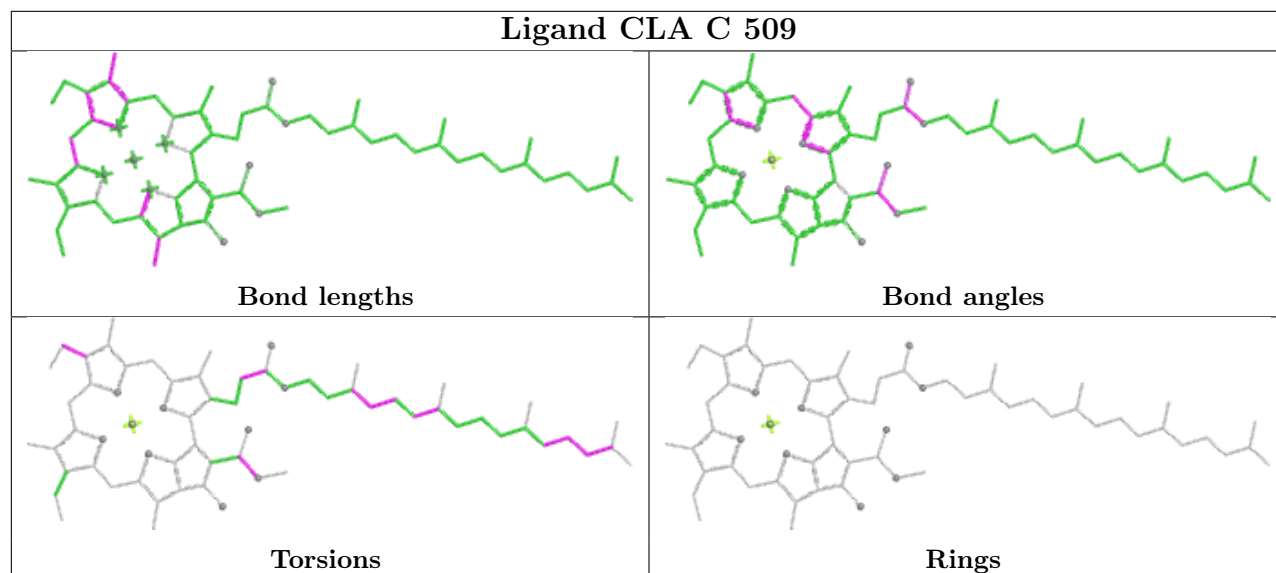
## Ligand CLA a 407



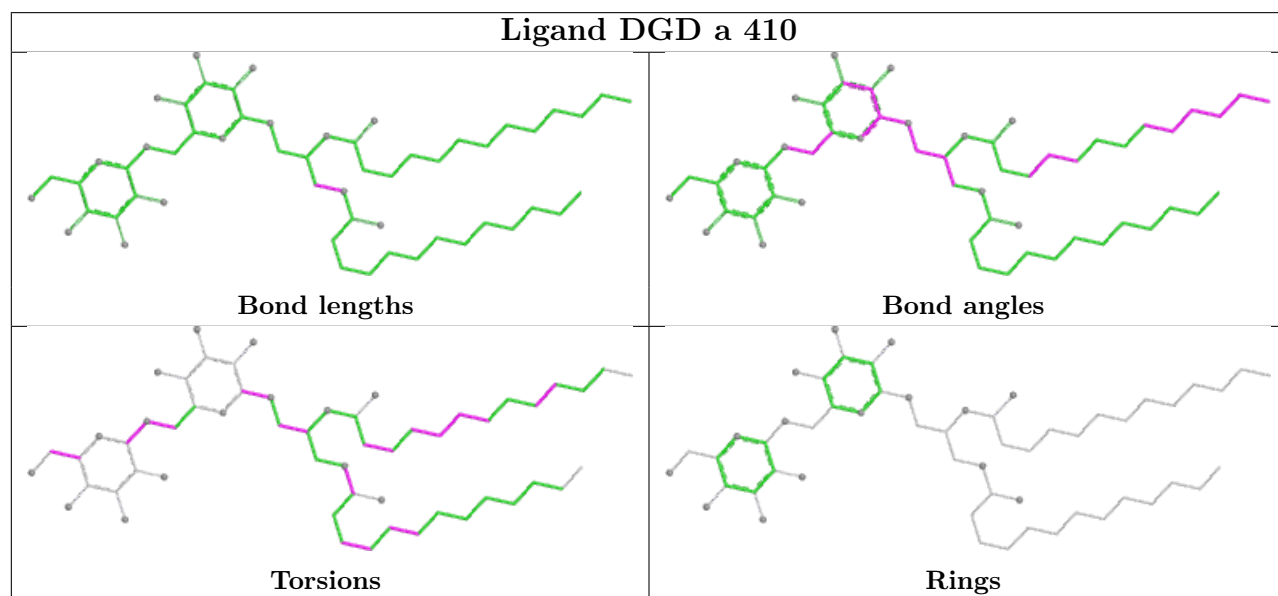
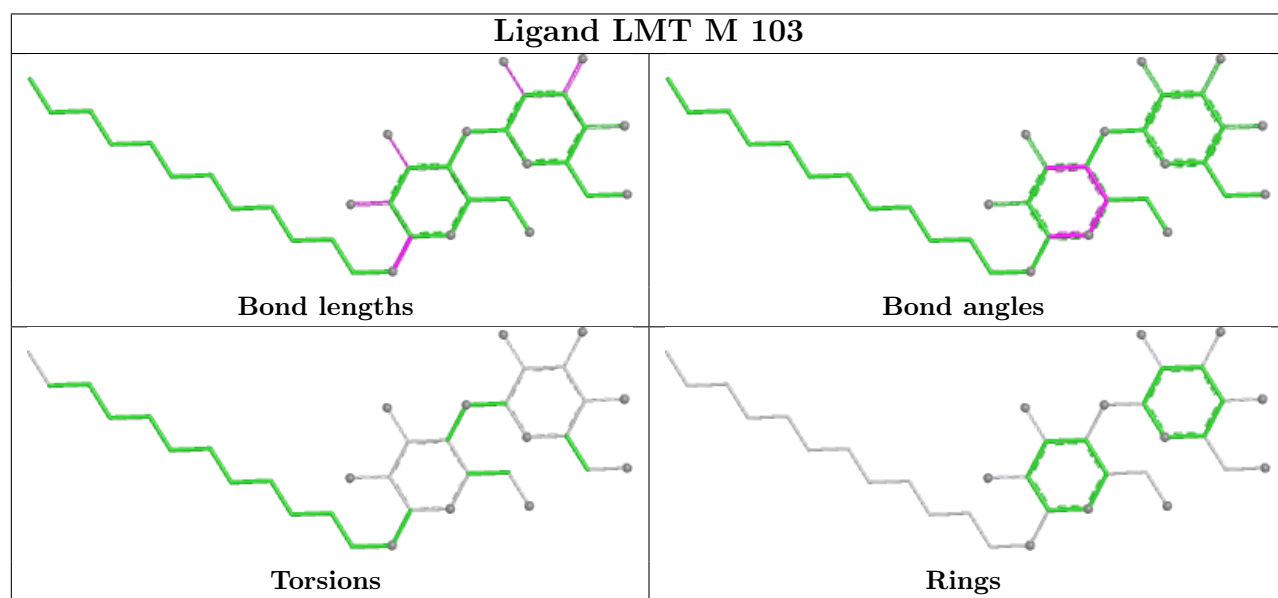
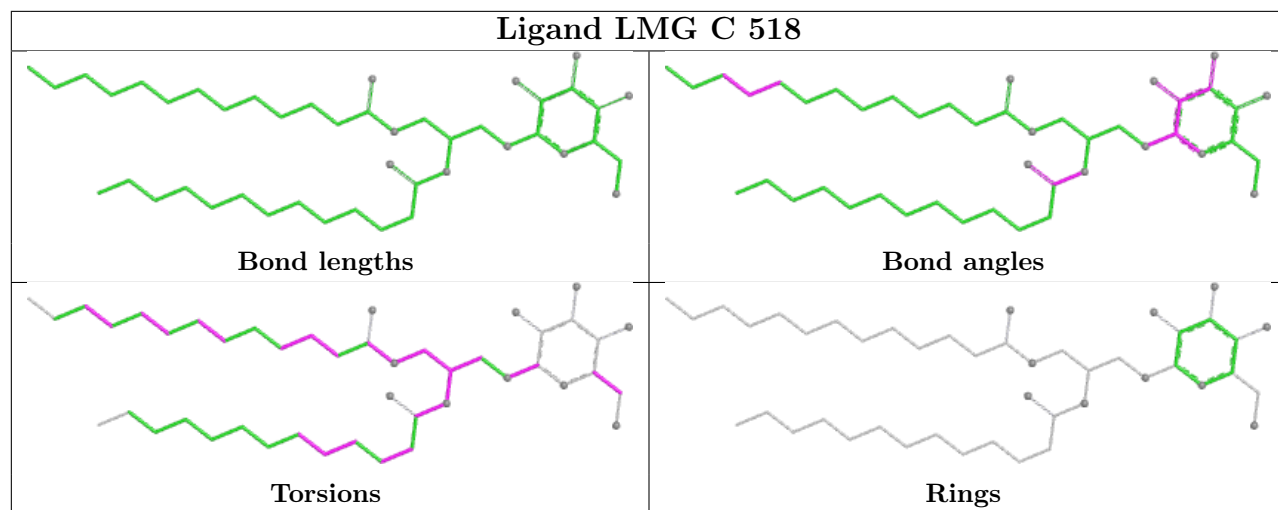
## Ligand BCR B 616

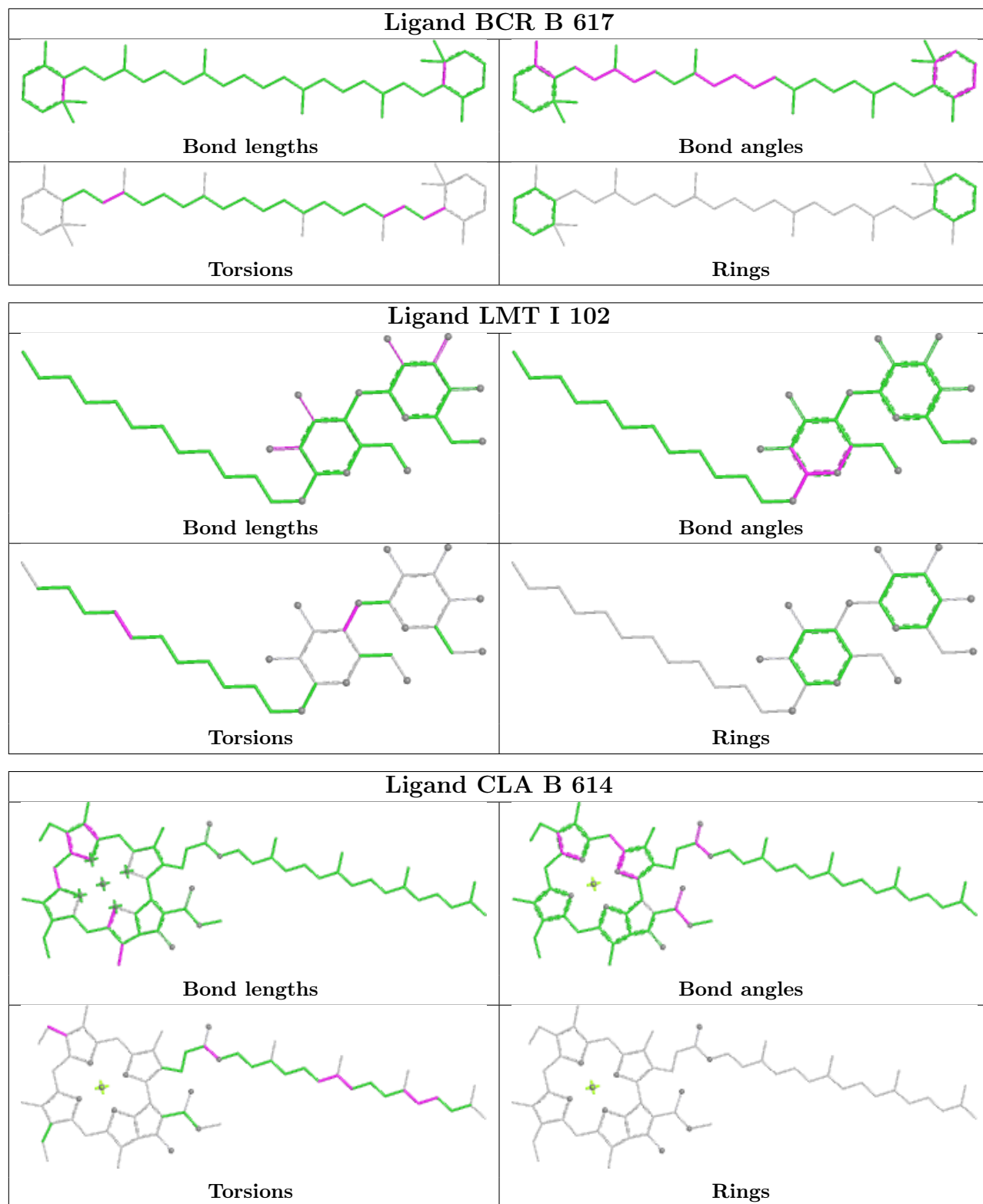


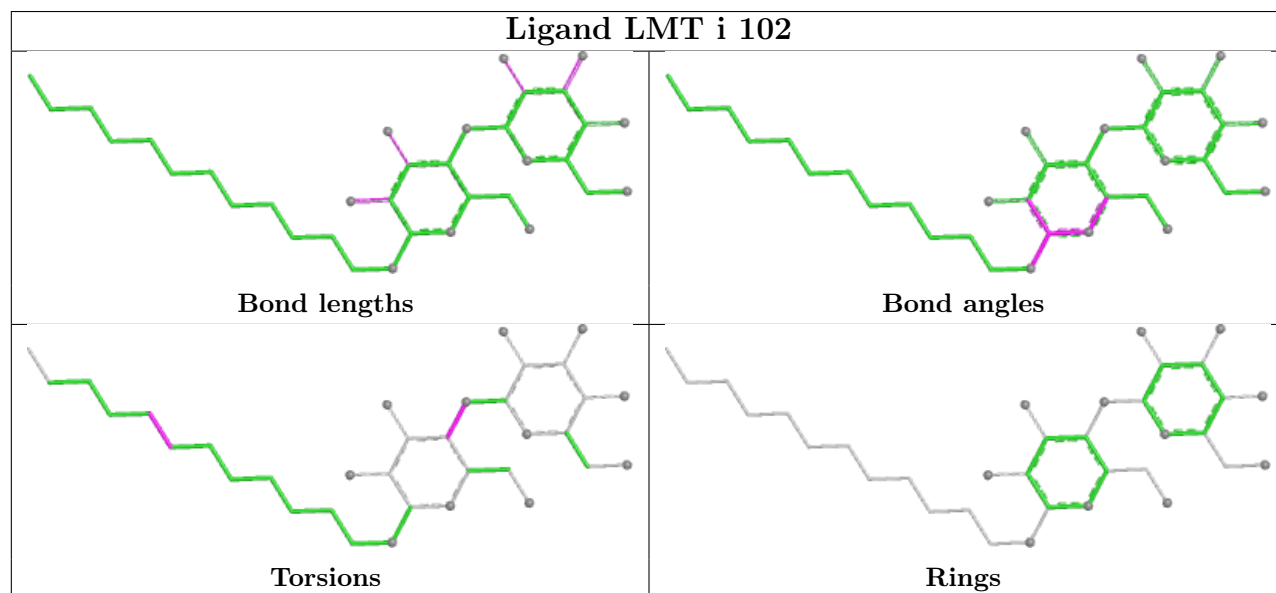
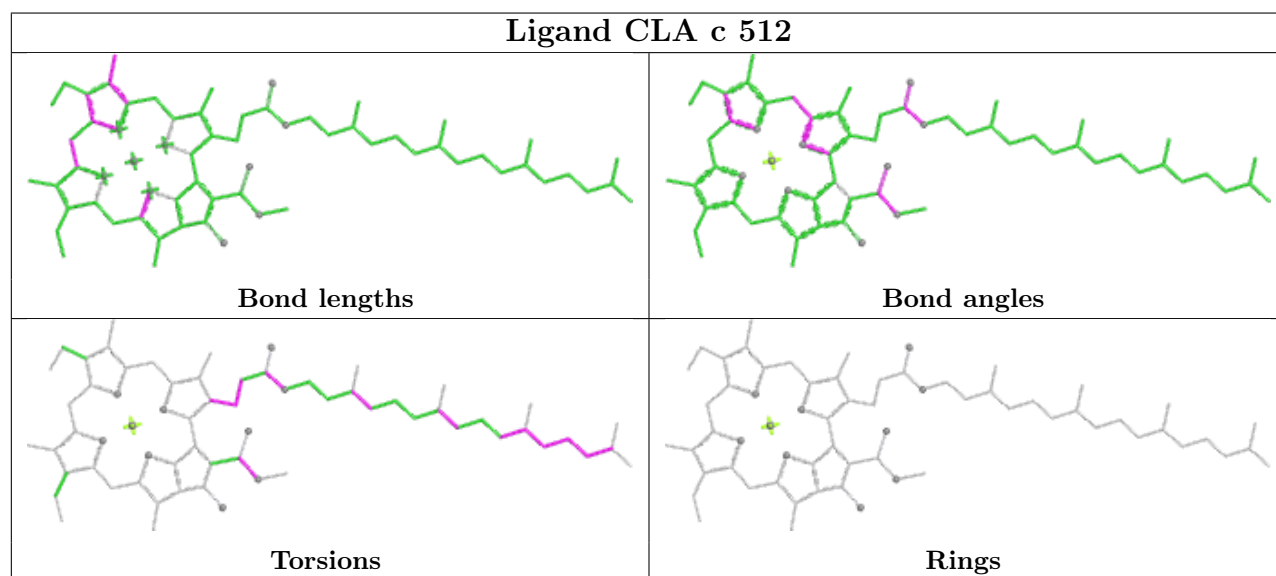
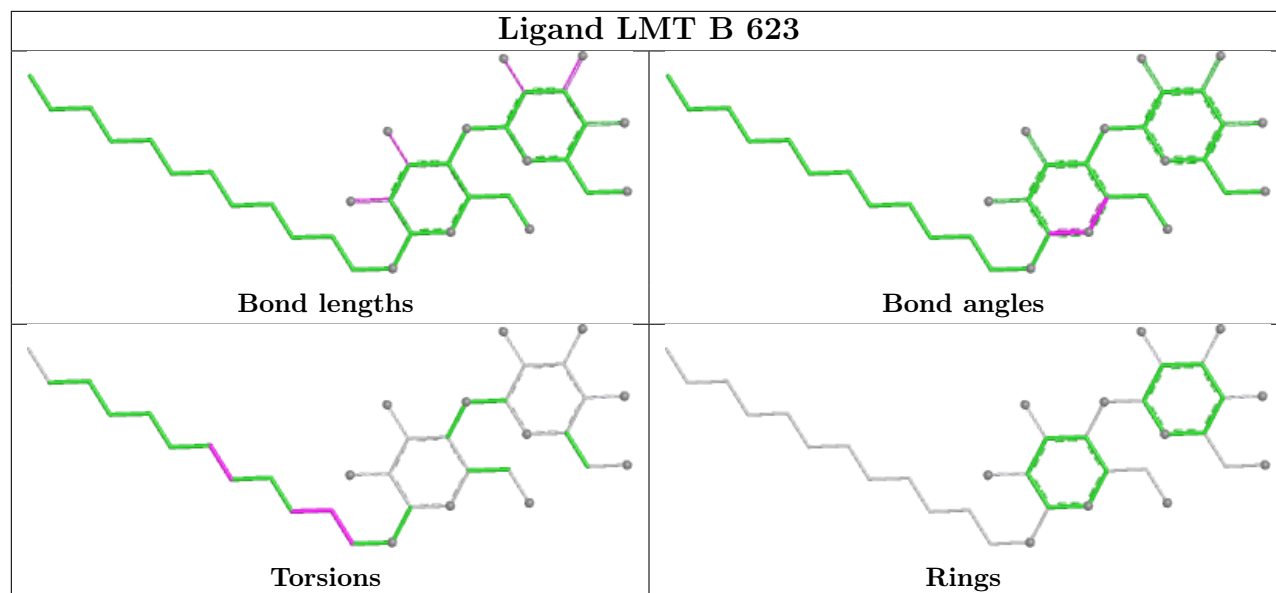
## Ligand CLA C 509

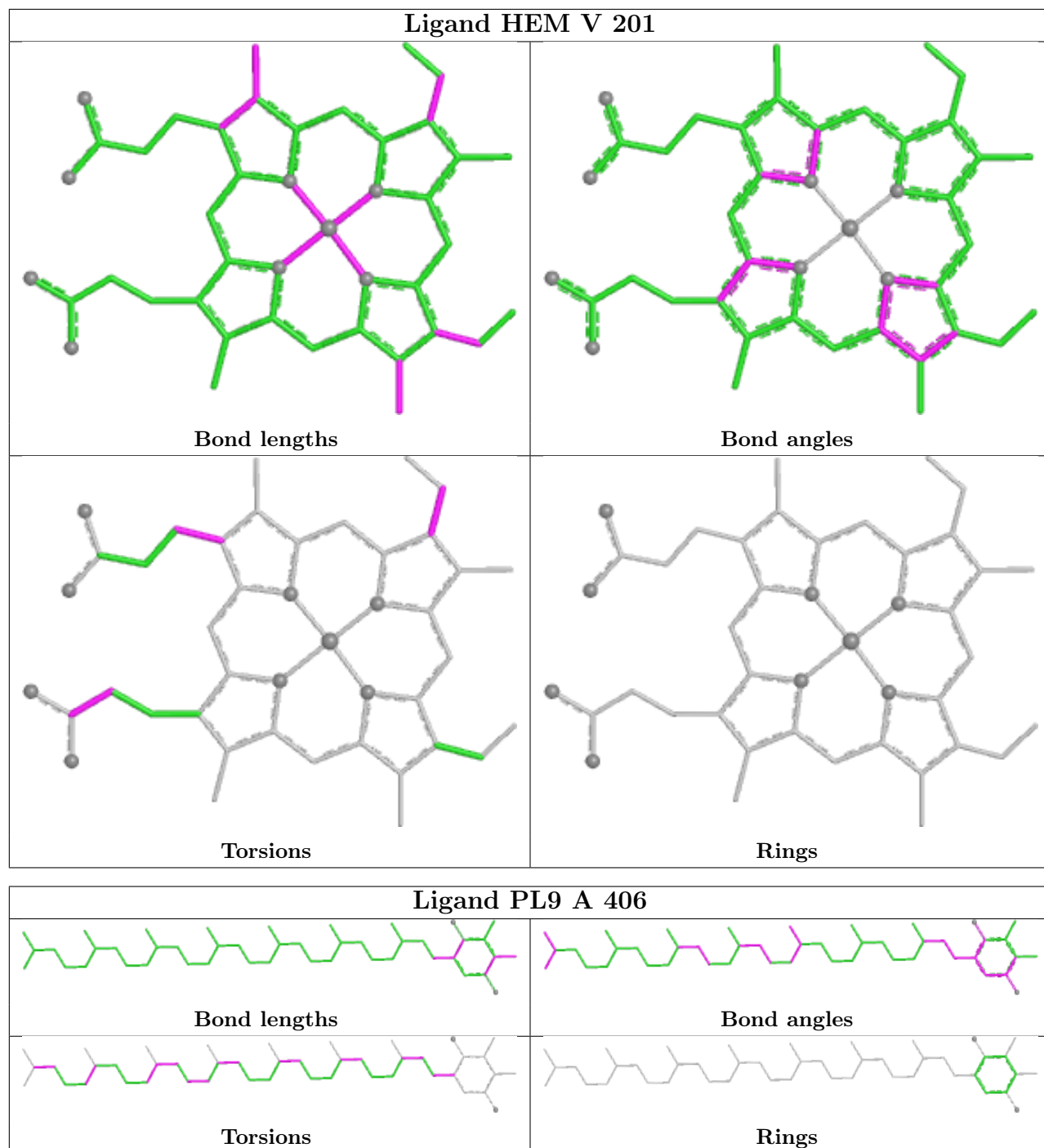




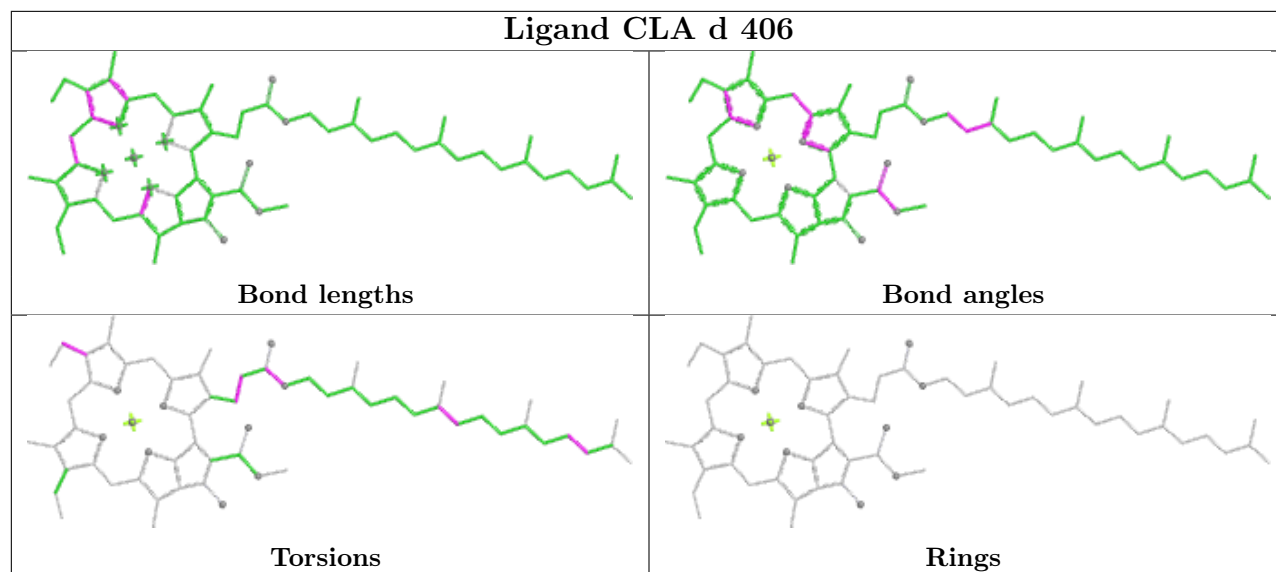




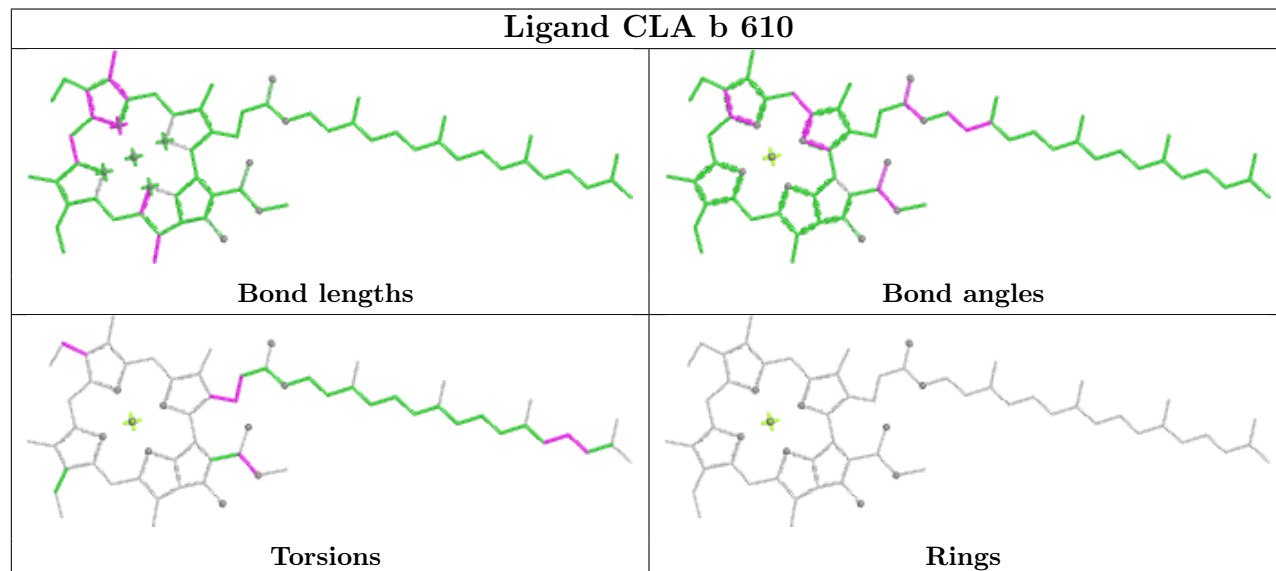




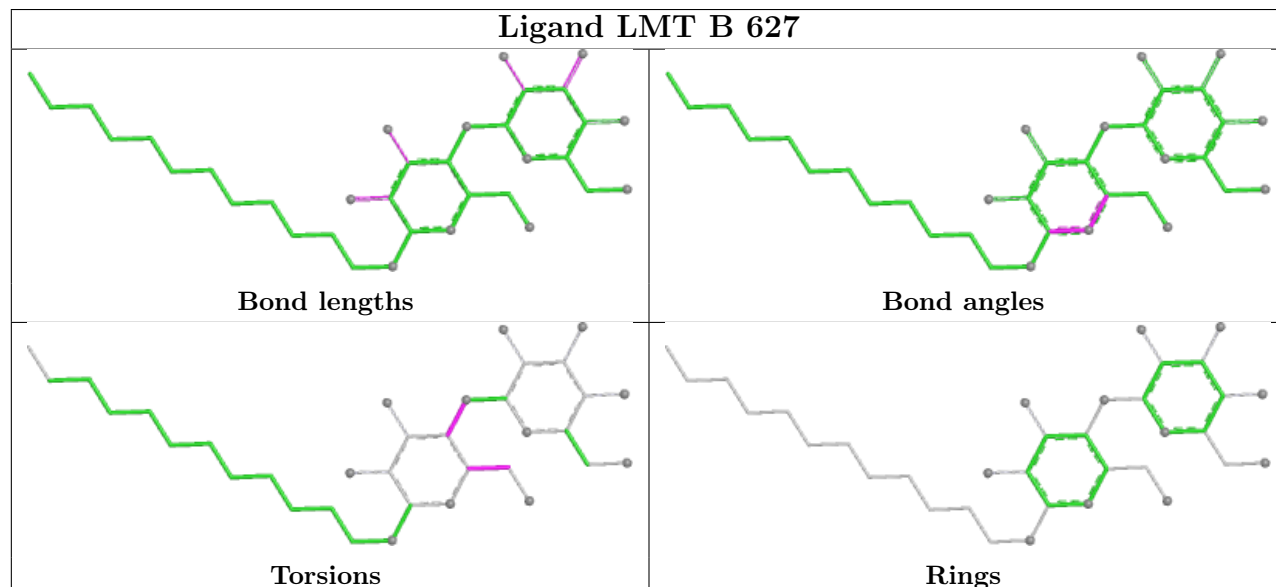
## Ligand CLA d 406

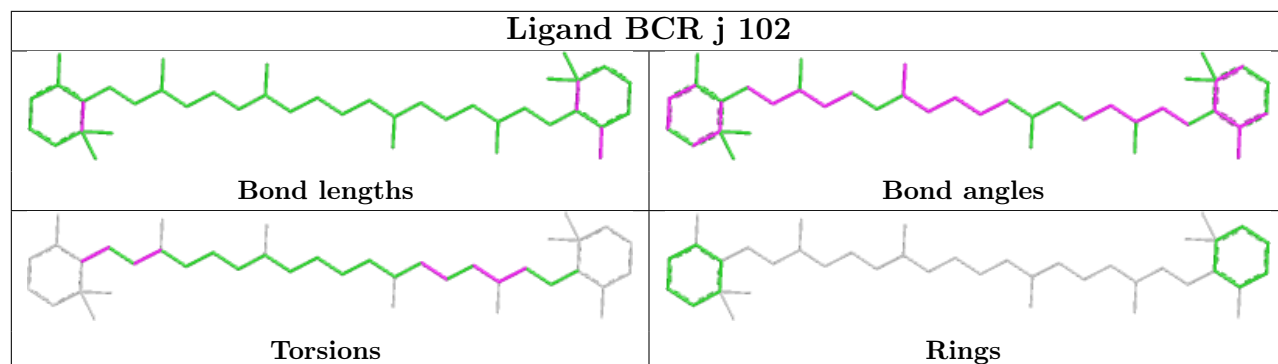
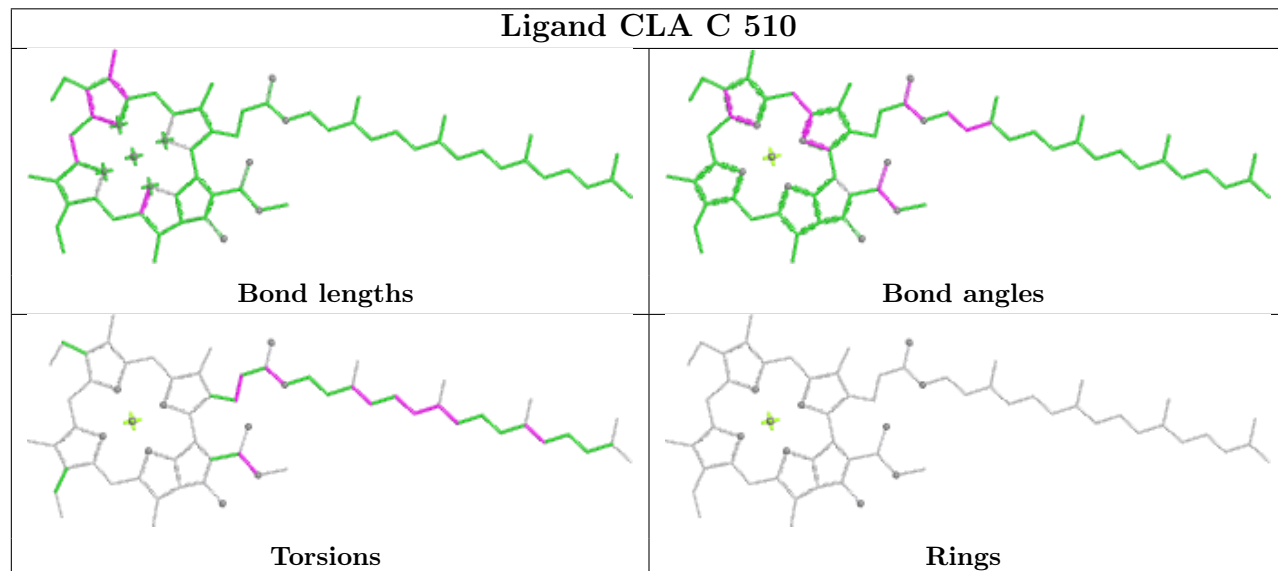
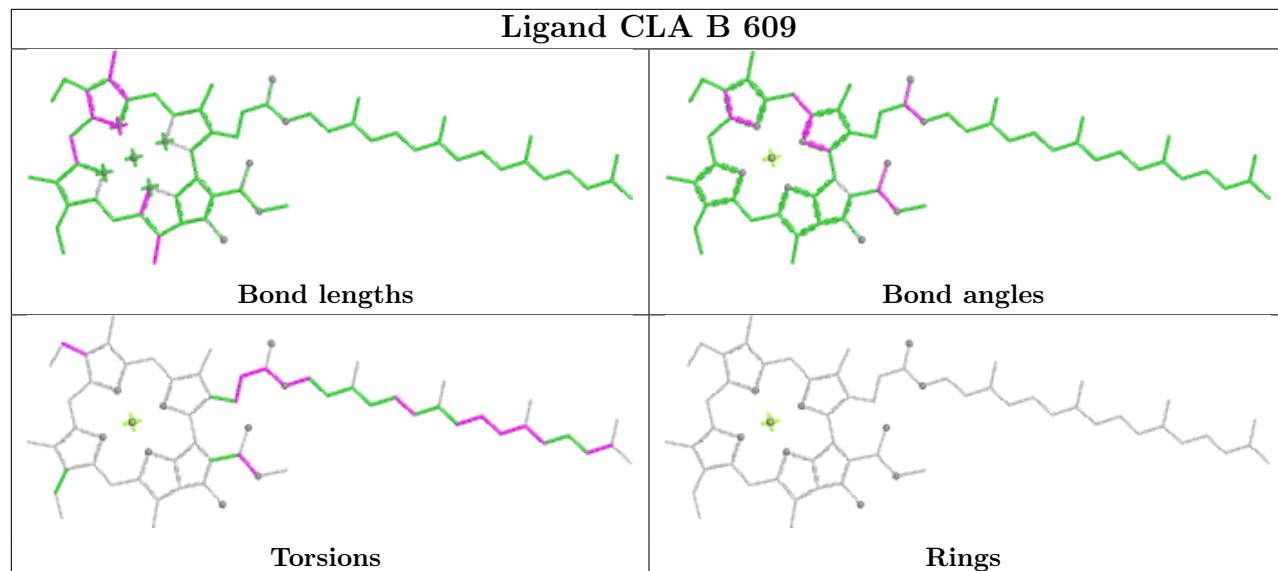


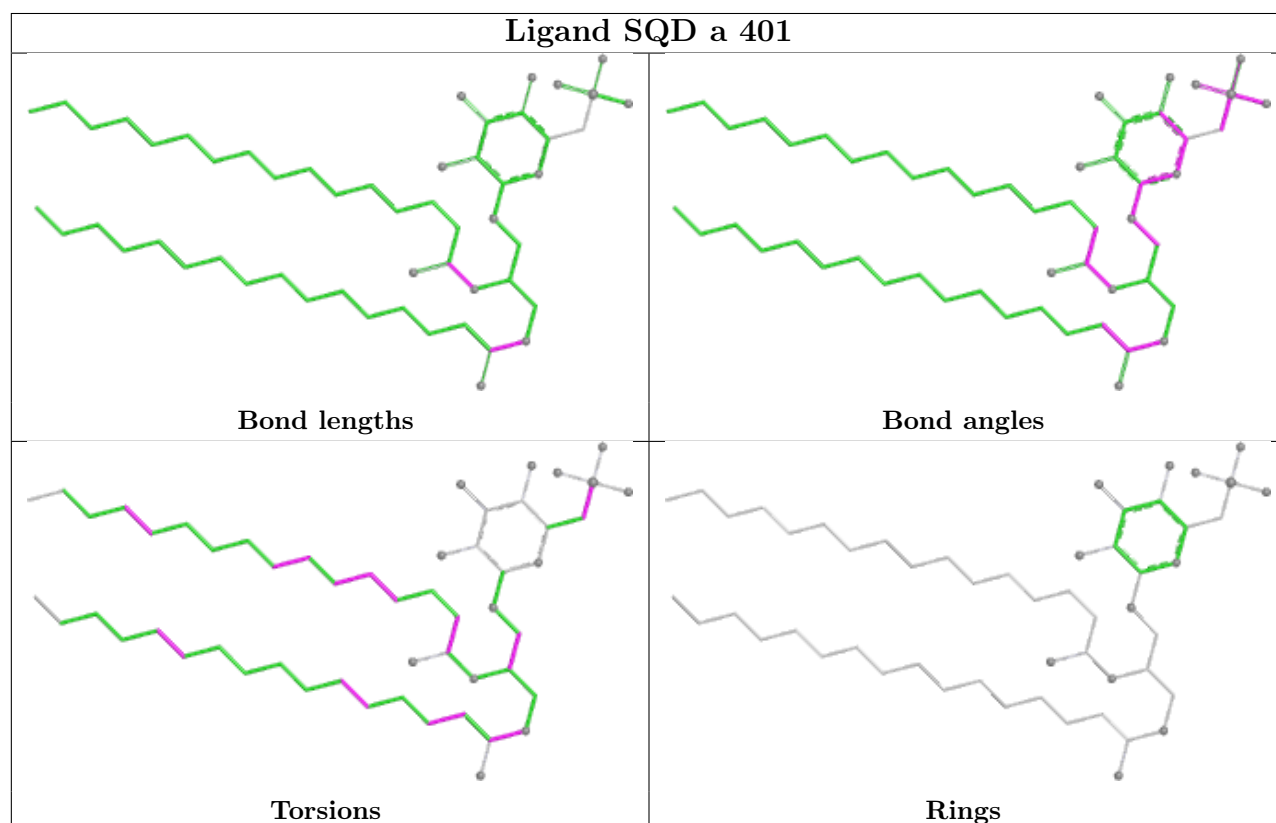
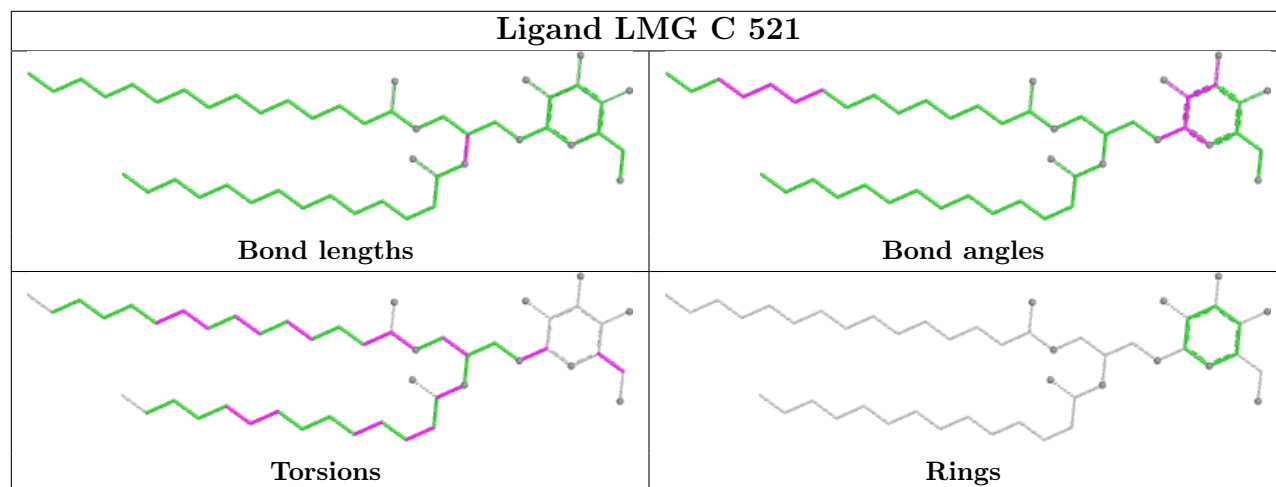
## Ligand CLA b 610



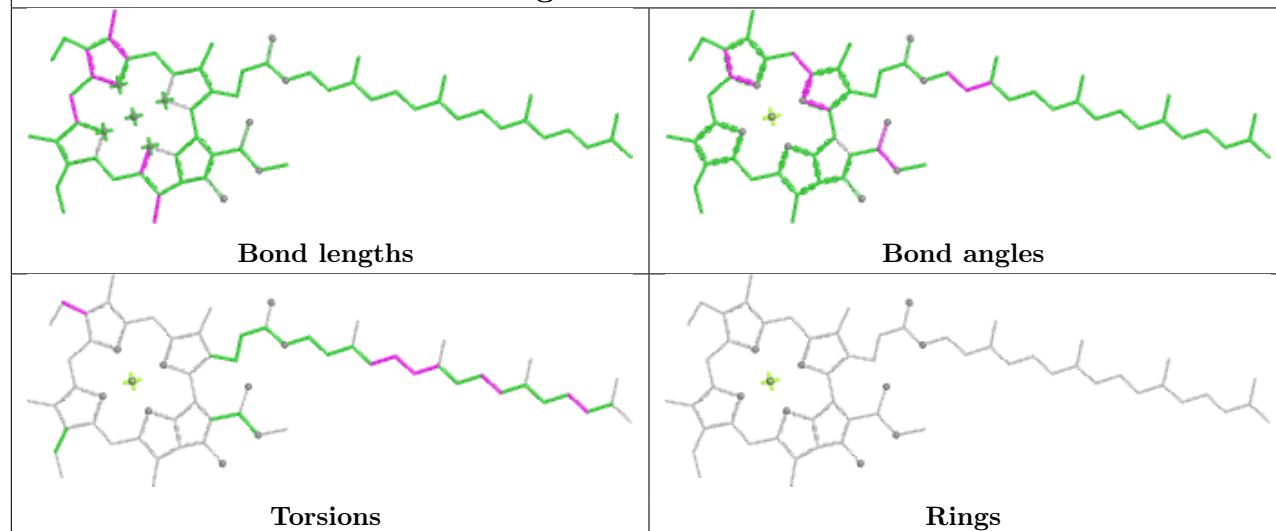
## Ligand LMT B 627



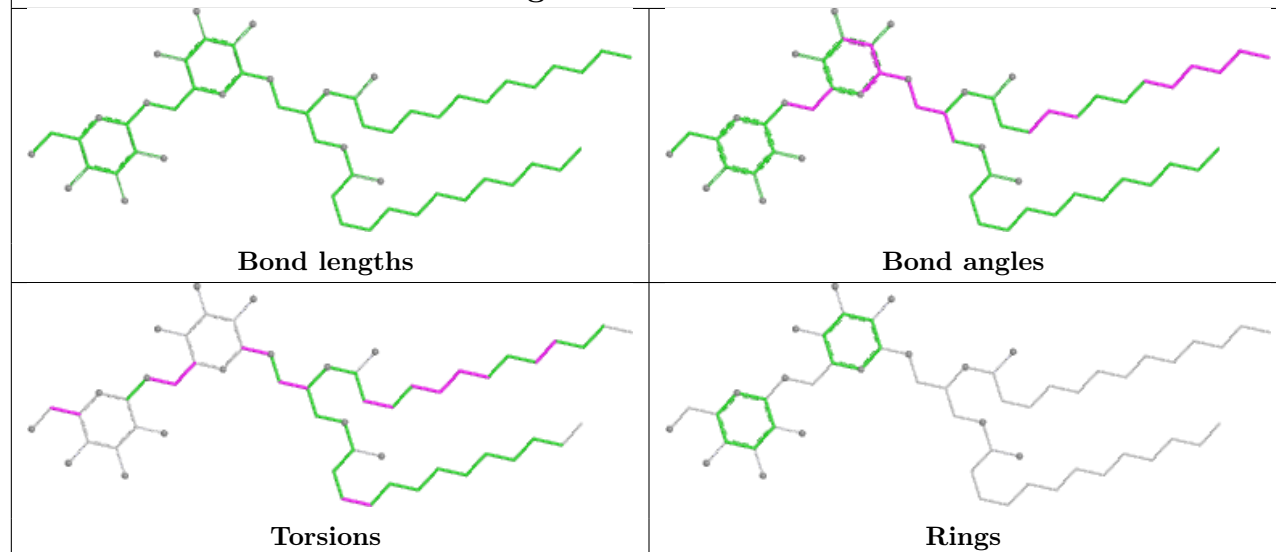
**Ligand BCR j 102****Ligand CLA C 510****Ligand CLA B 609**



