



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 05:12 PM JST

PDB ID : 8GN0 / pdb\_00008gn0  
Title : Crystal structure of DCBQ-bound photosystem II complex  
Authors : Kamada, S.; Nakajima, Y.; Shen, J.-R.  
Deposited on : 2022-08-22  
Resolution : 2.15 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:

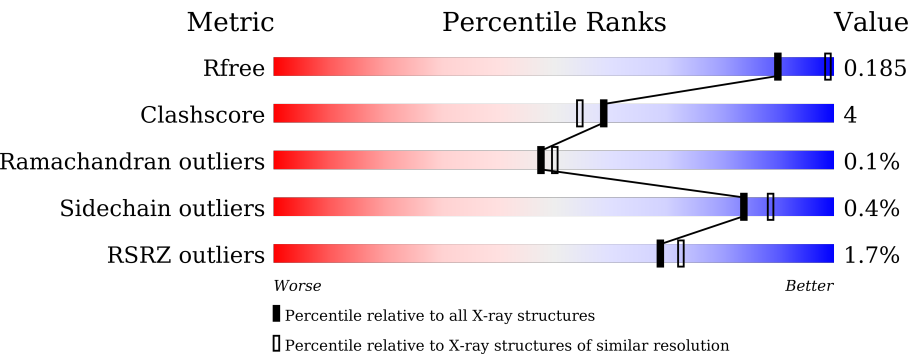
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.015 (Gargrove)  
Density-Fitness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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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                      | 2057 (2.16-2.16)                                      |
| Clashscore            | 190562                      | 2159 (2.16-2.16)                                      |
| Ramachandran outliers | 187476                      | 2134 (2.16-2.16)                                      |
| Sidechain outliers    | 187428                      | 2133 (2.16-2.16)                                      |
| RSRZ outliers         | 180081                      | 2059 (2.16-2.16)                                      |

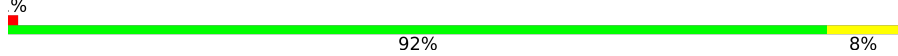
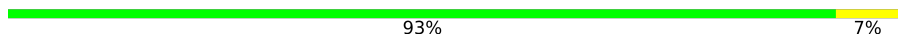
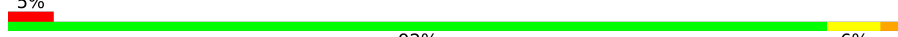
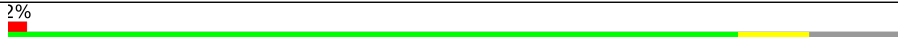
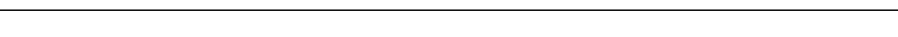
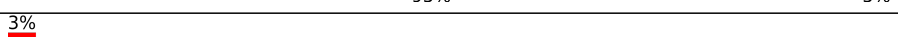
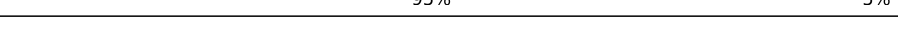
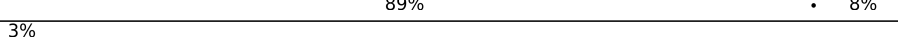
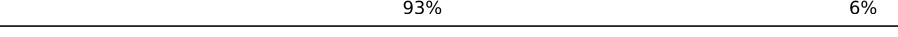
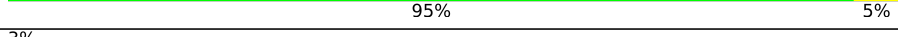
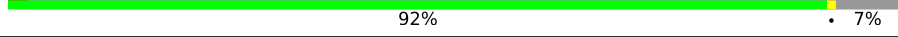
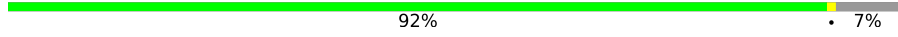
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 1   | A     | 344    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>88%9%</div></div> |
| 1   | a     | 344    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>90%7%</div></div> |
| 2   | B     | 505    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>94%6%</div></div> |
| 2   | b     | 505    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>86%9%</div></div> |
| 3   | C     | 455    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>92%7%</div></div> |
| 3   | c     | 455    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>92%8%</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D     | 342    |    |
| 4   | d     | 342    |    |
| 5   | E     | 83     |    |
| 5   | e     | 83     |    |
| 6   | F     | 44     |    |
| 6   | f     | 44     |    |
| 7   | H     | 63     |    |
| 7   | h     | 63     |    |
| 8   | I     | 38     |    |
| 8   | i     | 38     |    |
| 9   | J     | 40     |    |
| 9   | j     | 40     |    |
| 10  | K     | 37     |  |
| 10  | k     | 37     |  |
| 11  | L     | 37     |  |
| 11  | l     | 37     |  |
| 12  | M     | 36     |  |
| 12  | m     | 36     |  |
| 13  | O     | 244    |  |
| 13  | o     | 244    |  |
| 14  | T     | 32     |  |
| 14  | t     | 32     |  |
| 15  | U     | 104    |  |
| 15  | u     | 104    |  |
| 16  | V     | 137    |  |

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| Mol | Chain | Length | Quality of chain                                                    |
|-----|-------|--------|---------------------------------------------------------------------|
| 16  | v     | 137    | <div> <div></div> <div>96%</div> <div>.</div> </div>                |
| 17  | Y     | 30     | <div> <div></div> <div>100%</div> </div>                            |
| 17  | y     | 30     | <div> <div></div> <div>93%</div> <div>7%</div> </div>               |
| 18  | X     | 40     | <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> |
| 18  | x     | 40     | <div> <div></div> <div>88%</div> <div>12%</div> </div>              |
| 19  | Z     | 62     | <div> <div></div> <div>98%</div> <div>.</div> </div>                |
| 19  | z     | 62     | <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 31  | JOX  | a     | 2617 | -         | X        | -       | -                |
| 42  | HEC  | V     | 201  | X         | -        | -       | -                |
| 42  | HEC  | v     | 201  | X         | -        | -       | -                |

## 2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 53814 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 334      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2614  | 1715 | 428 | 456 | 15 |         |         |       |
| 1   | a     | 334      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2629  | 1722 | 432 | 460 | 15 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 279     | PRO      | ARG    | conflict | UNP P51765 |
| a     | 279     | PRO      | ARG    | conflict | UNP P51765 |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 505      | Total | C    | N   | O   | S  | 0       | 7       | 0     |
|     |       |          | 4005  | 2628 | 667 | 697 | 13 |         |         |       |
| 2   | b     | 483      | Total | C    | N   | O   | S  | 0       | 9       | 0     |
|     |       |          | 3833  | 2520 | 637 | 663 | 13 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 451      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 3494  | 2286 | 585 | 610 | 13 |         |         |       |
| 3   | c     | 455      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3518  | 2303 | 589 | 613 | 13 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 19      | ASN      | -      | expression tag | UNP D0VWR7 |
| C     | 20      | SER      | -      | expression tag | UNP D0VWR7 |

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 341      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 2726  | 1809 | 443 | 462 | 12 |         |         |       |
| 4   | d     | 342      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2738  | 1815 | 447 | 464 | 12 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 5   | E     | 80       | Total | C   | N   | O   |  | 0       | 1       | 0     |
|     |       |          | 643   | 422 | 101 | 120 |  |         |         |       |
| 5   | e     | 79       | Total | C   | N   | O   |  | 0       | 1       | 0     |
|     |       |          | 630   | 417 | 99  | 114 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | F     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 271   | 184 | 45 | 41 | 1 |         |         |       |
| 6   | f     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 255   | 173 | 43 | 38 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | H     | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 498   | 333 | 80 | 83 | 2 |         |         |       |
| 7   | h     | 63       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 506   | 338 | 83 | 83 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | I     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 256   | 177 | 37 | 41 | 1 |         |         |       |
| 8   | i     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 259   | 178 | 37 | 43 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | J     | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 251   | 171 | 37 | 42 | 1 |         |         |       |
| 9   | j     | 39       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 274   | 184 | 40 | 48 | 2 |         |         |       |

- 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       | 1       | 0     |
|     |       |          | 297   | 208 | 43 | 46 |         |         |       |
| 10  | k     | 37       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 289   | 201 | 42 | 46 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11  | L     | 37       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 303   | 204 | 45 | 53 | 1 |         |         |       |
| 11  | l     | 36       | Total | C   | N  | O  |   | 0       | 2       | 0     |
|     |       |          | 305   | 206 | 47 | 52 |   |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | M     | 33       | Total | C   | N  | O  | S | 0       | 2       | 0     |
|     |       |          | 267   | 180 | 38 | 48 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | m     | 34       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 270   | 182 | 39 | 48 | 1 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| M     | 8       | LEU      | PHE    | conflict | UNP P12312 |
| m     | 8       | LEU      | PHE    | conflict | UNP P12312 |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | O     | 244      | Total | C    | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1870  | 1171 | 314 | 380 | 5 |         |         |       |
| 13  | o     | 243      | Total | C    | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1874  | 1174 | 312 | 382 | 6 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 15  | U     | 97       | Total | C   | N   | O   |  | 0       | 1       | 0     |
|     |       |          | 776   | 493 | 130 | 153 |  |         |         |       |
| 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       | 1       | 0     |
|     |       |          | 1063  | 677 | 177 | 205 | 4 |         |         |       |
| 16  | v     | 137      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1058  | 671 | 175 | 208 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 17  | Y     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 218   | 144 | 35 | 36 | 3 |         |         |       |
| 17  | y     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 216   | 139 | 38 | 36 | 3 |         |         |       |

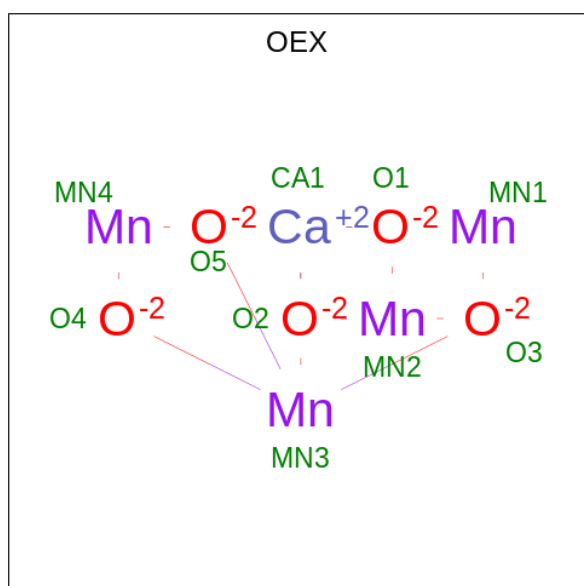
- Molecule 18 is a protein called Photosystem II reaction center protein X.

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 18  | X     | 38       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 275   | 185 | 44 | 46 |  |         |         |       |
| 18  | x     | 35       | Total | C   | N  | O  |  | 0       | 1       | 0     |
|     |       |          | 257   | 176 | 38 | 43 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 19  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 471   | 323 | 71 | 75 | 2 |         |         |       |
| 19  | z     | 61       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 456   | 312 | 70 | 72 | 2 |         |         |       |

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 20  | A     | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 20  | a     | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |

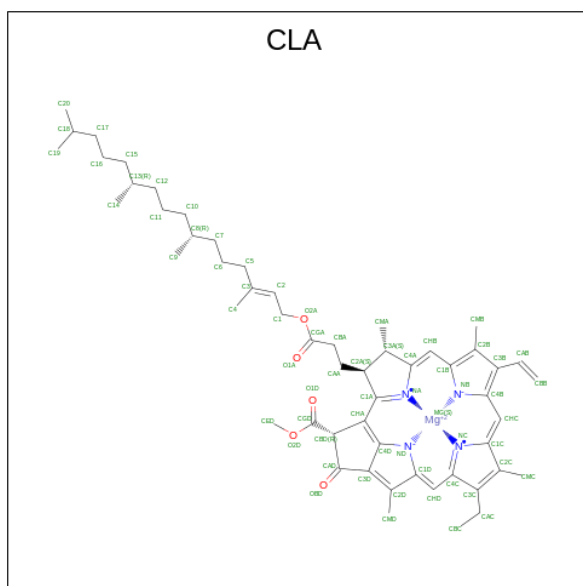
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| 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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    |  |  | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|--|--|---------|---------|
| 22  | A     | 2        | Total | Cl |  |  | 0       | 0       |
|     |       |          | 2     | 2  |  |  |         |         |
| 22  | a     | 2        | Total | Cl |  |  | 0       | 0       |
|     |       |          | 2     | 2  |  |  |         |         |

- Molecule 23 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 |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 23  | A     | 1        | Total | C  | Mg | N | O       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5       | 0       |
| 23  | A     | 1        | Total | C  | Mg | N | O       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5       | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 23  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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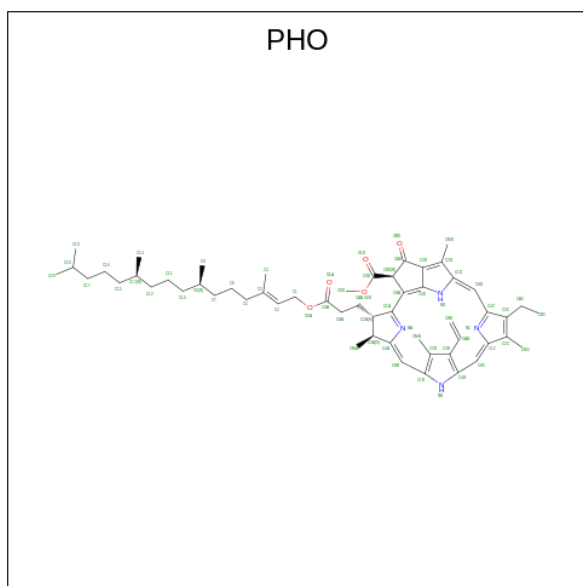
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 23  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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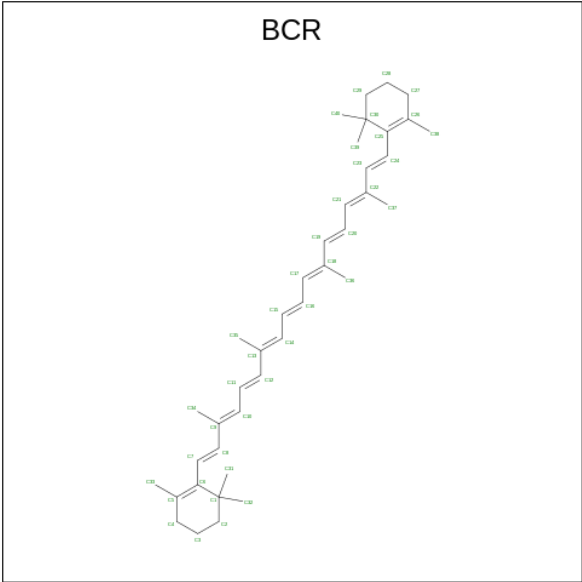
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 23  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 23  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 23  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 23  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 23  | d     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 24  | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 24  | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 24  | a     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 24  | a     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



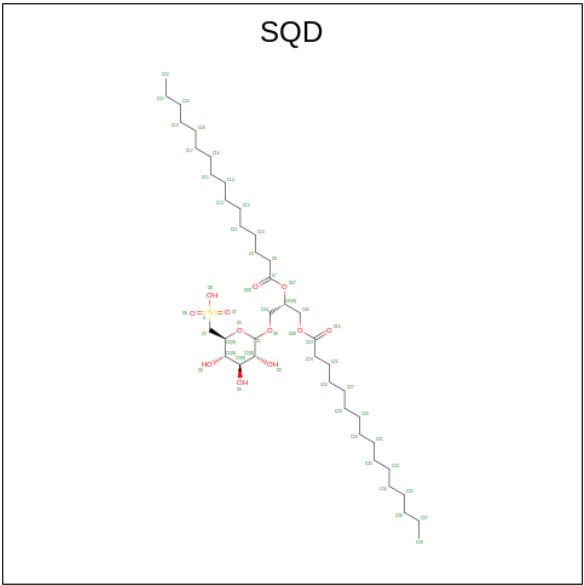
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 25  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | D     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | T     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | a     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | d     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | k     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | y     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | z     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



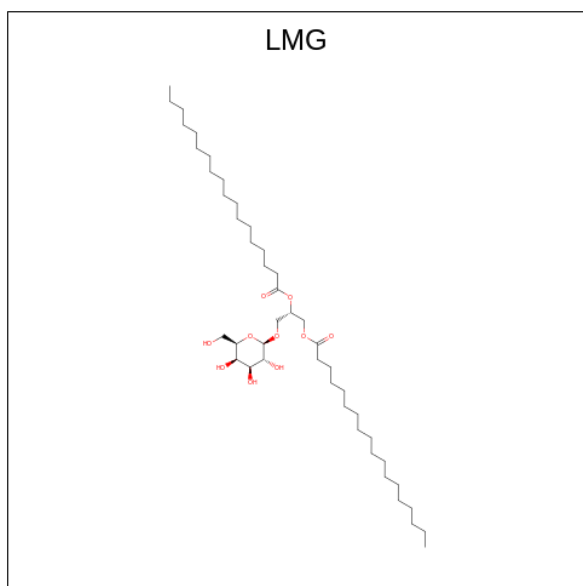
| Mol | Chain | Residues | Atoms                     | ZeroOcc | AltConf |
|-----|-------|----------|---------------------------|---------|---------|
| 26  | A     | 1        | Total C O S<br>46 33 12 1 | 0       | 0       |
| 26  | B     | 1        | Total C O S<br>54 41 12 1 | 0       | 0       |
| 26  | D     | 1        | Total C O S<br>54 41 12 1 | 0       | 0       |
| 26  | D     | 1        | Total C O S<br>45 32 12 1 | 0       | 0       |
| 26  | a     | 1        | Total C O S<br>54 41 12 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 48    | 35 | 12 | 1 |         |         |
| 26  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 48    | 35 | 12 | 1 |         |         |
| 26  | d     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 33    | 23 | 9  | 1 |         |         |
| 26  | l     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 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>).



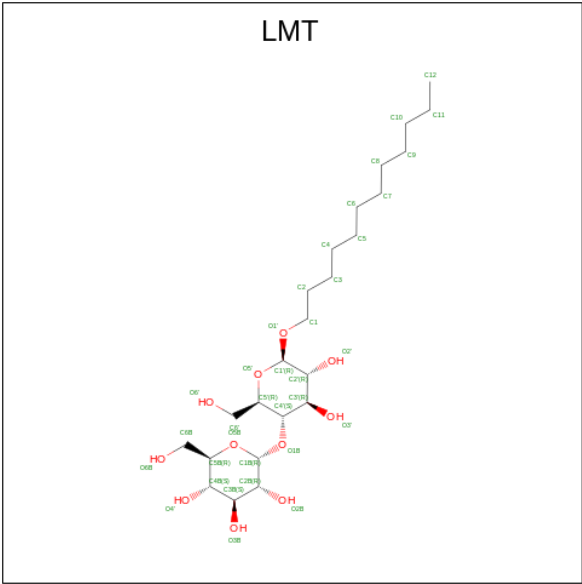
| Mol | Chain | Residues | Atoms |    |    |  | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|--|---------|---------|
| 27  | A     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |
| 27  | B     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |
| 27  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |
| 27  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |
| 27  | D     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 47    | 37 | 10 |  |         |         |
| 27  | c     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |  |         |         |
| 27  | c     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |  |         |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 27  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 27  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 27  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |

- Molecule 28 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 |
|-----|-------|----------|-------|----|----|---------|---------|
| 28  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 28  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 28  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 28  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 28  | F     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 28  | J     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 28  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 28  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

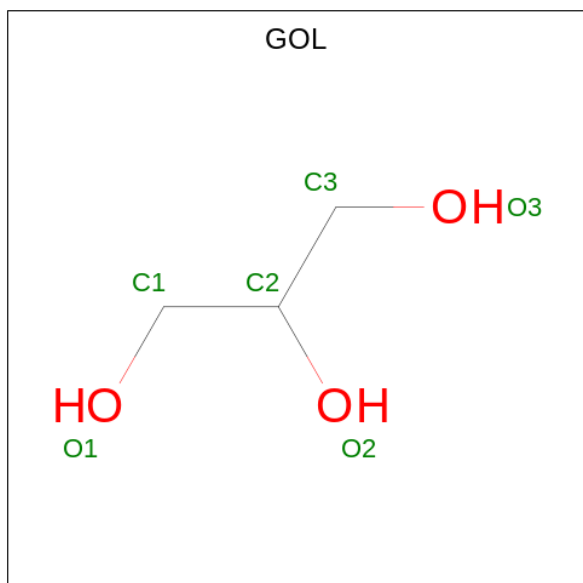
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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 28  | T     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 28  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 28  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 28  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 25    | 19 | 6  |         |         |
| 28  | f     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 28  | i     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 24    | 18 | 6  |         |         |
| 28  | j     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 34    | 23 | 11 |         |         |
| 28  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 28  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 28  | z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |

- Molecule 29 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 29  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 29  | A     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | B     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | B     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | B     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | D     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | E     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | J     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | O     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | O     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | O     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | O     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | U     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | U     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | V     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | a     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | a     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | b     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | b     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 29  | c     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 29  | c     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 29  | c     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 29  | d     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 29  | o     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 29  | u     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 29  | v     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 29  | v     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 29  | v     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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

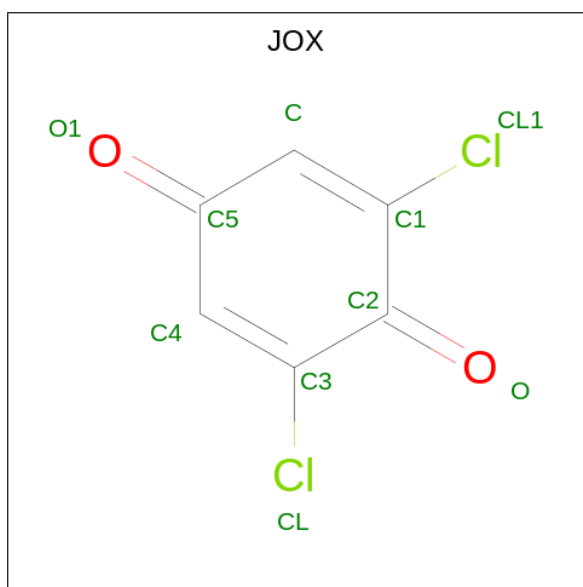
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 30  | A     | 2        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 32 | 5 |         |         |
| 30  | B     | 3        | Total | C  | O | 0       | 0       |
|     |       |          | 65    | 58 | 7 |         |         |
| 30  | C     | 2        | Total | C  | O | 0       | 0       |
|     |       |          | 50    | 45 | 5 |         |         |
| 30  | D     | 3        | Total | C  | O | 0       | 0       |
|     |       |          | 48    | 44 | 4 |         |         |
| 30  | E     | 2        | Total | C  |   | 0       | 0       |
|     |       |          | 15    | 15 |   |         |         |
| 30  | I     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 40    | 35 | 5 |         |         |
| 30  | J     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 5     | 5  |   |         |         |
| 30  | T     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 13    | 13 |   |         |         |
| 30  | Y     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 12    | 12 |   |         |         |
| 30  | a     | 2        | Total | C  | O | 0       | 0       |
|     |       |          | 42    | 37 | 5 |         |         |
| 30  | b     | 5        | Total | C  | O | 0       | 0       |
|     |       |          | 64    | 60 | 4 |         |         |

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| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 30  | c     | 4        | Total C O<br>59 54 5 | 0       | 0       |
| 30  | d     | 2        | Total C O<br>55 48 7 | 0       | 0       |
| 30  | e     | 1        | Total C<br>15 15     | 0       | 0       |
| 30  | i     | 1        | Total C O<br>19 15 4 | 0       | 0       |
| 30  | j     | 1        | Total C<br>16 16     | 0       | 0       |
| 30  | k     | 1        | Total C<br>16 16     | 0       | 0       |
| 30  | l     | 1        | Total C O<br>16 14 2 | 0       | 0       |
| 30  | m     | 1        | Total C O<br>15 13 2 | 0       | 0       |
| 30  | t     | 1        | Total C<br>8 8       | 0       | 0       |
| 30  | x     | 1        | Total C O<br>18 16 2 | 0       | 0       |

- Molecule 31 is 2,6-bis(chloranyl)cyclohexa-2,5-diene-1,4-dione (CCD ID: JOX) (formula:  $C_6H_2Cl_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



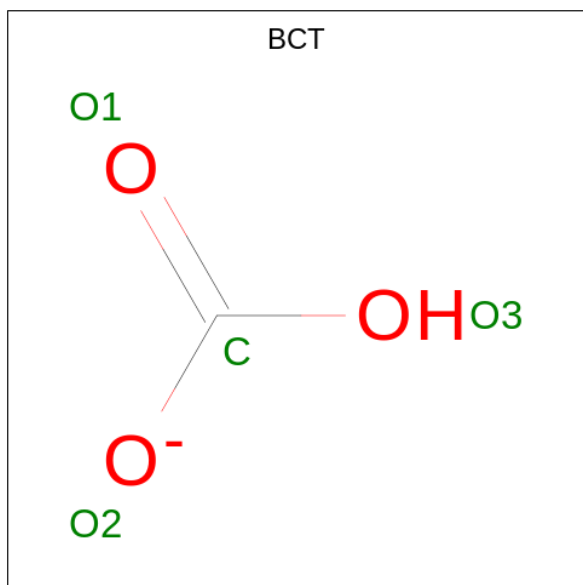
| Mol | Chain | Residues | Atoms                    | ZeroOcc | AltConf |
|-----|-------|----------|--------------------------|---------|---------|
| 31  | A     | 1        | Total C Cl O<br>10 6 2 2 | 0       | 0       |

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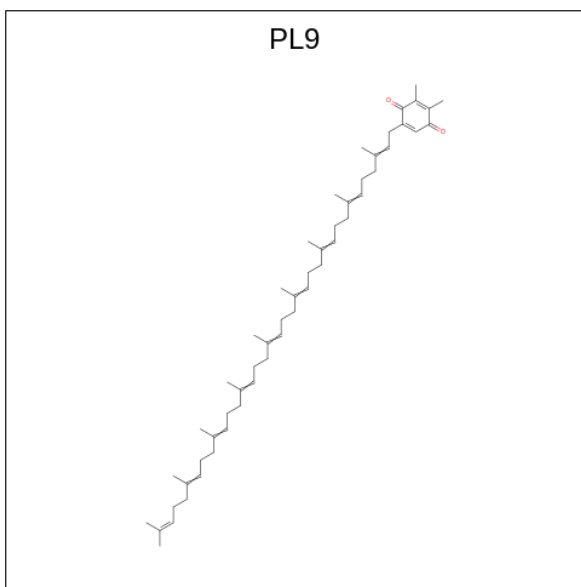
| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 31  | A     | 1        | Total | C | Cl | O | 0       | 0       |
|     |       |          | 10    | 6 | 2  | 2 |         |         |
| 31  | a     | 1        | Total | C | Cl | O | 0       | 0       |
|     |       |          | 10    | 6 | 2  | 2 |         |         |
| 31  | a     | 1        | Total | C | Cl | O | 0       | 0       |
|     |       |          | 10    | 6 | 2  | 2 |         |         |

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



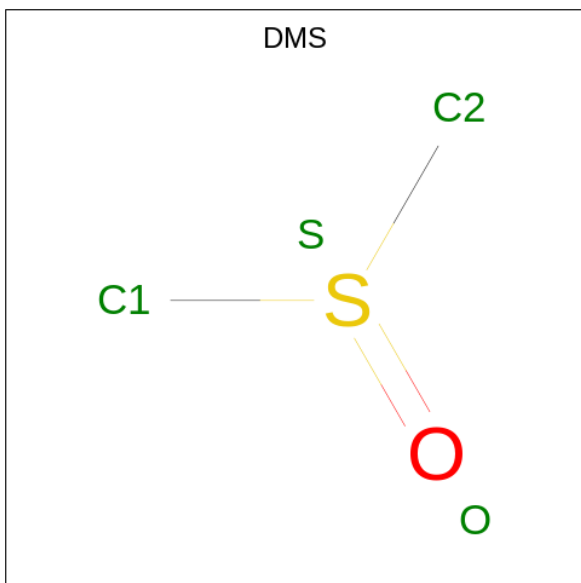
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 32  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 32  | a     | 1        | Total | C | O | 0    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

- Molecule 33 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:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 33  | A     | 1        | Total C<br>39 39     | 0       | 0       |
| 33  | D     | 1        | Total C O<br>55 53 2 | 0       | 0       |
| 33  | d     | 1        | Total C O<br>55 53 2 | 0       | 0       |
| 33  | x     | 1        | Total C<br>39 39     | 0       | 0       |

- Molecule 34 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula:  $C_2H_6OS$ ).



| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 34  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | A     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | B     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | C     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | D     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | H     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | O     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | T     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | T     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | U     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | U     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | U     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 34  | V     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | X     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | a     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | b     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | c     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | d     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 34  | l     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | o     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | t     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | u     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | u     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | u     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |
| 34  | v     | 1        | Total<br>4 | C<br>2 | O<br>1 | S<br>1 | 0       | 0       |

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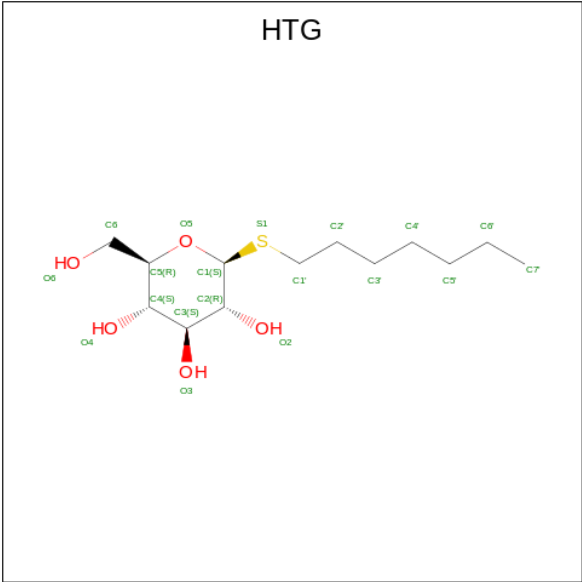
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| Mol | Chain | Residues | Atoms                  | ZeroOcc | AltConf |
|-----|-------|----------|------------------------|---------|---------|
| 34  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 34  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 34  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 34  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 34  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 34  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 34  | v     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |

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

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 35  | B     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 35  | O     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 35  | b     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 35  | c     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 35  | o     | 1        | Total Ca<br>1 1 | 0       | 0       |

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



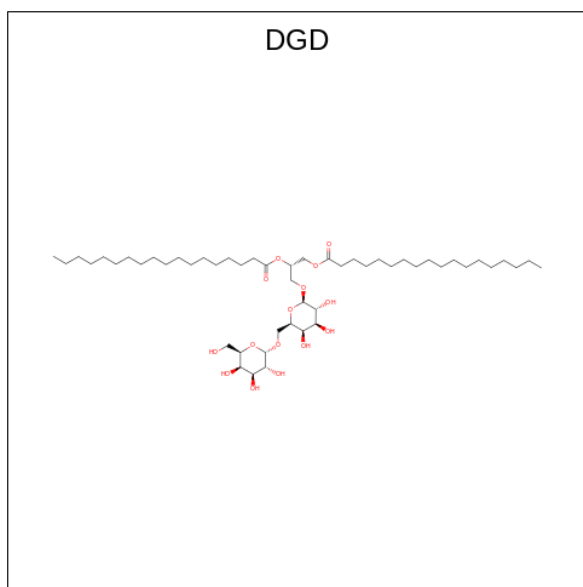
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 36  | B     | 1        | Total | C  | O  | S | 0       | 1       |
|     |       |          | 38    | 26 | 10 | 2 |         |         |
| 36  | B     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | B     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | B     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | C     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | C     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | C     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | H     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 17    | 12 | 4  | 1 |         |         |
| 36  | I     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | V     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |
| 36  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 19    | 13 | 5  | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 36  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 36  | c     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 36  | c     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 36  | c     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 36  | d     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 36  | d     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 36  | i     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 36  | o     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



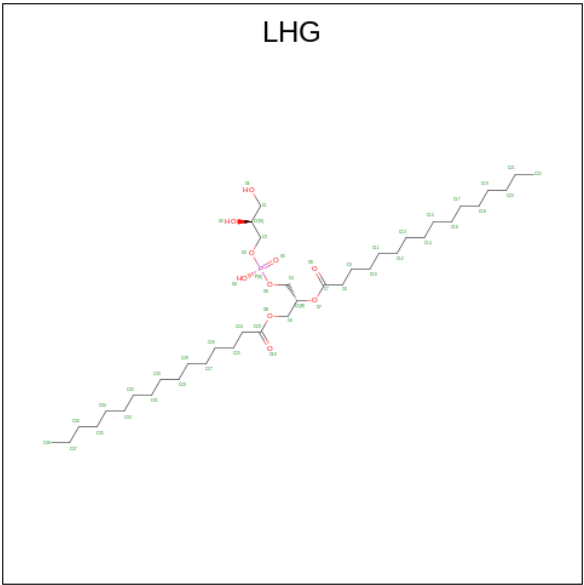
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 37  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 37  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 37  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 58    | 43 | 15 |         |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 37  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 53    | 42 | 11 |         |         |
| 37  | H     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 37  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 37  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 37  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 37  | h     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |

- Molecule 38 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 |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 38  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 38  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 38  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |         |
| 38  | E     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 40    | 29 | 10 | 1 |         |         |
| 38  | L     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |

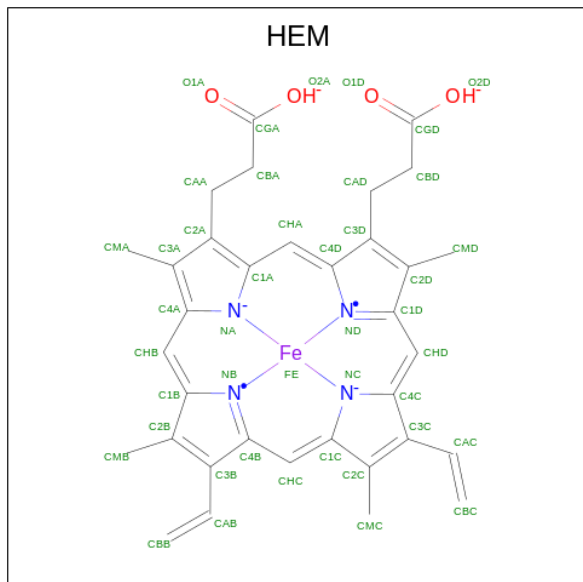
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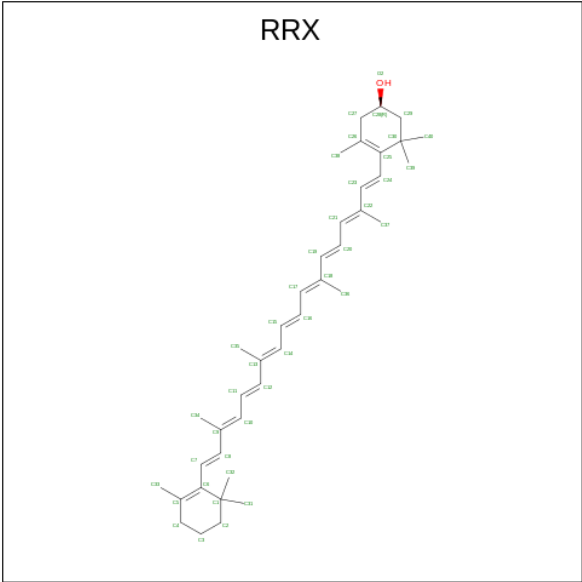
| Mol | Chain | Residues | Atoms       |         |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|
| 38  | d     | 1        | Total<br>43 | C<br>32 | O<br>10 | P<br>1 | 0       | 0       |
| 38  | d     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       | 0       |
| 38  | d     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       | 0       |
| 38  | e     | 1        | Total<br>40 | C<br>29 | O<br>10 | P<br>1 | 0       | 0       |
| 38  | l     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       | 0       |

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 39  | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 39  | e     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 40 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula:  $C_{40}H_{56}O$ ).

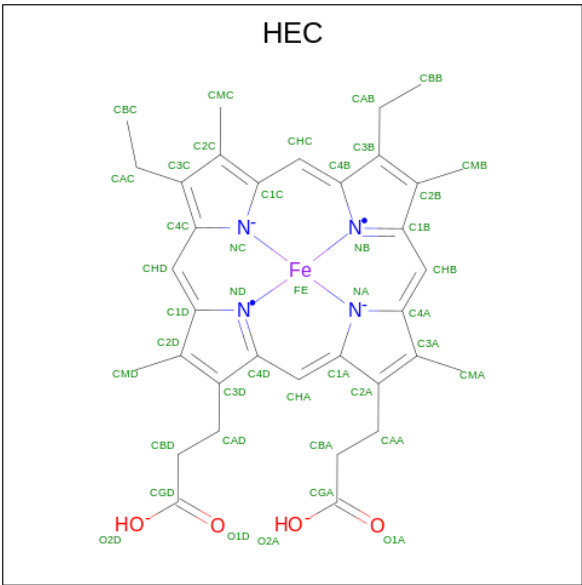


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 40  | H     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 41    | 40 | 1 |         |         |
| 40  | h     | 1        | Total | C  | O | 0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

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 41  | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 41  | K     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 41  | j     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 41  | k     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 42 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>36</sub>FeN<sub>4</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 42  | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 42  | v     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 43 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 43  | A     | 133      | Total | O   | 0       | 0       |
|     |       |          | 133   | 133 |         |         |
| 43  | B     | 302      | Total | O   | 0       | 0       |
|     |       |          | 302   | 302 |         |         |
| 43  | C     | 192      | Total | O   | 0       | 0       |
|     |       |          | 192   | 192 |         |         |
| 43  | D     | 146      | Total | O   | 0       | 1       |
|     |       |          | 147   | 147 |         |         |
| 43  | E     | 25       | Total | O   | 0       | 0       |
|     |       |          | 25    | 25  |         |         |
| 43  | F     | 9        | Total | O   | 0       | 0       |
|     |       |          | 9     | 9   |         |         |
| 43  | H     | 41       | Total | O   | 0       | 0       |
|     |       |          | 41    | 41  |         |         |
| 43  | I     | 8        | Total | O   | 0       | 0       |
|     |       |          | 8     | 8   |         |         |
| 43  | J     | 10       | Total | O   | 0       | 0       |
|     |       |          | 10    | 10  |         |         |
| 43  | K     | 10       | Total | O   | 0       | 0       |
|     |       |          | 10    | 10  |         |         |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 43  | L     | 15       | Total O<br>15 15   | 0       | 0       |
| 43  | M     | 12       | Total O<br>12 12   | 0       | 0       |
| 43  | O     | 144      | Total O<br>145 145 | 0       | 1       |
| 43  | T     | 12       | Total O<br>12 12   | 0       | 0       |
| 43  | U     | 79       | Total O<br>79 79   | 0       | 0       |
| 43  | V     | 113      | Total O<br>113 113 | 0       | 0       |
| 43  | Y     | 4        | Total O<br>4 4     | 0       | 0       |
| 43  | X     | 15       | Total O<br>15 15   | 0       | 0       |
| 43  | Z     | 8        | Total O<br>8 8     | 0       | 0       |
| 43  | a     | 122      | Total O<br>122 122 | 0       | 0       |
| 43  | b     | 250      | Total O<br>251 251 | 0       | 1       |
| 43  | c     | 211      | Total O<br>211 211 | 0       | 0       |
| 43  | d     | 146      | Total O<br>147 147 | 0       | 1       |
| 43  | e     | 19       | Total O<br>19 19   | 0       | 0       |
| 43  | f     | 7        | Total O<br>7 7     | 0       | 0       |
| 43  | h     | 27       | Total O<br>27 27   | 0       | 0       |
| 43  | i     | 8        | Total O<br>8 8     | 0       | 0       |
| 43  | j     | 10       | Total O<br>10 10   | 0       | 0       |
| 43  | k     | 5        | Total O<br>5 5     | 0       | 0       |
| 43  | l     | 20       | Total O<br>20 20   | 0       | 0       |
| 43  | m     | 11       | Total O<br>11 11   | 0       | 0       |

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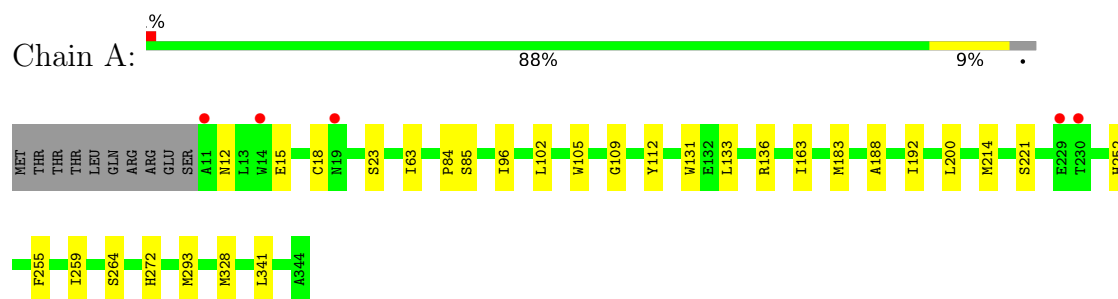
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 43  | o     | 143      | Total<br>144 | O<br>144 | 0       | 1       |
| 43  | t     | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 43  | u     | 78       | Total<br>78  | O<br>78  | 0       | 0       |
| 43  | v     | 93       | Total<br>93  | O<br>93  | 0       | 0       |
| 43  | y     | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 43  | x     | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 43  | z     | 6        | Total<br>6   | O<br>6   | 0       | 0       |

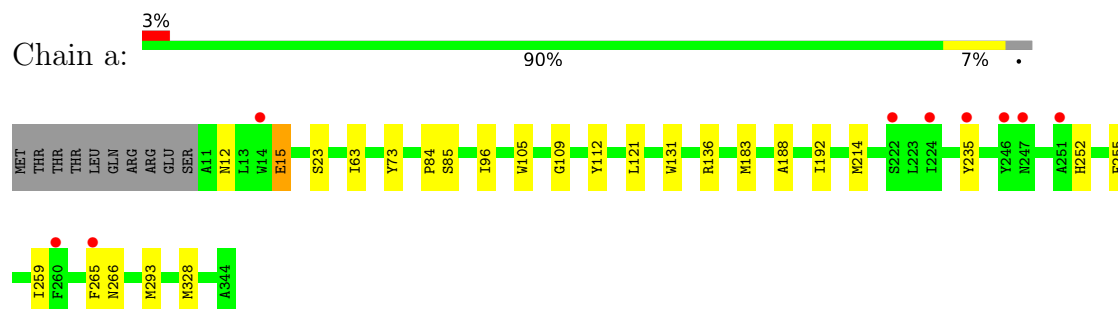
### 3 Residue-property plots [i](#)

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

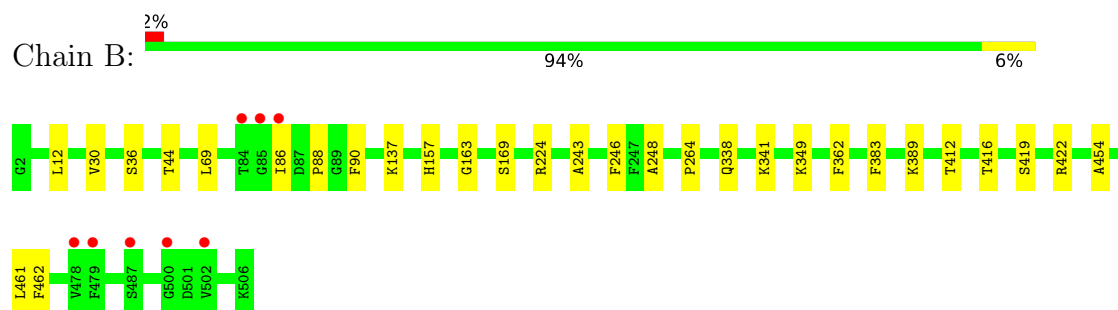
- Molecule 1: Photosystem II protein D1



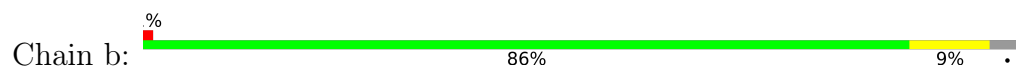
- Molecule 1: Photosystem II protein D1

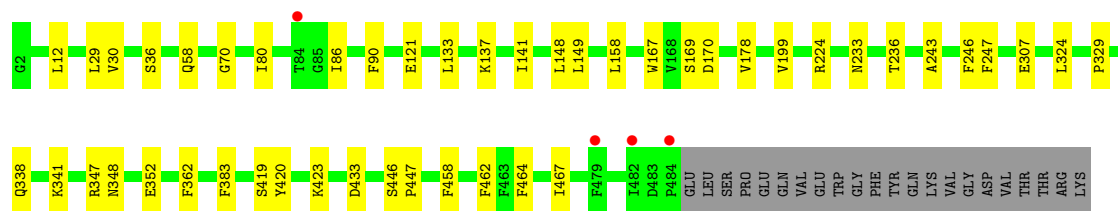


- Molecule 2: Photosystem II CP47 reaction center protein

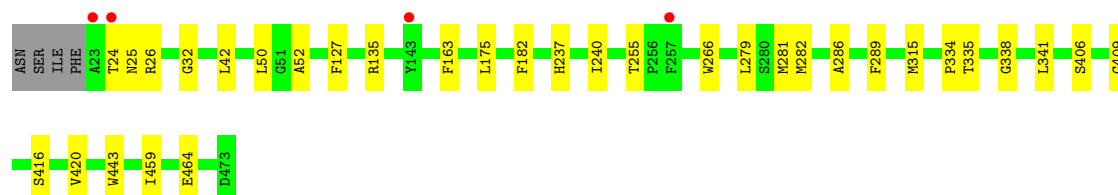
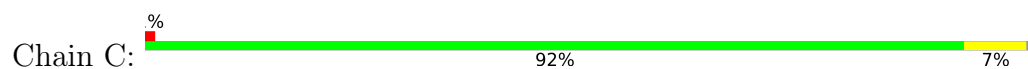


- Molecule 2: Photosystem II CP47 reaction center protein

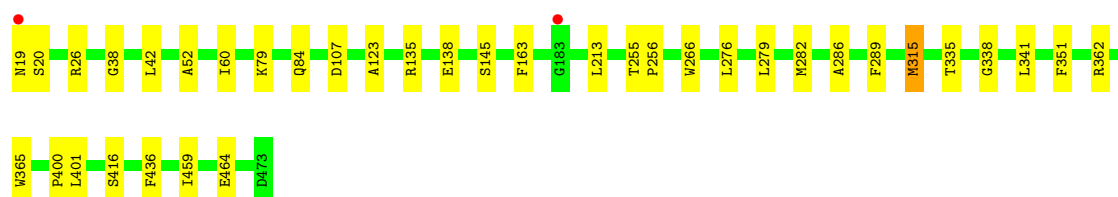
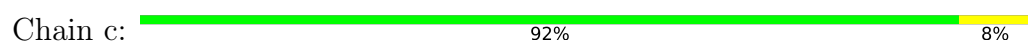




• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein



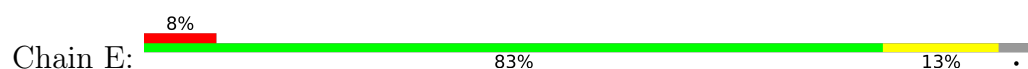
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein

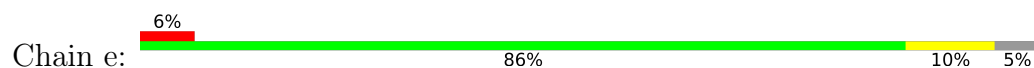


• Molecule 5: Cytochrome b559 subunit alpha

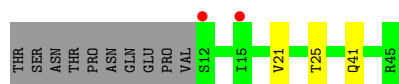




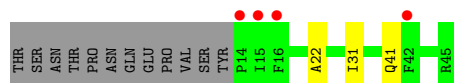
- Molecule 5: Cytochrome b559 subunit alpha



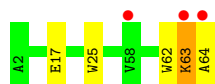
- Molecule 6: Cytochrome b559 subunit beta



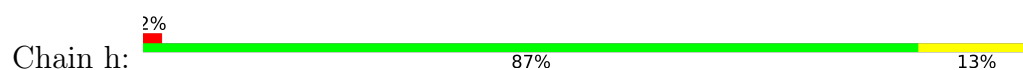
- Molecule 6: Cytochrome b559 subunit beta



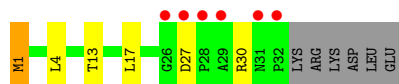
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

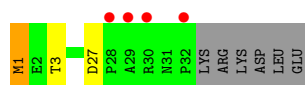
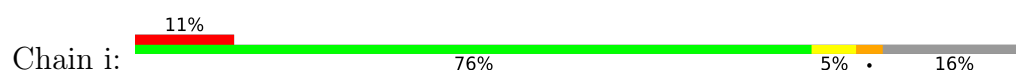


- Molecule 8: Photosystem II reaction center protein I

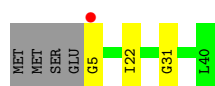
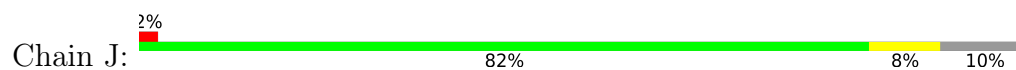


- Molecule 8: Photosystem II reaction center protein I

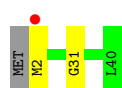
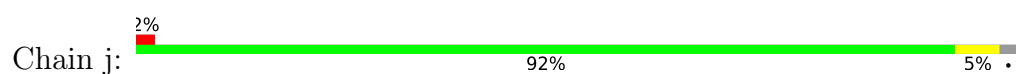




- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

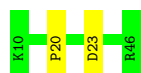


- Molecule 10: Photosystem II reaction center protein K

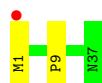


There are no outlier residues recorded for this chain.

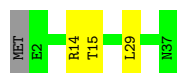
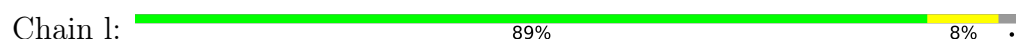
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



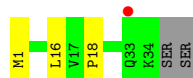
- Molecule 12: Photosystem II reaction center protein M

Chain M:  89% 8%

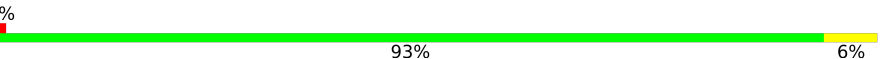


- Molecule 12: Photosystem II reaction center protein M

Chain m:  3% 86% 8% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  0% 93% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  95% 5%



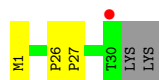
- Molecule 14: Photosystem II reaction center protein T

Chain T:  3% 81% 12% 6%

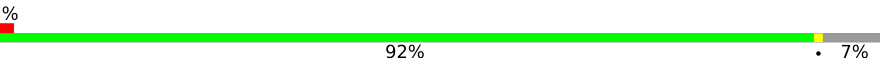


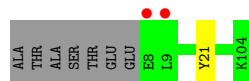
- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 84% 9% 6%



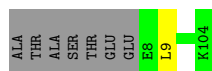
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  2% 92% 7%

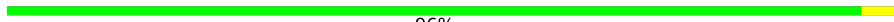


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  92% 7%

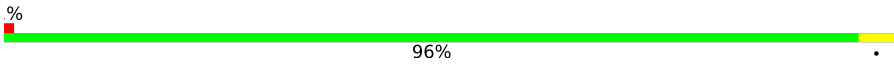


- Molecule 16: Cytochrome c-550

Chain V:  96%

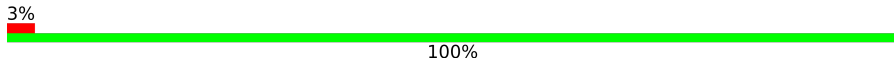


- Molecule 16: Cytochrome c-550

Chain v:  96%

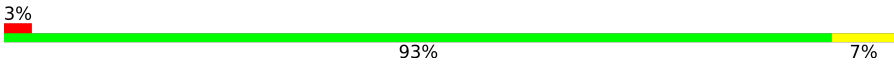


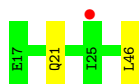
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  100%

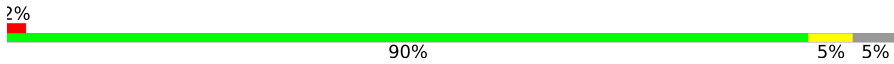


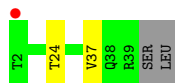
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  93% 7%



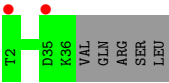
- Molecule 18: Photosystem II reaction center protein X

Chain X:  90% 5% 5%



- Molecule 18: Photosystem II reaction center protein X

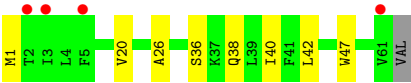
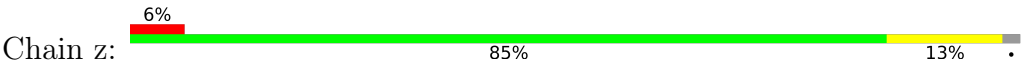
Chain x:  88% 12%



● Molecule 19: Photosystem II reaction center protein Z



● Molecule 19: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 121.22Å 228.21Å 287.00Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.00 – 2.15<br>49.00 – 2.15                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (49.00-2.15)<br>91.1 (49.00-2.15)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.06 (at 1.90Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.17.1 _3660                                         | Depositor        |
| R, $R_{free}$                                                           | 0.151 , 0.185<br>0.153 , 0.185                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 21442 reflections (3.43%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 37.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.401                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 69.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 53814                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 64.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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: RRX, BCR, SQD, OEX, HEM, CA, HEC, LHG, CLA, LMT, GOL, CL, PL9, BCT, HSK, FME, PHO, MG, JOX, HTG, UNL, LMG, DGD, FE2, DMS

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     | 0.37         | 0/2708  | 0.51        | 0/3695  |
| 1   | a     | 0.35         | 0/2725  | 0.53        | 0/3716  |
| 2   | B     | 0.35         | 0/4163  | 0.48        | 0/5672  |
| 2   | b     | 0.33         | 0/3994  | 0.48        | 0/5442  |
| 3   | C     | 0.29         | 0/3613  | 0.45        | 0/4919  |
| 3   | c     | 0.29         | 0/3632  | 0.46        | 0/4945  |
| 4   | D     | 0.37         | 0/2804  | 0.49        | 0/3820  |
| 4   | d     | 0.35         | 0/2819  | 0.47        | 0/3840  |
| 5   | E     | 0.23         | 0/665   | 0.41        | 0/911   |
| 5   | e     | 0.23         | 0/652   | 0.43        | 0/893   |
| 6   | F     | 0.23         | 0/280   | 0.43        | 0/382   |
| 6   | f     | 0.24         | 0/262   | 0.42        | 0/356   |
| 7   | H     | 0.25         | 0/511   | 0.41        | 0/697   |
| 7   | h     | 0.24         | 0/522   | 0.41        | 0/711   |
| 8   | I     | 0.21         | 0/253   | 0.37        | 0/345   |
| 8   | i     | 0.21         | 0/256   | 0.36        | 0/349   |
| 9   | J     | 0.25         | 0/257   | 0.37        | 0/349   |
| 9   | j     | 0.24         | 0/280   | 0.37        | 0/379   |
| 10  | K     | 0.23         | 0/310   | 0.39        | 0/426   |
| 10  | k     | 0.29         | 0/299   | 0.42        | 0/412   |
| 11  | L     | 0.41         | 0/313   | 0.41        | 0/426   |
| 11  | l     | 0.36         | 0/318   | 0.47        | 0/433   |
| 12  | M     | 0.31         | 0/266   | 0.47        | 0/364   |
| 12  | m     | 0.36         | 0/266   | 0.49        | 0/363   |
| 13  | O     | 0.31         | 0/1910  | 0.50        | 0/2592  |
| 13  | o     | 0.30         | 0/1917  | 0.50        | 0/2599  |
| 14  | T     | 0.36         | 0/257   | 0.41        | 0/349   |
| 14  | t     | 0.36         | 0/257   | 0.44        | 0/349   |
| 15  | U     | 0.34         | 0/790   | 0.48        | 0/1071  |
| 15  | u     | 0.33         | 0/785   | 0.50        | 0/1064  |
| 16  | V     | 0.32         | 0/1087  | 0.46        | 0/1475  |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 16  | v     | 0.27         | 0/1082  | 0.43        | 0/1472  |
| 17  | Y     | 0.20         | 0/219   | 0.32        | 0/293   |
| 17  | y     | 0.18         | 0/217   | 0.32        | 0/290   |
| 18  | X     | 0.18         | 0/278   | 0.29        | 0/376   |
| 18  | x     | 0.17         | 0/263   | 0.27        | 0/356   |
| 19  | Z     | 0.18         | 0/472   | 0.37        | 0/646   |
| 19  | z     | 0.18         | 0/457   | 0.36        | 0/626   |
| All | All   | 0.32         | 0/42159 | 0.47        | 0/57403 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2614  | 0        | 2510     | 21      | 0            |
| 1   | a     | 2629  | 0        | 2537     | 18      | 0            |
| 2   | B     | 4005  | 0        | 3863     | 26      | 0            |
| 2   | b     | 3833  | 0        | 3711     | 39      | 0            |
| 3   | C     | 3494  | 0        | 3418     | 24      | 0            |
| 3   | c     | 3518  | 0        | 3434     | 30      | 0            |
| 4   | D     | 2726  | 0        | 2629     | 22      | 0            |
| 4   | d     | 2738  | 0        | 2643     | 20      | 0            |
| 5   | E     | 643   | 0        | 618      | 8       | 0            |
| 5   | e     | 630   | 0        | 607      | 7       | 0            |
| 6   | F     | 271   | 0        | 270      | 2       | 0            |
| 6   | f     | 255   | 0        | 263      | 3       | 0            |
| 7   | H     | 498   | 0        | 518      | 7       | 0            |
| 7   | h     | 506   | 0        | 531      | 8       | 0            |
| 8   | I     | 256   | 0        | 266      | 6       | 0            |
| 8   | i     | 259   | 0        | 268      | 3       | 0            |
| 9   | J     | 251   | 0        | 257      | 3       | 0            |
| 9   | j     | 274   | 0        | 277      | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | K     | 297   | 0        | 314      | 0       | 0            |
| 10  | k     | 289   | 0        | 294      | 2       | 0            |
| 11  | L     | 303   | 0        | 316      | 2       | 0            |
| 11  | l     | 305   | 0        | 324      | 3       | 0            |
| 12  | M     | 267   | 0        | 288      | 1       | 0            |
| 12  | m     | 270   | 0        | 293      | 2       | 0            |
| 13  | O     | 1870  | 0        | 1843     | 13      | 0            |
| 13  | o     | 1874  | 0        | 1852     | 9       | 0            |
| 14  | T     | 258   | 0        | 261      | 2       | 0            |
| 14  | t     | 258   | 0        | 261      | 1       | 0            |
| 15  | U     | 776   | 0        | 777      | 1       | 0            |
| 15  | u     | 774   | 0        | 773      | 0       | 0            |
| 16  | V     | 1063  | 0        | 1078     | 4       | 0            |
| 16  | v     | 1058  | 0        | 1053     | 3       | 0            |
| 17  | Y     | 218   | 0        | 238      | 0       | 0            |
| 17  | y     | 216   | 0        | 227      | 3       | 0            |
| 18  | X     | 275   | 0        | 301      | 2       | 0            |
| 18  | x     | 257   | 0        | 288      | 0       | 0            |
| 19  | Z     | 471   | 0        | 498      | 0       | 0            |
| 19  | z     | 456   | 0        | 468      | 7       | 0            |
| 20  | A     | 10    | 0        | 0        | 0       | 0            |
| 20  | a     | 10    | 0        | 0        | 0       | 0            |
| 21  | A     | 1     | 0        | 0        | 0       | 0            |
| 21  | a     | 1     | 0        | 0        | 0       | 0            |
| 22  | A     | 2     | 0        | 0        | 0       | 0            |
| 22  | a     | 2     | 0        | 0        | 0       | 0            |
| 23  | A     | 260   | 0        | 288      | 10      | 0            |
| 23  | B     | 1040  | 0        | 1152     | 23      | 0            |
| 23  | C     | 845   | 0        | 936      | 40      | 0            |
| 23  | D     | 130   | 0        | 144      | 4       | 0            |
| 23  | a     | 195   | 0        | 216      | 6       | 0            |
| 23  | b     | 1040  | 0        | 1152     | 27      | 0            |
| 23  | c     | 845   | 0        | 936      | 31      | 0            |
| 23  | d     | 195   | 0        | 216      | 6       | 0            |
| 24  | A     | 128   | 0        | 148      | 4       | 0            |
| 24  | a     | 128   | 0        | 148      | 2       | 0            |
| 25  | A     | 40    | 0        | 56       | 0       | 0            |
| 25  | B     | 160   | 0        | 224      | 9       | 0            |
| 25  | C     | 80    | 0        | 112      | 5       | 0            |
| 25  | D     | 40    | 0        | 56       | 2       | 0            |
| 25  | K     | 40    | 0        | 56       | 1       | 0            |
| 25  | T     | 40    | 0        | 56       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25  | Y     | 40    | 0        | 56       | 2       | 0            |
| 25  | a     | 40    | 0        | 56       | 2       | 0            |
| 25  | b     | 120   | 0        | 168      | 7       | 0            |
| 25  | c     | 40    | 0        | 56       | 2       | 0            |
| 25  | d     | 40    | 0        | 56       | 2       | 0            |
| 25  | k     | 40    | 0        | 56       | 1       | 0            |
| 25  | y     | 40    | 0        | 56       | 2       | 0            |
| 25  | z     | 40    | 0        | 56       | 2       | 0            |
| 26  | A     | 46    | 0        | 59       | 2       | 0            |
| 26  | B     | 54    | 0        | 78       | 2       | 0            |
| 26  | D     | 99    | 0        | 135      | 4       | 0            |
| 26  | a     | 102   | 0        | 138      | 3       | 0            |
| 26  | b     | 48    | 0        | 63       | 1       | 0            |
| 26  | d     | 33    | 0        | 39       | 2       | 0            |
| 26  | l     | 54    | 0        | 78       | 4       | 0            |
| 27  | A     | 51    | 0        | 72       | 3       | 0            |
| 27  | B     | 51    | 0        | 72       | 1       | 0            |
| 27  | C     | 102   | 0        | 144      | 2       | 0            |
| 27  | D     | 47    | 0        | 64       | 2       | 0            |
| 27  | c     | 151   | 0        | 212      | 9       | 0            |
| 27  | d     | 51    | 0        | 72       | 4       | 0            |
| 27  | m     | 51    | 0        | 72       | 1       | 0            |
| 28  | A     | 57    | 0        | 74       | 9       | 0            |
| 28  | B     | 70    | 0        | 92       | 2       | 0            |
| 28  | F     | 24    | 0        | 35       | 0       | 0            |
| 28  | J     | 24    | 0        | 35       | 0       | 0            |
| 28  | M     | 70    | 0        | 92       | 1       | 0            |
| 28  | T     | 24    | 0        | 35       | 0       | 0            |
| 28  | Z     | 35    | 0        | 46       | 2       | 0            |
| 28  | d     | 60    | 0        | 81       | 7       | 0            |
| 28  | f     | 24    | 0        | 35       | 0       | 0            |
| 28  | i     | 24    | 0        | 35       | 1       | 0            |
| 28  | j     | 34    | 0        | 40       | 1       | 0            |
| 28  | m     | 70    | 0        | 92       | 1       | 0            |
| 28  | z     | 33    | 0        | 35       | 4       | 0            |
| 29  | A     | 12    | 0        | 16       | 0       | 0            |
| 29  | B     | 18    | 0        | 24       | 5       | 0            |
| 29  | C     | 12    | 0        | 16       | 2       | 0            |
| 29  | D     | 6     | 0        | 8        | 0       | 0            |
| 29  | E     | 6     | 0        | 8        | 0       | 0            |
| 29  | J     | 6     | 0        | 8        | 0       | 0            |
| 29  | O     | 24    | 0        | 32       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | U     | 12    | 0        | 15       | 0       | 0            |
| 29  | V     | 6     | 0        | 8        | 0       | 0            |
| 29  | a     | 12    | 0        | 16       | 1       | 0            |
| 29  | b     | 12    | 0        | 16       | 4       | 0            |
| 29  | c     | 18    | 0        | 24       | 1       | 0            |
| 29  | d     | 6     | 0        | 8        | 0       | 0            |
| 29  | o     | 6     | 0        | 8        | 0       | 0            |
| 29  | u     | 6     | 0        | 8        | 0       | 0            |
| 29  | v     | 18    | 0        | 24       | 0       | 0            |
| 30  | A     | 37    | 0        | 0        | 0       | 0            |
| 30  | B     | 65    | 0        | 0        | 0       | 0            |
| 30  | C     | 50    | 0        | 0        | 0       | 0            |
| 30  | D     | 48    | 0        | 0        | 0       | 0            |
| 30  | E     | 15    | 0        | 0        | 0       | 0            |
| 30  | I     | 40    | 0        | 0        | 0       | 0            |
| 30  | J     | 5     | 0        | 0        | 0       | 0            |
| 30  | T     | 13    | 0        | 0        | 0       | 0            |
| 30  | Y     | 12    | 0        | 0        | 0       | 0            |
| 30  | a     | 42    | 0        | 0        | 0       | 0            |
| 30  | b     | 64    | 0        | 0        | 0       | 0            |
| 30  | c     | 59    | 0        | 0        | 0       | 0            |
| 30  | d     | 55    | 0        | 0        | 0       | 0            |
| 30  | e     | 15    | 0        | 0        | 0       | 0            |
| 30  | i     | 19    | 0        | 0        | 0       | 0            |
| 30  | j     | 16    | 0        | 0        | 0       | 0            |
| 30  | k     | 16    | 0        | 0        | 0       | 0            |
| 30  | l     | 16    | 0        | 0        | 0       | 0            |
| 30  | m     | 15    | 0        | 0        | 0       | 0            |
| 30  | t     | 8     | 0        | 0        | 0       | 0            |
| 30  | x     | 18    | 0        | 0        | 0       | 0            |
| 31  | A     | 20    | 0        | 0        | 0       | 0            |
| 31  | a     | 20    | 0        | 0        | 0       | 0            |
| 32  | A     | 4     | 0        | 0        | 0       | 0            |
| 32  | a     | 4     | 0        | 0        | 0       | 0            |
| 33  | A     | 39    | 0        | 59       | 4       | 0            |
| 33  | D     | 55    | 0        | 80       | 0       | 0            |
| 33  | d     | 55    | 0        | 80       | 1       | 0            |
| 33  | x     | 39    | 0        | 59       | 2       | 0            |
| 34  | A     | 28    | 0        | 42       | 1       | 0            |
| 34  | B     | 52    | 0        | 78       | 6       | 0            |
| 34  | C     | 40    | 0        | 60       | 1       | 0            |
| 34  | D     | 20    | 0        | 30       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 34  | H     | 4     | 0        | 6        | 0       | 0            |
| 34  | O     | 56    | 0        | 84       | 1       | 0            |
| 34  | T     | 8     | 0        | 12       | 0       | 0            |
| 34  | U     | 12    | 0        | 18       | 1       | 0            |
| 34  | V     | 40    | 0        | 60       | 2       | 0            |
| 34  | X     | 4     | 0        | 6        | 0       | 0            |
| 34  | a     | 20    | 0        | 30       | 1       | 0            |
| 34  | b     | 44    | 0        | 66       | 1       | 0            |
| 34  | c     | 72    | 0        | 108      | 3       | 0            |
| 34  | d     | 24    | 0        | 36       | 1       | 0            |
| 34  | l     | 4     | 0        | 6        | 0       | 0            |
| 34  | o     | 52    | 0        | 78       | 3       | 0            |
| 34  | t     | 4     | 0        | 6        | 0       | 0            |
| 34  | u     | 12    | 0        | 18       | 0       | 0            |
| 34  | v     | 40    | 0        | 60       | 1       | 0            |
| 35  | B     | 1     | 0        | 0        | 0       | 0            |
| 35  | O     | 1     | 0        | 0        | 0       | 0            |
| 35  | b     | 1     | 0        | 0        | 0       | 0            |
| 35  | c     | 1     | 0        | 0        | 0       | 0            |
| 35  | o     | 1     | 0        | 0        | 0       | 0            |
| 36  | B     | 95    | 0        | 130      | 4       | 0            |
| 36  | C     | 57    | 0        | 78       | 3       | 0            |
| 36  | H     | 17    | 0        | 22       | 2       | 0            |
| 36  | I     | 19    | 0        | 26       | 2       | 0            |
| 36  | V     | 19    | 0        | 26       | 0       | 0            |
| 36  | b     | 95    | 0        | 130      | 10      | 0            |
| 36  | c     | 57    | 0        | 78       | 0       | 0            |
| 36  | d     | 38    | 0        | 52       | 3       | 0            |
| 36  | i     | 19    | 0        | 26       | 1       | 0            |
| 36  | o     | 19    | 0        | 26       | 2       | 0            |
| 37  | C     | 182   | 0        | 238      | 6       | 0            |
| 37  | D     | 53    | 0        | 71       | 3       | 0            |
| 37  | H     | 62    | 0        | 82       | 0       | 0            |
| 37  | c     | 186   | 0        | 246      | 2       | 0            |
| 37  | h     | 62    | 0        | 82       | 0       | 0            |
| 38  | D     | 137   | 0        | 196      | 4       | 0            |
| 38  | E     | 40    | 0        | 53       | 0       | 0            |
| 38  | L     | 49    | 0        | 74       | 1       | 0            |
| 38  | d     | 141   | 0        | 207      | 6       | 0            |
| 38  | e     | 40    | 0        | 53       | 1       | 0            |
| 38  | l     | 49    | 0        | 74       | 2       | 0            |
| 39  | F     | 43    | 0        | 30       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 39  | e     | 43    | 0        | 30       | 2       | 0            |
| 40  | H     | 41    | 0        | 56       | 3       | 0            |
| 40  | h     | 41    | 0        | 56       | 3       | 0            |
| 41  | J     | 1     | 0        | 0        | 0       | 0            |
| 41  | K     | 1     | 0        | 0        | 0       | 0            |
| 41  | j     | 1     | 0        | 0        | 0       | 0            |
| 41  | k     | 1     | 0        | 0        | 0       | 0            |
| 42  | V     | 43    | 0        | 30       | 0       | 0            |
| 42  | v     | 43    | 0        | 30       | 0       | 0            |
| 43  | A     | 133   | 0        | 0        | 0       | 0            |
| 43  | B     | 302   | 0        | 0        | 3       | 0            |
| 43  | C     | 192   | 0        | 0        | 0       | 0            |
| 43  | D     | 147   | 0        | 0        | 1       | 0            |
| 43  | E     | 25    | 0        | 0        | 0       | 0            |
| 43  | F     | 9     | 0        | 0        | 0       | 0            |
| 43  | H     | 41    | 0        | 0        | 1       | 0            |
| 43  | I     | 8     | 0        | 0        | 0       | 0            |
| 43  | J     | 10    | 0        | 0        | 0       | 0            |
| 43  | K     | 10    | 0        | 0        | 0       | 0            |
| 43  | L     | 15    | 0        | 0        | 0       | 0            |
| 43  | M     | 12    | 0        | 0        | 0       | 0            |
| 43  | O     | 145   | 0        | 0        | 2       | 0            |
| 43  | T     | 12    | 0        | 0        | 0       | 0            |
| 43  | U     | 79    | 0        | 0        | 0       | 0            |
| 43  | V     | 113   | 0        | 0        | 0       | 0            |
| 43  | X     | 15    | 0        | 0        | 0       | 0            |
| 43  | Y     | 4     | 0        | 0        | 0       | 0            |
| 43  | Z     | 8     | 0        | 0        | 0       | 0            |
| 43  | a     | 122   | 0        | 0        | 1       | 0            |
| 43  | b     | 251   | 0        | 0        | 1       | 0            |
| 43  | c     | 211   | 0        | 0        | 2       | 0            |
| 43  | d     | 147   | 0        | 0        | 1       | 0            |
| 43  | e     | 19    | 0        | 0        | 0       | 0            |
| 43  | f     | 7     | 0        | 0        | 0       | 0            |
| 43  | h     | 27    | 0        | 0        | 0       | 0            |
| 43  | i     | 8     | 0        | 0        | 0       | 0            |
| 43  | j     | 10    | 0        | 0        | 0       | 0            |
| 43  | k     | 5     | 0        | 0        | 0       | 0            |
| 43  | l     | 20    | 0        | 0        | 0       | 0            |
| 43  | m     | 11    | 0        | 0        | 0       | 0            |
| 43  | o     | 144   | 0        | 0        | 1       | 0            |
| 43  | t     | 10    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | u     | 78    | 0        | 0        | 0       | 0            |
| 43  | v     | 93    | 0        | 0        | 0       | 0            |
| 43  | x     | 4     | 0        | 0        | 0       | 0            |
| 43  | y     | 6     | 0        | 0        | 0       | 0            |
| 43  | z     | 6     | 0        | 0        | 0       | 0            |
| All | All   | 53814 | 0        | 52371    | 454     | 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 4.