## Ligand CLA a 406

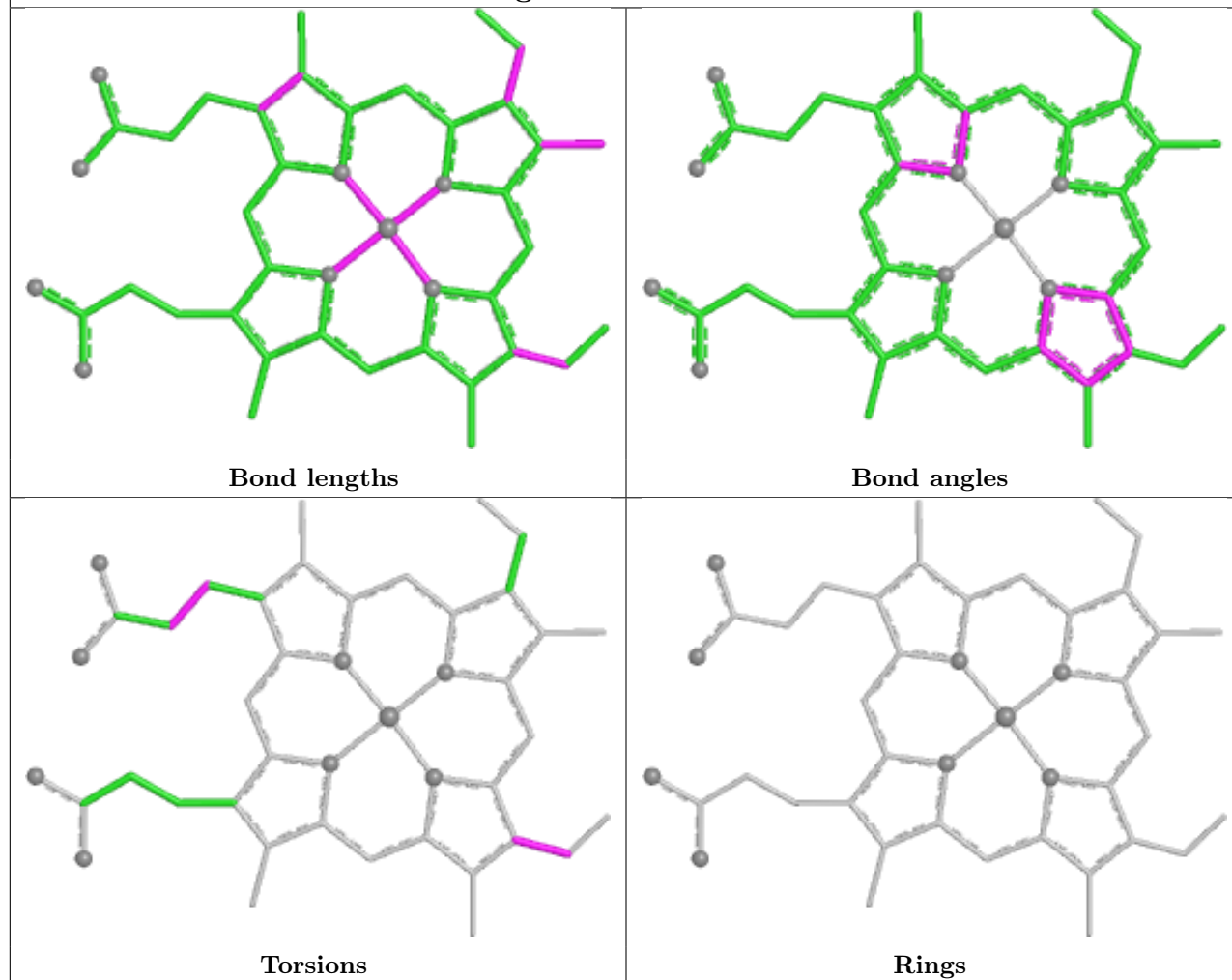


## Ligand DGD A 408

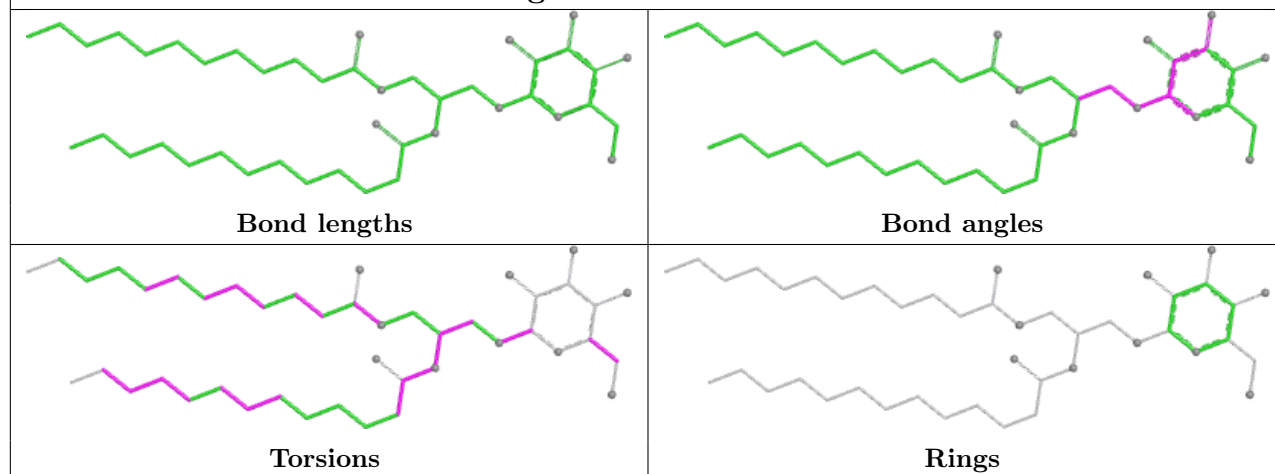


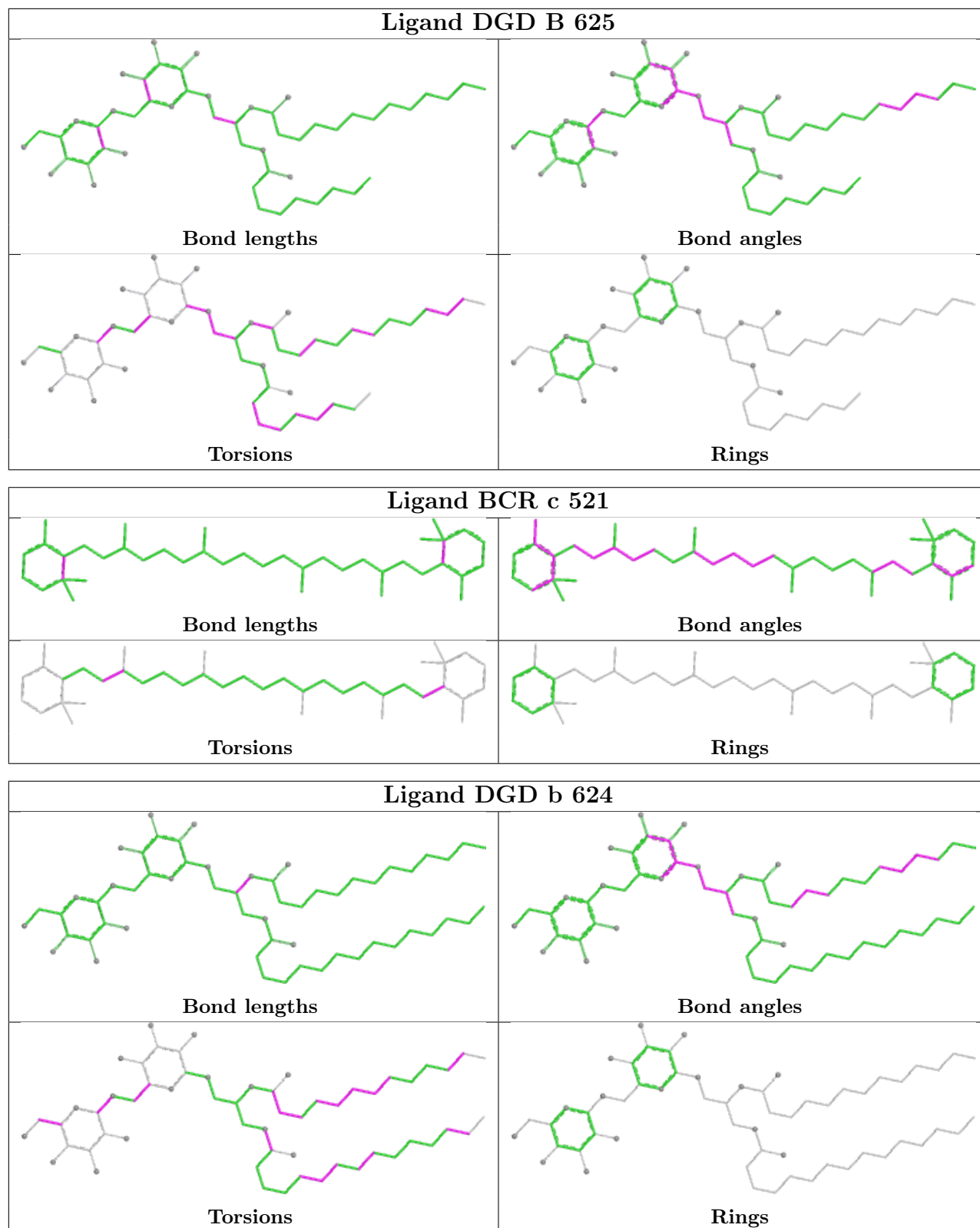


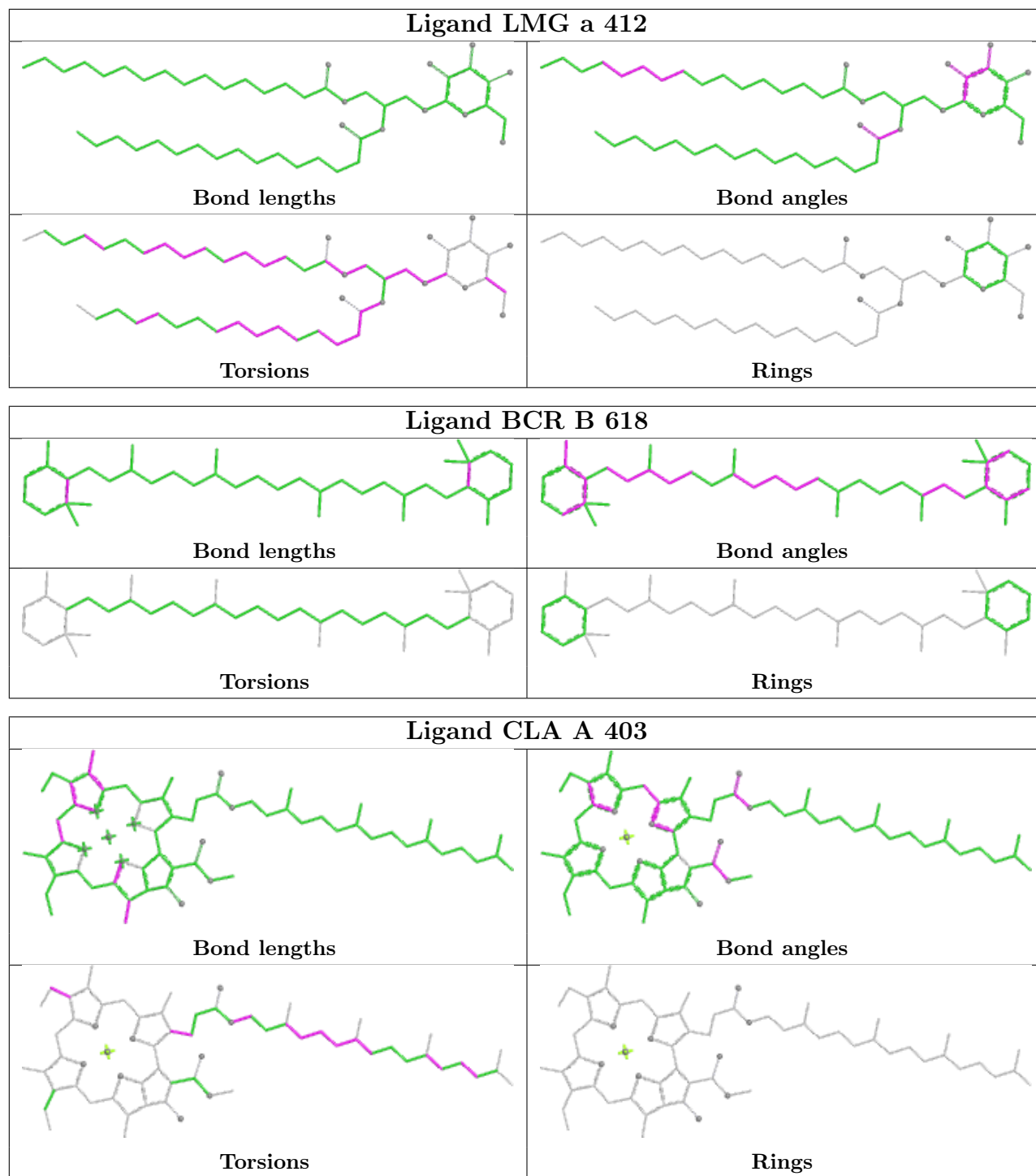
## Ligand HEM f 101



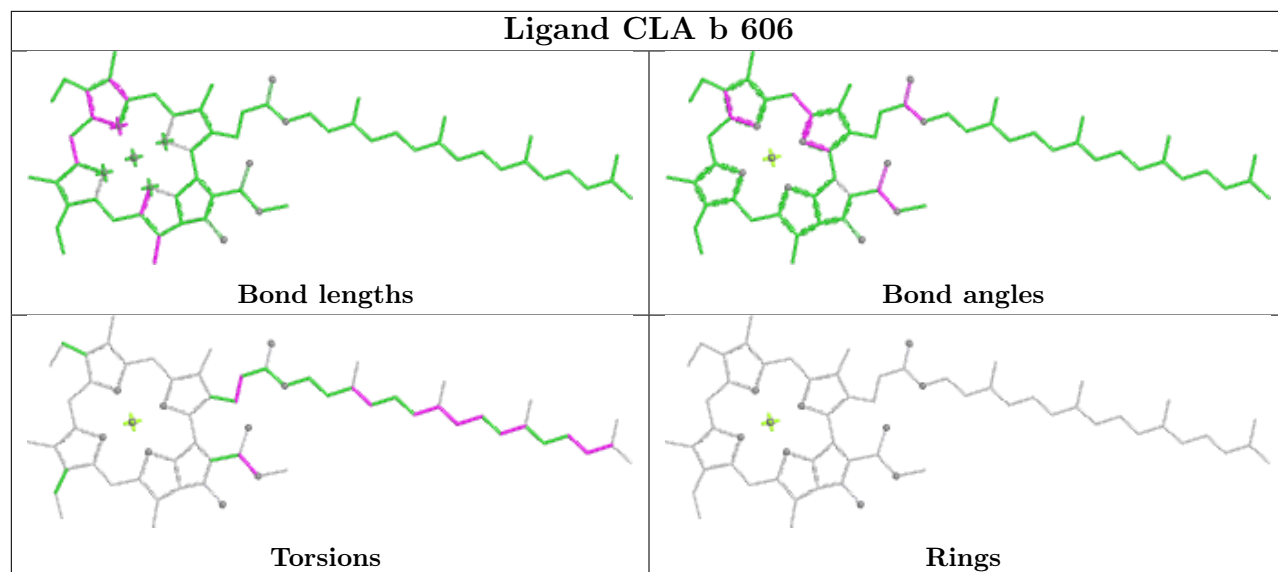
## Ligand LMG E 101



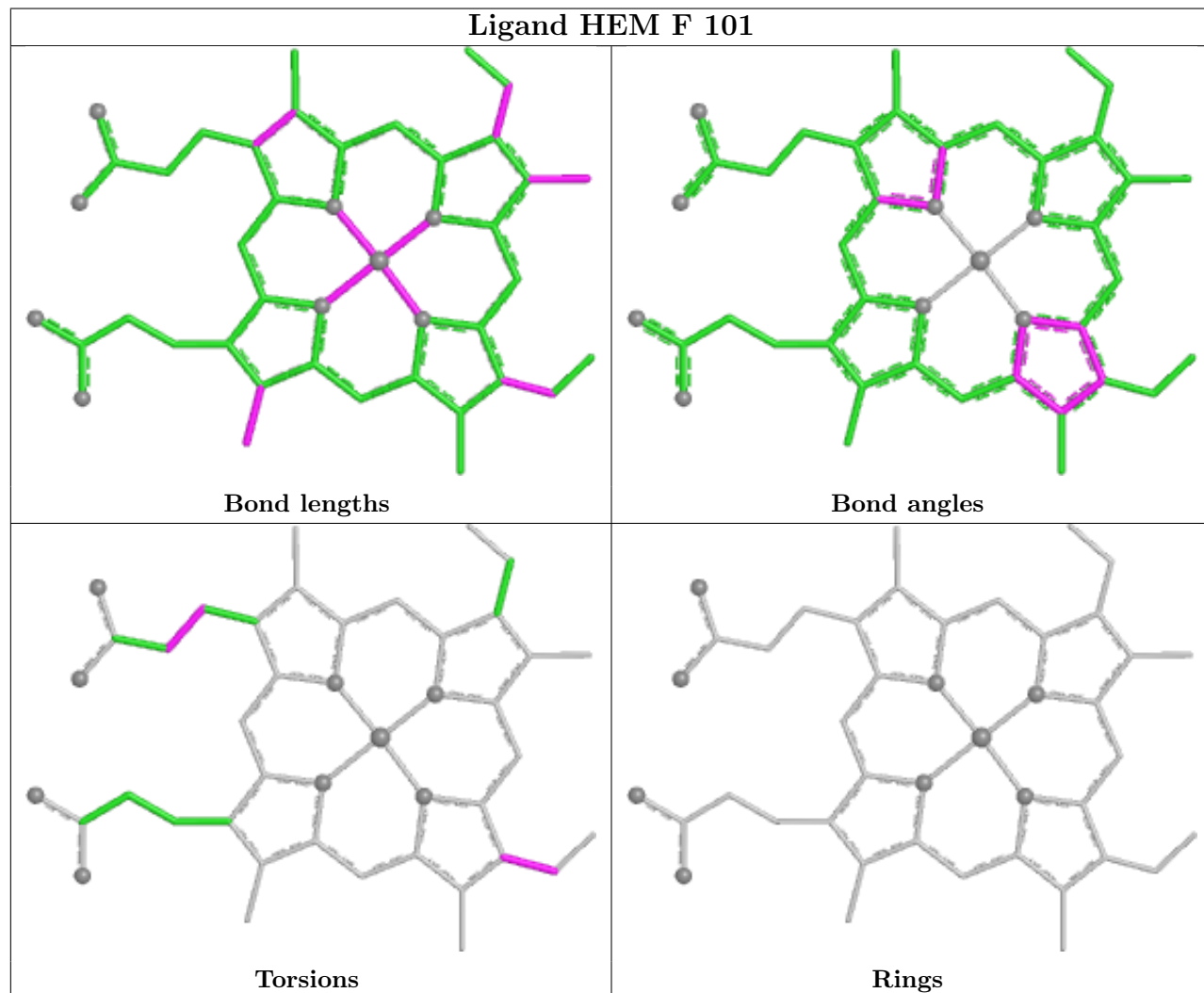




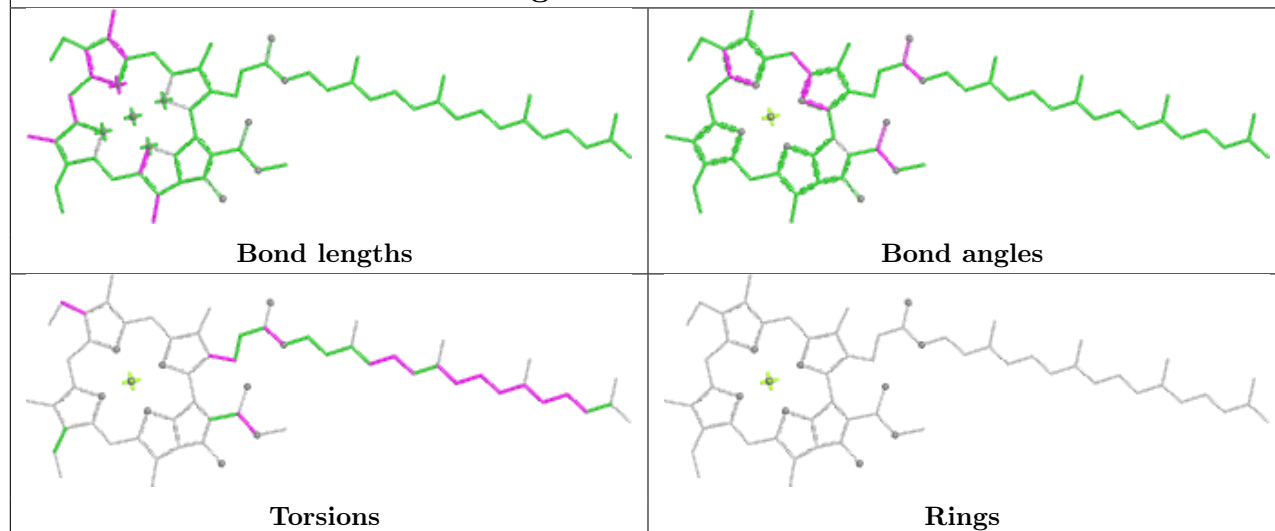
## Ligand CLA b 606



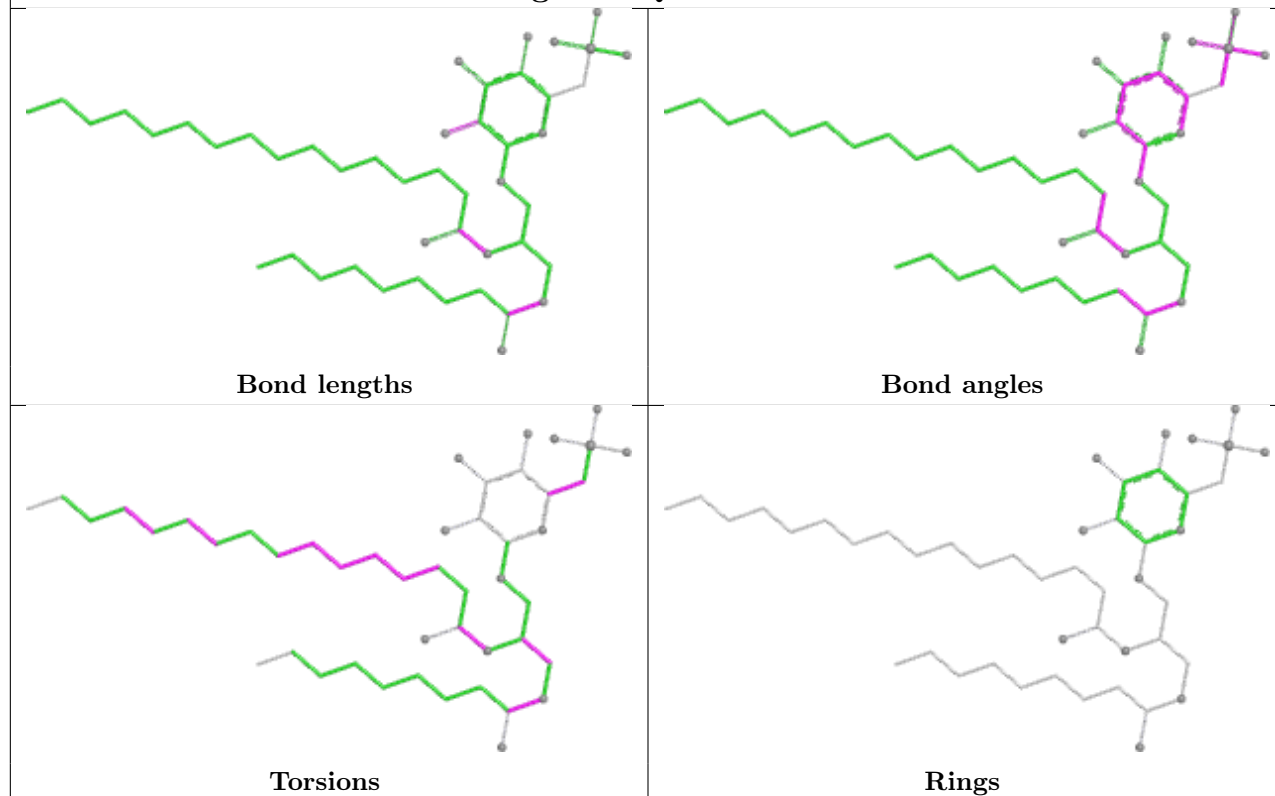
## Ligand HEM F 101



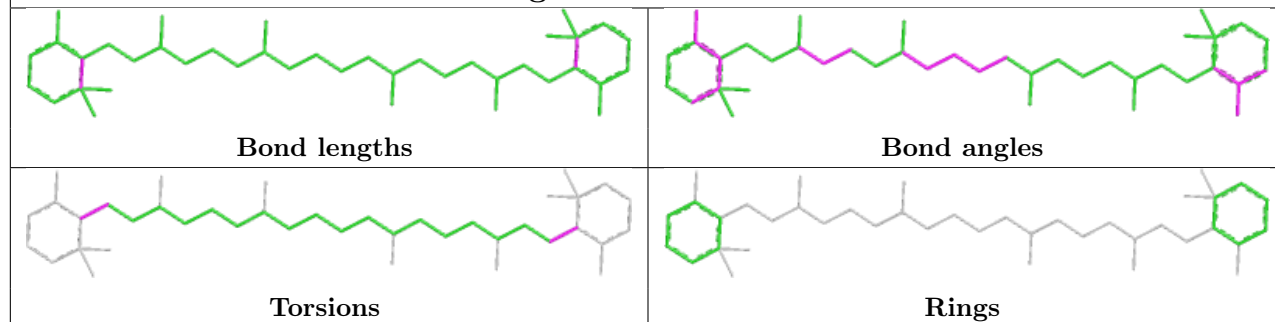
## Ligand CLA B 615

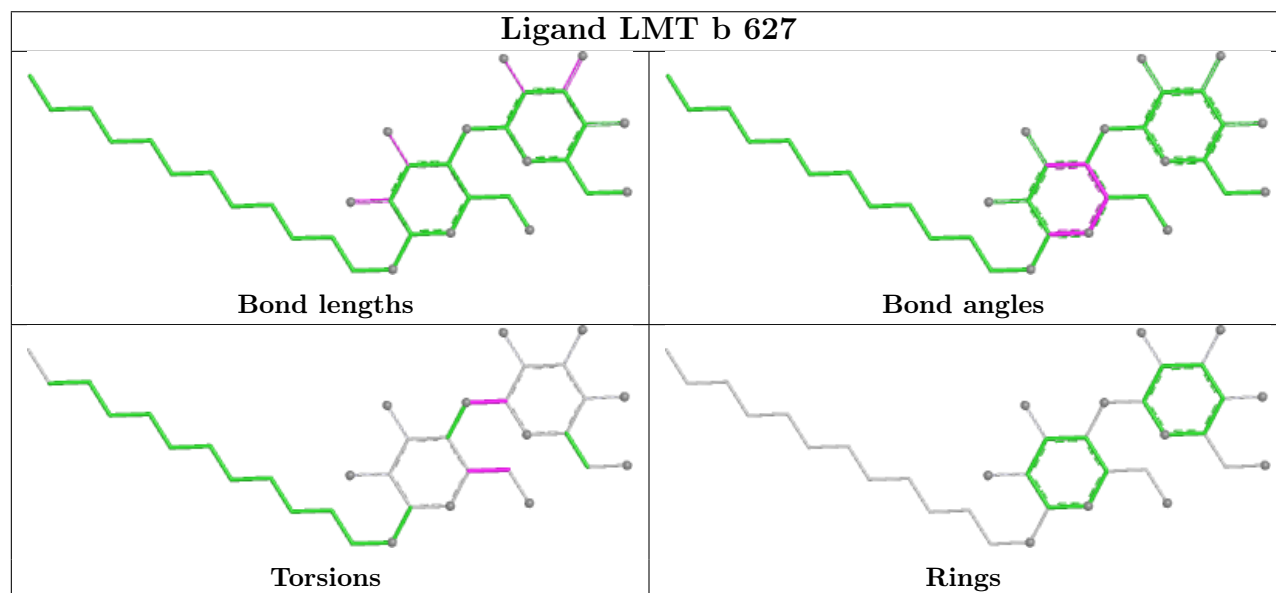
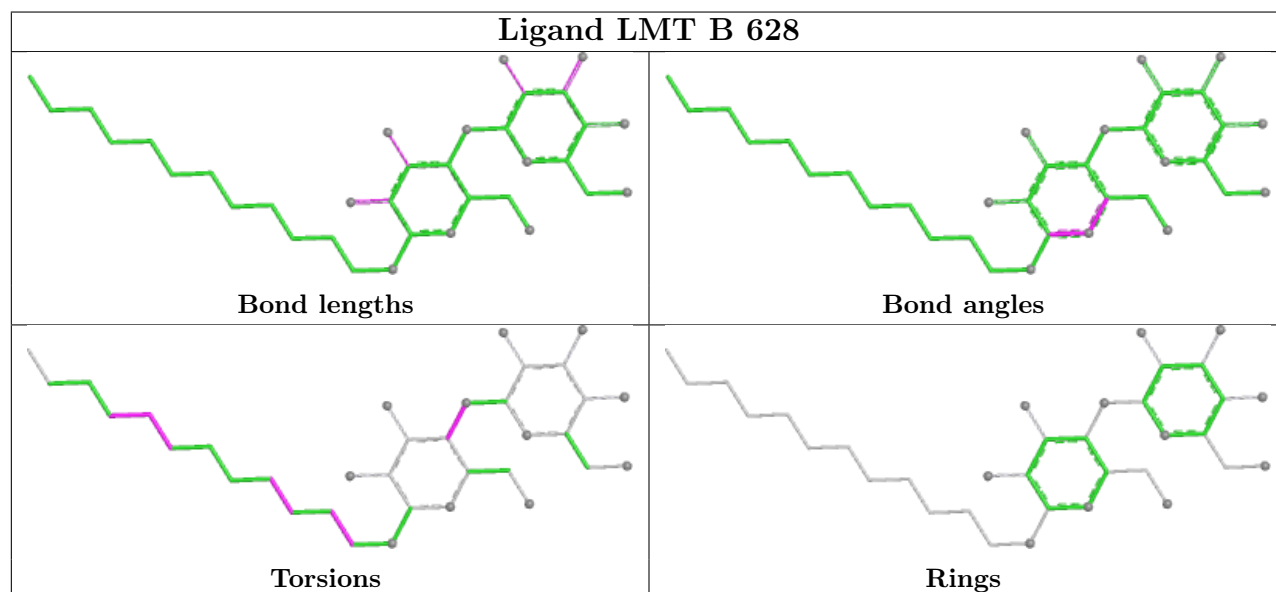
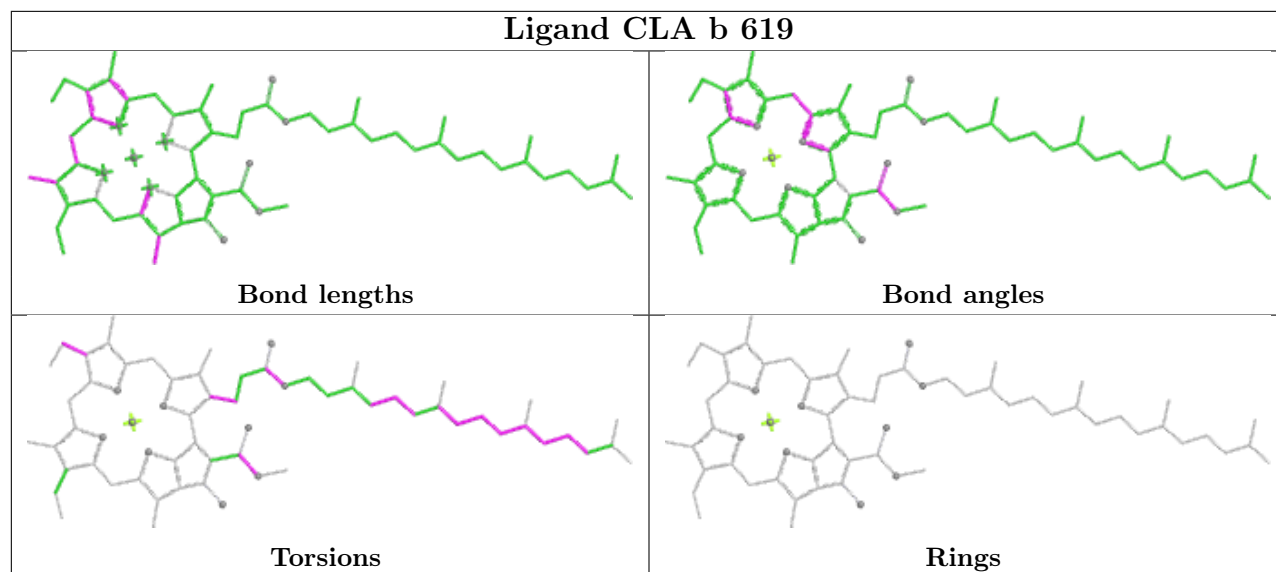


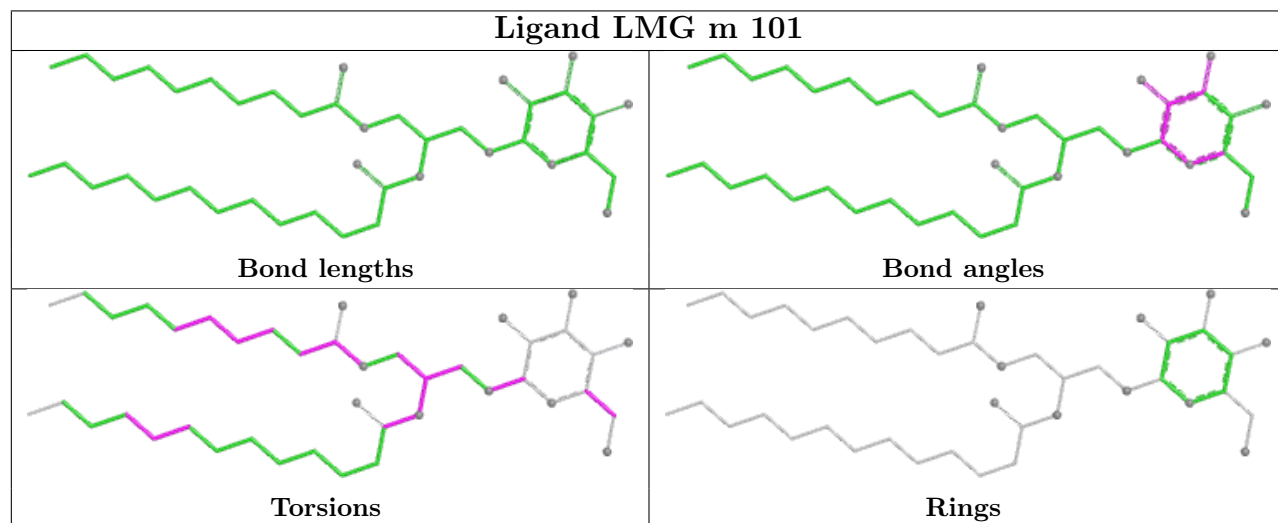
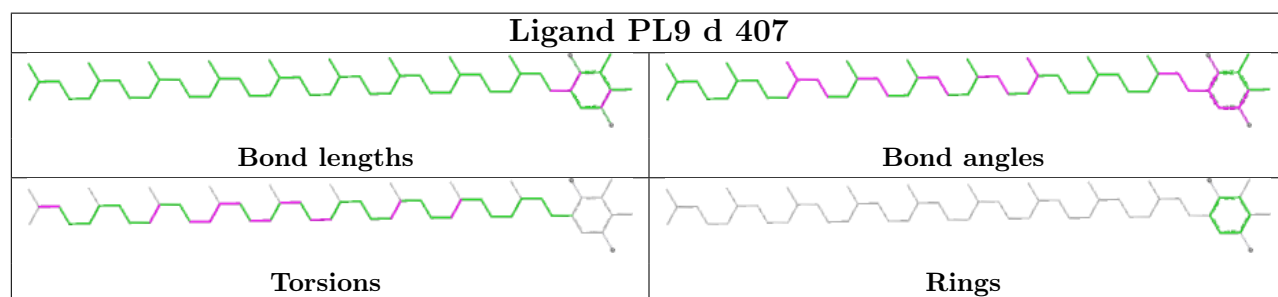
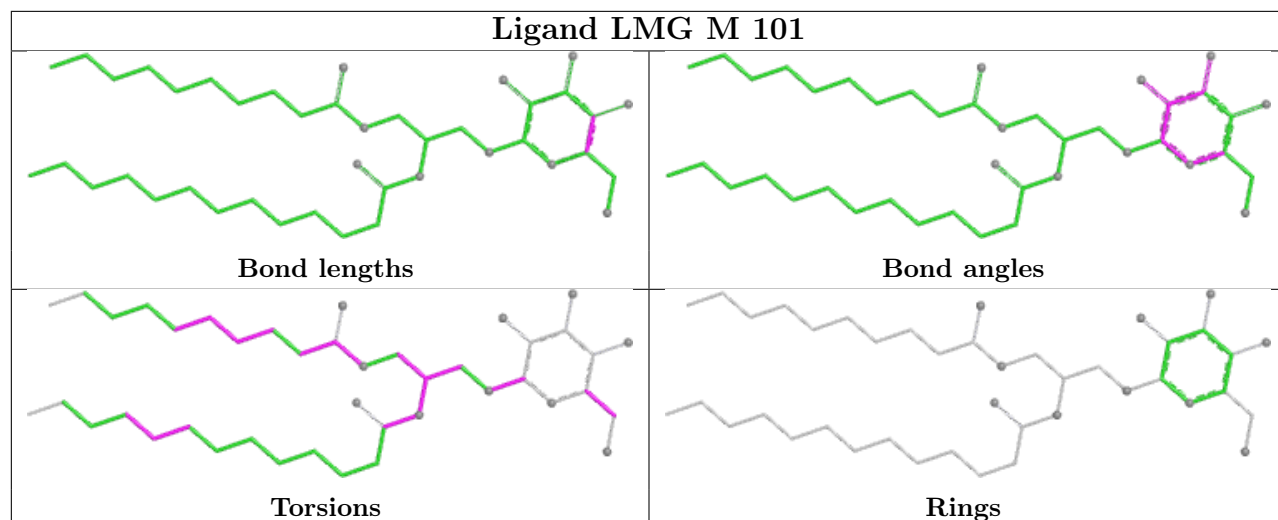
## Ligand SQD B 626