All (454) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:O:20:PRO:HG3    | 29:O:302:GOL:H12  | 1.64                     | 0.79              |
| 2:b:433:ASP:HB2    | 29:b:631:GOL:H11  | 1.66                     | 0.77              |
| 28:d:401:LMT:H22   | 36:o:301:HTG:H1   | 1.66                     | 0.76              |
| 4:d:192:THR:HG23   | 23:d:408:CLA:HBC2 | 1.71                     | 0.73              |
| 13:O:194:LYS:NZ    | 43:O:401:HOH:O    | 2.23                     | 0.70              |
| 23:c:506:CLA:HBB2  | 27:c:522:LMG:H412 | 1.72                     | 0.70              |
| 1:a:252:HIS:NE2    | 1:a:265:PHE:O     | 2.26                     | 0.69              |
| 1:A:12:ASN:HB3     | 1:A:15:GLU:HG3    | 1.73                     | 0.69              |
| 34:B:647:DMS:H12   | 28:d:401:LMT:H3'  | 1.75                     | 0.68              |
| 3:c:315:MET:HG2    | 3:c:351:PHE:CZ    | 2.29                     | 0.67              |
| 39:e:103:HEM:HMC2  | 39:e:103:HEM:HBC2 | 1.77                     | 0.67              |
| 26:D:2302:SQD:H252 | 26:D:2302:SQD:H92 | 1.77                     | 0.66              |
| 23:C:507:CLA:HMC2  | 23:C:508:CLA:H102 | 1.79                     | 0.65              |
| 5:e:18:ARG:HB2     | 9:j:2:MET:HB3     | 1.79                     | 0.65              |
| 2:B:169:SER:HB3    | 29:B:648:GOL:H2   | 1.79                     | 0.64              |
| 2:B:44:THR:HG22    | 28:B:634:LMT:H6D  | 1.78                     | 0.64              |
| 7:H:25:TRP:CD1     | 36:H:101:HTG:H1   | 2.32                     | 0.64              |
| 23:C:504:CLA:HBB1  | 27:C:527:LMG:H221 | 1.80                     | 0.63              |
| 23:c:504:CLA:C4D   | 23:c:506:CLA:H2   | 2.28                     | 0.62              |
| 4:D:24:ARG:HD3     | 18:X:37:VAL:HG22  | 1.80                     | 0.62              |
| 2:b:420:TYR:CE2    | 36:b:625:HTG:H2'1 | 2.34                     | 0.62              |
| 26:l:101:SQD:H462  | 26:l:101:SQD:H1   | 1.82                     | 0.62              |
| 2:b:133:LEU:HD12   | 34:b:639:DMS:H22  | 1.80                     | 0.62              |
| 5:e:8:ARG:HH21     | 5:e:12:ASP:HB3    | 1.65                     | 0.62              |
| 23:a:2610:CLA:H142 | 27:d:414:LMG:H241 | 1.81                     | 0.62              |
| 23:b:618:CLA:H18   | 38:d:412:LHG:H202 | 1.82                     | 0.61              |
| 5:E:27:ILE:HG12    | 39:F:101:HEM:HMC3 | 1.82                     | 0.61              |
| 28:A:414:LMT:H6'1  | 4:D:304:ARG:HH12  | 1.66                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:412:THR:N      | 34:B:642:DMS:O     | 2.34                     | 0.60              |
| 23:A:407:CLA:H192  | 33:A:422:PL9:H252  | 1.83                     | 0.59              |
| 34:B:644:DMS:H11   | 11:L:1:MET:HB3     | 1.84                     | 0.59              |
| 3:c:107:ASP:OD2    | 27:c:522:LMG:O2    | 2.20                     | 0.59              |
| 29:a:2602:GOL:H31  | 36:o:301:HTG:H1'1  | 1.85                     | 0.59              |
| 28:B:623:LMT:H42   | 26:D:2302:SQD:H241 | 1.85                     | 0.59              |
| 3:c:315:MET:HG3    | 3:c:365:TRP:HZ3    | 1.66                     | 0.59              |
| 2:B:90:PHE:H       | 36:B:627:HTG:H61   | 1.68                     | 0.59              |
| 25:T:102:BCR:H19C  | 25:b:623:BCR:H363  | 1.85                     | 0.59              |
| 23:C:503:CLA:H61   | 23:C:513:CLA:H42   | 1.85                     | 0.58              |
| 28:A:414:LMT:O4'   | 4:D:304:ARG:NH2    | 2.36                     | 0.58              |
| 25:B:633:BCR:HC8   | 25:B:633:BCR:H321  | 1.85                     | 0.58              |
| 23:b:620:CLA:H2    | 23:b:621:CLA:HBB2  | 1.85                     | 0.58              |
| 25:y:101:BCR:H321  | 25:y:101:BCR:HC8   | 1.86                     | 0.58              |
| 1:A:102:LEU:HD11   | 28:A:420:LMT:H42   | 1.85                     | 0.58              |
| 5:E:68:ASP:O       | 5:E:72:ALA:HB2     | 2.04                     | 0.57              |
| 19:z:47:TRP:CE2    | 28:z:102:LMT:H102  | 2.39                     | 0.57              |
| 2:B:12:LEU:HB2     | 23:B:613:CLA:HMC2  | 1.85                     | 0.57              |
| 2:B:248:ALA:HA     | 23:B:604:CLA:H42   | 1.86                     | 0.57              |
| 2:b:36:SER:OG      | 25:b:623:BCR:H362  | 2.05                     | 0.57              |
| 37:C:519:DGD:HA32  | 27:D:2312:LMG:H121 | 1.87                     | 0.56              |
| 4:D:61:HIS:HD2     | 43:D:2528:HOH:O    | 1.88                     | 0.56              |
| 28:d:404:LMT:H112  | 36:d:407:HTG:H6'2  | 1.87                     | 0.56              |
| 23:b:616:CLA:H101  | 23:b:618:CLA:H143  | 1.86                     | 0.56              |
| 1:A:183:MET:HA     | 23:A:405:CLA:HMD1  | 1.88                     | 0.56              |
| 4:D:192:THR:HG23   | 23:D:2303:CLA:HBC2 | 1.86                     | 0.56              |
| 2:b:341:LYS:NZ     | 36:b:625:HTG:S1    | 2.77                     | 0.56              |
| 26:A:412:SQD:H381  | 9:J:22:ILE:HD11    | 1.88                     | 0.55              |
| 37:C:518:DGD:HA82  | 37:C:518:DGD:HAF2  | 1.89                     | 0.55              |
| 3:C:50:LEU:HD11    | 23:C:514:CLA:HBB1  | 1.89                     | 0.55              |
| 3:C:279:LEU:HD22   | 23:C:510:CLA:HED2  | 1.88                     | 0.55              |
| 1:A:200:LEU:HG     | 37:C:519:DGD:HAT2  | 1.89                     | 0.55              |
| 26:B:621:SQD:H242  | 11:l:14:ARG:HD3    | 1.89                     | 0.54              |
| 3:C:182:PHE:HA     | 36:C:521:HTG:H61   | 1.88                     | 0.54              |
| 25:T:102:BCR:H321  | 25:T:102:BCR:HC8   | 1.88                     | 0.54              |
| 1:a:136:ARG:NH2    | 8:i:27:ASP:OD1     | 2.39                     | 0.54              |
| 1:a:192:ILE:HG13   | 1:a:293:MET:HE1    | 1.89                     | 0.54              |
| 2:b:347[A]:ARG:NH2 | 43:b:706:HOH:O     | 2.40                     | 0.54              |
| 23:C:502:CLA:HBB2  | 23:C:508:CLA:H92   | 1.90                     | 0.54              |
| 25:B:618:BCR:H383  | 26:B:621:SQD:H101  | 1.88                     | 0.54              |
| 28:A:414:LMT:O3'   | 28:A:414:LMT:O2B   | 2.23                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:B:619:BCR:H363  | 25:B:633:BCR:H19C  | 1.89                     | 0.54              |
| 25:Y:302:BCR:H321  | 25:Y:302:BCR:HC8   | 1.89                     | 0.54              |
| 6:f:41:GLN:OE1     | 9:j:31:GLY:HA3     | 2.07                     | 0.53              |
| 23:c:509:CLA:H2    | 25:c:517:BCR:H10C  | 1.91                     | 0.53              |
| 1:A:192:ILE:HG13   | 1:A:293:MET:HE1    | 1.91                     | 0.53              |
| 3:C:24:THR:O       | 3:C:26:ARG:N       | 2.42                     | 0.53              |
| 3:c:60:ILE:HG22    | 23:c:506:CLA:HHD   | 1.90                     | 0.53              |
| 24:A:409:PHO:HBC3  | 4:D:279:LEU:HD22   | 1.91                     | 0.52              |
| 3:C:286:ALA:HB2    | 23:C:503:CLA:HMD2  | 1.91                     | 0.52              |
| 5:E:60:GLN:NE2     | 5:E:62:SER:O       | 2.42                     | 0.52              |
| 23:B:616:CLA:H2    | 23:B:617:CLA:HBB2  | 1.91                     | 0.52              |
| 2:B:341:LYS:NZ     | 36:B:624[B]:HTG:S1 | 2.82                     | 0.52              |
| 23:C:502:CLA:C4D   | 23:C:504:CLA:H2    | 2.39                     | 0.52              |
| 23:C:510:CLA:HMB1  | 23:C:510:CLA:HBB1  | 1.92                     | 0.52              |
| 1:a:136:ARG:HD2    | 43:a:2769:HOH:O    | 2.09                     | 0.52              |
| 4:d:304:ARG:HH12   | 28:d:401:LMT:H6'1  | 1.74                     | 0.51              |
| 1:A:221[A]:SER:HB2 | 4:D:139:ARG:O      | 2.10                     | 0.51              |
| 25:D:2305:BCR:H383 | 27:D:2312:LMG:H171 | 1.90                     | 0.51              |
| 3:c:38:GLY:HA3     | 23:c:514:CLA:HMD2  | 1.92                     | 0.51              |
| 3:c:256:PRO:HA     | 23:c:509:CLA:HED2  | 1.92                     | 0.51              |
| 1:A:84:PRO:HA      | 1:A:112:TYR:CG     | 2.45                     | 0.51              |
| 23:c:504:CLA:H202  | 23:c:510:CLA:HBB1  | 1.92                     | 0.51              |
| 4:d:244:TYR:OH     | 4:d:264:LYS:HE2    | 2.11                     | 0.51              |
| 1:A:96:ILE:HG12    | 1:A:105:TRP:CE2    | 2.46                     | 0.51              |
| 5:E:16:SER:HB3     | 9:J:5:GLY:HA2      | 1.93                     | 0.51              |
| 1:a:183:MET:HA     | 23:a:2609:CLA:HMD1 | 1.91                     | 0.51              |
| 2:B:349:LYS:NZ     | 43:B:706:HOH:O     | 2.43                     | 0.51              |
| 34:B:637:DMS:H11   | 43:B:891:HOH:O     | 2.11                     | 0.51              |
| 23:B:606:CLA:C14   | 23:B:611:CLA:HED2  | 2.41                     | 0.51              |
| 1:a:84:PRO:HA      | 1:a:112:TYR:CG     | 2.46                     | 0.51              |
| 1:a:96:ILE:HG12    | 1:a:105:TRP:CE2    | 2.46                     | 0.51              |
| 19:z:26:ALA:HB1    | 19:z:36:SER:HB3    | 1.92                     | 0.51              |
| 1:A:214:MET:HE2    | 1:A:255:PHE:CE1    | 2.46                     | 0.51              |
| 23:c:514:CLA:H171  | 19:z:20:VAL:HA     | 1.92                     | 0.51              |
| 13:O:58:ASN:ND2    | 2:b:307[B]:GLU:OE2 | 2.44                     | 0.50              |
| 16:V:18:THR:O      | 34:V:206:DMS:H22   | 2.12                     | 0.50              |
| 23:d:402:CLA:HMB1  | 23:d:402:CLA:HBB1  | 1.93                     | 0.50              |
| 36:d:407:HTG:H2    | 7:h:25:TRP:NE1     | 2.26                     | 0.50              |
| 19:z:47:TRP:CE3    | 28:z:102:LMT:H81   | 2.47                     | 0.50              |
| 23:b:620:CLA:H2    | 23:b:621:CLA:CBB   | 2.41                     | 0.50              |
| 1:A:23:SER:HA      | 34:A:430:DMS:H13   | 1.94                     | 0.50              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 4:d:304:ARG:NH2    | 28:d:401:LMT:O4'     | 2.36                     | 0.50              |
| 23:B:617:CLA:HBB1  | 23:B:617:CLA:HMB3    | 1.94                     | 0.50              |
| 2:b:141:ILE:HG21   | 23:b:620:CLA:HBB1    | 1.93                     | 0.50              |
| 2:b:464:PHE:CZ     | 38:d:412:LHG:H252    | 2.46                     | 0.50              |
| 23:C:502:CLA:H193  | 23:C:508:CLA:HBB1    | 1.93                     | 0.50              |
| 26:a:2615:SQD:H262 | 38:d:403:LHG:H121    | 1.93                     | 0.49              |
| 3:c:459:ILE:HG21   | 3:c:464:GLU:HG3      | 1.95                     | 0.49              |
| 23:b:614:CLA:NC    | 40:h:101:RRX:H56     | 2.27                     | 0.49              |
| 23:A:407:CLA:H152  | 33:A:422:PL9:H222    | 1.95                     | 0.49              |
| 2:B:383:PHE:CZ     | 13:O:167:GLY:HA2     | 2.47                     | 0.49              |
| 28:A:420:LMT:H51   | 8:I:4:LEU:HD22       | 1.95                     | 0.49              |
| 8:I:13:THR:O       | 8:I:17:LEU:HG        | 2.12                     | 0.49              |
| 1:a:214:MET:HE2    | 1:a:255:PHE:CE1      | 2.48                     | 0.49              |
| 7:h:59:ASN:O       | 7:h:64:ALA:HB3       | 2.13                     | 0.49              |
| 26:D:2308:SQD:H321 | 18:X:24:THR:HA       | 1.94                     | 0.49              |
| 23:C:507:CLA:H51   | 23:C:507:CLA:H102    | 1.95                     | 0.49              |
| 8:i:1:FME:HG3      | 28:i:103:LMT:H6D     | 1.95                     | 0.49              |
| 2:b:383:PHE:CZ     | 13:o:167:GLY:HA2     | 2.48                     | 0.48              |
| 3:c:286:ALA:HB2    | 23:c:505:CLA:HMD2    | 1.93                     | 0.48              |
| 38:l:103:LHG:H321  | 12:m:18:PRO:HB3      | 1.96                     | 0.48              |
| 4:D:23:LYS:NZ      | 26:D:2302:SQD:H462   | 2.28                     | 0.48              |
| 7:h:38:PHE:HB2     | 40:h:101:RRX:C10     | 2.43                     | 0.48              |
| 2:B:416:THR:HG23   | 36:B:624[B]:HTG:H6'1 | 1.95                     | 0.48              |
| 23:c:508:CLA:HAA1  | 23:c:508:CLA:HBD     | 1.95                     | 0.48              |
| 4:d:335:PRO:HB2    | 5:e:65[B]:LEU:HD13   | 1.96                     | 0.48              |
| 23:C:504:CLA:HBB1  | 27:C:527:LMG:H391    | 1.96                     | 0.48              |
| 4:D:103:ARG:HH21   | 5:E:77:GLU:HG3       | 1.77                     | 0.48              |
| 4:D:126:MET:HE3    | 4:D:143:ALA:O        | 2.13                     | 0.48              |
| 37:D:2307:DGD:HBW2 | 37:D:2307:DGD:O1A    | 2.14                     | 0.48              |
| 3:c:279:LEU:HD22   | 23:c:512:CLA:HED2    | 1.96                     | 0.48              |
| 23:A:405:CLA:CBD   | 23:A:406:CLA:HAC2    | 2.43                     | 0.48              |
| 2:B:36[A]:SER:OG   | 25:B:619:BCR:H362    | 2.14                     | 0.48              |
| 2:b:70:GLY:HA2     | 2:b:178:VAL:HG21     | 1.96                     | 0.48              |
| 7:H:63:LYS:NZ      | 43:H:202:HOH:O       | 2.47                     | 0.48              |
| 2:b:12:LEU:HB2     | 23:b:617:CLA:HMC2    | 1.96                     | 0.48              |
| 23:c:505:CLA:H102  | 23:c:506:CLA:CHB     | 2.44                     | 0.48              |
| 27:c:521:LMG:O5    | 28:j:2701:LMT:H2B    | 2.14                     | 0.48              |
| 10:k:20:PRO:HB3    | 17:y:21:GLN:HG3      | 1.96                     | 0.48              |
| 23:a:2613:CLA:H161 | 23:a:2613:CLA:H122   | 1.71                     | 0.47              |
| 29:b:644:GOL:H31   | 7:h:62:TRP:CZ3       | 2.49                     | 0.47              |
| 34:o:307:DMS:H21   | 43:o:425:HOH:O       | 2.12                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 23:A:410:CLA:H18    | 23:C:506:CLA:H142  | 1.95                     | 0.47              |
| 2:B:461:LEU:HD22    | 38:D:2309:LHG:H301 | 1.96                     | 0.47              |
| 34:B:638:DMS:H21    | 15:U:21:TYR:CZ     | 2.49                     | 0.47              |
| 1:a:121[B]:LEU:HD11 | 23:c:508:CLA:H122  | 1.95                     | 0.47              |
| 2:b:58:GLN:C        | 2:b:329:PRO:HB3    | 2.40                     | 0.47              |
| 4:D:103:ARG:NH1     | 4:D:106:GLN:OE1    | 2.48                     | 0.47              |
| 4:d:61:HIS:HD2      | 43:d:627:HOH:O     | 1.95                     | 0.47              |
| 23:B:614:CLA:HBB1   | 23:B:614:CLA:HMB1  | 1.95                     | 0.47              |
| 1:A:63:ILE:HB       | 3:C:335:THR:HG21   | 1.97                     | 0.47              |
| 2:B:243:ALA:HA      | 2:B:246:PHE:CE2    | 2.50                     | 0.47              |
| 23:C:504:CLA:HAB    | 23:C:513:CLA:H41   | 1.97                     | 0.47              |
| 3:c:52:ALA:HB2      | 23:c:514:CLA:HMA2  | 1.96                     | 0.47              |
| 1:A:252:HIS:CE1     | 1:A:264:SER:HB3    | 2.49                     | 0.47              |
| 7:H:25:TRP:CD2      | 36:H:101:HTG:H1'2  | 2.50                     | 0.47              |
| 1:a:12[A]:ASN:OD1   | 1:a:15:GLU:HB2     | 2.13                     | 0.47              |
| 23:b:611:CLA:H72    | 25:b:624:BCR:H311  | 1.97                     | 0.47              |
| 2:B:86:ILE:HD12     | 2:B:88:PRO:HD3     | 1.97                     | 0.47              |
| 13:o:232:GLU:HG2    | 34:o:314:DMS:H11   | 1.96                     | 0.47              |
| 3:c:42:LEU:HD21     | 23:c:514:CLA:H2A   | 1.97                     | 0.47              |
| 3:c:79:LYS:HB3      | 3:c:84:GLN:NE2     | 2.30                     | 0.47              |
| 27:c:501:LMG:H382   | 37:c:518:DGD:HB52  | 1.98                     | 0.46              |
| 37:c:519:DGD:HA81   | 37:c:519:DGD:HAE2  | 1.46                     | 0.46              |
| 4:d:172:SER:HB2     | 4:d:177:ALA:HB1    | 1.97                     | 0.46              |
| 2:B:264:PRO:HB3     | 29:B:648:GOL:H11   | 1.96                     | 0.46              |
| 23:a:2610:CLA:HMD3  | 4:d:182:LEU:HD11   | 1.97                     | 0.46              |
| 23:c:509:CLA:HMC2   | 23:c:510:CLA:H102  | 1.96                     | 0.46              |
| 2:B:341:LYS:NZ      | 43:B:708:HOH:O     | 2.43                     | 0.46              |
| 19:z:47:TRP:CD2     | 28:z:102:LMT:H102  | 2.50                     | 0.46              |
| 23:A:406:CLA:H203   | 23:A:406:CLA:H162  | 1.70                     | 0.46              |
| 23:a:2609:CLA:CBD   | 23:d:402:CLA:HAC2  | 2.44                     | 0.46              |
| 3:C:163:PHE:CD2     | 23:C:513:CLA:HAB   | 2.51                     | 0.46              |
| 5:e:68:ASP:O        | 5:e:72:ALA:HB2     | 2.15                     | 0.46              |
| 23:B:610:CLA:HMA2   | 23:B:611:CLA:C2C   | 2.45                     | 0.46              |
| 23:c:504:CLA:C3D    | 23:c:506:CLA:H2    | 2.46                     | 0.46              |
| 19:z:26:ALA:HB3     | 19:z:40:ILE:HD11   | 1.97                     | 0.46              |
| 23:b:614:CLA:HMA3   | 23:b:615:CLA:C1C   | 2.46                     | 0.46              |
| 37:C:518:DGD:HBF1   | 37:C:518:DGD:HBE2  | 1.59                     | 0.46              |
| 38:L:101:LHG:H321   | 12:M:18:PRO:HB3    | 1.98                     | 0.46              |
| 23:b:618:CLA:H141   | 38:d:412:LHG:H182  | 1.97                     | 0.46              |
| 25:b:622:BCR:H313   | 27:m:2802:LMG:H111 | 1.97                     | 0.46              |
| 23:C:509:CLA:HBC3   | 23:C:511:CLA:H71   | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:K:101:BCR:H24C  | 25:K:101:BCR:H371  | 1.76                     | 0.45              |
| 2:b:80:ILE:HD11    | 2:b:167:TRP:CZ3    | 2.52                     | 0.45              |
| 2:b:149:LEU:HD21   | 23:b:611:CLA:HBB2  | 1.98                     | 0.45              |
| 2:b:423:LYS:HG3    | 36:b:625:HTG:H1'1  | 1.98                     | 0.45              |
| 23:B:615:CLA:H62   | 23:B:615:CLA:H41   | 1.63                     | 0.45              |
| 29:B:632:GOL:H2    | 34:U:503:DMS:H12   | 1.98                     | 0.45              |
| 4:D:172:SER:HB2    | 4:D:177:ALA:HB1    | 1.97                     | 0.45              |
| 13:O:57:LYS:HE2    | 2:b:338:GLN:HA     | 1.97                     | 0.45              |
| 23:C:511:CLA:H192  | 23:C:511:CLA:HBC3  | 1.97                     | 0.45              |
| 25:b:622:BCR:H24C  | 25:b:622:BCR:H371  | 1.77                     | 0.45              |
| 13:o:180:GLU:CD    | 13:o:180:GLU:H     | 2.24                     | 0.45              |
| 4:d:88:SER:HB2     | 5:e:69:ARG:CZ      | 2.46                     | 0.45              |
| 27:d:414:LMG:H292  | 27:d:414:LMG:H151  | 1.99                     | 0.45              |
| 23:B:616:CLA:H111  | 23:B:616:CLA:H152  | 1.56                     | 0.45              |
| 40:H:102:RRX:H47   | 40:H:102:RRX:H43   | 1.72                     | 0.45              |
| 4:d:61:HIS:HE1     | 4:d:80:THR:O       | 1.99                     | 0.45              |
| 1:A:272:HIS:CD2    | 4:D:218:VAL:HG21   | 2.51                     | 0.45              |
| 28:A:414:LMT:O2'   | 36:b:602:HTG:H5    | 2.17                     | 0.45              |
| 23:A:410:CLA:H151  | 23:A:410:CLA:H112  | 1.58                     | 0.45              |
| 25:C:516:BCR:H15C  | 25:C:516:BCR:H351  | 1.86                     | 0.45              |
| 2:b:233:ASN:O      | 2:b:236:THR:HG22   | 2.17                     | 0.45              |
| 23:b:606:CLA:HAA2  | 36:b:626:HTG:H62   | 1.97                     | 0.45              |
| 23:B:615:CLA:H71   | 23:B:615:CLA:H112  | 1.74                     | 0.45              |
| 25:B:633:BCR:H331  | 25:B:633:BCR:HC7   | 1.53                     | 0.45              |
| 3:C:42:LEU:HD21    | 23:C:512:CLA:H2A   | 1.99                     | 0.45              |
| 3:C:266:TRP:CZ3    | 23:C:508:CLA:HAC2  | 2.51                     | 0.45              |
| 11:L:9:PRO:HA      | 28:m:2803:LMT:H6D  | 1.98                     | 0.45              |
| 2:b:348:ASN:OD1    | 2:b:352[A]:GLU:HG2 | 2.17                     | 0.45              |
| 25:b:623:BCR:H331  | 25:b:623:BCR:C8    | 2.47                     | 0.45              |
| 25:c:517:BCR:H15C  | 25:c:517:BCR:H351  | 1.84                     | 0.45              |
| 23:C:510:CLA:H141  | 23:C:513:CLA:HMD3  | 1.99                     | 0.45              |
| 38:D:2311:LHG:H312 | 38:D:2311:LHG:H342 | 1.68                     | 0.45              |
| 33:A:422:PL9:H452  | 4:D:39:PRO:HG3     | 1.98                     | 0.44              |
| 23:B:607:CLA:H142  | 23:B:607:CLA:H111  | 1.73                     | 0.44              |
| 6:F:41:GLN:OE1     | 9:J:31:GLY:HA3     | 2.16                     | 0.44              |
| 1:a:131:TRP:CH2    | 23:c:508:CLA:HAA2  | 2.52                     | 0.44              |
| 23:c:514:CLA:HMB1  | 25:k:302:BCR:H382  | 1.98                     | 0.44              |
| 1:A:133:LEU:HD23   | 4:D:256:ILE:HG12   | 2.00                     | 0.44              |
| 4:D:88:SER:HB2     | 5:E:69:ARG:CZ      | 2.47                     | 0.44              |
| 27:c:501:LMG:O5    | 29:c:530:GOL:H31   | 2.17                     | 0.44              |
| 3:C:127:PHE:CZ     | 28:Z:101:LMT:H22   | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:334:PRO:HA     | 13:O:153:THR:OG1   | 2.17                     | 0.44              |
| 13:O:194:LYS:HE3   | 34:O:307:DMS:H11   | 2.00                     | 0.44              |
| 2:b:243:ALA:HA     | 2:b:246:PHE:CD2    | 2.53                     | 0.44              |
| 2:b:423:LYS:NZ     | 36:b:625:HTG:H62   | 2.32                     | 0.44              |
| 3:c:362:ARG:HD3    | 34:c:536:DMS:O     | 2.18                     | 0.44              |
| 13:o:196:GLN:NE2   | 34:o:314:DMS:O     | 2.50                     | 0.44              |
| 14:T:23:PHE:CD1    | 26:l:101:SQD:H45   | 2.52                     | 0.44              |
| 25:T:102:BCR:H11C  | 25:T:102:BCR:H341  | 1.87                     | 0.44              |
| 23:b:615:CLA:H92   | 23:b:615:CLA:H61   | 1.84                     | 0.44              |
| 6:f:22:ALA:HB2     | 33:x:1301:PL9:H353 | 1.99                     | 0.44              |
| 23:B:604:CLA:H143  | 23:B:609:CLA:HAC1  | 1.99                     | 0.44              |
| 3:C:443:TRP:CZ2    | 23:C:509:CLA:HMD1  | 2.52                     | 0.44              |
| 1:a:23:SER:HA      | 34:a:2624:DMS:S    | 2.56                     | 0.44              |
| 1:A:136:ARG:NH2    | 8:I:27:ASP:OD1     | 2.48                     | 0.44              |
| 13:O:40:ILE:HD12   | 13:O:95:PHE:CD1    | 2.53                     | 0.44              |
| 33:d:411:PL9:H411  | 11:l:29:LEU:HD23   | 1.99                     | 0.44              |
| 16:v:27:LEU:HD21   | 34:v:209:DMS:H23   | 1.98                     | 0.44              |
| 2:B:454:ALA:HB2    | 27:B:622:LMG:H172  | 1.99                     | 0.44              |
| 40:H:102:RRX:H26   | 40:H:102:RRX:H22   | 1.85                     | 0.44              |
| 3:c:123:ALA:HB1    | 28:z:102:LMT:H101  | 1.99                     | 0.44              |
| 23:B:606:CLA:H152  | 23:B:606:CLA:H112  | 1.77                     | 0.44              |
| 23:B:611:CLA:HHC   | 23:B:611:CLA:HBB1  | 2.00                     | 0.44              |
| 23:D:2303:CLA:HAA2 | 23:D:2303:CLA:HBD  | 2.00                     | 0.44              |
| 7:H:62:TRP:C       | 7:H:64:ALA:H       | 2.25                     | 0.44              |
| 28:M:101:LMT:H5'   | 43:t:208:HOH:O     | 2.18                     | 0.44              |
| 16:V:93:PRO:HA     | 16:V:101:PHE:CD2   | 2.53                     | 0.44              |
| 23:c:516:CLA:H61   | 23:c:516:CLA:H2    | 1.75                     | 0.44              |
| 4:d:49:LEU:HD13    | 25:d:410:BCR:C15   | 2.48                     | 0.44              |
| 19:z:38:GLN:O      | 19:z:42:LEU:HG     | 2.18                     | 0.44              |
| 23:B:614:CLA:H121  | 23:B:614:CLA:H162  | 1.66                     | 0.44              |
| 3:C:279:LEU:HD12   | 3:C:282:MET:HE3    | 1.99                     | 0.44              |
| 13:O:110:MET:HE2   | 13:O:110:MET:HB3   | 1.80                     | 0.44              |
| 3:c:145:SER:H      | 34:c:543:DMS:H13   | 1.83                     | 0.44              |
| 2:B:137:LYS:NZ     | 7:H:17:GLU:OE1     | 2.45                     | 0.43              |
| 3:C:459:ILE:HG21   | 3:C:464:GLU:HG3    | 2.00                     | 0.43              |
| 13:O:129:THR:HA    | 13:O:141:ASP:O     | 2.18                     | 0.43              |
| 1:a:63:ILE:HB      | 3:c:335:THR:HG21   | 1.99                     | 0.43              |
| 23:b:615:CLA:HHC   | 23:b:615:CLA:HBB1  | 2.00                     | 0.43              |
| 29:B:648:GOL:H32   | 7:H:62:TRP:CE3     | 2.53                     | 0.43              |
| 6:F:21:VAL:O       | 6:F:25:THR:HG23    | 2.18                     | 0.43              |
| 40:H:102:RRX:H32   | 40:H:102:RRX:H28   | 1.86                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:389:LYS:HZ1   | 29:B:632:GOL:H31   | 1.82                     | 0.43              |
| 3:C:175:LEU:HD23  | 3:C:237:HIS:CG     | 2.53                     | 0.43              |
| 23:b:612:CLA:H91  | 23:b:612:CLA:H112  | 1.82                     | 0.43              |
| 4:d:140:PRO:HD2   | 34:d:418:DMS:H23   | 1.99                     | 0.43              |
| 36:d:407:HTG:H3'2 | 36:d:407:HTG:H6'1  | 1.82                     | 0.43              |
| 1:A:188:ALA:HB2   | 1:A:328:MET:HB2    | 2.00                     | 0.43              |
| 33:A:422:PL9:H211 | 23:D:2303:CLA:H141 | 2.01                     | 0.43              |
| 26:b:601:SQD:H191 | 26:b:601:SQD:H161  | 1.70                     | 0.43              |
| 36:b:603:HTG:O2   | 36:b:604:HTG:S1    | 2.71                     | 0.43              |
| 27:c:501:LMG:H192 | 27:c:501:LMG:H161  | 1.77                     | 0.43              |
| 27:c:501:LMG:H202 | 27:c:501:LMG:H231  | 1.80                     | 0.43              |
| 5:e:8:ARG:NH2     | 5:e:12:ASP:HB3     | 2.33                     | 0.43              |
| 27:A:413:LMG:H372 | 37:C:517:DGD:HB32  | 2.00                     | 0.43              |
| 2:b:90:PHE:CE2    | 23:b:611:CLA:H151  | 2.54                     | 0.43              |
| 2:b:446:SER:HB2   | 2:b:447:PRO:HD2    | 2.00                     | 0.43              |
| 3:c:436:PHE:CE1   | 23:c:507:CLA:H202  | 2.53                     | 0.43              |
| 23:c:516:CLA:H172 | 27:c:522:LMG:H411  | 2.00                     | 0.43              |
| 23:B:611:CLA:H161 | 23:B:611:CLA:H203  | 1.80                     | 0.43              |
| 23:C:514:CLA:H171 | 25:C:515:BCR:H373  | 1.99                     | 0.43              |
| 2:B:419:SER:HA    | 2:B:422:ARG:NH1    | 2.34                     | 0.43              |
| 23:C:506:CLA:HBC2 | 25:C:516:BCR:H341  | 1.99                     | 0.43              |
| 1:a:73:TYR:HA     | 28:d:401:LMT:H4B   | 2.00                     | 0.43              |
| 2:b:341:LYS:NZ    | 36:b:625:HTG:O2    | 2.33                     | 0.43              |
| 7:h:20:LYS:HE3    | 7:h:20:LYS:HB2     | 1.77                     | 0.43              |
| 40:h:101:RRX:H32  | 40:h:101:RRX:H28   | 1.78                     | 0.43              |
| 2:B:462:PHE:CE2   | 23:B:614:CLA:HMB3  | 2.54                     | 0.43              |
| 25:Y:302:BCR:H351 | 25:Y:302:BCR:H15C  | 1.72                     | 0.43              |
| 2:b:137:LYS:HD2   | 7:h:14:LEU:O       | 2.17                     | 0.43              |
| 3:c:338:GLY:HA3   | 3:c:341:LEU:O      | 2.18                     | 0.43              |
| 4:d:26:ARG:NH2    | 26:d:417:SQD:O7    | 2.50                     | 0.43              |
| 25:B:633:BCR:H11C | 25:B:633:BCR:H341  | 1.84                     | 0.43              |
| 3:C:409:GLY:HA2   | 29:C:526:GOL:H2    | 2.01                     | 0.43              |
| 13:O:86:LYS:NZ    | 43:O:404:HOH:O     | 2.44                     | 0.43              |
| 14:t:26:PRO:HA    | 14:t:27:PRO:HD3    | 1.97                     | 0.43              |
| 28:A:414:LMT:H41  | 36:b:602:HTG:H3'2  | 2.00                     | 0.43              |
| 23:C:507:CLA:H43  | 23:C:507:CLA:H11   | 1.82                     | 0.43              |
| 23:C:507:CLA:HBA1 | 23:C:507:CLA:H3A   | 1.65                     | 0.43              |
| 2:b:170:ASP:O     | 29:b:644:GOL:H12   | 2.19                     | 0.43              |
| 3:c:279:LEU:HD12  | 3:c:282:MET:HE3    | 2.01                     | 0.43              |
| 23:c:506:CLA:H112 | 23:c:506:CLA:H72   | 1.76                     | 0.43              |
| 4:d:103:ARG:HG3   | 5:e:73:LYS:HG3     | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:i:3:THR:HB       | 36:i:102:HTG:H1'1  | 2.01                     | 0.43              |
| 8:I:1:FME:CN       | 36:I:101:HTG:H61   | 2.48                     | 0.42              |
| 1:a:252:HIS:CD2    | 1:a:266:ASN:HA     | 2.54                     | 0.42              |
| 3:c:26:ARG:NH2     | 17:y:46:LEU:OXT    | 2.38                     | 0.42              |
| 3:c:138:GLU:OE2    | 43:c:601:HOH:O     | 2.21                     | 0.42              |
| 23:c:506:CLA:HBB1  | 27:c:522:LMG:H231  | 2.01                     | 0.42              |
| 3:C:338:GLY:HA3    | 3:C:341:LEU:O      | 2.19                     | 0.42              |
| 23:C:504:CLA:HMC3  | 23:C:514:CLA:H191  | 2.00                     | 0.42              |
| 25:C:516:BCR:H341  | 25:C:516:BCR:H11C  | 1.90                     | 0.42              |
| 2:b:29:LEU:HD23    | 26:l:101:SQD:H211  | 2.00                     | 0.42              |
| 2:b:30:VAL:HG12    | 23:b:610:CLA:HHD   | 2.01                     | 0.42              |
| 3:c:163:PHE:CD1    | 23:c:515:CLA:H201  | 2.54                     | 0.42              |
| 4:d:73:PHE:CZ      | 27:d:414:LMG:H192  | 2.54                     | 0.42              |
| 23:d:402:CLA:H162  | 23:d:402:CLA:H203  | 1.71                     | 0.42              |
| 38:e:101:LHG:H222  | 33:x:1301:PL9:H221 | 2.02                     | 0.42              |
| 7:h:62:TRP:C       | 7:h:64:ALA:H       | 2.27                     | 0.42              |
| 23:A:407:CLA:H142  | 23:A:407:CLA:H112  | 1.86                     | 0.42              |
| 36:B:625:HTG:O6    | 36:B:625:HTG:O4    | 2.35                     | 0.42              |
| 2:b:158:LEU:HB3    | 2:b:199:VAL:HG22   | 2.00                     | 0.42              |
| 2:b:324:LEU:HA     | 4:d:293[A]:LEU:HG  | 2.00                     | 0.42              |
| 23:b:621:CLA:H151  | 23:b:621:CLA:H111  | 1.88                     | 0.42              |
| 24:A:408:PHO:H61   | 24:A:408:PHO:H2    | 1.90                     | 0.42              |
| 23:A:410:CLA:H152  | 23:C:507:CLA:H13   | 2.00                     | 0.42              |
| 25:B:620:BCR:H382  | 26:a:2603:SQD:H242 | 2.00                     | 0.42              |
| 4:D:84:SER:O       | 5:E:69:ARG:HB2     | 2.20                     | 0.42              |
| 2:b:462:PHE:CE2    | 23:b:618:CLA:HMB3  | 2.53                     | 0.42              |
| 1:A:131:TRP:CH2    | 23:C:506:CLA:HAA2  | 2.54                     | 0.42              |
| 25:B:620:BCR:H331  | 25:B:620:BCR:C8    | 2.50                     | 0.42              |
| 14:T:20:ALA:O      | 14:T:24:ARG:HB3    | 2.20                     | 0.42              |
| 3:c:135:ARG:O      | 3:c:135:ARG:HD3    | 2.20                     | 0.42              |
| 3:c:315:MET:HG2    | 3:c:351:PHE:HZ     | 1.78                     | 0.42              |
| 2:B:224:ARG:HG3    | 7:H:25:TRP:CD2     | 2.55                     | 0.42              |
| 23:C:505:CLA:H161  | 23:C:511:CLA:H93   | 2.02                     | 0.42              |
| 37:D:2307:DGD:HBW2 | 37:D:2307:DGD:HB92 | 1.86                     | 0.42              |
| 3:c:19:ASN:HB3     | 3:c:20:SER:H       | 1.68                     | 0.42              |
| 16:v:122:GLU:HG3   | 16:v:126:LEU:HD12  | 2.02                     | 0.42              |
| 25:z:101:BCR:H15C  | 25:z:101:BCR:H351  | 1.73                     | 0.42              |
| 23:B:605:CLA:H41   | 23:B:605:CLA:H62   | 1.88                     | 0.42              |
| 4:D:191:TRP:CE3    | 4:D:289:LEU:HD11   | 2.54                     | 0.42              |
| 24:a:2612:PHO:HMC2 | 4:d:279:LEU:HD21   | 2.02                     | 0.42              |
| 24:a:2612:PHO:ND   | 24:a:2612:PHO:NC   | 2.67                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:b:419:SER:OG      | 36:b:625:HTG:H2'2  | 2.20                     | 0.42              |
| 26:d:417:SQD:H462   | 26:d:417:SQD:O9    | 2.20                     | 0.42              |
| 13:o:99:ASP:OD1     | 13:o:100:GLY:N     | 2.50                     | 0.42              |
| 1:A:341:LEU:HD13    | 29:C:526:GOL:H32   | 2.01                     | 0.42              |
| 34:B:647:DMS:H23    | 28:d:401:LMT:H5'   | 2.02                     | 0.42              |
| 3:C:135:ARG:O       | 3:C:135:ARG:HD3    | 2.20                     | 0.42              |
| 16:V:41:HIS:HA      | 16:V:45:ILE:O      | 2.18                     | 0.42              |
| 23:b:611:CLA:H162   | 23:b:611:CLA:H122  | 1.63                     | 0.42              |
| 3:c:276:LEU:HD23    | 23:c:512:CLA:HED1  | 2.02                     | 0.42              |
| 3:C:32:GLY:HA3      | 34:C:536:DMS:H13   | 2.01                     | 0.42              |
| 23:C:514:CLA:HMD1   | 28:Z:101:LMT:H5'   | 2.01                     | 0.42              |
| 13:O:42:ARG:O       | 13:O:241:ALA:HA    | 2.20                     | 0.42              |
| 1:a:85:SER:HA       | 1:a:109:GLY:HA3    | 2.02                     | 0.42              |
| 23:b:608:CLA:CGA    | 23:b:608:CLA:H3A   | 2.50                     | 0.42              |
| 25:y:101:BCR:H11C   | 25:y:101:BCR:H341  | 1.92                     | 0.42              |
| 1:A:163:ILE:HD11    | 37:C:517:DGD:HA22  | 2.02                     | 0.41              |
| 4:D:225:ASP:HB3     | 34:D:2320:DMS:H13  | 2.02                     | 0.41              |
| 4:D:266:TRP:CG      | 38:D:2310:LHG:HC2  | 2.55                     | 0.41              |
| 8:I:4:LEU:HD13      | 36:I:101:HTG:H4'1  | 2.02                     | 0.41              |
| 1:a:188:ALA:HB2     | 1:a:328:MET:HB2    | 2.01                     | 0.41              |
| 1:A:18:CYS:SG       | 8:I:30:ARG:NH2     | 2.93                     | 0.41              |
| 3:C:406:SER:HA      | 3:C:420:VAL:HG23   | 2.01                     | 0.41              |
| 23:b:615:CLA:H203   | 23:b:615:CLA:H152  | 2.01                     | 0.41              |
| 23:c:508:CLA:H93    | 23:c:508:CLA:H111  | 1.91                     | 0.41              |
| 1:A:85:SER:HA       | 1:A:109:GLY:HA3    | 2.01                     | 0.41              |
| 23:C:514:CLA:HAA1   | 36:C:525:HTG:H1'2  | 2.02                     | 0.41              |
| 23:D:2304:CLA:H141  | 23:D:2304:CLA:H161 | 1.88                     | 0.41              |
| 3:c:213:LEU:HD12    | 23:c:509:CLA:H202  | 2.02                     | 0.41              |
| 3:c:266:TRP:CZ3     | 23:c:510:CLA:HAC2  | 2.55                     | 0.41              |
| 3:c:436:PHE:CZ      | 23:c:507:CLA:H202  | 2.55                     | 0.41              |
| 27:d:414:LMG:H191   | 27:d:414:LMG:H162  | 1.97                     | 0.41              |
| 16:v:93:PRO:HA      | 16:v:101:PHE:CD2   | 2.55                     | 0.41              |
| 23:C:502:CLA:C3D    | 23:C:504:CLA:H2    | 2.50                     | 0.41              |
| 13:O:51:LEU:HB3     | 13:O:65:PHE:HB3    | 2.03                     | 0.41              |
| 25:b:624:BCR:H15C   | 25:b:624:BCR:H351  | 1.93                     | 0.41              |
| 38:d:413:LHG:HC62   | 11:l:15:THR:HG23   | 2.02                     | 0.41              |
| 12:m:16[A]:LEU:HD23 | 12:m:16[A]:LEU:HA  | 1.90                     | 0.41              |
| 25:z:101:BCR:H11C   | 25:z:101:BCR:H341  | 1.90                     | 0.41              |
| 23:C:502:CLA:H42    | 23:C:503:CLA:HMD3  | 2.03                     | 0.41              |
| 23:C:505:CLA:H91    | 23:C:505:CLA:H112  | 1.82                     | 0.41              |
| 23:C:513:CLA:C1B    | 25:C:515:BCR:H401  | 2.50                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 37:D:2307:DGD:HA62  | 37:D:2307:DGD:HA92  | 1.76                     | 0.41              |
| 2:b:148[B]:LEU:HD23 | 23:b:609:CLA:H191   | 2.03                     | 0.41              |
| 4:d:293[A]:LEU:HD12 | 4:d:293[A]:LEU:HA   | 1.93                     | 0.41              |
| 24:A:409:PHO:ND     | 24:A:409:PHO:NC     | 2.69                     | 0.41              |
| 2:B:30:VAL:HG12     | 23:B:606:CLA:HHD    | 2.02                     | 0.41              |
| 4:D:210:LEU:HA      | 4:D:213:ILE:HG22    | 2.02                     | 0.41              |
| 4:d:191:TRP:CE3     | 4:d:289:LEU:HD11    | 2.55                     | 0.41              |
| 3:C:52:ALA:HB2      | 23:C:512:CLA:HMA2   | 2.03                     | 0.41              |
| 3:C:240:ILE:HD13    | 3:C:240:ILE:HA      | 1.88                     | 0.41              |
| 16:V:128:ASP:OD2    | 34:V:212:DMS:H12    | 2.21                     | 0.41              |
| 26:a:2603:SQD:H282  | 26:a:2603:SQD:H312  | 1.79                     | 0.41              |
| 3:c:400:PRO:C       | 3:c:401:LEU:HD12    | 2.45                     | 0.41              |
| 2:B:69:LEU:HD12     | 23:B:606:CLA:HBA1   | 2.02                     | 0.41              |
| 23:B:613:CLA:HAA1   | 23:B:613:CLA:HBD    | 2.03                     | 0.41              |
| 23:C:503:CLA:H193   | 36:C:521:HTG:H3'1   | 2.03                     | 0.41              |
| 1:a:235:TYR:HD1     | 1:a:235:TYR:HA      | 1.75                     | 0.41              |
| 25:a:2614:BCR:H11C  | 25:a:2614:BCR:H341  | 1.89                     | 0.41              |
| 25:a:2614:BCR:H24C  | 25:a:2614:BCR:H371  | 1.96                     | 0.41              |
| 2:b:243:ALA:HA      | 2:b:246:PHE:CE2     | 2.55                     | 0.41              |
| 23:b:608:CLA:CAD    | 23:b:610:CLA:H12    | 2.51                     | 0.41              |
| 34:c:535:DMS:H21    | 43:c:697:HOH:O      | 2.21                     | 0.41              |
| 5:E:27:ILE:HB       | 5:E:28:PRO:HD3      | 2.03                     | 0.41              |
| 28:A:420:LMT:H2'    | 28:A:420:LMT:H11    | 1.81                     | 0.40              |
| 23:B:602:CLA:H91    | 23:B:602:CLA:H112   | 1.85                     | 0.40              |
| 25:B:619:BCR:H20C   | 25:B:619:BCR:H361   | 1.98                     | 0.40              |
| 2:b:169:SER:HB3     | 29:b:644:GOL:H2     | 2.02                     | 0.40              |
| 2:b:458:PHE:HB3     | 23:b:609:CLA:HBC2   | 2.02                     | 0.40              |
| 38:d:412:LHG:O9     | 38:l:103:LHG:HC81   | 2.20                     | 0.40              |
| 39:e:103:HEM:HMC2   | 6:f:31:ILE:HG13     | 2.03                     | 0.40              |
| 13:o:83:GLY:HA2     | 13:o:98:GLU:HG2     | 2.02                     | 0.40              |
| 13:o:225[B]:MET:HE3 | 13:o:225[B]:MET:HB3 | 1.95                     | 0.40              |
| 28:A:414:LMT:H51    | 28:A:414:LMT:H22    | 1.74                     | 0.40              |
| 23:c:515:CLA:H3A    | 23:c:515:CLA:HBA2   | 1.80                     | 0.40              |
| 4:d:272:LEU:C       | 4:d:272:LEU:HD23    | 2.46                     | 0.40              |
| 27:A:413:LMG:H201   | 27:A:413:LMG:H231   | 2.00                     | 0.40              |
| 2:B:338:GLN:HA      | 13:o:57:LYS:HE2     | 2.04                     | 0.40              |
| 25:D:2305:BCR:H20C  | 25:D:2305:BCR:H361  | 1.93                     | 0.40              |
| 38:D:2311:LHG:H141  | 38:D:2311:LHG:H332  | 2.03                     | 0.40              |
| 23:a:2609:CLA:CAD   | 23:d:402:CLA:HAC2   | 2.51                     | 0.40              |
| 2:b:86:ILE:H        | 2:b:86:ILE:HG13     | 1.75                     | 0.40              |
| 2:b:224:ARG:HG3     | 7:h:25:TRP:CD2      | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:247:PHE:CD1   | 23:b:607:CLA:H121 | 2.56                     | 0.40              |
| 26:A:412:SQD:H302 | 23:C:509:CLA:H71  | 2.03                     | 0.40              |
| 27:A:413:LMG:H402 | 3:C:281:MET:HG3   | 2.04                     | 0.40              |
| 23:B:604:CLA:CGA  | 23:B:604:CLA:H3A  | 2.50                     | 0.40              |
| 4:D:244:TYR:OH    | 4:D:264:LYS:HE3   | 2.22                     | 0.40              |
| 23:b:620:CLA:H92  | 23:b:620:CLA:H61  | 1.88                     | 0.40              |
| 13:o:53:LYS:HE2   | 13:o:63:ALA:HB3   | 2.03                     | 0.40              |
| 24:A:409:PHO:H42  | 24:A:409:PHO:H11  | 1.83                     | 0.40              |
| 23:A:410:CLA:H18  | 23:C:506:CLA:C14  | 2.52                     | 0.40              |
| 2:B:157:HIS:HA    | 2:B:163:GLY:HA3   | 2.02                     | 0.40              |
| 3:C:24:THR:C      | 3:C:26:ARG:H      | 2.30                     | 0.40              |
| 23:C:514:CLA:H3A  | 23:C:514:CLA:HBA1 | 1.58                     | 0.40              |
| 23:d:402:CLA:C4A  | 23:d:402:CLA:HBA1 | 2.51                     | 0.40              |
| 25:d:410:BCR:H11C | 25:d:410:BCR:H341 | 1.95                     | 0.40              |
| 10:k:23:ASP:OD2   | 17:y:21:GLN:NE2   | 2.53                     | 0.40              |
| 26:l:101:SQD:H341 | 26:l:101:SQD:H311 | 1.79                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 335/344 (97%)  | 331 (99%) | 3 (1%)  | 1 (0%)   | 36          | 34  |
| 1   | a     | 336/344 (98%)  | 332 (99%) | 3 (1%)  | 1 (0%)   | 36          | 34  |
| 2   | B     | 510/505 (101%) | 501 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 2   | b     | 490/505 (97%)  | 484 (99%) | 6 (1%)  | 0        | 100         | 100 |
| 3   | C     | 451/455 (99%)  | 441 (98%) | 8 (2%)  | 2 (0%)   | 30          | 26  |
| 3   | c     | 453/455 (100%) | 444 (98%) | 8 (2%)  | 1 (0%)   | 43          | 44  |
| 4   | D     | 339/342 (99%)  | 332 (98%) | 7 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 4   | d     | 341/342 (100%) | 335 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 5   | E     | 79/83 (95%)    | 79 (100%) | 0       | 0        | 100         | 100 |
| 5   | e     | 78/83 (94%)    | 78 (100%) | 0       | 0        | 100         | 100 |
| 6   | F     | 32/44 (73%)    | 32 (100%) | 0       | 0        | 100         | 100 |
| 6   | f     | 30/44 (68%)    | 30 (100%) | 0       | 0        | 100         | 100 |
| 7   | H     | 61/63 (97%)    | 58 (95%)  | 2 (3%)  | 1 (2%)   | 7           | 3   |
| 7   | h     | 62/63 (98%)    | 59 (95%)  | 2 (3%)  | 1 (2%)   | 7           | 3   |
| 8   | I     | 30/38 (79%)    | 29 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 8   | i     | 30/38 (79%)    | 30 (100%) | 0       | 0        | 100         | 100 |
| 9   | J     | 34/40 (85%)    | 33 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 9   | j     | 37/40 (92%)    | 37 (100%) | 0       | 0        | 100         | 100 |
| 10  | K     | 36/37 (97%)    | 36 (100%) | 0       | 0        | 100         | 100 |
| 10  | k     | 35/37 (95%)    | 35 (100%) | 0       | 0        | 100         | 100 |
| 11  | L     | 36/37 (97%)    | 36 (100%) | 0       | 0        | 100         | 100 |
| 11  | l     | 36/37 (97%)    | 36 (100%) | 0       | 0        | 100         | 100 |
| 12  | M     | 33/36 (92%)    | 33 (100%) | 0       | 0        | 100         | 100 |
| 12  | m     | 33/36 (92%)    | 33 (100%) | 0       | 0        | 100         | 100 |
| 13  | O     | 245/244 (100%) | 240 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 13  | o     | 245/244 (100%) | 240 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 14  | T     | 28/32 (88%)    | 28 (100%) | 0       | 0        | 100         | 100 |
| 14  | t     | 28/32 (88%)    | 28 (100%) | 0       | 0        | 100         | 100 |
| 15  | U     | 96/104 (92%)   | 93 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 15  | u     | 95/104 (91%)   | 92 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 16  | V     | 136/137 (99%)  | 133 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 16  | v     | 136/137 (99%)  | 133 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 17  | Y     | 28/30 (93%)    | 28 (100%) | 0       | 0        | 100         | 100 |
| 17  | y     | 28/30 (93%)    | 28 (100%) | 0       | 0        | 100         | 100 |
| 18  | X     | 36/40 (90%)    | 36 (100%) | 0       | 0        | 100         | 100 |
| 18  | x     | 34/40 (85%)    | 34 (100%) | 0       | 0        | 100         | 100 |
| 19  | Z     | 60/62 (97%)    | 58 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 19  | z     | 59/62 (95%)    | 58 (98%)  | 1 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| All | All   | 5191/5346 (97%) | 5103 (98%) | 81 (2%) | 7 (0%)   | 48          | 50 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 25  | ASN  |
| 3   | C     | 416 | SER  |
| 3   | c     | 416 | SER  |
| 7   | H     | 63  | LYS  |
| 7   | h     | 63  | LYS  |
| 1   | A     | 259 | ILE  |
| 1   | a     | 259 | ILE  |

### 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     | 268/279 (96%)  | 268 (100%) | 0        | 100         | 100 |
| 1   | a     | 272/279 (98%)  | 271 (100%) | 1 (0%)   | 84          | 89  |
| 2   | B     | 406/403 (101%) | 405 (100%) | 1 (0%)   | 87          | 92  |
| 2   | b     | 389/403 (96%)  | 386 (99%)  | 3 (1%)   | 73          | 79  |
| 3   | C     | 354/356 (99%)  | 351 (99%)  | 3 (1%)   | 73          | 79  |
| 3   | c     | 355/356 (100%) | 352 (99%)  | 3 (1%)   | 73          | 79  |
| 4   | D     | 275/276 (100%) | 274 (100%) | 1 (0%)   | 84          | 89  |
| 4   | d     | 277/276 (100%) | 275 (99%)  | 2 (1%)   | 76          | 82  |
| 5   | E     | 69/72 (96%)    | 67 (97%)   | 2 (3%)   | 37          | 39  |
| 5   | e     | 66/72 (92%)    | 66 (100%)  | 0        | 100         | 100 |
| 6   | F     | 26/38 (68%)    | 26 (100%)  | 0        | 100         | 100 |
| 6   | f     | 25/38 (66%)    | 25 (100%)  | 0        | 100         | 100 |
| 7   | H     | 53/53 (100%)   | 53 (100%)  | 0        | 100         | 100 |
| 7   | h     | 54/53 (102%)   | 54 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 8   | I     | 27/34 (79%)     | 27 (100%)   | 0        | 100         | 100 |
| 8   | i     | 28/34 (82%)     | 28 (100%)   | 0        | 100         | 100 |
| 9   | J     | 23/28 (82%)     | 23 (100%)   | 0        | 100         | 100 |
| 9   | j     | 26/28 (93%)     | 26 (100%)   | 0        | 100         | 100 |
| 10  | K     | 31/30 (103%)    | 31 (100%)   | 0        | 100         | 100 |
| 10  | k     | 29/30 (97%)     | 29 (100%)   | 0        | 100         | 100 |
| 11  | L     | 35/35 (100%)    | 35 (100%)   | 0        | 100         | 100 |
| 11  | l     | 36/35 (103%)    | 36 (100%)   | 0        | 100         | 100 |
| 12  | M     | 30/32 (94%)     | 30 (100%)   | 0        | 100         | 100 |
| 12  | m     | 30/32 (94%)     | 30 (100%)   | 0        | 100         | 100 |
| 13  | O     | 206/207 (100%)  | 205 (100%)  | 1 (0%)   | 81          | 87  |
| 13  | o     | 208/207 (100%)  | 208 (100%)  | 0        | 100         | 100 |
| 14  | T     | 26/28 (93%)     | 26 (100%)   | 0        | 100         | 100 |
| 14  | t     | 26/28 (93%)     | 26 (100%)   | 0        | 100         | 100 |
| 15  | U     | 84/89 (94%)     | 84 (100%)   | 0        | 100         | 100 |
| 15  | u     | 84/89 (94%)     | 83 (99%)    | 1 (1%)   | 63          | 70  |
| 16  | V     | 116/117 (99%)   | 116 (100%)  | 0        | 100         | 100 |
| 16  | v     | 115/117 (98%)   | 115 (100%)  | 0        | 100         | 100 |
| 17  | Y     | 21/23 (91%)     | 21 (100%)   | 0        | 100         | 100 |
| 17  | y     | 20/23 (87%)     | 20 (100%)   | 0        | 100         | 100 |
| 18  | X     | 29/33 (88%)     | 29 (100%)   | 0        | 100         | 100 |
| 18  | x     | 28/33 (85%)     | 28 (100%)   | 0        | 100         | 100 |
| 19  | Z     | 48/51 (94%)     | 48 (100%)   | 0        | 100         | 100 |
| 19  | z     | 44/51 (86%)     | 44 (100%)   | 0        | 100         | 100 |
| All | All   | 4239/4368 (97%) | 4221 (100%) | 18 (0%)  | 84          | 89  |