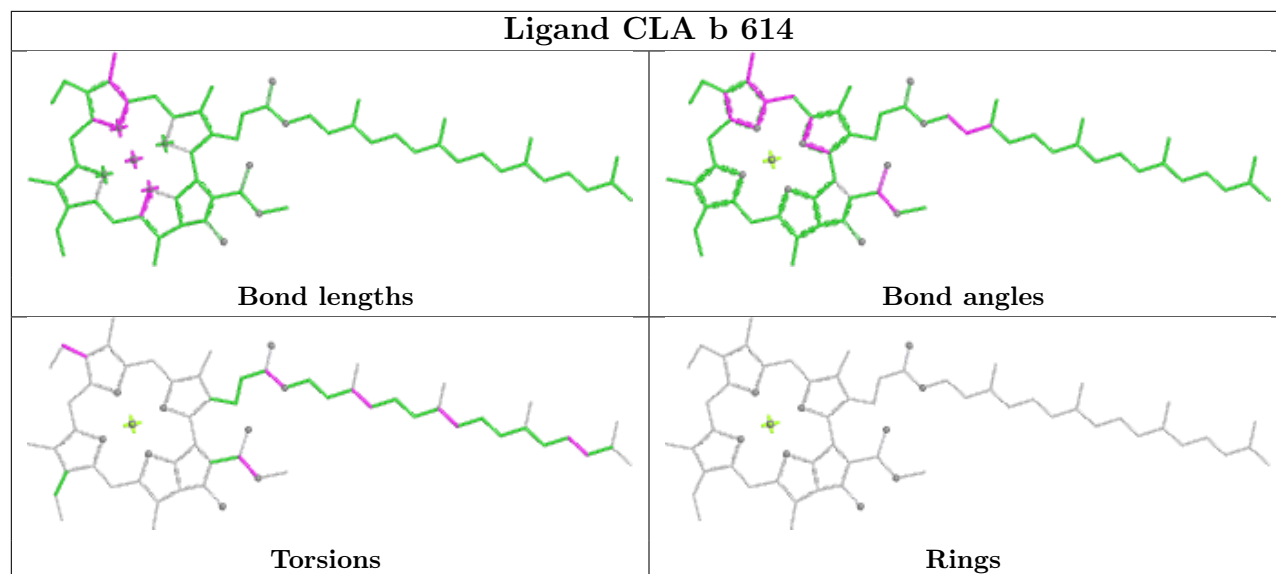
## Ligand BCR A 407



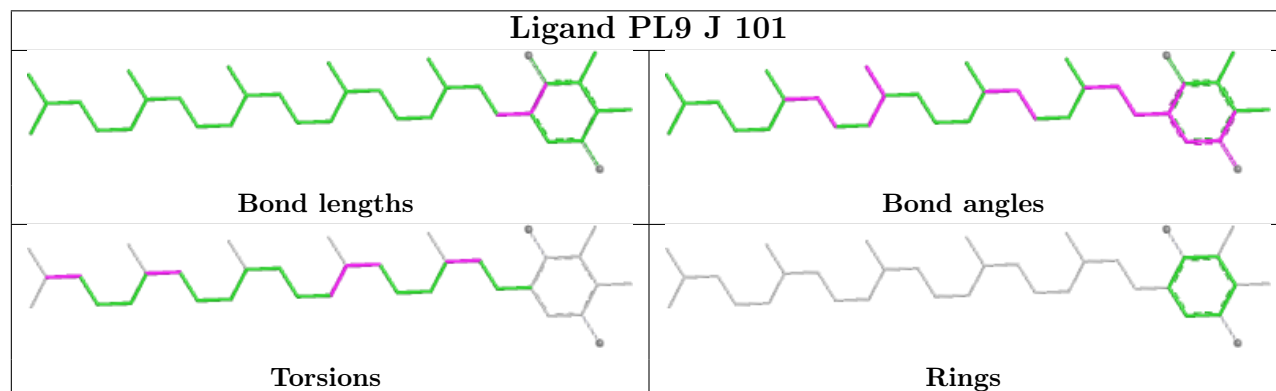




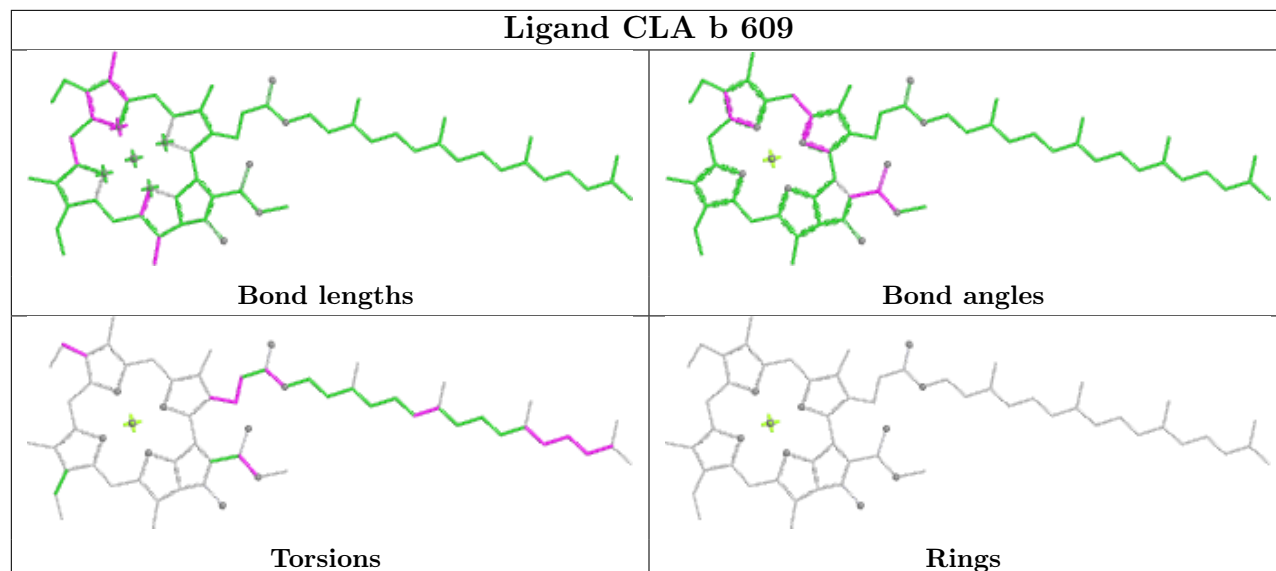
## Ligand CLA b 614



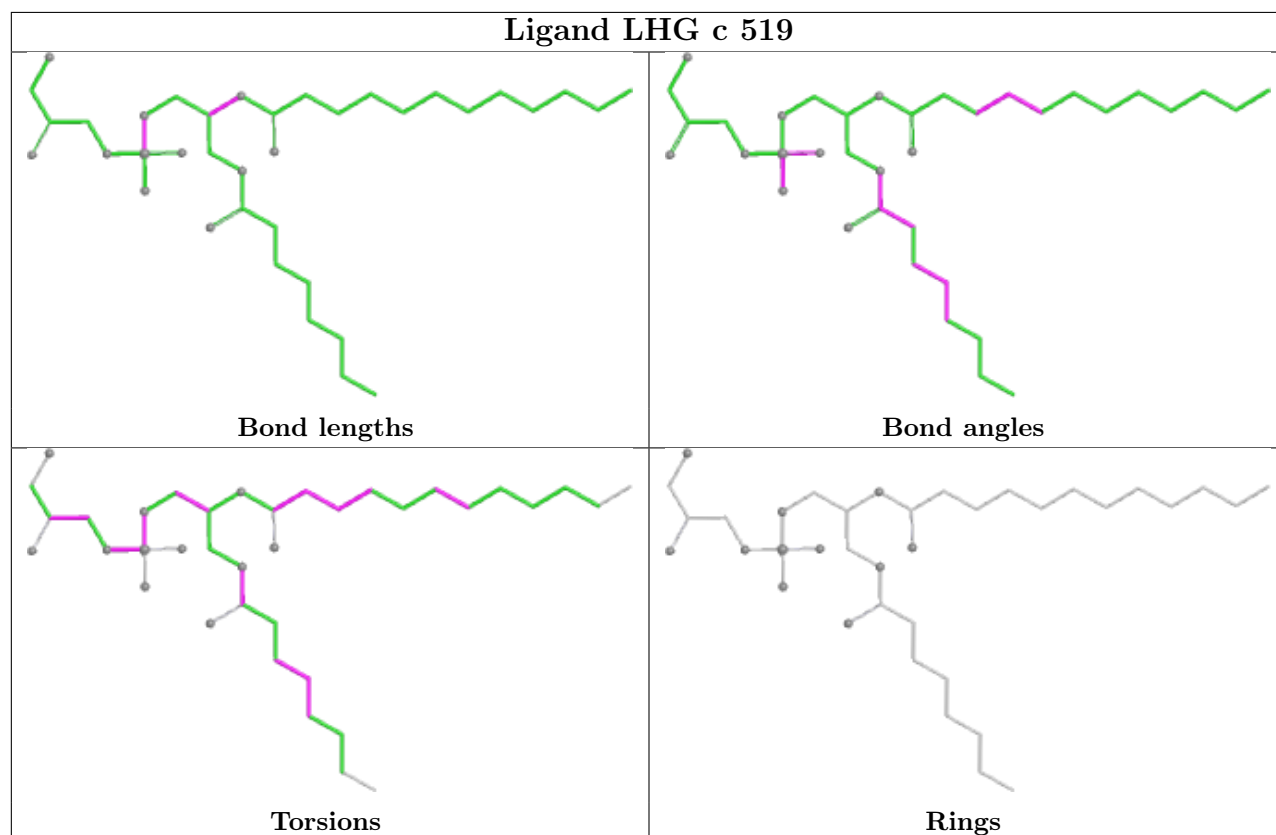
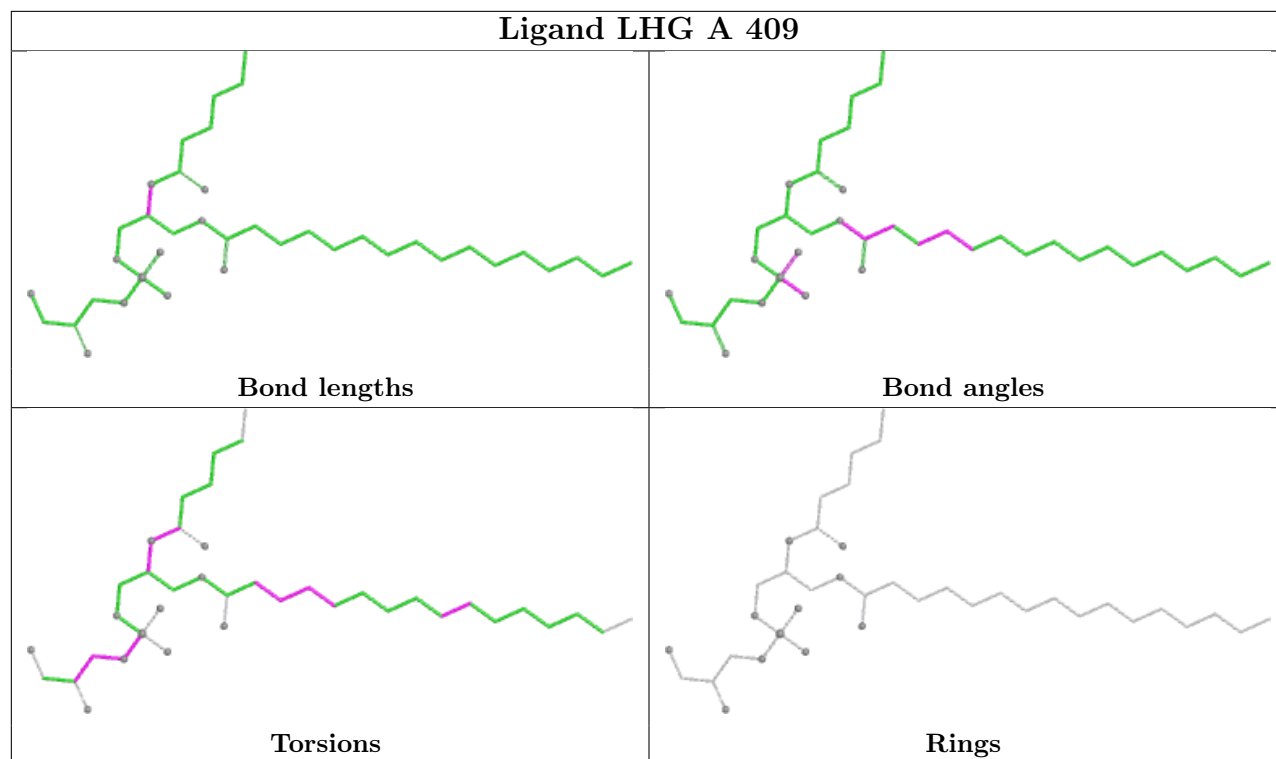
## Ligand PL9 J 101



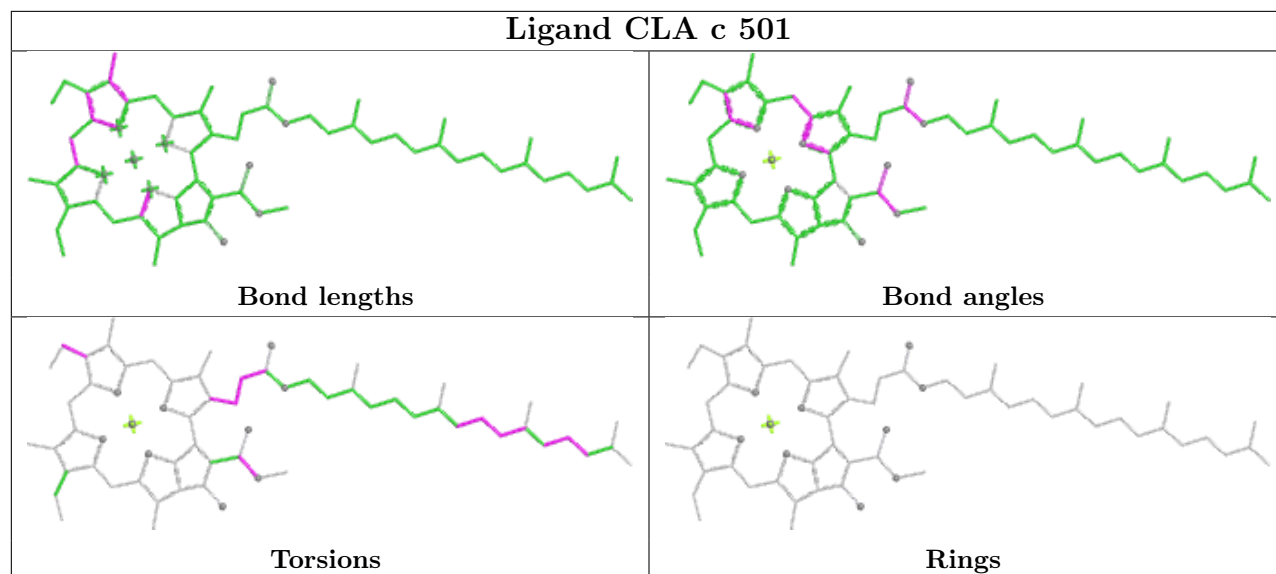
## Ligand CLA b 609



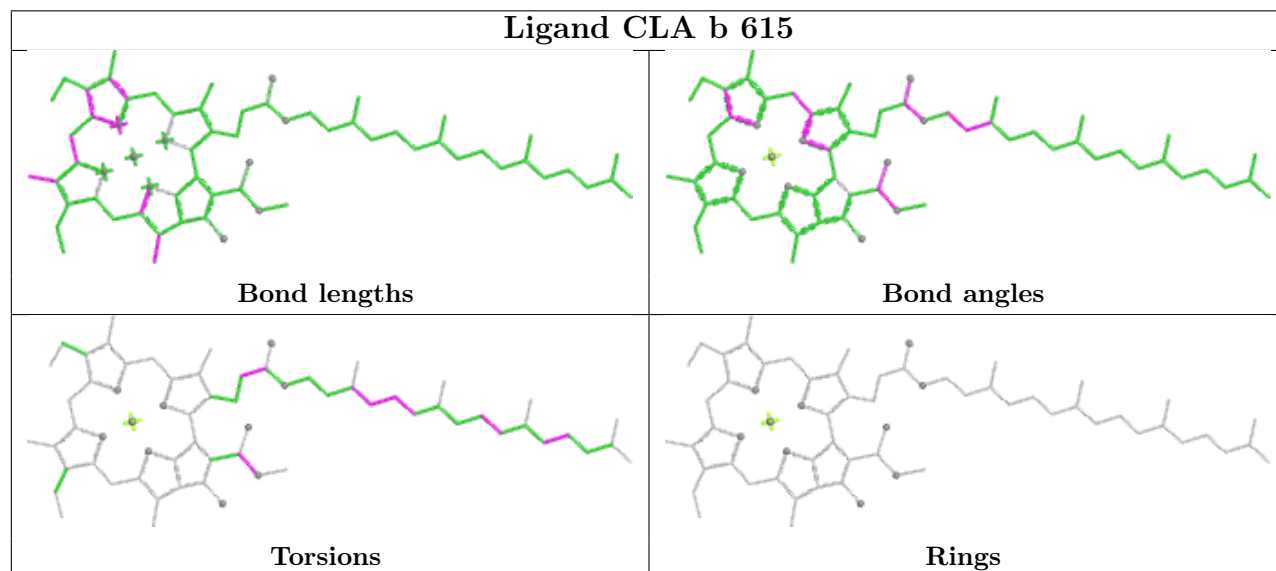




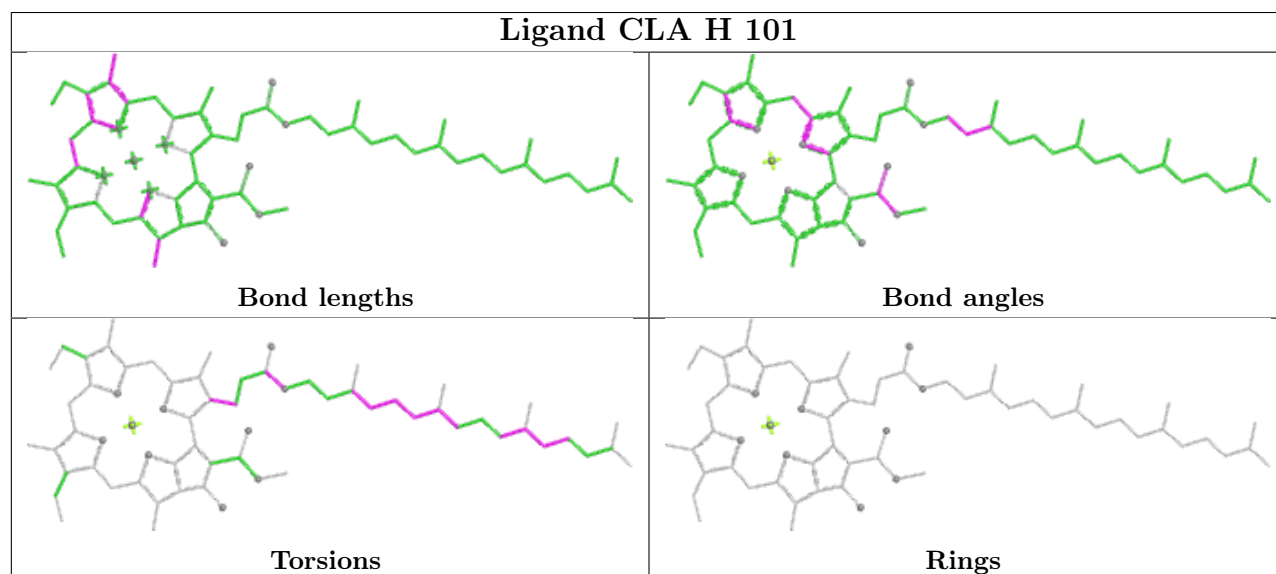
## Ligand CLA c 501

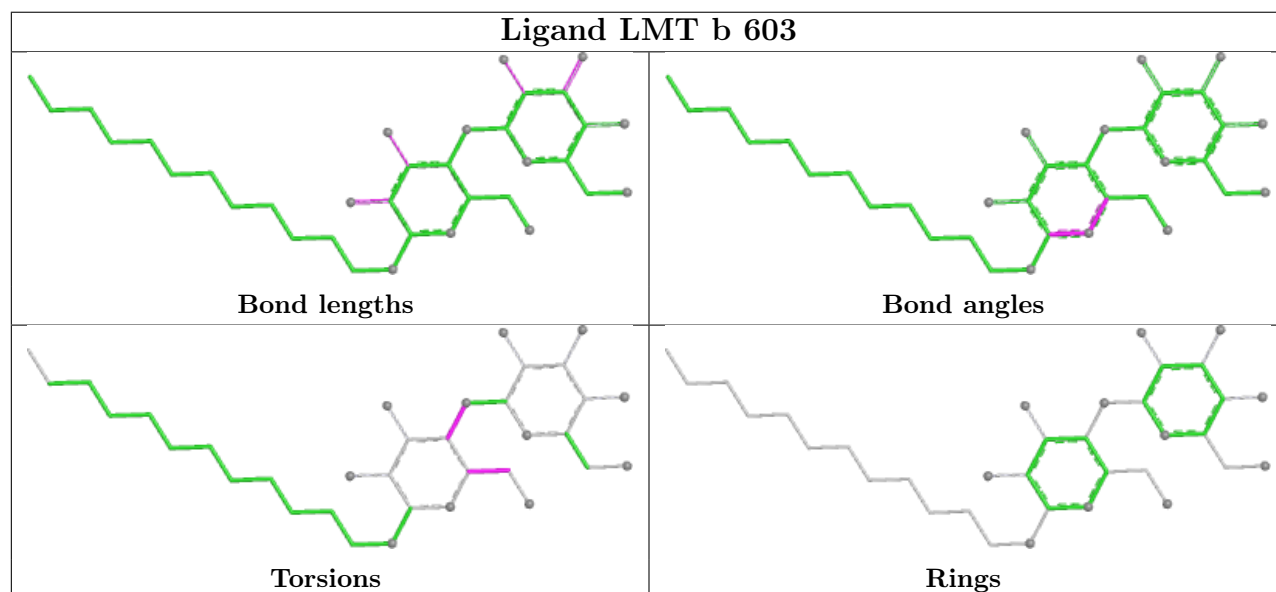
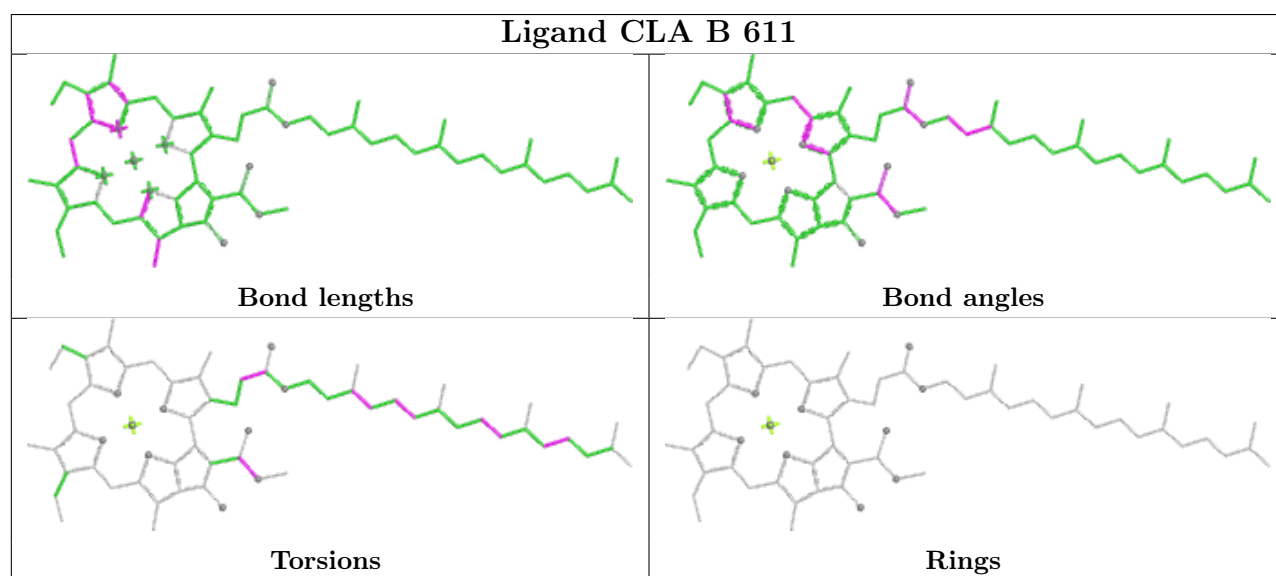
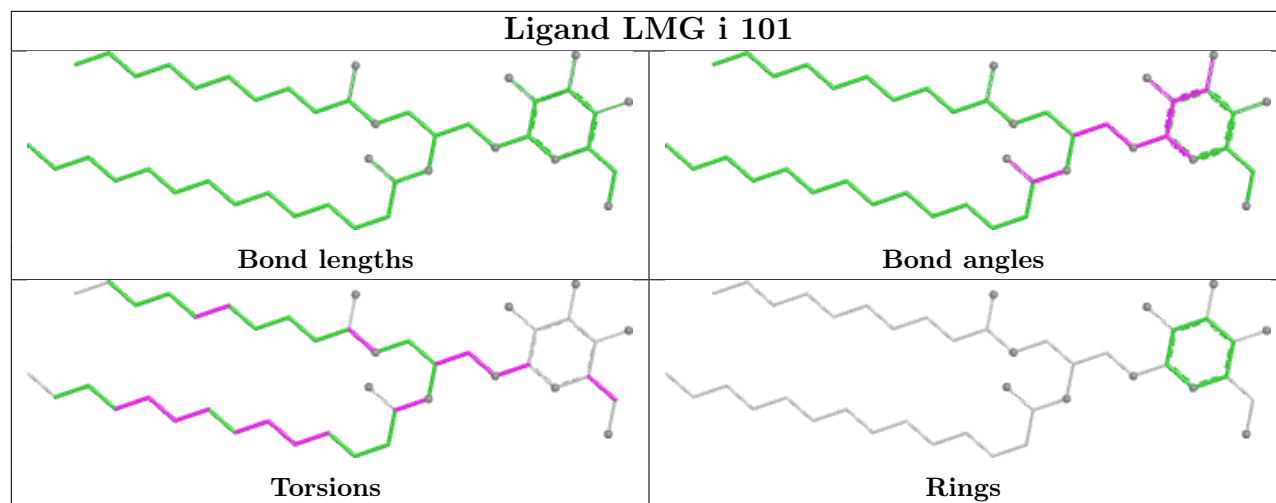


## Ligand CLA b 615

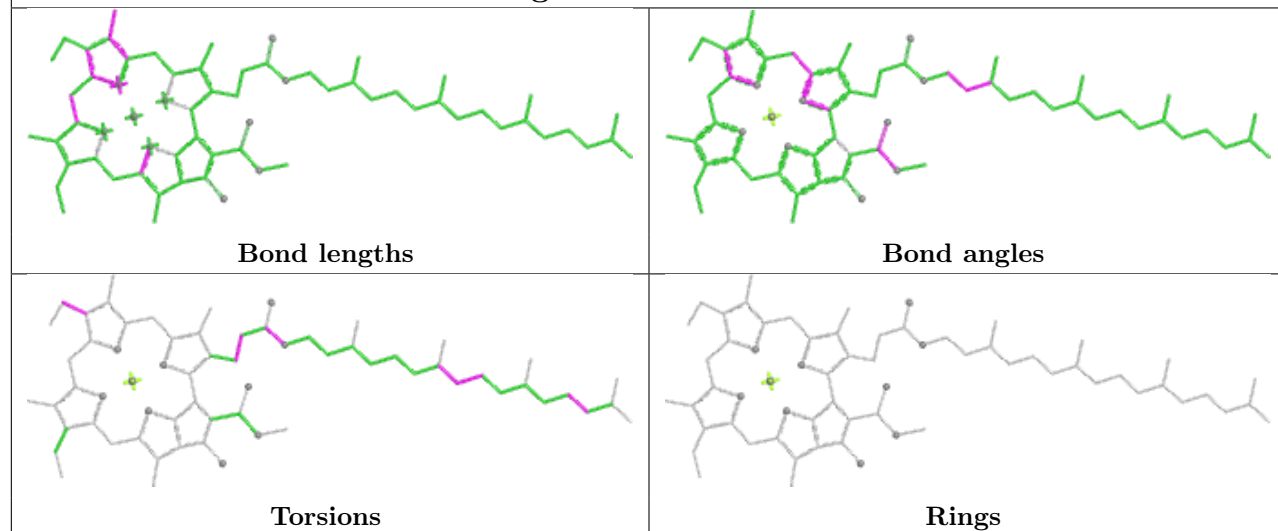


## Ligand CLA H 101

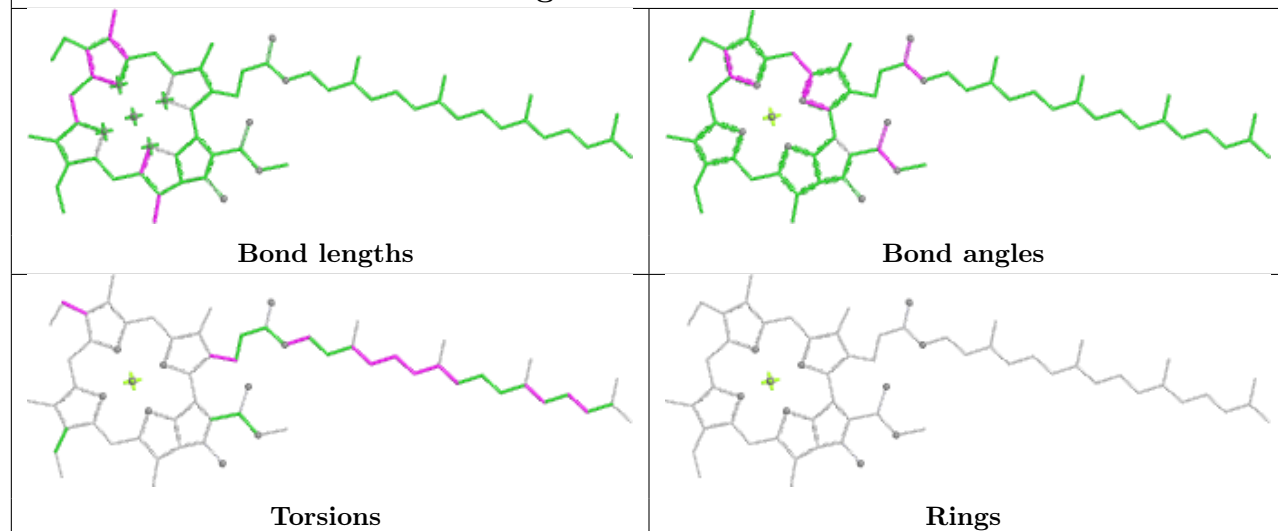




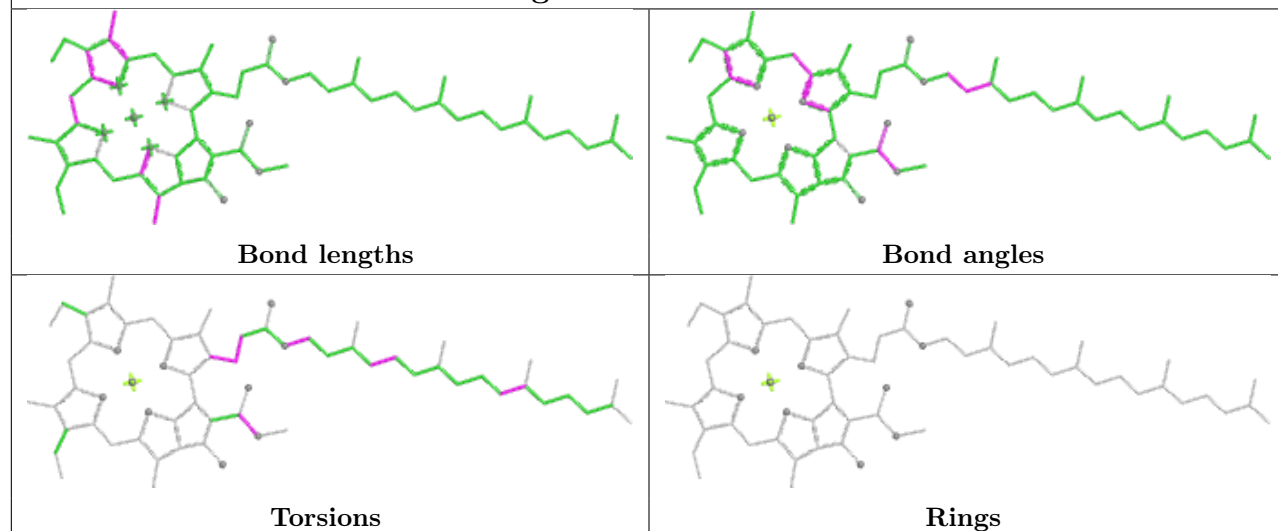
## Ligand CLA D 406

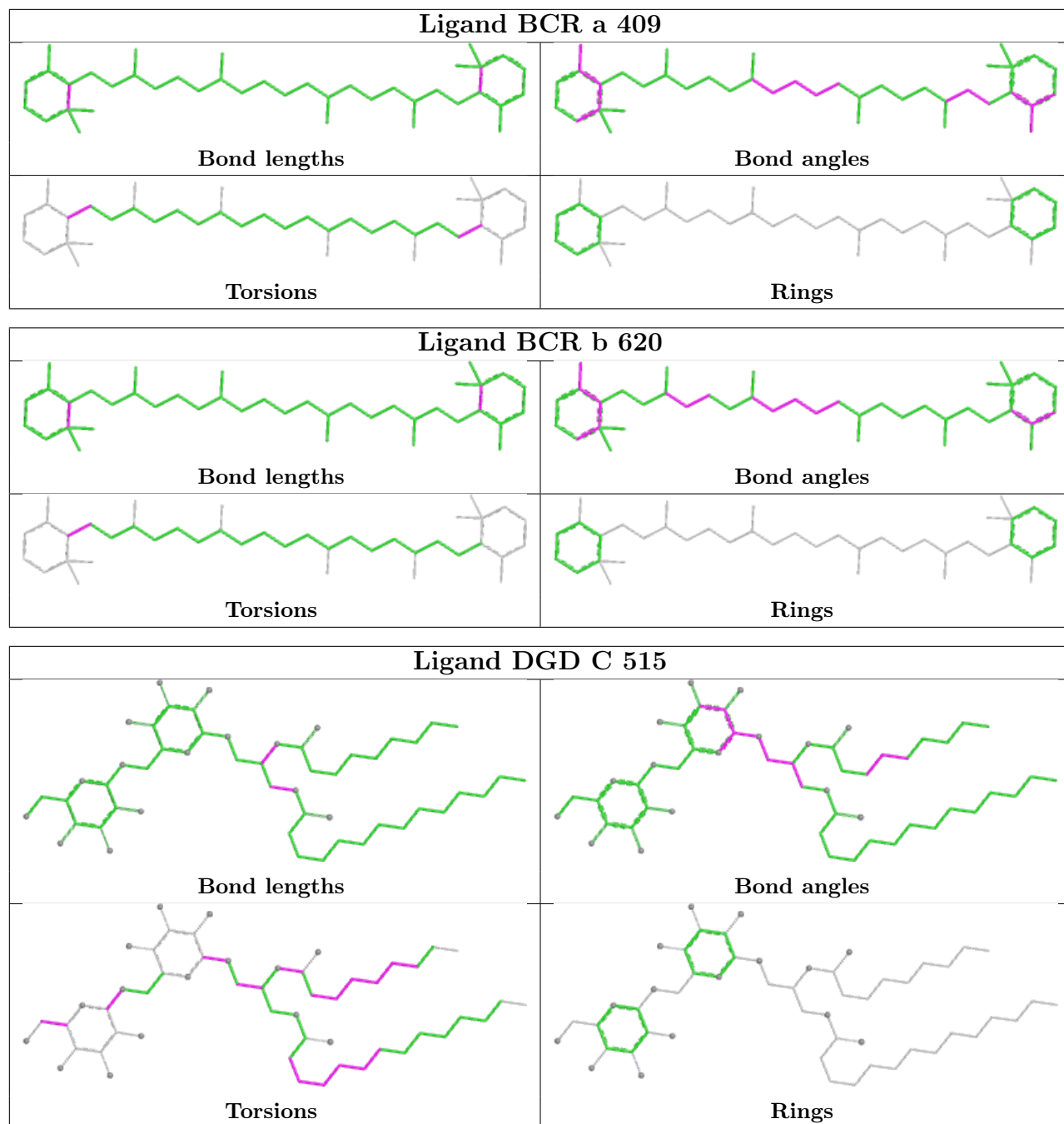


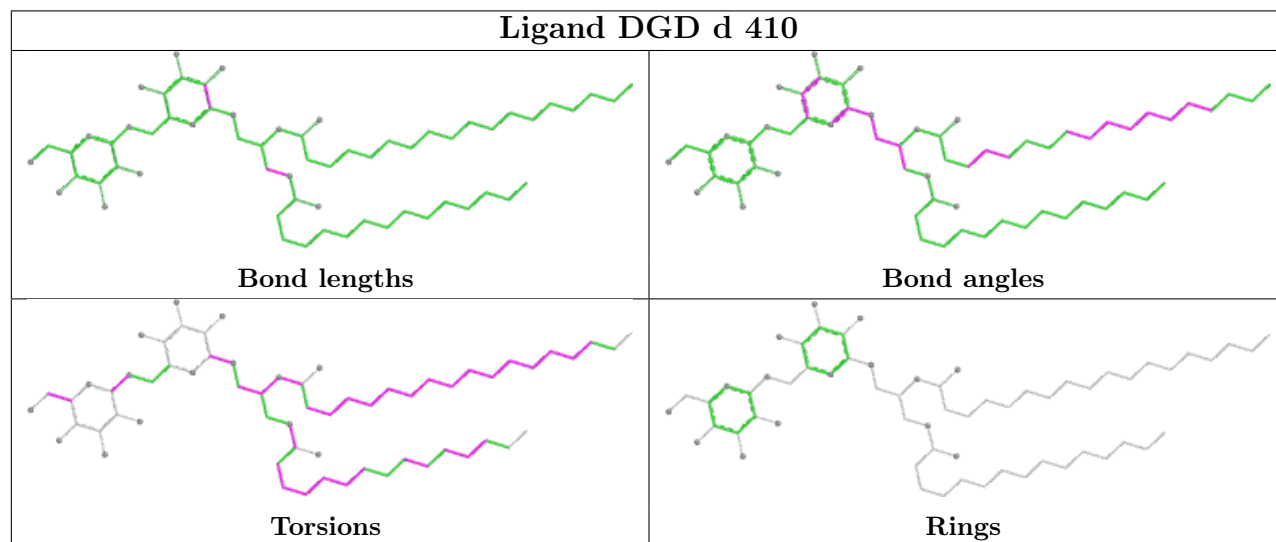
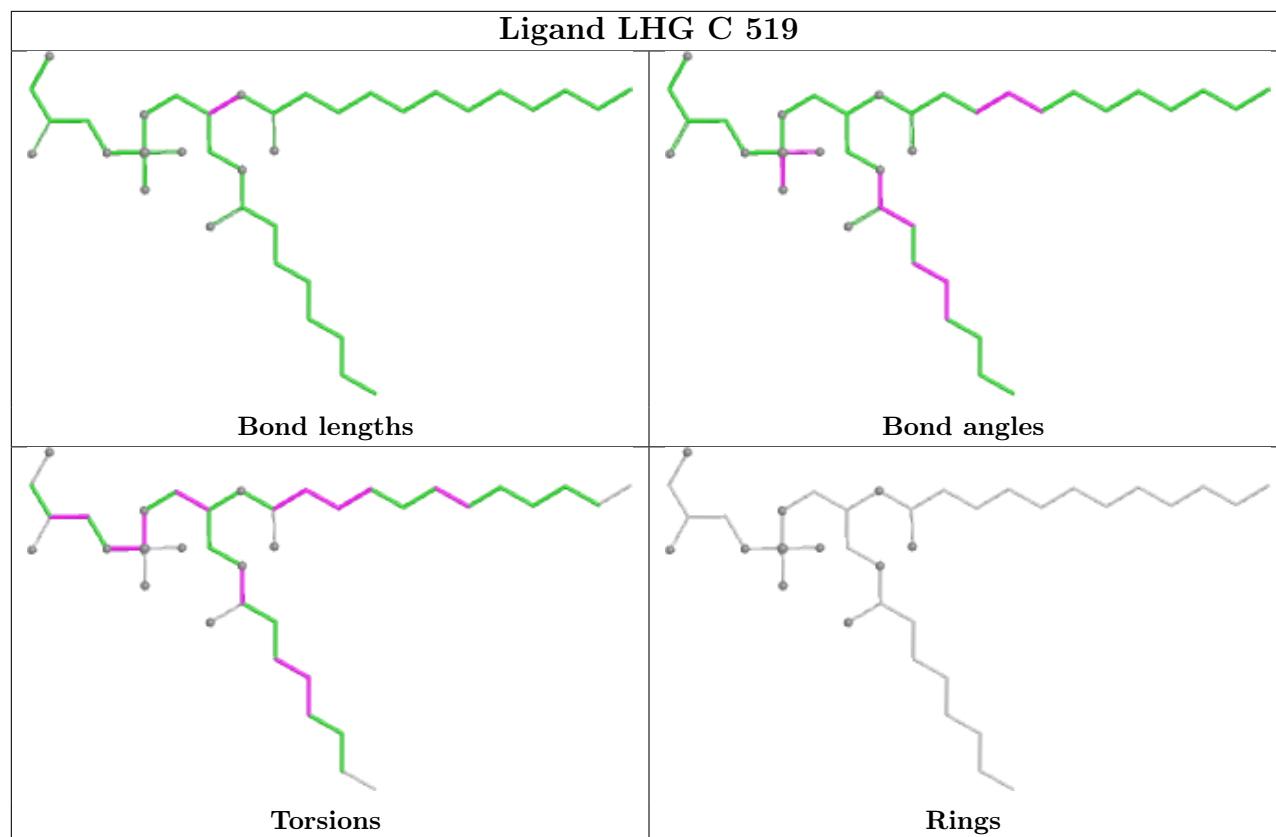
## Ligand CLA a 405

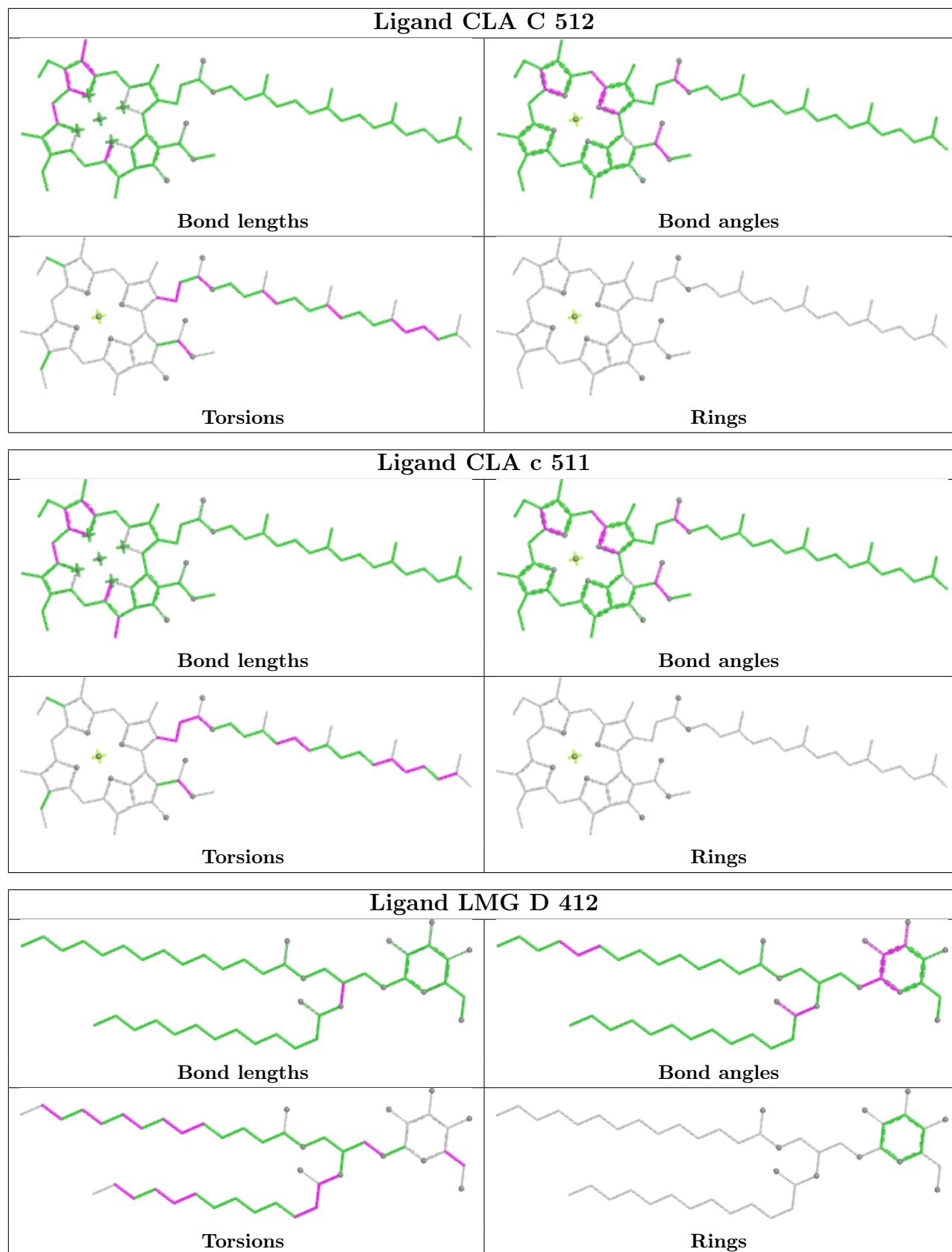


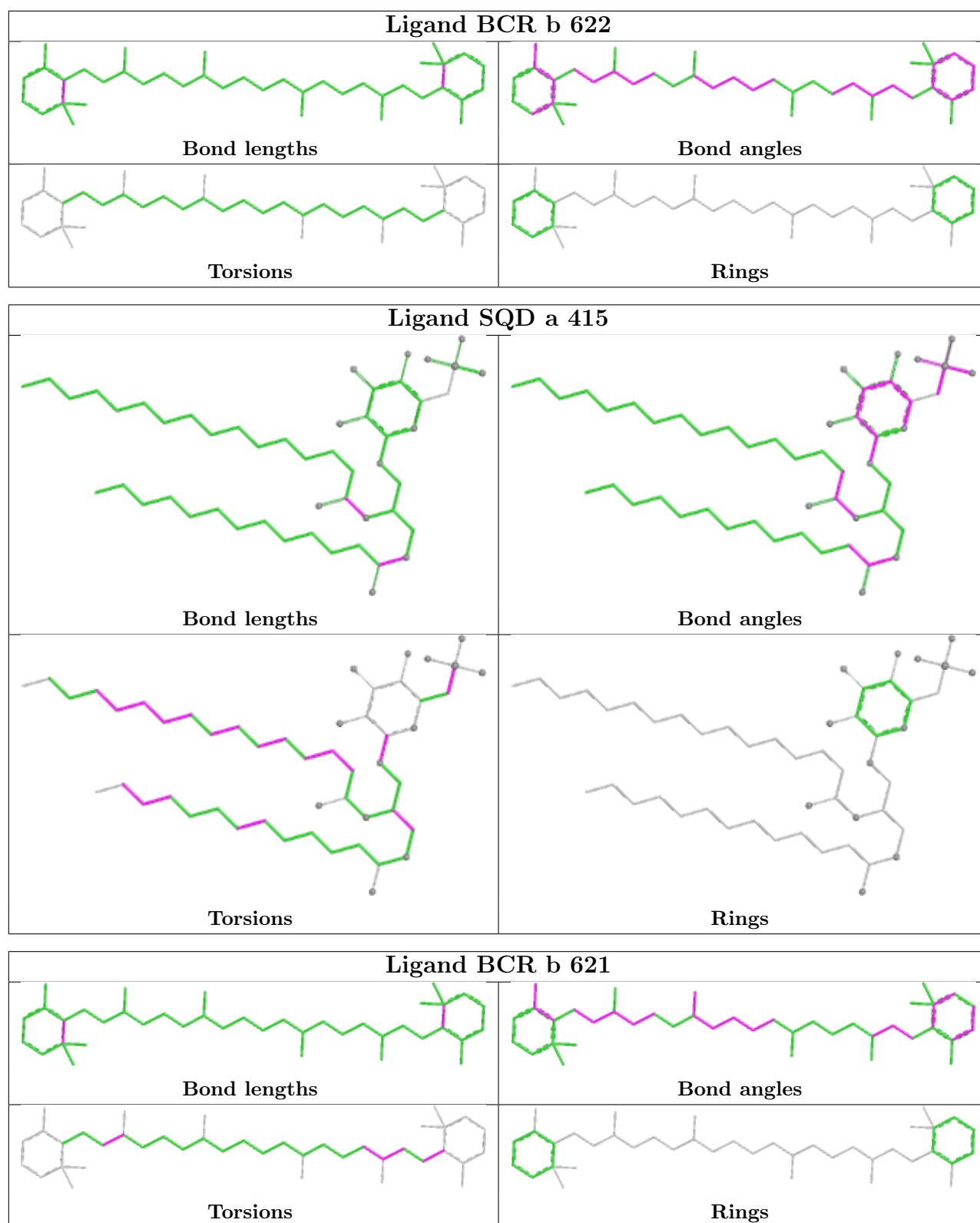
## Ligand CLA A 402











## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 335/344 (97%) | 0.14   | 8 (2%) 59 48  | 178, 179, 180, 181    | 0     |
| 1   | a     | 335/344 (97%) | 0.00   | 8 (2%) 59 48  | 178, 179, 180, 181    | 0     |
| 2   | B     | 490/510 (96%) | 0.03   | 7 (1%) 73 58  | 178, 179, 180, 181    | 0     |
| 2   | b     | 490/510 (96%) | 0.08   | 12 (2%) 59 48 | 178, 179, 180, 181    | 0     |
| 3   | C     | 447/461 (96%) | 0.05   | 5 (1%) 78 62  | 178, 179, 180, 181    | 0     |
| 3   | c     | 447/461 (96%) | -0.05  | 6 (1%) 75 60  | 178, 180, 180, 181    | 0     |
| 4   | D     | 340/352 (96%) | 0.14   | 7 (2%) 63 50  | 177, 179, 180, 181    | 0     |
| 4   | d     | 340/352 (96%) | -0.02  | 5 (1%) 72 57  | 177, 179, 180, 181    | 0     |
| 5   | E     | 82/84 (97%)   | -0.07  | 0 100 100     | 178, 180, 180, 181    | 0     |
| 5   | e     | 82/84 (97%)   | -0.04  | 2 (2%) 59 48  | 178, 180, 181, 181    | 0     |
| 6   | F     | 35/45 (77%)   | 0.19   | 3 (8%) 16 20  | 179, 179, 180, 180    | 0     |
| 6   | f     | 35/45 (77%)   | -0.12  | 0 100 100     | 179, 180, 181, 181    | 0     |
| 7   | H     | 65/66 (98%)   | 0.26   | 2 (3%) 51 41  | 179, 180, 180, 181    | 0     |
| 7   | h     | 65/66 (98%)   | 0.11   | 2 (3%) 51 41  | 179, 180, 181, 181    | 0     |
| 8   | I     | 35/38 (92%)   | -0.21  | 0 100 100     | 178, 179, 180, 181    | 0     |
| 8   | i     | 35/38 (92%)   | -0.08  | 0 100 100     | 179, 179, 181, 181    | 0     |
| 9   | J     | 34/40 (85%)   | -0.13  | 0 100 100     | 178, 179, 180, 180    | 0     |
| 9   | j     | 34/40 (85%)   | 0.06   | 0 100 100     | 179, 180, 181, 181    | 0     |
| 10  | K     | 37/46 (80%)   | 0.03   | 0 100 100     | 179, 180, 180, 180    | 0     |
| 10  | k     | 37/46 (80%)   | 0.04   | 0 100 100     | 179, 180, 181, 181    | 0     |
| 11  | L     | 37/37 (100%)  | 0.12   | 1 (2%) 56 44  | 178, 179, 180, 181    | 0     |
| 11  | l     | 37/37 (100%)  | -0.07  | 0 100 100     | 178, 179, 180, 181    | 0     |
| 12  | M     | 34/36 (94%)   | 0.27   | 0 100 100     | 178, 179, 180, 181    | 0     |
| 12  | m     | 34/36 (94%)   | 0.09   | 0 100 100     | 178, 179, 180, 181    | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | O     | 243/272 (89%)   | 0.13   | 3 (1%) 76 61  | 177, 179, 180, 181    | 0     |
| 13  | o     | 243/272 (89%)   | 0.05   | 2 (0%) 82 68  | 177, 179, 181, 181    | 0     |
| 14  | T     | 32/32 (100%)    | 0.08   | 0 100 100     | 178, 179, 181, 181    | 0     |
| 14  | t     | 32/32 (100%)    | 0.18   | 1 (3%) 51 41  | 178, 179, 180, 181    | 0     |
| 15  | U     | 97/134 (72%)    | 0.29   | 3 (3%) 51 41  | 178, 179, 180, 181    | 0     |
| 15  | u     | 97/134 (72%)    | 0.29   | 2 (2%) 63 50  | 178, 179, 180, 181    | 0     |
| 16  | V     | 137/163 (84%)   | 0.20   | 5 (3%) 46 39  | 178, 179, 180, 181    | 0     |
| 16  | v     | 137/163 (84%)   | 0.02   | 2 (1%) 72 57  | 178, 180, 181, 181    | 0     |
| 17  | g     | 28/46 (60%)     | 0.54   | 0 100 100     | 179, 180, 181, 182    | 0     |
| 17  | y     | 28/46 (60%)     | -0.13  | 0 100 100     | 178, 180, 181, 181    | 0     |
| 18  | X     | 37/41 (90%)     | -0.14  | 0 100 100     | 179, 179, 181, 181    | 0     |
| 18  | x     | 37/41 (90%)     | 0.19   | 0 100 100     | 179, 180, 180, 181    | 0     |
| 19  | G     | 0/28            | -      | -             | -                     | -     |
| 19  | Y     | 0/28            | -      | -             | -                     | -     |
| 20  | Z     | 62/62 (100%)    | -0.03  | 1 (1%) 70 55  | 179, 180, 181, 181    | 0     |
| 20  | z     | 62/62 (100%)    | -0.04  | 1 (1%) 70 55  | 179, 180, 181, 181    | 0     |
| All | All   | 5214/5674 (91%) | 0.06   | 88 (1%) 69 55 | 177, 179, 180, 182    | 0     |

All (88) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 16  | V     | 47  | LEU  | 5.1  |
| 2   | b     | 211 | ILE  | 5.0  |
| 2   | B     | 161 | LEU  | 4.5  |
| 13  | O     | 195 | ASP  | 4.4  |
| 2   | b     | 63  | LEU  | 4.3  |
| 1   | a     | 250 | ALA  | 4.3  |
| 2   | b     | 443 | PHE  | 4.3  |
| 15  | U     | 40  | VAL  | 4.1  |
| 20  | Z     | 17  | PHE  | 3.8  |
| 13  | o     | 213 | VAL  | 3.8  |
| 15  | U     | 39  | LEU  | 3.8  |
| 15  | u     | 47  | LEU  | 3.7  |
| 2   | b     | 302 | TRP  | 3.4  |
| 2   | B     | 411 | PHE  | 3.3  |
| 1   | A     | 19  | ASN  | 3.2  |
| 2   | b     | 393 | GLU  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 24  | ARG  | 3.1  |
| 2   | b     | 386 | ALA  | 3.1  |
| 4   | d     | 181 | PHE  | 3.1  |
| 2   | B     | 69  | LEU  | 2.9  |
| 7   | H     | 6   | TRP  | 2.9  |
| 3   | C     | 140 | LEU  | 2.9  |
| 15  | U     | 121 | LEU  | 2.9  |
| 2   | b     | 482 | ILE  | 2.8  |
| 1   | A     | 61  | ASP  | 2.8  |
| 6   | F     | 11  | VAL  | 2.8  |
| 16  | V     | 117 | VAL  | 2.8  |
| 5   | e     | 84  | LYS  | 2.8  |
| 2   | b     | 229 | LEU  | 2.7  |
| 3   | C     | 89  | ILE  | 2.6  |
| 1   | A     | 274 | PHE  | 2.6  |
| 4   | D     | 145 | ALA  | 2.6  |
| 3   | c     | 260 | ALA  | 2.6  |
| 1   | A     | 263 | ALA  | 2.5  |
| 16  | v     | 65  | SER  | 2.5  |
| 5   | e     | 82  | GLN  | 2.5  |
| 1   | a     | 50  | ILE  | 2.4  |
| 1   | a     | 280 | VAL  | 2.4  |
| 2   | b     | 78  | TRP  | 2.4  |
| 13  | o     | 202 | GLN  | 2.4  |
| 4   | D     | 311 | PHE  | 2.3  |
| 2   | b     | 64  | PRO  | 2.3  |
| 4   | d     | 136 | VAL  | 2.3  |
| 3   | c     | 401 | LEU  | 2.3  |
| 4   | d     | 122 | LEU  | 2.3  |
| 4   | D     | 13  | GLY  | 2.3  |
| 4   | D     | 276 | VAL  | 2.3  |
| 16  | V     | 69  | GLY  | 2.3  |
| 1   | A     | 103 | ASP  | 2.3  |
| 1   | a     | 294 | ALA  | 2.2  |
| 14  | t     | 29  | ILE  | 2.2  |
| 1   | A     | 185 | VAL  | 2.2  |
| 3   | C     | 266 | TRP  | 2.2  |
| 16  | V     | 52  | TYR  | 2.2  |
| 7   | H     | 30  | LEU  | 2.2  |
| 13  | O     | 41  | LEU  | 2.2  |
| 13  | O     | 141 | ARG  | 2.2  |
| 1   | A     | 218 | LEU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 11  | L     | 18  | TYR  | 2.2  |
| 3   | c     | 375 | LEU  | 2.2  |
| 16  | v     | 73  | LYS  | 2.2  |
| 2   | B     | 8   | VAL  | 2.2  |
| 1   | A     | 188 | ALA  | 2.2  |
| 2   | b     | 2   | GLY  | 2.2  |
| 1   | a     | 340 | PRO  | 2.2  |
| 4   | d     | 334 | GLN  | 2.2  |
| 4   | d     | 271 | MET  | 2.2  |
| 4   | D     | 203 | GLY  | 2.1  |
| 7   | h     | 14  | LEU  | 2.1  |
| 1   | a     | 222 | SER  | 2.1  |
| 7   | h     | 11  | LEU  | 2.1  |
| 15  | u     | 130 | ASN  | 2.1  |
| 6   | F     | 38  | ALA  | 2.1  |
| 3   | C     | 334 | PRO  | 2.1  |
| 3   | c     | 341 | LEU  | 2.1  |
| 20  | z     | 17  | PHE  | 2.1  |
| 3   | c     | 219 | GLY  | 2.1  |
| 6   | F     | 41  | GLN  | 2.1  |
| 2   | b     | 175 | THR  | 2.1  |
| 1   | a     | 279 | PRO  | 2.1  |
| 4   | D     | 274 | VAL  | 2.1  |
| 2   | B     | 320 | ALA  | 2.0  |
| 3   | C     | 43  | ILE  | 2.0  |
| 2   | B     | 472 | ARG  | 2.0  |
| 3   | c     | 143 | TYR  | 2.0  |
| 1   | a     | 292 | THR  | 2.0  |
| 2   | B     | 84  | THR  | 2.0  |
| 16  | V     | 147 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 30  | LMT  | I     | 102 | 35/35 | 0.49 | 0.17 | 178,180,182,183            | 0     |
| 30  | LMT  | d     | 411 | 31/35 | 0.52 | 0.18 | 178,181,182,183            | 0     |
| 35  | CA   | K     | 101 | 1/1   | 0.58 | 0.18 | 184,184,184,184            | 0     |
| 30  | LMT  | i     | 102 | 35/35 | 0.60 | 0.17 | 178,181,183,183            | 0     |
| 30  | LMT  | b     | 627 | 35/35 | 0.60 | 0.16 | 178,180,182,182            | 0     |
| 22  | CLA  | b     | 605 | 65/65 | 0.62 | 0.22 | 179,180,182,183            | 0     |
| 30  | LMT  | D     | 411 | 31/35 | 0.63 | 0.13 | 179,180,182,182            | 0     |
| 22  | CLA  | B     | 601 | 65/65 | 0.63 | 0.19 | 177,180,181,182            | 0     |
| 30  | LMT  | b     | 626 | 35/35 | 0.64 | 0.14 | 178,180,182,183            | 0     |
| 30  | LMT  | b     | 603 | 35/35 | 0.65 | 0.15 | 178,179,181,182            | 0     |
| 30  | LMT  | B     | 627 | 35/35 | 0.65 | 0.15 | 178,180,182,182            | 0     |
| 30  | LMT  | B     | 628 | 35/35 | 0.65 | 0.21 | 177,180,182,183            | 0     |
| 30  | LMT  | B     | 623 | 35/35 | 0.66 | 0.14 | 177,181,182,183            | 0     |
| 25  | DGD  | D     | 410 | 63/66 | 0.70 | 0.21 | 178,181,182,183            | 0     |
| 25  | DGD  | d     | 410 | 63/66 | 0.71 | 0.23 | 178,180,183,183            | 0     |
| 23  | PL9  | J     | 101 | 35/55 | 0.71 | 0.31 | 177,180,181,181            | 0     |
| 22  | CLA  | b     | 619 | 65/65 | 0.72 | 0.18 | 177,179,180,181            | 0     |
| 27  | LMG  | C     | 518 | 45/55 | 0.73 | 0.17 | 178,179,180,181            | 0     |
| 24  | BCR  | J     | 102 | 40/40 | 0.74 | 0.27 | 178,180,181,181            | 0     |
| 24  | BCR  | j     | 102 | 40/40 | 0.75 | 0.27 | 179,180,182,183            | 0     |
| 25  | DGD  | B     | 625 | 52/66 | 0.75 | 0.19 | 177,180,182,182            | 0     |
| 29  | SQD  | B     | 626 | 47/54 | 0.75 | 0.17 | 175,179,181,183            | 0     |
| 29  | SQD  | d     | 403 | 43/54 | 0.75 | 0.18 | 178,180,182,186            | 0     |
| 22  | CLA  | c     | 512 | 65/65 | 0.75 | 0.16 | 178,180,181,182            | 0     |
| 26  | LHG  | C     | 519 | 37/49 | 0.76 | 0.19 | 176,180,184,188            | 0     |
| 27  | LMG  | M     | 101 | 42/55 | 0.77 | 0.21 | 178,180,181,182            | 0     |
| 30  | LMT  | B     | 624 | 35/35 | 0.77 | 0.15 | 178,180,182,183            | 0     |
| 25  | DGD  | b     | 601 | 52/66 | 0.78 | 0.18 | 178,180,181,182            | 0     |
| 26  | LHG  | c     | 519 | 37/49 | 0.78 | 0.18 | 178,180,183,187            | 0     |
| 22  | CLA  | C     | 506 | 65/65 | 0.80 | 0.18 | 177,179,180,180            | 0     |
| 27  | LMG  | A     | 414 | 42/55 | 0.80 | 0.22 | 177,179,182,182            | 0     |
| 30  | LMT  | b     | 604 | 35/35 | 0.81 | 0.20 | 177,179,181,182            | 0     |
| 27  | LMG  | a     | 402 | 42/55 | 0.81 | 0.23 | 177,180,181,182            | 0     |
| 27  | LMG  | I     | 101 | 43/55 | 0.81 | 0.20 | 178,180,181,182            | 0     |
| 30  | LMT  | M     | 102 | 35/35 | 0.82 | 0.18 | 178,179,181,182            | 0     |
| 22  | CLA  | A     | 405 | 65/65 | 0.82 | 0.17 | 177,179,180,181            | 0     |
| 23  | PL9  | A     | 406 | 45/55 | 0.82 | 0.27 | 177,179,180,180            | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | DGD  | C     | 516 | 62/66 | 0.82 | 0.15 | 177,179,180,181             | 0     |
| 29  | SQD  | b     | 602 | 47/54 | 0.83 | 0.16 | 176,179,182,185             | 0     |
| 27  | LMG  | c     | 518 | 45/55 | 0.83 | 0.15 | 178,180,181,181             | 0     |
| 27  | LMG  | m     | 101 | 42/55 | 0.83 | 0.20 | 175,179,181,181             | 0     |
| 25  | DGD  | c     | 516 | 62/66 | 0.83 | 0.19 | 178,179,180,181             | 0     |
| 25  | DGD  | a     | 410 | 56/66 | 0.84 | 0.20 | 178,180,181,182             | 0     |
| 29  | SQD  | a     | 415 | 51/54 | 0.84 | 0.18 | 178,179,181,182             | 0     |
| 24  | BCR  | b     | 621 | 40/40 | 0.84 | 0.20 | 178,178,179,179             | 0     |
| 27  | LMG  | E     | 101 | 44/55 | 0.84 | 0.20 | 176,179,181,182             | 0     |
| 24  | BCR  | b     | 623 | 40/40 | 0.84 | 0.18 | 177,178,180,180             | 0     |
| 29  | SQD  | A     | 412 | 51/54 | 0.84 | 0.18 | 178,179,180,181             | 0     |
| 24  | BCR  | H     | 102 | 40/40 | 0.85 | 0.19 | 178,180,181,182             | 0     |
| 27  | LMG  | b     | 625 | 49/55 | 0.85 | 0.20 | 178,179,180,180             | 0     |
| 25  | DGD  | A     | 408 | 56/66 | 0.85 | 0.17 | 178,179,181,182             | 0     |
| 27  | LMG  | i     | 101 | 43/55 | 0.85 | 0.16 | 177,180,182,184             | 0     |
| 24  | BCR  | b     | 622 | 40/40 | 0.85 | 0.27 | 176,178,179,179             | 0     |
| 23  | PL9  | j     | 101 | 35/55 | 0.85 | 0.24 | 179,180,181,181             | 0     |
| 25  | DGD  | b     | 624 | 58/66 | 0.86 | 0.21 | 177,178,180,180             | 0     |
| 25  | DGD  | c     | 515 | 53/66 | 0.86 | 0.20 | 176,179,181,182             | 0     |
| 24  | BCR  | a     | 409 | 40/40 | 0.86 | 0.21 | 177,178,180,180             | 0     |
| 29  | SQD  | F     | 103 | 45/54 | 0.86 | 0.19 | 178,180,182,182             | 0     |
| 22  | CLA  | C     | 512 | 65/65 | 0.86 | 0.13 | 177,180,181,182             | 0     |
| 27  | LMG  | e     | 101 | 44/55 | 0.86 | 0.18 | 177,179,181,181             | 0     |
| 33  | BCT  | d     | 404 | 4/4   | 0.86 | 0.10 | 178,180,180,180             | 0     |
| 25  | DGD  | C     | 517 | 66/66 | 0.86 | 0.18 | 177,179,180,181             | 0     |
| 35  | CA   | O     | 301 | 1/1   | 0.86 | 0.08 | 182,182,182,182             | 0     |
| 35  | CA   | k     | 101 | 1/1   | 0.86 | 0.09 | 180,180,180,180             | 0     |
| 22  | CLA  | C     | 505 | 65/65 | 0.87 | 0.17 | 177,179,180,181             | 0     |
| 32  | CL   | D     | 403 | 1/1   | 0.87 | 0.33 | 180,180,180,180             | 0     |
| 24  | BCR  | K     | 102 | 40/40 | 0.87 | 0.20 | 178,180,181,182             | 0     |
| 25  | DGD  | c     | 517 | 66/66 | 0.87 | 0.17 | 177,179,181,181             | 0     |
| 24  | BCR  | c     | 514 | 40/40 | 0.87 | 0.22 | 177,179,180,180             | 0     |
| 29  | SQD  | a     | 401 | 54/54 | 0.87 | 0.15 | 178,180,181,183             | 0     |
| 35  | CA   | o     | 301 | 1/1   | 0.87 | 0.12 | 184,184,184,184             | 0     |
| 24  | BCR  | c     | 521 | 40/40 | 0.88 | 0.17 | 178,179,181,181             | 0     |
| 24  | BCR  | B     | 619 | 40/40 | 0.88 | 0.16 | 178,179,180,180             | 0     |
| 22  | CLA  | c     | 506 | 65/65 | 0.88 | 0.15 | 178,179,180,181             | 0     |
| 22  | CLA  | a     | 406 | 65/65 | 0.88 | 0.17 | 177,179,180,181             | 0     |
| 27  | LMG  | c     | 522 | 48/55 | 0.88 | 0.21 | 178,180,180,181             | 0     |
| 22  | CLA  | C     | 510 | 65/65 | 0.88 | 0.15 | 177,179,180,181             | 0     |
| 22  | CLA  | b     | 618 | 65/65 | 0.88 | 0.15 | 177,179,180,180             | 0     |
| 23  | PL9  | a     | 408 | 45/55 | 0.88 | 0.19 | 176,179,180,180             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 23  | PL9  | d     | 407 | 55/55 | 0.88 | 0.17 | 177,179,180,181             | 0     |
| 22  | CLA  | C     | 508 | 65/65 | 0.88 | 0.13 | 177,179,180,180             | 0     |
| 24  | BCR  | B     | 617 | 40/40 | 0.88 | 0.19 | 177,179,180,180             | 0     |
| 30  | LMT  | M     | 103 | 35/35 | 0.88 | 0.17 | 177,179,180,180             | 0     |
| 26  | LHG  | A     | 409 | 39/49 | 0.89 | 0.18 | 178,179,181,181             | 0     |
| 22  | CLA  | c     | 510 | 65/65 | 0.89 | 0.12 | 178,179,181,181             | 0     |
| 24  | BCR  | g     | 101 | 40/40 | 0.89 | 0.16 | 178,179,180,180             | 0     |
| 24  | BCR  | x     | 101 | 40/40 | 0.89 | 0.17 | 178,179,180,181             | 0     |
| 24  | BCR  | B     | 616 | 40/40 | 0.89 | 0.17 | 176,178,180,180             | 0     |
| 27  | LMG  | D     | 409 | 48/55 | 0.89 | 0.16 | 175,178,180,181             | 0     |
| 22  | CLA  | b     | 609 | 65/65 | 0.89 | 0.13 | 178,179,180,181             | 0     |
| 25  | DGD  | C     | 515 | 53/66 | 0.89 | 0.17 | 177,178,179,180             | 0     |
| 22  | CLA  | C     | 520 | 65/65 | 0.89 | 0.15 | 178,179,180,181             | 0     |
| 24  | BCR  | b     | 620 | 40/40 | 0.89 | 0.21 | 177,179,179,180             | 0     |
| 27  | LMG  | a     | 412 | 51/55 | 0.89 | 0.20 | 177,179,180,180             | 0     |
| 22  | CLA  | c     | 502 | 65/65 | 0.90 | 0.18 | 178,179,180,181             | 0     |
| 22  | CLA  | c     | 505 | 65/65 | 0.90 | 0.15 | 177,179,180,181             | 0     |
| 22  | CLA  | B     | 615 | 65/65 | 0.90 | 0.13 | 176,179,180,181             | 0     |
| 22  | CLA  | A     | 404 | 65/65 | 0.90 | 0.19 | 176,178,180,181             | 0     |
| 22  | CLA  | B     | 603 | 65/65 | 0.90 | 0.12 | 176,179,180,180             | 0     |
| 27  | LMG  | A     | 410 | 51/55 | 0.90 | 0.17 | 177,178,180,181             | 0     |
| 22  | CLA  | h     | 101 | 65/65 | 0.90 | 0.15 | 176,179,180,181             | 0     |
| 27  | LMG  | B     | 621 | 49/55 | 0.90 | 0.15 | 177,179,180,180             | 0     |
| 22  | CLA  | B     | 605 | 65/65 | 0.90 | 0.12 | 178,179,180,180             | 0     |
| 27  | LMG  | C     | 521 | 48/55 | 0.90 | 0.16 | 177,179,180,181             | 0     |
| 27  | LMG  | D     | 408 | 49/55 | 0.90 | 0.20 | 177,178,180,180             | 0     |
| 24  | BCR  | C     | 514 | 40/40 | 0.90 | 0.17 | 178,179,180,181             | 0     |
| 29  | SQD  | A     | 413 | 54/54 | 0.90 | 0.14 | 178,180,182,184             | 0     |
| 22  | CLA  | b     | 606 | 65/65 | 0.91 | 0.13 | 177,179,180,181             | 0     |
| 25  | DGD  | B     | 620 | 58/66 | 0.91 | 0.18 | 176,179,181,182             | 0     |
| 22  | CLA  | c     | 503 | 65/65 | 0.91 | 0.13 | 177,179,180,181             | 0     |
| 29  | SQD  | f     | 103 | 45/54 | 0.91 | 0.15 | 177,179,181,182             | 0     |
| 22  | CLA  | b     | 607 | 65/65 | 0.91 | 0.13 | 177,179,180,181             | 0     |
| 24  | BCR  | c     | 513 | 40/40 | 0.91 | 0.15 | 178,179,180,180             | 0     |
| 31  | PHO  | D     | 402 | 64/64 | 0.91 | 0.14 | 177,179,180,181             | 0     |
| 31  | PHO  | d     | 401 | 64/64 | 0.91 | 0.16 | 178,179,180,180             | 0     |
| 22  | CLA  | C     | 509 | 65/65 | 0.91 | 0.15 | 177,179,180,180             | 0     |
| 22  | CLA  | a     | 407 | 65/65 | 0.91 | 0.14 | 178,179,180,181             | 0     |
| 29  | SQD  | B     | 622 | 43/54 | 0.91 | 0.14 | 177,180,182,185             | 0     |
| 22  | CLA  | B     | 613 | 65/65 | 0.91 | 0.13 | 177,179,180,180             | 0     |
| 24  | BCR  | A     | 407 | 40/40 | 0.91 | 0.19 | 177,179,180,180             | 0     |
| 22  | CLA  | c     | 520 | 65/65 | 0.91 | 0.16 | 177,179,180,181             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 22  | CLA  | C     | 503 | 65/65 | 0.92 | 0.13 | 177,179,180,180             | 0     |
| 24  | BCR  | F     | 102 | 40/40 | 0.92 | 0.18 | 177,179,180,180             | 0     |
| 27  | LMG  | D     | 412 | 46/55 | 0.92 | 0.14 | 178,179,180,181             | 0     |
| 22  | CLA  | c     | 501 | 65/65 | 0.92 | 0.13 | 177,179,180,181             | 0     |
| 22  | CLA  | C     | 507 | 65/65 | 0.92 | 0.17 | 178,179,180,181             | 0     |
| 22  | CLA  | C     | 504 | 65/65 | 0.92 | 0.16 | 177,179,180,180             | 0     |
| 24  | BCR  | y     | 101 | 40/40 | 0.92 | 0.15 | 177,179,180,180             | 0     |
| 22  | CLA  | D     | 405 | 65/65 | 0.92 | 0.13 | 177,179,180,180             | 0     |
| 31  | PHO  | D     | 401 | 64/64 | 0.92 | 0.15 | 177,179,180,180             | 0     |
| 22  | CLA  | a     | 405 | 65/65 | 0.92 | 0.20 | 174,178,179,180             | 0     |
| 22  | CLA  | c     | 508 | 65/65 | 0.92 | 0.11 | 177,179,180,181             | 0     |
| 22  | CLA  | c     | 509 | 65/65 | 0.92 | 0.12 | 177,179,180,180             | 0     |
| 27  | LMG  | d     | 408 | 49/55 | 0.92 | 0.15 | 178,179,180,180             | 0     |
| 27  | LMG  | d     | 409 | 48/55 | 0.92 | 0.14 | 177,179,180,180             | 0     |
| 22  | CLA  | b     | 613 | 65/65 | 0.92 | 0.13 | 178,179,180,181             | 0     |
| 22  | CLA  | c     | 511 | 65/65 | 0.92 | 0.12 | 178,180,181,182             | 0     |
| 22  | CLA  | C     | 501 | 65/65 | 0.92 | 0.12 | 178,179,180,180             | 0     |
| 22  | CLA  | B     | 606 | 65/65 | 0.93 | 0.12 | 177,179,180,180             | 0     |
| 22  | CLA  | c     | 504 | 65/65 | 0.93 | 0.15 | 177,179,180,180             | 0     |
| 23  | PL9  | D     | 407 | 55/55 | 0.93 | 0.18 | 177,178,179,180             | 0     |
| 22  | CLA  | B     | 607 | 65/65 | 0.93 | 0.14 | 178,179,180,181             | 0     |
| 22  | CLA  | b     | 608 | 65/65 | 0.93 | 0.12 | 178,179,180,181             | 0     |
| 22  | CLA  | c     | 507 | 65/65 | 0.93 | 0.14 | 177,179,180,181             | 0     |
| 22  | CLA  | H     | 101 | 65/65 | 0.93 | 0.15 | 177,179,180,181             | 0     |
| 22  | CLA  | a     | 404 | 65/65 | 0.93 | 0.16 | 177,178,180,180             | 0     |
| 27  | LMG  | d     | 412 | 46/55 | 0.93 | 0.13 | 177,178,180,180             | 0     |
| 22  | CLA  | B     | 608 | 65/65 | 0.93 | 0.14 | 177,179,180,180             | 0     |
| 33  | BCT  | D     | 404 | 4/4   | 0.93 | 0.06 | 178,179,179,179             | 0     |
| 22  | CLA  | B     | 604 | 65/65 | 0.93 | 0.10 | 177,179,180,180             | 0     |
| 22  | CLA  | C     | 511 | 65/65 | 0.93 | 0.13 | 178,179,180,181             | 0     |
| 24  | BCR  | C     | 513 | 40/40 | 0.93 | 0.15 | 177,179,180,180             | 0     |
| 22  | CLA  | B     | 602 | 65/65 | 0.93 | 0.13 | 176,178,180,180             | 0     |
| 22  | CLA  | d     | 406 | 65/65 | 0.93 | 0.13 | 177,179,180,181             | 0     |
| 22  | CLA  | b     | 615 | 65/65 | 0.94 | 0.11 | 177,179,180,180             | 0     |
| 22  | CLA  | b     | 617 | 65/65 | 0.94 | 0.17 | 178,179,180,182             | 0     |
| 26  | LHG  | a     | 411 | 39/49 | 0.94 | 0.14 | 177,179,180,181             | 0     |
| 22  | CLA  | B     | 610 | 65/65 | 0.94 | 0.12 | 177,179,180,180             | 0     |
| 22  | CLA  | B     | 612 | 65/65 | 0.94 | 0.14 | 176,178,180,181             | 0     |
| 31  | PHO  | d     | 402 | 64/64 | 0.94 | 0.10 | 178,179,180,181             | 0     |
| 24  | BCR  | f     | 102 | 40/40 | 0.94 | 0.14 | 177,179,181,181             | 0     |
| 22  | CLA  | C     | 502 | 65/65 | 0.94 | 0.14 | 178,179,180,180             | 0     |
| 22  | CLA  | D     | 406 | 65/65 | 0.94 | 0.13 | 177,179,180,181             | 0     |

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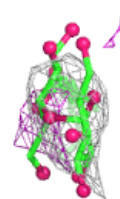
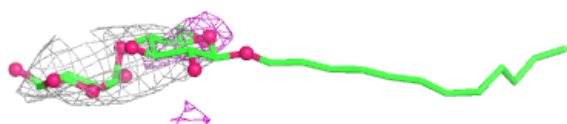
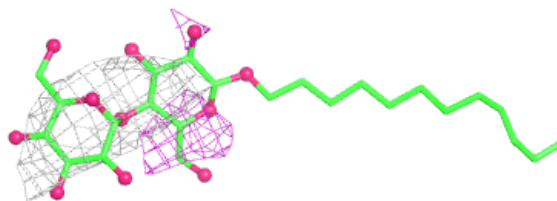
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 34  | HEM  | f     | 101 | 43/43 | 0.94 | 0.12 | 178,180,180,181             | 0     |
| 22  | CLA  | b     | 610 | 65/65 | 0.94 | 0.12 | 177,179,180,180             | 0     |
| 22  | CLA  | b     | 611 | 65/65 | 0.94 | 0.13 | 177,179,180,180             | 0     |
| 22  | CLA  | b     | 612 | 65/65 | 0.94 | 0.13 | 176,179,181,181             | 0     |
| 22  | CLA  | B     | 609 | 65/65 | 0.94 | 0.12 | 178,179,180,181             | 0     |
| 28  | OEX  | a     | 414 | 10/10 | 0.95 | 0.10 | 174,177,179,182             | 0     |
| 22  | CLA  | d     | 405 | 65/65 | 0.95 | 0.15 | 177,178,179,180             | 0     |
| 22  | CLA  | B     | 614 | 65/65 | 0.95 | 0.10 | 177,179,180,181             | 0     |
| 34  | HEM  | v     | 201 | 43/43 | 0.95 | 0.12 | 177,179,180,180             | 0     |
| 22  | CLA  | A     | 402 | 65/65 | 0.95 | 0.14 | 178,179,180,181             | 0     |
| 22  | CLA  | A     | 403 | 65/65 | 0.95 | 0.14 | 177,179,179,180             | 0     |
| 24  | BCR  | B     | 618 | 40/40 | 0.95 | 0.18 | 177,178,179,179             | 0     |
| 32  | CL   | a     | 413 | 1/1   | 0.95 | 0.15 | 177,177,177,177             | 0     |
| 22  | CLA  | b     | 614 | 65/65 | 0.96 | 0.13 | 178,179,180,180             | 0     |
| 22  | CLA  | B     | 611 | 65/65 | 0.96 | 0.12 | 177,179,180,180             | 0     |
| 28  | OEX  | A     | 411 | 10/10 | 0.96 | 0.09 | 172,175,178,178             | 0     |
| 22  | CLA  | b     | 616 | 65/65 | 0.96 | 0.13 | 177,179,180,180             | 0     |
| 34  | HEM  | F     | 101 | 43/43 | 0.96 | 0.11 | 178,180,181,182             | 0     |
| 34  | HEM  | V     | 201 | 43/43 | 0.96 | 0.14 | 176,178,180,180             | 0     |
| 21  | FE2  | A     | 401 | 1/1   | 0.97 | 0.07 | 176,176,176,176             | 0     |
| 21  | FE2  | a     | 403 | 1/1   | 0.97 | 0.10 | 182,182,182,182             | 0     |

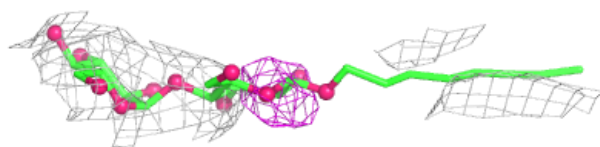
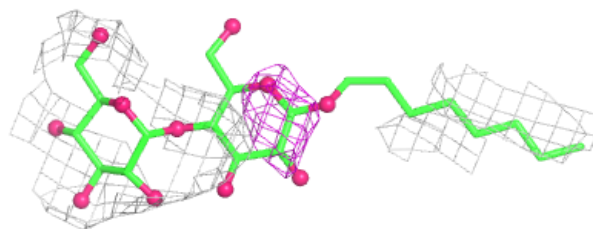
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMT I 102:**

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

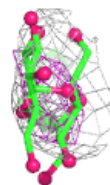
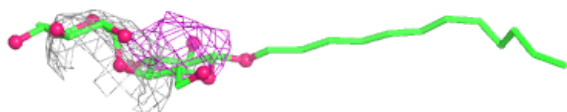
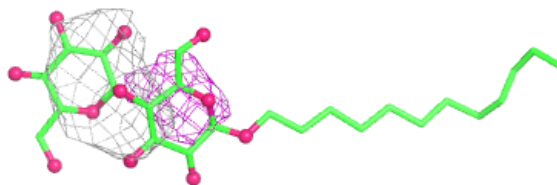
**Electron density around LMT d 411:**

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

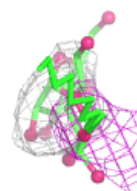
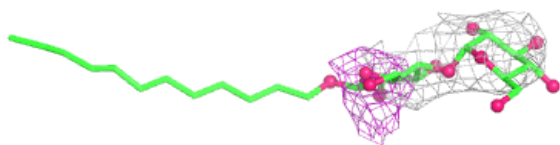
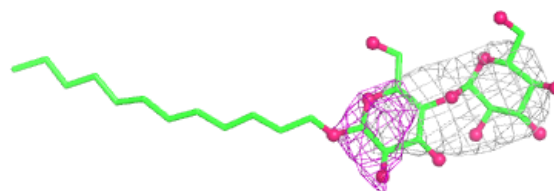


**Electron density around LMT i 102:**

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

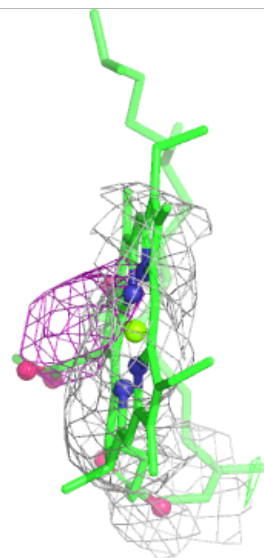
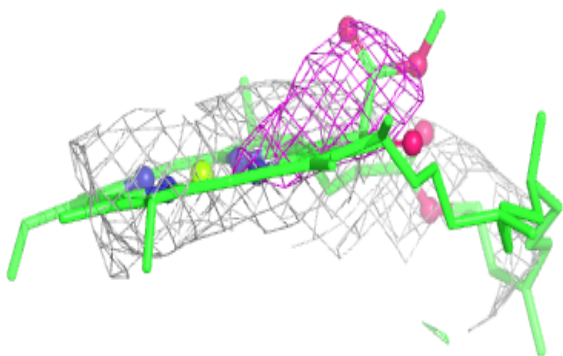
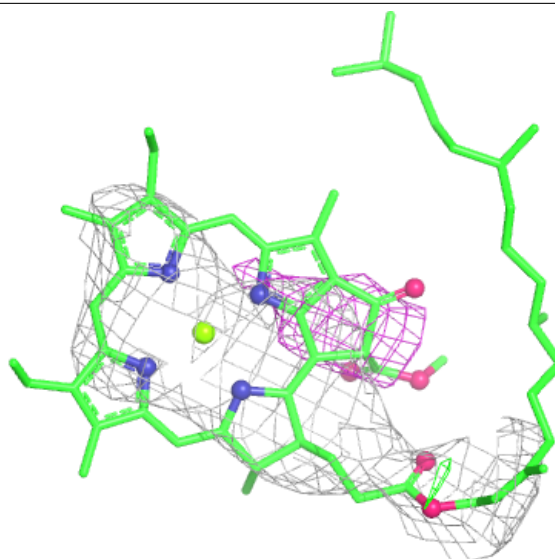
**Electron density around LMT b 627:**

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



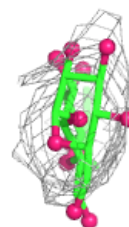
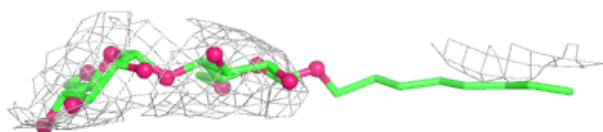
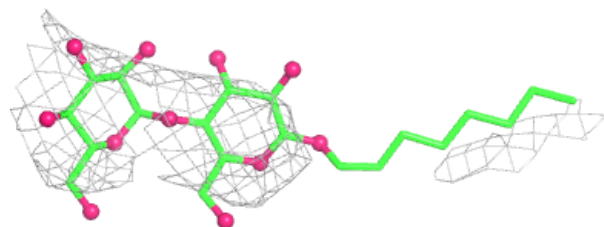
**Electron density around CLA b 605:**

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



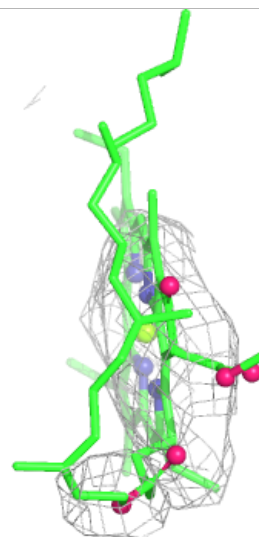
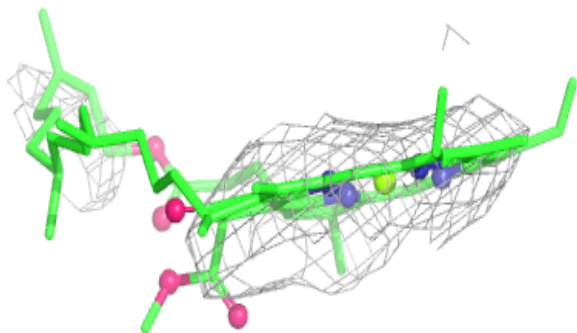
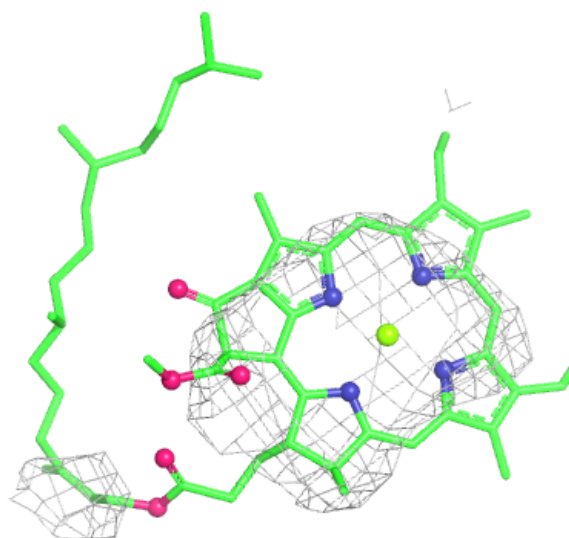
**Electron density around LMT D 411:**

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



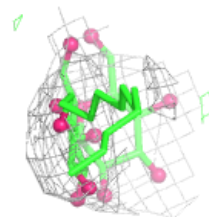
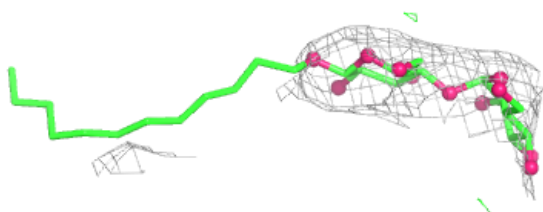
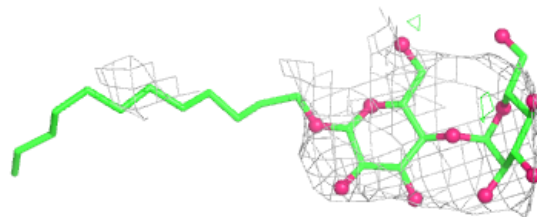
**Electron density around CLA B 601:**

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

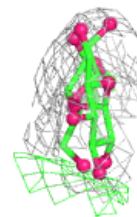
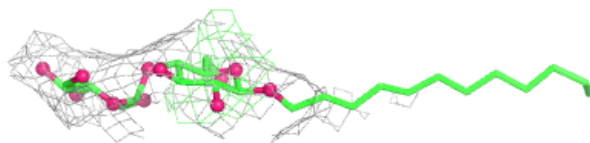
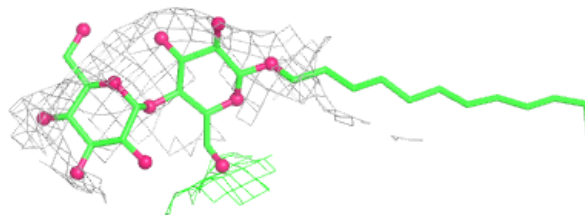


**Electron density around LMT b 626:**

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

**Electron density around LMT b 603:**

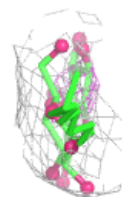
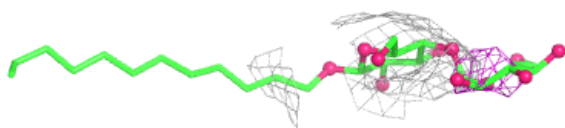
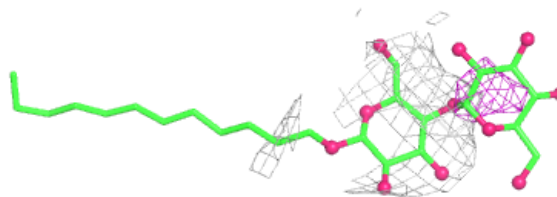
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



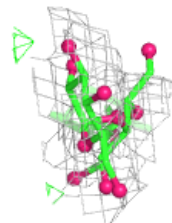
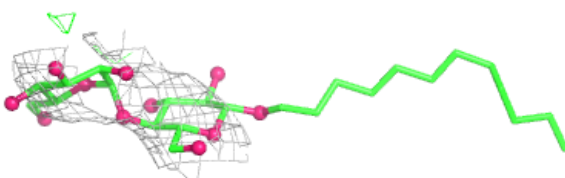
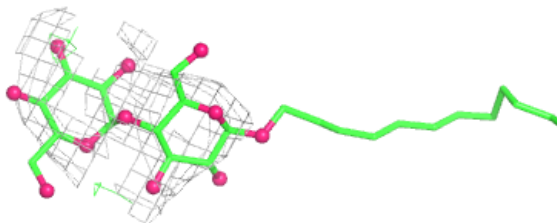


**Electron density around LMT B 627:**

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

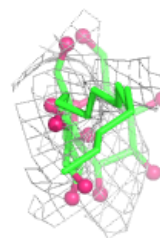
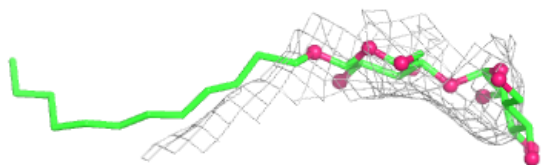
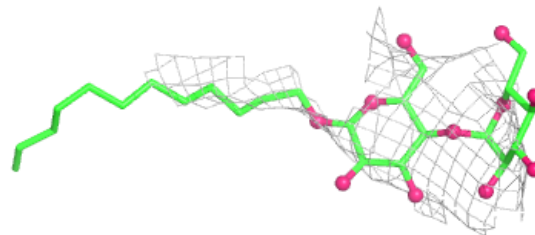
**Electron density around LMT B 628:**

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

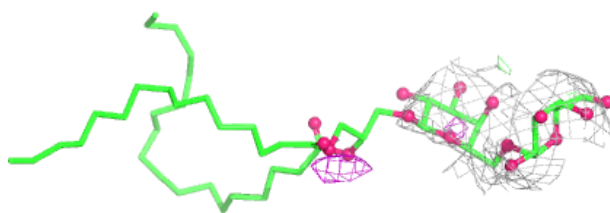
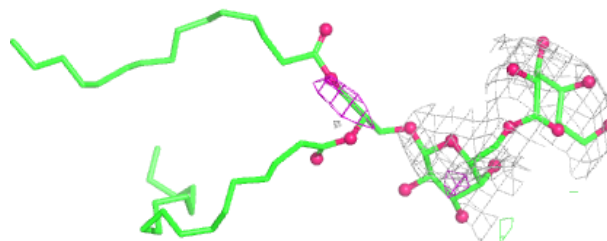


**Electron density around LMT B 623:**

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

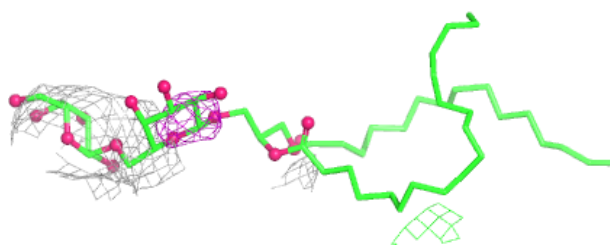
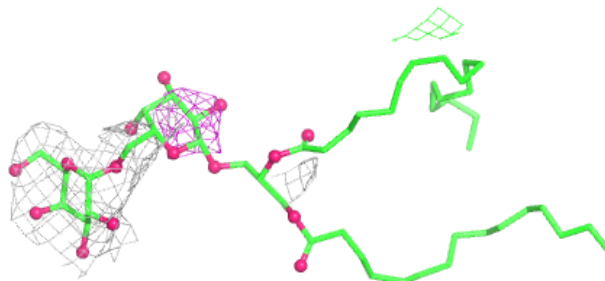
**Electron density around DGD D 410:**

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

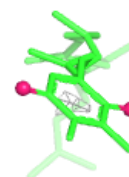
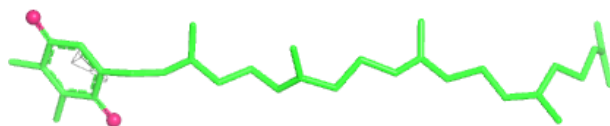
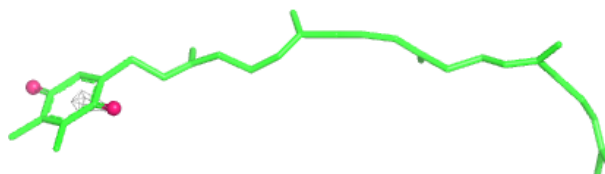