All (18) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 362 | PHE  |
| 3   | C     | 255 | THR  |
| 3   | C     | 289 | PHE  |
| 3   | C     | 315 | MET  |
| 4   | D     | 90  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 5   | THR  |
| 5   | E     | 65  | LEU  |
| 13  | O     | 110 | MET  |
| 1   | a     | 15  | GLU  |
| 2   | b     | 121 | GLU  |
| 2   | b     | 362 | PHE  |
| 2   | b     | 467 | ILE  |
| 3   | c     | 255 | THR  |
| 3   | c     | 289 | PHE  |
| 3   | c     | 315 | MET  |
| 4   | d     | 24  | ARG  |
| 4   | d     | 90  | LEU  |
| 15  | u     | 9   | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 75  | ASN  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 296 | ASN  |
| 2   | B     | 14  | ASN  |
| 2   | B     | 331 | ASN  |
| 2   | B     | 374 | ASN  |
| 3   | C     | 418 | ASN  |
| 4   | D     | 186 | GLN  |
| 4   | D     | 255 | GLN  |
| 4   | D     | 301 | GLN  |
| 5   | E     | 74  | GLN  |
| 19  | Z     | 58  | ASN  |
| 1   | a     | 165 | GLN  |
| 1   | a     | 252 | HIS  |
| 1   | a     | 296 | ASN  |
| 2   | b     | 282 | GLN  |
| 2   | b     | 394 | GLN  |
| 3   | c     | 19  | ASN  |
| 3   | c     | 201 | ASN  |
| 3   | c     | 415 | ASN  |
| 4   | d     | 186 | GLN  |
| 15  | u     | 78  | ASN  |
| 15  | u     | 81  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res    | Link | Bond lengths |       |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|-------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ  | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | FME  | m     | 1      | 12   | 8,9,10       | 0.53  | 0        | 7,9,11      | 1.36 | 1 (14%)  |
| 4   | HSK  | d     | 336[A] | -    | 9,10,12      | 13.41 | 1 (11%)  | 6,12,16     | 2.04 | 3 (50%)  |
| 4   | HSK  | d     | 336[B] | -    | 9,11,12      | 1.76  | 2 (22%)  | 6,14,16     | 4.06 | 4 (66%)  |
| 8   | FME  | I     | 1      | 8    | 8,9,10       | 0.57  | 0        | 7,9,11      | 1.72 | 3 (42%)  |
| 12  | FME  | M     | 1      | 12   | 8,9,10       | 0.65  | 0        | 7,9,11      | 1.15 | 0        |
| 19  | FME  | Z     | 1      | 19   | 8,9,10       | 0.62  | 0        | 7,9,11      | 1.80 | 3 (42%)  |
| 14  | FME  | T     | 1      | 14   | 8,9,10       | 0.79  | 0        | 7,9,11      | 1.73 | 2 (28%)  |
| 8   | FME  | i     | 1      | 8    | 8,9,10       | 0.64  | 0        | 7,9,11      | 1.69 | 3 (42%)  |
| 4   | HSK  | D     | 336[A] | -    | 9,10,12      | 13.04 | 1 (11%)  | 6,12,16     | 1.78 | 2 (33%)  |
| 14  | FME  | t     | 1      | 14   | 8,9,10       | 0.69  | 0        | 7,9,11      | 1.76 | 4 (57%)  |
| 4   | HSK  | D     | 336[B] | -    | 9,11,12      | 1.79  | 2 (22%)  | 6,14,16     | 3.83 | 4 (66%)  |
| 19  | FME  | z     | 1      | 19   | 8,9,10       | 0.58  | 0        | 7,9,11      | 1.70 | 3 (42%)  |

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   |
|-----|------|-------|--------|------|---------|----------|---------|
| 12  | FME  | m     | 1      | 12   | -       | 0/7/9/11 | -       |
| 4   | HSK  | d     | 336[A] | -    | -       | 0/5/6/8  | 0/1/1/1 |
| 4   | HSK  | d     | 336[B] | -    | -       | 0/5/6/8  | 0/1/1/1 |
| 8   | FME  | I     | 1      | 8    | -       | 2/7/9/11 | -       |
| 12  | FME  | M     | 1      | 12   | -       | 2/7/9/11 | -       |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions | Rings   |
|-----|------|-------|--------|------|---------|----------|---------|
| 19  | FME  | Z     | 1      | 19   | -       | 3/7/9/11 | -       |
| 14  | FME  | T     | 1      | 14   | -       | 3/7/9/11 | -       |
| 8   | FME  | i     | 1      | 8    | -       | 2/7/9/11 | -       |
| 4   | HSK  | D     | 336[A] | -    | -       | 0/5/6/8  | 0/1/1/1 |
| 14  | FME  | t     | 1      | 14   | -       | 3/7/9/11 | -       |
| 4   | HSK  | D     | 336[B] | -    | -       | 0/5/6/8  | 0/1/1/1 |
| 19  | FME  | z     | 1      | 19   | -       | 5/7/9/11 | -       |

All (6) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|--------|-------------|----------|
| 4   | d     | 336[A] | HSK  | OM-ND1  | -40.09 | 0.86        | 1.38     |
| 4   | D     | 336[A] | HSK  | OM-ND1  | -38.97 | 0.87        | 1.38     |
| 4   | D     | 336[B] | HSK  | OM-ND1  | 3.84   | 1.43        | 1.38     |
| 4   | d     | 336[B] | HSK  | OM-ND1  | 3.69   | 1.43        | 1.38     |
| 4   | d     | 336[B] | HSK  | CE1-ND1 | -2.36  | 1.33        | 1.37     |
| 4   | D     | 336[B] | HSK  | CE1-ND1 | -2.25  | 1.33        | 1.37     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 4   | d     | 336[B] | HSK  | ND1-CE1-NE2 | -6.13 | 104.09      | 111.75   |
| 4   | d     | 336[B] | HSK  | CE1-ND1-CG  | 6.00  | 115.05      | 107.37   |
| 4   | D     | 336[B] | HSK  | ND1-CE1-NE2 | -5.91 | 104.35      | 111.75   |
| 4   | D     | 336[B] | HSK  | CE1-ND1-CG  | 5.68  | 114.64      | 107.37   |
| 4   | d     | 336[B] | HSK  | CD2-NE2-CE1 | 3.53  | 109.51      | 105.22   |
| 4   | d     | 336[B] | HSK  | CB-CG-ND1   | 3.42  | 128.66      | 122.89   |
| 4   | D     | 336[B] | HSK  | CD2-NE2-CE1 | 3.36  | 109.31      | 105.22   |
| 4   | d     | 336[A] | HSK  | ND1-CE1-NE2 | -2.89 | 108.13      | 111.75   |
| 19  | z     | 1      | FME  | CE-SD-CG    | 2.89  | 110.32      | 100.40   |
| 12  | m     | 1      | FME  | CE-SD-CG    | 2.80  | 110.00      | 100.40   |
| 14  | T     | 1      | FME  | CE-SD-CG    | 2.73  | 109.79      | 100.40   |
| 19  | Z     | 1      | FME  | CE-SD-CG    | 2.68  | 109.61      | 100.40   |
| 4   | D     | 336[B] | HSK  | CB-CG-ND1   | 2.67  | 127.39      | 122.89   |
| 4   | d     | 336[A] | HSK  | CD2-NE2-CE1 | 2.62  | 108.41      | 105.22   |
| 4   | D     | 336[A] | HSK  | ND1-CE1-NE2 | -2.52 | 108.60      | 111.75   |
| 8   | i     | 1      | FME  | CA-N-CN     | -2.51 | 118.97      | 122.82   |
| 14  | t     | 1      | FME  | CE-SD-CG    | 2.49  | 108.94      | 100.40   |
| 19  | Z     | 1      | FME  | CA-N-CN     | -2.42 | 119.10      | 122.82   |
| 4   | D     | 336[A] | HSK  | CD2-NE2-CE1 | 2.38  | 108.11      | 105.22   |
| 19  | z     | 1      | FME  | O-C-CA      | -2.32 | 118.71      | 124.78   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 4   | d     | 336[A] | HSK  | CB-CG-ND1 | 2.28  | 126.74      | 122.89   |
| 14  | t     | 1      | FME  | O-C-CA    | -2.18 | 119.05      | 124.78   |
| 8   | I     | 1      | FME  | CE-SD-CG  | 2.18  | 107.89      | 100.40   |
| 19  | Z     | 1      | FME  | O1-CN-N   | -2.14 | 119.64      | 125.27   |
| 14  | t     | 1      | FME  | CA-N-CN   | -2.12 | 119.56      | 122.82   |
| 14  | t     | 1      | FME  | O1-CN-N   | -2.11 | 119.71      | 125.27   |
| 8   | I     | 1      | FME  | O-C-CA    | -2.10 | 119.29      | 124.78   |
| 14  | T     | 1      | FME  | O-C-CA    | -2.09 | 119.31      | 124.78   |
| 8   | i     | 1      | FME  | O1-CN-N   | -2.05 | 119.88      | 125.27   |
| 19  | z     | 1      | FME  | O1-CN-N   | -2.04 | 119.90      | 125.27   |
| 8   | i     | 1      | FME  | CE-SD-CG  | 2.02  | 107.34      | 100.40   |
| 8   | I     | 1      | FME  | CA-N-CN   | -2.02 | 119.72      | 122.82   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 14  | T     | 1   | FME  | N-CA-CB-CG  |
| 19  | Z     | 1   | FME  | O-C-CA-CB   |
| 19  | Z     | 1   | FME  | CA-CB-CG-SD |
| 8   | i     | 1   | FME  | O1-CN-N-CA  |
| 19  | z     | 1   | FME  | O1-CN-N-CA  |
| 19  | z     | 1   | FME  | CB-CA-N-CN  |
| 19  | z     | 1   | FME  | N-CA-CB-CG  |
| 14  | T     | 1   | FME  | CB-CG-SD-CE |
| 14  | t     | 1   | FME  | CB-CG-SD-CE |
| 14  | t     | 1   | FME  | N-CA-CB-CG  |
| 19  | Z     | 1   | FME  | CB-CG-SD-CE |
| 14  | T     | 1   | FME  | C-CA-CB-CG  |
| 14  | t     | 1   | FME  | C-CA-CB-CG  |
| 8   | I     | 1   | FME  | O1-CN-N-CA  |
| 12  | M     | 1   | FME  | O1-CN-N-CA  |
| 19  | z     | 1   | FME  | CB-CG-SD-CE |
| 19  | z     | 1   | FME  | C-CA-CB-CG  |
| 8   | I     | 1   | FME  | CB-CA-N-CN  |
| 12  | M     | 1   | FME  | CB-CA-N-CN  |
| 8   | i     | 1   | FME  | CB-CA-N-CN  |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 8   | I     | 1   | FME  | 1       | 0            |
| 8   | i     | 1   | FME  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 407 ligands modelled in this entry, 15 are monoatomic and 37 are unknown - leaving 355 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 | $\# Z  > 2$ |
| 34  | DMS  | O     | 311  | -    | 3,3,3        | 2.69 | 1 (33%)     | 3,3,3       | 0.58 | 0           |
| 38  | LHG  | D     | 2311 | -    | 38,38,48     | 0.95 | 2 (5%)      | 41,44,54    | 1.11 | 3 (7%)      |
| 38  | LHG  | L     | 101  | -    | 48,48,48     | 0.93 | 2 (4%)      | 51,54,54    | 1.06 | 5 (9%)      |
| 23  | CLA  | b     | 619  | 2    | 69,73,73     | 2.45 | 25 (36%)    | 83,113,113  | 2.63 | 32 (38%)    |
| 23  | CLA  | a     | 2609 | 1    | 69,73,73     | 2.52 | 24 (34%)    | 83,113,113  | 2.47 | 26 (31%)    |
| 34  | DMS  | c     | 541  | -    | 3,3,3        | 2.68 | 1 (33%)     | 3,3,3       | 0.60 | 0           |
| 25  | BCR  | b     | 623  | -    | 41,41,41     | 0.86 | 0           | 56,56,56    | 1.21 | 6 (10%)     |
| 37  | DGD  | c     | 519  | -    | 63,63,67     | 0.86 | 2 (3%)      | 77,77,81    | 1.14 | 6 (7%)      |
| 36  | HTG  | B     | 627  | -    | 19,19,19     | 1.02 | 2 (10%)     | 23,24,24    | 1.37 | 2 (8%)      |
| 34  | DMS  | O     | 307  | -    | 3,3,3        | 2.66 | 1 (33%)     | 3,3,3       | 0.53 | 0           |
| 34  | DMS  | b     | 637  | -    | 3,3,3        | 2.74 | 1 (33%)     | 3,3,3       | 0.67 | 0           |
| 36  | HTG  | c     | 524  | -    | 19,19,19     | 1.05 | 2 (10%)     | 23,24,24    | 1.44 | 2 (8%)      |
| 37  | DGD  | C     | 518  | -    | 63,63,67     | 0.87 | 2 (3%)      | 77,77,81    | 1.05 | 6 (7%)      |
| 29  | GOL  | C     | 526  | -    | 5,5,5        | 1.12 | 1 (20%)     | 5,5,5       | 0.96 | 0           |
| 38  | LHG  | D     | 2309 | -    | 48,48,48     | 0.90 | 2 (4%)      | 51,54,54    | 1.15 | 5 (9%)      |
| 23  | CLA  | b     | 615  | 43   | 69,73,73     | 2.52 | 25 (36%)    | 83,113,113  | 2.47 | 28 (33%)    |
| 23  | CLA  | b     | 616  | 2    | 69,73,73     | 2.35 | 25 (36%)    | 83,113,113  | 2.46 | 30 (36%)    |



| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | DMS  | b     | 640    | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 36  | HTG  | C     | 525    | -    | 19,19,19     | 1.10 | 2 (10%)  | 23,24,24    | 1.69 | 4 (17%)  |
| 42  | HEC  | V     | 201    | 16   | 50,50,50     | 1.90 | 10 (20%) | 68,82,82    | 1.49 | 8 (11%)  |
| 28  | LMT  | J     | 303    | -    | 24,24,36     | 0.54 | 0        | 29,29,47    | 0.94 | 1 (3%)   |
| 34  | DMS  | o     | 305    | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.50 | 0        |
| 23  | CLA  | B     | 617    | 2    | 69,73,73     | 2.54 | 22 (31%) | 83,113,113  | 2.49 | 29 (34%) |
| 34  | DMS  | B     | 646    | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.70 | 0        |
| 23  | CLA  | B     | 612    | 2    | 69,73,73     | 2.56 | 22 (31%) | 83,113,113  | 2.57 | 30 (36%) |
| 23  | CLA  | d     | 409    | 4    | 69,73,73     | 2.55 | 24 (34%) | 83,113,113  | 2.48 | 27 (32%) |
| 33  | PL9  | D     | 2306   | -    | 55,55,55     | 0.69 | 1 (1%)   | 68,69,69    | 1.60 | 18 (26%) |
| 34  | DMS  | o     | 306    | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 34  | DMS  | o     | 308    | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.46 | 0        |
| 23  | CLA  | C     | 504    | 3    | 69,73,73     | 2.51 | 22 (31%) | 83,113,113  | 2.39 | 27 (32%) |
| 23  | CLA  | d     | 402    | 43   | 69,73,73     | 2.48 | 22 (31%) | 83,113,113  | 2.57 | 28 (33%) |
| 26  | SQD  | d     | 417    | -    | 31,32,54     | 1.97 | 4 (12%)  | 34,36,65    | 1.57 | 4 (11%)  |
| 36  | HTG  | b     | 604    | -    | 19,19,19     | 1.07 | 2 (10%)  | 23,24,24    | 1.66 | 4 (17%)  |
| 34  | DMS  | V     | 211    | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 29  | GOL  | b     | 631    | -    | 5,5,5        | 1.07 | 0        | 5,5,5       | 0.60 | 0        |
| 23  | CLA  | a     | 2613   | 1    | 69,73,73     | 2.28 | 22 (31%) | 83,113,113  | 2.52 | 29 (34%) |
| 26  | SQD  | a     | 2615   | -    | 47,48,54     | 1.01 | 3 (6%)   | 56,59,65    | 1.79 | 12 (21%) |
| 29  | GOL  | E     | 104    | -    | 5,5,5        | 1.00 | 0        | 5,5,5       | 0.88 | 0        |
| 40  | RRX  | H     | 102    | -    | 42,42,42     | 0.69 | 0        | 57,58,58    | 1.47 | 9 (15%)  |
| 23  | CLA  | c     | 506    | 3    | 69,73,73     | 2.56 | 24 (34%) | 83,113,113  | 2.39 | 26 (31%) |
| 34  | DMS  | V     | 206    | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.73 | 0        |
| 26  | SQD  | D     | 2308   | -    | 44,45,54     | 1.12 | 3 (6%)   | 53,56,65    | 1.31 | 8 (15%)  |
| 34  | DMS  | B     | 636    | -    | 3,3,3        | 2.57 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 23  | CLA  | B     | 602    | 43   | 69,73,73     | 2.66 | 26 (37%) | 83,113,113  | 2.28 | 25 (30%) |
| 31  | JOX  | A     | 419    | -    | 10,10,10     | 1.98 | 4 (40%)  | 14,14,14    | 4.84 | 11 (78%) |
| 34  | DMS  | c     | 543    | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.50 | 0        |
| 25  | BCR  | c     | 517    | -    | 41,41,41     | 0.75 | 0        | 56,56,56    | 1.57 | 9 (16%)  |
| 34  | DMS  | C     | 535    | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 36  | HTG  | i     | 102    | -    | 19,19,19     | 1.13 | 2 (10%)  | 23,24,24    | 1.92 | 3 (13%)  |
| 23  | CLA  | C     | 513    | 3    | 69,73,73     | 2.86 | 24 (34%) | 83,113,113  | 2.45 | 28 (33%) |
| 36  | HTG  | B     | 624[A] | -    | 19,19,19     | 0.90 | 1 (5%)   | 23,24,24    | 1.25 | 4 (17%)  |
| 34  | DMS  | O     | 313    | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.60 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | DMS  | c     | 547  | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 34  | DMS  | A     | 427  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 34  | DMS  | d     | 422  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 28  | LMT  | M     | 101  | -    | 36,36,36     | 0.47 | 0        | 47,47,47    | 1.27 | 7 (14%)  |
| 24  | PHO  | a     | 2611 | -    | 58,69,69     | 2.62 | 11 (18%) | 56,99,99    | 2.76 | 17 (30%) |
| 25  | BCR  | k     | 302  | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 1.47 | 12 (21%) |
| 34  | DMS  | c     | 539  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 36  | HTG  | b     | 625  | -    | 19,19,19     | 0.89 | 1 (5%)   | 23,24,24    | 1.54 | 4 (17%)  |
| 29  | GOL  | V     | 203  | -    | 5,5,5        | 0.90 | 0        | 5,5,5       | 0.92 | 0        |
| 31  | JOX  | a     | 2619 | 1    | 10,10,10     | 1.91 | 6 (60%)  | 14,14,14    | 2.29 | 5 (35%)  |
| 25  | BCR  | d     | 410  | -    | 41,41,41     | 0.80 | 0        | 56,56,56    | 1.65 | 5 (8%)   |
| 34  | DMS  | B     | 645  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 34  | DMS  | a     | 2624 | -    | 3,3,3        | 2.74 | 1 (33%)  | 3,3,3       | 0.70 | 0        |
| 25  | BCR  | b     | 624  | -    | 41,41,41     | 0.72 | 0        | 56,56,56    | 1.59 | 12 (21%) |
| 34  | DMS  | C     | 533  | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.35 | 0        |
| 27  | LMG  | B     | 622  | -    | 51,51,55     | 0.94 | 2 (3%)   | 59,59,63    | 1.05 | 3 (5%)   |
| 34  | DMS  | O     | 314  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 34  | DMS  | b     | 634  | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.35 | 0        |
| 34  | DMS  | C     | 532  | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.72 | 0        |
| 23  | CLA  | b     | 617  | 2    | 69,73,73     | 2.36 | 22 (31%) | 83,113,113  | 2.58 | 26 (31%) |
| 34  | DMS  | O     | 312  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 34  | DMS  | c     | 544  | -    | 3,3,3        | 2.73 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 38  | LHG  | D     | 2310 | -    | 48,48,48     | 0.87 | 2 (4%)   | 51,54,54    | 0.95 | 3 (5%)   |
| 23  | CLA  | c     | 516  | 3    | 69,73,73     | 2.52 | 25 (36%) | 83,113,113  | 2.39 | 26 (31%) |
| 34  | DMS  | D     | 2316 | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 23  | CLA  | b     | 606  | 43   | 69,73,73     | 2.67 | 26 (37%) | 83,113,113  | 2.28 | 27 (32%) |
| 27  | LMG  | d     | 414  | 41   | 51,51,55     | 0.90 | 2 (3%)   | 59,59,63    | 0.86 | 1 (1%)   |
| 32  | BCT  | a     | 2608 | 21   | 2,3,3        | 0.67 | 0        | 2,3,3       | 1.05 | 0        |
| 29  | GOL  | O     | 305  | -    | 5,5,5        | 0.88 | 0        | 5,5,5       | 0.90 | 0        |
| 34  | DMS  | o     | 312  | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.49 | 0        |
| 34  | DMS  | v     | 210  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 28  | LMT  | Z     | 101  | -    | 36,36,36     | 0.45 | 0        | 47,47,47    | 0.91 | 2 (4%)   |
| 23  | CLA  | B     | 614  | 2    | 69,73,73     | 2.37 | 22 (31%) | 83,113,113  | 2.54 | 28 (33%) |
| 23  | CLA  | A     | 406  | 43   | 69,73,73     | 2.32 | 23 (33%) | 83,113,113  | 2.74 | 30 (36%) |
| 23  | CLA  | b     | 609  | 2    | 69,73,73     | 2.78 | 23 (33%) | 83,113,113  | 2.44 | 27 (32%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | DMS  | V     | 205  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 36  | HTG  | d     | 415  | -    | 19,19,19     | 1.05 | 2 (10%)  | 23,24,24    | 1.52 | 1 (4%)   |
| 29  | GOL  | B     | 632  | -    | 5,5,5        | 0.95 | 0        | 5,5,5       | 0.91 | 0        |
| 24  | PHO  | A     | 409  | -    | 58,69,69     | 2.79 | 16 (27%) | 56,99,99    | 2.88 | 13 (23%) |
| 23  | CLA  | A     | 407  | 43   | 69,73,73     | 2.24 | 23 (33%) | 83,113,113  | 2.58 | 32 (38%) |
| 31  | JOX  | A     | 418  | -    | 10,10,10     | 2.05 | 4 (40%)  | 14,14,14    | 3.36 | 10 (71%) |
| 23  | CLA  | a     | 2610 | 43   | 69,73,73     | 2.37 | 22 (31%) | 83,113,113  | 2.62 | 29 (34%) |
| 29  | GOL  | O     | 302  | -    | 5,5,5        | 0.92 | 0        | 5,5,5       | 1.03 | 0        |
| 34  | DMS  | a     | 2622 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.49 | 0        |
| 23  | CLA  | c     | 508  | 3    | 69,73,73     | 2.56 | 25 (36%) | 83,113,113  | 2.50 | 23 (27%) |
| 23  | CLA  | b     | 611  | 2    | 69,73,73     | 2.65 | 23 (33%) | 83,113,113  | 2.41 | 26 (31%) |
| 27  | LMG  | C     | 527  | -    | 51,51,55     | 0.96 | 2 (3%)   | 59,59,63    | 1.27 | 5 (8%)   |
| 23  | CLA  | A     | 405  | 1    | 69,73,73     | 2.36 | 23 (33%) | 83,113,113  | 2.49 | 29 (34%) |
| 23  | CLA  | D     | 2303 | 4    | 69,73,73     | 2.14 | 22 (31%) | 83,113,113  | 2.66 | 27 (32%) |
| 23  | CLA  | B     | 608  | 43   | 69,73,73     | 2.42 | 22 (31%) | 83,113,113  | 2.45 | 28 (33%) |
| 29  | GOL  | v     | 203  | -    | 5,5,5        | 0.93 | 0        | 5,5,5       | 1.14 | 1 (20%)  |
| 29  | GOL  | U     | 502  | -    | 5,5,5        | 1.29 | 1 (20%)  | 5,5,5       | 0.80 | 0        |
| 34  | DMS  | d     | 423  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.51 | 0        |
| 23  | CLA  | c     | 512  | 3    | 69,73,73     | 2.57 | 24 (34%) | 83,113,113  | 2.47 | 26 (31%) |
| 28  | LMT  | i     | 103  | -    | 24,24,36     | 0.51 | 0        | 29,29,47    | 1.08 | 2 (6%)   |
| 23  | CLA  | b     | 614  | 2    | 69,73,73     | 2.61 | 24 (34%) | 83,113,113  | 2.33 | 27 (32%) |
| 25  | BCR  | y     | 101  | -    | 41,41,41     | 0.76 | 0        | 56,56,56    | 1.56 | 12 (21%) |
| 27  | LMG  | c     | 522  | -    | 51,51,55     | 0.98 | 2 (3%)   | 59,59,63    | 1.34 | 6 (10%)  |
| 34  | DMS  | U     | 505  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.62 | 0        |
| 34  | DMS  | d     | 418  | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.62 | 0        |
| 34  | DMS  | B     | 640  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.51 | 0        |
| 23  | CLA  | C     | 511  | 3    | 69,73,73     | 2.64 | 25 (36%) | 83,113,113  | 2.47 | 30 (36%) |
| 34  | DMS  | B     | 642  | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 37  | DGD  | c     | 520  | -    | 63,63,67     | 0.88 | 3 (4%)   | 77,77,81    | 0.86 | 5 (6%)   |
| 38  | LHG  | l     | 103  | -    | 48,48,48     | 0.87 | 2 (4%)   | 51,54,54    | 1.02 | 3 (5%)   |
| 28  | LMT  | z     | 102  | -    | 33,33,36     | 0.54 | 0        | 43,43,47    | 1.06 | 4 (9%)   |
| 34  | DMS  | A     | 428  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 29  | GOL  | c     | 531  | -    | 5,5,5        | 0.95 | 0        | 5,5,5       | 0.86 | 0        |
| 28  | LMT  | B     | 634  | -    | 36,36,36     | 0.53 | 1 (2%)   | 47,47,47    | 0.85 | 0        |
| 23  | CLA  | B     | 603  | 2    | 69,73,73     | 2.55 | 24 (34%) | 83,113,113  | 2.48 | 29 (34%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | LMG  | c     | 521  | -    | 49,49,55     | 0.91 | 2 (4%)   | 57,57,63    | 1.13 | 5 (8%)   |
| 36  | HTG  | c     | 526  | -    | 19,19,19     | 1.00 | 2 (10%)  | 23,24,24    | 1.24 | 1 (4%)   |
| 34  | DMS  | O     | 317  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 37  | DGD  | h     | 102  | -    | 63,63,67     | 0.88 | 2 (3%)   | 77,77,81    | 1.03 | 5 (6%)   |
| 36  | HTG  | b     | 626  | -    | 19,19,19     | 1.14 | 2 (10%)  | 23,24,24    | 1.46 | 2 (8%)   |
| 25  | BCR  | T     | 102  | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 1.85 | 14 (25%) |
| 28  | LMT  | j     | 2701 | 41   | 34,34,36     | 0.56 | 1 (2%)   | 44,44,47    | 1.05 | 3 (6%)   |
| 34  | DMS  | U     | 504  | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 38  | LHG  | d     | 412  | -    | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.01 | 3 (5%)   |
| 34  | DMS  | C     | 536  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 23  | CLA  | b     | 621  | 2    | 69,73,73     | 2.57 | 23 (33%) | 83,113,113  | 2.63 | 28 (33%) |
| 25  | BCR  | a     | 2614 | -    | 41,41,41     | 0.80 | 0        | 56,56,56    | 1.31 | 6 (10%)  |
| 36  | HTG  | B     | 625  | -    | 19,19,19     | 1.05 | 1 (5%)   | 23,24,24    | 2.09 | 4 (17%)  |
| 23  | CLA  | c     | 513  | 3    | 69,73,73     | 2.61 | 25 (36%) | 83,113,113  | 2.35 | 28 (33%) |
| 34  | DMS  | c     | 534  | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.50 | 0        |
| 34  | DMS  | B     | 644  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.47 | 0        |
| 25  | BCR  | K     | 101  | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 1.33 | 9 (16%)  |
| 34  | DMS  | O     | 308  | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 33  | PL9  | A     | 422  | -    | 38,38,55     | 0.42 | 0        | 45,45,69    | 1.86 | 14 (31%) |
| 34  | DMS  | U     | 503  | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 23  | CLA  | c     | 507  | 43   | 69,73,73     | 2.28 | 22 (31%) | 83,113,113  | 2.64 | 25 (30%) |
| 38  | LHG  | d     | 403  | -    | 42,42,48     | 0.98 | 2 (4%)   | 45,48,54    | 0.91 | 3 (6%)   |
| 26  | SQD  | D     | 2302 | -    | 53,54,54     | 1.05 | 4 (7%)   | 62,65,65    | 1.42 | 9 (14%)  |
| 34  | DMS  | B     | 647  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 34  | DMS  | O     | 319  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.51 | 0        |
| 34  | DMS  | o     | 316  | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 34  | DMS  | d     | 420  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 36  | HTG  | b     | 602  | -    | 19,19,19     | 1.04 | 1 (5%)   | 23,24,24    | 1.04 | 2 (8%)   |
| 23  | CLA  | b     | 608  | 2    | 69,73,73     | 2.55 | 24 (34%) | 83,113,113  | 2.50 | 28 (33%) |
| 25  | BCR  | Y     | 302  | -    | 41,41,41     | 0.81 | 0        | 56,56,56    | 1.76 | 11 (19%) |
| 34  | DMS  | A     | 424  | -    | 3,3,3        | 2.61 | 1 (33%)  | 3,3,3       | 0.62 | 0        |
| 25  | BCR  | C     | 516  | -    | 41,41,41     | 0.74 | 0        | 56,56,56    | 1.53 | 7 (12%)  |
| 27  | LMG  | m     | 2802 | -    | 51,51,55     | 0.95 | 2 (3%)   | 59,59,63    | 1.06 | 2 (3%)   |
| 23  | CLA  | b     | 618  | 2    | 69,73,73     | 2.43 | 24 (34%) | 83,113,113  | 2.44 | 26 (31%) |
| 28  | LMT  | A     | 420  | -    | 24,24,36     | 0.42 | 0        | 29,29,47    | 0.96 | 0        |

| Mol | Type | Chain | Res  | Link   | Bond lengths |      |          | Bond angles |      |           |
|-----|------|-------|------|--------|--------------|------|----------|-------------|------|-----------|
|     |      |       |      |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2  |
| 34  | DMS  | D     | 2319 | -      | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.52 | 0         |
| 25  | BCR  | D     | 2305 | -      | 41,41,41     | 0.82 | 1 (2%)   | 56,56,56    | 1.63 | 8 (14%)   |
| 28  | LMT  | d     | 404  | -      | 25,25,36     | 0.52 | 0        | 30,30,47    | 0.90 | 2 (6%)    |
| 34  | DMS  | c     | 540  | -      | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.55 | 0         |
| 26  | SQD  | a     | 2603 | -      | 53,54,54     | 1.03 | 3 (5%)   | 62,65,65    | 1.14 | 3 (4%)    |
| 31  | JOX  | a     | 2617 | -      | 10,10,10     | 1.85 | 4 (40%)  | 14,14,14    | 4.93 | 14 (100%) |
| 28  | LMT  | A     | 414  | -      | 34,34,36     | 0.49 | 0        | 45,45,47    | 1.17 | 4 (8%)    |
| 29  | GOL  | A     | 417  | -      | 5,5,5        | 0.89 | 0        | 5,5,5       | 1.02 | 0         |
| 25  | BCR  | B     | 619  | -      | 41,41,41     | 0.81 | 0        | 56,56,56    | 1.20 | 5 (8%)    |
| 34  | DMS  | V     | 213  | -      | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.51 | 0         |
| 34  | DMS  | o     | 310  | -      | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.50 | 0         |
| 25  | BCR  | B     | 620  | -      | 41,41,41     | 0.74 | 0        | 56,56,56    | 1.17 | 6 (10%)   |
| 20  | OEX  | A     | 401  | 3,43,1 | 0,14,14      | -    | -        | -           | -    | -         |
| 24  | PHO  | A     | 408  | -      | 58,69,69     | 2.70 | 12 (20%) | 56,99,99    | 2.73 | 14 (25%)  |
| 34  | DMS  | c     | 537  | -      | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.56 | 0         |
| 34  | DMS  | O     | 315  | -      | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.52 | 0         |
| 23  | CLA  | b     | 620  | 2      | 69,73,73     | 2.49 | 24 (34%) | 83,113,113  | 2.27 | 31 (37%)  |
| 36  | HTG  | o     | 301  | -      | 19,19,19     | 0.88 | 1 (5%)   | 23,24,24    | 1.15 | 2 (8%)    |
| 29  | GOL  | C     | 524  | -      | 5,5,5        | 0.83 | 0        | 5,5,5       | 0.97 | 0         |
| 34  | DMS  | b     | 642  | -      | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.52 | 0         |
| 25  | BCR  | B     | 618  | -      | 41,41,41     | 0.76 | 0        | 56,56,56    | 1.28 | 5 (8%)    |
| 23  | CLA  | b     | 613  | 2      | 69,73,73     | 2.52 | 25 (36%) | 83,113,113  | 2.51 | 31 (37%)  |
| 34  | DMS  | o     | 314  | -      | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.50 | 0         |
| 29  | GOL  | v     | 204  | -      | 5,5,5        | 0.88 | 0        | 5,5,5       | 0.96 | 0         |
| 34  | DMS  | A     | 429  | -      | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.53 | 0         |
| 34  | DMS  | D     | 2317 | -      | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.55 | 0         |
| 25  | BCR  | B     | 633  | -      | 41,41,41     | 0.69 | 0        | 56,56,56    | 1.72 | 12 (21%)  |
| 23  | CLA  | c     | 515  | 3      | 69,73,73     | 2.65 | 25 (36%) | 83,113,113  | 2.52 | 30 (36%)  |
| 23  | CLA  | B     | 609  | 2      | 69,73,73     | 2.50 | 24 (34%) | 83,113,113  | 2.38 | 28 (33%)  |
| 34  | DMS  | O     | 309  | -      | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.52 | 0         |
| 29  | GOL  | c     | 530  | -      | 5,5,5        | 0.92 | 0        | 5,5,5       | 0.80 | 0         |
| 34  | DMS  | C     | 530  | -      | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.47 | 0         |
| 34  | DMS  | v     | 206  | -      | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.58 | 0         |
| 34  | DMS  | l     | 104  | -      | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.51 | 0         |
| 23  | CLA  | B     | 611  | 43     | 69,73,73     | 2.37 | 25 (36%) | 83,113,113  | 2.59 | 30 (36%)  |
| 23  | CLA  | d     | 408  | 4      | 69,73,73     | 2.41 | 24 (34%) | 83,113,113  | 2.55 | 27 (32%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | HTG  | C     | 521  | -    | 19,19,19     | 0.99 | 2 (10%)  | 23,24,24    | 1.04 | 1 (4%)   |
| 36  | HTG  | C     | 522  | -    | 19,19,19     | 0.97 | 2 (10%)  | 23,24,24    | 2.32 | 4 (17%)  |
| 34  | DMS  | B     | 635  | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 23  | CLA  | C     | 502  | 3    | 69,73,73     | 2.69 | 26 (37%) | 83,113,113  | 2.28 | 24 (28%) |
| 23  | CLA  | c     | 504  | 3    | 69,73,73     | 2.41 | 23 (33%) | 83,113,113  | 2.64 | 25 (30%) |
| 26  | SQD  | l     | 101  | -    | 53,54,54     | 1.05 | 4 (7%)   | 62,65,65    | 1.69 | 10 (16%) |
| 25  | BCR  | b     | 622  | -    | 41,41,41     | 0.78 | 0        | 56,56,56    | 1.39 | 9 (16%)  |
| 33  | PL9  | d     | 411  | -    | 55,55,55     | 0.69 | 1 (1%)   | 68,69,69    | 1.60 | 15 (22%) |
| 34  | DMS  | C     | 534  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 34  | DMS  | O     | 310  | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 23  | CLA  | C     | 507  | 3    | 69,73,73     | 2.58 | 23 (33%) | 83,113,113  | 2.61 | 29 (34%) |
| 23  | CLA  | C     | 510  | 3    | 69,73,73     | 2.57 | 26 (37%) | 83,113,113  | 2.49 | 27 (32%) |
| 23  | CLA  | c     | 505  | 3    | 69,73,73     | 2.45 | 25 (36%) | 83,113,113  | 2.38 | 24 (28%) |
| 27  | LMG  | c     | 501  | -    | 51,51,55     | 0.95 | 2 (3%)   | 59,59,63    | 1.12 | 3 (5%)   |
| 34  | DMS  | B     | 637  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.51 | 0        |
| 32  | BCT  | A     | 421  | 21   | 2,3,3        | 0.65 | 0        | 2,3,3       | 1.06 | 0        |
| 29  | GOL  | c     | 529  | -    | 5,5,5        | 0.91 | 0        | 5,5,5       | 0.98 | 0        |
| 29  | GOL  | a     | 2602 | -    | 5,5,5        | 0.85 | 0        | 5,5,5       | 1.03 | 0        |
| 24  | PHO  | a     | 2612 | -    | 58,69,69     | 2.69 | 13 (22%) | 56,99,99    | 3.01 | 15 (26%) |
| 34  | DMS  | b     | 639  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 34  | DMS  | V     | 209  | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 29  | GOL  | O     | 303  | -    | 5,5,5        | 0.93 | 0        | 5,5,5       | 0.94 | 0        |
| 34  | DMS  | u     | 502  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 36  | HTG  | b     | 603  | -    | 19,19,19     | 0.95 | 2 (10%)  | 23,24,24    | 2.00 | 4 (17%)  |
| 23  | CLA  | c     | 514  | 3    | 69,73,73     | 2.47 | 23 (33%) | 83,113,113  | 2.40 | 28 (33%) |
| 34  | DMS  | u     | 504  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 23  | CLA  | C     | 508  | 43   | 69,73,73     | 2.67 | 24 (34%) | 83,113,113  | 2.54 | 28 (33%) |
| 34  | DMS  | o     | 307  | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.50 | 0        |
| 36  | HTG  | H     | 101  | -    | 17,17,19     | 1.23 | 2 (11%)  | 19,21,24    | 1.61 | 4 (21%)  |
| 34  | DMS  | b     | 638  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 34  | DMS  | v     | 208  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 34  | DMS  | v     | 213  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.46 | 0        |
| 34  | DMS  | c     | 548  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 34  | DMS  | d     | 421  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 37  | DGD  | C     | 519  | -    | 59,59,67     | 0.92 | 2 (3%)   | 73,73,81    | 1.28 | 6 (8%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | LMT  | T     | 103  | -    | 24,24,36     | 0.60 | 1 (4%)   | 29,29,47    | 0.94 | 2 (6%)   |
| 42  | HEC  | v     | 201  | 16   | 50,50,50     | 1.92 | 9 (18%)  | 68,82,82    | 1.53 | 11 (16%) |
| 28  | LMT  | d     | 401  | -    | 36,36,36     | 0.47 | 0        | 47,47,47    | 0.81 | 1 (2%)   |
| 34  | DMS  | v     | 209  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.64 | 0        |
| 34  | DMS  | H     | 104  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 37  | DGD  | D     | 2307 | -    | 53,53,67     | 0.96 | 2 (3%)   | 60,61,81    | 1.20 | 5 (8%)   |
| 34  | DMS  | c     | 549  | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.62 | 0        |
| 34  | DMS  | V     | 210  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 34  | DMS  | o     | 304  | -    | 3,3,3        | 2.54 | 1 (33%)  | 3,3,3       | 0.32 | 0        |
| 23  | CLA  | C     | 506  | 3    | 69,73,73     | 2.70 | 25 (36%) | 83,113,113  | 2.27 | 27 (32%) |
| 34  | DMS  | c     | 545  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 28  | LMT  | f     | 101  | -    | 24,24,36     | 0.46 | 0        | 29,29,47    | 0.76 | 0        |
| 34  | DMS  | O     | 316  | -    | 3,3,3        | 2.63 | 1 (33%)  | 3,3,3       | 0.51 | 0        |
| 39  | HEM  | e     | 103  | 5,6  | 50,50,50     | 1.95 | 8 (16%)  | 66,82,82    | 1.52 | 7 (10%)  |
| 29  | GOL  | D     | 2301 | -    | 5,5,5        | 1.00 | 0        | 5,5,5       | 0.79 | 0        |
| 23  | CLA  | A     | 410  | 1    | 69,73,73     | 2.34 | 24 (34%) | 83,113,113  | 2.59 | 28 (33%) |
| 36  | HTG  | V     | 204  | -    | 19,19,19     | 0.96 | 1 (5%)   | 23,24,24    | 1.84 | 4 (17%)  |
| 34  | DMS  | a     | 2623 | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 34  | DMS  | B     | 643  | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 27  | LMG  | D     | 2312 | 41   | 47,47,55     | 0.90 | 2 (4%)   | 55,55,63    | 0.88 | 3 (5%)   |
| 23  | CLA  | C     | 512  | 3    | 69,73,73     | 2.58 | 23 (33%) | 83,113,113  | 2.39 | 27 (32%) |
| 40  | RRX  | h     | 101  | -    | 42,42,42     | 0.69 | 0        | 57,58,58    | 1.41 | 8 (14%)  |
| 34  | DMS  | c     | 532  | -    | 3,3,3        | 2.76 | 1 (33%)  | 3,3,3       | 0.80 | 0        |
| 27  | LMG  | A     | 413  | -    | 51,51,55     | 0.93 | 2 (3%)   | 59,59,63    | 1.24 | 6 (10%)  |
| 34  | DMS  | o     | 311  | -    | 3,3,3        | 2.75 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 36  | HTG  | I     | 101  | -    | 19,19,19     | 1.10 | 2 (10%)  | 23,24,24    | 1.81 | 4 (17%)  |
| 25  | BCR  | z     | 101  | -    | 41,41,41     | 0.74 | 0        | 56,56,56    | 1.52 | 12 (21%) |
| 34  | DMS  | C     | 529  | -    | 3,3,3        | 2.62 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 29  | GOL  | a     | 2618 | -    | 5,5,5        | 0.87 | 0        | 5,5,5       | 1.04 | 0        |
| 23  | CLA  | B     | 613  | 2    | 69,73,73     | 2.35 | 23 (33%) | 83,113,113  | 2.53 | 25 (30%) |
| 29  | GOL  | J     | 301  | -    | 5,5,5        | 0.96 | 0        | 5,5,5       | 0.89 | 0        |
| 34  | DMS  | c     | 538  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 37  | DGD  | C     | 517  | -    | 63,63,67     | 0.84 | 2 (3%)   | 77,77,81    | 0.97 | 5 (6%)   |
| 34  | DMS  | o     | 313  | -    | 3,3,3        | 2.71 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 34  | DMS  | c     | 533  | -    | 3,3,3        | 2.61 | 1 (33%)  | 3,3,3       | 0.39 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | CLA  | c     | 511  | 3    | 69,73,73     | 2.76 | 24 (34%) | 83,113,113  | 2.42 | 24 (28%) |
| 36  | HTG  | d     | 407  | -    | 19,19,19     | 1.15 | 2 (10%)  | 23,24,24    | 1.64 | 5 (21%)  |
| 28  | LMT  | F     | 102  | -    | 24,24,36     | 0.47 | 0        | 29,29,47    | 0.73 | 0        |
| 29  | GOL  | B     | 630  | -    | 5,5,5        | 0.98 | 0        | 5,5,5       | 0.93 | 0        |
| 34  | DMS  | T     | 104  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 38  | LHG  | d     | 413  | -    | 48,48,48     | 0.82 | 2 (4%)   | 51,54,54    | 0.99 | 3 (5%)   |
| 23  | CLA  | B     | 604  | 2    | 69,73,73     | 2.56 | 23 (33%) | 83,113,113  | 2.56 | 28 (33%) |
| 34  | DMS  | T     | 105  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 34  | DMS  | c     | 535  | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.47 | 0        |
| 23  | CLA  | B     | 605  | 2    | 69,73,73     | 2.45 | 23 (33%) | 83,113,113  | 2.45 | 28 (33%) |
| 37  | DGD  | H     | 103  | -    | 63,63,67     | 0.90 | 2 (3%)   | 77,77,81    | 1.09 | 7 (9%)   |
| 34  | DMS  | V     | 208  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 34  | DMS  | a     | 2620 | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 34  | DMS  | t     | 102  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.56 | 0        |
| 38  | LHG  | e     | 101  | -    | 39,39,48     | 1.08 | 2 (5%)   | 42,45,54    | 1.07 | 3 (7%)   |
| 27  | LMG  | C     | 520  | -    | 51,51,55     | 0.95 | 2 (3%)   | 59,59,63    | 1.07 | 4 (6%)   |
| 29  | GOL  | O     | 304  | -    | 5,5,5        | 0.86 | 0        | 5,5,5       | 0.99 | 0        |
| 29  | GOL  | b     | 644  | -    | 5,5,5        | 0.69 | 0        | 5,5,5       | 1.21 | 1 (20%)  |
| 34  | DMS  | C     | 531  | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.51 | 0        |
| 34  | DMS  | v     | 207  | -    | 3,3,3        | 2.64 | 1 (33%)  | 3,3,3       | 0.46 | 0        |
| 26  | SQD  | B     | 621  | -    | 53,54,54     | 1.05 | 4 (7%)   | 62,65,65    | 1.45 | 9 (14%)  |
| 34  | DMS  | V     | 207  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.55 | 0        |
| 28  | LMT  | m     | 2804 | -    | 36,36,36     | 0.45 | 0        | 47,47,47    | 1.13 | 6 (12%)  |
| 33  | PL9  | x     | 1301 | -    | 38,38,55     | 0.44 | 0        | 45,45,69    | 1.72 | 11 (24%) |
| 36  | HTG  | B     | 626  | -    | 19,19,19     | 1.01 | 2 (10%)  | 23,24,24    | 1.49 | 1 (4%)   |
| 36  | HTG  | c     | 523  | -    | 19,19,19     | 1.02 | 2 (10%)  | 23,24,24    | 1.49 | 2 (8%)   |
| 23  | CLA  | b     | 612  | 43   | 69,73,73     | 2.38 | 24 (34%) | 83,113,113  | 2.45 | 28 (33%) |
| 28  | LMT  | M     | 102  | -    | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.81 | 0        |
| 23  | CLA  | B     | 606  | 2    | 69,73,73     | 2.35 | 23 (33%) | 83,113,113  | 2.48 | 25 (30%) |
| 23  | CLA  | c     | 509  | 3    | 69,73,73     | 2.63 | 25 (36%) | 83,113,113  | 2.46 | 30 (36%) |
| 34  | DMS  | O     | 306  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 25  | BCR  | C     | 515  | -    | 41,41,41     | 0.76 | 0        | 56,56,56    | 1.49 | 8 (14%)  |
| 34  | DMS  | B     | 638  | -    | 3,3,3        | 2.54 | 1 (33%)  | 3,3,3       | 0.34 | 0        |
| 29  | GOL  | A     | 415  | -    | 5,5,5        | 0.82 | 0        | 5,5,5       | 1.08 | 0        |
| 34  | DMS  | A     | 426  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 34  | DMS  | b     | 641  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.40 | 0        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | DMS  | a     | 2621 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.46 | 0        |
| 34  | DMS  | o     | 309  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 34  | DMS  | c     | 542  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 34  | DMS  | b     | 643  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 34  | DMS  | A     | 430  | -    | 3,3,3        | 2.72 | 1 (33%)  | 3,3,3       | 0.60 | 0        |
| 34  | DMS  | v     | 212  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 34  | DMS  | c     | 536  | -    | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.47 | 0        |
| 34  | DMS  | O     | 318  | -    | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.49 | 0        |
| 29  | GOL  | o     | 303  | -    | 5,5,5        | 0.98 | 0        | 5,5,5       | 0.94 | 0        |
| 23  | CLA  | C     | 505  | 43   | 69,73,73     | 2.39 | 25 (36%) | 83,113,113  | 2.46 | 27 (32%) |
| 23  | CLA  | C     | 514  | 3    | 69,73,73     | 2.50 | 25 (36%) | 83,113,113  | 2.42 | 24 (28%) |
| 28  | LMT  | m     | 2803 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.83 | 0        |
| 29  | GOL  | v     | 202  | -    | 5,5,5        | 1.01 | 0        | 5,5,5       | 0.89 | 0        |
| 34  | DMS  | d     | 419  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.48 | 0        |
| 23  | CLA  | B     | 607  | 2    | 69,73,73     | 2.48 | 22 (31%) | 83,113,113  | 2.41 | 26 (31%) |
| 23  | CLA  | B     | 610  | 2    | 69,73,73     | 2.65 | 22 (31%) | 83,113,113  | 2.43 | 26 (31%) |
| 37  | DGD  | c     | 518  | -    | 63,63,67     | 0.84 | 2 (3%)   | 77,77,81    | 1.04 | 4 (5%)   |
| 34  | DMS  | b     | 636  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.50 | 0        |
| 34  | DMS  | D     | 2320 | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.44 | 0        |
| 34  | DMS  | b     | 633  | -    | 3,3,3        | 2.50 | 1 (33%)  | 3,3,3       | 0.35 | 0        |
| 25  | BCR  | A     | 411  | -    | 41,41,41     | 0.75 | 0        | 56,56,56    | 1.39 | 8 (14%)  |
| 34  | DMS  | o     | 315  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 38  | LHG  | E     | 101  | -    | 39,39,48     | 1.06 | 2 (5%)   | 42,45,54    | 1.12 | 3 (7%)   |
| 23  | CLA  | B     | 615  | 2    | 69,73,73     | 2.39 | 22 (31%) | 83,113,113  | 2.60 | 30 (36%) |
| 23  | CLA  | B     | 616  | 2    | 69,73,73     | 2.44 | 22 (31%) | 83,113,113  | 2.61 | 30 (36%) |
| 29  | GOL  | B     | 648  | -    | 5,5,5        | 0.89 | 0        | 5,5,5       | 0.94 | 0        |
| 34  | DMS  | C     | 528  | -    | 3,3,3        | 2.69 | 1 (33%)  | 3,3,3       | 0.58 | 0        |
| 34  | DMS  | V     | 212  | -    | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.63 | 0        |
| 34  | DMS  | B     | 639  | -    | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 34  | DMS  | u     | 503  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.59 | 0        |
| 34  | DMS  | D     | 2318 | -    | 3,3,3        | 2.57 | 1 (33%)  | 3,3,3       | 0.47 | 0        |
| 23  | CLA  | C     | 503  | 3    | 69,73,73     | 2.62 | 25 (36%) | 83,113,113  | 2.47 | 27 (32%) |
| 26  | SQD  | b     | 601  | -    | 47,48,54     | 1.04 | 3 (6%)   | 56,59,65    | 1.46 | 9 (16%)  |
| 34  | DMS  | A     | 425  | -    | 3,3,3        | 2.66 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 28  | LMT  | B     | 623  | -    | 36,36,36     | 0.41 | 0        | 47,47,47    | 1.35 | 4 (8%)   |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 34  | DMS  | X     | 101    | -      | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 34  | DMS  | V     | 202    | -      | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 26  | SQD  | A     | 412    | -      | 45,46,54     | 1.05 | 3 (6%)   | 54,57,65    | 1.55 | 11 (20%) |
| 34  | DMS  | b     | 635    | -      | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.61 | 0        |
| 29  | GOL  | d     | 416    | -      | 5,5,5        | 0.89 | 0        | 5,5,5       | 0.99 | 0        |
| 34  | DMS  | v     | 205    | -      | 3,3,3        | 2.65 | 1 (33%)  | 3,3,3       | 0.51 | 0        |
| 39  | HEM  | F     | 101    | 5,6    | 50,50,50     | 1.88 | 9 (18%)  | 66,82,82    | 1.47 | 7 (10%)  |
| 36  | HTG  | B     | 624[B] | -      | 19,19,19     | 0.96 | 1 (5%)   | 23,24,24    | 1.86 | 6 (26%)  |
| 23  | CLA  | C     | 509    | 3      | 69,73,73     | 2.52 | 23 (33%) | 83,113,113  | 2.44 | 27 (32%) |
| 34  | DMS  | C     | 537    | -      | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.52 | 0        |
| 23  | CLA  | c     | 510    | 43     | 69,73,73     | 2.54 | 23 (33%) | 83,113,113  | 2.62 | 32 (38%) |
| 34  | DMS  | v     | 214    | -      | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.53 | 0        |
| 23  | CLA  | D     | 2304   | 4      | 69,73,73     | 2.23 | 22 (31%) | 83,113,113  | 2.55 | 28 (33%) |
| 20  | OEX  | a     | 2604   | 3,43,1 | 0,14,14      | -    | -        | -           | -    | -        |
| 29  | GOL  | U     | 501    | -      | 5,5,5        | 1.02 | 0        | 5,5,5       | 0.93 | 0        |
| 34  | DMS  | v     | 211    | -      | 3,3,3        | 2.67 | 1 (33%)  | 3,3,3       | 0.54 | 0        |
| 34  | DMS  | c     | 546    | -      | 3,3,3        | 2.70 | 1 (33%)  | 3,3,3       | 0.57 | 0        |
| 29  | GOL  | u     | 501    | -      | 5,5,5        | 1.25 | 0        | 5,5,5       | 0.83 | 0        |
| 23  | CLA  | b     | 607    | 2      | 69,73,73     | 2.52 | 24 (34%) | 83,113,113  | 2.46 | 26 (31%) |
| 23  | CLA  | b     | 610    | 2      | 69,73,73     | 2.36 | 23 (33%) | 83,113,113  | 2.73 | 27 (32%) |
| 34  | DMS  | B     | 641    | -      | 3,3,3        | 2.68 | 1 (33%)  | 3,3,3       | 0.54 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|------|------|---------|--------------|---------|
| 38  | LHG  | D     | 2311 | -    | -       | 9/43/43/53   | -       |
| 38  | LHG  | L     | 101  | -    | -       | 15/53/53/53  | -       |
| 29  | GOL  | v     | 203  | -    | -       | 1/4/4/4      | -       |
| 38  | LHG  | e     | 101  | -    | -       | 14/44/44/53  | -       |
| 23  | CLA  | b     | 619  | 2    | -       | 8/39/115/115 | -       |
| 23  | CLA  | a     | 2609 | 1    | -       | 4/39/115/115 | -       |
| 27  | LMG  | C     | 520  | -    | -       | 13/46/66/70  | 0/1/1/1 |
| 29  | GOL  | O     | 304  | -    | -       | 2/4/4/4      | -       |
| 29  | GOL  | U     | 502  | -    | -       | 2/4/4/4      | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 29  | GOL  | b     | 644  | -    | -       | 2/4/4/4       | -       |
| 23  | CLA  | B     | 611  | 43   | -       | 5/39/115/115  | -       |
| 26  | SQD  | B     | 621  | -    | -       | 22/49/69/69   | 0/1/1/1 |
| 23  | CLA  | d     | 408  | 4    | -       | 3/39/115/115  | -       |
| 28  | LMT  | m     | 2804 | -    | -       | 10/21/61/61   | 0/2/2/2 |
| 25  | BCR  | b     | 623  | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 37  | DGD  | c     | 519  | -    | -       | 18/51/91/95   | 0/2/2/2 |
| 36  | HTG  | B     | 627  | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 23  | CLA  | c     | 512  | 3    | -       | 5/39/115/115  | -       |
| 33  | PL9  | x     | 1301 | -    | -       | 12/42/42/73   | -       |
| 36  | HTG  | B     | 626  | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 36  | HTG  | c     | 523  | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 36  | HTG  | C     | 521  | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 36  | HTG  | C     | 522  | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 37  | DGD  | C     | 518  | -    | -       | 17/51/91/95   | 0/2/2/2 |
| 36  | HTG  | c     | 524  | -    | -       | 0/10/30/30    | 0/1/1/1 |
| 23  | CLA  | C     | 502  | 3    | -       | 4/39/115/115  | -       |
| 23  | CLA  | b     | 612  | 43   | -       | 1/39/115/115  | -       |
| 28  | LMT  | i     | 103  | -    | -       | 8/15/35/61    | 0/1/1/2 |
| 29  | GOL  | C     | 526  | -    | -       | 2/4/4/4       | -       |
| 38  | LHG  | D     | 2309 | -    | -       | 13/53/53/53   | -       |
| 23  | CLA  | b     | 615  | 43   | -       | 6/39/115/115  | -       |
| 23  | CLA  | b     | 616  | 2    | -       | 4/39/115/115  | -       |
| 28  | LMT  | M     | 102  | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 23  | CLA  | B     | 606  | 2    | -       | 9/39/115/115  | -       |
| 23  | CLA  | b     | 614  | 2    | -       | 7/39/115/115  | -       |
| 23  | CLA  | c     | 504  | 3    | -       | 4/39/115/115  | -       |
| 25  | BCR  | y     | 101  | -    | -       | 6/29/63/63    | 0/2/2/2 |
| 36  | HTG  | C     | 525  | -    | -       | 0/10/30/30    | 0/1/1/1 |
| 27  | LMG  | c     | 522  | -    | -       | 5/46/66/70    | 0/1/1/1 |
| 42  | HEC  | V     | 201  | 16   | 1/1/3/7 | 6/14/54/54    | -       |
| 26  | SQD  | l     | 101  | -    | -       | 23/49/69/69   | 0/1/1/1 |
| 28  | LMT  | J     | 303  | -    | -       | 5/15/35/61    | 0/1/1/2 |
| 23  | CLA  | c     | 509  | 3    | -       | 11/39/115/115 | -       |
| 23  | CLA  | B     | 617  | 2    | -       | 9/39/115/115  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 25  | BCR  | b     | 622  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 33  | PL9  | d     | 411  | -    | -       | 4/53/73/73    | 0/1/1/1 |
| 25  | BCR  | C     | 515  | -    | -       | 7/29/63/63    | 0/2/2/2 |
| 23  | CLA  | B     | 612  | 2    | -       | 3/39/115/115  | -       |
| 29  | GOL  | A     | 415  | -    | -       | 2/4/4/4       | -       |
| 23  | CLA  | C     | 507  | 3    | -       | 14/39/115/115 | -       |
| 23  | CLA  | C     | 510  | 3    | -       | 6/39/115/115  | -       |
| 23  | CLA  | d     | 409  | 4    | -       | 6/39/115/115  | -       |
| 23  | CLA  | C     | 511  | 3    | -       | 6/39/115/115  | -       |
| 33  | PL9  | D     | 2306 | -    | -       | 3/53/73/73    | 0/1/1/1 |
| 37  | DGD  | c     | 520  | -    | -       | 10/51/91/95   | 0/2/2/2 |
| 23  | CLA  | C     | 504  | 3    | -       | 5/39/115/115  | -       |
| 38  | LHG  | l     | 103  | -    | -       | 13/53/53/53   | -       |
| 23  | CLA  | c     | 505  | 3    | -       | 6/39/115/115  | -       |
| 23  | CLA  | d     | 402  | 43   | -       | 5/39/115/115  | -       |
| 27  | LMG  | c     | 501  | -    | -       | 12/46/66/70   | 0/1/1/1 |
| 28  | LMT  | z     | 102  | -    | -       | 12/16/56/61   | 0/2/2/2 |
| 26  | SQD  | d     | 417  | -    | -       | 13/33/33/69   | -       |
| 29  | GOL  | c     | 531  | -    | -       | 2/4/4/4       | -       |
| 28  | LMT  | B     | 634  | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 23  | CLA  | B     | 603  | 2    | -       | 3/39/115/115  | -       |
| 27  | LMG  | c     | 521  | -    | -       | 14/44/64/70   | 0/1/1/1 |
| 29  | GOL  | c     | 529  | -    | -       | 0/4/4/4       | -       |
| 29  | GOL  | a     | 2602 | -    | -       | 4/4/4/4       | -       |
| 36  | HTG  | c     | 526  | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 29  | GOL  | o     | 303  | -    | -       | 0/4/4/4       | -       |
| 23  | CLA  | C     | 505  | 43   | -       | 8/39/115/115  | -       |
| 24  | PHO  | a     | 2612 | -    | -       | 1/37/103/103  | 0/5/6/6 |
| 36  | HTG  | b     | 604  | -    | -       | 1/10/30/30    | 0/1/1/1 |
| 37  | DGD  | h     | 102  | -    | -       | 12/51/91/95   | 0/2/2/2 |
| 23  | CLA  | C     | 514  | 3    | -       | 8/39/115/115  | -       |
| 36  | HTG  | b     | 626  | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 25  | BCR  | T     | 102  | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 28  | LMT  | j     | 2701 | 41   | -       | 3/17/57/61    | 0/2/2/2 |
| 29  | GOL  | O     | 303  | -    | -       | 0/4/4/4       | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 28  | LMT  | m     | 2803 | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 36  | HTG  | b     | 603  | -    | -       | 0/10/30/30    | 0/1/1/1 |
| 38  | LHG  | d     | 412  | -    | -       | 13/53/53/53   | -       |
| 23  | CLA  | c     | 514  | 3    | -       | 3/39/115/115  | -       |
| 29  | GOL  | b     | 631  | -    | -       | 0/4/4/4       | -       |
| 23  | CLA  | a     | 2613 | 1    | -       | 7/39/115/115  | -       |
| 29  | GOL  | v     | 202  | -    | -       | 2/4/4/4       | -       |
| 26  | SQD  | a     | 2615 | -    | -       | 8/43/63/69    | 0/1/1/1 |
| 29  | GOL  | E     | 104  | -    | -       | 0/4/4/4       | -       |
| 23  | CLA  | C     | 508  | 43   | -       | 9/39/115/115  | -       |
| 36  | HTG  | H     | 101  | -    | -       | 2/8/25/30     | 0/1/1/1 |
| 23  | CLA  | B     | 607  | 2    | -       | 6/39/115/115  | -       |
| 23  | CLA  | B     | 610  | 2    | -       | 5/39/115/115  | -       |
| 23  | CLA  | b     | 621  | 2    | -       | 12/39/115/115 | -       |
| 25  | BCR  | a     | 2614 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 37  | DGD  | c     | 518  | -    | -       | 17/51/91/95   | 0/2/2/2 |
| 36  | HTG  | B     | 625  | -    | -       | 1/10/30/30    | 0/1/1/1 |
| 40  | RRX  | H     | 102  | -    | -       | 1/29/65/65    | 0/2/2/2 |
| 23  | CLA  | c     | 506  | 3    | -       | 5/39/115/115  | -       |
| 23  | CLA  | c     | 513  | 3    | -       | 8/39/115/115  | -       |
| 37  | DGD  | C     | 519  | -    | -       | 14/47/87/95   | 0/2/2/2 |
| 25  | BCR  | K     | 101  | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 25  | BCR  | A     | 411  | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 26  | SQD  | D     | 2308 | -    | -       | 16/40/60/69   | 0/1/1/1 |
| 23  | CLA  | B     | 602  | 43   | -       | 10/39/115/115 | -       |
| 28  | LMT  | T     | 103  | -    | -       | 9/15/35/61    | 0/1/1/2 |
| 31  | JOX  | A     | 419  | -    | -       | -             | 0/1/1/1 |
| 42  | HEC  | v     | 201  | 16   | 1/1/3/7 | 6/14/54/54    | -       |
| 28  | LMT  | d     | 401  | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 33  | PL9  | A     | 422  | -    | -       | 10/42/42/73   | -       |
| 37  | DGD  | D     | 2307 | -    | -       | 23/47/68/95   | 0/1/1/2 |
| 23  | CLA  | c     | 507  | 43   | -       | 6/39/115/115  | -       |
| 25  | BCR  | c     | 517  | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 38  | LHG  | d     | 403  | -    | -       | 7/47/47/53    | -       |
| 38  | LHG  | E     | 101  | -    | -       | 13/44/44/53   | -       |
| 26  | SQD  | D     | 2302 | -    | -       | 14/49/69/69   | 0/1/1/1 |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|--------|------|---------|---------------|---------|
| 36  | HTG  | i     | 102    | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 23  | CLA  | C     | 513    | 3    | -       | 9/39/115/115  | -       |
| 23  | CLA  | C     | 506    | 3    | -       | 8/39/115/115  | -       |
| 36  | HTG  | B     | 624[A] | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 28  | LMT  | f     | 101    | -    | -       | 4/15/35/61    | 0/1/1/2 |
| 23  | CLA  | B     | 615    | 2    | -       | 12/39/115/115 | -       |
| 23  | CLA  | B     | 616    | 2    | -       | 7/39/115/115  | -       |
| 29  | GOL  | B     | 648    | -    | -       | 0/4/4/4       | -       |
| 36  | HTG  | b     | 602    | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 23  | CLA  | b     | 608    | 2    | -       | 4/39/115/115  | -       |
| 25  | BCR  | Y     | 302    | -    | -       | 5/29/63/63    | 0/2/2/2 |
| 39  | HEM  | e     | 103    | 5,6  | -       | 4/14/54/54    | -       |
| 25  | BCR  | C     | 516    | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 29  | GOL  | D     | 2301   | -    | -       | 2/4/4/4       | -       |
| 23  | CLA  | A     | 410    | 1    | -       | 10/39/115/115 | -       |
| 28  | LMT  | M     | 101    | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 36  | HTG  | V     | 204    | -    | -       | 5/10/30/30    | 0/1/1/1 |
| 27  | LMG  | m     | 2802   | -    | -       | 10/46/66/70   | 0/1/1/1 |
| 24  | PHO  | a     | 2611   | -    | -       | 3/37/103/103  | 0/5/6/6 |
| 25  | BCR  | k     | 302    | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 36  | HTG  | b     | 625    | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 29  | GOL  | V     | 203    | -    | -       | 0/4/4/4       | -       |
| 31  | JOX  | a     | 2619   | 1    | -       | -             | 0/1/1/1 |
| 25  | BCR  | d     | 410    | -    | -       | 8/29/63/63    | 0/2/2/2 |
| 23  | CLA  | b     | 618    | 2    | -       | 6/39/115/115  | -       |
| 28  | LMT  | A     | 420    | -    | -       | 6/15/35/61    | 0/1/1/2 |
| 25  | BCR  | D     | 2305   | -    | -       | 8/29/63/63    | 0/2/2/2 |
| 25  | BCR  | b     | 624    | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 27  | LMG  | D     | 2312   | 41   | -       | 6/42/62/70    | 0/1/1/1 |
| 28  | LMT  | d     | 404    | -    | -       | 5/17/37/61    | 0/1/1/2 |
| 23  | CLA  | C     | 503    | 3    | -       | 6/39/115/115  | -       |
| 27  | LMG  | B     | 622    | -    | -       | 16/46/66/70   | 0/1/1/1 |
| 26  | SQD  | a     | 2603   | -    | -       | 16/49/69/69   | 0/1/1/1 |
| 23  | CLA  | C     | 512    | 3    | -       | 2/39/115/115  | -       |
| 26  | SQD  | b     | 601    | -    | -       | 16/43/63/69   | 0/1/1/1 |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|--------|------|---------|---------------|---------|
| 40  | RRX  | h     | 101    | -    | -       | 2/29/65/65    | 0/2/2/2 |
| 31  | JOX  | a     | 2617   | -    | -       | -             | 0/1/1/1 |
| 28  | LMT  | B     | 623    | -    | -       | 12/21/61/61   | 0/2/2/2 |
| 28  | LMT  | A     | 414    | -    | -       | 8/19/59/61    | 0/2/2/2 |
| 27  | LMG  | A     | 413    | -    | -       | 20/46/66/70   | 0/1/1/1 |
| 29  | GOL  | A     | 417    | -    | -       | 3/4/4/4       | -       |
| 36  | HTG  | I     | 101    | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 25  | BCR  | B     | 619    | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 26  | SQD  | A     | 412    | -    | -       | 8/41/61/69    | 0/1/1/1 |
| 25  | BCR  | z     | 101    | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 23  | CLA  | b     | 617    | 2    | -       | 2/39/115/115  | -       |
| 38  | LHG  | D     | 2310   | -    | -       | 8/53/53/53    | -       |
| 29  | GOL  | d     | 416    | -    | -       | 2/4/4/4       | -       |
| 23  | CLA  | c     | 516    | 3    | -       | 10/39/115/115 | -       |
| 25  | BCR  | B     | 620    | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 24  | PHO  | A     | 408    | -    | -       | 4/37/103/103  | 0/5/6/6 |
| 23  | CLA  | b     | 606    | 43   | -       | 10/39/115/115 | -       |
| 29  | GOL  | a     | 2618   | -    | -       | 1/4/4/4       | -       |
| 27  | LMG  | d     | 414    | 41   | -       | 11/46/66/70   | 0/1/1/1 |
| 23  | CLA  | b     | 620    | 2    | -       | 5/39/115/115  | -       |
| 36  | HTG  | o     | 301    | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 29  | GOL  | C     | 524    | -    | -       | 2/4/4/4       | -       |
| 29  | GOL  | O     | 305    | -    | -       | 2/4/4/4       | -       |
| 23  | CLA  | B     | 613    | 2    | -       | 5/39/115/115  | -       |
| 29  | GOL  | J     | 301    | -    | -       | 4/4/4/4       | -       |
| 37  | DGD  | C     | 517    | -    | -       | 18/51/91/95   | 0/2/2/2 |
| 25  | BCR  | B     | 618    | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 28  | LMT  | Z     | 101    | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 23  | CLA  | B     | 614    | 2    | -       | 8/39/115/115  | -       |
| 23  | CLA  | c     | 511    | 3    | -       | 5/39/115/115  | -       |
| 23  | CLA  | A     | 406    | 43   | -       | 4/39/115/115  | -       |
| 23  | CLA  | b     | 609    | 2    | -       | 2/39/115/115  | -       |
| 39  | HEM  | F     | 101    | 5,6  | -       | 4/14/54/54    | -       |
| 23  | CLA  | b     | 613    | 2    | -       | 1/39/115/115  | -       |
| 36  | HTG  | B     | 624[B] | -    | -       | 4/10/30/30    | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 36  | HTG  | d     | 415  | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 36  | HTG  | d     | 407  | -    | -       | 7/10/30/30    | 0/1/1/1 |
| 29  | GOL  | B     | 632  | -    | -       | 3/4/4/4       | -       |
| 24  | PHO  | A     | 409  | -    | -       | 3/37/103/103  | 0/5/6/6 |
| 23  | CLA  | C     | 509  | 3    | -       | 6/39/115/115  | -       |
| 29  | GOL  | v     | 204  | -    | -       | 1/4/4/4       | -       |
| 23  | CLA  | A     | 407  | 43   | -       | 6/39/115/115  | -       |
| 23  | CLA  | c     | 510  | 43   | -       | 10/39/115/115 | -       |
| 25  | BCR  | B     | 633  | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 28  | LMT  | F     | 102  | -    | -       | 5/15/35/61    | 0/1/1/2 |
| 31  | JOX  | A     | 418  | -    | -       | -             | 0/1/1/1 |
| 23  | CLA  | a     | 2610 | 43   | -       | 13/39/115/115 | -       |
| 23  | CLA  | c     | 515  | 3    | -       | 8/39/115/115  | -       |
| 23  | CLA  | D     | 2304 | 4    | -       | 7/39/115/115  | -       |
| 29  | GOL  | O     | 302  | -    | -       | 2/4/4/4       | -       |
| 23  | CLA  | B     | 609  | 2    | -       | 1/39/115/115  | -       |
| 29  | GOL  | B     | 630  | -    | -       | 0/4/4/4       | -       |
| 29  | GOL  | U     | 501  | -    | -       | 0/4/4/4       | -       |
| 38  | LHG  | d     | 413  | -    | -       | 10/53/53/53   | -       |
| 23  | CLA  | c     | 508  | 3    | -       | 9/39/115/115  | -       |
| 23  | CLA  | B     | 604  | 2    | -       | 7/39/115/115  | -       |
| 23  | CLA  | B     | 605  | 2    | -       | 6/39/115/115  | -       |
| 29  | GOL  | u     | 501  | -    | -       | 1/4/4/4       | -       |
| 23  | CLA  | b     | 611  | 2    | -       | 11/39/115/115 | -       |
| 27  | LMG  | C     | 527  | -    | -       | 14/46/66/70   | 0/1/1/1 |
| 23  | CLA  | A     | 405  | 1    | -       | 2/39/115/115  | -       |
| 23  | CLA  | D     | 2303 | 4    | -       | 3/39/115/115  | -       |
| 23  | CLA  | b     | 607  | 2    | -       | 4/39/115/115  | -       |
| 23  | CLA  | B     | 608  | 43   | -       | 5/39/115/115  | -       |
| 23  | CLA  | b     | 610  | 2    | -       | 3/39/115/115  | -       |
| 29  | GOL  | c     | 530  | -    | -       | 4/4/4/4       | -       |
| 37  | DGD  | H     | 103  | -    | -       | 12/51/91/95   | 0/2/2/2 |

All (2032) bond length outliers are listed below:

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | C     | 508  | CLA  | MG-NA   | 10.59 | 2.31        | 2.06     |
| 23  | C     | 512  | CLA  | MG-NA   | 10.29 | 2.30        | 2.06     |
| 23  | c     | 506  | CLA  | MG-NA   | 10.17 | 2.30        | 2.06     |
| 23  | c     | 511  | CLA  | MG-ND   | -9.74 | 1.86        | 2.05     |
| 23  | b     | 609  | CLA  | MG-ND   | -9.39 | 1.87        | 2.05     |
| 24  | a     | 2611 | PHO  | C1D-C2D | 9.28  | 1.49        | 1.39     |
| 23  | C     | 513  | CLA  | MG-NA   | 9.27  | 2.28        | 2.06     |
| 23  | C     | 503  | CLA  | MG-NA   | 9.25  | 2.28        | 2.06     |
| 23  | c     | 514  | CLA  | MG-NA   | 9.22  | 2.28        | 2.06     |
| 23  | B     | 602  | CLA  | MG-NA   | 9.19  | 2.28        | 2.06     |
| 23  | B     | 612  | CLA  | MG-NA   | 9.16  | 2.28        | 2.06     |
| 24  | a     | 2612 | PHO  | C1D-C2D | 8.95  | 1.49        | 1.39     |
| 23  | b     | 621  | CLA  | MG-NA   | 8.95  | 2.27        | 2.06     |
| 23  | C     | 506  | CLA  | MG-NA   | 8.92  | 2.27        | 2.06     |
| 23  | b     | 621  | CLA  | MG-ND   | -8.84 | 1.88        | 2.05     |
| 23  | b     | 614  | CLA  | MG-NA   | 8.78  | 2.27        | 2.06     |
| 24  | A     | 408  | PHO  | C1D-C2D | 8.74  | 1.49        | 1.39     |
| 23  | B     | 616  | CLA  | MG-NA   | 8.69  | 2.26        | 2.06     |
| 23  | C     | 513  | CLA  | MG-ND   | -8.51 | 1.88        | 2.05     |
| 23  | c     | 504  | CLA  | MG-NA   | 8.51  | 2.26        | 2.06     |
| 23  | b     | 611  | CLA  | MG-ND   | -8.51 | 1.88        | 2.05     |
| 24  | A     | 408  | PHO  | C1B-C2B | 8.47  | 1.49        | 1.39     |
| 24  | A     | 409  | PHO  | C1B-C2B | 8.45  | 1.49        | 1.39     |
| 23  | b     | 609  | CLA  | MG-NA   | 8.38  | 2.26        | 2.06     |
| 23  | c     | 515  | CLA  | MG-ND   | -8.37 | 1.89        | 2.05     |
| 23  | B     | 617  | CLA  | MG-NA   | 8.34  | 2.26        | 2.06     |
| 24  | A     | 409  | PHO  | C1D-C2D | 8.33  | 1.48        | 1.39     |
| 23  | b     | 609  | CLA  | MG-NC   | 8.31  | 2.26        | 2.06     |
| 23  | C     | 502  | CLA  | MG-NC   | 8.29  | 2.26        | 2.06     |
| 23  | c     | 509  | CLA  | MG-ND   | -8.25 | 1.89        | 2.05     |
| 23  | B     | 608  | CLA  | MG-NA   | 8.23  | 2.25        | 2.06     |
| 24  | a     | 2612 | PHO  | C1B-C2B | 8.22  | 1.48        | 1.39     |
| 23  | C     | 504  | CLA  | MG-NA   | 8.19  | 2.25        | 2.06     |
| 23  | b     | 606  | CLA  | MG-NC   | 7.96  | 2.25        | 2.06     |
| 23  | C     | 511  | CLA  | MG-NA   | 7.96  | 2.25        | 2.06     |
| 23  | C     | 510  | CLA  | MG-NA   | 7.96  | 2.25        | 2.06     |
| 23  | a     | 2609 | CLA  | MG-ND   | -7.95 | 1.90        | 2.05     |
| 23  | b     | 620  | CLA  | MG-NA   | 7.92  | 2.25        | 2.06     |
| 23  | c     | 511  | CLA  | MG-NC   | 7.87  | 2.25        | 2.06     |
| 39  | F     | 101  | HEM  | C3D-C2D | 7.86  | 1.53        | 1.36     |
| 23  | B     | 610  | CLA  | MG-NC   | 7.84  | 2.24        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | b     | 608  | CLA  | MG-NA   | 7.84  | 2.24        | 2.06     |
| 39  | e     | 103  | HEM  | C3D-C2D | 7.80  | 1.53        | 1.36     |
| 42  | v     | 201  | HEC  | C3D-C2D | 7.80  | 1.53        | 1.36     |
| 23  | B     | 610  | CLA  | MG-ND   | -7.79 | 1.90        | 2.05     |
| 23  | B     | 603  | CLA  | MG-ND   | -7.73 | 1.90        | 2.05     |
| 23  | c     | 508  | CLA  | MG-NA   | 7.69  | 2.24        | 2.06     |
| 23  | B     | 607  | CLA  | MG-NA   | 7.68  | 2.24        | 2.06     |
| 23  | C     | 507  | CLA  | MG-ND   | -7.66 | 1.90        | 2.05     |
| 23  | c     | 513  | CLA  | MG-ND   | -7.66 | 1.90        | 2.05     |
| 23  | c     | 510  | CLA  | MG-NA   | 7.64  | 2.24        | 2.06     |
| 23  | B     | 604  | CLA  | MG-NA   | 7.63  | 2.24        | 2.06     |
| 24  | a     | 2611 | PHO  | C1B-C2B | 7.63  | 1.48        | 1.39     |
| 42  | V     | 201  | HEC  | C3D-C2D | 7.56  | 1.52        | 1.36     |
| 23  | C     | 504  | CLA  | MG-NC   | 7.54  | 2.24        | 2.06     |
| 23  | c     | 508  | CLA  | MG-ND   | -7.48 | 1.91        | 2.05     |
| 23  | B     | 603  | CLA  | MG-NA   | 7.46  | 2.24        | 2.06     |
| 23  | c     | 512  | CLA  | MG-NA   | 7.44  | 2.23        | 2.06     |
| 23  | B     | 604  | CLA  | MG-NC   | 7.41  | 2.23        | 2.06     |
| 23  | C     | 511  | CLA  | MG-ND   | -7.37 | 1.91        | 2.05     |
| 23  | B     | 617  | CLA  | MG-ND   | -7.35 | 1.91        | 2.05     |
| 24  | A     | 409  | PHO  | C3B-C4B | 7.34  | 1.49        | 1.41     |
| 23  | b     | 606  | CLA  | MG-NA   | 7.32  | 2.23        | 2.06     |
| 23  | b     | 613  | CLA  | MG-ND   | -7.31 | 1.91        | 2.05     |
| 23  | c     | 510  | CLA  | MG-ND   | -7.26 | 1.91        | 2.05     |
| 23  | C     | 506  | CLA  | MG-ND   | -7.25 | 1.91        | 2.05     |
| 23  | b     | 611  | CLA  | MG-NC   | 7.25  | 2.23        | 2.06     |
| 23  | C     | 514  | CLA  | MG-NC   | 7.22  | 2.23        | 2.06     |
| 23  | B     | 609  | CLA  | MG-ND   | -7.21 | 1.91        | 2.05     |
| 23  | b     | 618  | CLA  | MG-NC   | 7.20  | 2.23        | 2.06     |
| 23  | B     | 606  | CLA  | MG-NA   | 7.19  | 2.23        | 2.06     |
| 26  | d     | 417  | SQD  | C6-S    | -7.15 | 1.67        | 1.77     |
| 23  | c     | 513  | CLA  | MG-NA   | 7.12  | 2.23        | 2.06     |
| 23  | B     | 607  | CLA  | MG-NC   | 7.07  | 2.23        | 2.06     |
| 23  | d     | 408  | CLA  | MG-NA   | 7.04  | 2.23        | 2.06     |
| 23  | b     | 615  | CLA  | MG-NA   | 7.03  | 2.23        | 2.06     |
| 23  | b     | 619  | CLA  | MG-ND   | -7.02 | 1.91        | 2.05     |
| 23  | c     | 515  | CLA  | MG-NA   | 7.01  | 2.22        | 2.06     |
| 23  | b     | 611  | CLA  | MG-NA   | 6.97  | 2.22        | 2.06     |
| 23  | B     | 605  | CLA  | MG-NA   | 6.97  | 2.22        | 2.06     |
| 23  | d     | 402  | CLA  | MG-ND   | -6.93 | 1.92        | 2.05     |
| 23  | c     | 516  | CLA  | MG-NA   | 6.92  | 2.22        | 2.06     |
| 23  | C     | 503  | CLA  | MG-ND   | -6.91 | 1.92        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | a     | 2612 | PHO  | C3B-C4B | 6.90  | 1.49        | 1.41     |
| 23  | b     | 612  | CLA  | MG-NA   | 6.86  | 2.22        | 2.06     |
| 23  | c     | 509  | CLA  | MG-NA   | 6.76  | 2.22        | 2.06     |
| 23  | B     | 610  | CLA  | MG-NA   | 6.76  | 2.22        | 2.06     |
| 23  | b     | 613  | CLA  | MG-NA   | 6.75  | 2.22        | 2.06     |
| 23  | c     | 507  | CLA  | MG-NA   | 6.73  | 2.22        | 2.06     |
| 24  | A     | 409  | PHO  | C3B-C2B | 6.70  | 1.49        | 1.40     |
| 23  | b     | 614  | CLA  | MG-NC   | 6.70  | 2.22        | 2.06     |
| 23  | B     | 612  | CLA  | MG-ND   | -6.68 | 1.92        | 2.05     |
| 23  | b     | 607  | CLA  | MG-NC   | 6.68  | 2.22        | 2.06     |
| 23  | c     | 509  | CLA  | MG-NC   | 6.67  | 2.22        | 2.06     |
| 23  | C     | 513  | CLA  | MG-NB   | 6.65  | 2.19        | 2.05     |
| 24  | A     | 408  | PHO  | C4D-CHA | 6.63  | 1.50        | 1.39     |
| 23  | B     | 609  | CLA  | MG-NA   | 6.63  | 2.22        | 2.06     |
| 23  | c     | 512  | CLA  | MG-ND   | -6.63 | 1.92        | 2.05     |
| 23  | b     | 610  | CLA  | MG-NA   | 6.63  | 2.22        | 2.06     |
| 23  | B     | 610  | CLA  | C1D-ND  | 6.61  | 1.45        | 1.37     |
| 24  | a     | 2611 | PHO  | C3B-C2B | 6.59  | 1.49        | 1.40     |
| 23  | C     | 507  | CLA  | MG-NA   | 6.57  | 2.21        | 2.06     |
| 23  | C     | 506  | CLA  | MG-NC   | 6.53  | 2.21        | 2.06     |
| 23  | A     | 406  | CLA  | MG-ND   | -6.51 | 1.92        | 2.05     |
| 23  | d     | 409  | CLA  | MG-NC   | 6.49  | 2.21        | 2.06     |
| 23  | C     | 509  | CLA  | MG-ND   | -6.48 | 1.92        | 2.05     |
| 23  | B     | 613  | CLA  | MG-ND   | -6.45 | 1.93        | 2.05     |
| 23  | C     | 502  | CLA  | MG-NA   | 6.45  | 2.21        | 2.06     |
| 23  | C     | 510  | CLA  | MG-ND   | -6.43 | 1.93        | 2.05     |
| 23  | b     | 616  | CLA  | MG-NA   | 6.41  | 2.21        | 2.06     |
| 23  | b     | 615  | CLA  | MG-ND   | -6.40 | 1.93        | 2.05     |
| 24  | A     | 408  | PHO  | C3B-C2B | 6.40  | 1.49        | 1.40     |
| 23  | d     | 409  | CLA  | MG-NA   | 6.40  | 2.21        | 2.06     |
| 23  | b     | 607  | CLA  | MG-NA   | 6.39  | 2.21        | 2.06     |
| 23  | c     | 506  | CLA  | MG-NC   | 6.38  | 2.21        | 2.06     |
| 24  | A     | 409  | PHO  | C4D-CHA | 6.37  | 1.49        | 1.39     |
| 23  | C     | 507  | CLA  | MG-NC   | 6.36  | 2.21        | 2.06     |
| 23  | C     | 508  | CLA  | MG-NB   | -6.31 | 1.93        | 2.05     |
| 23  | d     | 409  | CLA  | MG-ND   | -6.31 | 1.93        | 2.05     |
| 23  | A     | 405  | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 23  | c     | 505  | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 23  | C     | 514  | CLA  | C1D-ND  | 6.28  | 1.45        | 1.37     |
| 23  | B     | 605  | CLA  | MG-ND   | -6.26 | 1.93        | 2.05     |
| 23  | D     | 2304 | CLA  | C3C-C2C | 6.22  | 1.50        | 1.36     |
| 23  | C     | 502  | CLA  | C1D-ND  | 6.21  | 1.45        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | B     | 614  | CLA  | MG-NA   | 6.20  | 2.21        | 2.06     |
| 23  | a     | 2610 | CLA  | MG-NA   | 6.20  | 2.21        | 2.06     |
| 23  | c     | 509  | CLA  | C1D-ND  | 6.18  | 1.45        | 1.37     |
| 23  | b     | 611  | CLA  | C1D-ND  | 6.18  | 1.45        | 1.37     |
| 23  | a     | 2609 | CLA  | MG-NC   | 6.17  | 2.20        | 2.06     |
| 24  | a     | 2612 | PHO  | C3B-C2B | 6.17  | 1.48        | 1.40     |
| 23  | c     | 515  | CLA  | C1D-ND  | 6.17  | 1.45        | 1.37     |
| 23  | c     | 512  | CLA  | MG-NC   | 6.16  | 2.20        | 2.06     |
| 23  | B     | 605  | CLA  | MG-NC   | 6.16  | 2.20        | 2.06     |
| 23  | b     | 615  | CLA  | C1D-ND  | 6.16  | 1.45        | 1.37     |
| 23  | b     | 606  | CLA  | C1D-ND  | 6.15  | 1.45        | 1.37     |
| 24  | a     | 2611 | PHO  | C4D-CHA | 6.13  | 1.49        | 1.39     |
| 23  | c     | 504  | CLA  | MG-ND   | -6.13 | 1.93        | 2.05     |
| 23  | d     | 408  | CLA  | MG-NC   | 6.13  | 2.20        | 2.06     |
| 23  | b     | 606  | CLA  | C3C-C2C | 6.11  | 1.49        | 1.36     |
| 23  | b     | 617  | CLA  | MG-ND   | -6.08 | 1.93        | 2.05     |
| 23  | b     | 608  | CLA  | MG-NC   | 6.08  | 2.20        | 2.06     |
| 23  | c     | 508  | CLA  | C1D-ND  | 6.06  | 1.45        | 1.37     |
| 23  | c     | 510  | CLA  | MG-NC   | 6.06  | 2.20        | 2.06     |
| 23  | B     | 602  | CLA  | C3C-C2C | 6.05  | 1.49        | 1.36     |
| 23  | b     | 609  | CLA  | C1D-ND  | 6.03  | 1.45        | 1.37     |
| 23  | C     | 513  | CLA  | MG-NC   | 6.03  | 2.20        | 2.06     |
| 23  | c     | 513  | CLA  | C1D-ND  | 6.03  | 1.45        | 1.37     |
| 23  | C     | 507  | CLA  | C1D-ND  | 6.01  | 1.45        | 1.37     |
| 23  | B     | 602  | CLA  | MG-NC   | 6.00  | 2.20        | 2.06     |
| 23  | b     | 610  | CLA  | MG-NC   | 5.99  | 2.20        | 2.06     |
| 23  | c     | 511  | CLA  | C3C-C2C | 5.99  | 1.49        | 1.36     |
| 23  | c     | 516  | CLA  | C1D-ND  | 5.99  | 1.45        | 1.37     |
| 23  | C     | 509  | CLA  | C3C-C2C | 5.99  | 1.49        | 1.36     |
| 23  | c     | 506  | CLA  | C3C-C2C | 5.98  | 1.49        | 1.36     |
| 23  | B     | 605  | CLA  | C1D-ND  | 5.97  | 1.45        | 1.37     |
| 23  | B     | 610  | CLA  | C3C-C2C | 5.97  | 1.49        | 1.36     |
| 23  | c     | 516  | CLA  | MG-NC   | 5.96  | 2.20        | 2.06     |
| 23  | b     | 619  | CLA  | C1D-ND  | 5.96  | 1.45        | 1.37     |
| 23  | d     | 409  | CLA  | C3C-C2C | 5.96  | 1.49        | 1.36     |
| 23  | B     | 604  | CLA  | C1D-ND  | 5.96  | 1.45        | 1.37     |
| 23  | C     | 502  | CLA  | MG-ND   | -5.95 | 1.94        | 2.05     |
| 23  | B     | 602  | CLA  | C1D-ND  | 5.94  | 1.45        | 1.37     |
| 23  | C     | 506  | CLA  | C1D-ND  | 5.94  | 1.45        | 1.37     |
| 23  | b     | 614  | CLA  | C1D-ND  | 5.94  | 1.45        | 1.37     |
| 23  | C     | 510  | CLA  | C1D-ND  | 5.94  | 1.45        | 1.37     |
| 23  | C     | 511  | CLA  | C3C-C2C | 5.92  | 1.49        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | a     | 2613 | CLA  | C3C-C2C | 5.91  | 1.49        | 1.36     |
| 23  | b     | 607  | CLA  | C1D-ND  | 5.91  | 1.45        | 1.37     |
| 23  | b     | 612  | CLA  | C3C-C2C | 5.90  | 1.49        | 1.36     |
| 23  | b     | 618  | CLA  | MG-NA   | 5.90  | 2.20        | 2.06     |
| 23  | C     | 513  | CLA  | C3C-C2C | 5.89  | 1.49        | 1.36     |
| 23  | c     | 512  | CLA  | C1D-ND  | 5.89  | 1.45        | 1.37     |
| 23  | C     | 503  | CLA  | C3C-C2C | 5.88  | 1.49        | 1.36     |
| 23  | C     | 505  | CLA  | MG-NC   | 5.87  | 2.20        | 2.06     |
| 23  | C     | 509  | CLA  | MG-NC   | 5.87  | 2.20        | 2.06     |
| 23  | b     | 614  | CLA  | C3C-C2C | 5.87  | 1.49        | 1.36     |
| 23  | c     | 505  | CLA  | C3C-C2C | 5.86  | 1.49        | 1.36     |
| 23  | B     | 617  | CLA  | C1D-ND  | 5.86  | 1.45        | 1.37     |
| 23  | B     | 611  | CLA  | C3C-C2C | 5.86  | 1.49        | 1.36     |
| 24  | A     | 409  | PHO  | C3C-C2C | 5.85  | 1.49        | 1.36     |
| 23  | B     | 616  | CLA  | MG-ND   | -5.85 | 1.94        | 2.05     |
| 23  | B     | 614  | CLA  | C1D-ND  | 5.85  | 1.45        | 1.37     |
| 23  | C     | 507  | CLA  | C3C-C2C | 5.85  | 1.49        | 1.36     |
| 23  | B     | 612  | CLA  | C1D-ND  | 5.85  | 1.45        | 1.37     |
| 23  | B     | 611  | CLA  | C1D-ND  | 5.84  | 1.45        | 1.37     |
| 23  | C     | 506  | CLA  | C3C-C2C | 5.84  | 1.49        | 1.36     |
| 23  | d     | 408  | CLA  | MG-ND   | -5.83 | 1.94        | 2.05     |
| 23  | c     | 515  | CLA  | C3C-C2C | 5.83  | 1.49        | 1.36     |
| 23  | b     | 608  | CLA  | C3C-C2C | 5.83  | 1.49        | 1.36     |
| 23  | D     | 2303 | CLA  | C3C-C2C | 5.83  | 1.49        | 1.36     |
| 23  | b     | 607  | CLA  | MG-ND   | -5.82 | 1.94        | 2.05     |
| 23  | B     | 607  | CLA  | C3C-C2C | 5.82  | 1.49        | 1.36     |
| 23  | b     | 618  | CLA  | C3C-C2C | 5.82  | 1.49        | 1.36     |
| 23  | a     | 2610 | CLA  | MG-ND   | -5.81 | 1.94        | 2.05     |
| 23  | c     | 516  | CLA  | MG-ND   | -5.81 | 1.94        | 2.05     |
| 23  | C     | 510  | CLA  | C3C-C2C | 5.81  | 1.49        | 1.36     |
| 23  | A     | 405  | CLA  | C3C-C2C | 5.81  | 1.49        | 1.36     |
| 26  | d     | 417  | SQD  | O47-C7  | 5.80  | 1.46        | 1.33     |
| 23  | b     | 615  | CLA  | C3C-C2C | 5.78  | 1.49        | 1.36     |
| 23  | C     | 513  | CLA  | C1D-ND  | 5.78  | 1.44        | 1.37     |
| 23  | a     | 2613 | CLA  | MG-NC   | 5.78  | 2.20        | 2.06     |
| 23  | c     | 509  | CLA  | C3C-C2C | 5.77  | 1.49        | 1.36     |
| 23  | C     | 504  | CLA  | C3C-C2C | 5.75  | 1.49        | 1.36     |
| 23  | c     | 511  | CLA  | C1D-ND  | 5.74  | 1.44        | 1.37     |
| 23  | d     | 409  | CLA  | C1D-ND  | 5.74  | 1.44        | 1.37     |
| 23  | b     | 610  | CLA  | C3C-C2C | 5.73  | 1.48        | 1.36     |
| 23  | b     | 613  | CLA  | C1D-ND  | 5.73  | 1.44        | 1.37     |
| 23  | b     | 620  | CLA  | C1D-ND  | 5.72  | 1.44        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | C     | 512  | CLA  | C3C-C2C | 5.71  | 1.48        | 1.36     |
| 23  | C     | 514  | CLA  | C3C-C2C | 5.71  | 1.48        | 1.36     |
| 23  | b     | 621  | CLA  | C1D-ND  | 5.71  | 1.44        | 1.37     |
| 24  | A     | 408  | PHO  | C3C-C2C | 5.70  | 1.48        | 1.36     |
| 23  | b     | 607  | CLA  | C3C-C2C | 5.69  | 1.48        | 1.36     |
| 23  | c     | 508  | CLA  | MG-NC   | 5.69  | 2.19        | 2.06     |
| 23  | B     | 607  | CLA  | C1D-ND  | 5.68  | 1.44        | 1.37     |
| 23  | B     | 615  | CLA  | MG-NA   | 5.68  | 2.19        | 2.06     |
| 23  | C     | 504  | CLA  | C1D-ND  | 5.68  | 1.44        | 1.37     |
| 23  | a     | 2609 | CLA  | C3C-C2C | 5.67  | 1.48        | 1.36     |
| 23  | b     | 620  | CLA  | MG-NC   | 5.67  | 2.19        | 2.06     |
| 23  | B     | 609  | CLA  | C1D-ND  | 5.67  | 1.44        | 1.37     |
| 23  | c     | 511  | CLA  | MG-NB   | 5.67  | 2.17        | 2.05     |
| 23  | B     | 603  | CLA  | C1D-ND  | 5.67  | 1.44        | 1.37     |
| 23  | B     | 611  | CLA  | MG-NC   | 5.66  | 2.19        | 2.06     |
| 23  | b     | 617  | CLA  | MG-NC   | 5.66  | 2.19        | 2.06     |
| 23  | C     | 514  | CLA  | MG-ND   | -5.66 | 1.94        | 2.05     |
| 23  | B     | 615  | CLA  | C3C-C2C | 5.66  | 1.48        | 1.36     |
| 23  | c     | 505  | CLA  | MG-NC   | 5.66  | 2.19        | 2.06     |
| 23  | d     | 402  | CLA  | MG-NA   | 5.65  | 2.19        | 2.06     |
| 23  | b     | 611  | CLA  | C3C-C2C | 5.64  | 1.48        | 1.36     |
| 24  | A     | 408  | PHO  | C3D-C2D | 5.64  | 1.49        | 1.39     |
| 23  | B     | 603  | CLA  | C3C-C2C | 5.63  | 1.48        | 1.36     |
| 23  | C     | 502  | CLA  | C3C-C2C | 5.63  | 1.48        | 1.36     |
| 23  | B     | 604  | CLA  | C3C-C2C | 5.62  | 1.48        | 1.36     |
| 23  | a     | 2610 | CLA  | C1D-ND  | 5.62  | 1.44        | 1.37     |
| 23  | b     | 617  | CLA  | C3C-C2C | 5.61  | 1.48        | 1.36     |
| 23  | a     | 2613 | CLA  | C1D-ND  | 5.60  | 1.44        | 1.37     |
| 23  | C     | 508  | CLA  | C1D-ND  | 5.60  | 1.44        | 1.37     |
| 23  | A     | 410  | CLA  | C1D-ND  | 5.59  | 1.44        | 1.37     |
| 23  | d     | 402  | CLA  | C3C-C2C | 5.59  | 1.48        | 1.36     |
| 23  | A     | 405  | CLA  | MG-ND   | -5.58 | 1.94        | 2.05     |
| 23  | B     | 609  | CLA  | C3C-C2C | 5.57  | 1.48        | 1.36     |
| 23  | b     | 609  | CLA  | C3C-C2C | 5.57  | 1.48        | 1.36     |
| 23  | b     | 608  | CLA  | C1D-ND  | 5.57  | 1.44        | 1.37     |
| 23  | c     | 516  | CLA  | C3C-C2C | 5.56  | 1.48        | 1.36     |
| 23  | B     | 608  | CLA  | C3C-C2C | 5.56  | 1.48        | 1.36     |
| 23  | c     | 513  | CLA  | C3C-C2C | 5.56  | 1.48        | 1.36     |
| 24  | a     | 2612 | PHO  | C3C-C2C | 5.54  | 1.48        | 1.36     |
| 23  | C     | 505  | CLA  | C1D-ND  | 5.54  | 1.44        | 1.37     |
| 23  | A     | 407  | CLA  | C3C-C2C | 5.53  | 1.48        | 1.36     |
| 23  | c     | 505  | CLA  | C1D-ND  | 5.53  | 1.44        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | b     | 608  | CLA  | MG-ND   | -5.53 | 1.94        | 2.05     |
| 23  | b     | 610  | CLA  | C1D-ND  | 5.53  | 1.44        | 1.37     |
| 23  | c     | 512  | CLA  | C3C-C2C | 5.52  | 1.48        | 1.36     |
| 23  | c     | 508  | CLA  | C3C-C2C | 5.52  | 1.48        | 1.36     |
| 23  | b     | 620  | CLA  | C3C-C2C | 5.51  | 1.48        | 1.36     |
| 23  | B     | 606  | CLA  | C1D-ND  | 5.51  | 1.44        | 1.37     |
| 24  | a     | 2612 | PHO  | C4D-CHA | 5.51  | 1.48        | 1.39     |
| 23  | b     | 613  | CLA  | C3C-C2C | 5.50  | 1.48        | 1.36     |
| 23  | d     | 402  | CLA  | C1D-ND  | 5.48  | 1.44        | 1.37     |
| 23  | c     | 514  | CLA  | C3C-C2C | 5.48  | 1.48        | 1.36     |
| 23  | b     | 616  | CLA  | C1D-ND  | 5.47  | 1.44        | 1.37     |
| 23  | C     | 505  | CLA  | C3C-C2C | 5.47  | 1.48        | 1.36     |
| 23  | b     | 619  | CLA  | C3C-C2C | 5.46  | 1.48        | 1.36     |
| 23  | b     | 618  | CLA  | C1D-ND  | 5.46  | 1.44        | 1.37     |
| 23  | B     | 613  | CLA  | MG-NA   | 5.45  | 2.19        | 2.06     |
| 23  | c     | 515  | CLA  | MG-NC   | 5.44  | 2.19        | 2.06     |
| 23  | a     | 2610 | CLA  | C3C-C2C | 5.44  | 1.48        | 1.36     |
| 23  | C     | 509  | CLA  | C1D-ND  | 5.44  | 1.44        | 1.37     |
| 23  | c     | 513  | CLA  | MG-NC   | 5.43  | 2.19        | 2.06     |
| 23  | B     | 615  | CLA  | C1D-ND  | 5.43  | 1.44        | 1.37     |
| 23  | C     | 508  | CLA  | C3C-C2C | 5.42  | 1.48        | 1.36     |
| 23  | C     | 513  | CLA  | CHC-C1C | 5.42  | 1.49        | 1.38     |
| 23  | d     | 408  | CLA  | C3C-C2C | 5.42  | 1.48        | 1.36     |
| 23  | A     | 410  | CLA  | C3C-C2C | 5.42  | 1.48        | 1.36     |
| 23  | A     | 410  | CLA  | MG-NA   | 5.41  | 2.19        | 2.06     |
| 23  | c     | 507  | CLA  | C3C-C2C | 5.41  | 1.48        | 1.36     |
| 23  | a     | 2609 | CLA  | MG-NA   | 5.40  | 2.19        | 2.06     |
| 23  | c     | 506  | CLA  | C1D-ND  | 5.39  | 1.44        | 1.37     |
| 23  | B     | 617  | CLA  | MG-NC   | 5.38  | 2.19        | 2.06     |
| 24  | a     | 2611 | PHO  | C3B-C4B | 5.38  | 1.47        | 1.41     |
| 23  | B     | 612  | CLA  | C3C-C2C | 5.37  | 1.48        | 1.36     |
| 23  | b     | 614  | CLA  | O2D-CGD | 5.36  | 1.46        | 1.33     |
| 23  | b     | 617  | CLA  | C1D-ND  | 5.35  | 1.44        | 1.37     |
| 23  | c     | 510  | CLA  | C1D-ND  | 5.35  | 1.44        | 1.37     |
| 23  | B     | 602  | CLA  | CHC-C1C | 5.35  | 1.49        | 1.38     |
| 23  | c     | 514  | CLA  | C1D-ND  | 5.34  | 1.44        | 1.37     |
| 23  | c     | 504  | CLA  | C3C-C2C | 5.34  | 1.48        | 1.36     |
| 23  | B     | 608  | CLA  | C1D-ND  | 5.34  | 1.44        | 1.37     |
| 23  | c     | 510  | CLA  | C3C-C2C | 5.34  | 1.48        | 1.36     |
| 23  | C     | 506  | CLA  | CHD-C1D | 5.33  | 1.48        | 1.38     |
| 23  | C     | 502  | CLA  | CHC-C1C | 5.33  | 1.49        | 1.38     |
| 23  | B     | 617  | CLA  | C3C-C2C | 5.31  | 1.48        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | b     | 610  | CLA  | MG-ND   | -5.31 | 1.95        | 2.05     |
| 23  | a     | 2609 | CLA  | C1D-ND  | 5.30  | 1.44        | 1.37     |
| 23  | b     | 606  | CLA  | CHD-C1D | 5.30  | 1.48        | 1.38     |
| 23  | b     | 616  | CLA  | C3C-C2C | 5.29  | 1.48        | 1.36     |
| 23  | B     | 605  | CLA  | C3C-C2C | 5.28  | 1.47        | 1.36     |
| 23  | B     | 614  | CLA  | C3C-C2C | 5.27  | 1.47        | 1.36     |
| 23  | b     | 620  | CLA  | CHC-C1C | 5.27  | 1.49        | 1.38     |
| 23  | C     | 505  | CLA  | MG-NA   | 5.27  | 2.18        | 2.06     |
| 23  | B     | 614  | CLA  | O2D-CGD | 5.26  | 1.46        | 1.33     |
| 23  | b     | 619  | CLA  | MG-NA   | 5.26  | 2.18        | 2.06     |
| 23  | D     | 2304 | CLA  | CHC-C1C | 5.26  | 1.49        | 1.38     |
| 23  | C     | 511  | CLA  | C1D-ND  | 5.25  | 1.44        | 1.37     |
| 23  | B     | 616  | CLA  | C1D-ND  | 5.24  | 1.44        | 1.37     |
| 24  | a     | 2611 | PHO  | C3D-C2D | 5.24  | 1.48        | 1.39     |
| 23  | B     | 610  | CLA  | O2D-CGD | 5.24  | 1.46        | 1.33     |
| 23  | A     | 406  | CLA  | C3C-C2C | 5.23  | 1.47        | 1.36     |
| 23  | C     | 508  | CLA  | MG-NC   | 5.23  | 2.18        | 2.06     |
| 23  | B     | 606  | CLA  | MG-NC   | 5.23  | 2.18        | 2.06     |
| 23  | C     | 503  | CLA  | C1D-ND  | 5.22  | 1.44        | 1.37     |
| 23  | C     | 512  | CLA  | C1D-ND  | 5.22  | 1.44        | 1.37     |
| 24  | A     | 409  | PHO  | C3D-C2D | 5.20  | 1.48        | 1.39     |
| 23  | b     | 606  | CLA  | CHC-C1C | 5.19  | 1.49        | 1.38     |
| 23  | C     | 507  | CLA  | O2D-CGD | 5.19  | 1.45        | 1.33     |
| 23  | A     | 407  | CLA  | C1D-ND  | 5.19  | 1.44        | 1.37     |
| 23  | B     | 616  | CLA  | C3C-C2C | 5.19  | 1.47        | 1.36     |
| 23  | B     | 606  | CLA  | C3C-C2C | 5.18  | 1.47        | 1.36     |
| 23  | C     | 514  | CLA  | CHC-C1C | 5.18  | 1.49        | 1.38     |
| 23  | B     | 607  | CLA  | CHC-C1C | 5.17  | 1.49        | 1.38     |
| 23  | b     | 621  | CLA  | C3C-C2C | 5.17  | 1.47        | 1.36     |
| 23  | B     | 613  | CLA  | C3C-C2C | 5.17  | 1.47        | 1.36     |
| 23  | c     | 509  | CLA  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 23  | c     | 516  | CLA  | CHC-C1C | 5.16  | 1.49        | 1.38     |
| 23  | B     | 602  | CLA  | CHD-C1D | 5.16  | 1.48        | 1.38     |
| 23  | A     | 406  | CLA  | MG-NA   | 5.15  | 2.18        | 2.06     |
| 23  | b     | 621  | CLA  | O2D-CGD | 5.15  | 1.45        | 1.33     |
| 23  | b     | 606  | CLA  | O2D-CGD | 5.15  | 1.45        | 1.33     |
| 24  | a     | 2612 | PHO  | C3D-C2D | 5.14  | 1.48        | 1.39     |
| 23  | A     | 405  | CLA  | C1D-ND  | 5.13  | 1.44        | 1.37     |
| 39  | F     | 101  | HEM  | FE-ND   | 5.13  | 2.10        | 1.94     |
| 23  | C     | 502  | CLA  | CHD-C1D | 5.13  | 1.48        | 1.38     |
| 23  | B     | 604  | CLA  | CHC-C1C | 5.12  | 1.48        | 1.38     |
| 23  | d     | 402  | CLA  | MG-NB   | 5.12  | 2.15        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | A     | 406  | CLA  | C1D-ND  | 5.10  | 1.44        | 1.37     |
| 24  | A     | 408  | PHO  | C3B-C4B | 5.09  | 1.47        | 1.41     |
| 24  | a     | 2611 | PHO  | C3C-C2C | 5.09  | 1.47        | 1.36     |
| 23  | B     | 614  | CLA  | MG-ND   | -5.09 | 1.95        | 2.05     |
| 23  | D     | 2303 | CLA  | MG-NC   | 5.09  | 2.18        | 2.06     |
| 23  | c     | 505  | CLA  | CHC-C1C | 5.09  | 1.48        | 1.38     |
| 23  | c     | 507  | CLA  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 23  | A     | 410  | CLA  | MG-NC   | 5.08  | 2.18        | 2.06     |
| 23  | C     | 506  | CLA  | CHC-C1C | 5.08  | 1.48        | 1.38     |
| 39  | e     | 103  | HEM  | FE-ND   | 5.08  | 2.10        | 1.94     |
| 23  | b     | 613  | CLA  | MG-NC   | 5.07  | 2.18        | 2.06     |
| 23  | b     | 615  | CLA  | CHC-C1C | 5.07  | 1.48        | 1.38     |
| 23  | B     | 602  | CLA  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 23  | b     | 613  | CLA  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 23  | b     | 614  | CLA  | CHD-C1D | 5.04  | 1.48        | 1.38     |
| 23  | b     | 619  | CLA  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 23  | c     | 506  | CLA  | CHC-C1C | 5.03  | 1.48        | 1.38     |
| 23  | b     | 606  | CLA  | MG-ND   | -5.03 | 1.95        | 2.05     |
| 23  | b     | 620  | CLA  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 23  | b     | 607  | CLA  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 23  | c     | 515  | CLA  | MG-NB   | 5.00  | 2.15        | 2.05     |
| 23  | B     | 609  | CLA  | CHC-C1C | 4.99  | 1.48        | 1.38     |
| 23  | c     | 505  | CLA  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 23  | b     | 614  | CLA  | CHC-C1C | 4.99  | 1.48        | 1.38     |
| 23  | c     | 513  | CLA  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 23  | a     | 2613 | CLA  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 23  | C     | 505  | CLA  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 23  | C     | 509  | CLA  | CHC-C1C | 4.98  | 1.48        | 1.38     |
| 23  | b     | 619  | CLA  | MG-NC   | 4.97  | 2.18        | 2.06     |
| 23  | c     | 515  | CLA  | CHC-C1C | 4.97  | 1.48        | 1.38     |
| 23  | c     | 511  | CLA  | CHC-C1C | 4.97  | 1.48        | 1.38     |
| 23  | B     | 615  | CLA  | CHC-C1C | 4.97  | 1.48        | 1.38     |
| 23  | C     | 507  | CLA  | CHC-C1C | 4.96  | 1.48        | 1.38     |
| 23  | B     | 613  | CLA  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 24  | A     | 409  | PHO  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 23  | c     | 514  | CLA  | CHD-C1D | 4.95  | 1.48        | 1.38     |
| 24  | a     | 2611 | PHO  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 23  | c     | 509  | CLA  | CHD-C1D | 4.94  | 1.48        | 1.38     |
| 23  | c     | 505  | CLA  | MG-ND   | -4.94 | 1.96        | 2.05     |
| 23  | d     | 409  | CLA  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 23  | B     | 616  | CLA  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 23  | a     | 2610 | CLA  | CHC-C1C | 4.93  | 1.48        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | c     | 507  | CLA  | MG-ND   | -4.92 | 1.96        | 2.05     |
| 23  | C     | 503  | CLA  | CHC-C1C | 4.92  | 1.48        | 1.38     |
| 23  | B     | 604  | CLA  | MG-ND   | -4.92 | 1.96        | 2.05     |
| 23  | C     | 511  | CLA  | MG-NB   | 4.92  | 2.15        | 2.05     |
| 23  | d     | 409  | CLA  | CHC-C1C | 4.91  | 1.48        | 1.38     |
| 23  | d     | 402  | CLA  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 23  | b     | 612  | CLA  | MG-ND   | -4.91 | 1.96        | 2.05     |
| 23  | C     | 509  | CLA  | MG-NB   | 4.91  | 2.15        | 2.05     |
| 23  | C     | 504  | CLA  | CHC-C1C | 4.90  | 1.48        | 1.38     |
| 23  | C     | 510  | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 23  | c     | 514  | CLA  | CHC-C1C | 4.90  | 1.48        | 1.38     |
| 23  | A     | 407  | CLA  | CHC-C1C | 4.90  | 1.48        | 1.38     |
| 23  | C     | 514  | CLA  | CHD-C1D | 4.89  | 1.47        | 1.38     |
| 23  | c     | 511  | CLA  | CHD-C1D | 4.89  | 1.47        | 1.38     |
| 23  | b     | 616  | CLA  | O2D-CGD | 4.88  | 1.45        | 1.33     |
| 23  | C     | 506  | CLA  | O2D-CGD | 4.88  | 1.45        | 1.33     |
| 23  | C     | 511  | CLA  | MG-NC   | 4.88  | 2.17        | 2.06     |
| 23  | C     | 514  | CLA  | O2D-CGD | 4.88  | 1.45        | 1.33     |
| 23  | B     | 611  | CLA  | CHC-C1C | 4.88  | 1.48        | 1.38     |
| 39  | e     | 103  | HEM  | FE-NB   | 4.87  | 2.09        | 1.94     |
| 23  | c     | 507  | CLA  | CHC-C1C | 4.87  | 1.48        | 1.38     |
| 24  | a     | 2612 | PHO  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 23  | c     | 513  | CLA  | CHC-C1C | 4.86  | 1.48        | 1.38     |
| 23  | B     | 603  | CLA  | CHD-C1D | 4.86  | 1.47        | 1.38     |
| 23  | b     | 618  | CLA  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 23  | A     | 410  | CLA  | CHC-C1C | 4.86  | 1.48        | 1.38     |
| 23  | b     | 619  | CLA  | CHC-C1C | 4.85  | 1.48        | 1.38     |
| 23  | A     | 407  | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 23  | b     | 607  | CLA  | CHD-C1D | 4.85  | 1.47        | 1.38     |
| 23  | C     | 505  | CLA  | CHC-C1C | 4.85  | 1.48        | 1.38     |
| 23  | B     | 617  | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 23  | c     | 507  | CLA  | C1D-ND  | 4.85  | 1.43        | 1.37     |
| 23  | B     | 606  | CLA  | CHC-C1C | 4.84  | 1.48        | 1.38     |
| 23  | B     | 607  | CLA  | CHD-C1D | 4.83  | 1.47        | 1.38     |
| 23  | B     | 613  | CLA  | CHB-C1B | 4.83  | 1.50        | 1.39     |
| 23  | B     | 610  | CLA  | CHC-C1C | 4.83  | 1.48        | 1.38     |
| 23  | A     | 410  | CLA  | CHD-C1D | 4.82  | 1.47        | 1.38     |
| 23  | C     | 508  | CLA  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 23  | c     | 516  | CLA  | CHD-C1D | 4.82  | 1.47        | 1.38     |
| 23  | C     | 511  | CLA  | CHC-C1C | 4.82  | 1.48        | 1.38     |
| 24  | A     | 408  | PHO  | O2D-CGD | 4.82  | 1.44        | 1.33     |
| 23  | D     | 2304 | CLA  | O2D-CGD | 4.81  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | c     | 512  | CLA  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 23  | b     | 615  | CLA  | MG-NC   | 4.80  | 2.17        | 2.06     |
| 23  | C     | 512  | CLA  | CHC-C1C | 4.80  | 1.48        | 1.38     |
| 23  | c     | 516  | CLA  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 23  | c     | 512  | CLA  | CHB-C1B | 4.80  | 1.50        | 1.39     |
| 23  | a     | 2613 | CLA  | CHC-C1C | 4.80  | 1.48        | 1.38     |
| 23  | C     | 502  | CLA  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 23  | b     | 609  | CLA  | CHC-C1C | 4.79  | 1.48        | 1.38     |
| 23  | c     | 504  | CLA  | C1D-ND  | 4.79  | 1.43        | 1.37     |
| 23  | C     | 513  | CLA  | O2D-CGD | 4.79  | 1.44        | 1.33     |
| 23  | B     | 612  | CLA  | CHC-C1C | 4.79  | 1.48        | 1.38     |
| 23  | b     | 611  | CLA  | O2D-CGD | 4.79  | 1.44        | 1.33     |
| 23  | b     | 617  | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 23  | c     | 504  | CLA  | CHC-C1C | 4.78  | 1.48        | 1.38     |
| 23  | b     | 607  | CLA  | CHC-C1C | 4.78  | 1.48        | 1.38     |
| 23  | b     | 616  | CLA  | CHD-C1D | 4.78  | 1.47        | 1.38     |
| 23  | b     | 612  | CLA  | MG-NC   | 4.78  | 2.17        | 2.06     |
| 23  | C     | 511  | CLA  | CHB-C1B | 4.78  | 1.50        | 1.39     |
| 23  | B     | 606  | CLA  | CHD-C1D | 4.77  | 1.47        | 1.38     |
| 23  | C     | 512  | CLA  | CHD-C1D | 4.77  | 1.47        | 1.38     |
| 23  | C     | 503  | CLA  | O2D-CGD | 4.77  | 1.44        | 1.33     |
| 23  | C     | 509  | CLA  | O2D-CGD | 4.76  | 1.44        | 1.33     |
| 23  | B     | 614  | CLA  | MG-NC   | 4.76  | 2.17        | 2.06     |
| 23  | b     | 618  | CLA  | CHC-C1C | 4.76  | 1.48        | 1.38     |
| 23  | B     | 614  | CLA  | CHC-C1C | 4.76  | 1.48        | 1.38     |
| 23  | b     | 608  | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 23  | C     | 513  | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 23  | B     | 613  | CLA  | CHC-C1C | 4.74  | 1.48        | 1.38     |
| 23  | b     | 612  | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 23  | c     | 508  | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 23  | B     | 603  | CLA  | CHC-C1C | 4.73  | 1.48        | 1.38     |
| 23  | C     | 503  | CLA  | CHD-C1D | 4.73  | 1.47        | 1.38     |
| 23  | b     | 608  | CLA  | CHC-C1C | 4.73  | 1.48        | 1.38     |
| 23  | A     | 410  | CLA  | MG-ND   | -4.73 | 1.96        | 2.05     |
| 23  | C     | 512  | CLA  | O2D-CGD | 4.72  | 1.44        | 1.33     |
| 23  | B     | 608  | CLA  | O2D-CGD | 4.72  | 1.44        | 1.33     |
| 23  | C     | 512  | CLA  | MG-ND   | -4.72 | 1.96        | 2.05     |
| 42  | v     | 201  | HEC  | FE-ND   | 4.72  | 2.09        | 1.94     |
| 23  | B     | 607  | CLA  | O2D-CGD | 4.72  | 1.44        | 1.33     |
| 23  | c     | 509  | CLA  | CHC-C1C | 4.71  | 1.48        | 1.38     |
| 23  | b     | 608  | CLA  | CHD-C1D | 4.71  | 1.47        | 1.38     |
| 23  | b     | 610  | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | B     | 607  | CLA  | CHC-C4B | 4.70  | 1.49        | 1.39     |
| 23  | B     | 610  | CLA  | CHD-C1D | 4.70  | 1.47        | 1.38     |
| 23  | c     | 510  | CLA  | O2D-CGD | 4.69  | 1.44        | 1.33     |
| 23  | C     | 505  | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 23  | c     | 513  | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 23  | B     | 606  | CLA  | O2D-CGD | 4.68  | 1.44        | 1.33     |
| 23  | B     | 604  | CLA  | CHC-C4B | 4.68  | 1.49        | 1.39     |
| 23  | b     | 609  | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 23  | c     | 506  | CLA  | CHB-C1B | 4.67  | 1.49        | 1.39     |
| 23  | A     | 405  | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 23  | C     | 502  | CLA  | CHC-C4B | 4.67  | 1.49        | 1.39     |
| 23  | c     | 504  | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 23  | b     | 611  | CLA  | CHC-C1C | 4.67  | 1.48        | 1.38     |
| 23  | d     | 408  | CLA  | CHC-C1C | 4.67  | 1.48        | 1.38     |
| 23  | c     | 515  | CLA  | O2D-CGD | 4.66  | 1.44        | 1.33     |
| 23  | b     | 613  | CLA  | CHC-C1C | 4.65  | 1.48        | 1.38     |
| 23  | C     | 510  | CLA  | CHC-C1C | 4.65  | 1.48        | 1.38     |
| 23  | B     | 603  | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 23  | B     | 604  | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 23  | C     | 511  | CLA  | O2D-CGD | 4.63  | 1.44        | 1.33     |
| 23  | C     | 509  | CLA  | MG-NA   | 4.63  | 2.17        | 2.06     |
| 23  | c     | 511  | CLA  | MG-NA   | 4.63  | 2.17        | 2.06     |
| 23  | B     | 608  | CLA  | CHC-C1C | 4.63  | 1.47        | 1.38     |
| 23  | b     | 613  | CLA  | CHD-C1D | 4.62  | 1.47        | 1.38     |
| 23  | d     | 402  | CLA  | CHD-C1D | 4.62  | 1.47        | 1.38     |
| 34  | c     | 532  | DMS  | O-S     | 4.62  | 1.81        | 1.50     |
| 23  | c     | 512  | CLA  | CHC-C1C | 4.62  | 1.47        | 1.38     |
| 34  | o     | 311  | DMS  | O-S     | 4.61  | 1.81        | 1.50     |
| 23  | A     | 410  | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 23  | c     | 508  | CLA  | CHC-C1C | 4.61  | 1.47        | 1.38     |
| 23  | B     | 608  | CLA  | MG-NC   | 4.60  | 2.17        | 2.06     |
| 23  | B     | 616  | CLA  | CHC-C1C | 4.60  | 1.47        | 1.38     |
| 23  | C     | 504  | CLA  | CHC-C4B | 4.60  | 1.49        | 1.39     |
| 23  | A     | 407  | CLA  | CHD-C1D | 4.60  | 1.47        | 1.38     |
| 23  | a     | 2610 | CLA  | O2D-CGD | 4.60  | 1.44        | 1.33     |
| 23  | c     | 512  | CLA  | CHD-C1D | 4.59  | 1.47        | 1.38     |
| 23  | D     | 2304 | CLA  | C1D-ND  | 4.59  | 1.43        | 1.37     |
| 23  | b     | 617  | CLA  | CHC-C1C | 4.59  | 1.47        | 1.38     |
| 23  | b     | 612  | CLA  | CHD-C1D | 4.59  | 1.47        | 1.38     |
| 23  | C     | 508  | CLA  | MG-ND   | -4.59 | 1.96        | 2.05     |
| 34  | b     | 637  | DMS  | O-S     | 4.59  | 1.81        | 1.50     |
| 23  | B     | 611  | CLA  | CHD-C1D | 4.59  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | a     | 2609 | CLA  | CHC-C1C | 4.59  | 1.47        | 1.38     |
| 34  | c     | 544  | DMS  | O-S     | 4.58  | 1.81        | 1.50     |
| 23  | b     | 614  | CLA  | CHB-C1B | 4.58  | 1.49        | 1.39     |
| 34  | a     | 2624 | DMS  | O-S     | 4.58  | 1.81        | 1.50     |
| 23  | B     | 611  | CLA  | MG-ND   | -4.58 | 1.96        | 2.05     |
| 23  | b     | 612  | CLA  | C1D-ND  | 4.58  | 1.43        | 1.37     |
| 23  | d     | 402  | CLA  | CHC-C1C | 4.57  | 1.47        | 1.38     |
| 23  | b     | 616  | CLA  | CHB-C1B | 4.57  | 1.49        | 1.39     |
| 23  | B     | 612  | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |
| 23  | B     | 602  | CLA  | O2A-CGA | 4.57  | 1.46        | 1.33     |
| 23  | C     | 508  | CLA  | CHD-C1D | 4.57  | 1.47        | 1.38     |
| 23  | b     | 616  | CLA  | CHC-C1C | 4.57  | 1.47        | 1.38     |
| 23  | d     | 408  | CLA  | O2A-CGA | 4.57  | 1.46        | 1.33     |
| 27  | m     | 2802 | LMG  | O8-C28  | 4.57  | 1.46        | 1.33     |
| 23  | c     | 513  | CLA  | CHB-C1B | 4.56  | 1.49        | 1.39     |
| 34  | A     | 430  | DMS  | O-S     | 4.56  | 1.81        | 1.50     |
| 23  | b     | 620  | CLA  | MG-ND   | -4.56 | 1.96        | 2.05     |
| 34  | B     | 643  | DMS  | O-S     | 4.56  | 1.81        | 1.50     |
| 23  | b     | 611  | CLA  | CHD-C1D | 4.56  | 1.47        | 1.38     |
| 34  | o     | 316  | DMS  | O-S     | 4.56  | 1.81        | 1.50     |
| 23  | B     | 617  | CLA  | CHC-C1C | 4.56  | 1.47        | 1.38     |
| 23  | B     | 609  | CLA  | CHD-C1D | 4.56  | 1.47        | 1.38     |
| 23  | C     | 507  | CLA  | CHD-C1D | 4.56  | 1.47        | 1.38     |
| 34  | c     | 549  | DMS  | O-S     | 4.56  | 1.81        | 1.50     |
| 34  | o     | 313  | DMS  | O-S     | 4.55  | 1.81        | 1.50     |
| 34  | D     | 2316 | DMS  | O-S     | 4.55  | 1.81        | 1.50     |
| 23  | A     | 406  | CLA  | O2D-CGD | 4.55  | 1.44        | 1.33     |
| 23  | b     | 620  | CLA  | CHD-C1D | 4.55  | 1.47        | 1.38     |
| 23  | B     | 615  | CLA  | CHB-C1B | 4.54  | 1.49        | 1.39     |
| 34  | V     | 206  | DMS  | O-S     | 4.54  | 1.80        | 1.50     |
| 23  | B     | 603  | CLA  | MG-NC   | 4.54  | 2.17        | 2.06     |
| 34  | C     | 531  | DMS  | O-S     | 4.54  | 1.80        | 1.50     |
| 34  | B     | 639  | DMS  | O-S     | 4.54  | 1.80        | 1.50     |
| 23  | C     | 510  | CLA  | MG-NC   | 4.53  | 2.17        | 2.06     |
| 23  | B     | 615  | CLA  | MG-NB   | 4.53  | 2.14        | 2.05     |
| 23  | C     | 504  | CLA  | CHB-C1B | 4.53  | 1.49        | 1.39     |
| 23  | C     | 512  | CLA  | CHB-C1B | 4.53  | 1.49        | 1.39     |
| 23  | d     | 409  | CLA  | CHD-C1D | 4.53  | 1.47        | 1.38     |
| 23  | B     | 605  | CLA  | CHD-C1D | 4.53  | 1.47        | 1.38     |
| 23  | c     | 508  | CLA  | CHD-C1D | 4.53  | 1.47        | 1.38     |
| 23  | c     | 511  | CLA  | O2D-CGD | 4.53  | 1.44        | 1.33     |
| 34  | O     | 313  | DMS  | O-S     | 4.53  | 1.80        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 34  | U     | 503  | DMS  | O-S     | 4.53 | 1.80        | 1.50     |
| 34  | T     | 105  | DMS  | O-S     | 4.53 | 1.80        | 1.50     |
| 34  | B     | 635  | DMS  | O-S     | 4.53 | 1.80        | 1.50     |
| 34  | O     | 314  | DMS  | O-S     | 4.53 | 1.80        | 1.50     |
| 34  | b     | 635  | DMS  | O-S     | 4.53 | 1.80        | 1.50     |
| 23  | c     | 510  | CLA  | CHD-C1D | 4.52 | 1.47        | 1.38     |
| 23  | b     | 615  | CLA  | O2D-CGD | 4.52 | 1.44        | 1.33     |
| 34  | O     | 308  | DMS  | O-S     | 4.52 | 1.80        | 1.50     |
| 34  | O     | 312  | DMS  | O-S     | 4.52 | 1.80        | 1.50     |
| 34  | c     | 546  | DMS  | O-S     | 4.52 | 1.80        | 1.50     |
| 23  | b     | 619  | CLA  | CHD-C1D | 4.52 | 1.47        | 1.38     |
| 34  | b     | 643  | DMS  | O-S     | 4.52 | 1.80        | 1.50     |
| 23  | B     | 613  | CLA  | CHD-C1D | 4.52 | 1.47        | 1.38     |
| 34  | v     | 206  | DMS  | O-S     | 4.52 | 1.80        | 1.50     |
| 23  | B     | 612  | CLA  | MG-NC   | 4.52 | 2.17        | 2.06     |
| 34  | l     | 104  | DMS  | O-S     | 4.52 | 1.80        | 1.50     |
| 34  | U     | 504  | DMS  | O-S     | 4.52 | 1.80        | 1.50     |
| 34  | A     | 428  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | c     | 547  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | D     | 2317 | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | O     | 315  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | V     | 205  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | C     | 528  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | b     | 641  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 23  | B     | 611  | CLA  | O2D-CGD | 4.51 | 1.44        | 1.33     |
| 23  | B     | 610  | CLA  | CHB-C1B | 4.51 | 1.49        | 1.39     |
| 34  | c     | 542  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | B     | 646  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | B     | 644  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | t     | 102  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | c     | 540  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | B     | 637  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | A     | 426  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | c     | 537  | DMS  | O-S     | 4.51 | 1.80        | 1.50     |
| 34  | o     | 309  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |
| 34  | c     | 538  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |
| 34  | A     | 429  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |
| 34  | B     | 641  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |
| 34  | B     | 645  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |
| 34  | b     | 636  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |
| 34  | V     | 208  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |
| 34  | o     | 306  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 34  | c     | 545  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |
| 23  | b     | 618  | CLA  | CHD-C1D | 4.50 | 1.47        | 1.38     |
| 34  | V     | 211  | DMS  | O-S     | 4.50 | 1.80        | 1.50     |
| 26  | l     | 101  | SQD  | O47-C7  | 4.50 | 1.47        | 1.34     |
| 23  | C     | 508  | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 34  | o     | 305  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | D     | 2319 | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | U     | 505  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | d     | 423  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 27  | c     | 522  | LMG  | O7-C10  | 4.49 | 1.47        | 1.34     |
| 34  | v     | 210  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | a     | 2620 | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 23  | C     | 509  | CLA  | CHD-C1D | 4.49 | 1.47        | 1.38     |
| 34  | C     | 537  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | O     | 317  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | B     | 647  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | v     | 214  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 23  | c     | 506  | CLA  | O2D-CGD | 4.49 | 1.44        | 1.33     |
| 23  | b     | 615  | CLA  | CHD-C1D | 4.49 | 1.47        | 1.38     |
| 34  | O     | 311  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | V     | 210  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | O     | 309  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | T     | 104  | DMS  | O-S     | 4.49 | 1.80        | 1.50     |
| 34  | v     | 208  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | o     | 315  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | X     | 101  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | V     | 212  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | v     | 211  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | v     | 212  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | O     | 319  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | H     | 104  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | c     | 541  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | b     | 639  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 34  | c     | 539  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 23  | B     | 605  | CLA  | O2D-CGD | 4.48 | 1.44        | 1.33     |
| 23  | c     | 505  | CLA  | CHD-C1D | 4.48 | 1.47        | 1.38     |
| 34  | c     | 548  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 23  | A     | 406  | CLA  | O2A-CGA | 4.48 | 1.46        | 1.33     |
| 34  | b     | 642  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 37  | C     | 519  | DGD  | O1G-C1A | 4.48 | 1.46        | 1.33     |
| 34  | o     | 310  | DMS  | O-S     | 4.48 | 1.80        | 1.50     |
| 27  | C     | 527  | LMG  | O7-C10  | 4.47 | 1.46        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 34  | C     | 536  | DMS  | O-S     | 4.47 | 1.80        | 1.50     |
| 34  | A     | 427  | DMS  | O-S     | 4.47 | 1.80        | 1.50     |
| 34  | b     | 638  | DMS  | O-S     | 4.47 | 1.80        | 1.50     |
| 34  | V     | 207  | DMS  | O-S     | 4.47 | 1.80        | 1.50     |
| 34  | a     | 2621 | DMS  | O-S     | 4.47 | 1.80        | 1.50     |
| 34  | V     | 213  | DMS  | O-S     | 4.47 | 1.80        | 1.50     |
| 34  | C     | 530  | DMS  | O-S     | 4.47 | 1.80        | 1.50     |
| 26  | a     | 2603 | SQD  | O47-C7  | 4.47 | 1.46        | 1.34     |
| 34  | O     | 318  | DMS  | O-S     | 4.47 | 1.80        | 1.50     |
| 34  | O     | 306  | DMS  | O-S     | 4.47 | 1.80        | 1.50     |
| 23  | B     | 602  | CLA  | CHB-C1B | 4.47 | 1.49        | 1.39     |
| 34  | d     | 419  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | D     | 2320 | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | v     | 209  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | v     | 213  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | o     | 308  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | d     | 421  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | u     | 504  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | u     | 502  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | a     | 2622 | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 26  | B     | 621  | SQD  | O47-C7  | 4.46 | 1.46        | 1.34     |
| 34  | d     | 420  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | O     | 310  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 23  | b     | 612  | CLA  | CHC-C1C | 4.46 | 1.47        | 1.38     |
| 34  | C     | 534  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | d     | 422  | DMS  | O-S     | 4.46 | 1.80        | 1.50     |
| 34  | B     | 640  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 34  | b     | 640  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 34  | o     | 314  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 34  | v     | 205  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 34  | V     | 202  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 23  | b     | 610  | CLA  | CHC-C1C | 4.45 | 1.47        | 1.38     |
| 34  | d     | 418  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 34  | V     | 209  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 23  | b     | 621  | CLA  | CHB-C1B | 4.45 | 1.49        | 1.39     |
| 23  | a     | 2609 | CLA  | CHD-C1D | 4.45 | 1.47        | 1.38     |
| 34  | c     | 543  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 23  | b     | 606  | CLA  | CHC-C4B | 4.45 | 1.49        | 1.39     |
| 38  | e     | 101  | LHG  | O8-C23  | 4.45 | 1.46        | 1.33     |
| 34  | A     | 425  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 34  | c     | 536  | DMS  | O-S     | 4.45 | 1.80        | 1.50     |
| 39  | e     | 103  | HEM  | FE-NA   | 4.45 | 2.10        | 1.95     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34  | C     | 535  | DMS  | O-S     | 4.45  | 1.80        | 1.50     |
| 34  | a     | 2623 | DMS  | O-S     | 4.44  | 1.80        | 1.50     |
| 34  | O     | 307  | DMS  | O-S     | 4.44  | 1.80        | 1.50     |
| 34  | c     | 535  | DMS  | O-S     | 4.44  | 1.80        | 1.50     |
| 34  | u     | 503  | DMS  | O-S     | 4.44  | 1.80        | 1.50     |
| 23  | b     | 614  | CLA  | O2A-CGA | 4.44  | 1.46        | 1.33     |
| 34  | C     | 533  | DMS  | O-S     | 4.44  | 1.80        | 1.50     |