**Electron density around DGD d 410:**

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

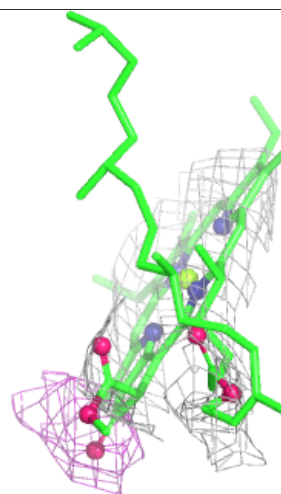
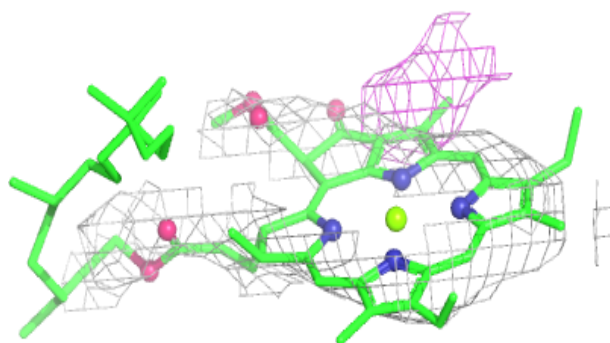
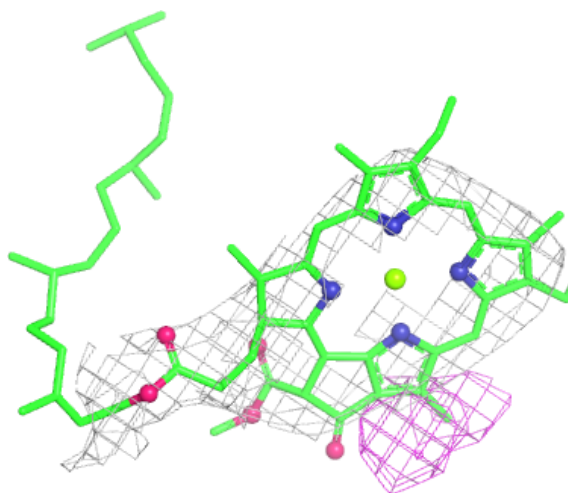
**Electron density around PL9 J 101:**

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



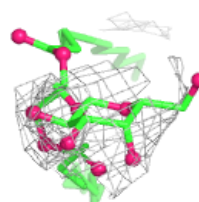
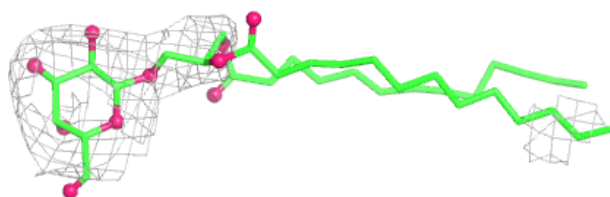
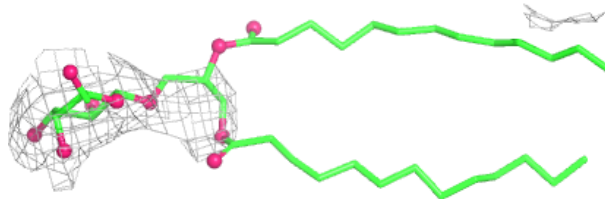
**Electron density around CLA b 619:**

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

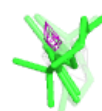
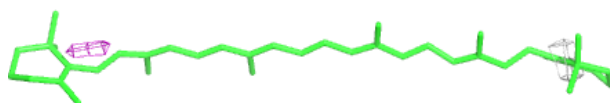
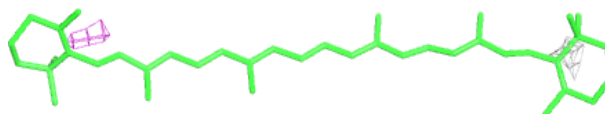


**Electron density around LMG C 518:**

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

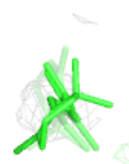
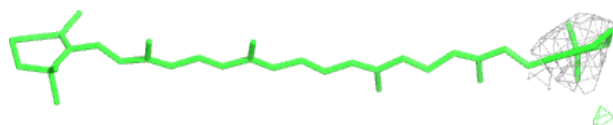
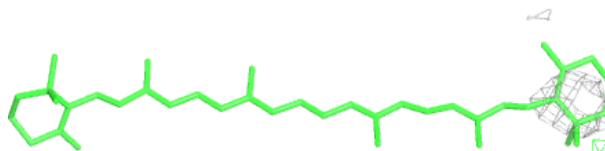
**Electron density around BCR J 102:**

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

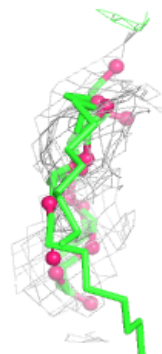
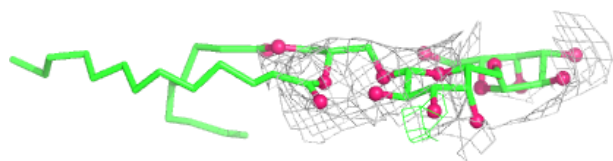
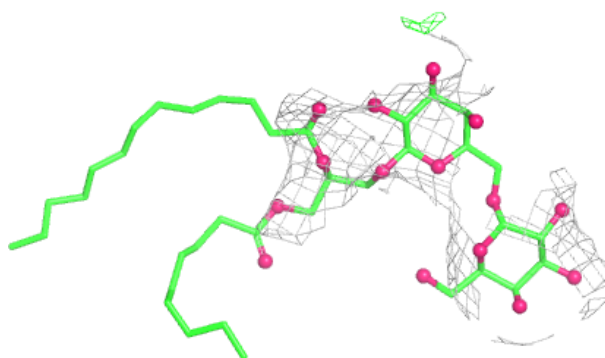


**Electron density around BCR j 102:**

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

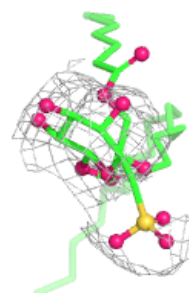
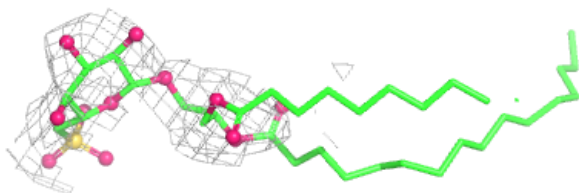
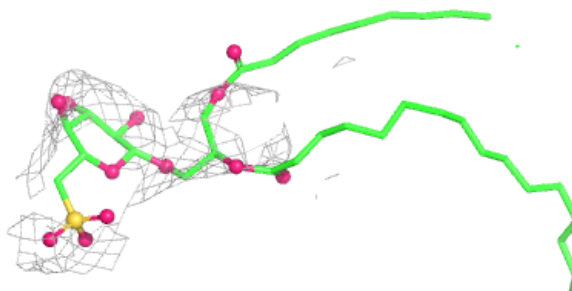
**Electron density around DGD B 625:**

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

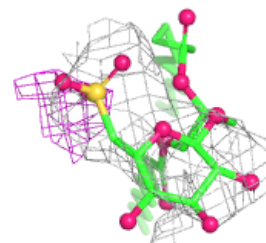
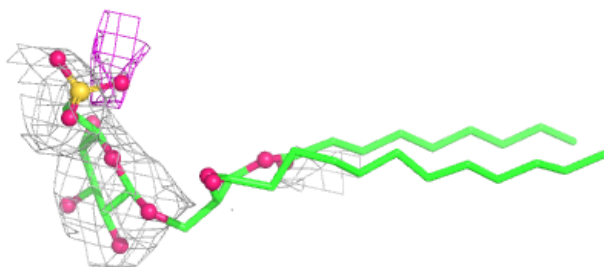
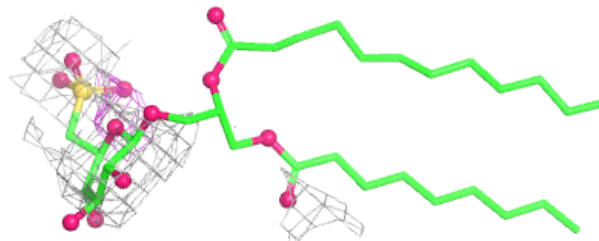


**Electron density around SQD B 626:**

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

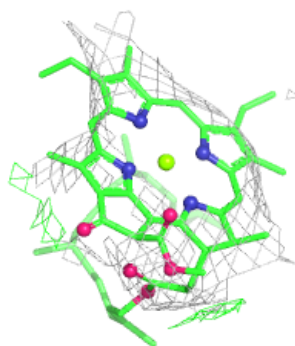
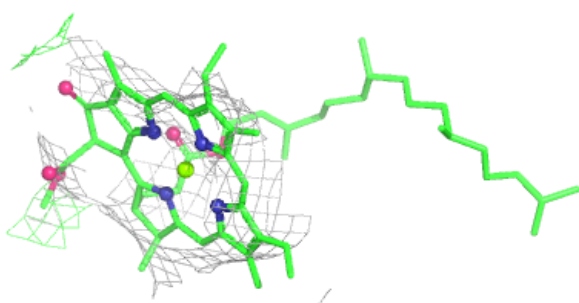
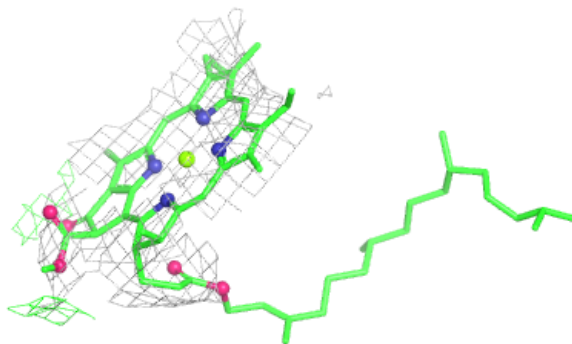
**Electron density around SQD d 403:**

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

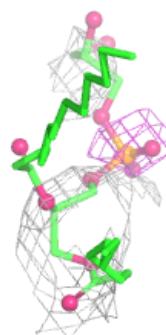
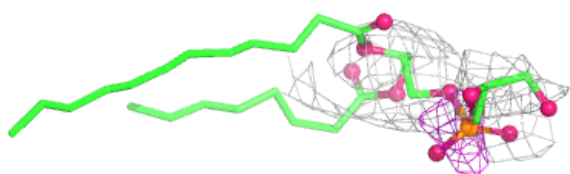
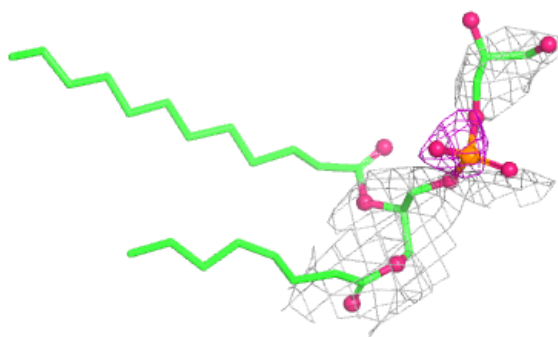


**Electron density around CLA c 512:**

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

**Electron density around LHG C 519:**

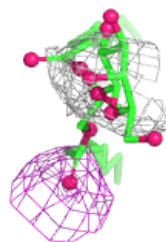
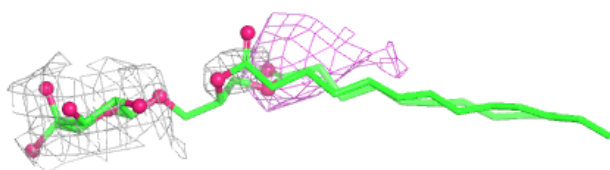
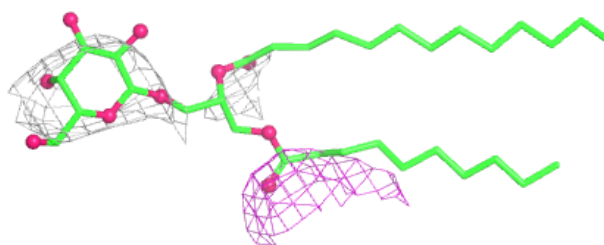
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



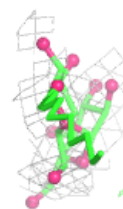
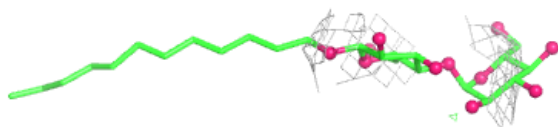
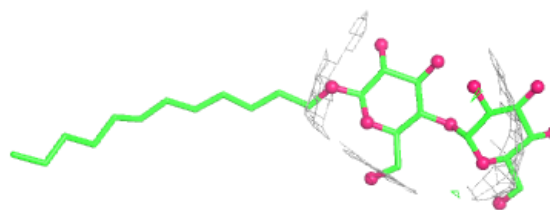


**Electron density around LMG M 101:**

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

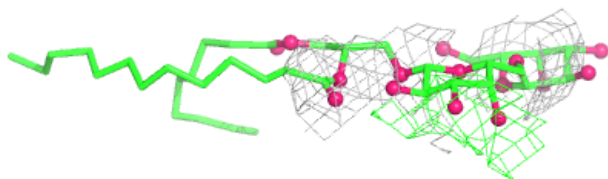
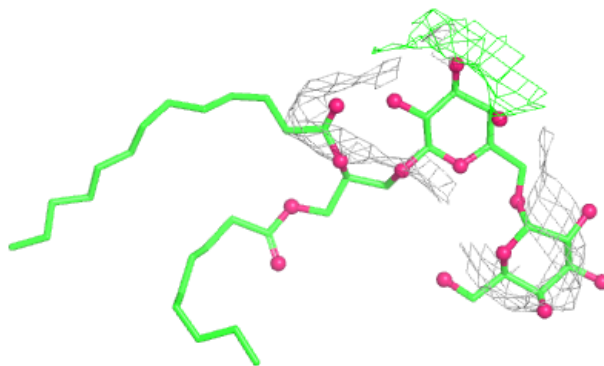
**Electron density around LMT B 624:**

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

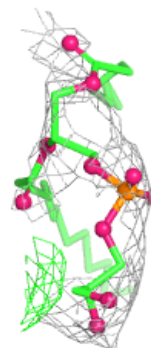
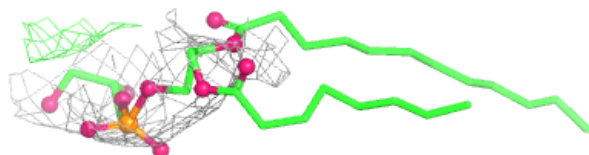
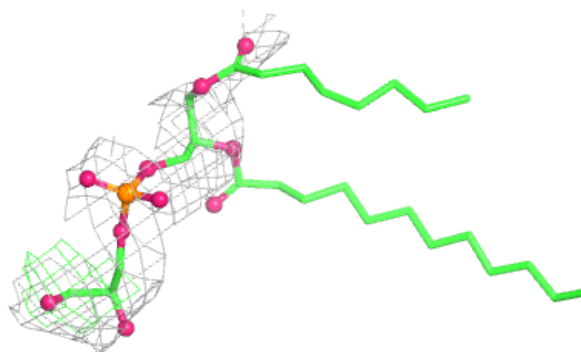


**Electron density around DGD b 601:**

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

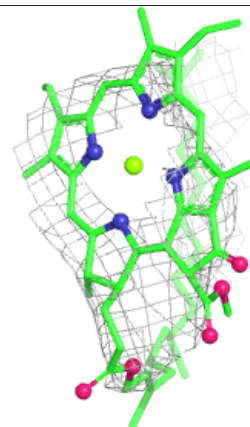
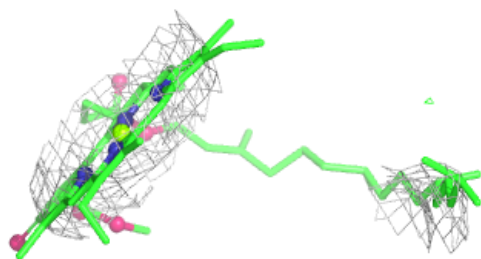
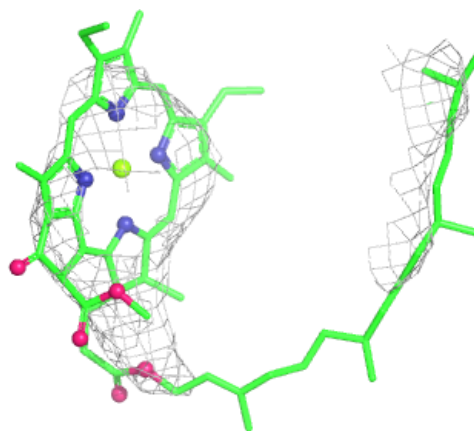
**Electron density around LHG c 519:**

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

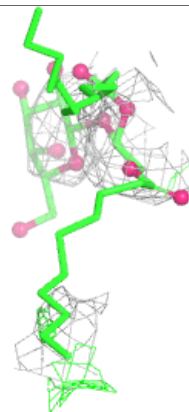
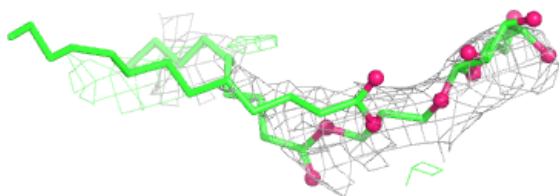


**Electron density around CLA C 506:**

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

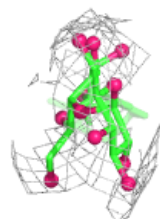
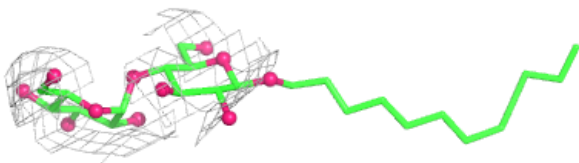
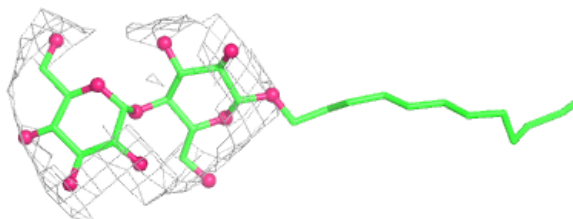
**Electron density around LMG A 414:**

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

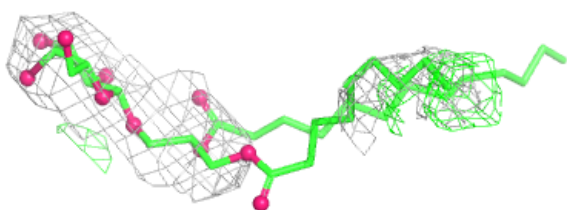
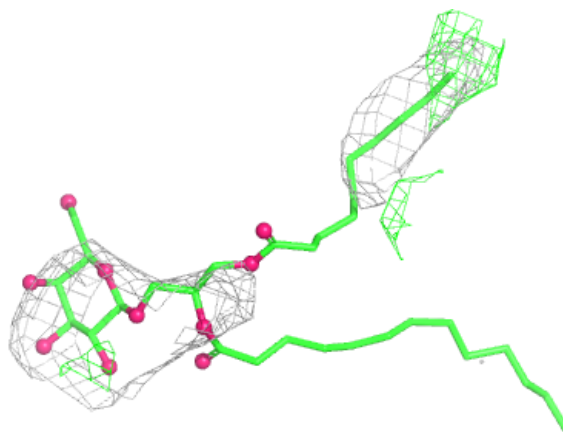


**Electron density around LMT b 604:**

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

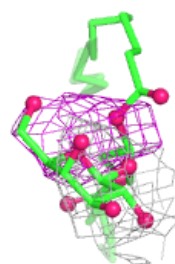
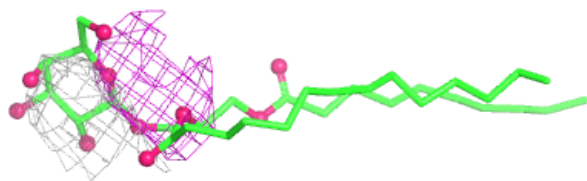
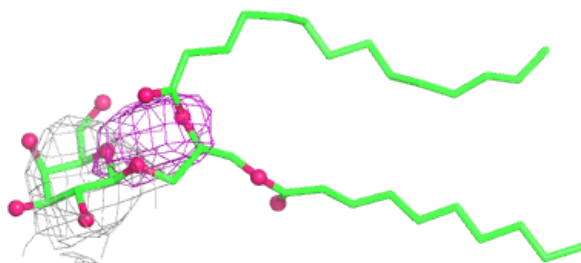
**Electron density around LMG a 402:**

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

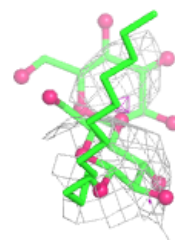
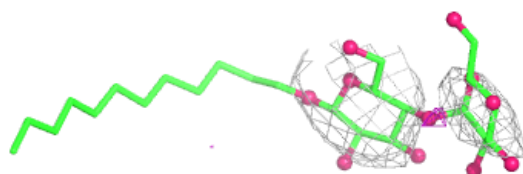
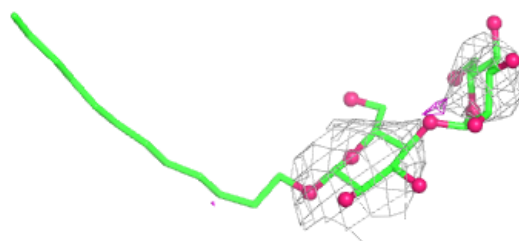


**Electron density around LMG I 101:**

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

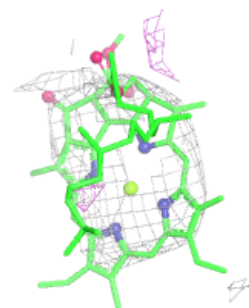
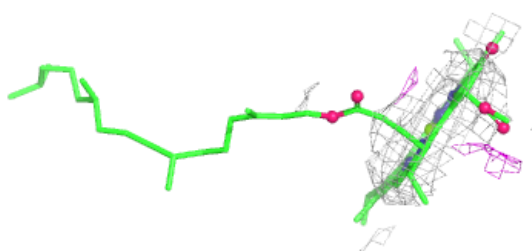
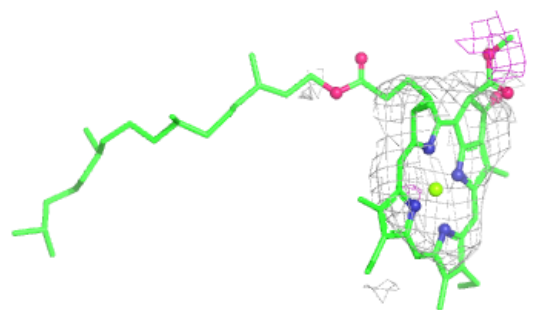
**Electron density around LMT M 102:**

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

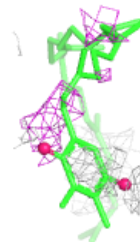
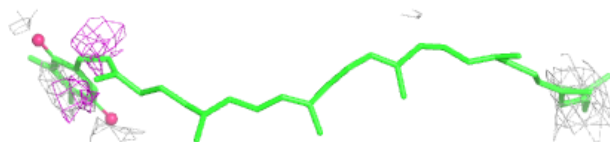
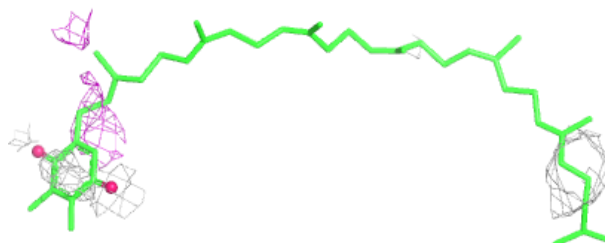


**Electron density around CLA A 405:**

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

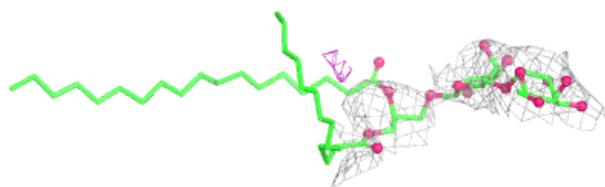
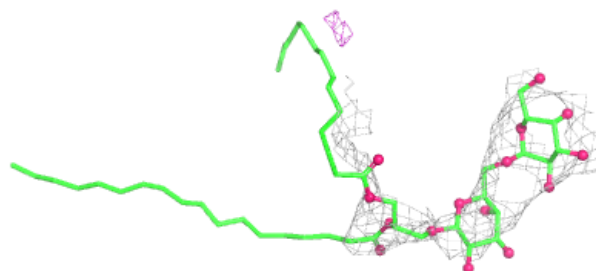
**Electron density around PL9 A 406:**

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

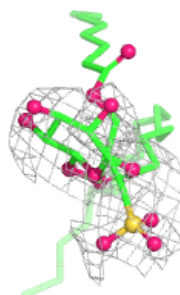
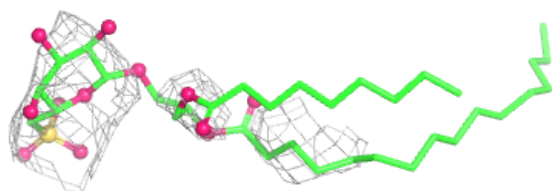
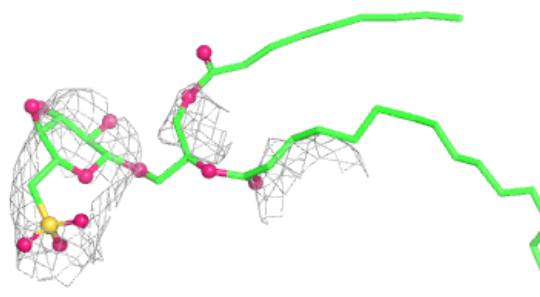


**Electron density around DGD C 516:**

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

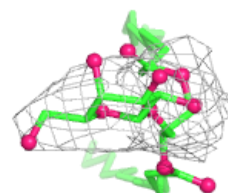
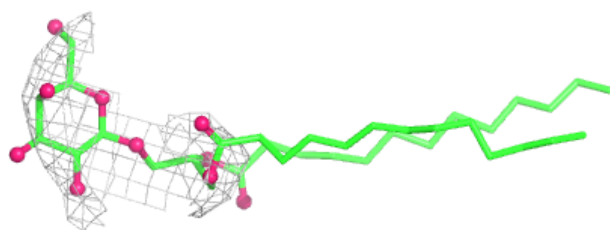
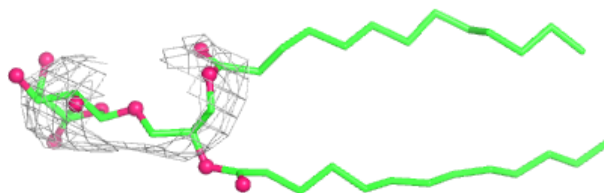
**Electron density around SQD b 602:**

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

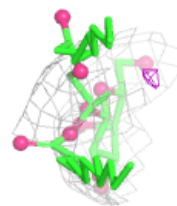
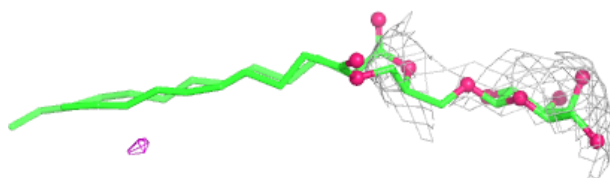
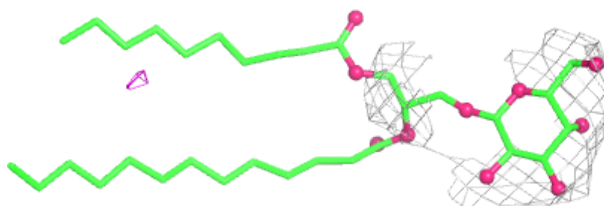


**Electron density around LMG c 518:**

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

**Electron density around LMG m 101:**

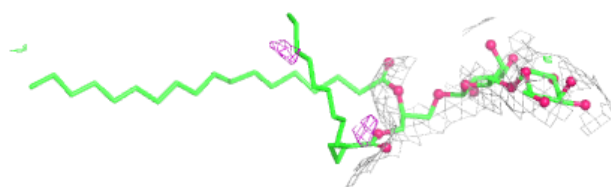
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



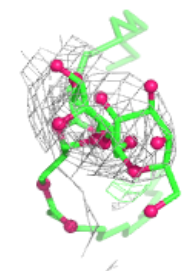
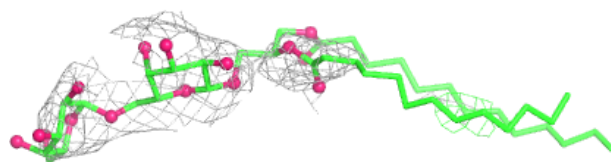


**Electron density around DGD c 516:**

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

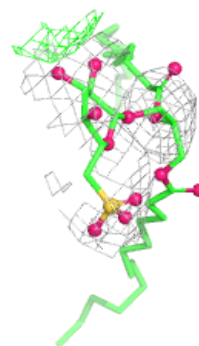
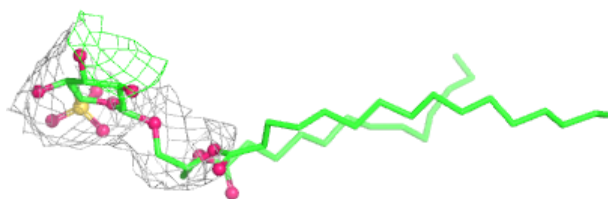
**Electron density around DGD a 410:**

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

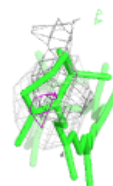
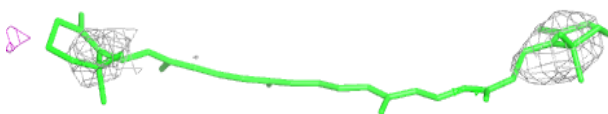
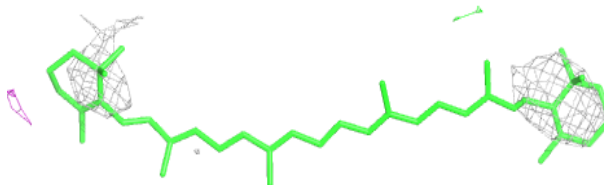


**Electron density around SQD a 415:**

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

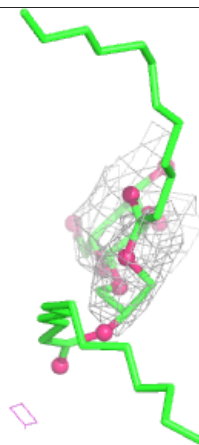
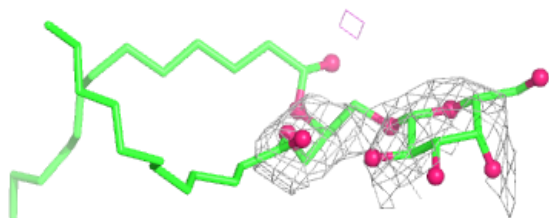
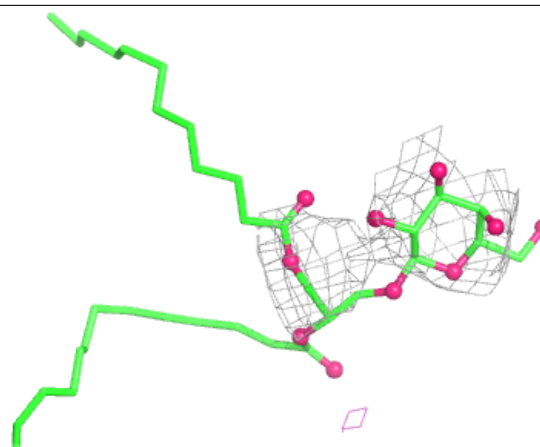
**Electron density around BCR b 621:**

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

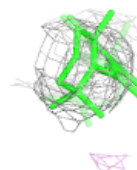
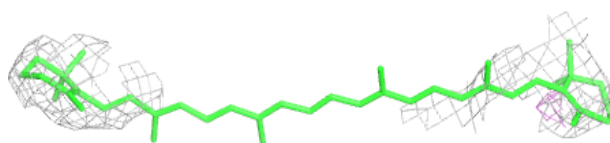
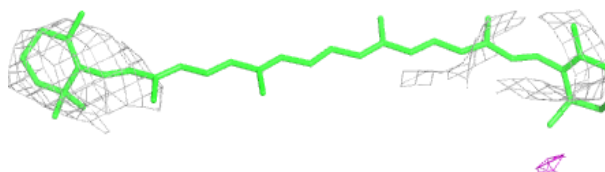


**Electron density around LMG E 101:**

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

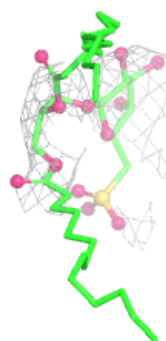
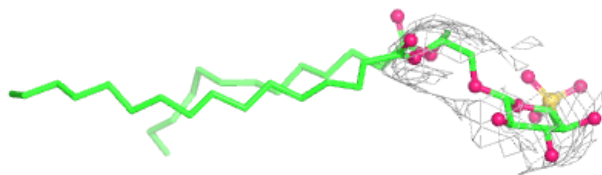
**Electron density around BCR b 623:**

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

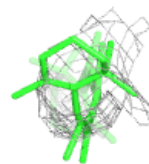
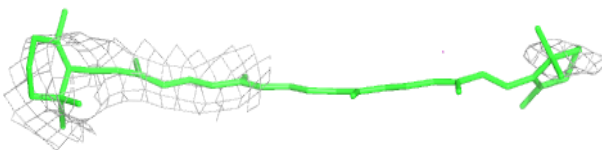
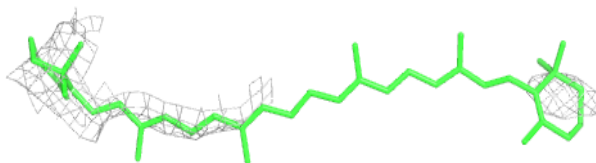


**Electron density around SQD A 412:**

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

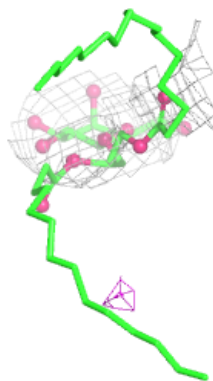
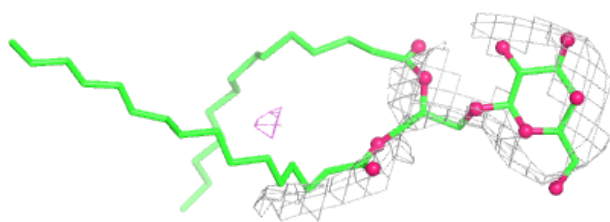
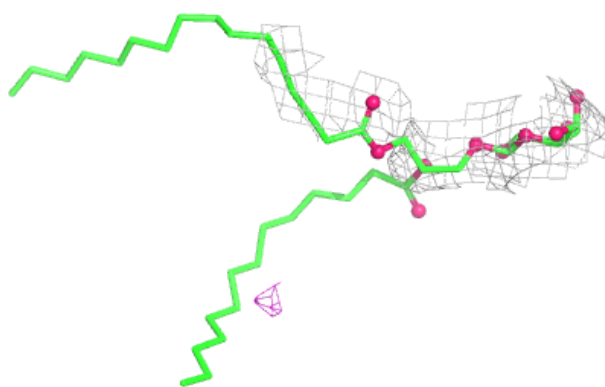
**Electron density around BCR H 102:**

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

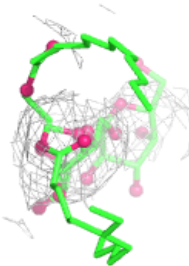
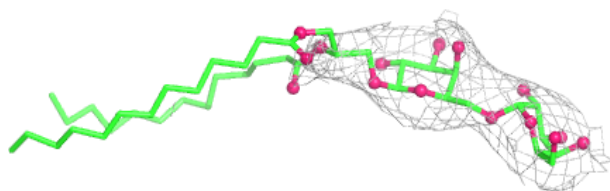
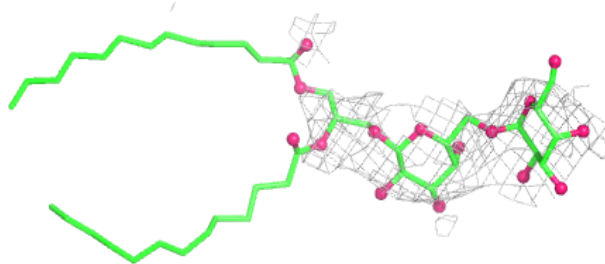


**Electron density around LMG b 625:**

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

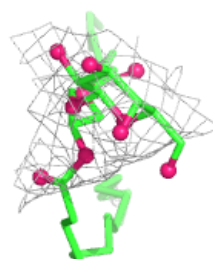
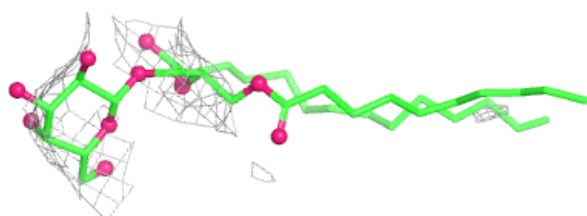
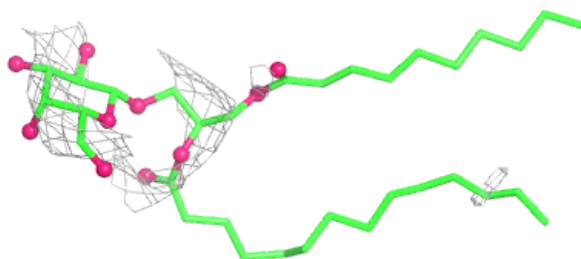
**Electron density around DGD A 408:**

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

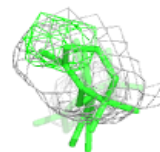
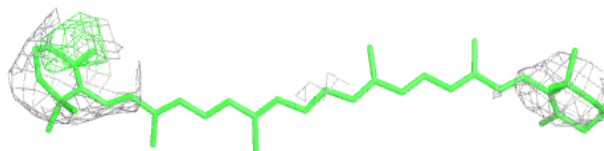


**Electron density around LMG i 101:**

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

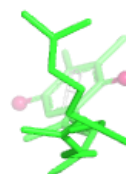
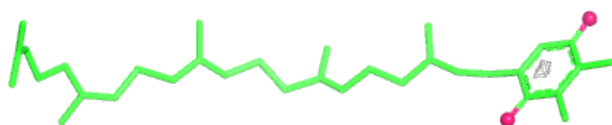
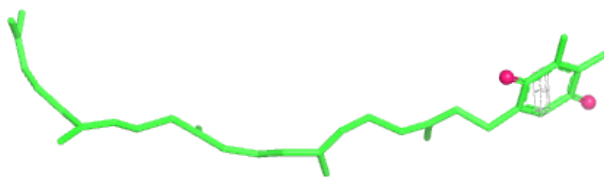
**Electron density around BCR b 622:**

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

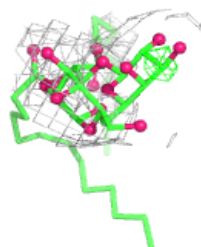
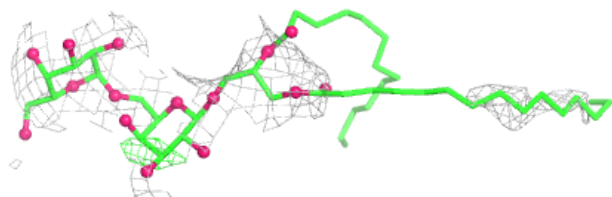


**Electron density around PL9 j 101:**

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

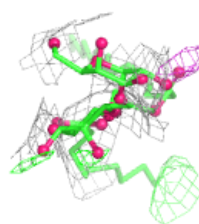
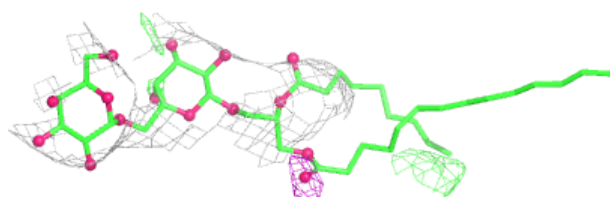
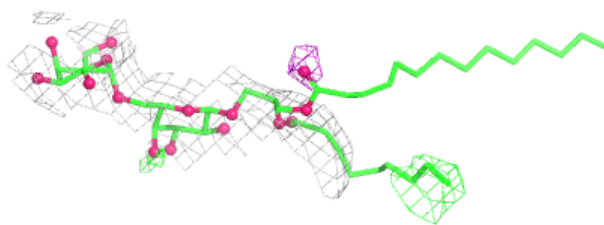
**Electron density around DGD b 624:**

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

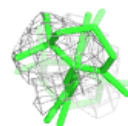
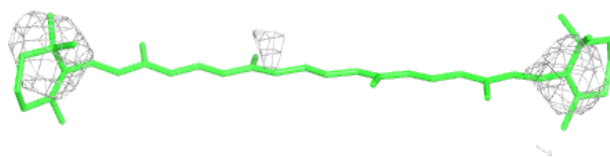
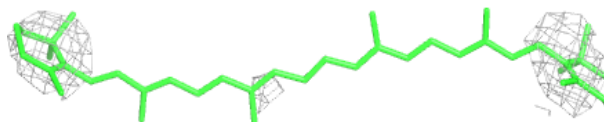


**Electron density around DGD c 515:**

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

**Electron density around BCR a 409:**

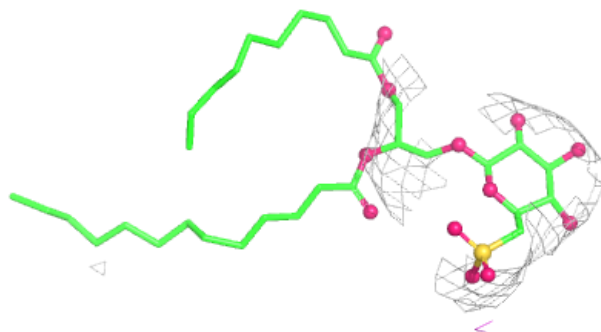
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



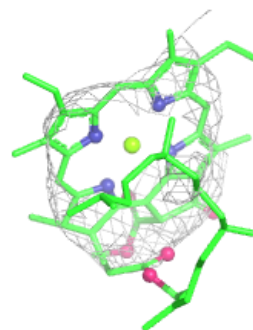
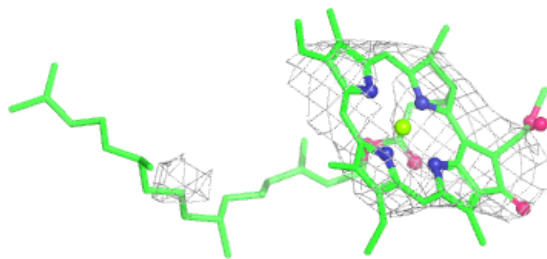
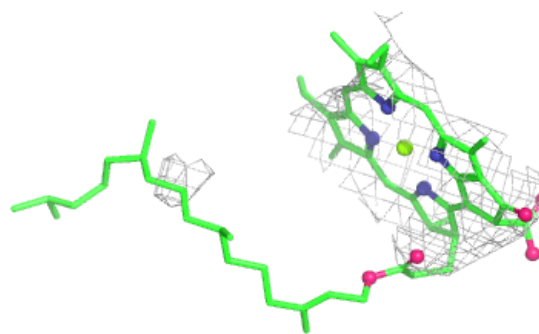


**Electron density around SQD F 103:**

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

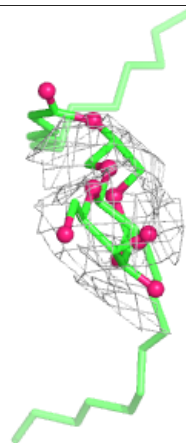
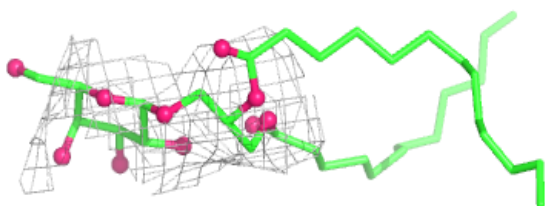
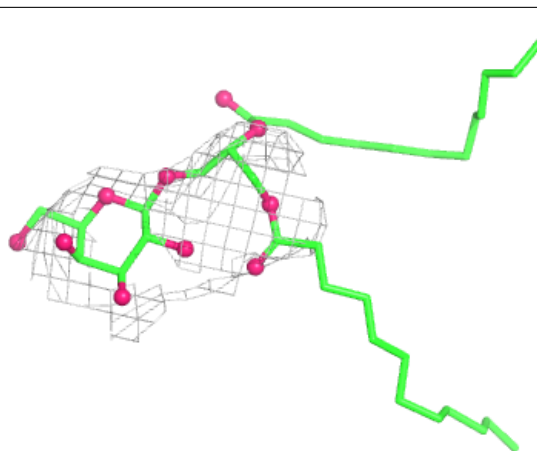
**Electron density around CLA C 512:**

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

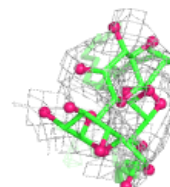
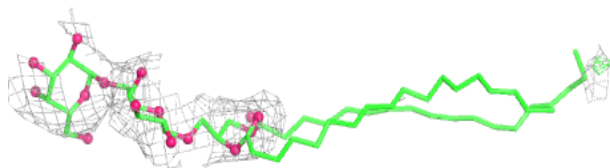