| 34  | b     | 634  | DMS  | O-S     | 4.43  | 1.80        | 1.50     |
| 23  | B     | 603  | CLA  | CHB-C1B | 4.43  | 1.49        | 1.39     |
| 34  | c     | 534  | DMS  | O-S     | 4.43  | 1.80        | 1.50     |
| 34  | v     | 207  | DMS  | O-S     | 4.43  | 1.80        | 1.50     |
| 34  | o     | 307  | DMS  | O-S     | 4.43  | 1.80        | 1.50     |
| 23  | C     | 510  | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 23  | C     | 514  | CLA  | CHC-C4B | 4.42  | 1.49        | 1.39     |
| 34  | o     | 312  | DMS  | O-S     | 4.42  | 1.80        | 1.50     |
| 37  | D     | 2307 | DGD  | O1G-C1A | 4.42  | 1.46        | 1.33     |
| 23  | C     | 503  | CLA  | CHB-C1B | 4.42  | 1.49        | 1.39     |
| 23  | C     | 513  | CLA  | CHB-C1B | 4.42  | 1.49        | 1.39     |
| 23  | B     | 615  | CLA  | MG-ND   | -4.42 | 1.97        | 2.05     |
| 23  | b     | 617  | CLA  | CHB-C1B | 4.42  | 1.49        | 1.39     |
| 23  | C     | 509  | CLA  | O2A-CGA | 4.42  | 1.46        | 1.33     |
| 34  | B     | 642  | DMS  | O-S     | 4.41  | 1.80        | 1.50     |
| 23  | D     | 2303 | CLA  | CHC-C1C | 4.41  | 1.47        | 1.38     |
| 26  | D     | 2302 | SQD  | O47-C7  | 4.41  | 1.46        | 1.34     |
| 23  | C     | 504  | CLA  | CHD-C1D | 4.41  | 1.46        | 1.38     |
| 34  | O     | 316  | DMS  | O-S     | 4.41  | 1.80        | 1.50     |
| 23  | C     | 502  | CLA  | CHB-C1B | 4.40  | 1.49        | 1.39     |
| 34  | C     | 529  | DMS  | O-S     | 4.40  | 1.80        | 1.50     |
| 23  | c     | 516  | CLA  | O2A-CGA | 4.39  | 1.46        | 1.33     |
| 23  | B     | 602  | CLA  | CHC-C4B | 4.39  | 1.49        | 1.39     |
| 23  | B     | 617  | CLA  | CHD-C1D | 4.39  | 1.46        | 1.38     |
| 27  | C     | 520  | LMG  | O8-C28  | 4.38  | 1.46        | 1.33     |
| 23  | a     | 2613 | CLA  | CHB-C1B | 4.38  | 1.49        | 1.39     |
| 34  | A     | 424  | DMS  | O-S     | 4.38  | 1.79        | 1.50     |
| 34  | C     | 532  | DMS  | O-S     | 4.37  | 1.79        | 1.50     |
| 23  | C     | 510  | CLA  | O2A-CGA | 4.37  | 1.46        | 1.33     |
| 23  | B     | 615  | CLA  | O2A-CGA | 4.37  | 1.46        | 1.33     |
| 34  | c     | 533  | DMS  | O-S     | 4.37  | 1.79        | 1.50     |
| 23  | B     | 602  | CLA  | CHD-C4C | 4.37  | 1.49        | 1.39     |
| 38  | E     | 101  | LHG  | O8-C23  | 4.37  | 1.46        | 1.33     |
| 23  | B     | 608  | CLA  | O2A-CGA | 4.37  | 1.46        | 1.33     |
| 23  | C     | 506  | CLA  | CHB-C1B | 4.36  | 1.49        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 23  | D     | 2303 | CLA  | O2D-CGD | 4.36 | 1.43        | 1.33     |
| 23  | B     | 613  | CLA  | C1D-ND  | 4.36 | 1.43        | 1.37     |
| 26  | d     | 417  | SQD  | O48-C23 | 4.36 | 1.46        | 1.33     |
| 23  | B     | 609  | CLA  | CHB-C1B | 4.36 | 1.49        | 1.39     |
| 23  | c     | 514  | CLA  | O2D-CGD | 4.36 | 1.43        | 1.33     |
| 23  | d     | 408  | CLA  | O2D-CGD | 4.36 | 1.43        | 1.33     |
| 26  | D     | 2308 | SQD  | O47-C7  | 4.35 | 1.46        | 1.34     |
| 23  | B     | 609  | CLA  | O2D-CGD | 4.35 | 1.43        | 1.33     |
| 38  | e     | 101  | LHG  | O7-C7   | 4.35 | 1.46        | 1.34     |
| 37  | D     | 2307 | DGD  | O2G-C1B | 4.35 | 1.46        | 1.34     |
| 23  | b     | 615  | CLA  | CHC-C4B | 4.35 | 1.49        | 1.39     |
| 23  | B     | 616  | CLA  | CHB-C1B | 4.35 | 1.49        | 1.39     |
| 27  | c     | 501  | LMG  | O8-C28  | 4.34 | 1.46        | 1.33     |
| 23  | D     | 2304 | CLA  | CHB-C1B | 4.34 | 1.49        | 1.39     |
| 23  | C     | 511  | CLA  | CHD-C1D | 4.34 | 1.46        | 1.38     |
| 34  | D     | 2318 | DMS  | O-S     | 4.34 | 1.79        | 1.50     |
| 23  | b     | 606  | CLA  | O2A-CGA | 4.33 | 1.46        | 1.33     |
| 23  | c     | 505  | CLA  | CHB-C1B | 4.33 | 1.49        | 1.39     |
| 23  | B     | 610  | CLA  | O2A-CGA | 4.33 | 1.46        | 1.33     |
| 23  | b     | 608  | CLA  | CHB-C1B | 4.33 | 1.49        | 1.39     |
| 23  | C     | 502  | CLA  | CHD-C4C | 4.33 | 1.49        | 1.39     |
| 23  | C     | 509  | CLA  | CHB-C1B | 4.33 | 1.49        | 1.39     |
| 23  | d     | 402  | CLA  | OBD-CAD | 4.33 | 1.29        | 1.22     |
| 23  | d     | 402  | CLA  | CHB-C1B | 4.32 | 1.49        | 1.39     |
| 23  | C     | 503  | CLA  | O2A-CGA | 4.32 | 1.46        | 1.33     |
| 23  | B     | 605  | CLA  | CHB-C1B | 4.32 | 1.49        | 1.39     |
| 23  | B     | 604  | CLA  | CHD-C1D | 4.32 | 1.46        | 1.38     |
| 23  | d     | 408  | CLA  | C1D-ND  | 4.32 | 1.43        | 1.37     |
| 37  | H     | 103  | DGD  | O1G-C1A | 4.32 | 1.46        | 1.33     |
| 23  | C     | 513  | CLA  | CHC-C4B | 4.31 | 1.49        | 1.39     |
| 23  | D     | 2303 | CLA  | O2A-CGA | 4.31 | 1.45        | 1.33     |
| 23  | B     | 614  | CLA  | CHD-C1D | 4.31 | 1.46        | 1.38     |
| 34  | B     | 636  | DMS  | O-S     | 4.31 | 1.79        | 1.50     |
| 23  | C     | 504  | CLA  | O2D-CGD | 4.30 | 1.43        | 1.33     |
| 23  | b     | 609  | CLA  | CHB-C1B | 4.30 | 1.49        | 1.39     |
| 23  | b     | 606  | CLA  | CHD-C4C | 4.30 | 1.49        | 1.39     |
| 23  | b     | 621  | CLA  | CHC-C1C | 4.30 | 1.47        | 1.38     |
| 23  | B     | 615  | CLA  | CHD-C1D | 4.30 | 1.46        | 1.38     |
| 23  | c     | 510  | CLA  | OBD-CAD | 4.29 | 1.29        | 1.22     |
| 23  | B     | 608  | CLA  | CHD-C1D | 4.29 | 1.46        | 1.38     |
| 23  | b     | 614  | CLA  | CHC-C4B | 4.29 | 1.49        | 1.39     |
| 23  | B     | 608  | CLA  | CHC-C4B | 4.29 | 1.49        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 23  | c     | 515  | CLA  | CHB-C1B | 4.29 | 1.49        | 1.39     |
| 23  | B     | 617  | CLA  | CHB-C1B | 4.29 | 1.49        | 1.39     |
| 26  | D     | 2308 | SQD  | O48-C23 | 4.28 | 1.45        | 1.33     |
| 34  | B     | 638  | DMS  | O-S     | 4.27 | 1.79        | 1.50     |
| 23  | B     | 608  | CLA  | CHB-C1B | 4.27 | 1.49        | 1.39     |
| 27  | B     | 622  | LMG  | O8-C28  | 4.27 | 1.45        | 1.33     |
| 23  | A     | 405  | CLA  | CHC-C1C | 4.27 | 1.47        | 1.38     |
| 23  | C     | 513  | CLA  | O2A-CGA | 4.27 | 1.45        | 1.33     |
| 23  | b     | 616  | CLA  | MG-NC   | 4.26 | 2.16        | 2.06     |
| 23  | d     | 408  | CLA  | CHB-C1B | 4.26 | 1.49        | 1.39     |
| 23  | C     | 508  | CLA  | CHC-C4B | 4.26 | 1.49        | 1.39     |
| 23  | b     | 618  | CLA  | CHB-C1B | 4.26 | 1.49        | 1.39     |
| 23  | b     | 619  | CLA  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 23  | b     | 618  | CLA  | CHD-C4C | 4.25 | 1.48        | 1.39     |
| 23  | c     | 506  | CLA  | CHD-C1D | 4.25 | 1.46        | 1.38     |
| 23  | b     | 621  | CLA  | O2A-CGA | 4.25 | 1.45        | 1.33     |
| 23  | C     | 510  | CLA  | CHB-C1B | 4.25 | 1.48        | 1.39     |
| 23  | a     | 2613 | CLA  | CHD-C1D | 4.25 | 1.46        | 1.38     |
| 23  | b     | 617  | CLA  | CHD-C1D | 4.25 | 1.46        | 1.38     |
| 38  | E     | 101  | LHG  | O7-C7   | 4.24 | 1.46        | 1.34     |
| 23  | b     | 609  | CLA  | CHD-C1D | 4.24 | 1.46        | 1.38     |
| 23  | A     | 405  | CLA  | OBD-CAD | 4.24 | 1.29        | 1.22     |
| 23  | C     | 514  | CLA  | CHB-C1B | 4.24 | 1.48        | 1.39     |
| 23  | b     | 611  | CLA  | CHB-C1B | 4.24 | 1.48        | 1.39     |
| 23  | B     | 615  | CLA  | CHC-C4B | 4.23 | 1.48        | 1.39     |
| 34  | o     | 304  | DMS  | O-S     | 4.23 | 1.78        | 1.50     |
| 23  | b     | 606  | CLA  | CHB-C1B | 4.23 | 1.48        | 1.39     |
| 42  | V     | 201  | HEC  | FE-ND   | 4.23 | 2.07        | 1.94     |
| 23  | b     | 620  | CLA  | C3D-C2D | 4.23 | 1.50        | 1.39     |
| 23  | b     | 609  | CLA  | CHC-C4B | 4.23 | 1.48        | 1.39     |
| 23  | C     | 506  | CLA  | O2A-CGA | 4.23 | 1.45        | 1.33     |
| 23  | D     | 2303 | CLA  | CHC-C4B | 4.22 | 1.48        | 1.39     |
| 23  | a     | 2610 | CLA  | CHB-C1B | 4.22 | 1.48        | 1.39     |
| 23  | C     | 503  | CLA  | CHC-C4B | 4.22 | 1.48        | 1.39     |
| 42  | V     | 201  | HEC  | FE-NB   | 4.22 | 2.07        | 1.94     |
| 23  | a     | 2610 | CLA  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 23  | c     | 504  | CLA  | CHB-C1B | 4.21 | 1.48        | 1.39     |
| 27  | c     | 501  | LMG  | O7-C10  | 4.21 | 1.46        | 1.34     |
| 23  | B     | 615  | CLA  | O2D-CGD | 4.21 | 1.43        | 1.33     |
| 23  | b     | 615  | CLA  | CHB-C1B | 4.21 | 1.48        | 1.39     |
| 23  | c     | 511  | CLA  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 27  | c     | 522  | LMG  | O8-C28  | 4.20 | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | B     | 614  | CLA  | CHB-C1B | 4.20  | 1.48        | 1.39     |
| 23  | C     | 508  | CLA  | CHB-C1B | 4.20  | 1.48        | 1.39     |
| 27  | C     | 527  | LMG  | O8-C28  | 4.20  | 1.45        | 1.33     |
| 23  | C     | 512  | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 23  | C     | 507  | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 23  | b     | 611  | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 26  | a     | 2603 | SQD  | O48-C23 | 4.19  | 1.45        | 1.33     |
| 34  | b     | 633  | DMS  | O-S     | 4.19  | 1.78        | 1.50     |
| 23  | b     | 621  | CLA  | CHD-C1D | 4.19  | 1.46        | 1.38     |
| 23  | b     | 613  | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 23  | B     | 605  | CLA  | CHC-C1C | 4.18  | 1.47        | 1.38     |
| 23  | c     | 514  | CLA  | CHB-C1B | 4.18  | 1.48        | 1.39     |
| 23  | A     | 405  | CLA  | CHB-C1B | 4.18  | 1.48        | 1.39     |
| 24  | A     | 409  | PHO  | OBD-CAD | 4.18  | 1.28        | 1.22     |
| 23  | c     | 505  | CLA  | CHC-C4B | 4.18  | 1.48        | 1.39     |
| 23  | B     | 604  | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 23  | c     | 516  | CLA  | CHB-C1B | 4.18  | 1.48        | 1.39     |
| 23  | b     | 618  | CLA  | MG-ND   | -4.18 | 1.97        | 2.05     |
| 23  | A     | 405  | CLA  | CHD-C1D | 4.17  | 1.46        | 1.38     |
| 23  | D     | 2304 | CLA  | MG-NC   | 4.17  | 2.16        | 2.06     |
| 23  | c     | 514  | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 23  | c     | 504  | CLA  | CHC-C4B | 4.17  | 1.48        | 1.39     |
| 23  | B     | 609  | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 23  | c     | 515  | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 23  | b     | 608  | CLA  | CHC-C4B | 4.17  | 1.48        | 1.39     |
| 23  | b     | 617  | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 23  | C     | 508  | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 24  | A     | 408  | PHO  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 27  | c     | 521  | LMG  | O8-C28  | 4.16  | 1.45        | 1.33     |
| 23  | B     | 612  | CLA  | CHD-C1D | 4.16  | 1.46        | 1.38     |
| 23  | c     | 510  | CLA  | CHB-C1B | 4.16  | 1.48        | 1.39     |
| 23  | c     | 504  | CLA  | CHD-C1D | 4.16  | 1.46        | 1.38     |
| 23  | B     | 614  | CLA  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 23  | C     | 505  | CLA  | CHD-C4C | 4.16  | 1.48        | 1.39     |
| 27  | A     | 413  | LMG  | O8-C28  | 4.16  | 1.45        | 1.33     |
| 23  | D     | 2303 | CLA  | CHB-C1B | 4.16  | 1.48        | 1.39     |
| 23  | c     | 514  | CLA  | CHD-C4C | 4.15  | 1.48        | 1.39     |
| 23  | C     | 507  | CLA  | CHB-C1B | 4.15  | 1.48        | 1.39     |
| 23  | a     | 2609 | CLA  | O2D-CGD | 4.15  | 1.43        | 1.33     |
| 27  | A     | 413  | LMG  | O7-C10  | 4.15  | 1.46        | 1.34     |
| 23  | c     | 507  | CLA  | CHC-C4B | 4.15  | 1.48        | 1.39     |
| 26  | B     | 621  | SQD  | O48-C23 | 4.15  | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 27  | B     | 622  | LMG  | O7-C10  | 4.15  | 1.46        | 1.34     |
| 24  | a     | 2611 | PHO  | OBD-CAD | 4.15  | 1.28        | 1.22     |
| 23  | D     | 2304 | CLA  | CHD-C4C | 4.15  | 1.48        | 1.39     |
| 23  | C     | 503  | CLA  | OBD-CAD | 4.15  | 1.29        | 1.22     |
| 23  | c     | 510  | CLA  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 23  | d     | 409  | CLA  | CHB-C1B | 4.14  | 1.48        | 1.39     |
| 23  | c     | 505  | CLA  | C3D-C2D | 4.14  | 1.50        | 1.39     |
| 23  | c     | 510  | CLA  | CHC-C1C | 4.14  | 1.46        | 1.38     |
| 23  | C     | 502  | CLA  | O2A-CGA | 4.13  | 1.45        | 1.33     |
| 23  | a     | 2610 | CLA  | CHD-C1D | 4.13  | 1.46        | 1.38     |
| 23  | b     | 607  | CLA  | CHB-C1B | 4.12  | 1.48        | 1.39     |
| 23  | c     | 507  | CLA  | CHD-C1D | 4.12  | 1.46        | 1.38     |
| 23  | b     | 611  | CLA  | CHC-C4B | 4.12  | 1.48        | 1.39     |
| 27  | m     | 2802 | LMG  | O7-C10  | 4.12  | 1.45        | 1.34     |
| 23  | a     | 2609 | CLA  | CHB-C1B | 4.11  | 1.48        | 1.39     |
| 23  | c     | 506  | CLA  | CHC-C4B | 4.11  | 1.48        | 1.39     |
| 23  | B     | 603  | CLA  | CHC-C4B | 4.11  | 1.48        | 1.39     |
| 23  | C     | 509  | CLA  | CHC-C4B | 4.11  | 1.48        | 1.39     |
| 23  | a     | 2613 | CLA  | O2A-CGA | 4.11  | 1.45        | 1.33     |
| 23  | b     | 613  | CLA  | CHB-C1B | 4.11  | 1.48        | 1.39     |
| 36  | d     | 407  | HTG  | C1'-S1  | -4.11 | 1.76        | 1.81     |
| 38  | d     | 412  | LHG  | O8-C23  | 4.11  | 1.45        | 1.33     |
| 23  | b     | 620  | CLA  | CHB-C1B | 4.11  | 1.48        | 1.39     |
| 23  | B     | 614  | CLA  | CHC-C4B | 4.10  | 1.48        | 1.39     |
| 23  | B     | 602  | CLA  | MG-ND   | -4.10 | 1.97        | 2.05     |
| 23  | c     | 509  | CLA  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 23  | c     | 513  | CLA  | OBD-CAD | 4.10  | 1.29        | 1.22     |
| 26  | D     | 2302 | SQD  | O48-C23 | 4.10  | 1.45        | 1.33     |
| 38  | L     | 101  | LHG  | O8-C23  | 4.10  | 1.45        | 1.33     |
| 23  | c     | 515  | CLA  | CHD-C1D | 4.10  | 1.46        | 1.38     |
| 23  | b     | 612  | CLA  | CHB-C1B | 4.10  | 1.48        | 1.39     |
| 23  | B     | 611  | CLA  | MG-NA   | 4.10  | 2.16        | 2.06     |
| 37  | c     | 520  | DGD  | O1G-C1A | 4.10  | 1.45        | 1.33     |
| 23  | b     | 607  | CLA  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 23  | C     | 505  | CLA  | CHB-C1B | 4.09  | 1.48        | 1.39     |
| 23  | c     | 508  | CLA  | CHB-C1B | 4.09  | 1.48        | 1.39     |
| 23  | c     | 511  | CLA  | CHC-C4B | 4.09  | 1.48        | 1.39     |
| 23  | c     | 512  | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 23  | d     | 402  | CLA  | C3D-C2D | 4.08  | 1.50        | 1.39     |
| 27  | d     | 414  | LMG  | O8-C28  | 4.08  | 1.45        | 1.33     |
| 36  | i     | 102  | HTG  | C1'-S1  | -4.08 | 1.76        | 1.81     |
| 23  | B     | 606  | CLA  | CHC-C4B | 4.08  | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | C     | 502  | CLA  | OBD-CAD | 4.07  | 1.29        | 1.22     |
| 23  | B     | 613  | CLA  | OBD-CAD | 4.07  | 1.29        | 1.22     |
| 36  | H     | 101  | HTG  | C1'-S1  | -4.07 | 1.76        | 1.81     |
| 23  | D     | 2303 | CLA  | MG-NA   | 4.07  | 2.15        | 2.06     |
| 23  | B     | 613  | CLA  | MG-NC   | 4.07  | 2.15        | 2.06     |
| 23  | c     | 514  | CLA  | OBD-CAD | 4.07  | 1.29        | 1.22     |
| 23  | C     | 514  | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 23  | c     | 513  | CLA  | CHC-C4B | 4.06  | 1.48        | 1.39     |
| 37  | h     | 102  | DGD  | O2G-C1B | 4.06  | 1.45        | 1.34     |
| 23  | B     | 605  | CLA  | OBD-CAD | 4.06  | 1.29        | 1.22     |
| 23  | C     | 504  | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 23  | c     | 516  | CLA  | CHC-C4B | 4.06  | 1.48        | 1.39     |
| 23  | C     | 514  | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 23  | b     | 614  | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 38  | D     | 2309 | LHG  | O8-C23  | 4.06  | 1.45        | 1.33     |
| 23  | c     | 509  | CLA  | CHB-C1B | 4.06  | 1.48        | 1.39     |
| 23  | D     | 2304 | CLA  | C3D-C2D | 4.06  | 1.50        | 1.39     |
| 26  | b     | 601  | SQD  | O48-C23 | 4.05  | 1.45        | 1.33     |
| 23  | B     | 609  | CLA  | MG-NB   | 4.05  | 2.13        | 2.05     |
| 23  | D     | 2304 | CLA  | CHC-C4B | 4.05  | 1.48        | 1.39     |
| 23  | b     | 608  | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 23  | d     | 409  | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 23  | A     | 407  | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 23  | C     | 506  | CLA  | CHC-C4B | 4.04  | 1.48        | 1.39     |
| 23  | B     | 612  | CLA  | CHB-C1B | 4.04  | 1.48        | 1.39     |
| 23  | B     | 611  | CLA  | CHC-C4B | 4.04  | 1.48        | 1.39     |
| 23  | D     | 2303 | CLA  | C1D-ND  | 4.04  | 1.42        | 1.37     |
| 23  | C     | 512  | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 23  | C     | 507  | CLA  | CHC-C4B | 4.03  | 1.48        | 1.39     |
| 26  | b     | 601  | SQD  | O47-C7  | 4.03  | 1.45        | 1.34     |
| 23  | a     | 2609 | CLA  | CHC-C4B | 4.03  | 1.48        | 1.39     |
| 38  | d     | 403  | LHG  | O7-C7   | 4.02  | 1.45        | 1.34     |
| 36  | b     | 626  | HTG  | C1'-S1  | -4.02 | 1.76        | 1.81     |
| 23  | D     | 2304 | CLA  | O2A-CGA | 4.01  | 1.45        | 1.33     |
| 23  | b     | 613  | CLA  | CHC-C4B | 4.01  | 1.48        | 1.39     |
| 37  | C     | 519  | DGD  | O2G-C1B | 4.01  | 1.45        | 1.34     |
| 23  | a     | 2613 | CLA  | C3D-C2D | 4.01  | 1.50        | 1.39     |
| 23  | c     | 504  | CLA  | O2A-CGA | 4.01  | 1.45        | 1.33     |
| 23  | b     | 620  | CLA  | O2A-CGA | 4.01  | 1.45        | 1.33     |
| 26  | l     | 101  | SQD  | O48-C23 | 4.01  | 1.45        | 1.33     |
| 24  | a     | 2612 | PHO  | OBD-CAD | 4.00  | 1.27        | 1.22     |
| 23  | D     | 2304 | CLA  | CHD-C1D | 4.00  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 23  | A     | 406  | CLA  | CHC-C1C | 4.00 | 1.46        | 1.38     |
| 23  | B     | 616  | CLA  | CHD-C1D | 4.00 | 1.46        | 1.38     |
| 23  | B     | 609  | CLA  | CHC-C4B | 4.00 | 1.48        | 1.39     |
| 38  | l     | 103  | LHG  | O8-C23  | 4.00 | 1.45        | 1.33     |
| 23  | d     | 408  | CLA  | CHD-C1D | 4.00 | 1.46        | 1.38     |
| 37  | c     | 519  | DGD  | O2G-C1B | 4.00 | 1.45        | 1.34     |
| 26  | A     | 412  | SQD  | O47-C7  | 3.99 | 1.45        | 1.34     |
| 23  | c     | 508  | CLA  | CHC-C4B | 3.99 | 1.48        | 1.39     |
| 23  | b     | 619  | CLA  | CHC-C4B | 3.99 | 1.48        | 1.39     |
| 23  | c     | 507  | CLA  | CHB-C1B | 3.98 | 1.48        | 1.39     |
| 23  | b     | 606  | CLA  | C3D-C2D | 3.98 | 1.50        | 1.39     |
| 23  | d     | 409  | CLA  | CHC-C4B | 3.98 | 1.48        | 1.39     |
| 26  | A     | 412  | SQD  | O48-C23 | 3.97 | 1.45        | 1.33     |
| 23  | c     | 515  | CLA  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 37  | h     | 102  | DGD  | O1G-C1A | 3.97 | 1.44        | 1.33     |
| 26  | a     | 2615 | SQD  | O48-C23 | 3.97 | 1.44        | 1.33     |
| 23  | c     | 505  | CLA  | O2A-CGA | 3.97 | 1.44        | 1.33     |
| 23  | d     | 409  | CLA  | OBD-CAD | 3.96 | 1.29        | 1.22     |
| 23  | A     | 407  | CLA  | OBD-CAD | 3.96 | 1.29        | 1.22     |
| 23  | c     | 515  | CLA  | C3D-C2D | 3.96 | 1.49        | 1.39     |
| 37  | H     | 103  | DGD  | O2G-C1B | 3.96 | 1.45        | 1.34     |
| 23  | B     | 617  | CLA  | O2A-CGA | 3.96 | 1.44        | 1.33     |
| 23  | C     | 506  | CLA  | OBD-CAD | 3.96 | 1.29        | 1.22     |
| 23  | B     | 606  | CLA  | O2A-CGA | 3.95 | 1.44        | 1.33     |
| 23  | C     | 513  | CLA  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 23  | B     | 605  | CLA  | CHC-C4B | 3.95 | 1.48        | 1.39     |
| 23  | a     | 2610 | CLA  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 23  | a     | 2613 | CLA  | CHD-C4C | 3.94 | 1.48        | 1.39     |
| 23  | C     | 512  | CLA  | C3D-C2D | 3.94 | 1.49        | 1.39     |
| 23  | A     | 406  | CLA  | CHB-C1B | 3.94 | 1.48        | 1.39     |
| 23  | c     | 509  | CLA  | CHD-C4C | 3.94 | 1.48        | 1.39     |
| 23  | a     | 2609 | CLA  | OBD-CAD | 3.94 | 1.29        | 1.22     |
| 23  | C     | 509  | CLA  | CHD-C4C | 3.94 | 1.48        | 1.39     |
| 23  | c     | 508  | CLA  | O2A-CGA | 3.94 | 1.44        | 1.33     |
| 27  | D     | 2312 | LMG  | O8-C28  | 3.94 | 1.44        | 1.33     |
| 23  | C     | 510  | CLA  | OBD-CAD | 3.94 | 1.29        | 1.22     |
| 23  | b     | 617  | CLA  | CHC-C4B | 3.93 | 1.48        | 1.39     |
| 23  | B     | 604  | CLA  | CHB-C1B | 3.93 | 1.48        | 1.39     |
| 37  | c     | 519  | DGD  | O1G-C1A | 3.93 | 1.44        | 1.33     |
| 23  | A     | 407  | CLA  | C3D-C2D | 3.93 | 1.49        | 1.39     |
| 23  | B     | 606  | CLA  | CHB-C1B | 3.92 | 1.48        | 1.39     |
| 23  | B     | 616  | CLA  | CHC-C4B | 3.92 | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | C     | 507  | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 23  | B     | 617  | CLA  | CHC-C4B | 3.92  | 1.48        | 1.39     |
| 36  | C     | 525  | HTG  | C1'-S1  | -3.92 | 1.76        | 1.81     |
| 23  | B     | 603  | CLA  | O2A-CGA | 3.92  | 1.44        | 1.33     |
| 37  | c     | 518  | DGD  | O1G-C1A | 3.92  | 1.44        | 1.33     |
| 23  | b     | 615  | CLA  | O2A-CGA | 3.92  | 1.44        | 1.33     |
| 23  | c     | 505  | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 23  | d     | 402  | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 23  | B     | 611  | CLA  | CHB-C1B | 3.91  | 1.48        | 1.39     |
| 23  | c     | 512  | CLA  | CHC-C4B | 3.91  | 1.48        | 1.39     |
| 23  | B     | 605  | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 38  | D     | 2310 | LHG  | O7-C7   | 3.91  | 1.45        | 1.34     |
| 23  | b     | 610  | CLA  | CHB-C1B | 3.91  | 1.48        | 1.39     |
| 36  | I     | 101  | HTG  | C1'-S1  | -3.91 | 1.76        | 1.81     |
| 23  | A     | 405  | CLA  | CHC-C4B | 3.90  | 1.48        | 1.39     |
| 23  | b     | 613  | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 23  | A     | 405  | CLA  | C3D-C2D | 3.90  | 1.49        | 1.39     |
| 23  | B     | 603  | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 23  | B     | 613  | CLA  | O2A-CGA | 3.90  | 1.44        | 1.33     |
| 24  | A     | 408  | PHO  | OBD-CAD | 3.90  | 1.27        | 1.22     |
| 23  | C     | 503  | CLA  | C3D-C2D | 3.90  | 1.49        | 1.39     |
| 23  | A     | 406  | CLA  | MG-NC   | 3.90  | 2.15        | 2.06     |
| 23  | C     | 508  | CLA  | OBD-CAD | 3.90  | 1.29        | 1.22     |
| 23  | c     | 506  | CLA  | O2A-CGA | 3.90  | 1.44        | 1.33     |
| 23  | b     | 618  | CLA  | CHC-C4B | 3.90  | 1.48        | 1.39     |
| 23  | D     | 2304 | CLA  | MG-NA   | 3.90  | 2.15        | 2.06     |
| 23  | A     | 407  | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 23  | A     | 407  | CLA  | C1B-NB  | -3.89 | 1.33        | 1.37     |
| 23  | B     | 615  | CLA  | C4B-NB  | -3.89 | 1.33        | 1.37     |
| 37  | c     | 520  | DGD  | O2G-C1B | 3.89  | 1.45        | 1.34     |
| 23  | B     | 609  | CLA  | C3D-C2D | 3.89  | 1.49        | 1.39     |
| 23  | b     | 612  | CLA  | O2A-CGA | 3.88  | 1.44        | 1.33     |
| 27  | C     | 520  | LMG  | O7-C10  | 3.88  | 1.45        | 1.34     |
| 23  | B     | 610  | CLA  | CHC-C4B | 3.88  | 1.48        | 1.39     |
| 23  | C     | 506  | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 23  | C     | 511  | CLA  | C3D-C2D | 3.88  | 1.49        | 1.39     |
| 23  | A     | 410  | CLA  | CHC-C4B | 3.88  | 1.48        | 1.39     |
| 23  | b     | 607  | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 23  | b     | 614  | CLA  | MG-ND   | -3.88 | 1.98        | 2.05     |
| 23  | C     | 511  | CLA  | CHC-C4B | 3.87  | 1.48        | 1.39     |
| 23  | b     | 616  | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 23  | A     | 410  | CLA  | O2A-CGA | 3.87  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | c     | 510  | CLA  | CHC-C4B | 3.87  | 1.48        | 1.39     |
| 23  | C     | 505  | CLA  | CHC-C4B | 3.87  | 1.48        | 1.39     |
| 23  | b     | 607  | CLA  | CHC-C4B | 3.87  | 1.48        | 1.39     |
| 23  | b     | 610  | CLA  | CHC-C4B | 3.87  | 1.48        | 1.39     |
| 23  | b     | 614  | CLA  | OBD-CAD | 3.87  | 1.29        | 1.22     |
| 23  | B     | 607  | CLA  | O2A-CGA | 3.87  | 1.44        | 1.33     |
| 23  | b     | 608  | CLA  | OBD-CAD | 3.86  | 1.29        | 1.22     |
| 23  | A     | 407  | CLA  | MG-NC   | 3.86  | 2.15        | 2.06     |
| 23  | d     | 409  | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 38  | d     | 403  | LHG  | O8-C23  | 3.86  | 1.44        | 1.33     |
| 23  | A     | 410  | CLA  | OBD-CAD | 3.86  | 1.29        | 1.22     |
| 23  | c     | 513  | CLA  | O2A-CGA | 3.86  | 1.44        | 1.33     |
| 23  | B     | 607  | CLA  | CHB-C1B | 3.86  | 1.48        | 1.39     |
| 23  | c     | 512  | CLA  | OBD-CAD | 3.86  | 1.29        | 1.22     |
| 23  | B     | 610  | CLA  | OBD-CAD | 3.86  | 1.29        | 1.22     |
| 37  | C     | 518  | DGD  | O2G-C1B | 3.86  | 1.45        | 1.34     |
| 23  | a     | 2609 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 27  | d     | 414  | LMG  | O7-C10  | 3.86  | 1.45        | 1.34     |
| 23  | b     | 609  | CLA  | O2A-CGA | 3.85  | 1.44        | 1.33     |
| 23  | b     | 607  | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 23  | A     | 410  | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 23  | C     | 503  | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 23  | d     | 402  | CLA  | C1B-NB  | -3.84 | 1.33        | 1.37     |
| 23  | B     | 612  | CLA  | CHC-C4B | 3.84  | 1.48        | 1.39     |
| 23  | c     | 514  | CLA  | CHC-C4B | 3.84  | 1.48        | 1.39     |
| 23  | b     | 620  | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 23  | c     | 512  | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 23  | B     | 602  | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 23  | C     | 509  | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 23  | B     | 616  | CLA  | OBD-CAD | 3.84  | 1.29        | 1.22     |
| 23  | B     | 608  | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 23  | b     | 612  | CLA  | CHC-C4B | 3.84  | 1.48        | 1.39     |
| 37  | C     | 518  | DGD  | O1G-C1A | 3.84  | 1.44        | 1.33     |
| 23  | C     | 510  | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 26  | a     | 2615 | SQD  | O47-C7  | 3.84  | 1.45        | 1.34     |
| 23  | B     | 616  | CLA  | O2A-CGA | 3.83  | 1.44        | 1.33     |
| 23  | C     | 511  | CLA  | OBD-CAD | 3.83  | 1.29        | 1.22     |
| 23  | C     | 511  | CLA  | CHD-C4C | 3.83  | 1.48        | 1.39     |
| 23  | b     | 617  | CLA  | MG-NA   | 3.83  | 2.15        | 2.06     |
| 23  | b     | 618  | CLA  | O2A-CGA | 3.83  | 1.44        | 1.33     |
| 23  | a     | 2610 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 23  | C     | 505  | CLA  | MG-ND   | -3.83 | 1.98        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | c     | 516  | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 27  | c     | 521  | LMG  | O7-C10  | 3.83  | 1.45        | 1.34     |
| 23  | C     | 505  | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 23  | B     | 612  | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 23  | B     | 607  | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 23  | A     | 410  | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 23  | c     | 505  | CLA  | OBD-CAD | 3.82  | 1.29        | 1.22     |
| 23  | C     | 510  | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 23  | c     | 511  | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 23  | C     | 503  | CLA  | MG-NC   | 3.82  | 2.15        | 2.06     |
| 24  | a     | 2612 | PHO  | O2A-CGA | 3.81  | 1.44        | 1.33     |
| 23  | b     | 614  | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 23  | C     | 505  | CLA  | O2A-CGA | 3.81  | 1.44        | 1.33     |
| 23  | C     | 514  | CLA  | MG-NB   | 3.81  | 2.13        | 2.05     |
| 23  | B     | 606  | CLA  | MG-ND   | -3.81 | 1.98        | 2.05     |
| 23  | c     | 509  | CLA  | CHC-C4B | 3.80  | 1.47        | 1.39     |
| 23  | b     | 610  | CLA  | O2A-CGA | 3.80  | 1.44        | 1.33     |
| 23  | D     | 2303 | CLA  | CHD-C1D | 3.80  | 1.45        | 1.38     |
| 23  | B     | 615  | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 42  | v     | 201  | HEC  | CBC-CAC | -3.79 | 1.34        | 1.51     |
| 36  | b     | 602  | HTG  | C1'-S1  | -3.79 | 1.76        | 1.81     |
| 23  | b     | 606  | CLA  | OBD-CAD | 3.79  | 1.29        | 1.22     |
| 23  | b     | 619  | CLA  | CHB-C1B | 3.79  | 1.47        | 1.39     |
| 23  | d     | 409  | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 23  | c     | 511  | CLA  | CHB-C1B | 3.79  | 1.47        | 1.39     |
| 23  | c     | 511  | CLA  | C1B-NB  | -3.79 | 1.33        | 1.37     |
| 23  | A     | 410  | CLA  | CHB-C1B | 3.79  | 1.47        | 1.39     |
| 23  | c     | 507  | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 23  | B     | 617  | CLA  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 23  | b     | 620  | CLA  | CHC-C4B | 3.78  | 1.47        | 1.39     |
| 38  | D     | 2311 | LHG  | O8-C23  | 3.78  | 1.44        | 1.33     |
| 23  | C     | 509  | CLA  | OBD-CAD | 3.78  | 1.29        | 1.22     |
| 23  | C     | 510  | CLA  | CHC-C4B | 3.78  | 1.47        | 1.39     |
| 23  | c     | 506  | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 23  | b     | 616  | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 23  | A     | 406  | CLA  | CHD-C1D | 3.77  | 1.45        | 1.38     |
| 23  | c     | 513  | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 23  | c     | 513  | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 23  | c     | 515  | CLA  | CHC-C4B | 3.76  | 1.47        | 1.39     |
| 23  | c     | 509  | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 23  | b     | 616  | CLA  | O2A-CGA | 3.76  | 1.44        | 1.33     |
| 23  | B     | 608  | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | b     | 619  | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 23  | D     | 2303 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 24  | A     | 409  | PHO  | O2A-CGA | 3.75  | 1.44        | 1.33     |
| 23  | B     | 610  | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 23  | C     | 502  | CLA  | C3D-C2D | 3.74  | 1.49        | 1.39     |
| 36  | d     | 415  | HTG  | C1'-S1  | -3.74 | 1.76        | 1.81     |
| 23  | B     | 612  | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 23  | B     | 615  | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 38  | d     | 413  | LHG  | O7-C7   | 3.74  | 1.44        | 1.34     |
| 42  | v     | 201  | HEC  | FE-NA   | 3.74  | 2.07        | 1.95     |
| 23  | b     | 617  | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 23  | C     | 512  | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 23  | b     | 616  | CLA  | MG-NB   | 3.73  | 2.13        | 2.05     |
| 23  | B     | 609  | CLA  | MG-NC   | 3.73  | 2.15        | 2.06     |
| 23  | c     | 514  | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 23  | b     | 615  | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 38  | d     | 412  | LHG  | O7-C7   | 3.73  | 1.44        | 1.34     |
| 23  | A     | 407  | CLA  | CHB-C1B | 3.72  | 1.47        | 1.39     |
| 23  | C     | 512  | CLA  | CHC-C4B | 3.72  | 1.47        | 1.39     |
| 23  | B     | 608  | CLA  | MG-ND   | -3.72 | 1.98        | 2.05     |
| 23  | C     | 513  | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 42  | V     | 201  | HEC  | CBC-CAC | -3.72 | 1.34        | 1.51     |
| 37  | C     | 517  | DGD  | O2G-C1B | 3.72  | 1.44        | 1.34     |
| 23  | b     | 611  | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 23  | B     | 614  | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 23  | c     | 504  | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 23  | c     | 507  | CLA  | O2A-CGA | 3.71  | 1.44        | 1.33     |
| 23  | b     | 609  | CLA  | C4D-CHA | 3.70  | 1.51        | 1.38     |
| 23  | A     | 406  | CLA  | CHC-C4B | 3.70  | 1.47        | 1.39     |
| 23  | b     | 610  | CLA  | CHD-C1D | 3.70  | 1.45        | 1.38     |
| 36  | B     | 625  | HTG  | C1'-S1  | -3.70 | 1.76        | 1.81     |
| 23  | c     | 516  | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 23  | c     | 515  | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 23  | b     | 616  | CLA  | C3D-C2D | 3.70  | 1.49        | 1.39     |
| 23  | A     | 407  | CLA  | CHC-C4B | 3.70  | 1.47        | 1.39     |
| 23  | B     | 616  | CLA  | C3D-C2D | 3.70  | 1.49        | 1.39     |
| 23  | A     | 405  | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 36  | c     | 524  | HTG  | C1'-S1  | -3.70 | 1.76        | 1.81     |
| 23  | A     | 406  | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 23  | B     | 614  | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 23  | B     | 604  | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 23  | B     | 613  | CLA  | C1B-NB  | -3.69 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | B     | 602  | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 23  | d     | 408  | CLA  | C3D-C2D | 3.68  | 1.49        | 1.39     |
| 36  | b     | 604  | HTG  | C1'-S1  | -3.68 | 1.76        | 1.81     |
| 23  | A     | 405  | CLA  | C1B-NB  | -3.68 | 1.33        | 1.37     |
| 23  | b     | 611  | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 23  | B     | 603  | CLA  | C3D-C2D | 3.68  | 1.49        | 1.39     |
| 23  | c     | 508  | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 23  | C     | 502  | CLA  | MG-NB   | 3.67  | 2.13        | 2.05     |
| 23  | B     | 612  | CLA  | O2A-CGA | 3.67  | 1.44        | 1.33     |
| 38  | L     | 101  | LHG  | O7-C7   | 3.67  | 1.44        | 1.34     |
| 23  | b     | 612  | CLA  | C3D-C2D | 3.67  | 1.49        | 1.39     |
| 23  | B     | 603  | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 23  | B     | 609  | CLA  | C1B-NB  | -3.67 | 1.33        | 1.37     |
| 23  | B     | 611  | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 24  | a     | 2611 | PHO  | O2A-CGA | 3.65  | 1.44        | 1.33     |
| 23  | C     | 513  | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 23  | B     | 608  | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 23  | C     | 514  | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 23  | b     | 609  | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 23  | c     | 511  | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 23  | b     | 615  | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 23  | B     | 611  | CLA  | C3D-C2D | 3.64  | 1.49        | 1.39     |
| 23  | b     | 609  | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 23  | C     | 508  | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 24  | A     | 409  | PHO  | CHA-CBD | -3.64 | 1.47        | 1.51     |
| 23  | d     | 402  | CLA  | O2A-CGA | 3.63  | 1.44        | 1.33     |
| 23  | b     | 617  | CLA  | C1B-NB  | -3.63 | 1.33        | 1.37     |
| 23  | d     | 402  | CLA  | CHC-C4B | 3.63  | 1.47        | 1.39     |
| 23  | B     | 617  | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 23  | A     | 406  | CLA  | C3D-C2D | 3.62  | 1.49        | 1.39     |
| 23  | a     | 2610 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 23  | b     | 612  | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 23  | B     | 607  | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 37  | C     | 517  | DGD  | O1G-C1A | 3.61  | 1.43        | 1.33     |
| 23  | b     | 617  | CLA  | C3D-C2D | 3.61  | 1.49        | 1.39     |
| 23  | B     | 609  | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 42  | v     | 201  | HEC  | CBB-CAB | -3.61 | 1.35        | 1.51     |
| 23  | C     | 511  | CLA  | O2A-CGA | 3.60  | 1.43        | 1.33     |
| 23  | b     | 613  | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 23  | B     | 615  | CLA  | C3D-C2D | 3.60  | 1.49        | 1.39     |
| 23  | b     | 621  | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 23  | b     | 609  | CLA  | C3D-C2D | 3.60  | 1.48        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 504    | CLA  | C3D-C2D | 3.60  | 1.48        | 1.39     |
| 23  | B     | 606    | CLA  | C3D-C2D | 3.60  | 1.48        | 1.39     |
| 23  | a     | 2610   | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 23  | b     | 620    | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 23  | D     | 2304   | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 23  | B     | 613    | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 37  | c     | 518    | DGD  | O2G-C1B | 3.58  | 1.44        | 1.34     |
| 23  | B     | 611    | CLA  | O2A-CGA | 3.58  | 1.43        | 1.33     |
| 23  | B     | 606    | CLA  | CHD-C4C | 3.57  | 1.47        | 1.39     |
| 23  | c     | 514    | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 23  | c     | 511    | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 23  | b     | 610    | CLA  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 23  | B     | 612    | CLA  | MG-NB   | 3.56  | 2.12        | 2.05     |
| 23  | c     | 510    | CLA  | CHD-C4C | 3.56  | 1.47        | 1.39     |
| 23  | c     | 507    | CLA  | C3D-C2D | 3.55  | 1.48        | 1.39     |
| 23  | b     | 616    | CLA  | CHC-C4B | 3.55  | 1.47        | 1.39     |
| 38  | D     | 2310   | LHG  | O8-C23  | 3.55  | 1.43        | 1.33     |
| 23  | B     | 615    | CLA  | C1B-NB  | -3.55 | 1.33        | 1.37     |
| 23  | B     | 607    | CLA  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 23  | a     | 2609   | CLA  | O2A-CGA | 3.54  | 1.43        | 1.33     |
| 36  | b     | 625    | HTG  | C1'-S1  | -3.54 | 1.76        | 1.81     |
| 23  | c     | 504    | CLA  | CHD-C4C | 3.54  | 1.47        | 1.39     |
| 23  | B     | 616    | CLA  | C4B-NB  | -3.54 | 1.33        | 1.37     |
| 38  | D     | 2311   | LHG  | O7-C7   | 3.53  | 1.44        | 1.34     |
| 23  | C     | 511    | CLA  | C1B-NB  | -3.53 | 1.33        | 1.37     |
| 36  | V     | 204    | HTG  | C1'-S1  | -3.53 | 1.76        | 1.81     |
| 23  | D     | 2304   | CLA  | C1B-NB  | -3.53 | 1.33        | 1.37     |
| 36  | B     | 627    | HTG  | C1'-S1  | -3.52 | 1.76        | 1.81     |
| 23  | A     | 405    | CLA  | MG-NC   | 3.52  | 2.14        | 2.06     |
| 23  | b     | 612    | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 23  | d     | 409    | CLA  | C1B-NB  | -3.52 | 1.33        | 1.37     |
| 31  | A     | 418    | JOX  | C1-CL1  | 3.52  | 1.80        | 1.73     |
| 23  | C     | 514    | CLA  | C3D-C2D | 3.52  | 1.48        | 1.39     |
| 23  | B     | 612    | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 23  | b     | 615    | CLA  | C3D-C2D | 3.51  | 1.48        | 1.39     |
| 23  | C     | 504    | CLA  | CHD-C4C | 3.51  | 1.47        | 1.39     |
| 23  | B     | 607    | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 23  | B     | 606    | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 36  | B     | 624[B] | HTG  | C1'-S1  | -3.51 | 1.76        | 1.81     |
| 23  | b     | 619    | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 23  | C     | 505    | CLA  | C1B-NB  | -3.50 | 1.33        | 1.37     |
| 23  | b     | 608    | CLA  | CHD-C4C | 3.50  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | c     | 512  | CLA  | C3D-C2D | 3.50  | 1.48        | 1.39     |
| 23  | B     | 616  | CLA  | CHD-C4C | 3.50  | 1.47        | 1.39     |
| 23  | B     | 604  | CLA  | C3D-C2D | 3.50  | 1.48        | 1.39     |
| 23  | D     | 2303 | CLA  | C3D-C2D | 3.50  | 1.48        | 1.39     |
| 23  | c     | 508  | CLA  | C3D-C2D | 3.50  | 1.48        | 1.39     |
| 23  | A     | 405  | CLA  | O2A-CGA | 3.49  | 1.43        | 1.33     |
| 23  | b     | 608  | CLA  | C3D-C2D | 3.49  | 1.48        | 1.39     |
| 23  | A     | 407  | CLA  | MG-NA   | 3.49  | 2.14        | 2.06     |
| 27  | D     | 2312 | LMG  | O7-C10  | 3.49  | 1.44        | 1.34     |
| 36  | c     | 526  | HTG  | C1'-S1  | -3.48 | 1.77        | 1.81     |
| 23  | c     | 510  | CLA  | C3D-C2D | 3.48  | 1.48        | 1.39     |
| 23  | b     | 618  | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 23  | a     | 2609 | CLA  | C1B-NB  | -3.48 | 1.33        | 1.37     |
| 23  | b     | 608  | CLA  | MG-NB   | -3.47 | 1.98        | 2.05     |
| 23  | a     | 2613 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 31  | A     | 418  | JOX  | C3-CL   | 3.47  | 1.79        | 1.73     |
| 23  | b     | 611  | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 23  | c     | 504  | CLA  | C3D-C2D | 3.46  | 1.48        | 1.39     |
| 23  | c     | 508  | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 23  | d     | 408  | CLA  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 23  | b     | 613  | CLA  | C3D-C2D | 3.44  | 1.48        | 1.39     |
| 23  | B     | 605  | CLA  | C3D-C2D | 3.44  | 1.48        | 1.39     |
| 36  | c     | 523  | HTG  | C1'-S1  | -3.44 | 1.77        | 1.81     |
| 23  | a     | 2613 | CLA  | C1B-NB  | -3.44 | 1.33        | 1.37     |
| 23  | C     | 510  | CLA  | C4B-NB  | -3.44 | 1.33        | 1.37     |
| 23  | B     | 613  | CLA  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 38  | D     | 2309 | LHG  | O7-C7   | 3.43  | 1.44        | 1.34     |
| 23  | b     | 617  | CLA  | CHD-C4C | 3.42  | 1.47        | 1.39     |
| 23  | d     | 408  | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 31  | A     | 419  | JOX  | C1-CL1  | 3.41  | 1.79        | 1.73     |
| 23  | C     | 512  | CLA  | C4B-NB  | -3.41 | 1.33        | 1.37     |
| 23  | B     | 614  | CLA  | C3D-C2D | 3.41  | 1.48        | 1.39     |
| 23  | b     | 607  | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 23  | b     | 618  | CLA  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 23  | B     | 605  | CLA  | O2A-CGA | 3.40  | 1.43        | 1.33     |
| 23  | c     | 506  | CLA  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 23  | B     | 611  | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 36  | B     | 626  | HTG  | C1'-S1  | -3.40 | 1.77        | 1.81     |
| 23  | c     | 507  | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 23  | a     | 2609 | CLA  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 23  | d     | 408  | CLA  | CHC-C4B | 3.40  | 1.47        | 1.39     |
| 23  | C     | 508  | CLA  | C3D-C2D | 3.38  | 1.48        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 507    | CLA  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 23  | b     | 612    | CLA  | C1B-NB  | -3.38 | 1.33        | 1.37     |
| 23  | A     | 406    | CLA  | CHD-C4C | 3.38  | 1.46        | 1.39     |
| 23  | B     | 612    | CLA  | C1B-NB  | -3.37 | 1.33        | 1.37     |
| 23  | b     | 610    | CLA  | CHD-C4C | 3.37  | 1.46        | 1.39     |
| 23  | B     | 611    | CLA  | C4B-NB  | -3.37 | 1.33        | 1.37     |
| 42  | V     | 201    | HEC  | CBB-CAB | -3.37 | 1.36        | 1.51     |
| 23  | b     | 621    | CLA  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 23  | B     | 610    | CLA  | CHD-C4C | 3.35  | 1.46        | 1.39     |
| 36  | C     | 521    | HTG  | C1'-S1  | -3.35 | 1.77        | 1.81     |
| 23  | a     | 2613   | CLA  | CHC-C4B | 3.35  | 1.46        | 1.39     |
| 38  | l     | 103    | LHG  | O7-C7   | 3.35  | 1.43        | 1.34     |
| 23  | B     | 613    | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 23  | b     | 615    | CLA  | C1B-NB  | -3.33 | 1.33        | 1.37     |
| 23  | b     | 613    | CLA  | C4B-NB  | -3.33 | 1.33        | 1.37     |
| 23  | c     | 510    | CLA  | C4B-NB  | -3.33 | 1.33        | 1.37     |
| 23  | c     | 506    | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 23  | C     | 507    | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 23  | a     | 2610   | CLA  | MG-NC   | 3.32  | 2.14        | 2.06     |
| 23  | b     | 621    | CLA  | MG-NC   | 3.32  | 2.14        | 2.06     |
| 23  | c     | 509    | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 23  | b     | 619    | CLA  | C3D-C2D | 3.30  | 1.48        | 1.39     |
| 23  | B     | 609    | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 23  | b     | 616    | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 23  | C     | 507    | CLA  | C1B-NB  | -3.29 | 1.33        | 1.37     |
| 23  | C     | 508    | CLA  | C4D-CHA | 3.29  | 1.50        | 1.38     |
| 23  | c     | 516    | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 39  | F     | 101    | HEM  | FE-NA   | 3.28  | 2.06        | 1.95     |
| 23  | C     | 506    | CLA  | C3D-C2D | 3.28  | 1.48        | 1.39     |
| 23  | c     | 512    | CLA  | C1B-C2B | 3.27  | 1.50        | 1.43     |
| 23  | A     | 406    | CLA  | C1B-NB  | -3.27 | 1.33        | 1.37     |
| 36  | b     | 603    | HTG  | C1'-S1  | -3.26 | 1.77        | 1.81     |
| 23  | C     | 514    | CLA  | MG-NA   | 3.26  | 2.14        | 2.06     |
| 23  | A     | 406    | CLA  | C4B-NB  | -3.26 | 1.33        | 1.37     |
| 36  | B     | 624[A] | HTG  | C1'-S1  | -3.25 | 1.77        | 1.81     |
| 23  | B     | 612    | CLA  | C4D-CHA | 3.25  | 1.49        | 1.38     |
| 23  | B     | 611    | CLA  | C3B-C4B | 3.25  | 1.50        | 1.42     |
| 23  | B     | 617    | CLA  | C4D-CHA | 3.24  | 1.49        | 1.38     |
| 36  | C     | 522    | HTG  | C1'-S1  | -3.24 | 1.77        | 1.81     |
| 23  | c     | 506    | CLA  | C4D-CHA | 3.23  | 1.49        | 1.38     |
| 23  | c     | 513    | CLA  | MG-NB   | 3.22  | 2.12        | 2.05     |
| 23  | B     | 616    | CLA  | C1B-C2B | 3.22  | 1.50        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | b     | 610  | CLA  | C4B-NB  | -3.21 | 1.33        | 1.37     |
| 39  | F     | 101  | HEM  | FE-NB   | 3.21  | 2.04        | 1.94     |
| 23  | a     | 2613 | CLA  | MG-ND   | -3.19 | 1.99        | 2.05     |
| 23  | B     | 614  | CLA  | C1B-NB  | -3.19 | 1.33        | 1.37     |
| 23  | C     | 504  | CLA  | OBD-CAD | 3.19  | 1.28        | 1.22     |
| 23  | B     | 615  | CLA  | MG-NC   | 3.19  | 2.13        | 2.06     |
| 23  | a     | 2609 | CLA  | MG-NB   | 3.19  | 2.12        | 2.05     |
| 23  | B     | 608  | CLA  | C4D-CHA | 3.19  | 1.49        | 1.38     |
| 23  | b     | 621  | CLA  | CHD-C4C | 3.19  | 1.46        | 1.39     |
| 23  | C     | 505  | CLA  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 23  | b     | 619  | CLA  | C1B-NB  | -3.18 | 1.33        | 1.37     |
| 23  | b     | 615  | CLA  | C4D-CHA | 3.17  | 1.49        | 1.38     |
| 23  | B     | 608  | CLA  | C1B-C2B | 3.17  | 1.50        | 1.43     |
| 23  | a     | 2610 | CLA  | C1B-NB  | -3.16 | 1.33        | 1.37     |
| 23  | C     | 511  | CLA  | C1C-C2C | 3.15  | 1.50        | 1.44     |
| 23  | b     | 621  | CLA  | C1B-C2B | 3.15  | 1.50        | 1.43     |
| 23  | b     | 620  | CLA  | C4D-CHA | 3.15  | 1.49        | 1.38     |
| 38  | d     | 413  | LHG  | O8-C23  | 3.14  | 1.42        | 1.33     |
| 42  | V     | 201  | HEC  | FE-NA   | 3.14  | 2.05        | 1.95     |
| 26  | d     | 417  | SQD  | O47-C45 | -3.14 | 1.43        | 1.46     |
| 23  | d     | 402  | CLA  | C1B-C2B | 3.13  | 1.50        | 1.43     |
| 23  | C     | 512  | CLA  | C4D-CHA | 3.13  | 1.49        | 1.38     |
| 23  | c     | 508  | CLA  | C4B-NB  | -3.13 | 1.33        | 1.37     |
| 23  | B     | 616  | CLA  | C1B-NB  | -3.12 | 1.33        | 1.37     |
| 23  | b     | 621  | CLA  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 23  | B     | 604  | CLA  | C1C-C2C | 3.12  | 1.50        | 1.44     |
| 23  | b     | 612  | CLA  | C1B-C2B | 3.11  | 1.50        | 1.43     |
| 23  | D     | 2303 | CLA  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 23  | d     | 408  | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 23  | B     | 604  | CLA  | OBD-CAD | 3.10  | 1.27        | 1.22     |
| 23  | B     | 602  | CLA  | C4D-CHA | 3.10  | 1.49        | 1.38     |
| 23  | c     | 510  | CLA  | C4D-CHA | 3.10  | 1.49        | 1.38     |
| 23  | c     | 514  | CLA  | C3B-C4B | 3.09  | 1.50        | 1.42     |
| 23  | B     | 604  | CLA  | C4D-CHA | 3.09  | 1.49        | 1.38     |
| 23  | B     | 611  | CLA  | C1B-NB  | -3.08 | 1.34        | 1.37     |
| 23  | B     | 602  | CLA  | C3B-C4B | 3.08  | 1.50        | 1.42     |
| 23  | B     | 615  | CLA  | C1B-C2B | 3.07  | 1.50        | 1.43     |
| 23  | C     | 504  | CLA  | C1B-C2B | 3.07  | 1.50        | 1.43     |
| 23  | a     | 2613 | CLA  | C4B-NB  | -3.07 | 1.34        | 1.37     |
| 23  | b     | 615  | CLA  | C3B-C4B | 3.07  | 1.49        | 1.42     |
| 23  | c     | 514  | CLA  | MG-NC   | 3.07  | 2.13        | 2.06     |
| 23  | c     | 504  | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | B     | 609  | CLA  | C4B-NB  | -3.06 | 1.34        | 1.37     |
| 23  | b     | 621  | CLA  | C4B-NB  | -3.06 | 1.34        | 1.37     |
| 23  | C     | 510  | CLA  | C4D-CHA | 3.06  | 1.49        | 1.38     |
| 23  | b     | 620  | CLA  | C3B-C4B | 3.05  | 1.49        | 1.42     |
| 23  | C     | 503  | CLA  | C4D-CHA | 3.04  | 1.49        | 1.38     |
| 23  | C     | 513  | CLA  | C3B-C4B | 3.04  | 1.49        | 1.42     |
| 23  | C     | 502  | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 23  | b     | 606  | CLA  | C3B-C4B | 3.03  | 1.49        | 1.42     |
| 23  | B     | 615  | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 23  | A     | 410  | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 23  | c     | 515  | CLA  | C4D-CHA | 3.02  | 1.49        | 1.38     |