**Electron density around LMG e 101:**

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

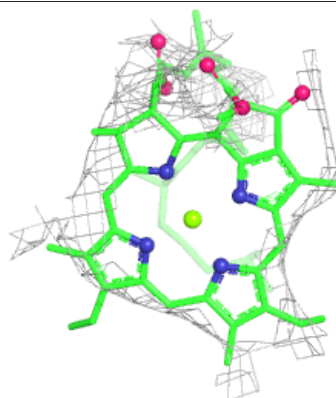
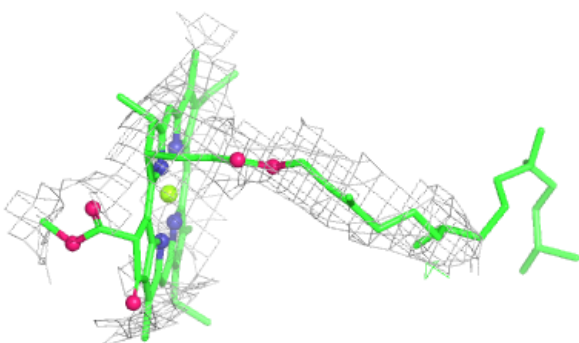
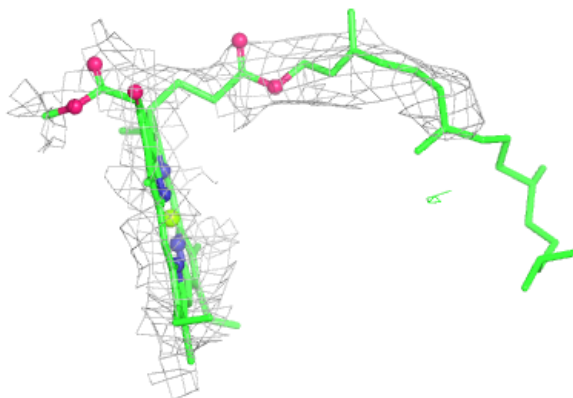
**Electron density around DGD C 517:**

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

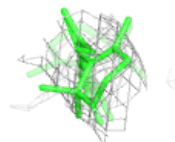
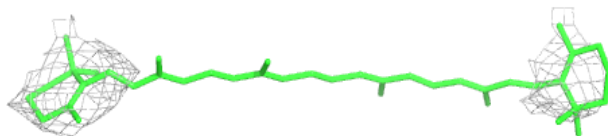
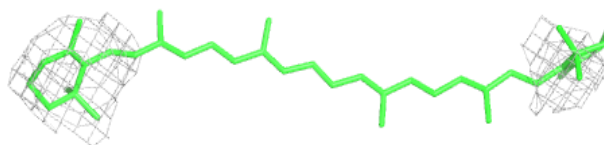


**Electron density around CLA C 505:**

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

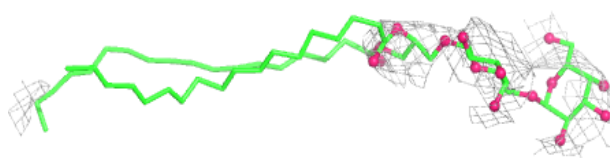
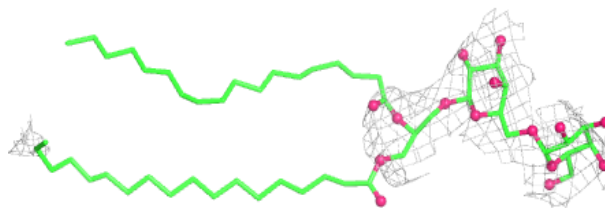
**Electron density around BCR K 102:**

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

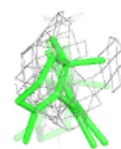
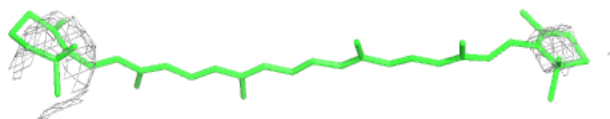
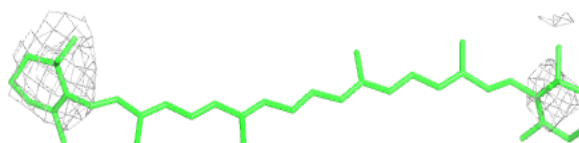


**Electron density around DGD c 517:**

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

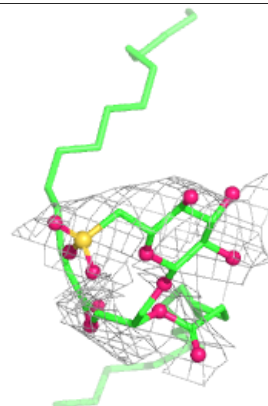
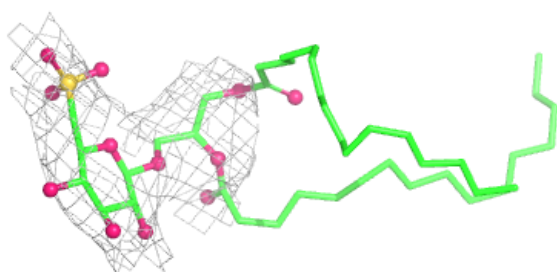
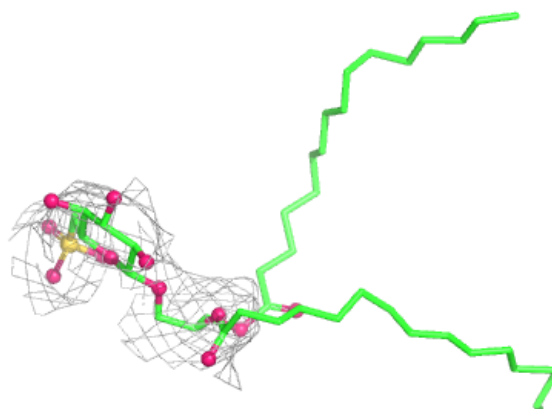
**Electron density around BCR c 514:**

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

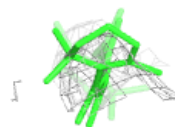
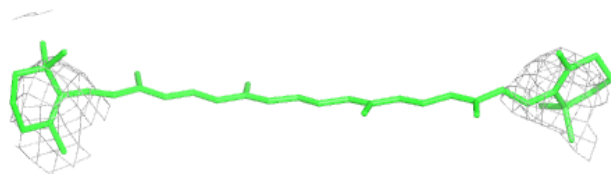
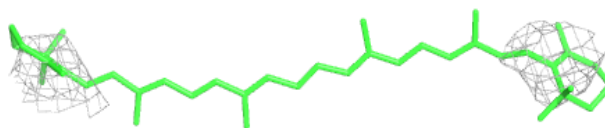


**Electron density around SQD a 401:**

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

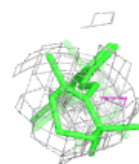
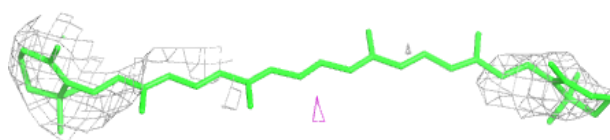
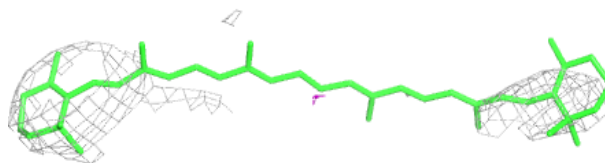
**Electron density around BCR c 521:**

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

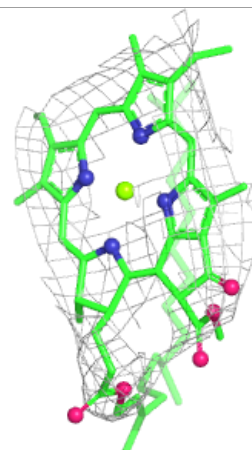
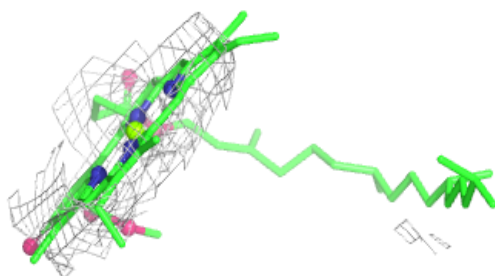
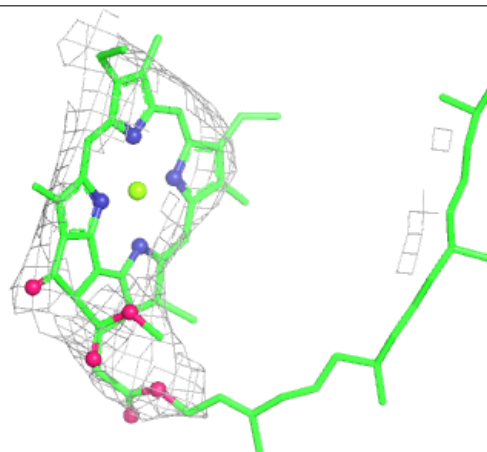


**Electron density around BCR B 619:**

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

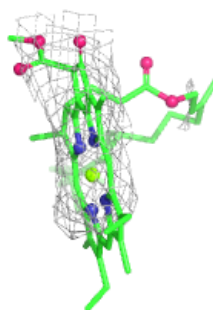
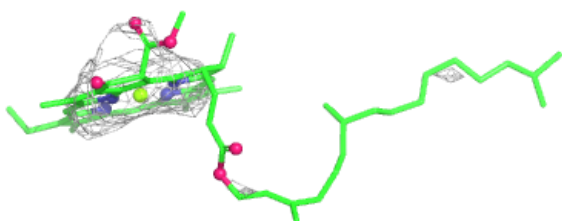
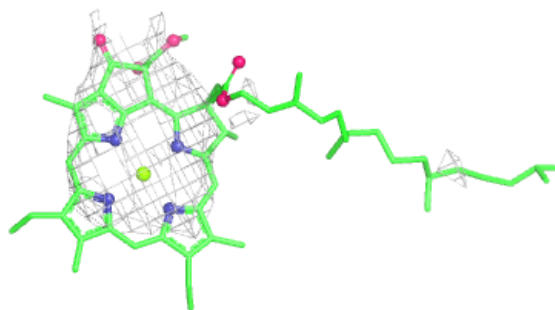
**Electron density around CLA c 506:**

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

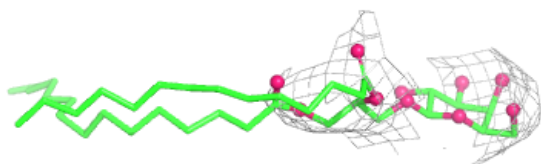


**Electron density around CLA a 406:**

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

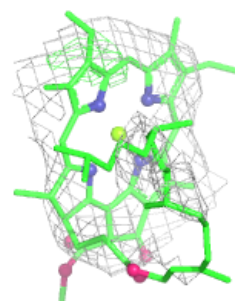
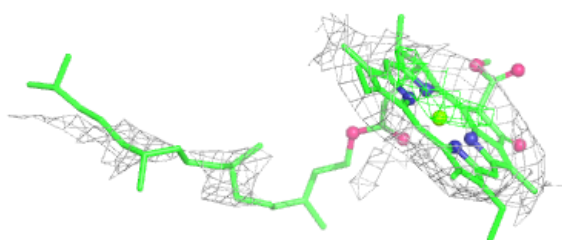
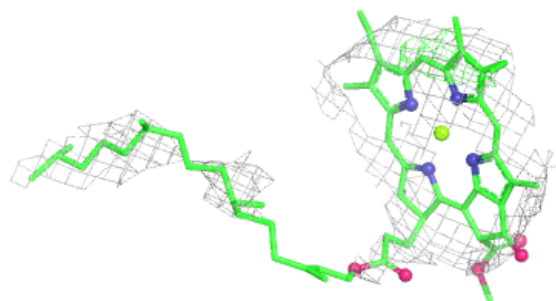
**Electron density around LMG c 522:**

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



**Electron density around CLA C 510:**

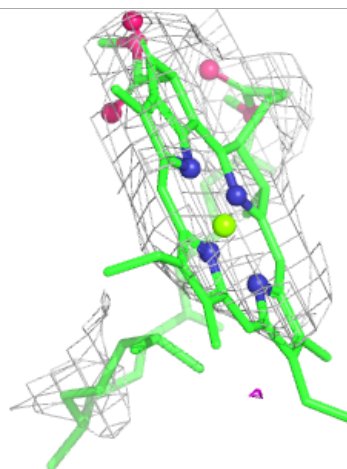
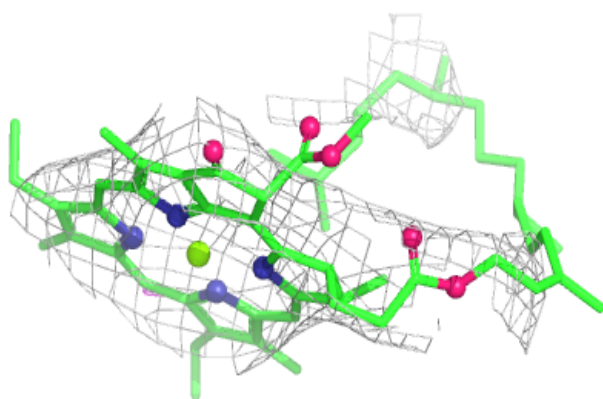
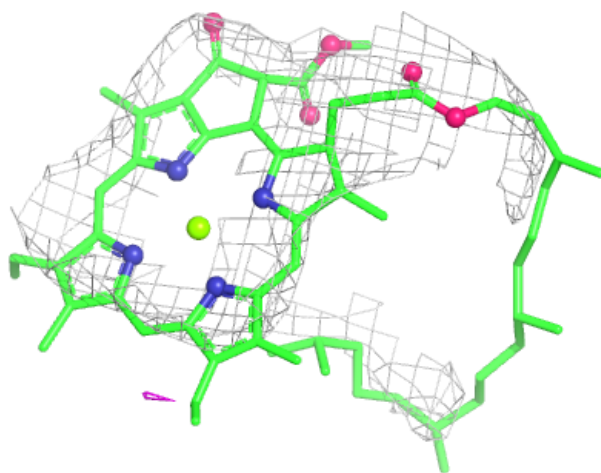
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





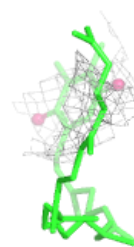
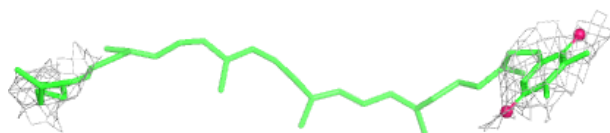
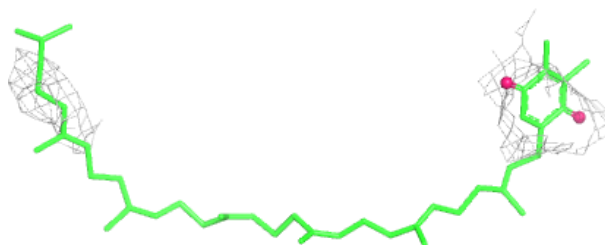
**Electron density around CLA b 618:**

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

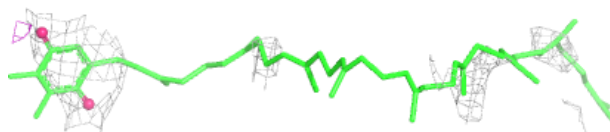
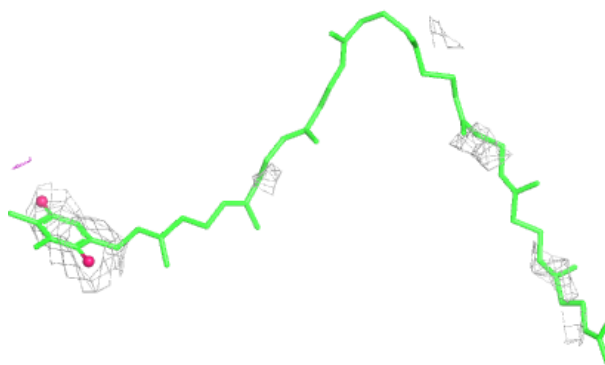


**Electron density around PL9 a 408:**

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

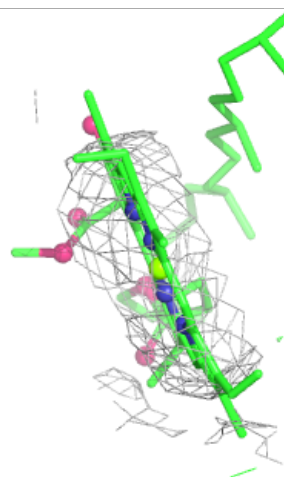
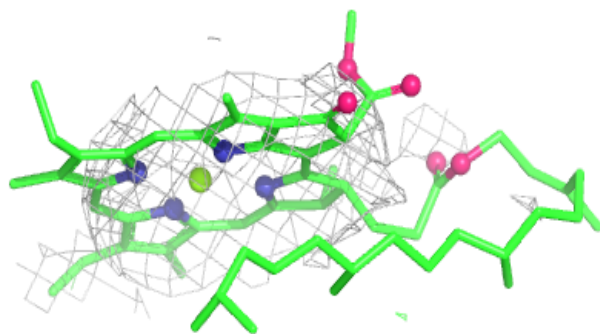
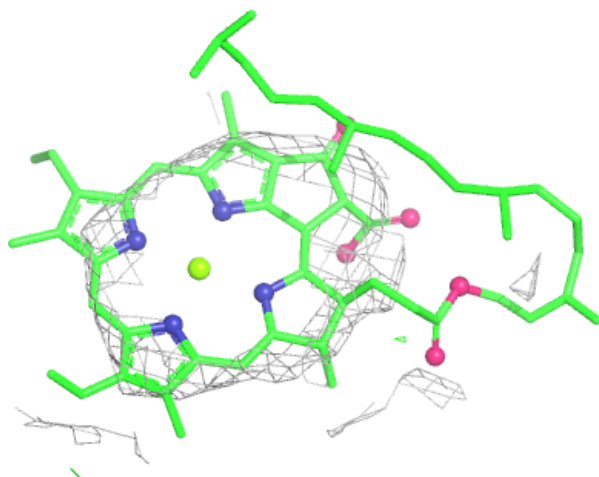
**Electron density around PL9 d 407:**

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



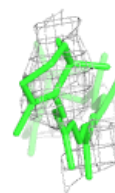
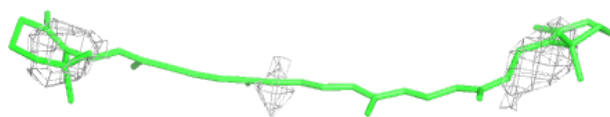
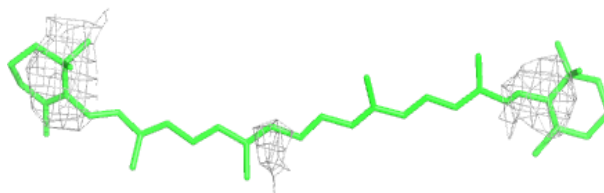
**Electron density around CLA C 508:**

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

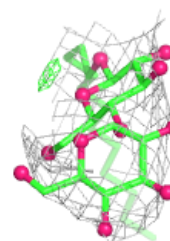
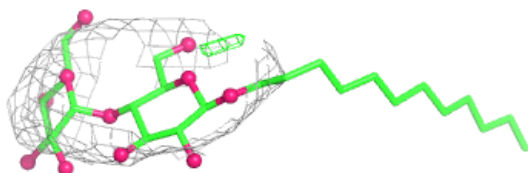
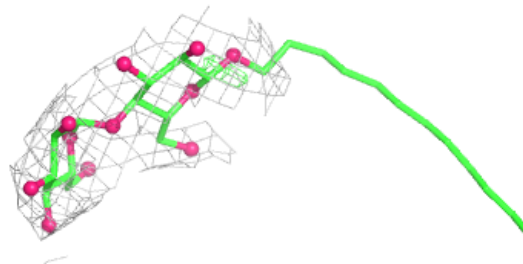


**Electron density around BCR B 617:**

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

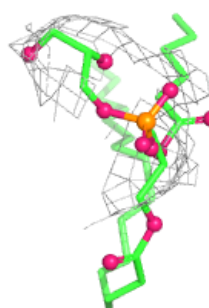
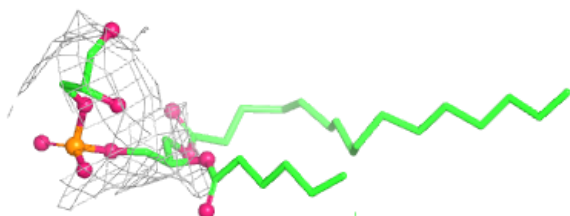
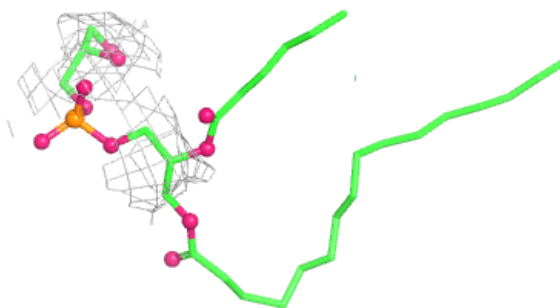
**Electron density around LMT M 103:**

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

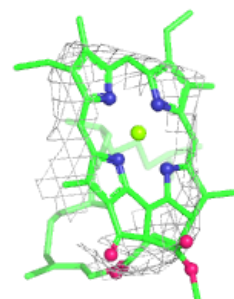
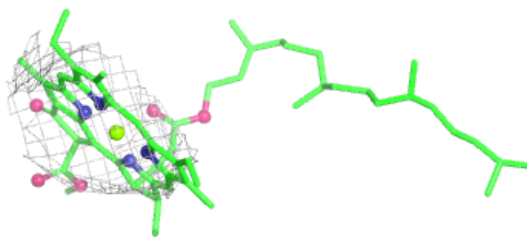
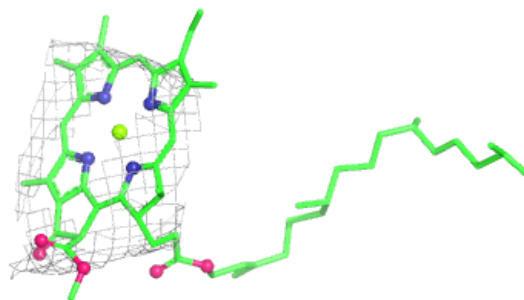


**Electron density around LHG A 409:**

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

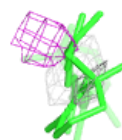
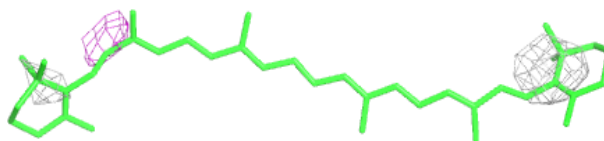
**Electron density around CLA c 510:**

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

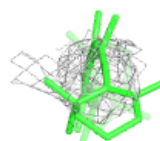
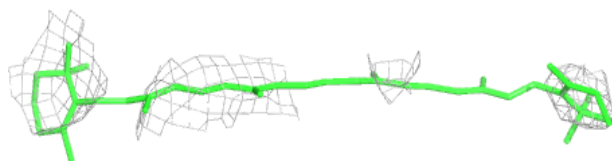
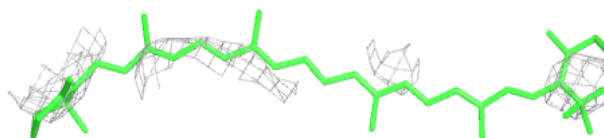


**Electron density around BCR g 101:**

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

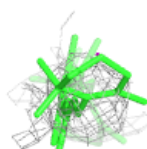
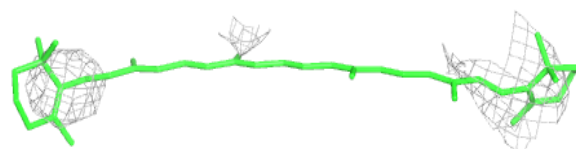
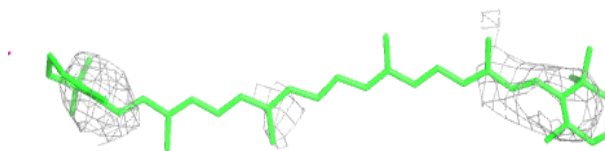
**Electron density around BCR x 101:**

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

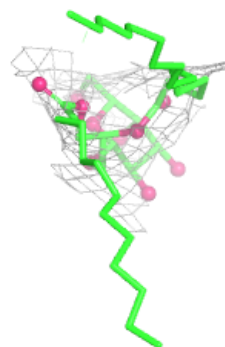
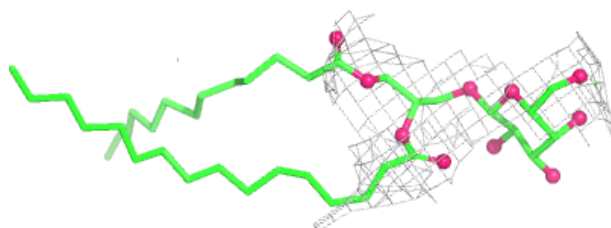
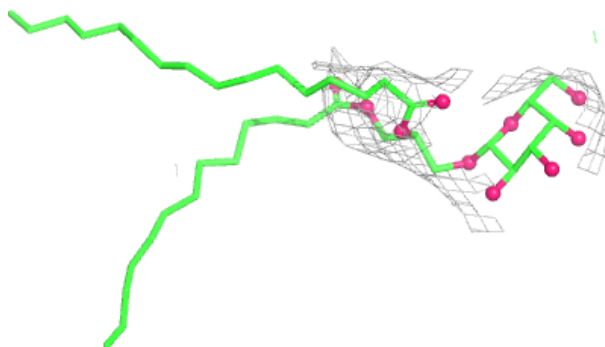


**Electron density around BCR B 616:**

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

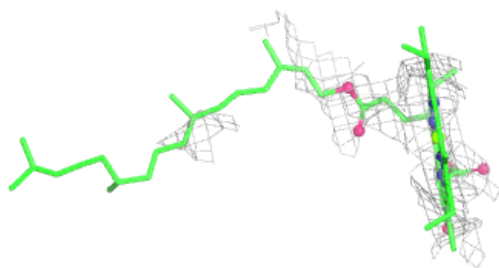
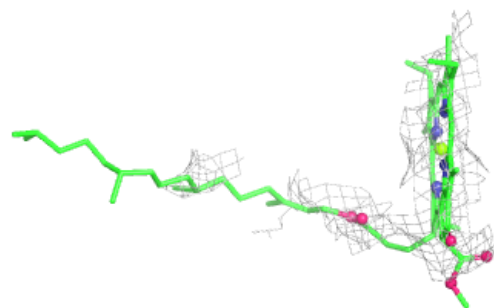
**Electron density around LMG D 409:**

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

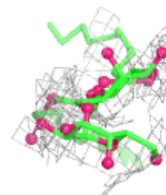
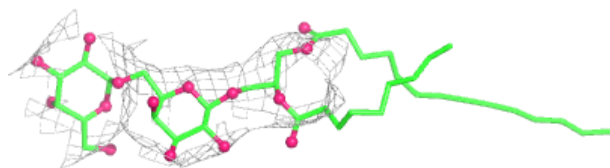


**Electron density around CLA b 609:**

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

**Electron density around DGD C 515:**

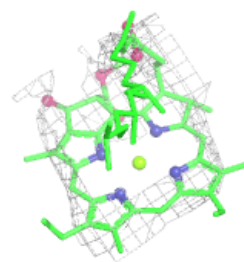
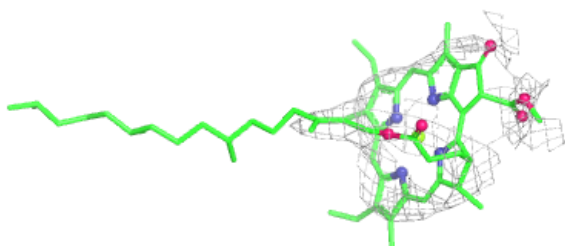
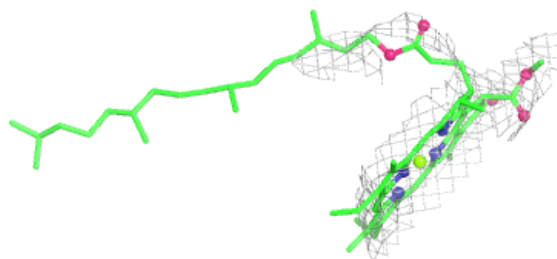
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



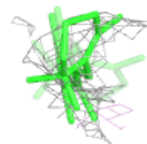
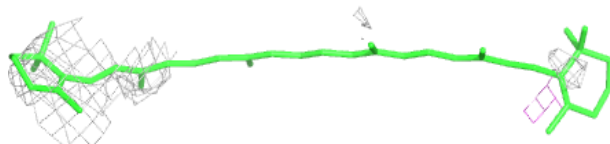
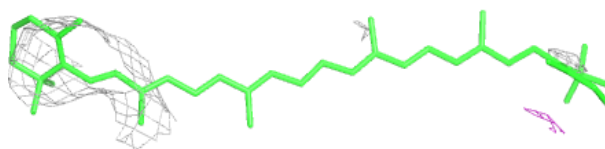


**Electron density around CLA C 520:**

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

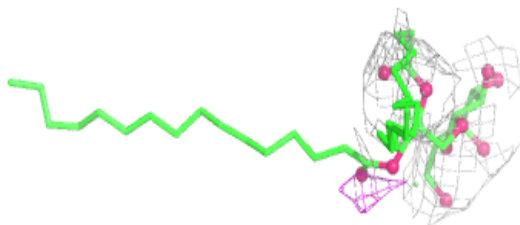
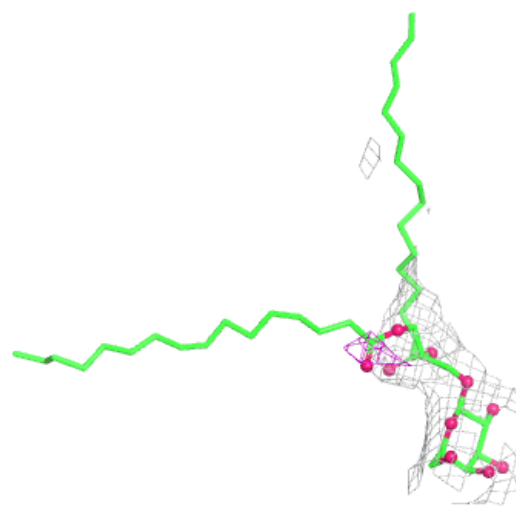
**Electron density around BCR b 620:**

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



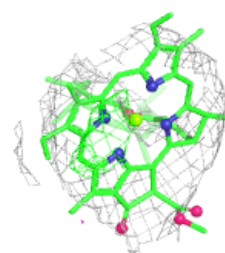
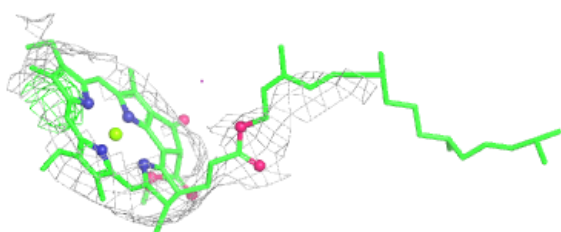
**Electron density around LMG a 412:**

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

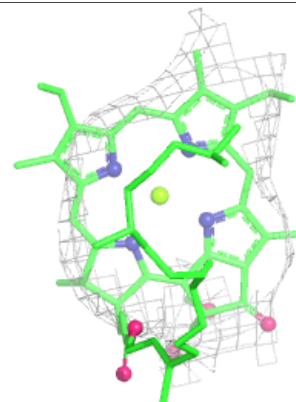
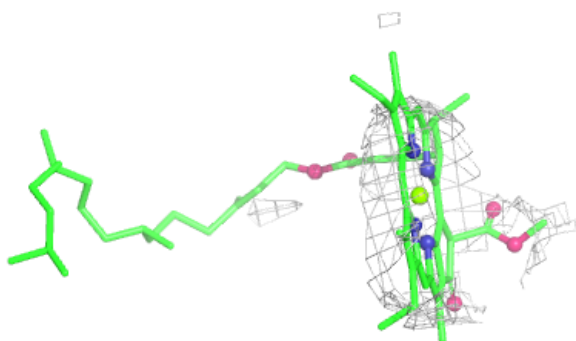
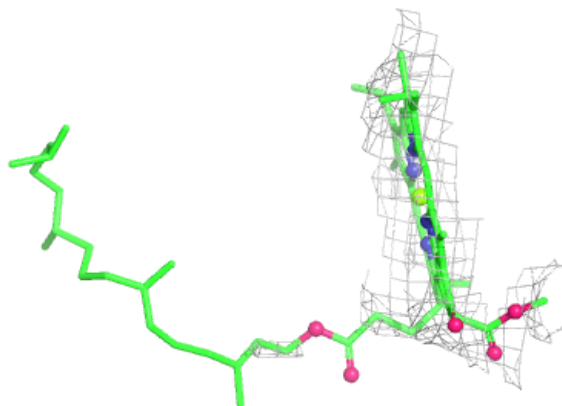


**Electron density around CLA c 502:**

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

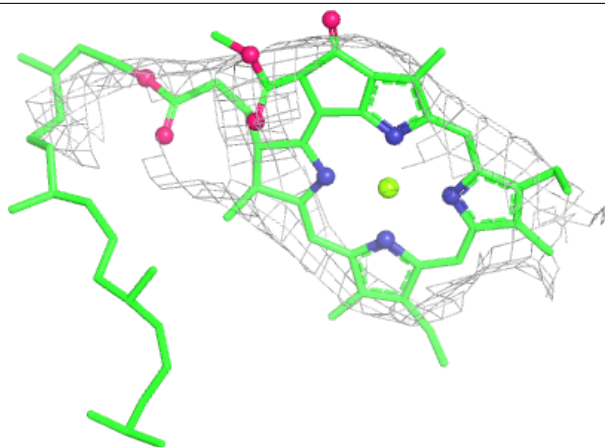
**Electron density around CLA c 505:**

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



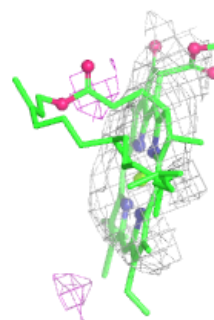
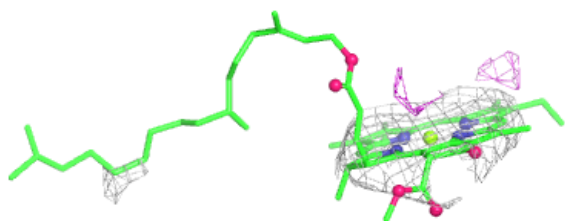
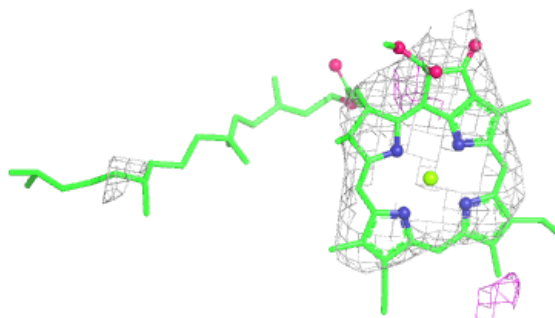
**Electron density around CLA B 615:**

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

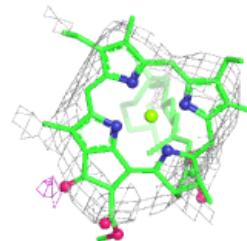
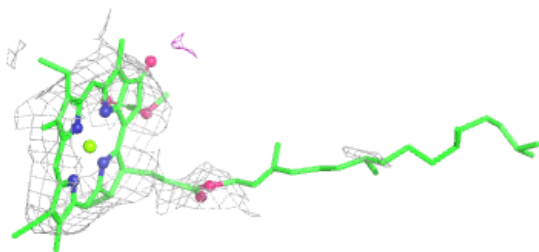
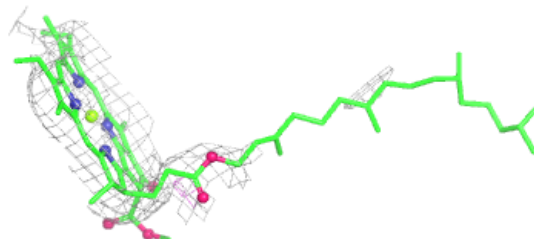


**Electron density around CLA A 404:**

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

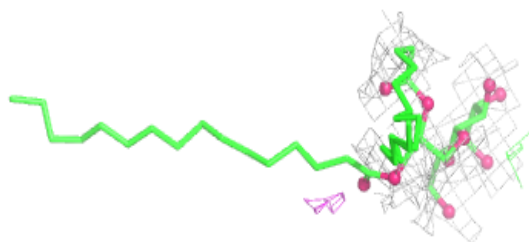
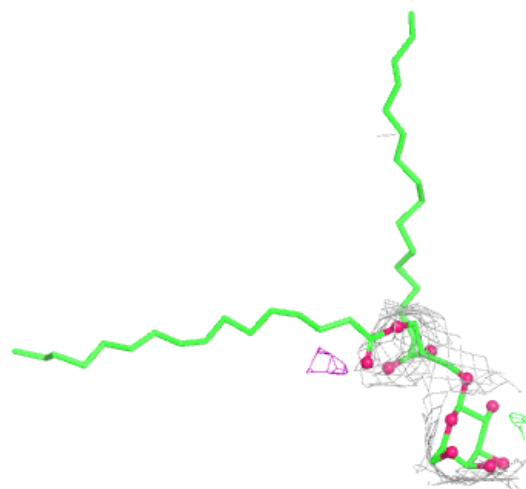
**Electron density around CLA B 603:**

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



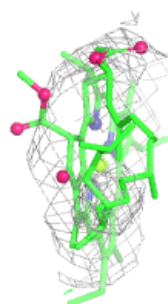
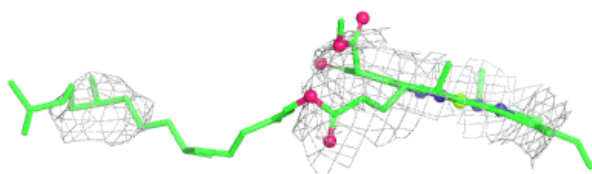
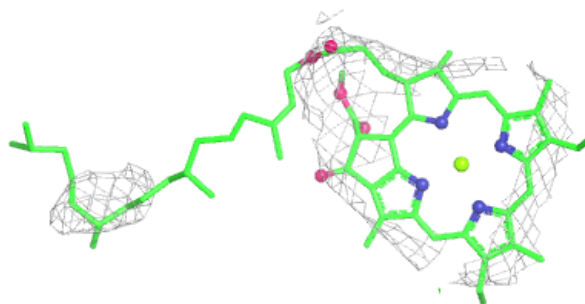
**Electron density around LMG A 410:**

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

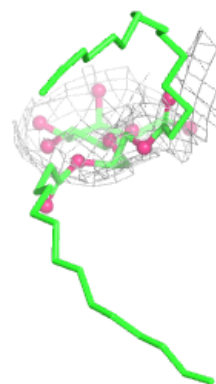


**Electron density around CLA h 101:**

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

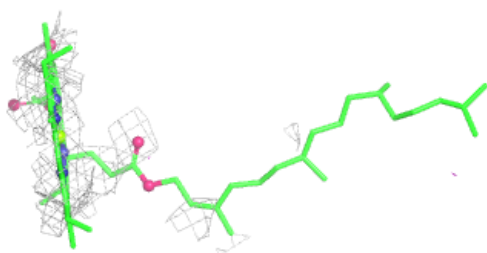
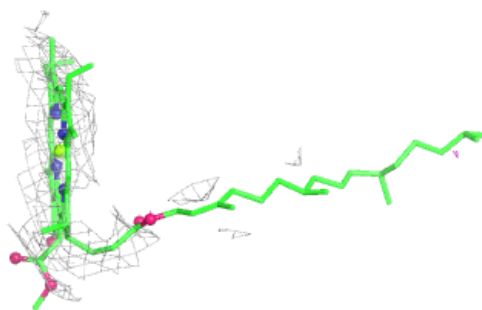
**Electron density around LMG B 621:**

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

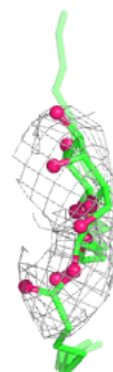
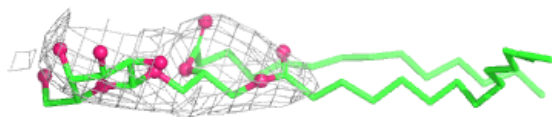
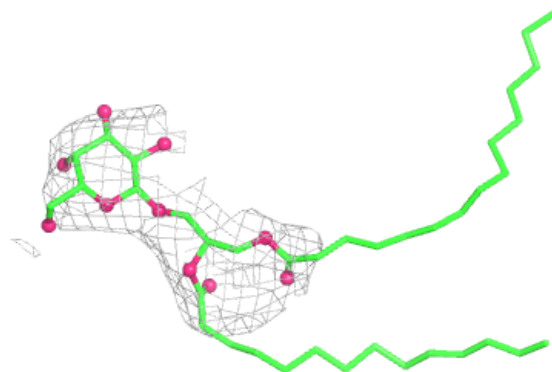


**Electron density around CLA B 605:**

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

**Electron density around LMG C 521:**

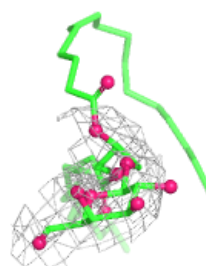
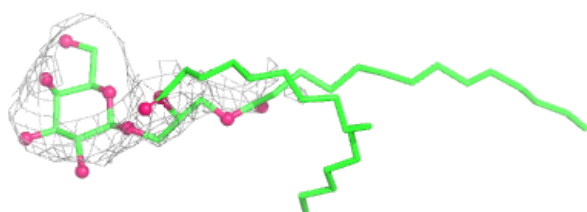
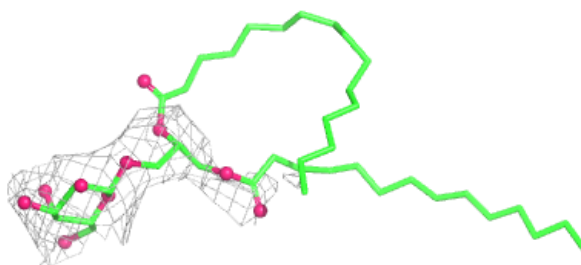
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



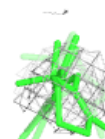
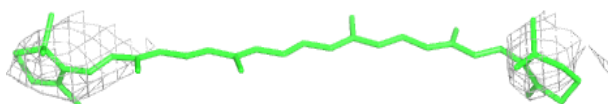
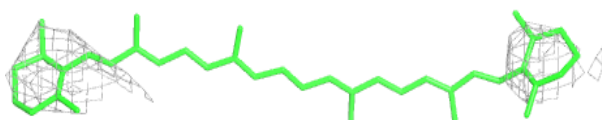


**Electron density around LMG D 408:**

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

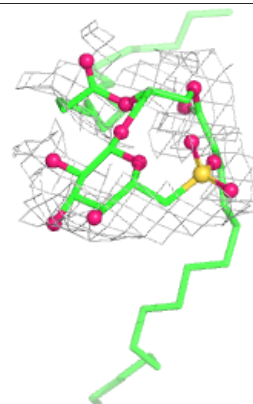
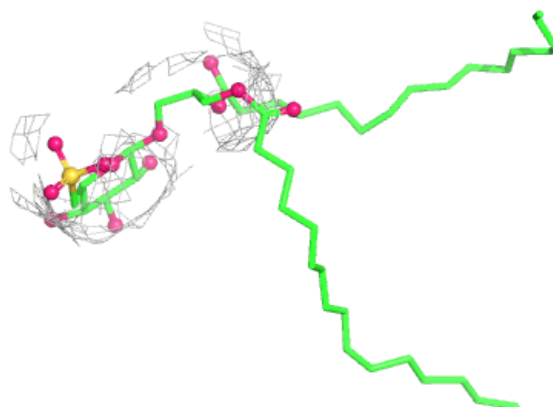
**Electron density around BCR C 514:**

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

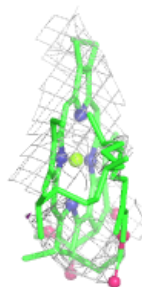
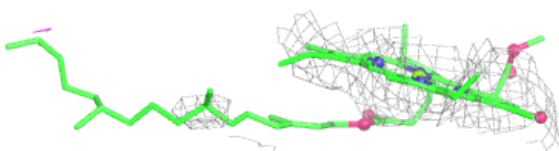
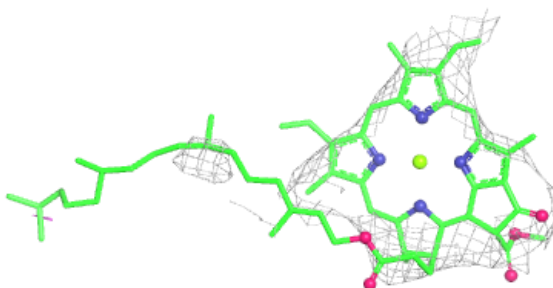


**Electron density around SQD A 413:**

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

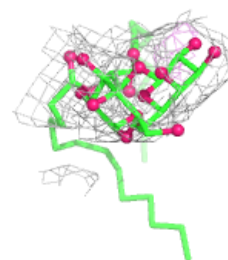
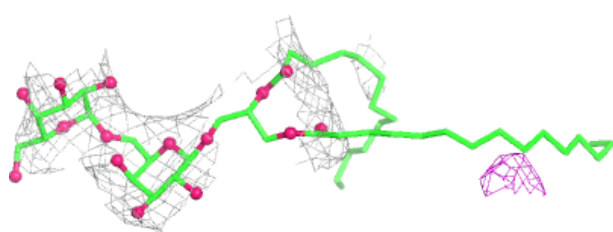
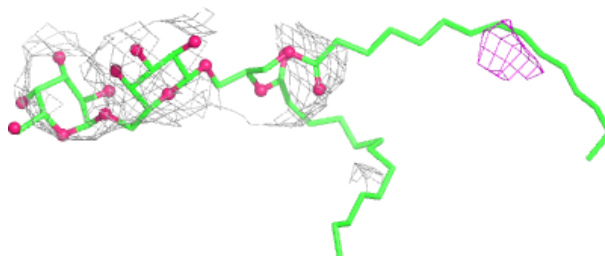
**Electron density around CLA b 606:**

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

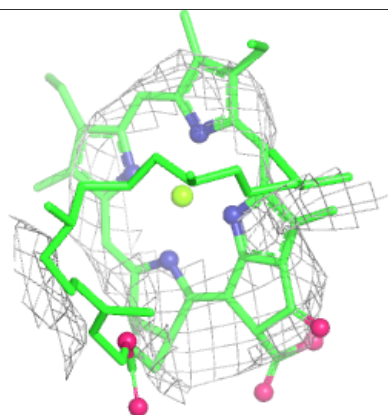
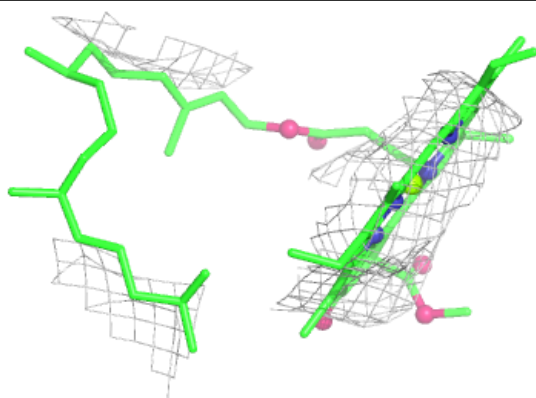
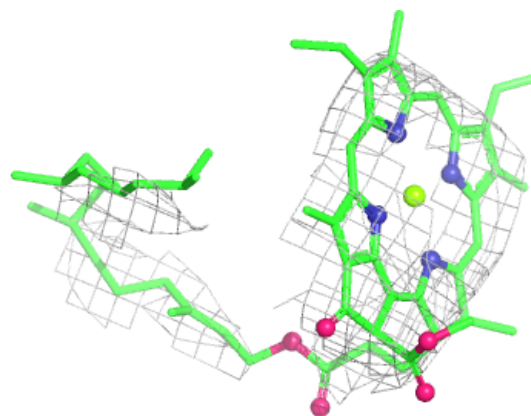


**Electron density around DGD B 620:**

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

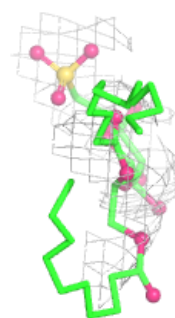
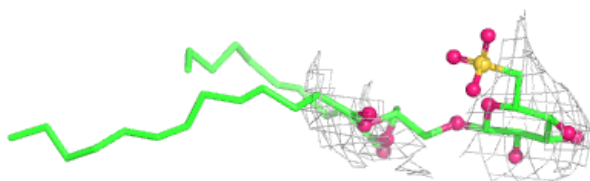
**Electron density around CLA c 503:**

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

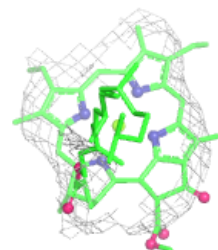


**Electron density around SQD f 103:**

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

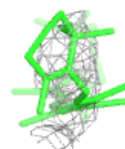
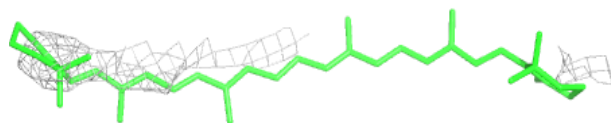
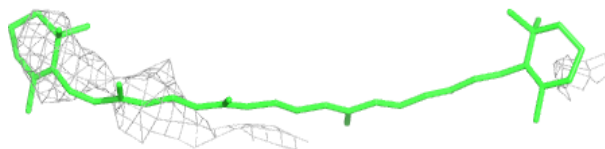
**Electron density around CLA b 607:**

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

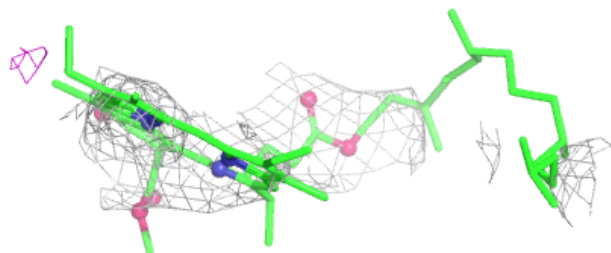
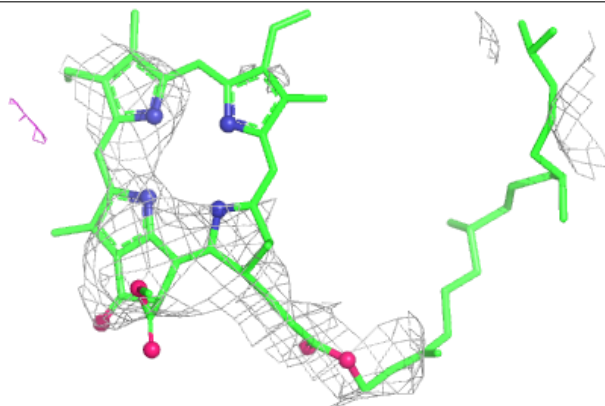


**Electron density around BCR c 513:**

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

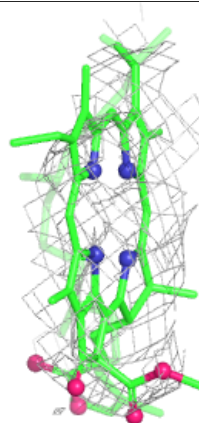
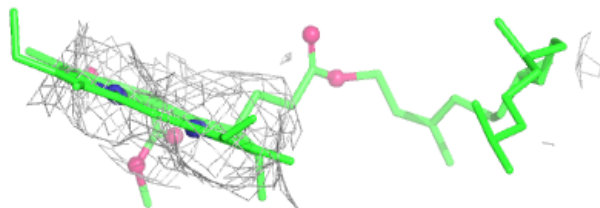
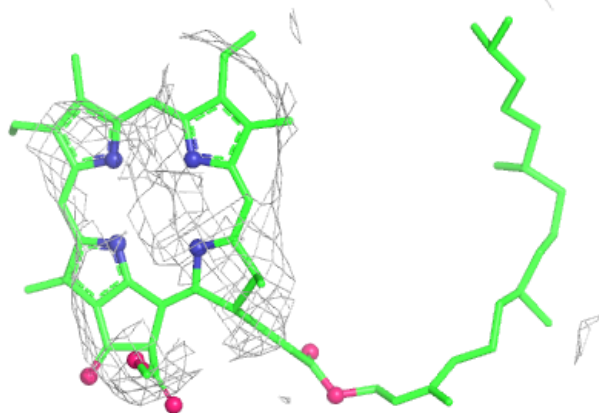
**Electron density around PHO D 402:**

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



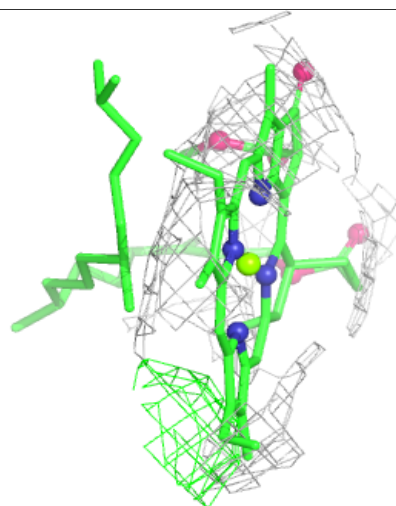
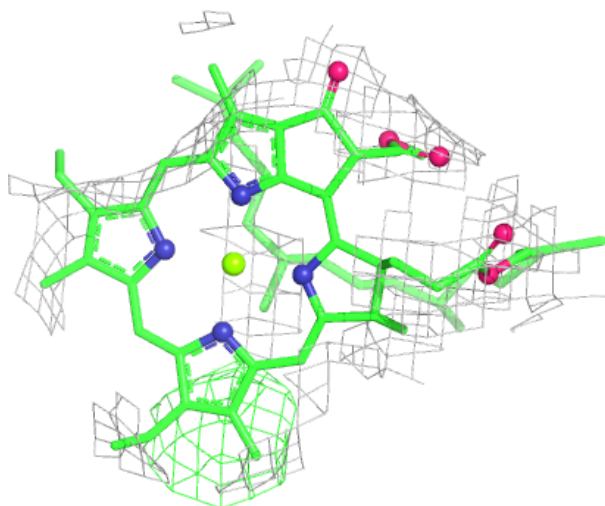
**Electron density around PHO d 401:**

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



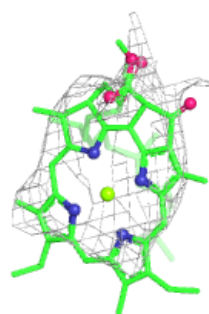
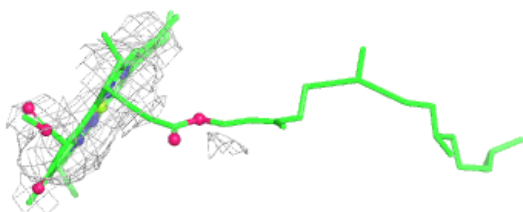
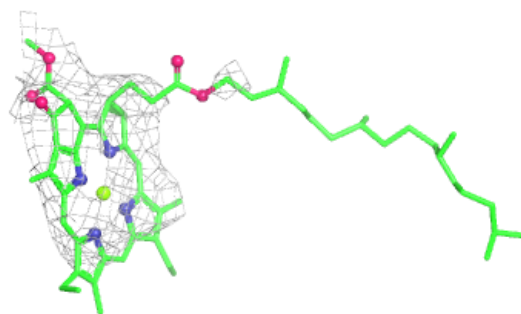
**Electron density around CLA C 509:**

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

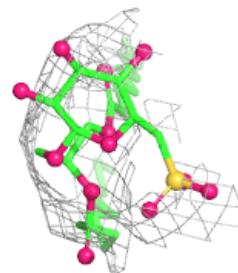
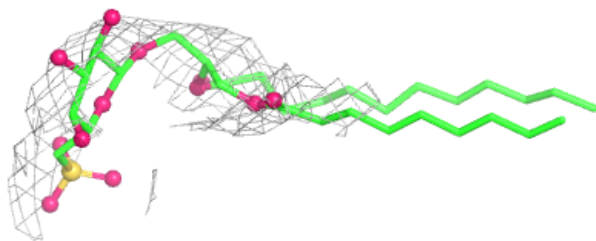


**Electron density around CLA a 407:**

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

**Electron density around SQD B 622:**

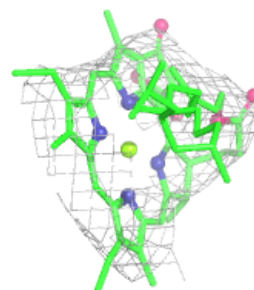
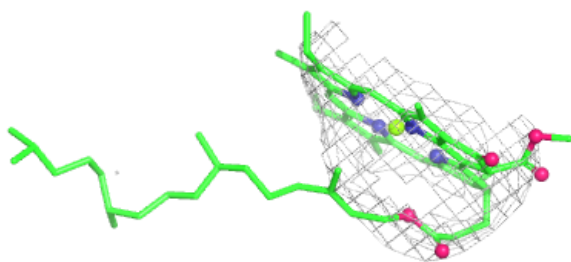
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



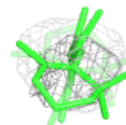
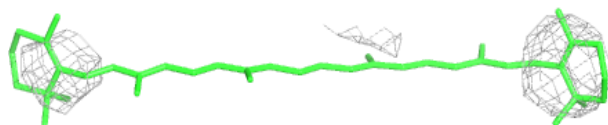
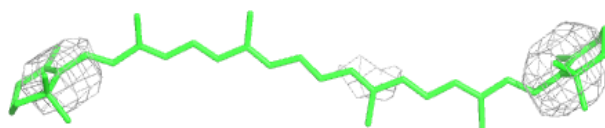


**Electron density around CLA B 613:**

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

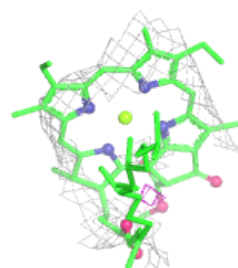
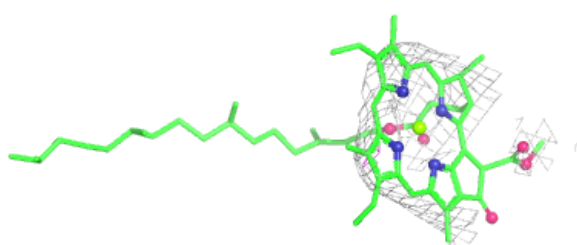
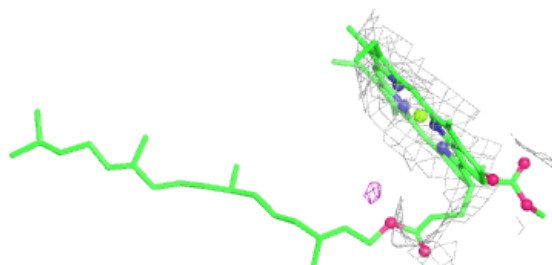
**Electron density around BCR A 407:**

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

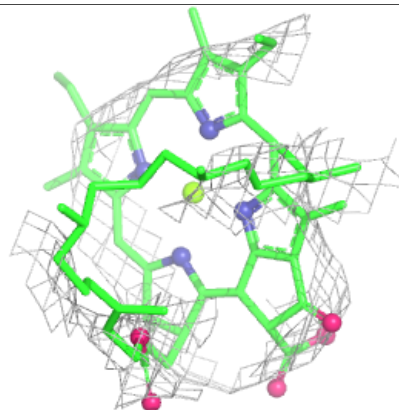
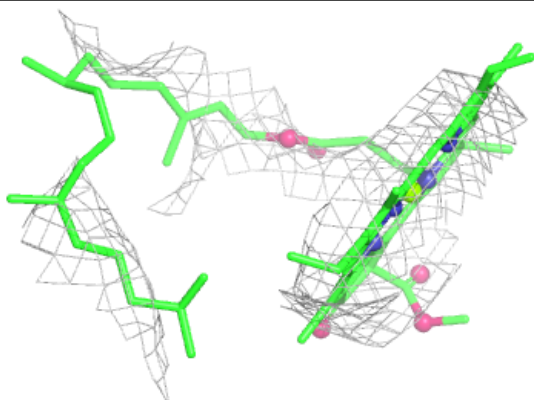
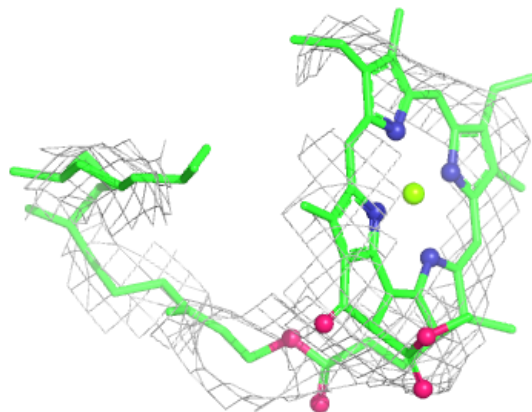


**Electron density around CLA c 520:**

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

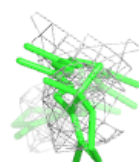
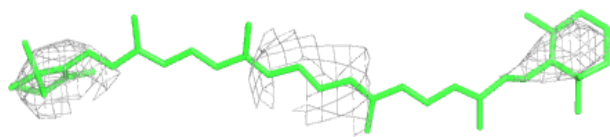
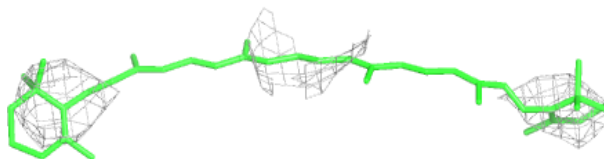
**Electron density around CLA C 503:**

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

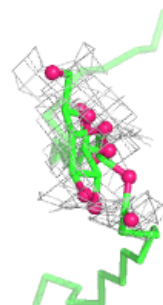
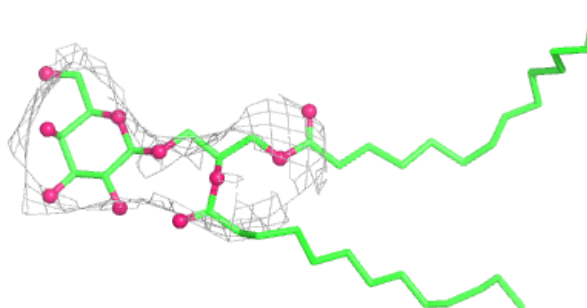


**Electron density around BCR F 102:**

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

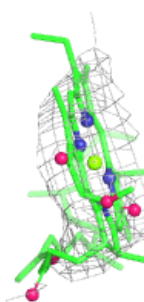
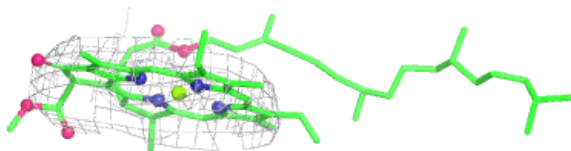
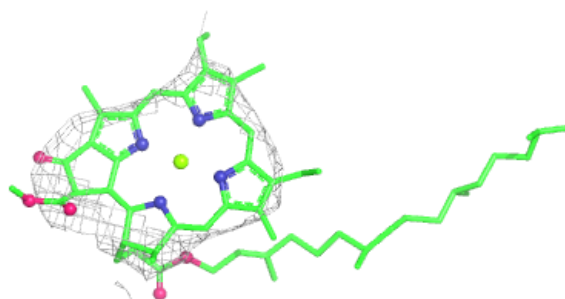
**Electron density around LMG D 412:**

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

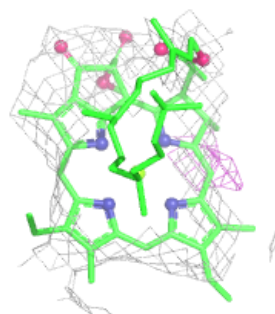
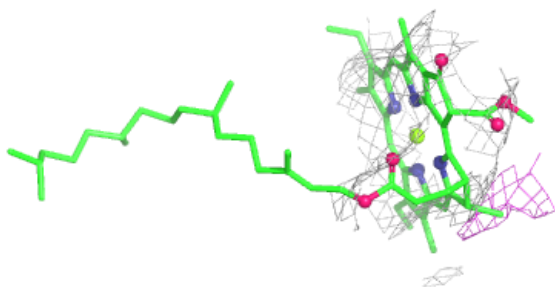
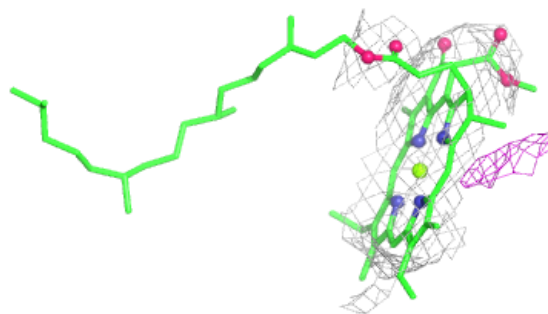


**Electron density around CLA c 501:**

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

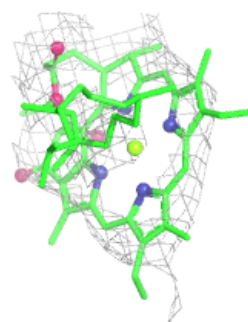
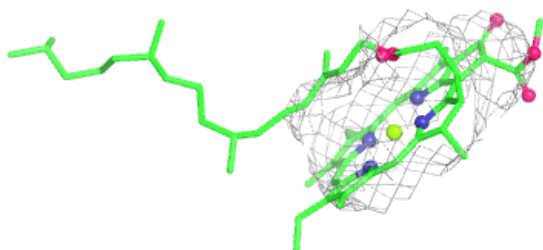
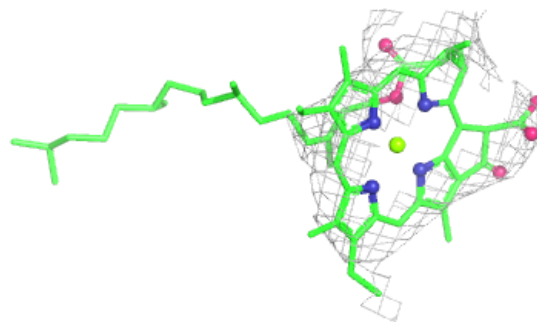
**Electron density around CLA C 507:**

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

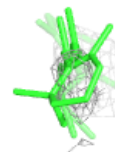
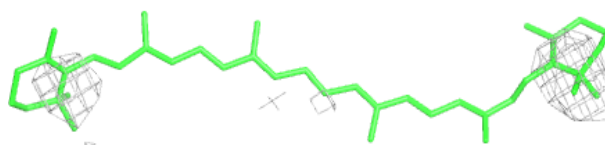


**Electron density around CLA C 504:**

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

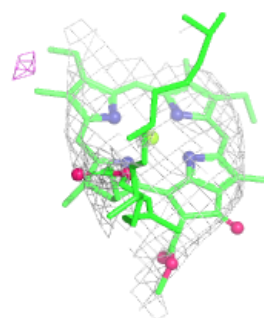
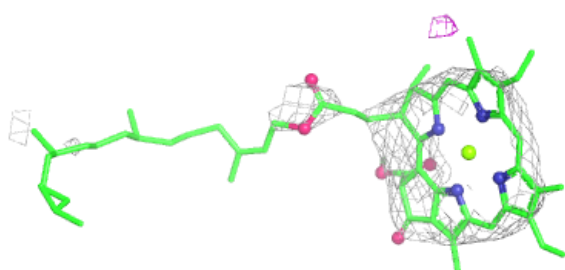
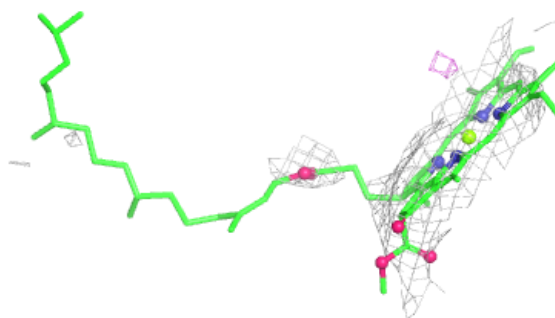
**Electron density around BCR y 101:**

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

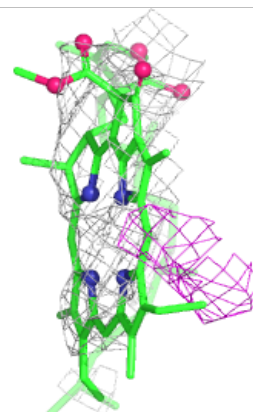
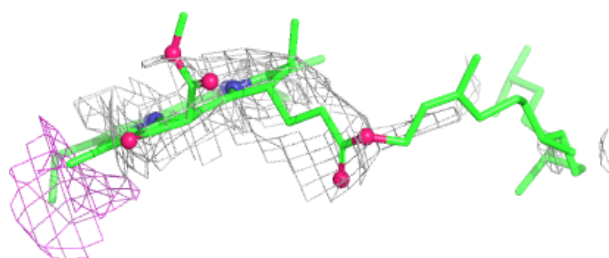
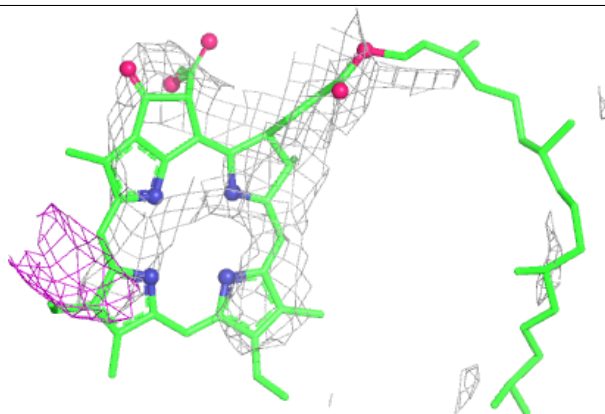


**Electron density around CLA D 405:**

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

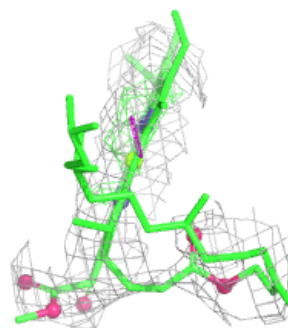
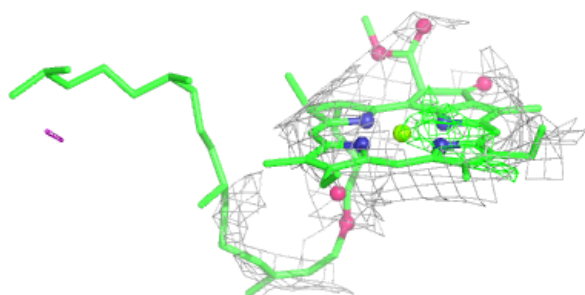
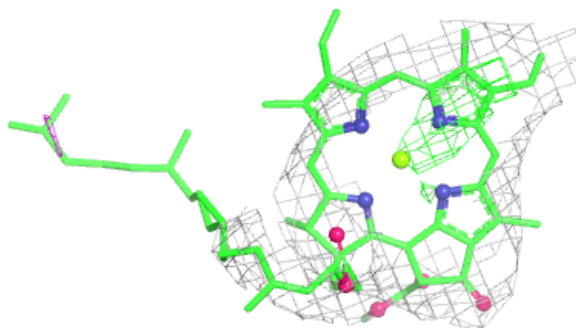
**Electron density around PHO D 401:**

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



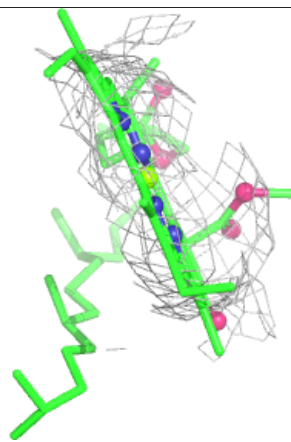
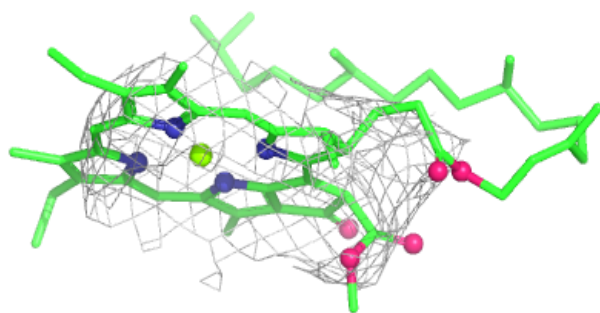
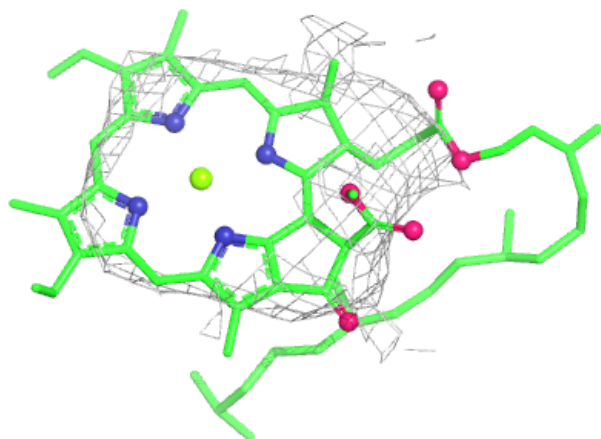
**Electron density around CLA a 405:**

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



**Electron density around CLA c 508:**

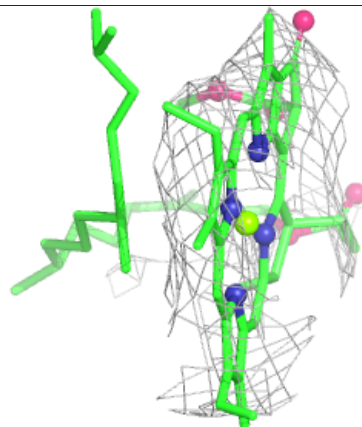
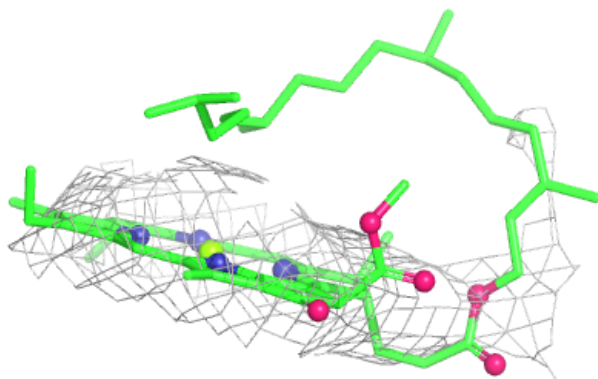
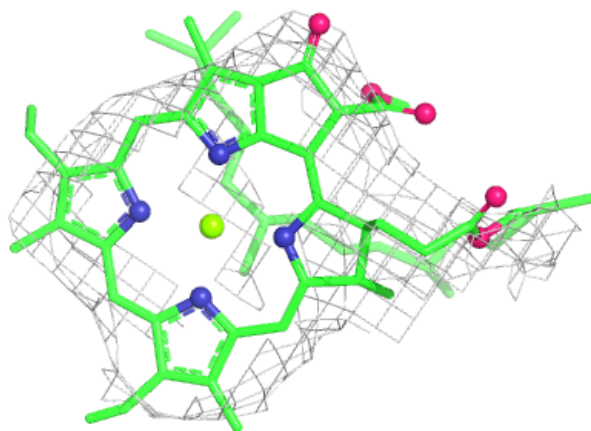
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



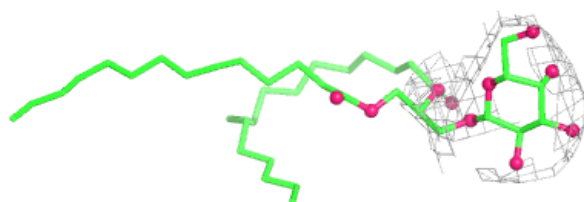
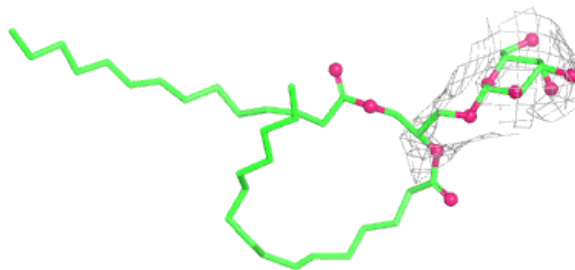


**Electron density around CLA c 509:**

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

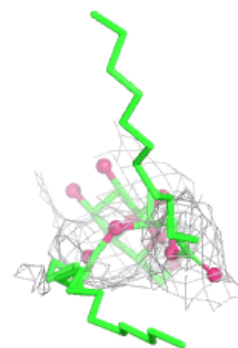
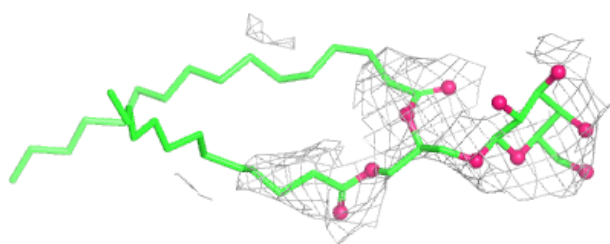
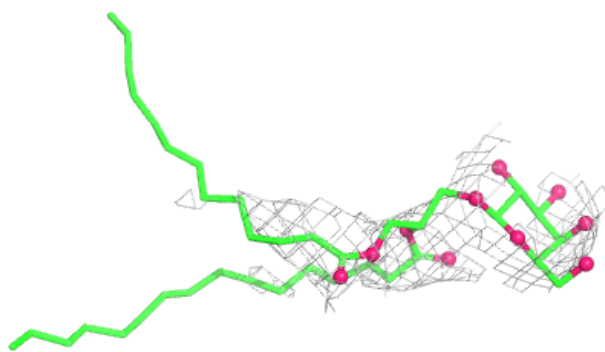
**Electron density around LMG d 408:**

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

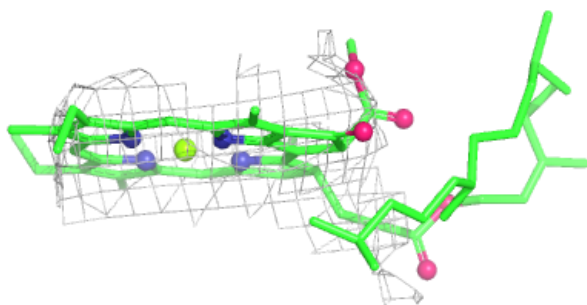
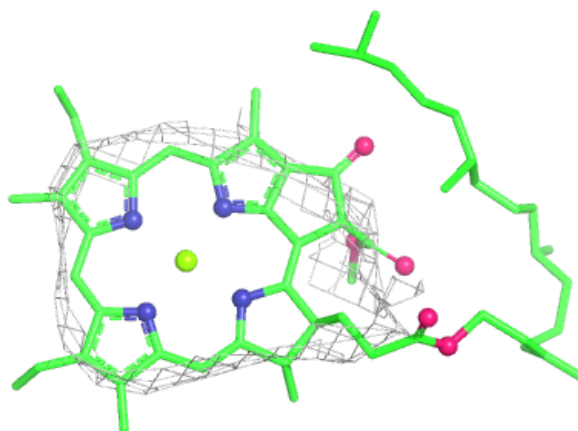


**Electron density around LMG d 409:**

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

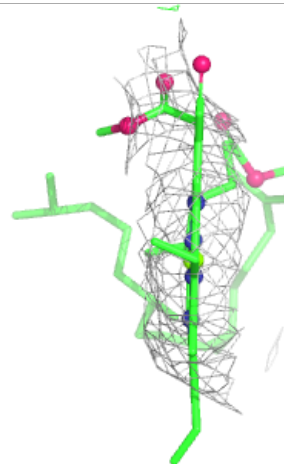
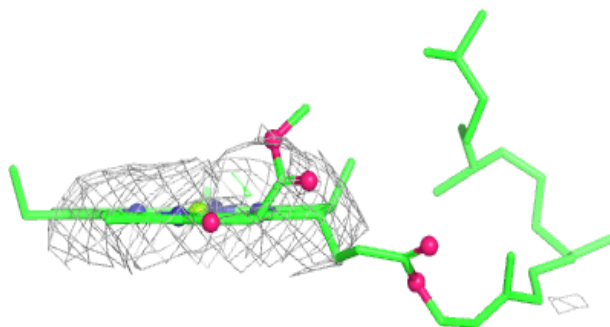
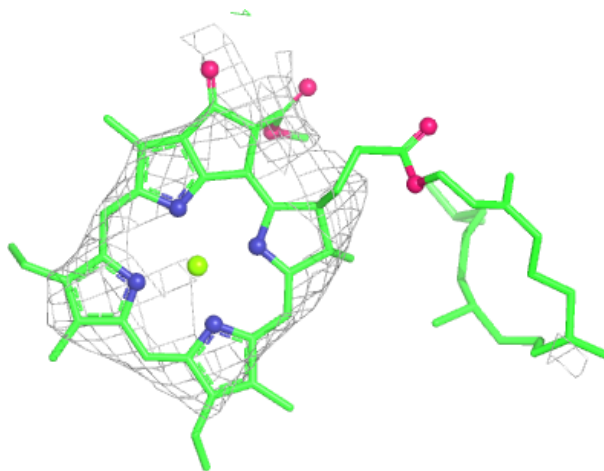
**Electron density around CLA b 613:**

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



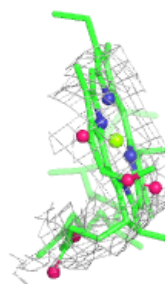
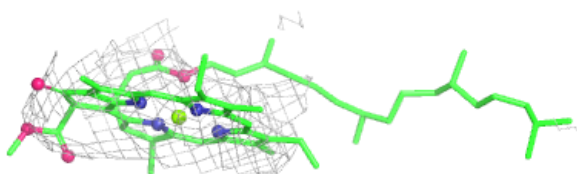
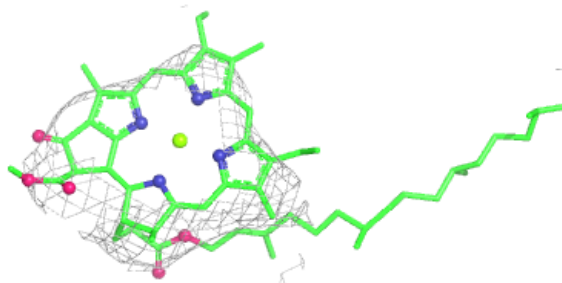
**Electron density around CLA c 511:**

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

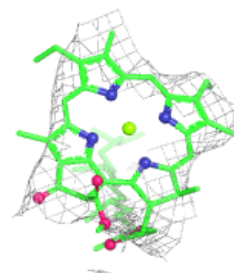
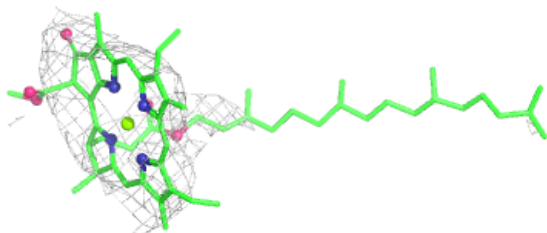
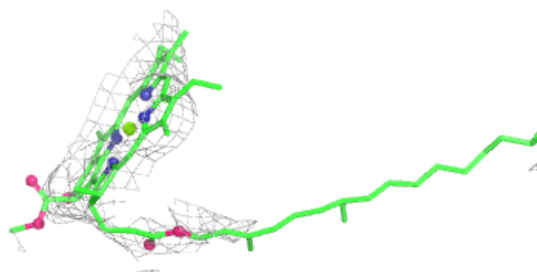


**Electron density around CLA C 501:**

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

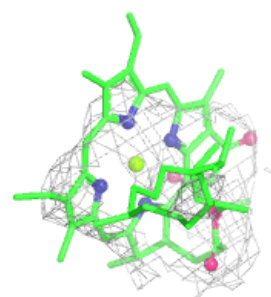
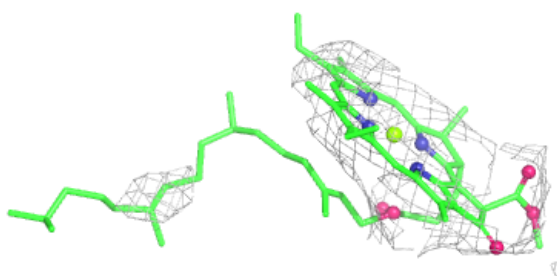
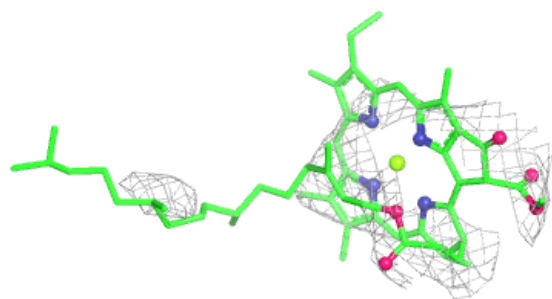
**Electron density around CLA B 606:**

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

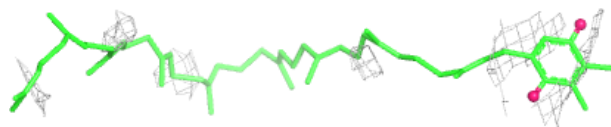
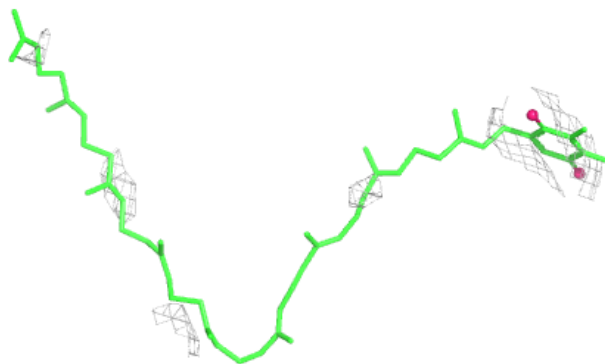


**Electron density around CLA c 504:**

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

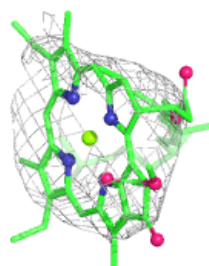
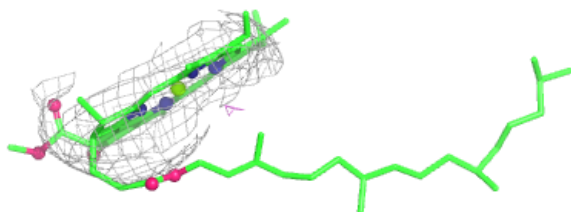
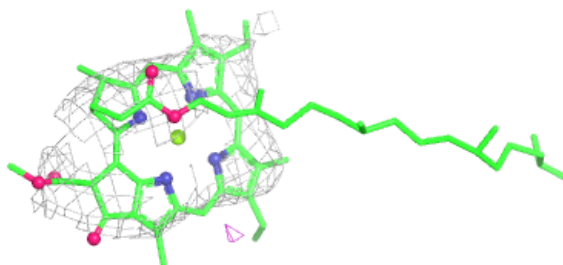
**Electron density around PL9 D 407:**

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

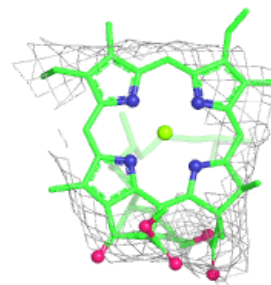
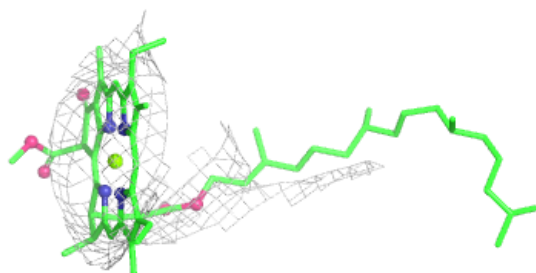
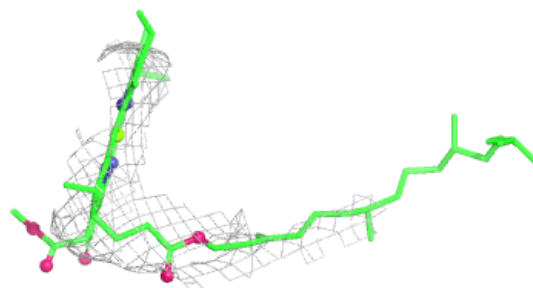


**Electron density around CLA B 607:**

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

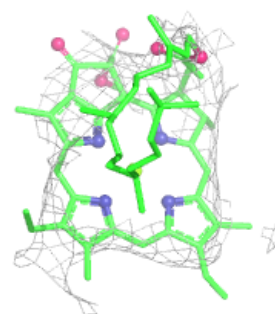
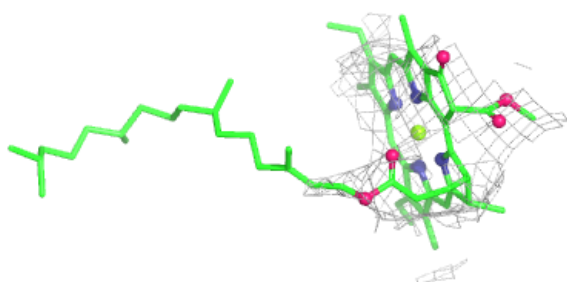
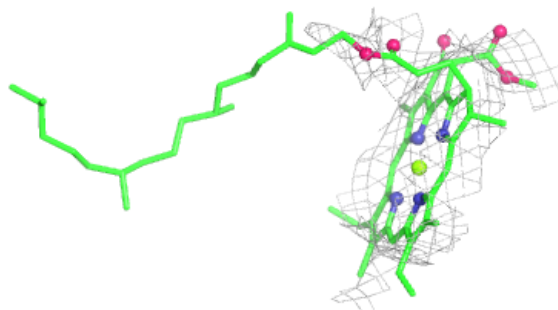
**Electron density around CLA b 608:**

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

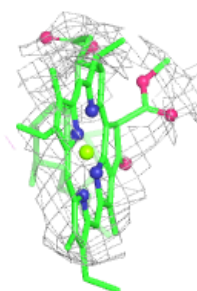
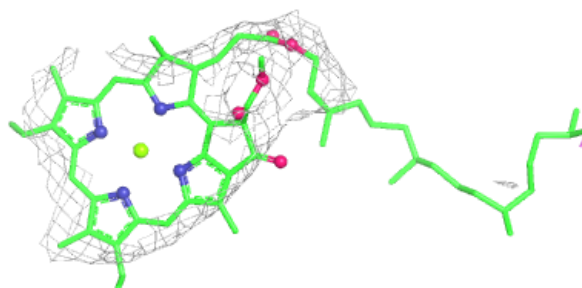


**Electron density around CLA c 507:**

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

**Electron density around CLA H 101:**

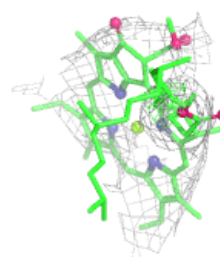
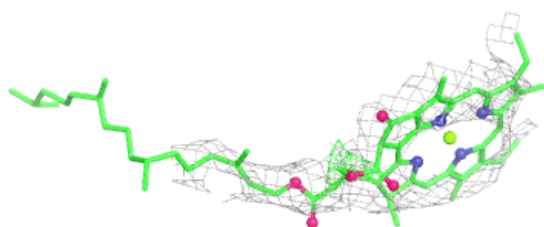
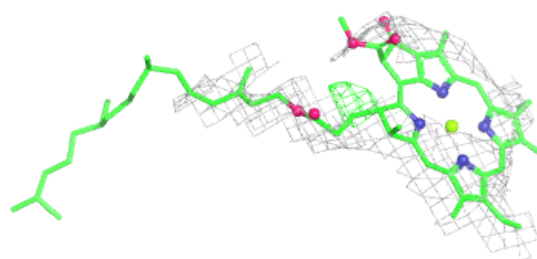
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