| 23  | C     | 512  | CLA  | C1B-C2B | 3.02  | 1.50        | 1.43     |
| 23  | A     | 407  | CLA  | MG-NB   | -3.02 | 1.99        | 2.05     |
| 39  | e     | 103  | HEM  | CAB-C3B | 3.02  | 1.55        | 1.47     |
| 23  | c     | 513  | CLA  | C1B-NB  | -3.02 | 1.34        | 1.37     |
| 23  | C     | 505  | CLA  | C4B-NB  | -3.02 | 1.34        | 1.37     |
| 23  | B     | 605  | CLA  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 23  | b     | 606  | CLA  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 36  | o     | 301  | HTG  | C1'-S1  | -3.01 | 1.77        | 1.81     |
| 23  | b     | 615  | CLA  | MG-NB   | 3.01  | 2.11        | 2.05     |
| 23  | c     | 512  | CLA  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 23  | B     | 607  | CLA  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 23  | b     | 611  | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 23  | b     | 616  | CLA  | C4B-NB  | -3.00 | 1.34        | 1.37     |
| 23  | C     | 513  | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 23  | C     | 502  | CLA  | C3B-C4B | 3.00  | 1.49        | 1.42     |
| 23  | C     | 506  | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 23  | b     | 612  | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 23  | c     | 513  | CLA  | C4B-NB  | -2.99 | 1.34        | 1.37     |
| 23  | B     | 603  | CLA  | C1B-C2B | 2.98  | 1.50        | 1.43     |
| 23  | b     | 621  | CLA  | C4D-CHA | 2.98  | 1.49        | 1.38     |
| 23  | d     | 402  | CLA  | C4B-NB  | -2.98 | 1.34        | 1.37     |
| 23  | c     | 514  | CLA  | C1B-C2B | 2.98  | 1.50        | 1.43     |
| 23  | C     | 510  | CLA  | C1B-C2B | 2.98  | 1.50        | 1.43     |
| 39  | F     | 101  | HEM  | CAC-C3C | 2.98  | 1.55        | 1.47     |
| 39  | e     | 103  | HEM  | CAC-C3C | 2.97  | 1.55        | 1.47     |
| 23  | c     | 515  | CLA  | C1B-C2B | 2.97  | 1.50        | 1.43     |
| 23  | b     | 621  | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 23  | c     | 509  | CLA  | C1B-NB  | -2.97 | 1.34        | 1.37     |
| 23  | a     | 2610 | CLA  | C3B-C4B | 2.97  | 1.49        | 1.42     |
| 23  | c     | 508  | CLA  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 23  | d     | 408  | CLA  | C1B-C2B | 2.97  | 1.50        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | C     | 511  | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 23  | B     | 604  | CLA  | C1B-C2B | 2.96  | 1.50        | 1.43     |
| 23  | c     | 507  | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 23  | c     | 515  | CLA  | C1B-NB  | -2.96 | 1.34        | 1.37     |
| 23  | C     | 505  | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 23  | a     | 2613 | CLA  | C1B-C2B | 2.95  | 1.50        | 1.43     |
| 23  | b     | 610  | CLA  | OBD-CAD | 2.95  | 1.27        | 1.22     |
| 23  | C     | 504  | CLA  | C1C-C2C | 2.95  | 1.50        | 1.44     |
| 23  | A     | 407  | CLA  | C3B-C4B | 2.95  | 1.49        | 1.42     |
| 23  | B     | 606  | CLA  | C1B-C2B | 2.94  | 1.50        | 1.43     |
| 23  | C     | 502  | CLA  | C1B-NB  | -2.94 | 1.34        | 1.37     |
| 23  | d     | 408  | CLA  | C1B-NB  | -2.94 | 1.34        | 1.37     |
| 23  | C     | 504  | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 23  | d     | 409  | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 39  | F     | 101  | HEM  | FE-NC   | 2.94  | 2.05        | 1.95     |
| 23  | c     | 510  | CLA  | C1B-C2B | 2.93  | 1.50        | 1.43     |
| 23  | B     | 616  | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 23  | c     | 508  | CLA  | C1B-C2B | 2.93  | 1.50        | 1.43     |
| 23  | C     | 503  | CLA  | C1B-NB  | -2.93 | 1.34        | 1.37     |
| 23  | A     | 407  | CLA  | MG-ND   | -2.93 | 2.00        | 2.05     |
| 23  | b     | 607  | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 23  | d     | 402  | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 23  | b     | 610  | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 23  | b     | 619  | CLA  | C1B-C2B | 2.92  | 1.50        | 1.43     |
| 23  | C     | 511  | CLA  | C1B-C2B | 2.92  | 1.50        | 1.43     |
| 23  | c     | 513  | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 23  | b     | 618  | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 23  | c     | 507  | CLA  | C1B-NB  | -2.91 | 1.34        | 1.37     |
| 23  | C     | 512  | CLA  | MG-NB   | 2.91  | 2.11        | 2.05     |
| 23  | B     | 617  | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 23  | c     | 514  | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 23  | B     | 605  | CLA  | C1B-C2B | 2.91  | 1.50        | 1.43     |
| 23  | b     | 607  | CLA  | C3B-C4B | 2.90  | 1.49        | 1.42     |
| 23  | c     | 512  | CLA  | C1C-C2C | 2.89  | 1.50        | 1.44     |
| 23  | b     | 616  | CLA  | C1B-NB  | -2.89 | 1.34        | 1.37     |
| 23  | B     | 604  | CLA  | C3B-C4B | 2.89  | 1.49        | 1.42     |
| 23  | C     | 512  | CLA  | C1B-NB  | -2.89 | 1.34        | 1.37     |
| 23  | c     | 504  | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 31  | a     | 2619 | JOX  | C3-CL   | 2.89  | 1.78        | 1.73     |
| 23  | C     | 509  | CLA  | C3B-C4B | 2.89  | 1.49        | 1.42     |
| 23  | c     | 508  | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 23  | B     | 611  | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | C     | 514  | CLA  | C3B-C4B | 2.88  | 1.49        | 1.42     |
| 23  | B     | 606  | CLA  | C3B-C4B | 2.88  | 1.49        | 1.42     |
| 39  | F     | 101  | HEM  | CAB-C3B | 2.88  | 1.55        | 1.47     |
| 23  | C     | 507  | CLA  | C4D-CHA | 2.87  | 1.48        | 1.38     |
| 23  | b     | 608  | CLA  | C3B-C4B | 2.87  | 1.49        | 1.42     |
| 23  | B     | 611  | CLA  | MG-NB   | 2.87  | 2.11        | 2.05     |
| 23  | B     | 614  | CLA  | C4D-CHA | 2.87  | 1.48        | 1.38     |
| 23  | B     | 613  | CLA  | C1B-C2B | 2.87  | 1.50        | 1.43     |
| 23  | c     | 506  | CLA  | C1B-C2B | 2.87  | 1.50        | 1.43     |
| 23  | c     | 516  | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 23  | a     | 2609 | CLA  | C1B-C2B | 2.86  | 1.50        | 1.43     |
| 23  | c     | 516  | CLA  | C1B-C2B | 2.86  | 1.50        | 1.43     |
| 23  | b     | 611  | CLA  | MG-NB   | 2.86  | 2.11        | 2.05     |
| 23  | b     | 613  | CLA  | C1B-NB  | -2.86 | 1.34        | 1.37     |
| 23  | b     | 612  | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 23  | b     | 616  | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 23  | B     | 605  | CLA  | C1B-NB  | -2.85 | 1.34        | 1.37     |
| 23  | C     | 503  | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 23  | B     | 617  | CLA  | OBD-CAD | 2.85  | 1.27        | 1.22     |
| 23  | a     | 2613 | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 23  | b     | 607  | CLA  | C1C-NC  | -2.84 | 1.33        | 1.37     |
| 26  | a     | 2603 | SQD  | C6-S    | -2.84 | 1.66        | 1.77     |
| 23  | b     | 610  | CLA  | C1B-C2B | 2.84  | 1.49        | 1.43     |
| 23  | b     | 614  | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 23  | C     | 509  | CLA  | C1B-NB  | -2.84 | 1.34        | 1.37     |
| 26  | A     | 412  | SQD  | C6-S    | -2.84 | 1.66        | 1.77     |
| 23  | C     | 513  | CLA  | C1C-C2C | 2.84  | 1.50        | 1.44     |
| 23  | C     | 506  | CLA  | C4C-C3C | 2.84  | 1.49        | 1.45     |
| 23  | A     | 406  | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 23  | b     | 608  | CLA  | C1B-C2B | 2.84  | 1.49        | 1.43     |
| 23  | c     | 509  | CLA  | C3B-C4B | 2.84  | 1.49        | 1.42     |
| 23  | b     | 618  | CLA  | C1B-NB  | -2.83 | 1.34        | 1.37     |
| 23  | D     | 2303 | CLA  | C1B-NB  | -2.83 | 1.34        | 1.37     |
| 23  | d     | 409  | CLA  | C1B-C2B | 2.83  | 1.49        | 1.43     |
| 23  | b     | 613  | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 23  | B     | 603  | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 23  | b     | 607  | CLA  | C1B-C2B | 2.83  | 1.49        | 1.43     |
| 23  | C     | 506  | CLA  | C1B-C2B | 2.83  | 1.49        | 1.43     |
| 23  | B     | 617  | CLA  | C1C-NC  | -2.83 | 1.33        | 1.37     |
| 23  | C     | 510  | CLA  | C1B-NB  | -2.82 | 1.34        | 1.37     |
| 23  | b     | 619  | CLA  | MG-NB   | 2.82  | 2.11        | 2.05     |
| 23  | b     | 607  | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | D     | 2304 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 23  | b     | 612  | CLA  | C3B-C4B | 2.81  | 1.49        | 1.42     |
| 23  | b     | 617  | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 23  | b     | 618  | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 23  | D     | 2304 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 23  | d     | 408  | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 23  | B     | 614  | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 23  | b     | 609  | CLA  | C1B-NB  | -2.79 | 1.34        | 1.37     |
| 23  | A     | 405  | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 23  | C     | 510  | CLA  | C1C-C2C | 2.78  | 1.50        | 1.44     |
| 23  | C     | 512  | CLA  | C3B-C4B | 2.78  | 1.49        | 1.42     |
| 23  | c     | 507  | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 23  | c     | 513  | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 23  | c     | 516  | CLA  | C1B-NB  | -2.78 | 1.34        | 1.37     |
| 31  | a     | 2619 | JOX  | C1-CL1  | 2.78  | 1.78        | 1.73     |
| 23  | B     | 609  | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 23  | b     | 617  | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 23  | B     | 603  | CLA  | C3B-C4B | 2.78  | 1.49        | 1.42     |
| 23  | c     | 504  | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 23  | b     | 610  | CLA  | C1C-NC  | -2.78 | 1.33        | 1.37     |
| 23  | A     | 407  | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 23  | C     | 509  | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 23  | B     | 616  | CLA  | MG-NC   | 2.77  | 2.12        | 2.06     |
| 23  | b     | 616  | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 23  | a     | 2613 | CLA  | C3B-C4B | 2.77  | 1.49        | 1.42     |
| 23  | b     | 612  | CLA  | MG-NB   | 2.77  | 2.11        | 2.05     |
| 23  | A     | 410  | CLA  | C1B-NB  | -2.77 | 1.34        | 1.37     |
| 23  | B     | 607  | CLA  | C1B-NB  | -2.77 | 1.34        | 1.37     |
| 23  | b     | 609  | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 23  | D     | 2303 | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 23  | b     | 614  | CLA  | C1B-NB  | -2.77 | 1.34        | 1.37     |
| 23  | A     | 405  | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 23  | c     | 505  | CLA  | C1C-C2C | 2.77  | 1.49        | 1.44     |
| 23  | C     | 505  | CLA  | C3B-C4B | 2.76  | 1.49        | 1.42     |
| 23  | C     | 507  | CLA  | C3B-C4B | 2.76  | 1.49        | 1.42     |
| 23  | b     | 620  | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 23  | A     | 406  | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 23  | a     | 2610 | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 23  | B     | 608  | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 23  | a     | 2609 | CLA  | C3B-C4B | 2.76  | 1.49        | 1.42     |
| 23  | C     | 503  | CLA  | MG-NB   | 2.75  | 2.11        | 2.05     |
| 23  | D     | 2304 | CLA  | C3B-C4B | 2.75  | 1.49        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | b     | 608  | CLA  | C4D-CHA | 2.75  | 1.48        | 1.38     |
| 23  | b     | 617  | CLA  | C1C-C2C | 2.75  | 1.49        | 1.44     |
| 26  | a     | 2615 | SQD  | C6-S    | -2.75 | 1.67        | 1.77     |
| 23  | B     | 606  | CLA  | C4D-CHA | 2.75  | 1.48        | 1.38     |
| 23  | B     | 603  | CLA  | C1B-NB  | -2.75 | 1.34        | 1.37     |
| 23  | D     | 2303 | CLA  | C4D-CHA | 2.75  | 1.48        | 1.38     |
| 23  | b     | 619  | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 23  | C     | 513  | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 23  | b     | 614  | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 23  | c     | 511  | CLA  | C3B-C4B | 2.74  | 1.49        | 1.42     |
| 23  | B     | 613  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 23  | C     | 508  | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 23  | b     | 606  | CLA  | C1B-NB  | -2.74 | 1.34        | 1.37     |
| 23  | a     | 2613 | CLA  | MG-NA   | 2.73  | 2.12        | 2.06     |
| 23  | b     | 610  | CLA  | C3B-C4B | 2.73  | 1.49        | 1.42     |
| 23  | B     | 612  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 23  | C     | 509  | CLA  | C4D-CHA | 2.73  | 1.48        | 1.38     |
| 23  | C     | 507  | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 23  | C     | 507  | CLA  | C1C-NC  | -2.72 | 1.33        | 1.37     |
| 23  | c     | 505  | CLA  | C4D-CHA | 2.72  | 1.48        | 1.38     |
| 23  | C     | 504  | CLA  | C3B-C4B | 2.72  | 1.49        | 1.42     |
| 42  | v     | 201  | HEC  | FE-NB   | 2.72  | 2.03        | 1.94     |
| 26  | b     | 601  | SQD  | C6-S    | -2.71 | 1.67        | 1.77     |
| 23  | b     | 615  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 23  | B     | 610  | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 23  | c     | 509  | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 23  | b     | 615  | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 26  | D     | 2302 | SQD  | C6-S    | -2.71 | 1.67        | 1.77     |
| 23  | d     | 409  | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 23  | C     | 514  | CLA  | C1B-NB  | -2.70 | 1.34        | 1.37     |
| 23  | b     | 613  | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 23  | c     | 505  | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 23  | C     | 514  | CLA  | C1C-C2C | 2.70  | 1.49        | 1.44     |
| 23  | b     | 617  | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 23  | c     | 505  | CLA  | C3B-C4B | 2.70  | 1.49        | 1.42     |
| 23  | c     | 516  | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 24  | a     | 2612 | PHO  | C3A-C2A | -2.69 | 1.52        | 1.54     |
| 23  | c     | 509  | CLA  | C1C-NC  | -2.69 | 1.33        | 1.37     |
| 23  | d     | 408  | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 26  | D     | 2308 | SQD  | C6-S    | -2.69 | 1.67        | 1.77     |
| 23  | C     | 511  | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 23  | B     | 610  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | c     | 506  | CLA  | C1C-C2C | 2.68  | 1.49        | 1.44     |
| 23  | c     | 514  | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 23  | b     | 619  | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 23  | d     | 409  | CLA  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 23  | C     | 508  | CLA  | C1C-NC  | -2.67 | 1.33        | 1.37     |
| 23  | d     | 402  | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 23  | a     | 2609 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 23  | a     | 2610 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 23  | c     | 507  | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 23  | c     | 510  | CLA  | C1C-NC  | -2.67 | 1.33        | 1.37     |
| 23  | c     | 506  | CLA  | MG-ND   | -2.67 | 2.00        | 2.05     |
| 23  | C     | 514  | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 23  | C     | 507  | CLA  | C1C-C2C | 2.66  | 1.49        | 1.44     |
| 23  | A     | 410  | CLA  | C3B-C4B | 2.66  | 1.49        | 1.42     |
| 23  | c     | 511  | CLA  | C1C-C2C | 2.66  | 1.49        | 1.44     |
| 23  | b     | 607  | CLA  | C4C-C3C | 2.66  | 1.49        | 1.45     |
| 36  | b     | 626  | HTG  | C1-S1   | -2.66 | 1.76        | 1.80     |
| 23  | c     | 504  | CLA  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 23  | A     | 410  | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 23  | b     | 607  | CLA  | C1B-NB  | -2.65 | 1.34        | 1.37     |
| 23  | c     | 512  | CLA  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 23  | B     | 608  | CLA  | C3B-C4B | 2.65  | 1.49        | 1.42     |
| 23  | C     | 506  | CLA  | C1B-NB  | -2.65 | 1.34        | 1.37     |
| 23  | c     | 515  | CLA  | C3B-C4B | 2.64  | 1.49        | 1.42     |
| 26  | B     | 621  | SQD  | C6-S    | -2.64 | 1.67        | 1.77     |
| 23  | c     | 505  | CLA  | C1B-NB  | -2.64 | 1.34        | 1.37     |
| 33  | D     | 2306 | PL9  | C6-C5   | 2.64  | 1.49        | 1.35     |
| 31  | a     | 2617 | JOX  | C3-CL   | 2.64  | 1.78        | 1.73     |
| 23  | C     | 506  | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 23  | a     | 2609 | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 23  | c     | 516  | CLA  | C3B-C4B | 2.63  | 1.48        | 1.42     |
| 23  | d     | 409  | CLA  | C3B-C4B | 2.63  | 1.48        | 1.42     |
| 23  | c     | 511  | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 23  | C     | 503  | CLA  | C1C-C2C | 2.63  | 1.49        | 1.44     |
| 23  | c     | 508  | CLA  | C1C-C2C | 2.63  | 1.49        | 1.44     |
| 23  | C     | 513  | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 23  | A     | 405  | CLA  | C1C-C2C | 2.62  | 1.49        | 1.44     |
| 23  | b     | 609  | CLA  | C1C-C2C | 2.62  | 1.49        | 1.44     |
| 23  | A     | 406  | CLA  | C3B-C4B | 2.62  | 1.48        | 1.42     |
| 23  | B     | 609  | CLA  | C3B-C4B | 2.62  | 1.48        | 1.42     |
| 23  | b     | 619  | CLA  | C3B-C4B | 2.62  | 1.48        | 1.42     |
| 23  | C     | 503  | CLA  | C3B-C4B | 2.62  | 1.48        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | c     | 513  | CLA  | C3B-C4B | 2.62  | 1.48        | 1.42     |
| 23  | c     | 504  | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 31  | A     | 419  | JOX  | C3-CL   | 2.61  | 1.78        | 1.73     |
| 23  | c     | 516  | CLA  | C1C-C2C | 2.61  | 1.49        | 1.44     |
| 23  | B     | 602  | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 23  | C     | 503  | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 23  | D     | 2303 | CLA  | C3B-C4B | 2.61  | 1.48        | 1.42     |
| 23  | B     | 614  | CLA  | C1C-C2C | 2.60  | 1.49        | 1.44     |
| 23  | C     | 502  | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 26  | l     | 101  | SQD  | C6-S    | -2.60 | 1.67        | 1.77     |
| 23  | b     | 614  | CLA  | C1C-C2C | 2.60  | 1.49        | 1.44     |
| 23  | C     | 512  | CLA  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 23  | b     | 606  | CLA  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 42  | V     | 201  | HEC  | FE-NC   | 2.59  | 2.03        | 1.95     |
| 23  | c     | 512  | CLA  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 23  | C     | 510  | CLA  | C3B-C4B | 2.59  | 1.48        | 1.42     |
| 23  | b     | 609  | CLA  | C4B-NB  | -2.59 | 1.34        | 1.37     |
| 23  | B     | 603  | CLA  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 23  | C     | 510  | CLA  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 23  | B     | 612  | CLA  | C3B-C4B | 2.59  | 1.48        | 1.42     |
| 23  | d     | 409  | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 23  | b     | 608  | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 23  | C     | 514  | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 23  | B     | 609  | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 23  | B     | 608  | CLA  | C1B-NB  | -2.58 | 1.34        | 1.37     |
| 24  | a     | 2612 | PHO  | C4B-NB  | -2.58 | 1.33        | 1.38     |
| 23  | b     | 611  | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 23  | c     | 508  | CLA  | C1B-NB  | -2.57 | 1.34        | 1.37     |
| 23  | C     | 504  | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 23  | A     | 410  | CLA  | C4B-NB  | -2.57 | 1.34        | 1.37     |
| 23  | b     | 614  | CLA  | C3B-C4B | 2.57  | 1.48        | 1.42     |
| 23  | b     | 618  | CLA  | C1C-NC  | -2.56 | 1.34        | 1.37     |
| 23  | A     | 406  | CLA  | C1C-NC  | -2.56 | 1.34        | 1.37     |
| 23  | C     | 502  | CLA  | C1C-C2C | 2.56  | 1.49        | 1.44     |
| 23  | b     | 606  | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 23  | B     | 602  | CLA  | C1C-C2C | 2.56  | 1.49        | 1.44     |
| 23  | b     | 621  | CLA  | C1B-NB  | -2.55 | 1.34        | 1.37     |
| 23  | C     | 505  | CLA  | C1C-C2C | 2.55  | 1.49        | 1.44     |
| 23  | b     | 611  | CLA  | C3B-C4B | 2.55  | 1.48        | 1.42     |
| 23  | c     | 512  | CLA  | C3B-C4B | 2.55  | 1.48        | 1.42     |
| 23  | c     | 507  | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 23  | c     | 504  | CLA  | C1C-C2C | 2.55  | 1.49        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | c     | 506  | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 23  | c     | 511  | CLA  | C4B-NB  | -2.55 | 1.34        | 1.37     |
| 24  | a     | 2611 | PHO  | C4B-NB  | -2.54 | 1.33        | 1.38     |
| 23  | b     | 607  | CLA  | C1C-C2C | 2.54  | 1.49        | 1.44     |
| 23  | C     | 506  | CLA  | C1C-NC  | -2.54 | 1.34        | 1.37     |
| 23  | B     | 610  | CLA  | C3B-C4B | 2.54  | 1.48        | 1.42     |
| 23  | A     | 410  | CLA  | C4C-C3C | 2.54  | 1.49        | 1.45     |
| 23  | b     | 606  | CLA  | C1C-C2C | 2.54  | 1.49        | 1.44     |
| 23  | c     | 515  | CLA  | C1C-C2C | 2.54  | 1.49        | 1.44     |
| 23  | c     | 512  | CLA  | C4B-NB  | -2.54 | 1.34        | 1.37     |
| 23  | B     | 611  | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 23  | c     | 512  | CLA  | C1B-NB  | -2.53 | 1.34        | 1.37     |
| 23  | b     | 617  | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 23  | d     | 408  | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 23  | B     | 606  | CLA  | C1C-C2C | 2.53  | 1.49        | 1.44     |
| 23  | B     | 613  | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 23  | a     | 2610 | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 23  | c     | 510  | CLA  | C1B-NB  | -2.52 | 1.34        | 1.37     |
| 23  | b     | 619  | CLA  | C4C-C3C | 2.52  | 1.49        | 1.45     |
| 23  | c     | 511  | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 23  | D     | 2303 | CLA  | C1C-C2C | 2.52  | 1.49        | 1.44     |
| 23  | c     | 509  | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 23  | B     | 613  | CLA  | C1C-NC  | -2.52 | 1.34        | 1.37     |
| 23  | b     | 613  | CLA  | C1C-NC  | -2.52 | 1.34        | 1.37     |
| 23  | A     | 405  | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 23  | D     | 2304 | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 24  | A     | 409  | PHO  | C4B-NB  | -2.52 | 1.33        | 1.38     |
| 23  | C     | 502  | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 29  | U     | 502  | GOL  | O2-C2   | -2.50 | 1.35        | 1.43     |
| 23  | B     | 607  | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 23  | B     | 617  | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 23  | B     | 607  | CLA  | C1C-C2C | 2.49  | 1.49        | 1.44     |
| 23  | C     | 514  | CLA  | C3D-C4D | -2.49 | 1.38        | 1.44     |
| 23  | a     | 2609 | CLA  | C1C-C2C | 2.49  | 1.49        | 1.44     |
| 23  | b     | 614  | CLA  | C1D-C2D | 2.49  | 1.50        | 1.45     |
| 23  | b     | 616  | CLA  | C3B-C2B | 2.49  | 1.49        | 1.41     |
| 23  | b     | 620  | CLA  | C1B-NB  | -2.49 | 1.34        | 1.37     |
| 23  | B     | 609  | CLA  | C1C-C2C | 2.49  | 1.49        | 1.44     |
| 23  | b     | 618  | CLA  | C3B-C4B | 2.48  | 1.48        | 1.42     |
| 23  | c     | 514  | CLA  | C1C-C2C | 2.48  | 1.49        | 1.44     |
| 36  | H     | 101  | HTG  | C1-S1   | -2.48 | 1.76        | 1.80     |
| 23  | b     | 610  | CLA  | C1B-NB  | -2.48 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | C     | 513 | CLA  | C1B-NB  | -2.47 | 1.34        | 1.37     |
| 23  | B     | 605 | CLA  | C3B-C4B | 2.47  | 1.48        | 1.42     |
| 23  | B     | 615 | CLA  | C3B-C4B | 2.47  | 1.48        | 1.42     |
| 23  | C     | 506 | CLA  | C1C-C2C | 2.47  | 1.49        | 1.44     |
| 23  | b     | 618 | CLA  | C3B-C2B | 2.47  | 1.49        | 1.41     |
| 23  | C     | 505 | CLA  | C1B-C2B | 2.47  | 1.49        | 1.43     |
| 23  | b     | 619 | CLA  | C1C-C2C | 2.46  | 1.49        | 1.44     |
| 23  | B     | 617 | CLA  | C1B-NB  | -2.46 | 1.34        | 1.37     |
| 23  | b     | 608 | CLA  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 23  | c     | 508 | CLA  | C3B-C4B | 2.46  | 1.48        | 1.42     |
| 23  | b     | 616 | CLA  | C3B-C4B | 2.46  | 1.48        | 1.42     |
| 23  | B     | 602 | CLA  | C4B-NB  | -2.46 | 1.34        | 1.37     |
| 23  | b     | 611 | CLA  | C1B-NB  | -2.46 | 1.34        | 1.37     |
| 23  | C     | 509 | CLA  | C4B-NB  | -2.45 | 1.34        | 1.37     |
| 23  | A     | 406 | CLA  | MG-NB   | 2.45  | 2.10        | 2.05     |
| 31  | A     | 419 | JOX  | C-C1    | 2.45  | 1.40        | 1.35     |
| 23  | c     | 514 | CLA  | C1B-NB  | -2.45 | 1.34        | 1.37     |
| 23  | A     | 406 | CLA  | C1C-C2C | 2.45  | 1.49        | 1.44     |
| 23  | B     | 615 | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 23  | B     | 613 | CLA  | C1C-C2C | 2.45  | 1.49        | 1.44     |
| 23  | B     | 606 | CLA  | C4B-NB  | -2.45 | 1.34        | 1.37     |
| 23  | c     | 509 | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 23  | c     | 511 | CLA  | C3B-C2B | 2.45  | 1.49        | 1.41     |
| 23  | C     | 502 | CLA  | C4B-NB  | -2.44 | 1.34        | 1.37     |
| 23  | A     | 410 | CLA  | C1C-C2C | 2.44  | 1.49        | 1.44     |
| 23  | A     | 407 | CLA  | C3D-C4D | -2.44 | 1.38        | 1.44     |
| 36  | d     | 407 | HTG  | C1-S1   | -2.44 | 1.77        | 1.80     |
| 36  | b     | 604 | HTG  | C1-S1   | -2.44 | 1.77        | 1.80     |
| 23  | B     | 604 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 23  | B     | 604 | CLA  | C1B-NB  | -2.44 | 1.34        | 1.37     |
| 23  | B     | 611 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 23  | A     | 406 | CLA  | C3B-C2B | 2.44  | 1.49        | 1.41     |
| 23  | b     | 613 | CLA  | MG-NB   | 2.44  | 2.10        | 2.05     |
| 23  | C     | 514 | CLA  | C4B-NB  | -2.44 | 1.34        | 1.37     |
| 23  | B     | 616 | CLA  | C3B-C4B | 2.43  | 1.48        | 1.42     |
| 23  | C     | 511 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 36  | c     | 524 | HTG  | C1-S1   | -2.43 | 1.77        | 1.80     |
| 36  | B     | 626 | HTG  | C1-S1   | -2.43 | 1.77        | 1.80     |
| 23  | c     | 506 | CLA  | C4B-NB  | -2.43 | 1.34        | 1.37     |
| 33  | d     | 411 | PL9  | C6-C5   | 2.43  | 1.48        | 1.35     |
| 23  | B     | 606 | CLA  | C1B-NB  | -2.43 | 1.34        | 1.37     |
| 23  | b     | 609 | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | B     | 614  | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 23  | C     | 511  | CLA  | C3B-C4B | 2.43  | 1.48        | 1.42     |
| 23  | B     | 602  | CLA  | C3B-C2B | 2.42  | 1.49        | 1.41     |
| 23  | d     | 408  | CLA  | C3D-C4D | -2.42 | 1.38        | 1.44     |
| 23  | C     | 505  | CLA  | MG-NB   | 2.42  | 2.10        | 2.05     |
| 23  | C     | 509  | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | a     | 2617 | JOX  | C1-CL1  | 2.42  | 1.77        | 1.73     |
| 23  | C     | 510  | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 23  | c     | 504  | CLA  | C3B-C4B | 2.42  | 1.48        | 1.42     |
| 23  | c     | 515  | CLA  | C4B-NB  | -2.42 | 1.34        | 1.37     |
| 23  | B     | 612  | CLA  | C1B-C2B | 2.42  | 1.49        | 1.43     |
| 23  | b     | 613  | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 23  | C     | 510  | CLA  | C3B-C2B | 2.42  | 1.49        | 1.41     |
| 23  | B     | 611  | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | a     | 2617 | JOX  | C4-C3   | 2.41  | 1.40        | 1.35     |
| 23  | B     | 617  | CLA  | C3B-C2B | 2.41  | 1.49        | 1.41     |
| 23  | B     | 603  | CLA  | C4B-NB  | -2.40 | 1.34        | 1.37     |
| 23  | a     | 2609 | CLA  | C1C-NC  | -2.40 | 1.34        | 1.37     |
| 23  | B     | 613  | CLA  | C3B-C2B | 2.40  | 1.49        | 1.41     |
| 23  | B     | 613  | CLA  | C3D-C4D | -2.40 | 1.38        | 1.44     |
| 23  | C     | 511  | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 24  | A     | 409  | PHO  | C1D-ND  | -2.40 | 1.34        | 1.38     |
| 23  | b     | 616  | CLA  | C3D-C4D | -2.39 | 1.38        | 1.44     |
| 31  | a     | 2619 | JOX  | C4-C3   | 2.39  | 1.40        | 1.35     |
| 23  | B     | 602  | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 23  | b     | 615  | CLA  | C1C-C2C | 2.38  | 1.49        | 1.44     |
| 23  | b     | 612  | CLA  | C1C-C2C | 2.38  | 1.49        | 1.44     |
| 23  | B     | 607  | CLA  | C3B-C4B | 2.38  | 1.48        | 1.42     |
| 23  | A     | 405  | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 23  | B     | 617  | CLA  | C3D-C4D | -2.38 | 1.38        | 1.44     |
| 23  | A     | 407  | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 23  | b     | 621  | CLA  | C3B-C2B | 2.38  | 1.49        | 1.41     |
| 24  | a     | 2612 | PHO  | CHA-CBD | -2.38 | 1.48        | 1.51     |
| 23  | B     | 610  | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 23  | b     | 618  | CLA  | C1C-C2C | 2.38  | 1.49        | 1.44     |
| 31  | a     | 2617 | JOX  | C-C1    | 2.38  | 1.40        | 1.35     |
| 23  | b     | 613  | CLA  | C3B-C4B | 2.38  | 1.48        | 1.42     |
| 23  | b     | 609  | CLA  | C1C-NC  | -2.38 | 1.34        | 1.37     |
| 24  | A     | 408  | PHO  | C1B-NB  | -2.38 | 1.34        | 1.38     |
| 23  | C     | 508  | CLA  | C1C-C2C | 2.37  | 1.49        | 1.44     |
| 23  | a     | 2609 | CLA  | C3B-C2B | 2.37  | 1.49        | 1.41     |
| 23  | a     | 2610 | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | a     | 2613 | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 23  | b     | 618  | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 23  | b     | 617  | CLA  | C3B-C2B | 2.37  | 1.49        | 1.41     |
| 28  | j     | 2701 | LMT  | O1'-C1' | 2.37  | 1.44        | 1.40     |
| 23  | C     | 505  | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 23  | A     | 410  | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 23  | b     | 610  | CLA  | C3B-C2B | 2.37  | 1.49        | 1.41     |
| 23  | A     | 407  | CLA  | C4B-NB  | -2.37 | 1.34        | 1.37     |
| 23  | B     | 605  | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 23  | b     | 617  | CLA  | C3B-C4B | 2.37  | 1.48        | 1.42     |
| 23  | b     | 611  | CLA  | C1C-C2C | 2.37  | 1.49        | 1.44     |
| 23  | B     | 610  | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 23  | c     | 508  | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 23  | c     | 512  | CLA  | C3B-C2B | 2.36  | 1.49        | 1.41     |
| 23  | C     | 503  | CLA  | C3B-C2B | 2.36  | 1.49        | 1.41     |
| 23  | B     | 605  | CLA  | C1C-C2C | 2.36  | 1.49        | 1.44     |
| 23  | C     | 505  | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 24  | A     | 409  | PHO  | C3D-C4D | -2.36 | 1.37        | 1.41     |
| 23  | c     | 507  | CLA  | C1C-C2C | 2.36  | 1.49        | 1.44     |
| 23  | c     | 510  | CLA  | C3B-C2B | 2.36  | 1.49        | 1.41     |
| 23  | C     | 502  | CLA  | C3D-C4D | -2.35 | 1.38        | 1.44     |
| 23  | C     | 512  | CLA  | C3B-C2B | 2.35  | 1.49        | 1.41     |
| 23  | B     | 614  | CLA  | C3B-C4B | 2.35  | 1.48        | 1.42     |
| 23  | c     | 506  | CLA  | C3B-C4B | 2.35  | 1.48        | 1.42     |
| 23  | C     | 512  | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 23  | c     | 509  | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 23  | C     | 504  | CLA  | MG-ND   | -2.35 | 2.01        | 2.05     |
| 23  | C     | 506  | CLA  | C3B-C4B | 2.35  | 1.48        | 1.42     |
| 23  | c     | 507  | CLA  | C3B-C4B | 2.35  | 1.48        | 1.42     |
| 23  | C     | 504  | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 23  | c     | 505  | CLA  | C4B-NB  | -2.34 | 1.34        | 1.37     |
| 23  | b     | 614  | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 23  | B     | 612  | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 23  | B     | 607  | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 23  | C     | 507  | CLA  | C3D-C4D | -2.34 | 1.38        | 1.44     |
| 23  | B     | 605  | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 23  | b     | 611  | CLA  | C4B-NB  | -2.34 | 1.34        | 1.37     |
| 23  | B     | 610  | CLA  | C1B-NB  | -2.34 | 1.34        | 1.37     |
| 26  | D     | 2302 | SQD  | O6-C1   | 2.33  | 1.44        | 1.40     |
| 23  | b     | 608  | CLA  | C1B-NB  | -2.33 | 1.34        | 1.37     |
| 23  | c     | 516  | CLA  | MG-NB   | 2.33  | 2.10        | 2.05     |
| 23  | C     | 509  | CLA  | C3B-C2B | 2.33  | 1.49        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 31  | A     | 418  | JOX  | C-C1    | 2.33  | 1.39        | 1.35     |
| 36  | C     | 521  | HTG  | C1-S1   | -2.32 | 1.77        | 1.80     |
| 23  | c     | 511  | CLA  | C3D-C4D | -2.32 | 1.38        | 1.44     |
| 36  | c     | 523  | HTG  | C1-S1   | -2.32 | 1.77        | 1.80     |
| 23  | B     | 611  | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 23  | c     | 509  | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 23  | b     | 618  | CLA  | C4B-NB  | -2.32 | 1.34        | 1.37     |
| 23  | b     | 611  | CLA  | C3B-C2B | 2.32  | 1.49        | 1.41     |
| 23  | c     | 510  | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 23  | B     | 606  | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 23  | b     | 607  | CLA  | C3B-C2B | 2.31  | 1.49        | 1.41     |
| 23  | c     | 513  | CLA  | C3B-C2B | 2.31  | 1.49        | 1.41     |
| 23  | A     | 405  | CLA  | C3B-C4B | 2.31  | 1.48        | 1.42     |
| 23  | b     | 614  | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 23  | B     | 604  | CLA  | C4B-NB  | -2.31 | 1.34        | 1.37     |
| 23  | c     | 514  | CLA  | C3B-C2B | 2.31  | 1.49        | 1.41     |
| 23  | C     | 508  | CLA  | C3B-C2B | 2.31  | 1.49        | 1.41     |
| 28  | B     | 634  | LMT  | O1'-C1' | 2.30  | 1.44        | 1.40     |
| 23  | d     | 408  | CLA  | C3B-C4B | 2.30  | 1.48        | 1.42     |
| 23  | C     | 510  | CLA  | C4D-ND  | 2.30  | 1.40        | 1.37     |
| 23  | B     | 614  | CLA  | C4B-NB  | -2.30 | 1.35        | 1.37     |
| 23  | C     | 509  | CLA  | C1C-C2C | 2.30  | 1.49        | 1.44     |
| 23  | B     | 614  | CLA  | C3B-C2B | 2.30  | 1.49        | 1.41     |
| 23  | C     | 508  | CLA  | C4B-NB  | -2.29 | 1.35        | 1.37     |
| 23  | b     | 609  | CLA  | C3B-C2B | 2.29  | 1.49        | 1.41     |
| 23  | C     | 503  | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |
| 26  | B     | 621  | SQD  | O6-C1   | 2.29  | 1.44        | 1.40     |
| 31  | A     | 419  | JOX  | C4-C3   | 2.29  | 1.39        | 1.35     |
| 23  | D     | 2304 | CLA  | C3B-C2B | 2.29  | 1.48        | 1.41     |
| 23  | C     | 504  | CLA  | C1B-NB  | -2.29 | 1.35        | 1.37     |
| 23  | B     | 604  | CLA  | C4C-C3C | 2.28  | 1.49        | 1.45     |
| 23  | b     | 606  | CLA  | C3B-C2B | 2.28  | 1.48        | 1.41     |
| 23  | B     | 602  | CLA  | C1D-C2D | 2.28  | 1.49        | 1.45     |
| 23  | c     | 515  | CLA  | C3B-C2B | 2.28  | 1.48        | 1.41     |
| 23  | c     | 505  | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 23  | D     | 2303 | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 42  | V     | 201  | HEC  | CAB-C3B | 2.27  | 1.56        | 1.51     |
| 23  | c     | 507  | CLA  | C4C-C3C | 2.27  | 1.49        | 1.45     |
| 23  | b     | 620  | CLA  | C4D-ND  | 2.27  | 1.40        | 1.37     |
| 23  | c     | 509  | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 23  | c     | 516  | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 23  | a     | 2609 | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | C     | 506  | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 23  | B     | 603  | CLA  | C1C-C2C | 2.27  | 1.49        | 1.44     |
| 23  | B     | 602  | CLA  | C1C-NC  | -2.27 | 1.34        | 1.37     |
| 36  | C     | 525  | HTG  | C1-S1   | -2.27 | 1.77        | 1.80     |
| 28  | T     | 103  | LMT  | O1'-C1' | 2.27  | 1.44        | 1.40     |
| 23  | C     | 505  | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 23  | b     | 621  | CLA  | C3B-C4B | 2.26  | 1.48        | 1.42     |
| 23  | b     | 613  | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 23  | b     | 621  | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 42  | v     | 201  | HEC  | CMC-C2C | 2.26  | 1.55        | 1.50     |
| 23  | B     | 604  | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 42  | v     | 201  | HEC  | CMD-C2D | 2.26  | 1.55        | 1.50     |
| 23  | B     | 603  | CLA  | C3B-C2B | 2.26  | 1.48        | 1.41     |
| 23  | c     | 516  | CLA  | C3B-C2B | 2.26  | 1.48        | 1.41     |
| 23  | c     | 509  | CLA  | C3B-C2B | 2.26  | 1.48        | 1.41     |
| 23  | b     | 606  | CLA  | C1C-NC  | -2.25 | 1.34        | 1.37     |
| 36  | d     | 415  | HTG  | C1-S1   | -2.25 | 1.77        | 1.80     |
| 23  | B     | 610  | CLA  | C1C-C2C | 2.25  | 1.48        | 1.44     |
| 23  | d     | 408  | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 23  | b     | 608  | CLA  | C4D-ND  | 2.25  | 1.40        | 1.37     |
| 23  | A     | 405  | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 23  | B     | 605  | CLA  | C4B-NB  | -2.24 | 1.35        | 1.37     |
| 23  | d     | 409  | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 23  | A     | 410  | CLA  | C3D-C4D | -2.24 | 1.39        | 1.44     |
| 23  | b     | 620  | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 23  | c     | 504  | CLA  | C1B-NB  | -2.24 | 1.35        | 1.37     |
| 39  | F     | 101  | HEM  | CMB-C2B | 2.24  | 1.55        | 1.50     |
| 23  | c     | 507  | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 23  | B     | 606  | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 23  | a     | 2610 | CLA  | C1C-C2C | 2.23  | 1.48        | 1.44     |
| 23  | c     | 514  | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 23  | B     | 613  | CLA  | C3B-C4B | 2.23  | 1.48        | 1.42     |
| 23  | b     | 608  | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 23  | C     | 513  | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 23  | B     | 608  | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 36  | c     | 526  | HTG  | C1-S1   | -2.22 | 1.77        | 1.80     |
| 42  | V     | 201  | HEC  | CMC-C2C | 2.22  | 1.55        | 1.50     |
| 23  | C     | 506  | CLA  | C4D-ND  | 2.22  | 1.40        | 1.37     |
| 24  | A     | 408  | PHO  | C4B-NB  | -2.22 | 1.34        | 1.38     |
| 23  | B     | 617  | CLA  | C4D-ND  | 2.22  | 1.40        | 1.37     |
| 23  | b     | 606  | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 23  | b     | 614  | CLA  | C4B-NB  | -2.22 | 1.35        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | a     | 2610 | CLA  | MG-NB   | 2.22  | 2.10        | 2.05     |
| 23  | D     | 2303 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 36  | I     | 101  | HTG  | C1-S1   | -2.21 | 1.77        | 1.80     |
| 23  | B     | 609  | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 23  | c     | 510  | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 23  | b     | 620  | CLA  | MG-NB   | 2.21  | 2.10        | 2.05     |
| 23  | b     | 619  | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 23  | c     | 511  | CLA  | C1C-NC  | -2.21 | 1.34        | 1.37     |
| 23  | C     | 513  | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 23  | b     | 610  | CLA  | C1C-C2C | 2.20  | 1.48        | 1.44     |
| 23  | B     | 603  | CLA  | MG-NB   | 2.20  | 2.10        | 2.05     |
| 23  | c     | 505  | CLA  | MG-NB   | 2.20  | 2.10        | 2.05     |
| 23  | b     | 612  | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 23  | c     | 506  | CLA  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 23  | C     | 511  | CLA  | C3B-C2B | 2.19  | 1.48        | 1.41     |
| 23  | B     | 612  | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 23  | C     | 503  | CLA  | C1C-NC  | -2.19 | 1.34        | 1.37     |
| 23  | B     | 616  | CLA  | C1C-NC  | -2.19 | 1.34        | 1.37     |
| 23  | B     | 607  | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 23  | b     | 615  | CLA  | C3B-C2B | 2.19  | 1.48        | 1.41     |
| 23  | c     | 510  | CLA  | C4D-ND  | 2.18  | 1.40        | 1.37     |
| 23  | C     | 508  | CLA  | C3B-C4B | 2.18  | 1.47        | 1.42     |
| 23  | B     | 615  | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 23  | C     | 503  | CLA  | C4D-ND  | 2.18  | 1.40        | 1.37     |
| 23  | a     | 2613 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 23  | B     | 608  | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 23  | C     | 504  | CLA  | C4B-NB  | -2.18 | 1.35        | 1.37     |
| 23  | b     | 613  | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 23  | c     | 504  | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 23  | c     | 506  | CLA  | C1B-NB  | -2.17 | 1.35        | 1.37     |
| 23  | b     | 612  | CLA  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 23  | b     | 620  | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 23  | D     | 2303 | CLA  | C4B-NB  | -2.17 | 1.35        | 1.37     |
| 23  | c     | 513  | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 36  | b     | 603  | HTG  | C1-S1   | -2.17 | 1.77        | 1.80     |
| 23  | C     | 506  | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 23  | A     | 407  | CLA  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 23  | b     | 615  | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 23  | B     | 610  | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 23  | C     | 514  | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 23  | C     | 514  | CLA  | C4C-C3C | 2.16  | 1.48        | 1.45     |
| 23  | A     | 410  | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 31  | A     | 418  | JOX  | C4-C5   | -2.16 | 1.40        | 1.45     |
| 23  | b     | 619  | CLA  | C1C-NC  | -2.16 | 1.34        | 1.37     |
| 23  | C     | 502  | CLA  | C4D-ND  | 2.16  | 1.40        | 1.37     |
| 23  | b     | 613  | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 23  | b     | 619  | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 23  | D     | 2303 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 23  | d     | 408  | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 23  | C     | 510  | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 23  | C     | 505  | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 36  | B     | 627  | HTG  | C1-S1   | -2.15 | 1.77        | 1.80     |
| 23  | c     | 508  | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 23  | c     | 516  | CLA  | C1C-NC  | -2.14 | 1.34        | 1.37     |
| 23  | A     | 407  | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 31  | a     | 2619 | JOX  | C4-C5   | -2.14 | 1.40        | 1.45     |
| 23  | b     | 612  | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 23  | C     | 511  | CLA  | C4D-ND  | 2.13  | 1.40        | 1.37     |
| 23  | B     | 607  | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 23  | a     | 2613 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 42  | V     | 201  | HEC  | CMD-C2D | 2.13  | 1.55        | 1.50     |
| 24  | A     | 409  | PHO  | C1B-NB  | -2.13 | 1.34        | 1.38     |
| 23  | B     | 603  | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 23  | d     | 402  | CLA  | C3B-C4B | 2.12  | 1.47        | 1.42     |
| 23  | B     | 606  | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 23  | D     | 2304 | CLA  | MG-NB   | 2.12  | 2.10        | 2.05     |
| 23  | c     | 508  | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 23  | c     | 505  | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 23  | b     | 618  | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 23  | C     | 508  | CLA  | C4D-ND  | 2.11  | 1.40        | 1.37     |
| 23  | c     | 514  | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 23  | b     | 615  | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 23  | d     | 409  | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 23  | d     | 402  | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 23  | b     | 620  | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 23  | C     | 514  | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 23  | c     | 505  | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 23  | b     | 611  | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 31  | a     | 2619 | JOX  | C-C1    | 2.10  | 1.39        | 1.35     |
| 23  | B     | 602  | CLA  | C4D-ND  | 2.10  | 1.40        | 1.37     |
| 23  | C     | 507  | CLA  | C1B-C2B | 2.09  | 1.48        | 1.43     |
| 23  | b     | 609  | CLA  | C3B-C4B | 2.09  | 1.47        | 1.42     |
| 37  | c     | 520  | DGD  | O2G-C2G | -2.09 | 1.41        | 1.46     |
| 23  | c     | 513  | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36  | i     | 102  | HTG  | C1-S1   | -2.09 | 1.77        | 1.80     |
| 36  | C     | 522  | HTG  | C1-S1   | -2.08 | 1.77        | 1.80     |
| 24  | A     | 409  | PHO  | C3A-C2A | -2.08 | 1.52        | 1.54     |
| 23  | C     | 513  | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 23  | b     | 606  | CLA  | C1D-C2D | 2.08  | 1.49        | 1.45     |
| 23  | b     | 606  | CLA  | C4B-NB  | -2.08 | 1.35        | 1.37     |
| 31  | a     | 2619 | JOX  | C-C5    | -2.08 | 1.40        | 1.45     |
| 23  | b     | 606  | CLA  | C4D-ND  | 2.08  | 1.40        | 1.37     |
| 23  | b     | 616  | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 26  | l     | 101  | SQD  | O6-C1   | 2.08  | 1.43        | 1.40     |
| 23  | C     | 508  | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 23  | A     | 405  | CLA  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 23  | D     | 2304 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 23  | B     | 616  | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 23  | D     | 2304 | CLA  | C1D-C2D | 2.07  | 1.49        | 1.45     |
| 23  | c     | 515  | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 23  | b     | 616  | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 23  | c     | 513  | CLA  | C4D-ND  | 2.07  | 1.40        | 1.37     |
| 42  | v     | 201  | HEC  | FE-NC   | 2.07  | 2.02        | 1.95     |
| 39  | e     | 103  | HEM  | CMC-C2C | 2.07  | 1.55        | 1.50     |
| 23  | b     | 608  | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 23  | c     | 515  | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 23  | c     | 513  | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 29  | C     | 526  | GOL  | O2-C2   | -2.06 | 1.37        | 1.43     |
| 23  | B     | 609  | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 23  | c     | 506  | CLA  | C3B-C2B | 2.05  | 1.48        | 1.41     |
| 23  | c     | 516  | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 23  | B     | 611  | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 23  | c     | 508  | CLA  | C4D-ND  | 2.05  | 1.40        | 1.37     |
| 23  | c     | 505  | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 23  | d     | 402  | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 23  | C     | 512  | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 23  | C     | 510  | CLA  | MG-NB   | 2.04  | 2.09        | 2.05     |
| 23  | b     | 621  | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 23  | c     | 515  | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 23  | B     | 616  | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 25  | D     | 2305 | BCR  | C30-C25 | -2.03 | 1.51        | 1.53     |
| 23  | B     | 605  | CLA  | C4D-ND  | 2.03  | 1.40        | 1.37     |
| 23  | B     | 602  | CLA  | C1B-NB  | -2.03 | 1.35        | 1.37     |
| 23  | B     | 611  | CLA  | C1D-C2D | 2.03  | 1.49        | 1.45     |
| 23  | c     | 504  | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 23  | c     | 512  | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | b     | 616 | CLA  | C1C-NC  | -2.02 | 1.34        | 1.37     |
| 23  | c     | 509 | CLA  | C1D-C2D | 2.02  | 1.49        | 1.45     |
| 23  | B     | 609 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 23  | b     | 607 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 23  | b     | 610 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 23  | b     | 615 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 23  | b     | 620 | CLA  | C4B-NB  | -2.02 | 1.35        | 1.37     |
| 23  | c     | 506 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 23  | C     | 502 | CLA  | C3B-C2B | 2.01  | 1.48        | 1.41     |
| 23  | d     | 409 | CLA  | C4D-ND  | 2.01  | 1.40        | 1.37     |
| 39  | e     | 103 | HEM  | CMA-C3A | 2.01  | 1.55        | 1.50     |
| 23  | C     | 502 | CLA  | C1D-C2D | 2.01  | 1.49        | 1.45     |
| 23  | C     | 507 | CLA  | C3B-C2B | 2.01  | 1.48        | 1.41     |
| 23  | B     | 608 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 39  | F     | 101 | HEM  | CMA-C3A | 2.01  | 1.55        | 1.50     |
| 23  | b     | 614 | CLA  | C3B-C2B | 2.01  | 1.48        | 1.41     |
| 23  | B     | 602 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |

All (2621) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | A     | 408  | PHO  | C2D-C1D-ND | 11.71  | 117.61      | 109.53   |
| 24  | A     | 409  | PHO  | C2D-C1D-ND | 11.34  | 117.35      | 109.53   |
| 24  | a     | 2612 | PHO  | C2D-C1D-ND | 11.01  | 117.13      | 109.53   |
| 23  | c     | 504  | CLA  | C1D-ND-C4D | -10.80 | 98.66       | 106.33   |
| 24  | a     | 2611 | PHO  | C2D-C1D-ND | 10.60  | 116.84      | 109.53   |
| 23  | b     | 617  | CLA  | C1D-ND-C4D | -10.14 | 99.13       | 106.33   |
| 23  | B     | 613  | CLA  | C1D-ND-C4D | -10.14 | 99.14       | 106.33   |
| 23  | a     | 2610 | CLA  | C1D-ND-C4D | -10.08 | 99.17       | 106.33   |
| 23  | a     | 2609 | CLA  | C1D-ND-C4D | -9.95  | 99.27       | 106.33   |
| 31  | A     | 419  | JOX  | C2-C3-CL   | -9.95  | 107.56      | 115.84   |
| 23  | A     | 406  | CLA  | C1D-ND-C4D | -9.93  | 99.28       | 106.33   |
| 23  | c     | 507  | CLA  | C1D-ND-C4D | -9.88  | 99.32       | 106.33   |
| 23  | b     | 610  | CLA  | C1D-ND-C4D | -9.88  | 99.32       | 106.33   |
| 23  | D     | 2303 | CLA  | C1D-ND-C4D | -9.75  | 99.41       | 106.33   |
| 23  | B     | 610  | CLA  | C1D-ND-C4D | -9.72  | 99.43       | 106.33   |
| 23  | B     | 614  | CLA  | C1D-ND-C4D | -9.69  | 99.45       | 106.33   |
| 23  | b     | 621  | CLA  | C1D-ND-C4D | -9.68  | 99.46       | 106.33   |
| 23  | c     | 511  | CLA  | C1D-ND-C4D | -9.57  | 99.54       | 106.33   |
| 23  | d     | 408  | CLA  | C1D-ND-C4D | -9.45  | 99.62       | 106.33   |
| 23  | c     | 504  | CLA  | C2D-C1D-ND | 9.37   | 117.01      | 110.10   |
| 23  | C     | 514  | CLA  | C1D-ND-C4D | -9.32  | 99.71       | 106.33   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23  | A     | 406  | CLA  | C2D-C1D-ND | 9.32  | 116.97      | 110.10   |
| 23  | b     | 619  | CLA  | C1D-ND-C4D | -9.31 | 99.72       | 106.33   |
| 23  | b     | 608  | CLA  | C1D-ND-C4D | -9.31 | 99.72       | 106.33   |
| 23  | C     | 507  | CLA  | C1D-ND-C4D | -9.31 | 99.72       | 106.33   |
| 23  | b     | 613  | CLA  | C1D-ND-C4D | -9.29 | 99.73       | 106.33   |
| 23  | B     | 609  | CLA  | C1D-ND-C4D | -9.29 | 99.74       | 106.33   |
| 23  | B     | 616  | CLA  | C1D-ND-C4D | -9.27 | 99.75       | 106.33   |
| 23  | C     | 509  | CLA  | C1D-ND-C4D | -9.26 | 99.76       | 106.33   |
| 23  | B     | 615  | CLA  | C1D-ND-C4D | -9.23 | 99.78       | 106.33   |
| 23  | c     | 512  | CLA  | C1D-ND-C4D | -9.21 | 99.79       | 106.33   |
| 23  | A     | 407  | CLA  | C1D-ND-C4D | -9.19 | 99.81       | 106.33   |
| 23  | b     | 610  | CLA  | C2D-C1D-ND | 9.15  | 116.85      | 110.10   |
| 23  | C     | 511  | CLA  | C1D-ND-C4D | -9.15 | 99.83       | 106.33   |
| 23  | c     | 505  | CLA  | C1D-ND-C4D | -9.14 | 99.84       | 106.33   |
| 23  | B     | 612  | CLA  | C1D-ND-C4D | -9.12 | 99.86       | 106.33   |
| 23  | b     | 618  | CLA  | C1D-ND-C4D | -9.05 | 99.91       | 106.33   |
| 23  | A     | 410  | CLA  | C1D-ND-C4D | -9.02 | 99.93       | 106.33   |
| 23  | d     | 409  | CLA  | C1D-ND-C4D | -9.00 | 99.94       | 106.33   |
| 23  | B     | 606  | CLA  | C1D-ND-C4D | -9.00 | 99.94       | 106.33   |
| 31  | a     | 2617 | JOX  | C2-C1-CL1  | -8.99 | 108.36      | 115.84   |
| 23  | D     | 2304 | CLA  | C1D-ND-C4D | -8.97 | 99.97       | 106.33   |
| 23  | B     | 605  | CLA  | C1D-ND-C4D | -8.96 | 99.97       | 106.33   |
| 23  | B     | 614  | CLA  | C2D-C1D-ND | 8.95  | 116.70      | 110.10   |
| 23  | a     | 2613 | CLA  | C1D-ND-C4D | -8.93 | 99.99       | 106.33   |
| 23  | b     | 621  | CLA  | C2D-C1D-ND | 8.92  | 116.68      | 110.10   |
| 23  | A     | 405  | CLA  | C1D-ND-C4D | -8.92 | 100.00      | 106.33   |
| 23  | c     | 508  | CLA  | C1D-ND-C4D | -8.91 | 100.01      | 106.33   |
| 23  | D     | 2303 | CLA  | C2D-C1D-ND | 8.91  | 116.67      | 110.10   |
| 23  | B     | 616  | CLA  | C2D-C1D-ND | 8.88  | 116.65      | 110.10   |
| 23  | C     | 503  | CLA  | C1D-ND-C4D | -8.87 | 100.04      | 106.33   |
| 23  | c     | 515  | CLA  | C1D-ND-C4D | -8.80 | 100.08      | 106.33   |
| 23  | d     | 402  | CLA  | C1D-ND-C4D | -8.78 | 100.10      | 106.33   |
| 23  | B     | 604  | CLA  | C1D-ND-C4D | -8.78 | 100.10      | 106.33   |
| 23  | b     | 615  | CLA  | C1D-ND-C4D | -8.75 | 100.12      | 106.33   |
| 23  | c     | 516  | CLA  | C1D-ND-C4D | -8.74 | 100.12      | 106.33   |
| 23  | c     | 507  | CLA  | C2D-C1D-ND | 8.73  | 116.53      | 110.10   |
| 23  | c     | 509  | CLA  | C1D-ND-C4D | -8.70 | 100.15      | 106.33   |
| 23  | a     | 2610 | CLA  | C2D-C1D-ND | 8.69  | 116.51      | 110.10   |
| 23  | b     | 611  | CLA  | C1D-ND-C4D | -8.69 | 100.16      | 106.33   |
| 36  | C     | 522  | HTG  | C1'-S1-C1  | 8.66  | 116.30      | 100.09   |
| 23  | c     | 510  | CLA  | C1D-ND-C4D | -8.66 | 100.18      | 106.33   |
| 23  | B     | 612  | CLA  | C2D-C1D-ND | 8.66  | 116.49      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | b     | 616  | CLA  | C1D-ND-C4D  | -8.65 | 100.19      | 106.33   |
| 23  | c     | 514  | CLA  | C1D-ND-C4D  | -8.65 | 100.19      | 106.33   |
| 23  | C     | 504  | CLA  | C1D-ND-C4D  | -8.62 | 100.21      | 106.33   |
| 23  | B     | 611  | CLA  | C1D-ND-C4D  | -8.62 | 100.21      | 106.33   |
| 23  | b     | 617  | CLA  | C2D-C1D-ND  | 8.60  | 116.44      | 110.10   |
| 23  | b     | 614  | CLA  | C1D-ND-C4D  | -8.59 | 100.23      | 106.33   |
| 23  | B     | 603  | CLA  | C1D-ND-C4D  | -8.58 | 100.24      | 106.33   |
| 23  | B     | 608  | CLA  | C1D-ND-C4D  | -8.55 | 100.26      | 106.33   |
| 23  | B     | 617  | CLA  | C1D-ND-C4D  | -8.52 | 100.28      | 106.33   |
| 23  | c     | 513  | CLA  | C1D-ND-C4D  | -8.51 | 100.29      | 106.33   |
| 23  | C     | 508  | CLA  | C1D-ND-C4D  | -8.46 | 100.33      | 106.33   |
| 23  | C     | 513  | CLA  | C1D-ND-C4D  | -8.45 | 100.33      | 106.33   |
| 23  | B     | 613  | CLA  | C2D-C1D-ND  | 8.42  | 116.31      | 110.10   |
| 23  | C     | 505  | CLA  | C1D-ND-C4D  | -8.39 | 100.38      | 106.33   |
| 23  | c     | 506  | CLA  | C1D-ND-C4D  | -8.36 | 100.39      | 106.33   |
| 24  | a     | 2612 | PHO  | C2B-C1B-NB  | 8.33  | 115.28      | 109.53   |
| 23  | C     | 510  | CLA  | C1D-ND-C4D  | -8.33 | 100.42      | 106.33   |
| 23  | b     | 607  | CLA  | C1D-ND-C4D  | -8.33 | 100.42      | 106.33   |
| 23  | b     | 612  | CLA  | C1D-ND-C4D  | -8.29 | 100.45      | 106.33   |
| 23  | d     | 408  | CLA  | C2D-C1D-ND  | 8.26  | 116.19      | 110.10   |
| 23  | B     | 607  | CLA  | C1D-ND-C4D  | -8.20 | 100.51      | 106.33   |
| 23  | B     | 608  | CLA  | C2D-C1D-ND  | 8.16  | 116.12      | 110.10   |
| 23  | C     | 502  | CLA  | C1D-ND-C4D  | -8.11 | 100.57      | 106.33   |
| 23  | B     | 609  | CLA  | C2D-C1D-ND  | 8.06  | 116.04      | 110.10   |
| 23  | c     | 515  | CLA  | C2D-C1D-ND  | 8.03  | 116.02      | 110.10   |
| 23  | C     | 512  | CLA  | C1D-ND-C4D  | -8.00 | 100.65      | 106.33   |
| 23  | B     | 606  | CLA  | C2D-C1D-ND  | 8.00  | 116.00      | 110.10   |
| 23  | c     | 512  | CLA  | C2D-C1D-ND  | 7.97  | 115.97      | 110.10   |
| 23  | b     | 609  | CLA  | C1D-ND-C4D  | -7.97 | 100.68      | 106.33   |
| 23  | b     | 612  | CLA  | C2D-C1D-ND  | 7.95  | 115.96      | 110.10   |
| 23  | C     | 508  | CLA  | C2D-C1D-ND  | 7.94  | 115.96      | 110.10   |
| 23  | C     | 504  | CLA  | C2D-C1D-ND  | 7.93  | 115.95      | 110.10   |
| 23  | C     | 503  | CLA  | C2D-C1D-ND  | 7.92  | 115.94      | 110.10   |
| 23  | A     | 410  | CLA  | C2D-C1D-ND  | 7.87  | 115.91      | 110.10   |
| 23  | c     | 506  | CLA  | C2D-C1D-ND  | 7.83  | 115.88      | 110.10   |
| 24  | a     | 2611 | PHO  | O2D-CGD-CBD | 7.83  | 120.91      | 111.00   |
| 23  | D     | 2304 | CLA  | C2D-C1D-ND  | 7.82  | 115.87      | 110.10   |
| 23  | d     | 402  | CLA  | C2D-C1D-ND  | 7.82  | 115.87      | 110.10   |
| 23  | c     | 511  | CLA  | C2D-C1D-ND  | 7.81  | 115.86      | 110.10   |
| 23  | C     | 506  | CLA  | C1D-ND-C4D  | -7.80 | 100.79      | 106.33   |
| 23  | C     | 509  | CLA  | C2D-C1D-ND  | 7.78  | 115.84      | 110.10   |
| 23  | a     | 2609 | CLA  | C2D-C1D-ND  | 7.77  | 115.83      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36  | b     | 603  | HTG  | C1'-S1-C1   | 7.76  | 114.61      | 100.09   |
| 23  | b     | 615  | CLA  | C2D-C1D-ND  | 7.76  | 115.82      | 110.10   |
| 23  | a     | 2613 | CLA  | C2D-C1D-ND  | 7.75  | 115.82      | 110.10   |
| 23  | b     | 620  | CLA  | C1D-ND-C4D  | -7.75 | 100.83      | 106.33   |
| 31  | a     | 2617 | JOX  | C2-C3-CL    | -7.74 | 109.39      | 115.84   |
| 23  | c     | 505  | CLA  | C2D-C1D-ND  | 7.68  | 115.77      | 110.10   |
| 23  | B     | 610  | CLA  | C2D-C1D-ND  | 7.66  | 115.75      | 110.10   |
| 23  | B     | 615  | CLA  | C2D-C1D-ND  | 7.65  | 115.74      | 110.10   |
| 23  | A     | 405  | CLA  | C2D-C1D-ND  | 7.60  | 115.70      | 110.10   |
| 23  | b     | 616  | CLA  | C2D-C1D-ND  | 7.59  | 115.70      | 110.10   |
| 23  | C     | 511  | CLA  | C2D-C1D-ND  | 7.58  | 115.69      | 110.10   |
| 23  | d     | 409  | CLA  | C2D-C1D-ND  | 7.55  | 115.67      | 110.10   |
| 23  | b     | 606  | CLA  | C1D-ND-C4D  | -7.55 | 100.97      | 106.33   |
| 23  | b     | 611  | CLA  | C2D-C1D-ND  | 7.54  | 115.66      | 110.10   |
| 23  | b     | 618  | CLA  | C2D-C1D-ND  | 7.52  | 115.65      | 110.10   |
| 23  | B     | 617  | CLA  | C2D-C1D-ND  | 7.51  | 115.64      | 110.10   |
| 23  | B     | 602  | CLA  | C1D-ND-C4D  | -7.50 | 101.01      | 106.33   |
| 23  | b     | 619  | CLA  | C2D-C1D-ND  | 7.48  | 115.61      | 110.10   |
| 23  | b     | 613  | CLA  | C2D-C1D-ND  | 7.46  | 115.60      | 110.10   |
| 23  | C     | 512  | CLA  | C2D-C1D-ND  | 7.42  | 115.57      | 110.10   |
| 23  | c     | 510  | CLA  | C2D-C1D-ND  | 7.41  | 115.56      | 110.10   |
| 23  | A     | 407  | CLA  | C2D-C1D-ND  | 7.40  | 115.56      | 110.10   |
| 23  | C     | 507  | CLA  | C1-C2-C3    | -7.40 | 113.24      | 126.04   |
| 23  | B     | 607  | CLA  | C2D-C1D-ND  | 7.35  | 115.52      | 110.10   |
| 23  | c     | 514  | CLA  | C2D-C1D-ND  | 7.33  | 115.50      | 110.10   |
| 23  | c     | 516  | CLA  | C2D-C1D-ND  | 7.32  | 115.50      | 110.10   |
| 23  | B     | 605  | CLA  | C2D-C1D-ND  | 7.31  | 115.49      | 110.10   |
| 23  | C     | 513  | CLA  | C2D-C1D-ND  | 7.31  | 115.49      | 110.10   |
| 23  | b     | 608  | CLA  | C2D-C1D-ND  | 7.29  | 115.48      | 110.10   |
| 23  | C     | 507  | CLA  | C2D-C1D-ND  | 7.29  | 115.48      | 110.10   |
| 23  | b     | 609  | CLA  | C2D-C1D-ND  | 7.27  | 115.46      | 110.10   |
| 23  | b     | 619  | CLA  | CMD-C2D-C1D | 7.25  | 137.50      | 124.71   |
| 23  | B     | 603  | CLA  | C2D-C1D-ND  | 7.25  | 115.45      | 110.10   |
| 23  | B     | 611  | CLA  | C2D-C1D-ND  | 7.22  | 115.43      | 110.10   |
| 23  | C     | 507  | CLA  | CMD-C2D-C1D | 7.21  | 137.41      | 124.71   |
| 23  | B     | 604  | CLA  | C2D-C1D-ND  | 7.20  | 115.41      | 110.10   |
| 23  | C     | 505  | CLA  | C2D-C1D-ND  | 7.19  | 115.41      | 110.10   |
| 23  | C     | 510  | CLA  | C2D-C1D-ND  | 7.18  | 115.40      | 110.10   |
| 24  | a     | 2612 | PHO  | C4D-ND-C1D  | -7.14 | 101.57      | 108.83   |
| 36  | i     | 102  | HTG  | C1'-S1-C1   | 7.12  | 113.40      | 100.09   |
| 23  | b     | 607  | CLA  | C2D-C1D-ND  | 7.08  | 115.32      | 110.10   |
| 23  | c     | 508  | CLA  | C2D-C1D-ND  | 7.04  | 115.30      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | a     | 2611 | PHO  | C1C-C2C-C3C | -7.03 | 102.77      | 108.61   |
| 31  | A     | 419  | JOX  | C3-C4-C5    | -7.03 | 117.45      | 120.54   |
| 24  | A     | 408  | PHO  | C4D-ND-C1D  | -7.00 | 101.70      | 108.83   |
| 23  | b     | 620  | CLA  | C2D-C1D-ND  | 6.96  | 115.23      | 110.10   |
| 23  | B     | 604  | CLA  | O2D-CGD-CBD | 6.96  | 123.63      | 111.27   |
| 23  | A     | 407  | CLA  | C2B-C1B-NB  | 6.95  | 114.89      | 110.23   |
| 23  | b     | 614  | CLA  | C2D-C1D-ND  | 6.90  | 115.19      | 110.10   |
| 23  | C     | 514  | CLA  | CMD-C2D-C1D | 6.88  | 136.84      | 124.71   |
| 23  | B     | 605  | CLA  | CMD-C2D-C1D | 6.88  | 136.84      | 124.71   |
| 23  | c     | 510  | CLA  | O2D-CGD-CBD | 6.86  | 123.46      | 111.27   |
| 23  | A     | 410  | CLA  | C2B-C1B-NB  | 6.84  | 114.82      | 110.23   |
| 23  | b     | 615  | CLA  | CMD-C2D-C1D | 6.83  | 136.76      | 124.71   |
| 23  | C     | 502  | CLA  | CMD-C2D-C1D | 6.83  | 136.74      | 124.71   |
| 26  | l     | 101  | SQD  | O6-C1-C2    | 6.82  | 118.95      | 108.30   |
| 24  | A     | 409  | PHO  | C1-C2-C3    | -6.79 | 114.30      | 126.04   |
| 24  | A     | 409  | PHO  | C4D-ND-C1D  | -6.78 | 101.93      | 108.83   |
| 24  | A     | 409  | PHO  | O2D-CGD-CBD | 6.75  | 119.55      | 111.00   |
| 24  | A     | 409  | PHO  | C2B-C1B-NB  | 6.72  | 114.17      | 109.53   |
| 23  | b     | 614  | CLA  | CMD-C2D-C1D | 6.71  | 136.54      | 124.71   |
| 36  | B     | 625  | HTG  | C1'-S1-C1   | 6.64  | 112.52      | 100.09   |
| 23  | B     | 602  | CLA  | CMD-C2D-C1D | 6.64  | 136.41      | 124.71   |
| 23  | C     | 514  | CLA  | C2D-C1D-ND  | 6.63  | 114.99      | 110.10   |
| 24  | A     | 408  | PHO  | C1C-C2C-C3C | -6.59 | 103.13      | 108.61   |
| 24  | a     | 2611 | PHO  | C4D-ND-C1D  | -6.59 | 102.13      | 108.83   |
| 23  | b     | 618  | CLA  | CMD-C2D-C1D | 6.58  | 136.31      | 124.71   |
| 23  | c     | 508  | CLA  | CMD-C2D-C1D | 6.57  | 136.28      | 124.71   |
| 23  | b     | 613  | CLA  | CMD-C2D-C1D | 6.55  | 136.25      | 124.71   |
| 31  | a     | 2617 | JOX  | C1-C-C5     | -6.54 | 117.66      | 120.54   |
| 24  | a     | 2612 | PHO  | O2D-CGD-CBD | 6.54  | 119.29      | 111.00   |
| 23  | C     | 506  | CLA  | CMD-C2D-C1D | 6.53  | 136.23      | 124.71   |
| 42  | v     | 201  | HEC  | C1D-ND-C4D  | 6.52  | 111.81      | 105.07   |
| 23  | c     | 509  | CLA  | CMD-C2D-C1D | 6.51  | 136.19      | 124.71   |
| 23  | c     | 513  | CLA  | C2D-C1D-ND  | 6.51  | 114.90      | 110.10   |
| 23  | b     | 610  | CLA  | C2B-C1B-NB  | 6.49  | 114.58      | 110.23   |
| 23  | c     | 509  | CLA  | C2D-C1D-ND  | 6.46  | 114.86      | 110.10   |
| 24  | a     | 2612 | PHO  | C1C-C2C-C3C | -6.44 | 103.26      | 108.61   |
| 23  | C     | 505  | CLA  | CMD-C2D-C1D | 6.43  | 136.05      | 124.71   |
| 31  | A     | 419  | JOX  | C1-C2-C3    | 6.43  | 120.02      | 114.18   |
| 23  | B     | 604  | CLA  | CMD-C2D-C1D | 6.43  | 136.04      | 124.71   |
| 23  | c     | 508  | CLA  | O2D-CGD-CBD | 6.40  | 122.64      | 111.27   |
| 23  | B     | 610  | CLA  | CMD-C2D-C1D | 6.40  | 135.99      | 124.71   |
| 23  | C     | 508  | CLA  | O2D-CGD-CBD | 6.39  | 122.61      | 111.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36  | d     | 415  | HTG  | C1'-S1-C1   | 6.38  | 112.02      | 100.09   |
| 23  | b     | 606  | CLA  | CMD-C2D-C1D | 6.31  | 135.84      | 124.71   |
| 23  | b     | 606  | CLA  | O2D-CGD-CBD | 6.31  | 122.48      | 111.27   |
| 24  | a     | 2611 | PHO  | C2B-C1B-NB  | 6.30  | 113.88      | 109.53   |
| 23  | d     | 409  | CLA  | CMD-C2D-C1D | 6.30  | 135.81      | 124.71   |
| 23  | B     | 615  | CLA  | CMD-C2D-C1D | 6.29  | 135.80      | 124.71   |
| 23  | c     | 516  | CLA  | CMD-C2D-C1D | 6.29  | 135.79      | 124.71   |
| 23  | C     | 508  | CLA  | CMD-C2D-C1D | 6.27  | 135.77      | 124.71   |
| 39  | F     | 101  | HEM  | C4D-ND-C1D  | 6.27  | 111.55      | 105.07   |
| 23  | b     | 608  | CLA  | CMD-C2D-C1D | 6.26  | 135.75      | 124.71   |
| 23  | C     | 510  | CLA  | O2D-CGD-CBD | 6.25  | 122.38      | 111.27   |
| 23  | d     | 408  | CLA  | CMD-C2D-C1D | 6.25  | 135.72      | 124.71   |
| 39  | e     | 103  | HEM  | C4D-ND-C1D  | 6.24  | 111.52      | 105.07   |
| 23  | C     | 504  | CLA  | CMD-C2D-C1D | 6.23  | 135.70      | 124.71   |
| 31  | A     | 419  | JOX  | C-C1-C2     | -6.23 | 118.17      | 123.18   |
| 23  | B     | 614  | CLA  | CMD-C2D-C1D | 6.23  | 135.68      | 124.71   |
| 23  | c     | 506  | CLA  | CMD-C2D-C1D | 6.23  | 135.68      | 124.71   |
| 23  | b     | 621  | CLA  | CMD-C2D-C1D | 6.21  | 135.66      | 124.71   |
| 23  | D     | 2303 | CLA  | CMD-C2D-C1D | 6.20  | 135.64      | 124.71   |
| 23  | C     | 513  | CLA  | O2D-CGD-CBD | 6.18  | 122.24      | 111.27   |
| 23  | c     | 510  | CLA  | CMD-C2D-C1D | 6.17  | 135.59      | 124.71   |
| 23  | C     | 510  | CLA  | CMD-C2D-C1D | 6.17  | 135.59      | 124.71   |
| 23  | C     | 502  | CLA  | O2D-CGD-CBD | 6.17  | 122.23      | 111.27   |
| 23  | B     | 603  | CLA  | CMD-C2D-C1D | 6.16  | 135.57      | 124.71   |
| 23  | c     | 515  | CLA  | O2D-CGD-CBD | 6.16  | 122.21      | 111.27   |
| 23  | B     | 612  | CLA  | CMD-C2D-C1D | 6.15  | 135.55      | 124.71   |
| 23  | d     | 409  | CLA  | C2B-C1B-NB  | 6.15  | 114.35      | 110.23   |
| 23  | c     | 507  | CLA  | CMD-C2D-C1D | 6.14  | 135.53      | 124.71   |
| 23  | B     | 611  | CLA  | CMD-C2D-C1D | 6.13  | 135.51      | 124.71   |
| 24  | A     | 408  | PHO  | C2B-C1B-NB  | 6.09  | 113.73      | 109.53   |
| 36  | I     | 101  | HTG  | C1'-S1-C1   | 6.09  | 111.47      | 100.09   |
| 23  | b     | 616  | CLA  | CMD-C2D-C1D | 6.08  | 135.43      | 124.71   |
| 23  | b     | 609  | CLA  | CMD-C2D-C1D | 6.07  | 135.41      | 124.71   |
| 23  | A     | 410  | CLA  | CMD-C2D-C1D | 6.06  | 135.40      | 124.71   |
| 23  | B     | 607  | CLA  | CMD-C2D-C1D | 6.06  | 135.39      | 124.71   |
| 31  | A     | 418  | JOX  | C1-C2-C3    | 6.05  | 119.68      | 114.18   |
| 23  | B     | 617  | CLA  | O2D-CGD-CBD | 6.04  | 122.00      | 111.27   |
| 23  | c     | 513  | CLA  | CMD-C2D-C1D | 6.03  | 135.34      | 124.71   |
| 23  | C     | 513  | CLA  | CMD-C2D-C1D | 6.02  | 135.33      | 124.71   |
| 23  | b     | 611  | CLA  | CMD-C2D-C1D | 6.01  | 135.31      | 124.71   |
| 23  | C     | 502  | CLA  | C2D-C1D-ND  | 6.01  | 114.53      | 110.10   |
| 36  | B     | 626  | HTG  | C1'-S1-C1   | 6.01  | 111.32      | 100.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | B     | 602  | CLA  | C2D-C1D-ND  | 6.00  | 114.53      | 110.10   |
| 23  | b     | 615  | CLA  | C2B-C1B-NB  | 5.98  | 114.24      | 110.23   |
| 23  | a     | 2610 | CLA  | CMD-C2D-C1D | 5.98  | 135.25      | 124.71   |
| 23  | a     | 2610 | CLA  | C2B-C1B-NB  | 5.98  | 114.24      | 110.23   |
| 26  | a     | 2615 | SQD  | O6-C1-C2    | 5.98  | 117.64      | 108.30   |
| 23  | C     | 503  | CLA  | O2D-CGD-CBD | 5.97  | 121.87      | 111.27   |
| 23  | B     | 611  | CLA  | C2B-C1B-NB  | 5.96  | 114.23      | 110.23   |
| 23  | c     | 511  | CLA  | C2B-C1B-NB  | 5.96  | 114.23      | 110.23   |
| 23  | A     | 407  | CLA  | CMD-C2D-C1D | 5.95  | 135.21      | 124.71   |
| 23  | C     | 511  | CLA  | O2D-CGD-CBD | 5.95  | 121.85      | 111.27   |
| 23  | b     | 607  | CLA  | O2D-CGD-CBD | 5.95  | 121.84      | 111.27   |
| 23  | b     | 607  | CLA  | CMD-C2D-C1D | 5.95  | 135.20      | 124.71   |
| 31  | a     | 2617 | JOX  | C1-C2-C3    | 5.94  | 119.58      | 114.18   |
| 23  | b     | 619  | CLA  | C2B-C1B-NB  | 5.93  | 114.21      | 110.23   |
| 23  | C     | 512  | CLA  | CMD-C2D-C1D | 5.93  | 135.16      | 124.71   |
| 23  | B     | 617  | CLA  | CMD-C2D-C1D | 5.92  | 135.15      | 124.71   |
| 23  | c     | 512  | CLA  | CMD-C2D-C1D | 5.92  | 135.14      | 124.71   |
| 23  | b     | 610  | CLA  | CMD-C2D-C1D | 5.89  | 135.09      | 124.71   |
| 23  | C     | 509  | CLA  | O2D-CGD-CBD | 5.87  | 121.70      | 111.27   |
| 23  | b     | 607  | CLA  | C2B-C1B-NB  | 5.84  | 114.15      | 110.23   |
| 23  | c     | 508  | CLA  | C2B-C1B-NB  | 5.83  | 114.14      | 110.23   |
| 24  | A     | 408  | PHO  | O2D-CGD-CBD | 5.82  | 118.37      | 111.00   |
| 23  | B     | 602  | CLA  | O2D-CGD-CBD | 5.81  | 121.59      | 111.27   |
| 23  | b     | 606  | CLA  | C2D-C1D-ND  | 5.81  | 114.39      | 110.10   |
| 23  | D     | 2304 | CLA  | O2D-CGD-CBD | 5.80  | 121.58      | 111.27   |
| 23  | b     | 612  | CLA  | CMD-C2D-C1D | 5.79  | 134.93      | 124.71   |
| 23  | B     | 604  | CLA  | C2B-C1B-NB  | 5.78  | 114.11      | 110.23   |
| 23  | b     | 621  | CLA  | O2D-CGD-CBD | 5.78  | 121.53      | 111.27   |
| 23  | A     | 406  | CLA  | C2B-C1B-NB  | 5.77  | 114.10      | 110.23   |
| 23  | b     | 613  | CLA  | C2B-C1B-NB  | 5.77  | 114.10      | 110.23   |
| 31  | A     | 418  | JOX  | C4-C3-C2    | -5.77 | 118.55      | 123.18   |
| 23  | b     | 619  | CLA  | O2D-CGD-CBD | 5.76  | 121.51      | 111.27   |
| 23  | A     | 405  | CLA  | CMD-C2D-C1D | 5.76  | 134.87      | 124.71   |
| 23  | C     | 514  | CLA  | C2B-C1B-NB  | 5.76  | 114.09      | 110.23   |
| 36  | C     | 525  | HTG  | C1'-S1-C1   | 5.75  | 110.85      | 100.09   |
| 42  | V     | 201  | HEC  | C1D-ND-C4D  | 5.74  | 111.00      | 105.07   |
| 23  | b     | 606  | CLA  | C2B-C1B-NB  | 5.71  | 114.06      | 110.23   |
| 26  | D     | 2302 | SQD  | O47-C7-C8   | 5.70  | 123.80      | 111.50   |
| 23  | c     | 507  | CLA  | O2D-CGD-CBD | 5.70  | 121.40      | 111.27   |
| 23  | B     | 616  | CLA  | CMD-C2D-C1D | 5.69  | 134.74      | 124.71   |
| 23  | D     | 2304 | CLA  | CHD-C1D-ND  | -5.68 | 119.24      | 124.45   |
| 31  | A     | 418  | JOX  | C-C1-C2     | -5.67 | 118.62      | 123.18   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36  | V     | 204  | HTG  | C1'-S1-C1   | 5.67  | 110.70      | 100.09   |
| 23  | a     | 2609 | CLA  | CMD-C2D-C1D | 5.67  | 134.70      | 124.71   |
| 23  | c     | 510  | CLA  | C2B-C1B-NB  | 5.67  | 114.03      | 110.23   |
| 23  | B     | 615  | CLA  | O2D-CGD-CBD | 5.65  | 121.31      | 111.27   |
| 23  | b     | 610  | CLA  | O2D-CGD-CBD | 5.63  | 121.28      | 111.27   |
| 23  | c     | 516  | CLA  | C2B-C1B-NB  | 5.63  | 114.01      | 110.23   |
| 23  | C     | 506  | CLA  | O2D-CGD-CBD | 5.59  | 121.21      | 111.27   |
| 23  | b     | 609  | CLA  | C1-C2-C3    | -5.59 | 116.37      | 126.04   |
| 25  | d     | 410  | BCR  | C24-C23-C22 | -5.59 | 117.80      | 126.23   |
| 23  | c     | 504  | CLA  | CMD-C2D-C1D | 5.58  | 134.55      | 124.71   |
| 36  | c     | 524  | HTG  | C1'-S1-C1   | 5.58  | 110.53      | 100.09   |
| 24  | A     | 409  | PHO  | C1C-C2C-C3C | -5.55 | 103.99      | 108.61   |
| 23  | D     | 2304 | CLA  | CMD-C2D-C1D | 5.52  | 134.45      | 124.71   |
| 23  | c     | 514  | CLA  | CMD-C2D-C1D | 5.52  | 134.44      | 124.71   |
| 23  | a     | 2610 | CLA  | CHD-C1D-ND  | -5.51 | 119.39      | 124.45   |
| 23  | a     | 2613 | CLA  | C2B-C1B-NB  | 5.51  | 113.93      | 110.23   |
| 23  | B     | 612  | CLA  | C2B-C1B-NB  | 5.50  | 113.92      | 110.23   |
| 24  | a     | 2612 | PHO  | C1-C2-C3    | -5.46 | 116.59      | 126.04   |
| 23  | c     | 509  | CLA  | C2B-C1B-NB  | 5.46  | 113.89      | 110.23   |
| 36  | b     | 604  | HTG  | C1'-S1-C1   | 5.46  | 110.30      | 100.09   |
| 23  | C     | 505  | CLA  | O2D-CGD-CBD | 5.43  | 120.92      | 111.27   |
| 24  | a     | 2612 | PHO  | C3D-C4D-ND  | 5.42  | 115.10      | 107.72   |
| 23  | B     | 607  | CLA  | O2D-CGD-CBD | 5.40  | 120.86      | 111.27   |
| 23  | D     | 2303 | CLA  | O2D-CGD-CBD | 5.39  | 120.85      | 111.27   |
| 23  | B     | 606  | CLA  | CMD-C2D-C1D | 5.39  | 134.20      | 124.71   |
| 23  | B     | 613  | CLA  | CMD-C2D-C1D | 5.38  | 134.20      | 124.71   |
| 36  | d     | 407  | HTG  | C1'-S1-C1   | 5.38  | 110.15      | 100.09   |
| 23  | B     | 606  | CLA  | C2B-C1B-NB  | 5.37  | 113.83      | 110.23   |
| 36  | b     | 626  | HTG  | C1'-S1-C1   | 5.37  | 110.14      | 100.09   |
| 23  | C     | 510  | CLA  | C2B-C1B-NB  | 5.37  | 113.83      | 110.23   |
| 23  | D     | 2304 | CLA  | C2B-C1B-NB  | 5.36  | 113.83      | 110.23   |
| 23  | c     | 514  | CLA  | C2B-C1B-NB  | 5.35  | 113.82      | 110.23   |
| 23  | C     | 507  | CLA  | C2B-C1B-NB  | 5.34  | 113.81      | 110.23   |
| 23  | C     | 503  | CLA  | CMD-C2D-C1D | 5.34  | 134.12      | 124.71   |
| 23  | A     | 406  | CLA  | CMD-C2D-C1D | 5.34  | 134.12      | 124.71   |
| 23  | B     | 616  | CLA  | C2B-C1B-NB  | 5.34  | 113.81      | 110.23   |
| 36  | c     | 523  | HTG  | C1'-S1-C1   | 5.33  | 110.07      | 100.09   |
| 23  | c     | 507  | CLA  | C2B-C1B-NB  | 5.30  | 113.79      | 110.23   |
| 23  | a     | 2609 | CLA  | C2B-C1B-NB  | 5.26  | 113.76      | 110.23   |
| 23  | B     | 607  | CLA  | C2B-C1B-NB  | 5.25  | 113.75      | 110.23   |
| 25  | B     | 633  | BCR  | C33-C5-C6   | -5.25 | 118.63      | 124.53   |
| 23  | C     | 508  | CLA  | C2B-C1B-NB  | 5.24  | 113.74      | 110.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | B     | 608  | CLA  | CMD-C2D-C1D | 5.23  | 133.94      | 124.71   |
| 23  | C     | 513  | CLA  | C2B-C1B-NB  | 5.22  | 113.73      | 110.23   |
| 23  | B     | 612  | CLA  | C3D-C2D-C1D | -5.22 | 98.71       | 105.83   |
| 23  | b     | 620  | CLA  | C2B-C1B-NB  | 5.22  | 113.73      | 110.23   |
| 23  | c     | 511  | CLA  | O2D-CGD-CBD | 5.20  | 120.51      | 111.27   |
| 23  | b     | 618  | CLA  | C2B-C1B-NB  | 5.19  | 113.71      | 110.23   |
| 23  | c     | 513  | CLA  | C2B-C1B-NB  | 5.18  | 113.71      | 110.23   |
| 24  | A     | 409  | PHO  | C3D-C4D-ND  | 5.18  | 114.78      | 107.72   |
| 23  | b     | 609  | CLA  | O2D-CGD-CBD | 5.18  | 120.47      | 111.27   |
| 23  | b     | 617  | CLA  | C2B-C1B-NB  | 5.17  | 113.70      | 110.23   |
| 23  | c     | 510  | CLA  | C3B-C2B-C1B | -5.17 | 100.93      | 107.16   |
| 23  | C     | 506  | CLA  | C2D-C1D-ND  | 5.16  | 113.91      | 110.10   |
| 23  | A     | 406  | CLA  | C1C-C2C-C3C | -5.15 | 101.54      | 106.96   |
| 23  | b     | 608  | CLA  | O2D-CGD-CBD | 5.14  | 120.41      | 111.27   |
| 36  | c     | 526  | HTG  | C1'-S1-C1   | 5.14  | 109.71      | 100.09   |
| 23  | B     | 608  | CLA  | O2D-CGD-CBD | 5.14  | 120.40      | 111.27   |
| 23  | b     | 611  | CLA  | O2D-CGD-CBD | 5.14  | 120.40      | 111.27   |
| 24  | a     | 2611 | PHO  | C3D-C4D-ND  | 5.14  | 114.72      | 107.72   |
| 23  | B     | 603  | CLA  | C2B-C1B-NB  | 5.13  | 113.67      | 110.23   |
| 23  | d     | 402  | CLA  | C2B-C1B-NB  | 5.13  | 113.67      | 110.23   |
| 26  | l     | 101  | SQD  | O47-C7-C8   | 5.13  | 122.55      | 111.50   |
| 36  | B     | 625  | HTG  | O5-C1-C2    | 5.12  | 116.75      | 110.31   |
| 23  | A     | 406  | CLA  | C3D-C2D-C1D | -5.11 | 98.86       | 105.83   |
| 23  | c     | 515  | CLA  | C2B-C1B-NB  | 5.10  | 113.65      | 110.23   |
| 37  | C     | 519  | DGD  | O2G-C1B-C2B | 5.08  | 122.45      | 111.50   |
| 23  | C     | 511  | CLA  | CMD-C2D-C1D | 5.06  | 133.63      | 124.71   |
| 23  | B     | 612  | CLA  | O2D-CGD-CBD | 5.06  | 120.26      | 111.27   |
| 23  | b     | 621  | CLA  | C3D-C2D-C1D | -5.05 | 98.94       | 105.83   |
| 23  | B     | 615  | CLA  | C2B-C1B-NB  | 5.04  | 113.61      | 110.23   |
| 23  | B     | 613  | CLA  | C2B-C1B-NB  | 5.04  | 113.61      | 110.23   |
| 23  | a     | 2613 | CLA  | CMD-C2D-C1D | 5.03  | 133.58      | 124.71   |
| 23  | c     | 504  | CLA  | C2B-C1B-NB  | 5.03  | 113.60      | 110.23   |
| 24  | A     | 408  | PHO  | C3D-C4D-ND  | 5.03  | 114.57      | 107.72   |
| 26  | B     | 621  | SQD  | O47-C7-C8   | 5.02  | 122.33      | 111.50   |
| 23  | b     | 610  | CLA  | C3D-C2D-C1D | -5.02 | 98.98       | 105.83   |
| 23  | b     | 621  | CLA  | C2B-C1B-NB  | 5.01  | 113.59      | 110.23   |
| 26  | d     | 417  | SQD  | O47-C7-O49  | -5.01 | 119.19      | 125.57   |
| 23  | A     | 406  | CLA  | C2C-C1C-NC  | 5.01  | 114.67      | 109.97   |
| 23  | b     | 612  | CLA  | C2B-C1B-NB  | 5.00  | 113.58      | 110.23   |
| 23  | B     | 611  | CLA  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 23  | C     | 509  | CLA  | C2B-C1B-NB  | 4.99  | 113.58      | 110.23   |
| 36  | B     | 627  | HTG  | C1'-S1-C1   | 4.99  | 109.42      | 100.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | d     | 408  | CLA  | C2C-C1C-NC  | 4.98  | 114.64      | 109.97   |
| 23  | c     | 505  | CLA  | C2B-C1B-NB  | 4.98  | 113.57      | 110.23   |
| 23  | C     | 506  | CLA  | C2B-C1B-NB  | 4.98  | 113.57      | 110.23   |
| 23  | C     | 503  | CLA  | C2B-C1B-NB  | 4.98  | 113.57      | 110.23   |
| 25  | Y     | 302  | BCR  | C15-C14-C13 | -4.98 | 120.21      | 127.31   |
| 23  | B     | 617  | CLA  | C2B-C1B-NB  | 4.97  | 113.57      | 110.23   |
| 36  | H     | 101  | HTG  | C1'-S1-C1   | 4.97  | 109.39      | 100.09   |
| 23  | C     | 512  | CLA  | C2B-C1B-NB  | 4.96  | 113.56      | 110.23   |
| 23  | C     | 505  | CLA  | C2B-C1B-NB  | 4.96  | 113.55      | 110.23   |
| 27  | C     | 527  | LMG  | O7-C10-C11  | 4.95  | 122.16      | 111.50   |
| 26  | b     | 601  | SQD  | O8-S-C6     | 4.95  | 113.62      | 105.74   |
| 23  | B     | 605  | CLA  | C2B-C1B-NB  | 4.94  | 113.54      | 110.23   |
| 23  | B     | 614  | CLA  | C2B-C1B-NB  | 4.94  | 113.54      | 110.23   |
| 23  | B     | 614  | CLA  | C3D-C2D-C1D | -4.93 | 99.10       | 105.83   |
| 23  | b     | 608  | CLA  | C2B-C1B-NB  | 4.93  | 113.54      | 110.23   |
| 23  | b     | 617  | CLA  | O2D-CGD-CBD | 4.93  | 120.03      | 111.27   |
| 23  | b     | 615  | CLA  | C3D-C2D-C1D | -4.93 | 99.10       | 105.83   |
| 23  | b     | 611  | CLA  | C2B-C1B-NB  | 4.93  | 113.54      | 110.23   |
| 23  | A     | 406  | CLA  | CBC-CAC-C3C | -4.92 | 98.85       | 112.43   |
| 23  | d     | 402  | CLA  | CMD-C2D-C1D | 4.91  | 133.37      | 124.71   |
| 23  | b     | 610  | CLA  | C3B-C2B-C1B | -4.91 | 101.24      | 107.16   |
| 23  | c     | 515  | CLA  | CMD-C2D-C1D | 4.91  | 133.36      | 124.71   |
| 23  | B     | 608  | CLA  | C2B-C1B-NB  | 4.88  | 113.50      | 110.23   |
| 23  | B     | 602  | CLA  | C2B-C1B-NB  | 4.88  | 113.50      | 110.23   |
| 23  | b     | 620  | CLA  | CMD-C2D-C1D | 4.87  | 133.30      | 124.71   |
| 27  | A     | 413  | LMG  | O7-C10-C11  | 4.87  | 122.00      | 111.50   |
| 23  | B     | 611  | CLA  | C1-C2-C3    | -4.87 | 117.63      | 126.04   |
| 23  | B     | 616  | CLA  | CHD-C4C-C3C | -4.86 | 117.69      | 124.84   |
| 23  | c     | 504  | CLA  | CHD-C1D-ND  | -4.86 | 119.98      | 124.45   |
| 23  | D     | 2303 | CLA  | O2D-CGD-O1D | -4.86 | 114.33      | 123.84   |
| 23  | D     | 2303 | CLA  | CHD-C4C-C3C | -4.85 | 117.72      | 124.84   |
| 23  | c     | 512  | CLA  | O2D-CGD-CBD | 4.84  | 119.88      | 111.27   |
| 23  | A     | 405  | CLA  | C2B-C1B-NB  | 4.84  | 113.48      | 110.23   |
| 23  | B     | 613  | CLA  | O2D-CGD-CBD | 4.84  | 119.87      | 111.27   |
| 23  | B     | 609  | CLA  | C2B-C1B-NB  | 4.83  | 113.47      | 110.23   |
| 23  | c     | 506  | CLA  | C3D-C2D-C1D | -4.82 | 99.25       | 105.83   |
| 23  | B     | 603  | CLA  | O2D-CGD-CBD | 4.82  | 119.83      | 111.27   |
| 31  | a     | 2617 | JOX  | C3-C4-C5    | -4.81 | 118.42      | 120.54   |
| 23  | D     | 2304 | CLA  | CHD-C4C-C3C | -4.81 | 117.77      | 124.84   |
| 23  | D     | 2303 | CLA  | C3D-C2D-C1D | -4.80 | 99.29       | 105.83   |
| 23  | a     | 2610 | CLA  | C3D-C2D-C1D | -4.79 | 99.29       | 105.83   |
| 23  | C     | 509  | CLA  | CMD-C2D-C1D | 4.79  | 133.16      | 124.71   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | D     | 2303   | CLA  | C2B-C1B-NB  | 4.78  | 113.44      | 110.23   |
| 23  | c     | 508    | CLA  | C3B-C2B-C1B | -4.78 | 101.39      | 107.16   |
| 23  | D     | 2303   | CLA  | CHD-C1D-ND  | -4.78 | 120.06      | 124.45   |
| 23  | A     | 406    | CLA  | O2D-CGD-CBD | 4.78  | 119.75      | 111.27   |
| 23  | c     | 507    | CLA  | CHD-C1D-ND  | -4.76 | 120.08      | 124.45   |
| 23  | B     | 616    | CLA  | C3D-C2D-C1D | -4.76 | 99.34       | 105.83   |
| 23  | B     | 606    | CLA  | C3D-C2D-C1D | -4.75 | 99.34       | 105.83   |
| 23  | b     | 617    | CLA  | CHD-C4C-C3C | -4.75 | 117.85      | 124.84   |
| 23  | c     | 509    | CLA  | O2D-CGD-CBD | 4.75  | 119.71      | 111.27   |
| 23  | b     | 610    | CLA  | CHD-C4C-C3C | -4.75 | 117.85      | 124.84   |
| 23  | c     | 505    | CLA  | CMD-C2D-C1D | 4.75  | 133.09      | 124.71   |
| 23  | b     | 612    | CLA  | C3D-C2D-C1D | -4.75 | 99.35       | 105.83   |
| 23  | c     | 510    | CLA  | C2C-C1C-NC  | 4.75  | 114.42      | 109.97   |
| 25  | T     | 102    | BCR  | C33-C5-C6   | -4.73 | 119.21      | 124.53   |
| 23  | b     | 617    | CLA  | CMD-C2D-C1D | 4.73  | 133.06      | 124.71   |
| 23  | c     | 504    | CLA  | O2D-CGD-CBD | 4.73  | 119.67      | 111.27   |
| 23  | a     | 2613   | CLA  | O2D-CGD-CBD | 4.72  | 119.66      | 111.27   |
| 23  | B     | 615    | CLA  | CHD-C4C-C3C | -4.71 | 117.91      | 124.84   |
| 36  | B     | 624[B] | HTG  | C1'-S1-C1   | 4.70  | 108.87      | 100.09   |
| 23  | d     | 408    | CLA  | C2B-C1B-NB  | 4.69  | 113.38      | 110.23   |
| 23  | C     | 504    | CLA  | CHD-C4C-C3C | -4.68 | 117.96      | 124.84   |
| 23  | C     | 508    | CLA  | C3B-C2B-C1B | -4.68 | 101.51      | 107.16   |
| 31  | A     | 419    | JOX  | C4-C3-CL    | 4.66  | 131.29      | 120.02   |
| 23  | b     | 612    | CLA  | O2D-CGD-CBD | 4.65  | 119.54      | 111.27   |
| 23  | d     | 409    | CLA  | O2D-CGD-CBD | 4.65  | 119.53      | 111.27   |
| 37  | D     | 2307   | DGD  | O2G-C1B-C2B | 4.65  | 121.52      | 111.50   |
| 23  | A     | 407    | CLA  | CHD-C4C-C3C | -4.63 | 118.03      | 124.84   |
| 23  | b     | 619    | CLA  | C3B-C2B-C1B | -4.63 | 101.58      | 107.16   |
| 23  | b     | 616    | CLA  | C3D-C2D-C1D | -4.62 | 99.53       | 105.83   |
| 23  | a     | 2613   | CLA  | C1C-C2C-C3C | -4.62 | 102.10      | 106.96   |
| 23  | B     | 614    | CLA  | CHD-C4C-C3C | -4.61 | 118.06      | 124.84   |
| 23  | B     | 608    | CLA  | C3D-C2D-C1D | -4.60 | 99.56       | 105.83   |
| 23  | B     | 605    | CLA  | C2C-C1C-NC  | 4.60  | 114.28      | 109.97   |
| 23  | b     | 614    | CLA  | C2B-C1B-NB  | 4.60  | 113.31      | 110.23   |
| 23  | c     | 505    | CLA  | O2D-CGD-CBD | 4.59  | 119.43      | 111.27   |
| 25  | C     | 516    | BCR  | C7-C8-C9    | -4.59 | 119.29      | 126.23   |
| 23  | D     | 2303   | CLA  | C2C-C1C-NC  | 4.59  | 114.27      | 109.97   |
| 23  | C     | 508    | CLA  | C3D-C2D-C1D | -4.59 | 99.57       | 105.83   |
| 25  | D     | 2305   | BCR  | C24-C23-C22 | -4.59 | 119.30      | 126.23   |
| 23  | B     | 615    | CLA  | C3D-C2D-C1D | -4.59 | 99.57       | 105.83   |
| 23  | d     | 402    | CLA  | O2D-CGD-CBD | 4.58  | 119.40      | 111.27   |
| 23  | b     | 613    | CLA  | C3B-C2B-C1B | -4.57 | 101.64      | 107.16   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | c     | 501  | LMG  | O7-C10-C11  | 4.57  | 121.35      | 111.50   |
| 23  | C     | 514  | CLA  | C3B-C2B-C1B | -4.57 | 101.65      | 107.16   |
| 23  | B     | 616  | CLA  | C3B-C2B-C1B | -4.56 | 101.65      | 107.16   |
| 23  | C     | 504  | CLA  | C3D-C2D-C1D | -4.56 | 99.61       | 105.83   |
| 23  | c     | 516  | CLA  | C3B-C2B-C1B | -4.55 | 101.66      | 107.16   |
| 23  | A     | 410  | CLA  | C3D-C2D-C1D | -4.55 | 99.62       | 105.83   |
| 23  | B     | 604  | CLA  | C3B-C2B-C1B | -4.55 | 101.67      | 107.16   |
| 23  | B     | 610  | CLA  | C2B-C1B-NB  | 4.54  | 113.28      | 110.23   |
| 23  | B     | 609  | CLA  | CMD-C2D-C1D | 4.54  | 132.71      | 124.71   |
| 23  | A     | 410  | CLA  | C3B-C2B-C1B | -4.54 | 101.69      | 107.16   |
| 23  | d     | 402  | CLA  | C2C-C1C-NC  | 4.53  | 114.22      | 109.97   |
| 23  | B     | 611  | CLA  | C3D-C2D-C1D | -4.53 | 99.64       | 105.83   |
| 23  | d     | 409  | CLA  | C3B-C2B-C1B | -4.53 | 101.69      | 107.16   |
| 23  | c     | 515  | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 23  | B     | 617  | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 23  | c     | 504  | CLA  | C3D-C2D-C1D | -4.53 | 99.66       | 105.83   |
| 23  | B     | 606  | CLA  | CHD-C4C-C3C | -4.52 | 118.19      | 124.84   |
| 23  | b     | 621  | CLA  | CHD-C4C-C3C | -4.52 | 118.19      | 124.84   |
| 26  | A     | 412  | SQD  | O47-C7-C8   | 4.52  | 121.23      | 111.50   |
| 25  | D     | 2305 | BCR  | C38-C26-C25 | -4.51 | 119.46      | 124.53   |
| 36  | C     | 522  | HTG  | C1-O5-C5    | 4.51  | 120.90      | 112.58   |
| 23  | B     | 607  | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 31  | a     | 2619 | JOX  | C-C1-C2     | -4.51 | 119.56      | 123.18   |
| 25  | D     | 2305 | BCR  | C7-C8-C9    | -4.51 | 119.42      | 126.23   |
| 23  | b     | 609  | CLA  | C2B-C1B-NB  | 4.51  | 113.25      | 110.23   |
| 27  | c     | 522  | LMG  | O7-C10-C11  | 4.51  | 121.21      | 111.50   |
| 23  | b     | 619  | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 23  | c     | 507  | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 23  | c     | 512  | CLA  | C2B-C1B-NB  | 4.49  | 113.24      | 110.23   |
| 23  | C     | 510  | CLA  | C3B-C2B-C1B | -4.49 | 101.74      | 107.16   |
| 23  | a     | 2609 | CLA  | C3D-C4D-ND  | 4.48  | 117.49      | 110.24   |
| 23  | b     | 611  | CLA  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 31  | a     | 2617 | JOX  | C-C1-CL1    | 4.48  | 130.84      | 120.02   |
| 23  | C     | 503  | CLA  | O2D-CGD-O1D | -4.47 | 115.09      | 123.84   |
| 23  | C     | 513  | CLA  | C3B-C2B-C1B | -4.47 | 101.76      | 107.16   |
| 23  | c     | 512  | CLA  | C3D-C2D-C1D | -4.47 | 99.73       | 105.83   |
| 23  | c     | 511  | CLA  | CMD-C2D-C1D | 4.46  | 132.58      | 124.71   |
| 23  | b     | 614  | CLA  | CHD-C1D-ND  | -4.46 | 120.35      | 124.45   |
| 23  | B     | 606  | CLA  | C3B-C2B-C1B | -4.46 | 101.78      | 107.16   |
| 23  | b     | 616  | CLA  | C2B-C1B-NB  | 4.46  | 113.22      | 110.23   |
| 23  | d     | 408  | CLA  | C3D-C2D-C1D | -4.45 | 99.76       | 105.83   |
| 23  | a     | 2613 | CLA  | C3D-C2D-C1D | -4.45 | 99.76       | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | b     | 621  | CLA  | C1D-CHD-C4C | -4.45 | 116.47      | 126.06   |
| 23  | c     | 504  | CLA  | C3D-C4D-ND  | 4.45  | 117.43      | 110.24   |
| 23  | A     | 410  | CLA  | C2C-C1C-NC  | 4.45  | 114.14      | 109.97   |
| 23  | a     | 2610 | CLA  | C3D-C4D-ND  | 4.44  | 117.42      | 110.24   |
| 23  | C     | 507  | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 23  | A     | 407  | CLA  | C3D-C4D-ND  | 4.44  | 117.42      | 110.24   |
| 23  | d     | 402  | CLA  | C1C-C2C-C3C | -4.44 | 102.29      | 106.96   |
| 23  | C     | 505  | CLA  | C3D-C2D-C1D | -4.43 | 99.78       | 105.83   |
| 23  | b     | 618  | CLA  | C3D-C2D-C1D | -4.43 | 99.78       | 105.83   |
| 23  | b     | 615  | CLA  | C3B-C2B-C1B | -4.43 | 101.81      | 107.16   |
| 23  | c     | 506  | CLA  | O2D-CGD-CBD | 4.43  | 119.14      | 111.27   |
| 23  | B     | 615  | CLA  | O2D-CGD-O1D | -4.43 | 115.18      | 123.84   |
| 23  | d     | 408  | CLA  | C1C-C2C-C3C | -4.43 | 102.30      | 106.96   |
| 25  | Y     | 302  | BCR  | C38-C26-C25 | -4.42 | 119.56      | 124.53   |
| 23  | A     | 405  | CLA  | CHD-C1D-ND  | -4.42 | 120.39      | 124.45   |
| 23  | d     | 409  | CLA  | C3D-C2D-C1D | -4.42 | 99.81       | 105.83   |
| 23  | C     | 505  | CLA  | C1C-C2C-C3C | -4.41 | 102.31      | 106.96   |
| 23  | B     | 615  | CLA  | C3B-C2B-C1B | -4.41 | 101.83      | 107.16   |
| 25  | z     | 101  | BCR  | C15-C14-C13 | -4.41 | 121.01      | 127.31   |
| 23  | B     | 605  | CLA  | C1C-C2C-C3C | -4.41 | 102.32      | 106.96   |
| 23  | C     | 509  | CLA  | C3D-C2D-C1D | -4.40 | 99.82       | 105.83   |
| 31  | a     | 2617 | JOX  | C4-C3-CL    | 4.40  | 130.66      | 120.02   |
| 23  | C     | 513  | CLA  | C3D-C2D-C1D | -4.40 | 99.83       | 105.83   |
| 23  | c     | 507  | CLA  | C2C-C1C-NC  | 4.39  | 114.08      | 109.97   |
| 26  | a     | 2603 | SQD  | O47-C7-C8   | 4.39  | 120.96      | 111.50   |
| 23  | b     | 607  | CLA  | C3B-C2B-C1B | -4.39 | 101.86      | 107.16   |
| 23  | c     | 514  | CLA  | CHD-C1D-ND  | -4.38 | 120.42      | 124.45   |
| 26  | a     | 2615 | SQD  | O47-C7-C8   | 4.38  | 120.95      | 111.50   |
| 23  | B     | 611  | CLA  | C3B-C2B-C1B | -4.38 | 101.87      | 107.16   |
| 23  | c     | 504  | CLA  | CHD-C4C-C3C | -4.38 | 118.40      | 124.84   |
| 23  | b     | 617  | CLA  | C3D-C4D-ND  | 4.38  | 117.32      | 110.24   |
| 23  | C     | 512  | CLA  | CHD-C1D-ND  | -4.38 | 120.43      | 124.45   |
| 23  | a     | 2613 | CLA  | C2C-C1C-NC  | 4.38  | 114.07      | 109.97   |
| 25  | c     | 517  | BCR  | C33-C5-C6   | -4.38 | 119.61      | 124.53   |
| 23  | b     | 616  | CLA  | CHD-C4C-C3C | -4.37 | 118.41      | 124.84   |
| 23  | A     | 406  | CLA  | CHD-C4C-C3C | -4.37 | 118.42      | 124.84   |
| 25  | d     | 410  | BCR  | C7-C8-C9    | -4.37 | 119.64      | 126.23   |
| 23  | b     | 610  | CLA  | C1C-C2C-C3C | -4.37 | 102.37      | 106.96   |
| 23  | B     | 604  | CLA  | O2D-CGD-O1D | -4.36 | 115.31      | 123.84   |
| 23  | d     | 402  | CLA  | C3D-C2D-C1D | -4.36 | 99.88       | 105.83   |
| 23  | C     | 514  | CLA  | C3D-C4D-ND  | 4.35  | 117.27      | 110.24   |
| 25  | d     | 410  | BCR  | C33-C5-C6   | -4.35 | 119.65      | 124.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | c     | 516  | CLA  | O2D-CGD-CBD | 4.35  | 118.99      | 111.27   |
| 23  | b     | 613  | CLA  | C3D-C2D-C1D | -4.34 | 99.90       | 105.83   |
| 23  | B     | 615  | CLA  | CHD-C1D-ND  | -4.34 | 120.46      | 124.45   |
| 23  | C     | 506  | CLA  | C3B-C2B-C1B | -4.34 | 101.92      | 107.16   |
| 31  | A     | 419  | JOX  | O-C2-C3     | -4.34 | 118.80      | 122.76   |
| 23  | c     | 516  | CLA  | C3D-C2D-C1D | -4.33 | 99.92       | 105.83   |
| 23  | b     | 607  | CLA  | C3D-C2D-C1D | -4.33 | 99.92       | 105.83   |
| 23  | c     | 505  | CLA  | CHD-C4C-C3C | -4.33 | 118.48      | 124.84   |
| 25  | T     | 102  | BCR  | C7-C8-C9    | -4.33 | 119.70      | 126.23   |
| 23  | c     | 508  | CLA  | C2C-C1C-NC  | 4.33  | 114.02      | 109.97   |
| 23  | d     | 402  | CLA  | CHD-C4C-C3C | -4.32 | 118.48      | 124.84   |
| 23  | B     | 603  | CLA  | C2C-C1C-NC  | 4.32  | 114.02      | 109.97   |
| 23  | B     | 613  | CLA  | C3D-C4D-ND  | 4.32  | 117.23      | 110.24   |
| 23  | c     | 505  | CLA  | C3D-C4D-ND  | 4.32  | 117.23      | 110.24   |
| 23  | B     | 610  | CLA  | O2D-CGD-CBD | 4.32  | 118.95      | 111.27   |
| 25  | T     | 102  | BCR  | C15-C16-C17 | -4.32 | 114.62      | 123.47   |
| 23  | C     | 504  | CLA  | C2B-C1B-NB  | 4.32  | 113.13      | 110.23   |
| 23  | D     | 2304 | CLA  | C3D-C4D-ND  | 4.32  | 117.22      | 110.24   |
| 23  | c     | 507  | CLA  | CHD-C4C-C3C | -4.31 | 118.50      | 124.84   |
| 23  | c     | 510  | CLA  | C1C-C2C-C3C | -4.31 | 102.43      | 106.96   |
| 23  | c     | 504  | CLA  | C1C-C2C-C3C | -4.31 | 102.43      | 106.96   |
| 23  | B     | 603  | CLA  | C3D-C2D-C1D | -4.31 | 99.96       | 105.83   |
| 23  | B     | 617  | CLA  | C3B-C2B-C1B | -4.30 | 101.97      | 107.16   |
| 23  | D     | 2304 | CLA  | C3D-C2D-C1D | -4.30 | 99.97       | 105.83   |
| 23  | C     | 512  | CLA  | C3D-C2D-C1D | -4.30 | 99.97       | 105.83   |
| 25  | B     | 618  | BCR  | C33-C5-C6   | -4.29 | 119.70      | 124.53   |
| 23  | B     | 610  | CLA  | C3D-C2D-C1D | -4.29 | 99.98       | 105.83   |
| 23  | c     | 507  | CLA  | C1C-C2C-C3C | -4.29 | 102.45      | 106.96   |
| 23  | b     | 621  | CLA  | C3C-C4C-NC  | 4.29  | 115.38      | 110.57   |
| 23  | c     | 511  | CLA  | C3D-C4D-ND  | 4.29  | 117.17      | 110.24   |
| 23  | c     | 511  | CLA  | C3D-C2D-C1D | -4.29 | 99.98       | 105.83   |
| 23  | A     | 407  | CLA  | C3D-C2D-C1D | -4.28 | 99.98       | 105.83   |
| 23  | B     | 611  | CLA  | CAC-C3C-C4C | 4.28  | 130.36      | 124.81   |
| 23  | A     | 405  | CLA  | C2C-C1C-NC  | 4.28  | 113.98      | 109.97   |
| 23  | b     | 612  | CLA  | CHD-C4C-C3C | -4.28 | 118.55      | 124.84   |
| 23  | b     | 610  | CLA  | O2D-CGD-O1D | -4.28 | 115.48      | 123.84   |
| 23  | A     | 406  | CLA  | C3B-C2B-C1B | -4.27 | 102.00      | 107.16   |
| 23  | C     | 510  | CLA  | C3D-C2D-C1D | -4.27 | 100.00      | 105.83   |
| 23  | A     | 407  | CLA  | O2D-CGD-CBD | 4.27  | 118.86      | 111.27   |
| 23  | c     | 513  | CLA  | O2D-CGD-CBD | 4.27  | 118.86      | 111.27   |
| 23  | D     | 2303 | CLA  | C3D-C4D-ND  | 4.27  | 117.14      | 110.24   |
| 23  | d     | 409  | CLA  | C1C-C2C-C3C | -4.27 | 102.47      | 106.96   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | B     | 613  | CLA  | C3D-C2D-C1D | -4.27 | 100.01      | 105.83   |
| 23  | c     | 507  | CLA  | C3B-C2B-C1B | -4.26 | 102.01      | 107.16   |
| 25  | T     | 102  | BCR  | C12-C13-C14 | -4.26 | 112.40      | 118.94   |
| 28  | M     | 101  | LMT  | O5'-C5'-C4' | 4.26  | 118.74      | 109.75   |
| 23  | c     | 511  | CLA  | C3B-C2B-C1B | -4.26 | 102.02      | 107.16   |
| 25  | Y     | 302  | BCR  | C33-C5-C6   | -4.26 | 119.74      | 124.53   |
| 23  | B     | 616  | CLA  | O2D-CGD-CBD | 4.26  | 118.84      | 111.27   |
| 23  | b     | 621  | CLA  | C3B-C2B-C1B | -4.26 | 102.02      | 107.16   |
| 37  | C     | 519  | DGD  | O1G-C1A-C2A | 4.25  | 125.26      | 111.91   |
| 25  | d     | 410  | BCR  | C38-C26-C25 | -4.25 | 119.75      | 124.53   |
| 23  | B     | 609  | CLA  | C3D-C2D-C1D | -4.25 | 100.03      | 105.83   |
| 23  | A     | 410  | CLA  | O2D-CGD-CBD | 4.25  | 118.82      | 111.27   |
| 23  | c     | 504  | CLA  | C3B-C2B-C1B | -4.25 | 102.03      | 107.16   |
| 31  | A     | 419  | JOX  | C2-C1-CL1   | -4.24 | 112.31      | 115.84   |
| 23  | d     | 402  | CLA  | CBC-CAC-C3C | -4.24 | 100.73      | 112.43   |
| 23  | C     | 509  | CLA  | C3D-C4D-ND  | 4.24  | 117.10      | 110.24   |
| 25  | b     | 624  | BCR  | C38-C26-C25 | -4.24 | 119.77      | 124.53   |
| 23  | b     | 620  | CLA  | O2D-CGD-CBD | 4.24  | 118.80      | 111.27   |
| 23  | C     | 503  | CLA  | C3D-C2D-C1D | -4.23 | 100.05      | 105.83   |
| 23  | C     | 511  | CLA  | C2B-C1B-NB  | 4.23  | 113.07      | 110.23   |
| 23  | B     | 612  | CLA  | CAC-C3C-C4C | 4.23  | 130.30      | 124.81   |
| 23  | B     | 605  | CLA  | O2D-CGD-CBD | 4.23  | 118.79      | 111.27   |
| 23  | b     | 609  | CLA  | C3D-C2D-C1D | -4.23 | 100.06      | 105.83   |
| 23  | c     | 505  | CLA  | C3B-C2B-C1B | -4.22 | 102.06      | 107.16   |
| 23  | A     | 405  | CLA  | C3D-C4D-ND  | 4.22  | 117.07      | 110.24   |
| 23  | b     | 617  | CLA  | C3D-C2D-C1D | -4.22 | 100.08      | 105.83   |
| 28  | B     | 623  | LMT  | C1B-O5B-C5B | 4.22  | 121.97      | 113.69   |
| 23  | B     | 604  | CLA  | C3D-C2D-C1D | -4.22 | 100.08      | 105.83   |
| 25  | y     | 101  | BCR  | C33-C5-C6   | -4.21 | 119.80      | 124.53   |
| 26  | b     | 601  | SQD  | O47-C7-C8   | 4.21  | 120.57      | 111.50   |
| 23  | D     | 2304 | CLA  | C3B-C2B-C1B | -4.20 | 102.09      | 107.16   |
| 23  | d     | 408  | CLA  | O2D-CGD-CBD | 4.20  | 118.73      | 111.27   |
| 23  | B     | 608  | CLA  | C3B-C2B-C1B | -4.20 | 102.09      | 107.16   |
| 23  | b     | 614  | CLA  | C3D-C2D-C1D | -4.20 | 100.10      | 105.83   |
| 23  | d     | 402  | CLA  | C3B-C2B-C1B | -4.20 | 102.09      | 107.16   |
| 26  | D     | 2308 | SQD  | O47-C7-C8   | 4.20  | 120.55      | 111.50   |
| 23  | d     | 409  | CLA  | C2C-C1C-NC  | 4.20  | 113.90      | 109.97   |
| 23  | C     | 503  | CLA  | C3B-C2B-C1B | -4.19 | 102.10      | 107.16   |
| 23  | b     | 606  | CLA  | C3B-C2B-C1B | -4.19 | 102.10      | 107.16   |
| 23  | C     | 504  | CLA  | C3B-C2B-C1B | -4.19 | 102.10      | 107.16   |
| 23  | c     | 507  | CLA  | C3D-C4D-ND  | 4.19  | 117.01      | 110.24   |
| 23  | B     | 608  | CLA  | C2C-C1C-NC  | 4.19  | 113.89      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | b     | 612  | CLA  | C1C-C2C-C3C | -4.18 | 102.56      | 106.96   |
| 26  | d     | 417  | SQD  | O8-S-C6     | 4.17  | 112.52      | 105.77   |
| 25  | c     | 517  | BCR  | C7-C8-C9    | -4.17 | 119.93      | 126.23   |
| 23  | c     | 505  | CLA  | C3D-C2D-C1D | -4.17 | 100.14      | 105.83   |
| 23  | C     | 514  | CLA  | O2D-CGD-CBD | 4.17  | 118.67      | 111.27   |
| 23  | B     | 613  | CLA  | CHD-C4C-C3C | -4.16 | 118.72      | 124.84   |
| 24  | a     | 2612 | PHO  | C4-C3-C5    | 4.16  | 122.28      | 115.27   |
| 23  | c     | 509  | CLA  | C3D-C4D-ND  | 4.16  | 116.97      | 110.24   |
| 26  | a     | 2615 | SQD  | O9-S-C6     | 4.16  | 111.89      | 106.94   |