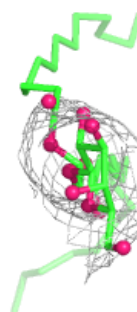
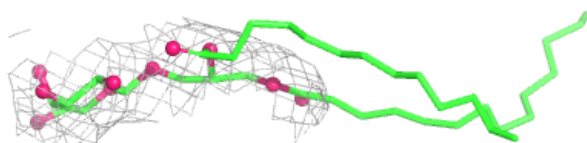
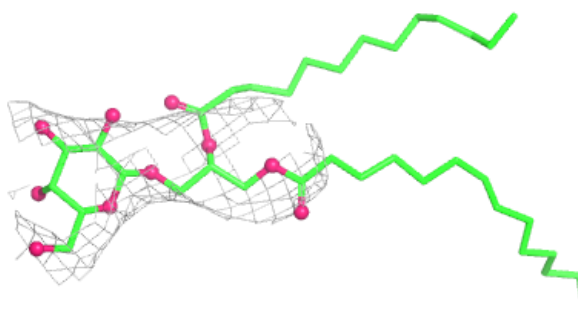


**Electron density around CLA a 404:**

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

**Electron density around LMG d 412:**

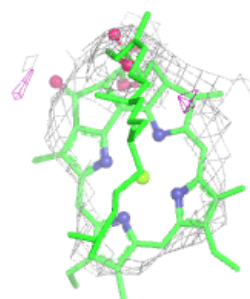
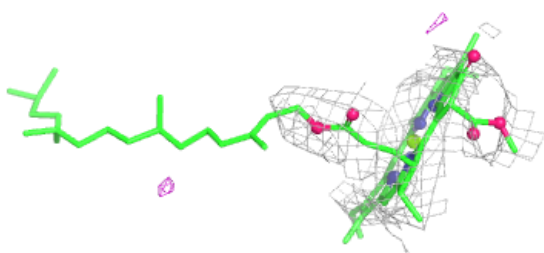
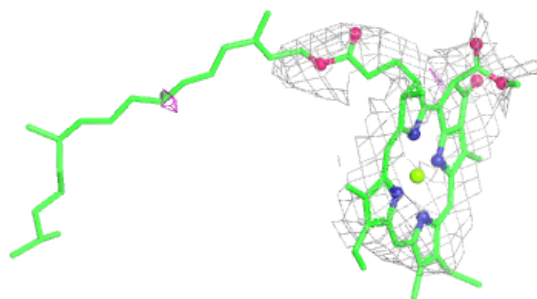
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



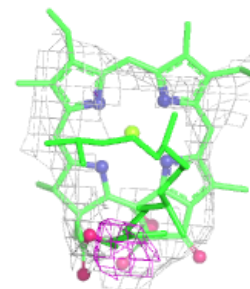
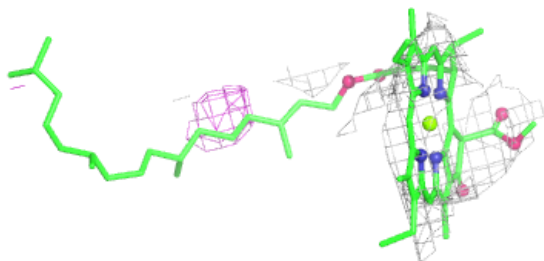
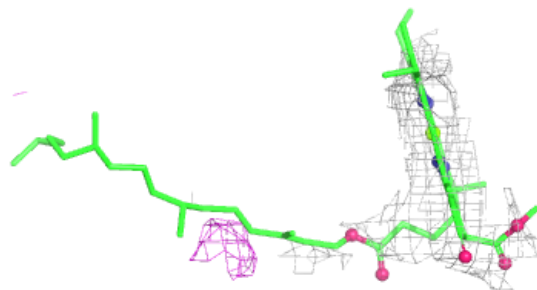


**Electron density around CLA B 608:**

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

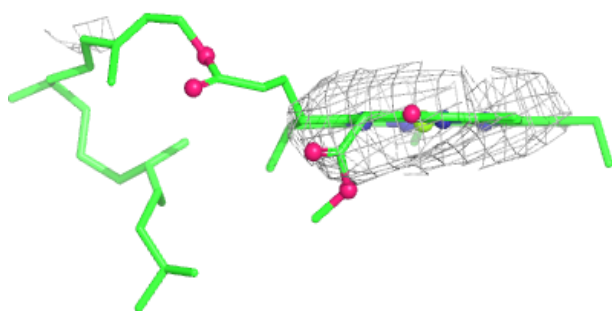
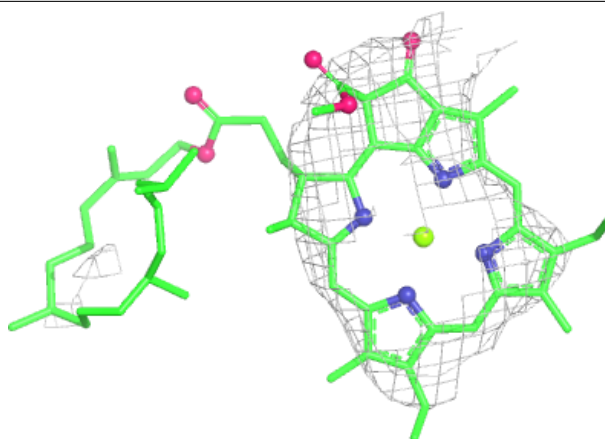
**Electron density around CLA B 604:**

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

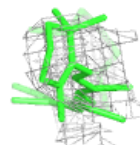
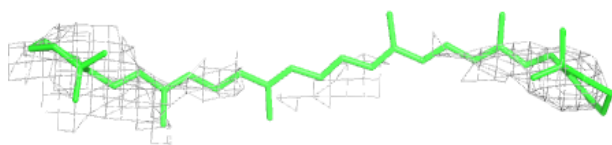
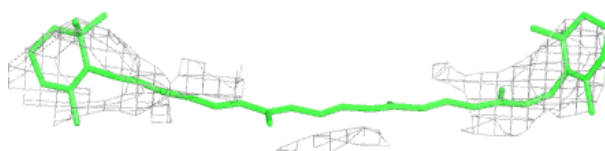


**Electron density around CLA C 511:**

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

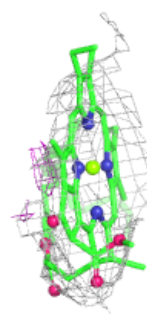
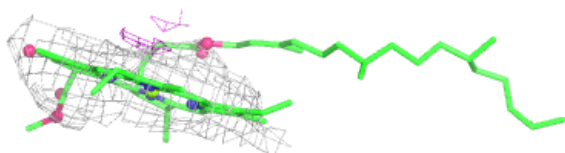
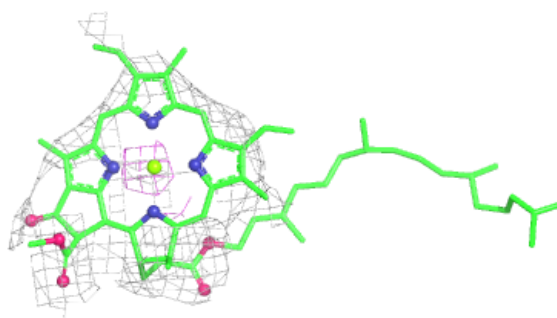
**Electron density around BCR C 513:**

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

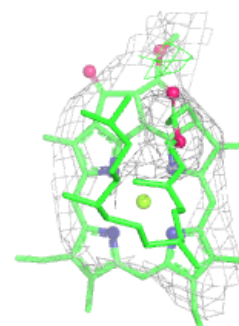
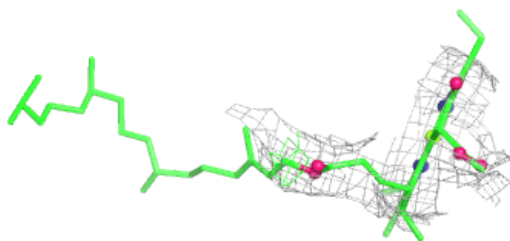
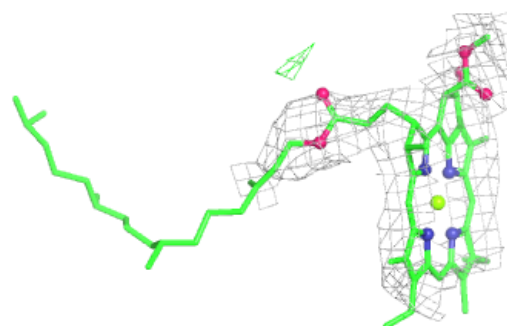


**Electron density around CLA B 602:**

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

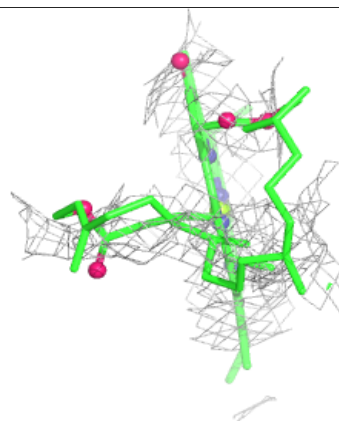
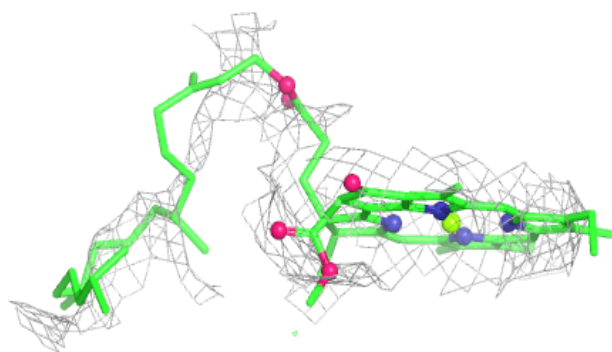
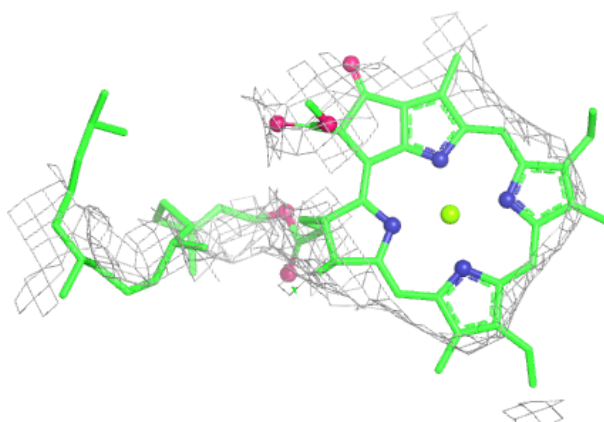
**Electron density around CLA d 406:**

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

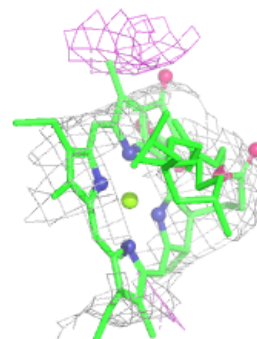
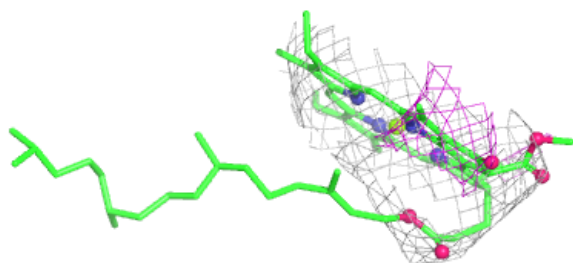
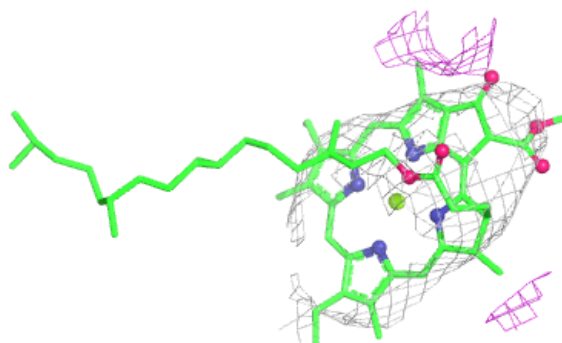


**Electron density around CLA b 615:**

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

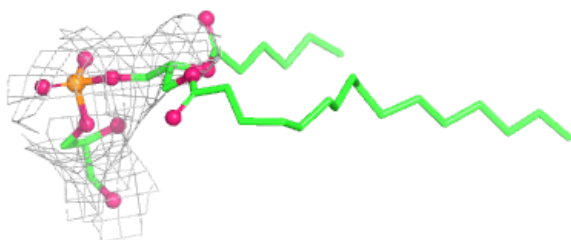
**Electron density around CLA b 617:**

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



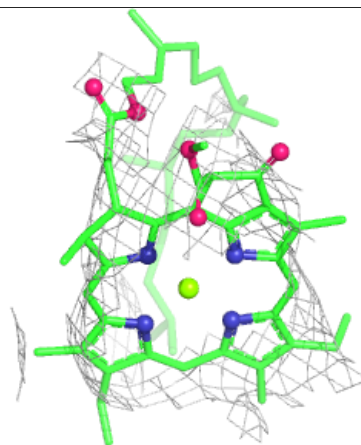
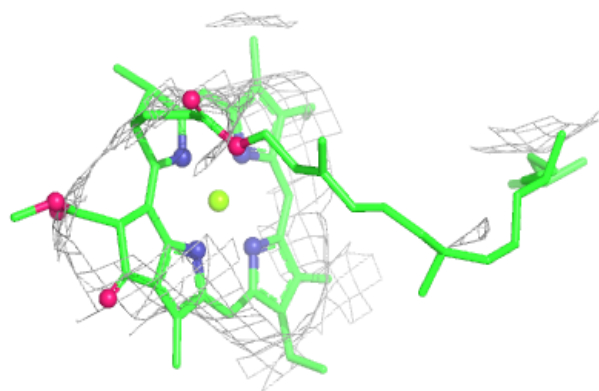
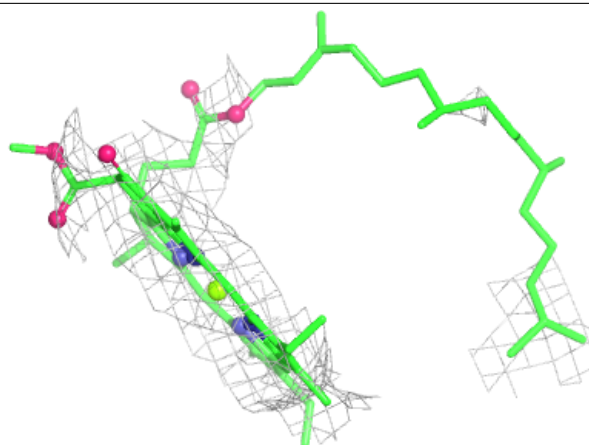
**Electron density around LHG a 411:**

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



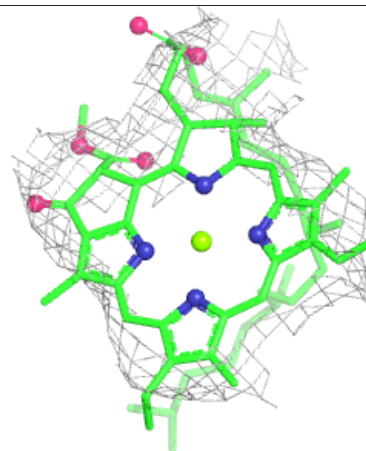
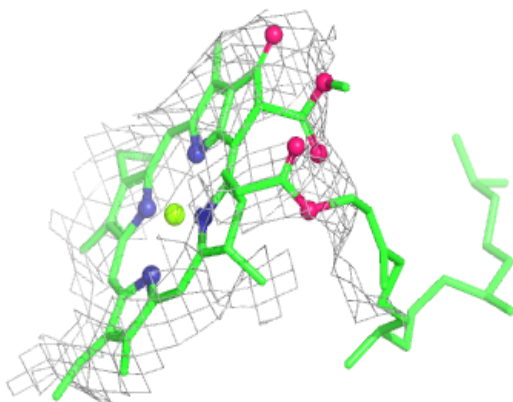
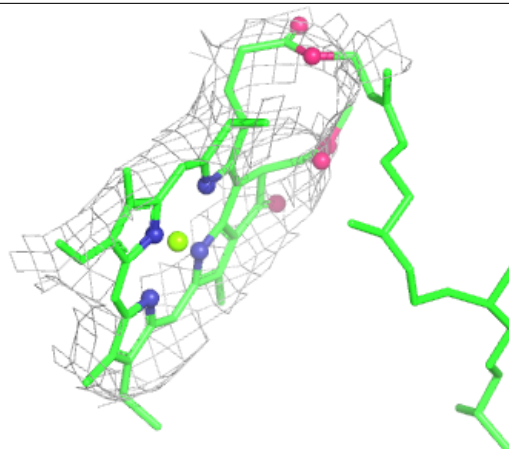
**Electron density around CLA B 610:**

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



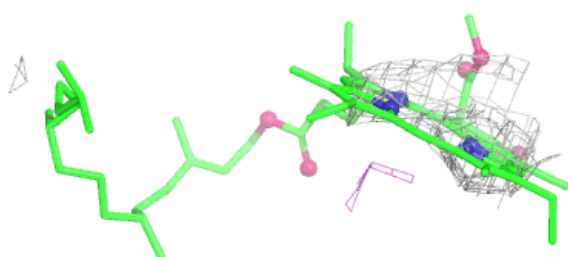
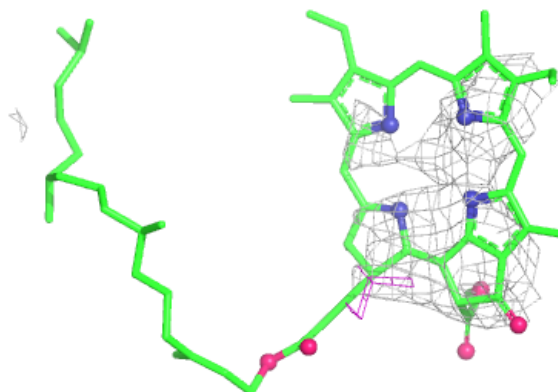
**Electron density around CLA B 612:**

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

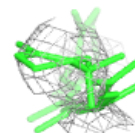
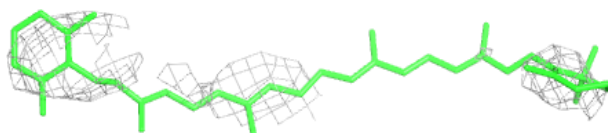
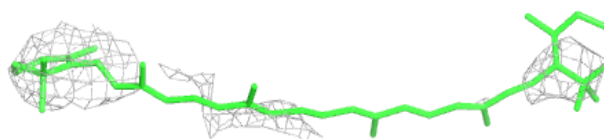


**Electron density around PHO d 402:**

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

**Electron density around BCR f 102:**

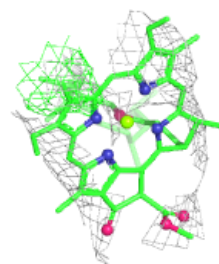
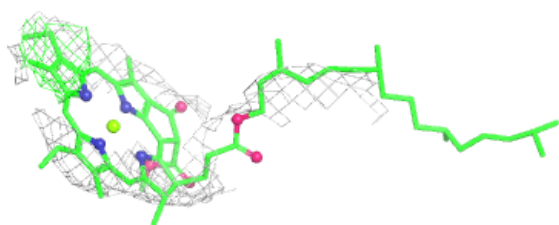
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



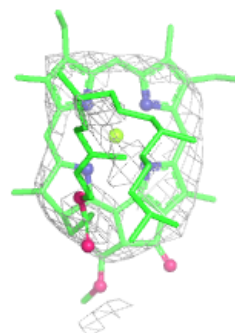
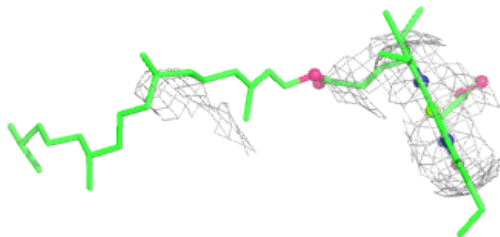
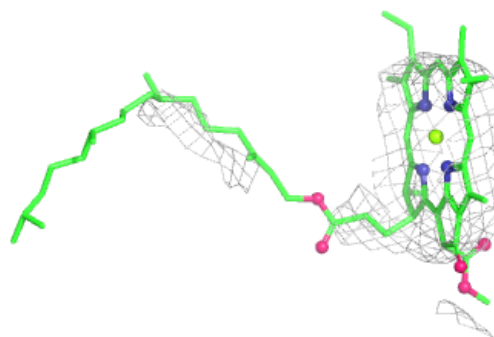


**Electron density around CLA C 502:**

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

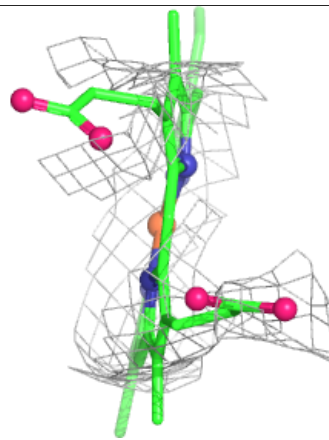
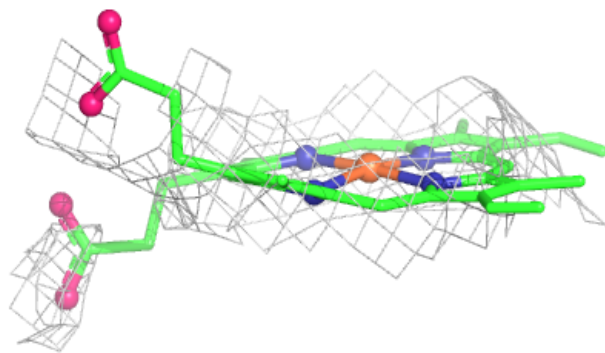
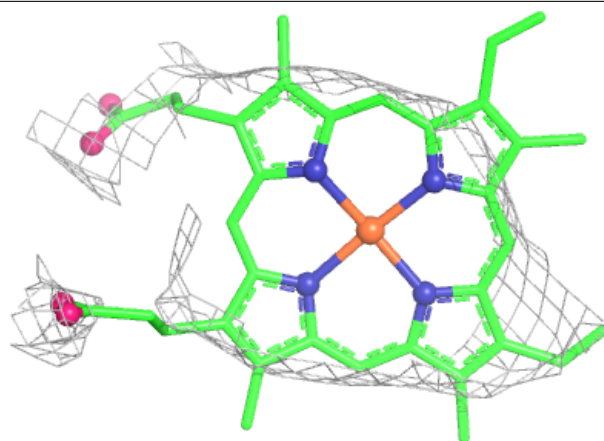
**Electron density around CLA D 406:**

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



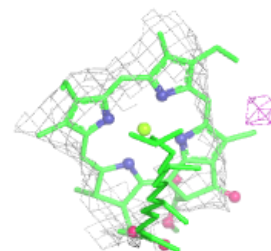
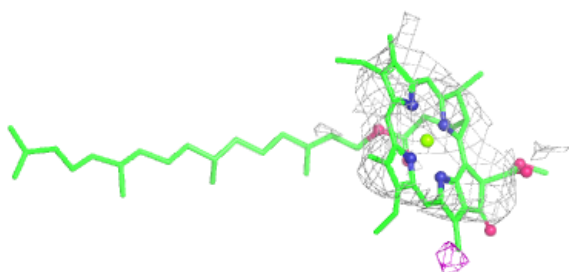
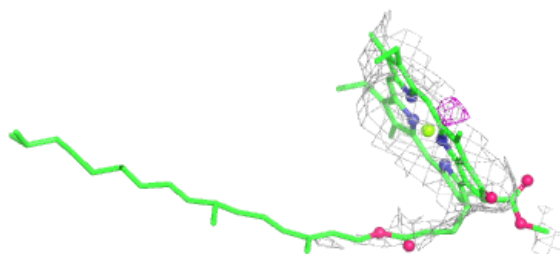
**Electron density around HEM f 101:**

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

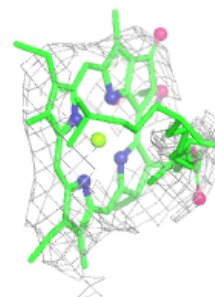
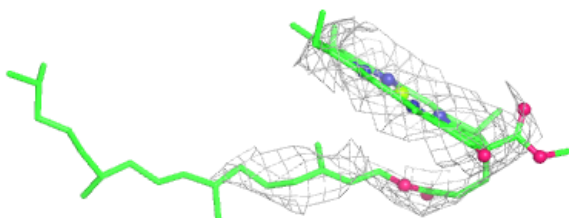
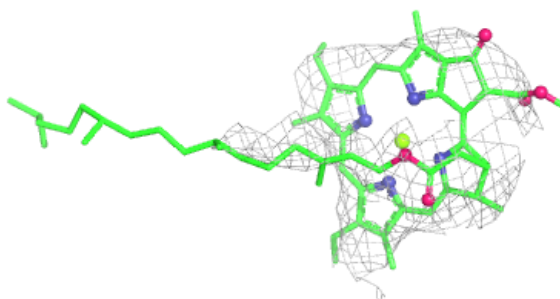


**Electron density around CLA b 610:**

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

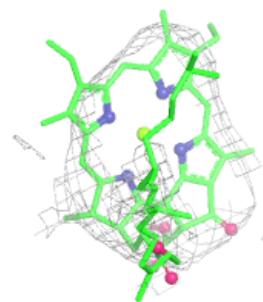
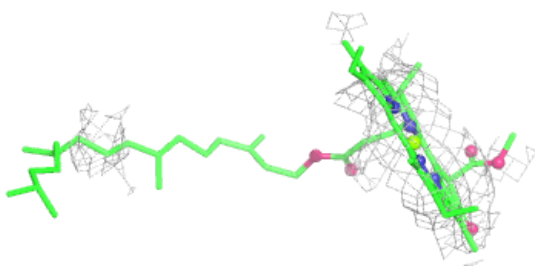
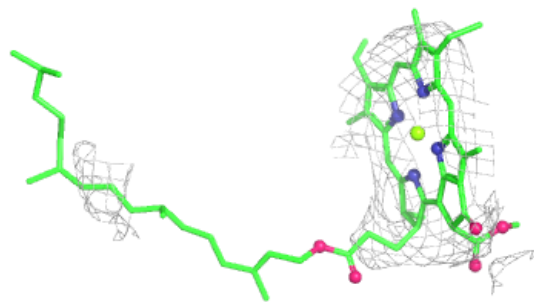
**Electron density around CLA b 611:**

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



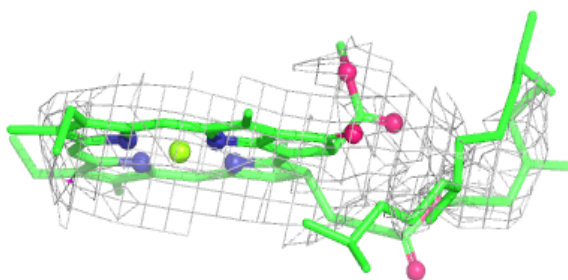
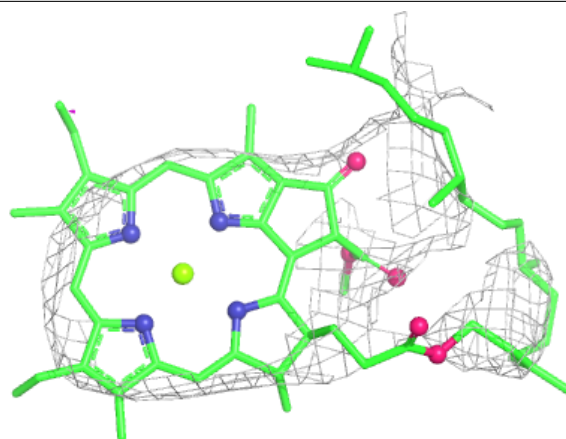
**Electron density around CLA b 612:**

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



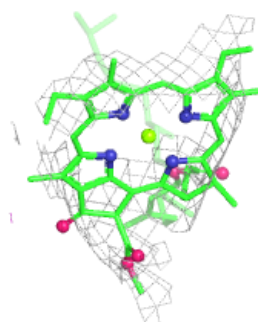
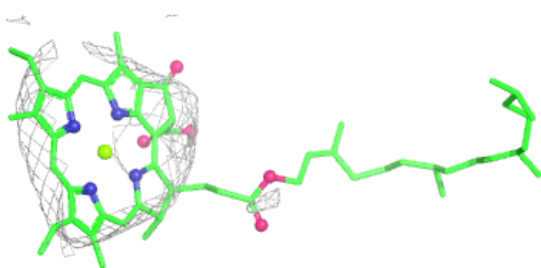
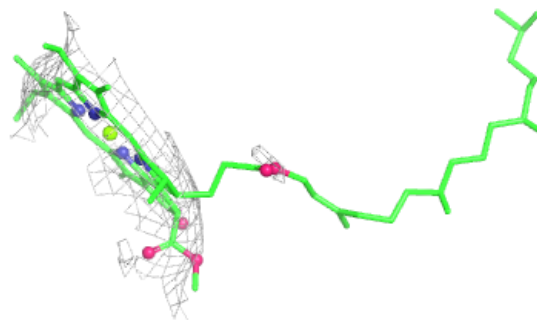
**Electron density around CLA B 609:**

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



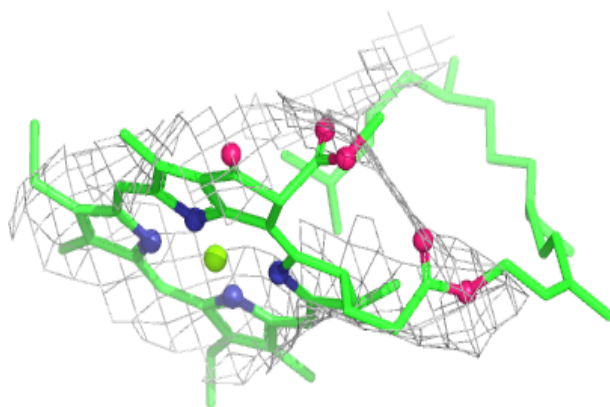
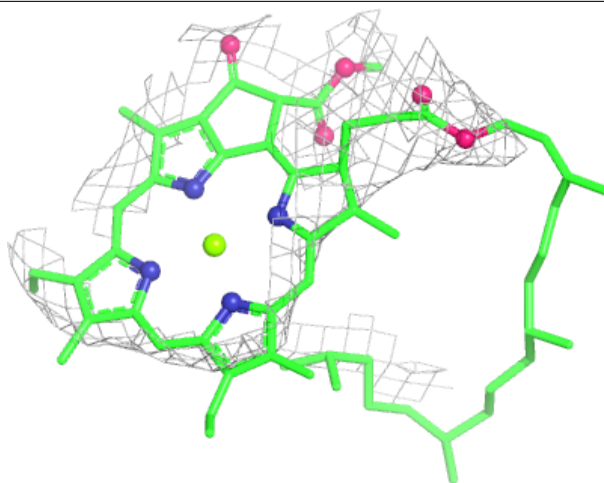
**Electron density around CLA d 405:**

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



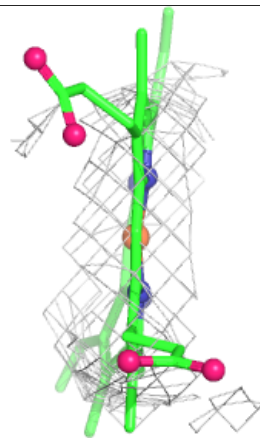
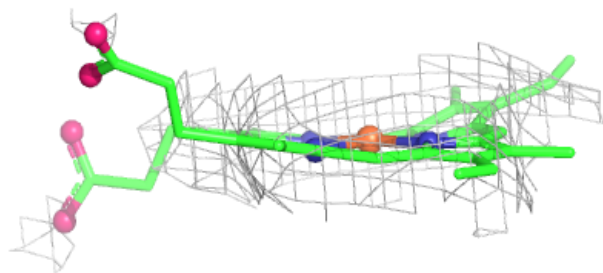
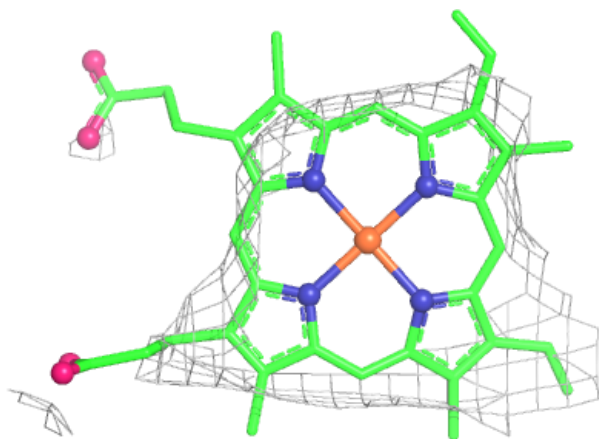
**Electron density around CLA B 614:**

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



**Electron density around HEM v 201:**

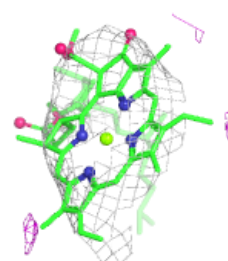
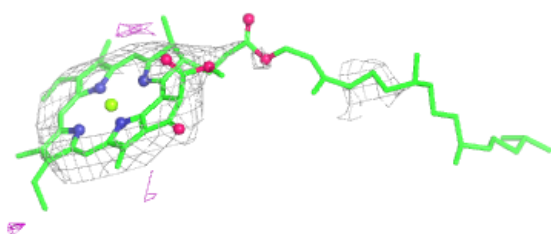
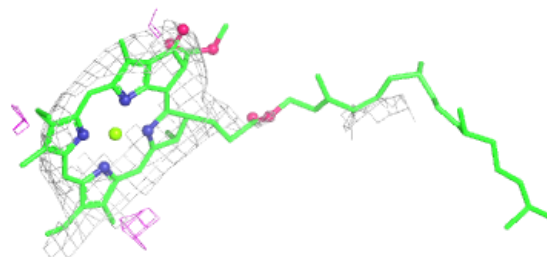
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



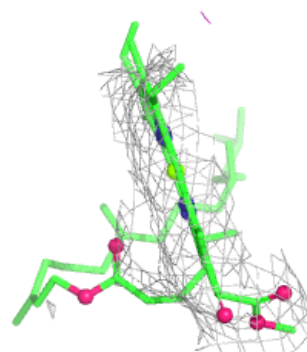
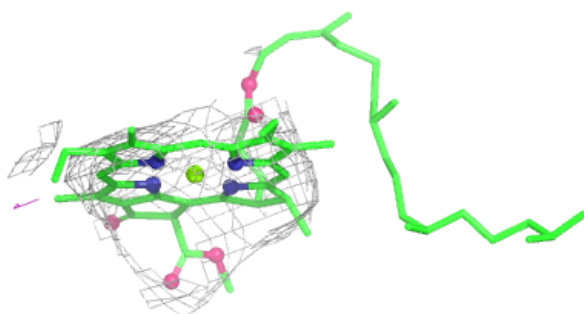
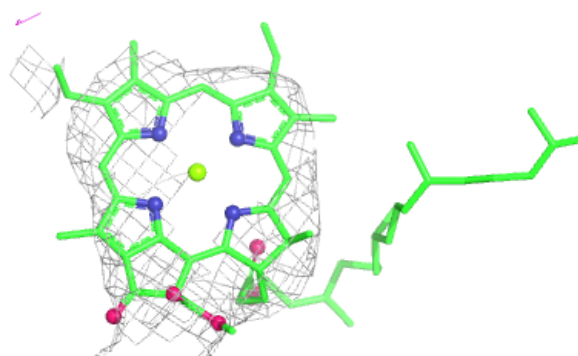


**Electron density around CLA A 402:**

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

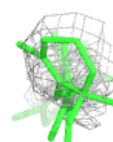
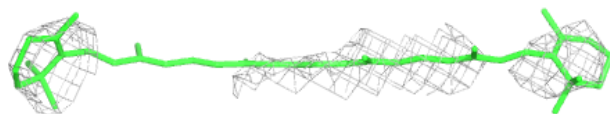
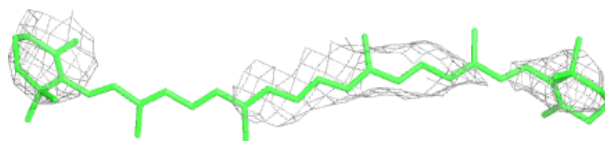
**Electron density around CLA A 403:**

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

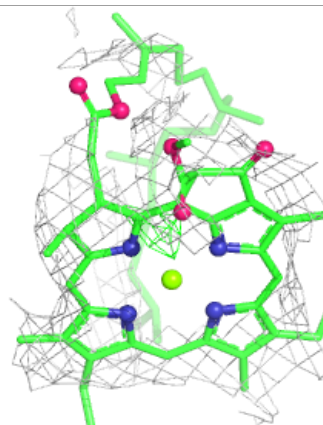
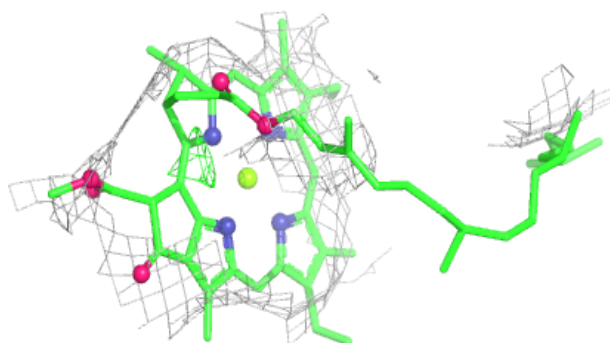
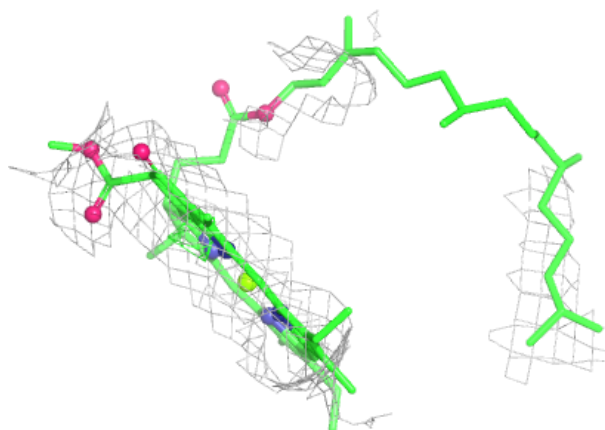


**Electron density around BCR B 618:**

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

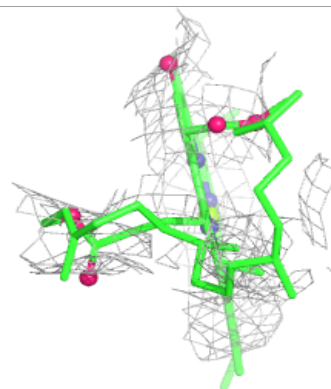
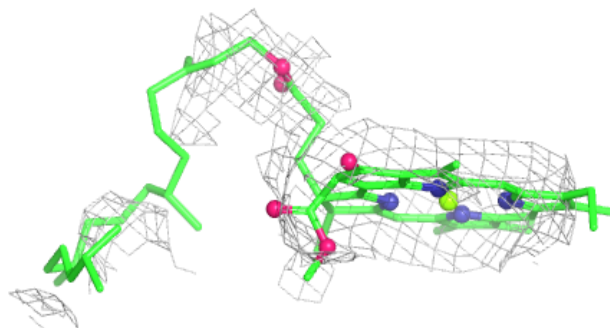
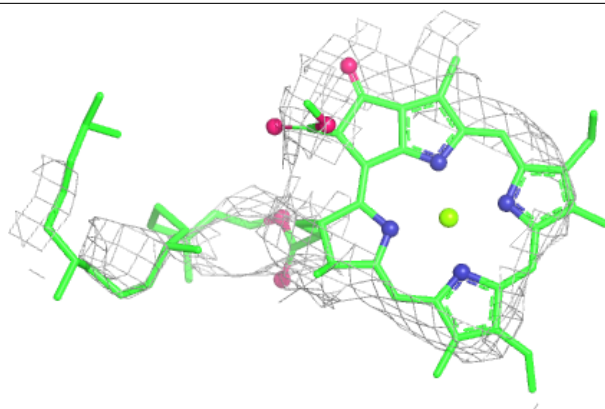
**Electron density around CLA b 614:**

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



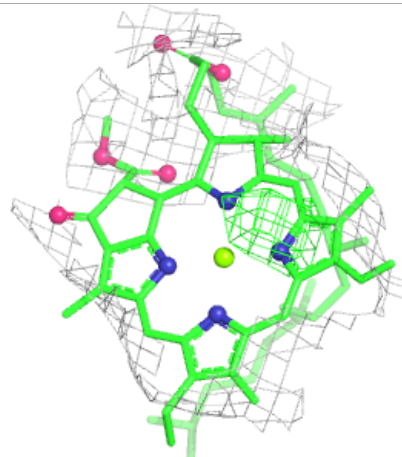
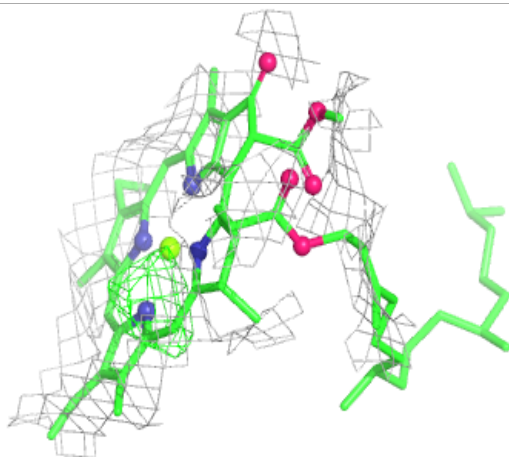
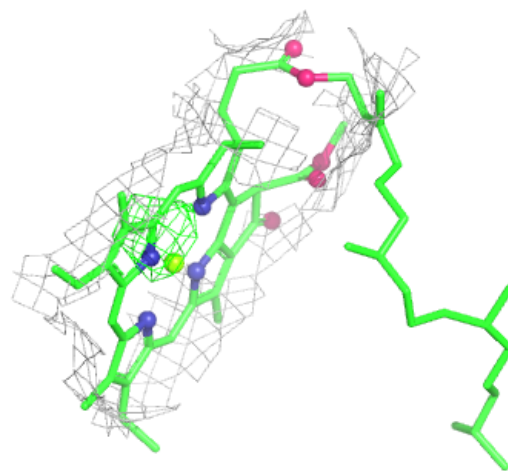
**Electron density around CLA B 611:**

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



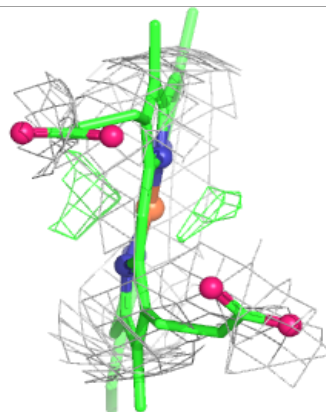
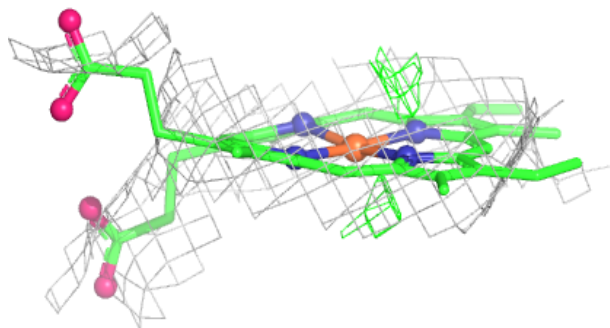
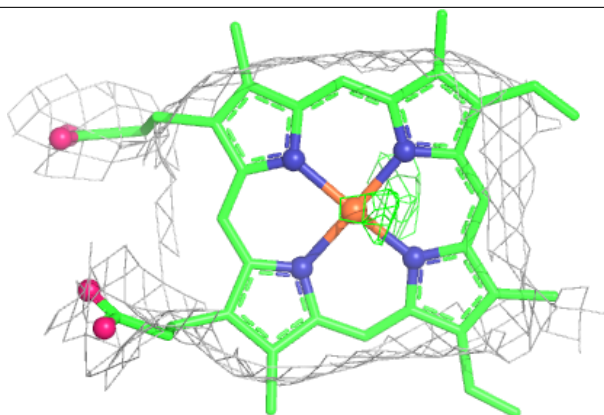
**Electron density around CLA b 616:**

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

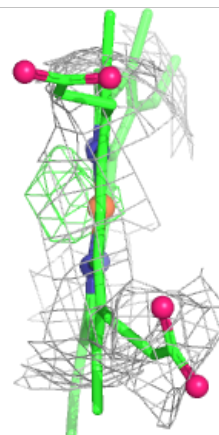
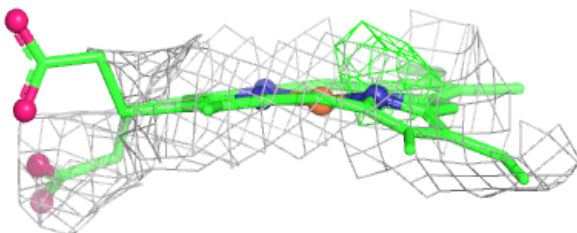
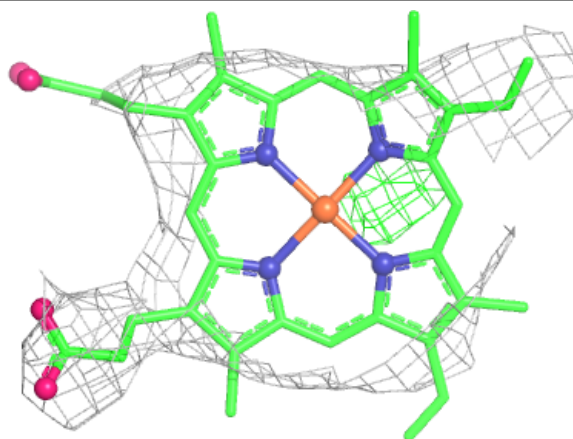


**Electron density around HEM F 101:**

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

**Electron density around HEM V 201:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.