| 23  | C     | 510  | CLA  | C2C-C1C-NC  | 4.16  | 113.87      | 109.97   |
| 23  | C     | 504  | CLA  | O2D-CGD-CBD | 4.16  | 118.66      | 111.27   |
| 23  | a     | 2613 | CLA  | CHD-C4C-C3C | -4.16 | 118.73      | 124.84   |
| 23  | c     | 509  | CLA  | C3D-C2D-C1D | -4.16 | 100.16      | 105.83   |
| 27  | c     | 522  | LMG  | O6-C5-C4    | 4.15  | 117.24      | 109.69   |
| 23  | d     | 408  | CLA  | C3D-C4D-ND  | 4.15  | 116.96      | 110.24   |
| 23  | b     | 618  | CLA  | C2C-C1C-NC  | 4.15  | 113.86      | 109.97   |
| 23  | C     | 511  | CLA  | C3D-C4D-ND  | 4.15  | 116.95      | 110.24   |
| 23  | B     | 609  | CLA  | CHD-C4C-C3C | -4.15 | 118.74      | 124.84   |
| 23  | C     | 505  | CLA  | C2C-C1C-NC  | 4.15  | 113.86      | 109.97   |
| 23  | c     | 515  | CLA  | C3B-C2B-C1B | -4.15 | 102.15      | 107.16   |
| 23  | b     | 616  | CLA  | O2D-CGD-CBD | 4.15  | 118.63      | 111.27   |
| 23  | A     | 406  | CLA  | C3D-C4D-ND  | 4.14  | 116.94      | 110.24   |
| 23  | b     | 609  | CLA  | C3B-C2B-C1B | -4.14 | 102.16      | 107.16   |
| 23  | c     | 506  | CLA  | CMB-C2B-C1B | 4.14  | 131.68      | 125.37   |
| 23  | B     | 616  | CLA  | C2C-C1C-NC  | 4.14  | 113.85      | 109.97   |
| 23  | B     | 612  | CLA  | C3B-C2B-C1B | -4.14 | 102.17      | 107.16   |
| 23  | b     | 610  | CLA  | C2C-C1C-NC  | 4.14  | 113.85      | 109.97   |
| 23  | b     | 617  | CLA  | C3B-C2B-C1B | -4.13 | 102.17      | 107.16   |
| 33  | A     | 422  | PL9  | C27-C28-C29 | -4.13 | 117.71      | 127.66   |
| 23  | b     | 615  | CLA  | CHD-C4C-C3C | -4.13 | 118.77      | 124.84   |
| 23  | C     | 502  | CLA  | C2B-C1B-NB  | 4.12  | 113.00      | 110.23   |
| 23  | B     | 605  | CLA  | C3D-C2D-C1D | -4.12 | 100.20      | 105.83   |
| 23  | B     | 610  | CLA  | C3D-C4D-ND  | 4.12  | 116.90      | 110.24   |
| 23  | d     | 408  | CLA  | C1-C2-C3    | -4.12 | 118.92      | 126.04   |
| 38  | E     | 101  | LHG  | O7-C7-C8    | 4.12  | 120.38      | 111.50   |
| 23  | a     | 2609 | CLA  | C3D-C2D-C1D | -4.12 | 100.21      | 105.83   |
| 23  | a     | 2610 | CLA  | C3B-C2B-C1B | -4.12 | 102.19      | 107.16   |
| 23  | b     | 621  | CLA  | C2C-C1C-NC  | 4.11  | 113.82      | 109.97   |
| 37  | c     | 518  | DGD  | O2G-C1B-C2B | 4.11  | 120.36      | 111.50   |
| 23  | b     | 614  | CLA  | C3D-C4D-ND  | 4.11  | 116.89      | 110.24   |
| 37  | C     | 518  | DGD  | O2G-C1B-C2B | 4.11  | 120.36      | 111.50   |
| 23  | b     | 619  | CLA  | C1-C2-C3    | -4.11 | 118.94      | 126.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | c     | 510  | CLA  | C3D-C2D-C1D | -4.11 | 100.23      | 105.83   |
| 23  | a     | 2613 | CLA  | C3D-C4D-ND  | 4.11  | 116.88      | 110.24   |
| 23  | A     | 407  | CLA  | CHD-C1D-ND  | -4.10 | 120.69      | 124.45   |
| 23  | C     | 514  | CLA  | C3D-C2D-C1D | -4.09 | 100.25      | 105.83   |
| 23  | B     | 602  | CLA  | C3B-C2B-C1B | -4.09 | 102.22      | 107.16   |
| 26  | a     | 2615 | SQD  | C1-O5-C5    | -4.09 | 105.66      | 113.69   |
| 23  | A     | 406  | CLA  | CHD-C1D-ND  | -4.09 | 120.69      | 124.45   |
| 23  | b     | 616  | CLA  | CHD-C1D-ND  | -4.09 | 120.70      | 124.45   |
| 26  | A     | 412  | SQD  | O6-C1-C2    | 4.09  | 114.69      | 108.30   |
| 23  | C     | 508  | CLA  | CHD-C4C-C3C | -4.09 | 118.83      | 124.84   |
| 40  | H     | 102  | RRX  | C7-C8-C9    | -4.09 | 120.06      | 126.23   |
| 23  | C     | 505  | CLA  | CHD-C1D-ND  | -4.08 | 120.70      | 124.45   |
| 23  | B     | 615  | CLA  | C3D-C4D-ND  | 4.08  | 116.84      | 110.24   |
| 23  | D     | 2303 | CLA  | C1C-C2C-C3C | -4.08 | 102.67      | 106.96   |
| 23  | b     | 620  | CLA  | C3D-C2D-C1D | -4.08 | 100.27      | 105.83   |
| 23  | A     | 405  | CLA  | C3D-C2D-C1D | -4.07 | 100.28      | 105.83   |
| 23  | b     | 613  | CLA  | O2D-CGD-CBD | 4.07  | 118.50      | 111.27   |
| 23  | B     | 609  | CLA  | C3B-C2B-C1B | -4.07 | 102.25      | 107.16   |
| 23  | b     | 612  | CLA  | C3B-C2B-C1B | -4.07 | 102.25      | 107.16   |
| 23  | B     | 609  | CLA  | C3D-C4D-ND  | 4.07  | 116.82      | 110.24   |
| 23  | B     | 607  | CLA  | C3B-C2B-C1B | -4.07 | 102.25      | 107.16   |
| 23  | c     | 504  | CLA  | O2D-CGD-O1D | -4.06 | 115.90      | 123.84   |
| 23  | c     | 513  | CLA  | C3B-C2B-C1B | -4.06 | 102.26      | 107.16   |
| 23  | C     | 512  | CLA  | C3B-C2B-C1B | -4.06 | 102.27      | 107.16   |
| 23  | b     | 611  | CLA  | C3B-C2B-C1B | -4.05 | 102.27      | 107.16   |
| 23  | b     | 617  | CLA  | C3C-C4C-NC  | 4.05  | 115.12      | 110.57   |
| 23  | b     | 618  | CLA  | C3B-C2B-C1B | -4.05 | 102.27      | 107.16   |
| 23  | C     | 508  | CLA  | C2C-C1C-NC  | 4.05  | 113.76      | 109.97   |
| 23  | A     | 407  | CLA  | C3B-C2B-C1B | -4.05 | 102.28      | 107.16   |
| 23  | A     | 407  | CLA  | C1C-C2C-C3C | -4.04 | 102.70      | 106.96   |
| 23  | c     | 512  | CLA  | C3B-C2B-C1B | -4.04 | 102.28      | 107.16   |
| 23  | C     | 503  | CLA  | C1-C2-C3    | -4.03 | 119.06      | 126.04   |
| 23  | B     | 616  | CLA  | C1D-CHD-C4C | -4.03 | 117.36      | 126.06   |
| 23  | B     | 613  | CLA  | C3B-C2B-C1B | -4.03 | 102.29      | 107.16   |
| 23  | b     | 613  | CLA  | C3D-C4D-ND  | 4.03  | 116.76      | 110.24   |
| 23  | d     | 402  | CLA  | C3D-C4D-ND  | 4.03  | 116.76      | 110.24   |
| 36  | I     | 101  | HTG  | C1-O5-C5    | 4.03  | 120.01      | 112.58   |
| 23  | B     | 603  | CLA  | C3B-C2B-C1B | -4.03 | 102.30      | 107.16   |
| 31  | a     | 2617 | JOX  | C4-C3-C2    | -4.03 | 119.94      | 123.18   |
| 27  | m     | 2802 | LMG  | O7-C10-C11  | 4.03  | 120.18      | 111.50   |
| 23  | a     | 2609 | CLA  | C3B-C2B-C1B | -4.02 | 102.30      | 107.16   |
| 23  | b     | 619  | CLA  | O2D-CGD-O1D | -4.02 | 115.98      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | c     | 508  | CLA  | C3D-C2D-C1D | -4.02 | 100.34      | 105.83   |
| 23  | C     | 512  | CLA  | C2C-C1C-NC  | 4.02  | 113.74      | 109.97   |
| 23  | A     | 407  | CLA  | C1D-CHD-C4C | -4.02 | 117.39      | 126.06   |
| 23  | b     | 612  | CLA  | CHD-C1D-ND  | -4.02 | 120.76      | 124.45   |
| 23  | b     | 619  | CLA  | C2C-C1C-NC  | 4.01  | 113.73      | 109.97   |
| 23  | c     | 514  | CLA  | C3D-C2D-C1D | -4.01 | 100.36      | 105.83   |
| 23  | D     | 2304 | CLA  | O2D-CGD-O1D | -4.01 | 116.00      | 123.84   |
| 40  | h     | 101  | RRX  | C16-C17-C18 | -4.00 | 121.60      | 127.31   |
| 23  | b     | 616  | CLA  | C3B-C2B-C1B | -4.00 | 102.33      | 107.16   |
| 23  | c     | 514  | CLA  | C3B-C2B-C1B | -4.00 | 102.33      | 107.16   |
| 23  | A     | 410  | CLA  | C1C-C2C-C3C | -4.00 | 102.75      | 106.96   |
| 23  | B     | 603  | CLA  | CAA-C2A-C3A | -3.99 | 101.84      | 112.78   |
| 23  | B     | 608  | CLA  | CAA-C2A-C3A | -3.99 | 101.84      | 112.78   |
| 23  | a     | 2613 | CLA  | C3B-C2B-C1B | -3.99 | 102.34      | 107.16   |
| 25  | k     | 302  | BCR  | C24-C23-C22 | -3.99 | 120.21      | 126.23   |
| 23  | b     | 608  | CLA  | C1C-C2C-C3C | -3.99 | 102.77      | 106.96   |
| 23  | C     | 507  | CLA  | C1C-C2C-C3C | -3.98 | 102.77      | 106.96   |
| 23  | C     | 507  | CLA  | C3D-C4D-ND  | 3.98  | 116.68      | 110.24   |
| 37  | c     | 519  | DGD  | O2G-C1B-C2B | 3.98  | 120.08      | 111.50   |
| 23  | B     | 602  | CLA  | C3D-C2D-C1D | -3.98 | 100.40      | 105.83   |
| 23  | c     | 506  | CLA  | C3B-C2B-C1B | -3.98 | 102.36      | 107.16   |
| 23  | b     | 616  | CLA  | CBC-CAC-C3C | -3.97 | 101.48      | 112.43   |
| 23  | B     | 609  | CLA  | O2D-CGD-CBD | 3.97  | 118.33      | 111.27   |
| 23  | c     | 514  | CLA  | CHD-C4C-C3C | -3.97 | 119.00      | 124.84   |
| 23  | b     | 618  | CLA  | C1C-C2C-C3C | -3.97 | 102.78      | 106.96   |
| 27  | c     | 522  | LMG  | C1-O6-C5    | 3.96  | 121.46      | 113.69   |
| 23  | b     | 614  | CLA  | C3B-C2B-C1B | -3.96 | 102.38      | 107.16   |
| 23  | c     | 515  | CLA  | C1-O2A-CGA  | 3.96  | 126.84      | 116.44   |
| 23  | b     | 608  | CLA  | C3D-C4D-ND  | 3.96  | 116.64      | 110.24   |
| 23  | b     | 616  | CLA  | C2C-C1C-NC  | 3.95  | 113.68      | 109.97   |
| 23  | B     | 606  | CLA  | O2A-CGA-O1A | -3.95 | 113.61      | 123.59   |
| 23  | d     | 408  | CLA  | C3B-C2B-C1B | -3.95 | 102.39      | 107.16   |
| 23  | B     | 602  | CLA  | CHD-C1D-ND  | -3.95 | 120.82      | 124.45   |
| 23  | c     | 513  | CLA  | C3D-C4D-ND  | 3.95  | 116.63      | 110.24   |
| 23  | B     | 603  | CLA  | C1C-C2C-C3C | -3.94 | 102.81      | 106.96   |
| 23  | B     | 614  | CLA  | C2C-C1C-NC  | 3.94  | 113.66      | 109.97   |
| 23  | b     | 607  | CLA  | O2D-CGD-O1D | -3.94 | 116.14      | 123.84   |
| 31  | A     | 419  | JOX  | C-C1-CL1    | 3.93  | 129.52      | 120.02   |
| 23  | c     | 514  | CLA  | C1C-C2C-C3C | -3.93 | 102.83      | 106.96   |
| 23  | A     | 407  | CLA  | C2C-C1C-NC  | 3.93  | 113.65      | 109.97   |
| 23  | B     | 614  | CLA  | C1C-C2C-C3C | -3.93 | 102.83      | 106.96   |
| 23  | B     | 611  | CLA  | CMB-C2B-C1B | 3.93  | 131.35      | 125.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | b     | 609  | CLA  | C1C-C2C-C3C | -3.92 | 102.83      | 106.96   |
| 23  | d     | 409  | CLA  | C3D-C4D-ND  | 3.92  | 116.59      | 110.24   |
| 23  | C     | 502  | CLA  | O2D-CGD-O1D | -3.92 | 116.17      | 123.84   |
| 23  | C     | 510  | CLA  | C1C-C2C-C3C | -3.92 | 102.83      | 106.96   |
| 23  | B     | 606  | CLA  | C3D-C4D-ND  | 3.92  | 116.58      | 110.24   |
| 24  | A     | 408  | PHO  | C1A-C2A-C3A | -3.92 | 99.11       | 102.84   |
| 23  | b     | 608  | CLA  | C2C-C1C-NC  | 3.92  | 113.64      | 109.97   |
| 23  | b     | 612  | CLA  | C2C-C1C-NC  | 3.92  | 113.64      | 109.97   |
| 23  | c     | 515  | CLA  | C1D-CHD-C4C | -3.91 | 117.61      | 126.06   |
| 23  | a     | 2613 | CLA  | CBC-CAC-C3C | -3.91 | 101.64      | 112.43   |
| 23  | a     | 2609 | CLA  | C2C-C1C-NC  | 3.91  | 113.64      | 109.97   |
| 23  | B     | 611  | CLA  | CHD-C4C-C3C | -3.91 | 119.10      | 124.84   |
| 23  | a     | 2610 | CLA  | CHD-C4C-C3C | -3.91 | 119.10      | 124.84   |
| 23  | b     | 620  | CLA  | C3B-C2B-C1B | -3.90 | 102.45      | 107.16   |
| 23  | b     | 609  | CLA  | C2C-C1C-NC  | 3.90  | 113.63      | 109.97   |
| 26  | D     | 2302 | SQD  | C1-O5-C5    | 3.90  | 121.34      | 113.69   |
| 23  | b     | 616  | CLA  | C1C-C2C-C3C | -3.90 | 102.86      | 106.96   |
| 39  | F     | 101  | HEM  | CBD-CAD-C3D | -3.90 | 101.80      | 112.63   |
| 23  | C     | 510  | CLA  | O2D-CGD-O1D | -3.90 | 116.22      | 123.84   |
| 23  | B     | 605  | CLA  | C3B-C2B-C1B | -3.89 | 102.46      | 107.16   |
| 23  | B     | 611  | CLA  | C3D-C4D-ND  | 3.89  | 116.53      | 110.24   |
| 23  | C     | 508  | CLA  | C1-C2-C3    | -3.89 | 119.32      | 126.04   |
| 23  | C     | 508  | CLA  | C1C-C2C-C3C | -3.89 | 102.87      | 106.96   |
| 23  | B     | 607  | CLA  | CHD-C4C-C3C | -3.88 | 119.13      | 124.84   |
| 36  | o     | 301  | HTG  | C1'-S1-C1   | 3.88  | 107.36      | 100.09   |
| 33  | x     | 1301 | PL9  | C27-C28-C29 | -3.88 | 118.31      | 127.66   |
| 23  | c     | 514  | CLA  | C2C-C1C-NC  | 3.88  | 113.61      | 109.97   |
| 23  | A     | 410  | CLA  | C3D-C4D-ND  | 3.88  | 116.51      | 110.24   |
| 23  | C     | 502  | CLA  | C3D-C2D-C1D | -3.88 | 100.54      | 105.83   |
| 23  | b     | 608  | CLA  | C3D-C2D-C1D | -3.88 | 100.54      | 105.83   |
| 23  | b     | 606  | CLA  | C3D-C2D-C1D | -3.88 | 100.54      | 105.83   |
| 23  | c     | 508  | CLA  | C3C-C4C-NC  | 3.87  | 114.91      | 110.57   |
| 25  | C     | 515  | BCR  | C38-C26-C25 | -3.87 | 120.18      | 124.53   |
| 23  | c     | 514  | CLA  | C3D-C4D-ND  | 3.87  | 116.49      | 110.24   |
| 23  | B     | 608  | CLA  | C1C-C2C-C3C | -3.86 | 102.89      | 106.96   |
| 23  | A     | 405  | CLA  | CHD-C4C-C3C | -3.86 | 119.17      | 124.84   |
| 23  | c     | 516  | CLA  | C3D-C4D-ND  | 3.86  | 116.48      | 110.24   |
| 23  | C     | 512  | CLA  | C1-O2A-CGA  | 3.86  | 126.57      | 116.44   |
| 23  | c     | 512  | CLA  | C2C-C1C-NC  | 3.86  | 113.58      | 109.97   |
| 23  | d     | 408  | CLA  | CHD-C1D-ND  | -3.86 | 120.91      | 124.45   |
| 23  | b     | 619  | CLA  | C3D-C4D-ND  | 3.86  | 116.47      | 110.24   |
| 33  | A     | 422  | PL9  | C32-C33-C34 | -3.85 | 118.38      | 127.66   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | B     | 614  | CLA  | C3B-C2B-C1B | -3.85 | 102.51      | 107.16   |
| 37  | H     | 103  | DGD  | O2G-C1B-C2B | 3.85  | 119.80      | 111.50   |
| 23  | b     | 611  | CLA  | CHD-C4C-C3C | -3.85 | 119.18      | 124.84   |
| 27  | C     | 520  | LMG  | O7-C10-C11  | 3.85  | 119.80      | 111.50   |
| 38  | e     | 101  | LHG  | O7-C7-C8    | 3.85  | 119.80      | 111.50   |
| 23  | C     | 512  | CLA  | CHD-C4C-C3C | -3.85 | 119.18      | 124.84   |
| 23  | B     | 615  | CLA  | C2C-C1C-NC  | 3.85  | 113.58      | 109.97   |
| 23  | C     | 511  | CLA  | CBC-CAC-C3C | -3.85 | 101.82      | 112.43   |
| 23  | B     | 617  | CLA  | C1D-CHD-C4C | -3.85 | 117.76      | 126.06   |
| 23  | B     | 613  | CLA  | C3C-C4C-NC  | 3.84  | 114.88      | 110.57   |
| 23  | D     | 2304 | CLA  | C1-C2-C3    | -3.84 | 119.41      | 126.04   |
| 23  | B     | 617  | CLA  | C2C-C1C-NC  | 3.84  | 113.57      | 109.97   |
| 23  | c     | 509  | CLA  | C2C-C1C-NC  | 3.84  | 113.57      | 109.97   |
| 23  | A     | 410  | CLA  | CHD-C1D-ND  | -3.83 | 120.93      | 124.45   |
| 23  | d     | 402  | CLA  | C1D-CHD-C4C | -3.83 | 117.79      | 126.06   |
| 23  | B     | 613  | CLA  | C2C-C1C-NC  | 3.83  | 113.56      | 109.97   |
| 23  | D     | 2303 | CLA  | C3B-C2B-C1B | -3.83 | 102.54      | 107.16   |
| 23  | C     | 503  | CLA  | CHD-C4C-C3C | -3.83 | 119.21      | 124.84   |
| 39  | e     | 103  | HEM  | CBD-CAD-C3D | -3.83 | 101.99      | 112.63   |
| 23  | C     | 509  | CLA  | C3B-C2B-C1B | -3.83 | 102.54      | 107.16   |
| 23  | a     | 2609 | CLA  | CAA-C2A-C3A | -3.83 | 102.30      | 112.78   |
| 23  | C     | 511  | CLA  | C1C-C2C-C3C | -3.82 | 102.94      | 106.96   |
| 28  | B     | 623  | LMT  | C1-O1'-C1'  | -3.82 | 107.50      | 113.84   |
| 23  | c     | 505  | CLA  | C1C-C2C-C3C | -3.82 | 102.94      | 106.96   |
| 23  | b     | 618  | CLA  | C3D-C4D-ND  | 3.82  | 116.42      | 110.24   |
| 23  | a     | 2613 | CLA  | C1-C2-C3    | -3.82 | 119.44      | 126.04   |
| 25  | C     | 516  | BCR  | C33-C5-C6   | -3.81 | 120.25      | 124.53   |
| 23  | C     | 503  | CLA  | C3D-C4D-ND  | 3.81  | 116.40      | 110.24   |
| 36  | V     | 204  | HTG  | O5-C1-C2    | -3.81 | 105.52      | 110.31   |
| 23  | b     | 617  | CLA  | CMC-C2C-C1C | 3.80  | 130.83      | 125.04   |
| 23  | c     | 513  | CLA  | CBC-CAC-C3C | -3.80 | 101.95      | 112.43   |
| 23  | b     | 616  | CLA  | C3D-C4D-ND  | 3.80  | 116.38      | 110.24   |
| 23  | C     | 507  | CLA  | O2D-CGD-CBD | 3.80  | 118.02      | 111.27   |
| 23  | C     | 513  | CLA  | CHD-C4C-C3C | -3.80 | 119.26      | 124.84   |
| 23  | c     | 515  | CLA  | CHD-C4C-C3C | -3.79 | 119.26      | 124.84   |
| 23  | d     | 402  | CLA  | CAA-C2A-C3A | -3.79 | 102.39      | 112.78   |
| 23  | b     | 621  | CLA  | C3B-C4B-NB  | 3.79  | 114.03      | 110.52   |
| 23  | b     | 610  | CLA  | C3D-C4D-ND  | 3.79  | 116.37      | 110.24   |
| 23  | a     | 2609 | CLA  | C1C-C2C-C3C | -3.79 | 102.97      | 106.96   |
| 23  | C     | 502  | CLA  | C3D-C4D-ND  | 3.79  | 116.37      | 110.24   |
| 23  | A     | 405  | CLA  | C3B-C2B-C1B | -3.78 | 102.59      | 107.16   |
| 23  | C     | 511  | CLA  | C3D-C2D-C1D | -3.78 | 100.67      | 105.83   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 608    | CLA  | CHD-C4C-C3C | -3.78 | 119.29      | 124.84   |
| 23  | C     | 505    | CLA  | C3D-C4D-ND  | 3.78  | 116.35      | 110.24   |
| 23  | C     | 509    | CLA  | C2C-C1C-NC  | 3.77  | 113.51      | 109.97   |
| 36  | b     | 625    | HTG  | C1'-S1-C1   | 3.77  | 107.14      | 100.09   |
| 23  | C     | 514    | CLA  | CHD-C4C-C3C | -3.77 | 119.30      | 124.84   |
| 23  | c     | 504    | CLA  | C2C-C1C-NC  | 3.77  | 113.50      | 109.97   |
| 36  | B     | 624[B] | HTG  | C1-O5-C5    | 3.76  | 119.52      | 112.58   |
| 23  | B     | 612    | CLA  | CHD-C1D-ND  | -3.76 | 121.00      | 124.45   |
| 23  | B     | 614    | CLA  | CHD-C1D-ND  | -3.76 | 121.00      | 124.45   |
| 23  | c     | 513    | CLA  | C3D-C2D-C1D | -3.76 | 100.70      | 105.83   |
| 33  | d     | 411    | PL9  | C7-C8-C9    | -3.75 | 120.54      | 126.79   |
| 23  | B     | 607    | CLA  | O2D-CGD-O1D | -3.75 | 116.50      | 123.84   |
| 38  | D     | 2309   | LHG  | O8-C23-C24  | 3.75  | 123.68      | 111.91   |
| 23  | C     | 507    | CLA  | CHD-C4C-C3C | -3.75 | 119.33      | 124.84   |
| 23  | c     | 511    | CLA  | O2D-CGD-O1D | -3.75 | 116.51      | 123.84   |
| 25  | b     | 624    | BCR  | C24-C23-C22 | -3.75 | 120.58      | 126.23   |
| 23  | C     | 505    | CLA  | C3B-C2B-C1B | -3.75 | 102.64      | 107.16   |
| 25  | a     | 2614   | BCR  | C33-C5-C6   | -3.74 | 120.33      | 124.53   |
| 23  | B     | 610    | CLA  | CMB-C2B-C1B | 3.74  | 131.07      | 125.37   |
| 23  | C     | 507    | CLA  | C2C-C1C-NC  | 3.73  | 113.47      | 109.97   |
| 28  | B     | 623    | LMT  | O5B-C5B-C4B | 3.73  | 116.47      | 109.69   |
| 23  | c     | 508    | CLA  | C3D-C4D-ND  | 3.73  | 116.27      | 110.24   |
| 23  | b     | 621    | CLA  | C4C-C3C-C2C | -3.73 | 101.46      | 106.90   |
| 23  | a     | 2609   | CLA  | C1D-CHD-C4C | -3.73 | 118.02      | 126.06   |
| 23  | B     | 605    | CLA  | C1-C2-C3    | -3.73 | 119.60      | 126.04   |
| 23  | B     | 615    | CLA  | C1D-CHD-C4C | -3.72 | 118.03      | 126.06   |
| 23  | b     | 607    | CLA  | C3D-C4D-ND  | 3.72  | 116.25      | 110.24   |
| 23  | D     | 2303   | CLA  | C3C-C4C-NC  | 3.71  | 114.74      | 110.57   |
| 38  | D     | 2309   | LHG  | O7-C7-C8    | 3.71  | 119.50      | 111.50   |
| 25  | b     | 622    | BCR  | C24-C23-C22 | -3.71 | 120.63      | 126.23   |
| 23  | B     | 604    | CLA  | C3D-C4D-ND  | 3.71  | 116.23      | 110.24   |
| 23  | c     | 513    | CLA  | C1C-C2C-C3C | -3.71 | 103.06      | 106.96   |
| 23  | c     | 507    | CLA  | CBC-CAC-C3C | -3.70 | 102.22      | 112.43   |
| 36  | B     | 624[B] | HTG  | O5-C1-C2    | 3.70  | 114.97      | 110.31   |
| 23  | C     | 506    | CLA  | C2C-C1C-NC  | 3.70  | 113.44      | 109.97   |
| 23  | c     | 514    | CLA  | O2D-CGD-CBD | 3.70  | 117.84      | 111.27   |
| 23  | A     | 410    | CLA  | C1-C2-C3    | -3.70 | 119.65      | 126.04   |
| 23  | A     | 410    | CLA  | CHD-C4C-C3C | -3.70 | 119.41      | 124.84   |
| 23  | c     | 506    | CLA  | C2B-C1B-NB  | 3.69  | 112.71      | 110.23   |
| 23  | B     | 609    | CLA  | C1D-CHD-C4C | -3.69 | 118.09      | 126.06   |
| 23  | a     | 2613   | CLA  | C1D-CHD-C4C | -3.69 | 118.09      | 126.06   |
| 23  | c     | 506    | CLA  | C2C-C1C-NC  | 3.69  | 113.43      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | c     | 513  | CLA  | C2C-C1C-NC  | 3.69  | 113.43      | 109.97   |
| 23  | c     | 509  | CLA  | C3B-C2B-C1B | -3.69 | 102.71      | 107.16   |
| 23  | c     | 512  | CLA  | C3D-C4D-ND  | 3.69  | 116.20      | 110.24   |
| 23  | B     | 603  | CLA  | C3D-C4D-ND  | 3.69  | 116.20      | 110.24   |
| 23  | B     | 605  | CLA  | C3D-C4D-ND  | 3.69  | 116.20      | 110.24   |
| 26  | d     | 417  | SQD  | O9-S-C6     | 3.68  | 111.35      | 106.92   |
| 23  | b     | 606  | CLA  | C3D-C4D-ND  | 3.68  | 116.18      | 110.24   |
| 26  | l     | 101  | SQD  | C1-C2-C3    | -3.67 | 102.36      | 110.00   |
| 23  | b     | 617  | CLA  | C2C-C1C-NC  | 3.67  | 113.41      | 109.97   |
| 23  | B     | 608  | CLA  | CBC-CAC-C3C | -3.67 | 102.32      | 112.43   |
| 26  | a     | 2615 | SQD  | O8-S-C6     | 3.67  | 111.58      | 105.74   |
| 23  | b     | 609  | CLA  | CAC-C3C-C4C | 3.66  | 129.56      | 124.81   |
| 23  | c     | 515  | CLA  | C3D-C4D-ND  | 3.66  | 116.16      | 110.24   |
| 23  | c     | 508  | CLA  | CHD-C4C-C3C | -3.66 | 119.46      | 124.84   |
| 31  | a     | 2619 | JOX  | C4-C3-C2    | -3.66 | 120.24      | 123.18   |
| 25  | b     | 622  | BCR  | C33-C5-C6   | -3.66 | 120.42      | 124.53   |
| 26  | a     | 2615 | SQD  | C1-C2-C3    | -3.66 | 102.38      | 110.00   |
| 23  | C     | 511  | CLA  | C4-C3-C5    | 3.66  | 121.42      | 115.27   |
| 23  | B     | 606  | CLA  | C3C-C4C-NC  | 3.66  | 114.67      | 110.57   |
| 23  | B     | 614  | CLA  | C4-C3-C5    | 3.65  | 121.42      | 115.27   |
| 23  | A     | 410  | CLA  | CMA-C3A-C4A | -3.65 | 101.95      | 111.77   |
| 23  | B     | 609  | CLA  | C3C-C4C-NC  | 3.65  | 114.66      | 110.57   |
| 23  | d     | 402  | CLA  | C3B-C4B-NB  | 3.65  | 113.90      | 110.52   |
| 23  | B     | 604  | CLA  | C1C-C2C-C3C | -3.65 | 103.12      | 106.96   |
| 23  | A     | 405  | CLA  | CAA-C2A-C3A | -3.65 | 102.79      | 112.78   |
| 23  | A     | 405  | CLA  | C3C-C4C-NC  | 3.64  | 114.66      | 110.57   |
| 23  | a     | 2610 | CLA  | O2D-CGD-CBD | 3.64  | 117.74      | 111.27   |
| 40  | H     | 102  | RRX  | C24-C23-C22 | -3.64 | 120.74      | 126.23   |
| 23  | b     | 608  | CLA  | C3B-C2B-C1B | -3.64 | 102.77      | 107.16   |
| 23  | b     | 608  | CLA  | C1D-CHD-C4C | -3.63 | 118.22      | 126.06   |
| 23  | C     | 507  | CLA  | C3B-C2B-C1B | -3.63 | 102.77      | 107.16   |
| 23  | B     | 604  | CLA  | C4-C3-C5    | 3.63  | 121.39      | 115.27   |
| 23  | B     | 614  | CLA  | C3D-C4D-ND  | 3.63  | 116.12      | 110.24   |
| 33  | d     | 411  | PL9  | C42-C43-C44 | -3.63 | 118.91      | 127.66   |
| 23  | C     | 514  | CLA  | CHD-C1D-ND  | -3.62 | 121.12      | 124.45   |
| 23  | b     | 607  | CLA  | C2C-C1C-NC  | 3.62  | 113.37      | 109.97   |
| 23  | C     | 502  | CLA  | C1C-C2C-C3C | -3.62 | 103.15      | 106.96   |
| 23  | B     | 612  | CLA  | C2C-C1C-NC  | 3.62  | 113.36      | 109.97   |
| 23  | C     | 506  | CLA  | C3D-C4D-ND  | 3.62  | 116.09      | 110.24   |
| 23  | c     | 505  | CLA  | CHD-C1D-ND  | -3.62 | 121.13      | 124.45   |
| 23  | b     | 613  | CLA  | C2C-C1C-NC  | 3.62  | 113.36      | 109.97   |
| 23  | c     | 509  | CLA  | C1C-C2C-C3C | -3.61 | 103.16      | 106.96   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | c     | 511  | CLA  | C3C-C4C-NC  | 3.61  | 114.62      | 110.57   |
| 23  | c     | 515  | CLA  | C1C-C2C-C3C | -3.61 | 103.16      | 106.96   |
| 27  | c     | 521  | LMG  | O7-C10-C11  | 3.61  | 119.28      | 111.50   |
| 26  | l     | 101  | SQD  | C3-C4-C5    | 3.61  | 116.68      | 110.24   |
| 23  | d     | 409  | CLA  | CHD-C1D-ND  | -3.61 | 121.14      | 124.45   |
| 23  | c     | 514  | CLA  | CBC-CAC-C3C | -3.61 | 102.49      | 112.43   |
| 25  | B     | 633  | BCR  | C15-C14-C13 | 3.60  | 132.45      | 127.31   |
| 25  | B     | 633  | BCR  | C15-C16-C17 | -3.60 | 116.11      | 123.47   |
| 23  | C     | 502  | CLA  | C3B-C2B-C1B | -3.59 | 102.82      | 107.16   |
| 23  | c     | 510  | CLA  | O2D-CGD-O1D | -3.59 | 116.81      | 123.84   |
| 23  | B     | 616  | CLA  | C1C-C2C-C3C | -3.59 | 103.18      | 106.96   |
| 33  | D     | 2306 | PL9  | C40-C39-C41 | 3.59  | 121.31      | 115.27   |
| 23  | c     | 508  | CLA  | C1C-C2C-C3C | -3.59 | 103.18      | 106.96   |
| 23  | b     | 613  | CLA  | C1C-C2C-C3C | -3.59 | 103.19      | 106.96   |
| 27  | B     | 622  | LMG  | O7-C10-C11  | 3.59  | 119.23      | 111.50   |
| 23  | C     | 505  | CLA  | C1D-CHD-C4C | -3.58 | 118.33      | 126.06   |
| 23  | c     | 506  | CLA  | CHD-C4C-C3C | -3.58 | 119.57      | 124.84   |
| 23  | C     | 513  | CLA  | C3D-C4D-ND  | 3.58  | 116.03      | 110.24   |
| 23  | b     | 610  | CLA  | C3C-C4C-NC  | 3.58  | 114.59      | 110.57   |
| 23  | b     | 612  | CLA  | C3D-C4D-ND  | 3.58  | 116.03      | 110.24   |
| 23  | B     | 608  | CLA  | C3D-C4D-ND  | 3.58  | 116.02      | 110.24   |
| 23  | A     | 405  | CLA  | C1C-C2C-C3C | -3.57 | 103.20      | 106.96   |
| 23  | B     | 617  | CLA  | C4-C3-C5    | 3.57  | 121.27      | 115.27   |
| 23  | B     | 610  | CLA  | C1D-CHD-C4C | -3.57 | 118.36      | 126.06   |
| 23  | B     | 610  | CLA  | C2C-C1C-NC  | 3.57  | 113.31      | 109.97   |
| 23  | B     | 602  | CLA  | C3D-C4D-ND  | 3.56  | 116.00      | 110.24   |
| 23  | b     | 614  | CLA  | C1C-C2C-C3C | -3.56 | 103.21      | 106.96   |
| 23  | C     | 504  | CLA  | C1-C2-C3    | -3.56 | 119.88      | 126.04   |
| 23  | c     | 506  | CLA  | CHD-C1D-ND  | -3.56 | 121.18      | 124.45   |
| 26  | D     | 2308 | SQD  | O7-S-C6     | 3.56  | 111.17      | 106.94   |
| 23  | A     | 405  | CLA  | O2D-CGD-CBD | 3.56  | 117.59      | 111.27   |
| 23  | B     | 610  | CLA  | C1-C2-C3    | -3.56 | 119.89      | 126.04   |
| 23  | c     | 511  | CLA  | CHD-C4C-C3C | -3.56 | 119.61      | 124.84   |
| 23  | B     | 615  | CLA  | C1C-C2C-C3C | -3.55 | 103.22      | 106.96   |
| 23  | c     | 510  | CLA  | C3D-C4D-ND  | 3.55  | 115.98      | 110.24   |
| 24  | a     | 2612 | PHO  | C4D-CHA-CBD | 3.55  | 110.12      | 108.52   |
| 23  | B     | 611  | CLA  | C4C-C3C-C2C | -3.55 | 101.73      | 106.90   |
| 23  | B     | 611  | CLA  | O2D-CGD-O1D | -3.54 | 116.92      | 123.84   |
| 23  | b     | 611  | CLA  | C1C-C2C-C3C | -3.54 | 103.24      | 106.96   |
| 23  | c     | 510  | CLA  | CHC-C4B-NB  | 3.54  | 128.00      | 124.26   |
| 25  | T     | 102  | BCR  | C35-C13-C12 | 3.54  | 123.65      | 118.08   |
| 23  | B     | 612  | CLA  | C3D-C4D-ND  | 3.53  | 115.95      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 38  | L     | 101  | LHG  | O8-C23-C24  | 3.53  | 122.98      | 111.91   |
| 23  | B     | 605  | CLA  | C1D-CHD-C4C | -3.53 | 118.45      | 126.06   |
| 23  | c     | 514  | CLA  | C1-O2A-CGA  | 3.53  | 125.70      | 116.44   |
| 23  | b     | 613  | CLA  | CHD-C1D-ND  | -3.53 | 121.21      | 124.45   |
| 23  | c     | 507  | CLA  | C1D-CHD-C4C | -3.52 | 118.45      | 126.06   |
| 31  | a     | 2619 | JOX  | C1-C2-C3    | 3.52  | 117.38      | 114.18   |
| 23  | c     | 512  | CLA  | C1-C2-C3    | -3.52 | 119.95      | 126.04   |
| 23  | C     | 511  | CLA  | CHD-C4C-C3C | -3.52 | 119.67      | 124.84   |
| 23  | c     | 515  | CLA  | CBC-CAC-C3C | -3.52 | 102.73      | 112.43   |
| 23  | b     | 620  | CLA  | C3D-C4D-ND  | 3.52  | 115.93      | 110.24   |
| 23  | C     | 504  | CLA  | C3D-C4D-ND  | 3.52  | 115.92      | 110.24   |
| 23  | b     | 610  | CLA  | C1D-CHD-C4C | -3.52 | 118.47      | 126.06   |
| 23  | d     | 402  | CLA  | CHD-C1D-ND  | -3.51 | 121.22      | 124.45   |
| 23  | c     | 504  | CLA  | CBC-CAC-C3C | -3.51 | 102.74      | 112.43   |
| 23  | C     | 514  | CLA  | C1C-C2C-C3C | -3.51 | 103.26      | 106.96   |
| 23  | C     | 509  | CLA  | O2D-CGD-O1D | -3.51 | 116.98      | 123.84   |
| 23  | C     | 512  | CLA  | C1C-C2C-C3C | -3.51 | 103.27      | 106.96   |
| 23  | B     | 606  | CLA  | C1D-CHD-C4C | -3.51 | 118.49      | 126.06   |
| 23  | C     | 508  | CLA  | CHC-C4B-NB  | 3.51  | 127.97      | 124.26   |
| 23  | b     | 606  | CLA  | C1C-C2C-C3C | -3.50 | 103.27      | 106.96   |
| 23  | B     | 616  | CLA  | O2D-CGD-O1D | -3.50 | 116.99      | 123.84   |
| 26  | B     | 621  | SQD  | C1-O5-C5    | 3.50  | 120.56      | 113.69   |
| 23  | b     | 611  | CLA  | C3D-C4D-ND  | 3.50  | 115.90      | 110.24   |
| 23  | b     | 618  | CLA  | O2D-CGD-CBD | 3.50  | 117.48      | 111.27   |
| 23  | B     | 616  | CLA  | C3D-C4D-ND  | 3.50  | 115.90      | 110.24   |
| 23  | C     | 512  | CLA  | C3D-C4D-ND  | 3.50  | 115.90      | 110.24   |
| 23  | b     | 611  | CLA  | C1D-CHD-C4C | -3.50 | 118.52      | 126.06   |
| 23  | B     | 603  | CLA  | C1D-CHD-C4C | -3.49 | 118.52      | 126.06   |
| 23  | b     | 608  | CLA  | C4-C3-C5    | 3.49  | 121.15      | 115.27   |
| 23  | C     | 511  | CLA  | C3B-C2B-C1B | -3.49 | 102.94      | 107.16   |
| 23  | C     | 502  | CLA  | CMB-C2B-C1B | 3.49  | 130.69      | 125.37   |
| 23  | c     | 512  | CLA  | C1D-CHD-C4C | -3.49 | 118.53      | 126.06   |
| 25  | D     | 2305 | BCR  | C33-C5-C6   | -3.49 | 120.61      | 124.53   |
| 23  | B     | 617  | CLA  | CHD-C4C-C3C | -3.49 | 119.72      | 124.84   |
| 23  | C     | 509  | CLA  | C1C-C2C-C3C | -3.49 | 103.29      | 106.96   |
| 23  | B     | 613  | CLA  | CHD-C1D-ND  | -3.49 | 121.25      | 124.45   |
| 23  | C     | 509  | CLA  | CHD-C1D-ND  | -3.48 | 121.25      | 124.45   |
| 37  | C     | 517  | DGD  | O2G-C1B-C2B | 3.48  | 119.01      | 111.50   |
| 26  | B     | 621  | SQD  | C3-C4-C5    | 3.48  | 116.45      | 110.24   |
| 23  | B     | 602  | CLA  | C1C-C2C-C3C | -3.48 | 103.30      | 106.96   |
| 23  | a     | 2610 | CLA  | C1C-C2C-C3C | -3.48 | 103.30      | 106.96   |
| 23  | B     | 610  | CLA  | C3B-C2B-C1B | -3.48 | 102.96      | 107.16   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | B     | 617  | CLA  | CBC-CAC-C3C | -3.48 | 102.84      | 112.43   |
| 26  | a     | 2603 | SQD  | O7-S-C6     | 3.48  | 111.07      | 106.94   |
| 36  | b     | 625  | HTG  | C6-C5-C4    | -3.48 | 104.86      | 113.00   |
| 23  | d     | 408  | CLA  | C3C-C4C-NC  | 3.48  | 114.47      | 110.57   |
| 23  | b     | 617  | CLA  | C1C-C2C-C3C | -3.47 | 103.30      | 106.96   |
| 23  | b     | 617  | CLA  | C1D-CHD-C4C | -3.47 | 118.57      | 126.06   |
| 23  | c     | 509  | CLA  | C16-C15-C13 | -3.47 | 104.70      | 115.92   |
| 23  | C     | 506  | CLA  | C1D-CHD-C4C | -3.47 | 118.57      | 126.06   |
| 25  | C     | 515  | BCR  | C33-C5-C6   | -3.47 | 120.63      | 124.53   |
| 23  | c     | 510  | CLA  | C4A-NA-C1A  | 3.47  | 108.27      | 106.71   |
| 23  | c     | 506  | CLA  | C1C-C2C-C3C | -3.47 | 103.31      | 106.96   |
| 23  | B     | 611  | CLA  | CHD-C1D-ND  | -3.47 | 121.27      | 124.45   |
| 23  | C     | 512  | CLA  | C4A-NA-C1A  | 3.47  | 108.26      | 106.71   |
| 23  | C     | 510  | CLA  | C1-C2-C3    | -3.46 | 120.05      | 126.04   |
| 23  | B     | 603  | CLA  | O2D-CGD-O1D | -3.46 | 117.07      | 123.84   |
| 23  | C     | 509  | CLA  | CHD-C4C-C3C | -3.46 | 119.76      | 124.84   |
| 36  | C     | 521  | HTG  | C1'-S1-C1   | 3.46  | 106.56      | 100.09   |
| 23  | B     | 613  | CLA  | C1C-C2C-C3C | -3.46 | 103.32      | 106.96   |
| 23  | b     | 615  | CLA  | C3D-C4D-ND  | 3.46  | 115.83      | 110.24   |
| 23  | C     | 510  | CLA  | C3D-C4D-ND  | 3.45  | 115.82      | 110.24   |
| 23  | b     | 619  | CLA  | C1D-CHD-C4C | -3.45 | 118.62      | 126.06   |
| 23  | b     | 614  | CLA  | CBC-CAC-C3C | -3.45 | 102.92      | 112.43   |
| 23  | B     | 612  | CLA  | O2D-CGD-O1D | -3.45 | 117.10      | 123.84   |
| 23  | b     | 619  | CLA  | CHD-C1D-ND  | -3.45 | 121.29      | 124.45   |
| 23  | A     | 410  | CLA  | CBC-CAC-C3C | -3.45 | 102.93      | 112.43   |
| 23  | C     | 511  | CLA  | C1-C2-C3    | -3.44 | 120.09      | 126.04   |
| 37  | h     | 102  | DGD  | O2G-C1B-C2B | 3.44  | 118.92      | 111.50   |
| 23  | C     | 504  | CLA  | C1C-C2C-C3C | -3.44 | 103.34      | 106.96   |
| 23  | b     | 619  | CLA  | CAC-C3C-C4C | 3.44  | 129.27      | 124.81   |
| 23  | B     | 614  | CLA  | C3C-C4C-NC  | 3.44  | 114.43      | 110.57   |
| 36  | i     | 102  | HTG  | C3-C4-C5    | 3.44  | 116.38      | 110.24   |
| 23  | c     | 512  | CLA  | CHD-C4C-C3C | -3.44 | 119.78      | 124.84   |
| 23  | b     | 613  | CLA  | C1-C2-C3    | -3.44 | 120.09      | 126.04   |
| 23  | b     | 620  | CLA  | C1D-CHD-C4C | -3.44 | 118.64      | 126.06   |
| 23  | c     | 512  | CLA  | C1C-C2C-C3C | -3.44 | 103.34      | 106.96   |
| 27  | C     | 520  | LMG  | O8-C28-C29  | 3.44  | 122.70      | 111.91   |
| 23  | C     | 510  | CLA  | CHD-C4C-C3C | -3.44 | 119.79      | 124.84   |
| 23  | B     | 613  | CLA  | CMC-C2C-C1C | 3.44  | 130.27      | 125.04   |
| 23  | C     | 508  | CLA  | O2D-CGD-O1D | -3.44 | 117.12      | 123.84   |
| 37  | D     | 2307 | DGD  | O1G-C1A-C2A | 3.43  | 122.68      | 111.91   |
| 23  | b     | 611  | CLA  | C3C-C4C-NC  | 3.43  | 114.42      | 110.57   |
| 33  | A     | 422  | PL9  | C32-C31-C29 | -3.43 | 101.69      | 112.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | C     | 507  | CLA  | CHD-C1D-ND  | -3.43 | 121.30      | 124.45   |
| 38  | D     | 2309 | LHG  | O8-C23-O10  | -3.43 | 114.94      | 123.59   |
| 39  | e     | 103  | HEM  | C4C-NC-C1C  | 3.43  | 108.71      | 105.35   |
| 23  | b     | 615  | CLA  | C1D-CHD-C4C | -3.43 | 118.67      | 126.06   |
| 23  | c     | 516  | CLA  | C1D-CHD-C4C | -3.43 | 118.67      | 126.06   |
| 23  | B     | 604  | CLA  | CHD-C4C-C3C | -3.42 | 119.81      | 124.84   |
| 25  | B     | 618  | BCR  | C7-C8-C9    | -3.42 | 121.07      | 126.23   |
| 23  | B     | 611  | CLA  | C2C-C1C-NC  | 3.42  | 113.17      | 109.97   |
| 23  | a     | 2609 | CLA  | C3C-C4C-NC  | 3.42  | 114.41      | 110.57   |
| 23  | c     | 516  | CLA  | CHD-C1D-ND  | -3.42 | 121.31      | 124.45   |
| 23  | A     | 406  | CLA  | C1D-CHD-C4C | -3.41 | 118.70      | 126.06   |
| 23  | b     | 614  | CLA  | C2C-C1C-NC  | 3.41  | 113.17      | 109.97   |
| 25  | c     | 517  | BCR  | C38-C26-C25 | -3.41 | 120.70      | 124.53   |
| 25  | C     | 515  | BCR  | C11-C10-C9  | -3.41 | 122.45      | 127.31   |
| 23  | a     | 2613 | CLA  | C3B-C4B-NB  | 3.41  | 113.67      | 110.52   |
| 23  | b     | 621  | CLA  | C3D-C4D-ND  | 3.40  | 115.75      | 110.24   |
| 23  | b     | 612  | CLA  | C3C-C4C-NC  | 3.40  | 114.39      | 110.57   |
| 23  | c     | 513  | CLA  | C1D-CHD-C4C | -3.40 | 118.72      | 126.06   |
| 23  | c     | 512  | CLA  | CAC-C3C-C4C | 3.40  | 129.23      | 124.81   |
| 23  | D     | 2304 | CLA  | C1C-C2C-C3C | -3.40 | 103.38      | 106.96   |
| 23  | b     | 609  | CLA  | C1D-CHD-C4C | -3.40 | 118.72      | 126.06   |
| 23  | B     | 606  | CLA  | O2D-CGD-CBD | 3.40  | 117.31      | 111.27   |
| 24  | a     | 2612 | PHO  | O2D-CGD-O1D | -3.40 | 117.19      | 123.84   |
| 23  | C     | 511  | CLA  | C2C-C1C-NC  | 3.40  | 113.16      | 109.97   |
| 23  | b     | 614  | CLA  | CHD-C4C-C3C | -3.40 | 119.85      | 124.84   |
| 23  | b     | 615  | CLA  | CHD-C1D-ND  | -3.40 | 121.33      | 124.45   |
| 25  | z     | 101  | BCR  | C16-C17-C18 | -3.39 | 122.47      | 127.31   |
| 23  | c     | 511  | CLA  | C1D-CHD-C4C | -3.39 | 118.74      | 126.06   |
| 23  | B     | 617  | CLA  | C3D-C4D-ND  | 3.39  | 115.72      | 110.24   |
| 25  | A     | 411  | BCR  | C33-C5-C6   | -3.39 | 120.72      | 124.53   |
| 23  | C     | 505  | CLA  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 23  | B     | 617  | CLA  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 38  | d     | 412  | LHG  | O8-C23-C24  | 3.39  | 122.54      | 111.91   |
| 23  | B     | 611  | CLA  | C1D-CHD-C4C | -3.39 | 118.75      | 126.06   |
| 23  | b     | 608  | CLA  | O2A-CGA-O1A | -3.39 | 115.04      | 123.59   |
| 23  | A     | 406  | CLA  | C3B-C4B-NB  | 3.39  | 113.66      | 110.52   |
| 23  | b     | 619  | CLA  | C1C-C2C-C3C | -3.39 | 103.40      | 106.96   |
| 23  | b     | 610  | CLA  | C4-C3-C5    | 3.39  | 120.97      | 115.27   |
| 23  | c     | 505  | CLA  | C2C-C1C-NC  | 3.39  | 113.14      | 109.97   |
| 28  | z     | 102  | LMT  | O1B-C1B-C2B | 3.39  | 116.87      | 108.10   |
| 24  | a     | 2612 | PHO  | CMB-C2B-C3B | 3.38  | 131.01      | 124.68   |
| 23  | c     | 512  | CLA  | O2D-CGD-O1D | -3.38 | 117.22      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | C     | 527  | LMG  | O8-C28-C29  | 3.38  | 122.52      | 111.91   |
| 23  | B     | 612  | CLA  | C1C-C2C-C3C | -3.38 | 103.41      | 106.96   |
| 40  | H     | 102  | RRX  | C10-C11-C12 | -3.38 | 112.68      | 123.22   |
| 23  | c     | 515  | CLA  | C2C-C1C-NC  | 3.38  | 113.14      | 109.97   |
| 23  | b     | 618  | CLA  | CHD-C1D-ND  | -3.38 | 121.35      | 124.45   |
| 23  | C     | 506  | CLA  | CAC-C3C-C4C | 3.37  | 129.19      | 124.81   |
| 23  | c     | 508  | CLA  | C4C-C3C-C2C | -3.37 | 101.98      | 106.90   |
| 23  | C     | 503  | CLA  | C1C-C2C-C3C | -3.37 | 103.41      | 106.96   |
| 23  | B     | 617  | CLA  | C1C-C2C-C3C | -3.37 | 103.41      | 106.96   |
| 23  | b     | 606  | CLA  | O2D-CGD-O1D | -3.37 | 117.25      | 123.84   |
| 26  | b     | 601  | SQD  | O5-C5-C4    | 3.37  | 115.81      | 109.69   |
| 23  | b     | 615  | CLA  | C3C-C4C-NC  | 3.37  | 114.35      | 110.57   |
| 26  | l     | 101  | SQD  | O7-S-C6     | 3.37  | 110.94      | 106.94   |
| 27  | C     | 527  | LMG  | O6-C5-C4    | 3.36  | 115.80      | 109.69   |
| 23  | B     | 605  | CLA  | CHD-C4C-C3C | -3.36 | 119.90      | 124.84   |
| 23  | b     | 618  | CLA  | C1-C2-C3    | -3.36 | 120.23      | 126.04   |
| 23  | B     | 608  | CLA  | CAC-C3C-C4C | 3.36  | 129.17      | 124.81   |
| 23  | b     | 619  | CLA  | CHD-C4C-C3C | -3.36 | 119.91      | 124.84   |
| 23  | b     | 610  | CLA  | CHD-C1D-ND  | -3.35 | 121.37      | 124.45   |
| 23  | c     | 510  | CLA  | CMB-C2B-C1B | 3.35  | 130.48      | 125.37   |
| 23  | C     | 504  | CLA  | C4A-NA-C1A  | 3.35  | 108.21      | 106.71   |
| 23  | a     | 2610 | CLA  | C2C-C1C-NC  | 3.35  | 113.11      | 109.97   |
| 23  | c     | 515  | CLA  | CBA-CAA-C2A | -3.35 | 103.97      | 113.86   |
| 23  | C     | 507  | CLA  | C1D-CHD-C4C | -3.35 | 118.83      | 126.06   |
| 23  | c     | 508  | CLA  | C1D-CHD-C4C | -3.35 | 118.83      | 126.06   |
| 23  | B     | 604  | CLA  | CMB-C2B-C1B | 3.35  | 130.47      | 125.37   |
| 23  | b     | 611  | CLA  | C2C-C1C-NC  | 3.35  | 113.11      | 109.97   |
| 23  | B     | 612  | CLA  | CHD-C4C-C3C | -3.35 | 119.92      | 124.84   |
| 23  | b     | 607  | CLA  | C4C-C3C-C2C | -3.35 | 102.02      | 106.90   |
| 23  | b     | 607  | CLA  | CAC-C3C-C4C | 3.34  | 129.15      | 124.81   |
| 23  | C     | 513  | CLA  | C1D-CHD-C4C | -3.34 | 118.84      | 126.06   |
| 23  | b     | 618  | CLA  | CHD-C4C-C3C | -3.34 | 119.93      | 124.84   |
| 23  | C     | 504  | CLA  | C1D-CHD-C4C | -3.34 | 118.85      | 126.06   |
| 23  | B     | 606  | CLA  | C4C-C3C-C2C | -3.34 | 102.03      | 106.90   |
| 23  | C     | 505  | CLA  | CHD-C4C-C3C | -3.34 | 119.93      | 124.84   |
| 23  | a     | 2609 | CLA  | CHD-C4C-C3C | -3.34 | 119.93      | 124.84   |
| 23  | B     | 616  | CLA  | C3C-C4C-NC  | 3.34  | 114.31      | 110.57   |
| 23  | b     | 616  | CLA  | C1D-CHD-C4C | -3.34 | 118.86      | 126.06   |
| 23  | C     | 503  | CLA  | C2C-C1C-NC  | 3.33  | 113.10      | 109.97   |
| 23  | B     | 607  | CLA  | C3D-C4D-ND  | 3.33  | 115.63      | 110.24   |
| 23  | A     | 407  | CLA  | CMB-C2B-C1B | 3.33  | 130.44      | 125.37   |
| 23  | B     | 611  | CLA  | C3C-C4C-NC  | 3.33  | 114.31      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | C     | 512  | CLA  | C1D-CHD-C4C | -3.33 | 118.88      | 126.06   |
| 23  | A     | 410  | CLA  | C4-C3-C5    | 3.33  | 120.87      | 115.27   |
| 23  | c     | 509  | CLA  | CBC-CAC-C3C | -3.33 | 103.26      | 112.43   |
| 23  | b     | 609  | CLA  | CMB-C2B-C1B | 3.33  | 130.43      | 125.37   |
| 23  | b     | 620  | CLA  | CHD-C4C-C3C | -3.32 | 119.95      | 124.84   |
| 23  | B     | 606  | CLA  | O2D-CGD-O1D | -3.32 | 117.34      | 123.84   |
| 23  | c     | 505  | CLA  | O2D-CGD-O1D | -3.32 | 117.35      | 123.84   |
| 23  | c     | 511  | CLA  | C4C-C3C-C2C | -3.32 | 102.06      | 106.90   |
| 24  | A     | 409  | PHO  | C4-C3-C5    | 3.32  | 120.85      | 115.27   |
| 25  | K     | 101  | BCR  | C24-C23-C22 | -3.32 | 121.22      | 126.23   |
| 23  | C     | 506  | CLA  | C4C-C3C-C2C | -3.32 | 102.06      | 106.90   |
| 28  | M     | 101  | LMT  | C1'-O5'-C5' | 3.31  | 120.19      | 113.69   |
| 25  | B     | 633  | BCR  | C11-C10-C9  | -3.31 | 122.58      | 127.31   |
| 23  | B     | 613  | CLA  | C3B-C4B-NB  | 3.31  | 113.59      | 110.52   |
| 23  | C     | 512  | CLA  | C3B-C4B-NB  | 3.31  | 113.59      | 110.52   |
| 23  | b     | 608  | CLA  | C3C-C4C-NC  | 3.31  | 114.28      | 110.57   |
| 23  | c     | 516  | CLA  | C1-C2-C3    | -3.31 | 120.32      | 126.04   |
| 23  | c     | 506  | CLA  | C3D-C4D-ND  | 3.31  | 115.59      | 110.24   |
| 23  | c     | 512  | CLA  | C3C-C4C-NC  | 3.31  | 114.28      | 110.57   |
| 36  | V     | 204  | HTG  | C1-C2-C3    | -3.30 | 104.07      | 110.59   |
| 23  | c     | 509  | CLA  | O2D-CGD-O1D | -3.30 | 117.39      | 123.84   |
| 23  | c     | 516  | CLA  | CHD-C4C-C3C | -3.30 | 119.99      | 124.84   |
| 23  | C     | 508  | CLA  | C1D-CHD-C4C | -3.30 | 118.94      | 126.06   |
| 23  | a     | 2613 | CLA  | CMA-C3A-C2A | -3.30 | 100.53      | 113.83   |
| 23  | C     | 508  | CLA  | C3C-C4C-NC  | 3.29  | 114.27      | 110.57   |
| 23  | A     | 407  | CLA  | CBC-CAC-C3C | -3.29 | 103.35      | 112.43   |
| 23  | c     | 510  | CLA  | C3C-C4C-NC  | 3.29  | 114.26      | 110.57   |
| 23  | C     | 509  | CLA  | C1-C2-C3    | -3.29 | 120.35      | 126.04   |
| 23  | c     | 514  | CLA  | C4-C3-C5    | 3.29  | 120.80      | 115.27   |
| 23  | C     | 514  | CLA  | C1D-CHD-C4C | -3.29 | 118.97      | 126.06   |
| 23  | b     | 614  | CLA  | CMB-C2B-C1B | 3.29  | 130.37      | 125.37   |
| 23  | b     | 615  | CLA  | O2D-CGD-CBD | 3.29  | 117.11      | 111.27   |
| 40  | H     | 102  | RRX  | C38-C26-C25 | -3.29 | 120.84      | 124.53   |
| 23  | B     | 610  | CLA  | C4C-C3C-C2C | -3.28 | 102.11      | 106.90   |
| 23  | d     | 409  | CLA  | O2D-CGD-O1D | -3.28 | 117.42      | 123.84   |
| 23  | a     | 2613 | CLA  | C4-C3-C5    | 3.28  | 120.79      | 115.27   |
| 25  | B     | 633  | BCR  | C12-C13-C14 | -3.28 | 113.91      | 118.94   |
| 23  | C     | 507  | CLA  | CBC-CAC-C3C | -3.28 | 103.39      | 112.43   |
| 23  | A     | 407  | CLA  | C4-C3-C5    | 3.27  | 120.78      | 115.27   |
| 23  | c     | 506  | CLA  | C3C-C4C-NC  | 3.27  | 114.24      | 110.57   |
| 23  | b     | 608  | CLA  | O2D-CGD-O1D | -3.27 | 117.45      | 123.84   |
| 23  | A     | 410  | CLA  | C1D-CHD-C4C | -3.27 | 119.01      | 126.06   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | C     | 511  | CLA  | C3B-C4B-NB  | 3.26  | 113.54      | 110.52   |
| 23  | B     | 616  | CLA  | C3B-C4B-NB  | 3.26  | 113.54      | 110.52   |
| 23  | B     | 607  | CLA  | C2C-C1C-NC  | 3.26  | 113.03      | 109.97   |
| 23  | D     | 2303 | CLA  | O2A-CGA-CBA | 3.26  | 122.14      | 111.91   |
| 23  | d     | 402  | CLA  | C3C-C4C-NC  | 3.26  | 114.23      | 110.57   |
| 23  | c     | 513  | CLA  | CHD-C4C-C3C | -3.26 | 120.05      | 124.84   |
| 23  | c     | 509  | CLA  | C1D-CHD-C4C | -3.26 | 119.03      | 126.06   |
| 23  | b     | 617  | CLA  | C4C-C3C-C2C | -3.26 | 102.15      | 106.90   |
| 33  | D     | 2306 | PL9  | C7-C8-C9    | -3.26 | 121.37      | 126.79   |
| 23  | B     | 604  | CLA  | C2C-C1C-NC  | 3.26  | 113.02      | 109.97   |
| 23  | C     | 505  | CLA  | CBC-CAC-C3C | -3.25 | 103.46      | 112.43   |
| 23  | c     | 516  | CLA  | C1C-C2C-C3C | -3.25 | 103.54      | 106.96   |
| 42  | V     | 201  | HEC  | CBD-CAD-C3D | -3.25 | 103.60      | 112.63   |
| 33  | A     | 422  | PL9  | C17-C18-C19 | -3.25 | 119.84      | 127.66   |
| 33  | d     | 411  | PL9  | C37-C38-C39 | -3.25 | 119.84      | 127.66   |
| 23  | A     | 407  | CLA  | CAA-C2A-C3A | -3.25 | 103.89      | 112.78   |
| 23  | A     | 405  | CLA  | CAA-C2A-C1A | -3.25 | 101.33      | 111.97   |
| 23  | B     | 607  | CLA  | C3C-C4C-NC  | 3.25  | 114.21      | 110.57   |
| 25  | c     | 517  | BCR  | C15-C14-C13 | -3.25 | 122.68      | 127.31   |
| 23  | b     | 619  | CLA  | C3C-C4C-NC  | 3.24  | 114.21      | 110.57   |
| 25  | y     | 101  | BCR  | C38-C26-C25 | -3.24 | 120.89      | 124.53   |
| 23  | B     | 607  | CLA  | C1D-CHD-C4C | -3.24 | 119.06      | 126.06   |
| 23  | B     | 606  | CLA  | O2A-CGA-CBA | 3.24  | 122.08      | 111.91   |
| 23  | d     | 409  | CLA  | C4-C3-C5    | 3.24  | 120.72      | 115.27   |
| 23  | C     | 504  | CLA  | CMC-C2C-C1C | 3.24  | 129.97      | 125.04   |
| 23  | c     | 515  | CLA  | CMB-C2B-C1B | 3.24  | 130.30      | 125.37   |
| 38  | d     | 412  | LHG  | O8-C23-O10  | -3.24 | 115.43      | 123.59   |
| 23  | B     | 610  | CLA  | C1C-C2C-C3C | -3.23 | 103.56      | 106.96   |
| 23  | b     | 615  | CLA  | C4C-C3C-C2C | -3.23 | 102.19      | 106.90   |
| 23  | b     | 612  | CLA  | CMC-C2C-C1C | 3.23  | 129.96      | 125.04   |
| 23  | B     | 609  | CLA  | C4C-C3C-C2C | -3.23 | 102.19      | 106.90   |
| 23  | B     | 606  | CLA  | CHD-C1D-ND  | -3.23 | 121.49      | 124.45   |
| 23  | C     | 510  | CLA  | C1D-CHD-C4C | -3.23 | 119.09      | 126.06   |
| 23  | C     | 503  | CLA  | CHD-C1D-ND  | -3.23 | 121.49      | 124.45   |
| 23  | c     | 505  | CLA  | C1D-CHD-C4C | -3.23 | 119.09      | 126.06   |
| 23  | B     | 606  | CLA  | CAC-C3C-C4C | 3.23  | 129.00      | 124.81   |
| 23  | c     | 508  | CLA  | CMB-C2B-C1B | 3.22  | 130.28      | 125.37   |
| 23  | B     | 604  | CLA  | C3C-C4C-NC  | 3.22  | 114.19      | 110.57   |
| 23  | d     | 408  | CLA  | C3B-C4B-NB  | 3.22  | 113.50      | 110.52   |
| 31  | A     | 418  | JOX  | O1-C5-C4    | -3.21 | 116.81      | 121.41   |
| 23  | a     | 2609 | CLA  | CAA-C2A-C1A | -3.21 | 101.44      | 111.97   |
| 23  | c     | 514  | CLA  | C1D-CHD-C4C | -3.21 | 119.13      | 126.06   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | b     | 615  | CLA  | C2C-C1C-NC  | 3.21  | 112.98      | 109.97   |
| 23  | c     | 510  | CLA  | CHD-C4C-C3C | -3.21 | 120.12      | 124.84   |
| 23  | b     | 613  | CLA  | CHD-C4C-C3C | -3.20 | 120.13      | 124.84   |
| 23  | b     | 608  | CLA  | O2A-CGA-CBA | 3.20  | 121.96      | 111.91   |
| 23  | c     | 516  | CLA  | C2C-C1C-NC  | 3.20  | 112.97      | 109.97   |
| 23  | B     | 616  | CLA  | CBC-CAC-C3C | -3.20 | 103.60      | 112.43   |
| 27  | c     | 521  | LMG  | O8-C28-C29  | 3.20  | 121.96      | 111.91   |
| 23  | B     | 602  | CLA  | O2D-CGD-O1D | -3.20 | 117.58      | 123.84   |
| 23  | C     | 503  | CLA  | C1D-CHD-C4C | -3.20 | 119.16      | 126.06   |
| 23  | B     | 608  | CLA  | C1D-CHD-C4C | -3.20 | 119.16      | 126.06   |
| 23  | B     | 602  | CLA  | O2A-CGA-CBA | 3.20  | 121.94      | 111.91   |
| 23  | B     | 610  | CLA  | C3C-C4C-NC  | 3.20  | 114.16      | 110.57   |
| 23  | C     | 510  | CLA  | C3C-C4C-NC  | 3.19  | 114.15      | 110.57   |
| 23  | B     | 613  | CLA  | C4C-C3C-C2C | -3.19 | 102.24      | 106.90   |
| 33  | A     | 422  | PL9  | C12-C13-C14 | -3.19 | 119.97      | 127.66   |
| 23  | b     | 612  | CLA  | C1D-CHD-C4C | -3.19 | 119.17      | 126.06   |
| 25  | B     | 633  | BCR  | C7-C8-C9    | -3.19 | 121.41      | 126.23   |
| 23  | B     | 603  | CLA  | CHD-C1D-ND  | -3.19 | 121.52      | 124.45   |
| 23  | A     | 406  | CLA  | CAA-C2A-C3A | -3.19 | 104.05      | 112.78   |
| 25  | b     | 624  | BCR  | C15-C14-C13 | -3.19 | 122.76      | 127.31   |
| 23  | B     | 607  | CLA  | CAC-C3C-C4C | 3.19  | 128.94      | 124.81   |
| 23  | b     | 609  | CLA  | CHC-C4B-NB  | 3.19  | 127.63      | 124.26   |
| 23  | b     | 610  | CLA  | CMC-C2C-C1C | 3.19  | 129.89      | 125.04   |
| 25  | A     | 411  | BCR  | C38-C26-C25 | -3.18 | 120.95      | 124.53   |
| 23  | c     | 510  | CLA  | C1-C2-C3    | -3.18 | 120.54      | 126.04   |
| 40  | H     | 102  | RRX  | C16-C17-C18 | -3.18 | 122.77      | 127.31   |
| 24  | a     | 2612 | PHO  | C1A-C2A-C3A | -3.18 | 99.81       | 102.84   |
| 23  | c     | 506  | CLA  | C1D-CHD-C4C | -3.18 | 119.20      | 126.06   |
| 37  | c     | 519  | DGD  | O1G-C1A-C2A | 3.18  | 121.88      | 111.91   |
| 23  | b     | 609  | CLA  | C3C-C4C-NC  | 3.18  | 114.13      | 110.57   |
| 23  | b     | 606  | CLA  | C2C-C1C-NC  | 3.18  | 112.95      | 109.97   |
| 23  | b     | 613  | CLA  | O2A-CGA-CBA | 3.18  | 121.88      | 111.91   |
| 23  | C     | 504  | CLA  | C3C-C4C-NC  | 3.17  | 114.13      | 110.57   |
| 33  | d     | 411  | PL9  | C40-C39-C41 | 3.17  | 120.61      | 115.27   |
| 23  | C     | 511  | CLA  | CHD-C1D-ND  | -3.17 | 121.54      | 124.45   |
| 25  | b     | 622  | BCR  | C7-C8-C9    | -3.16 | 121.45      | 126.23   |
| 33  | x     | 1301 | PL9  | C12-C13-C14 | -3.16 | 120.04      | 127.66   |
| 23  | C     | 509  | CLA  | C3C-C4C-NC  | 3.16  | 114.12      | 110.57   |
| 23  | b     | 607  | CLA  | CHD-C1D-ND  | -3.16 | 121.55      | 124.45   |
| 23  | b     | 608  | CLA  | CAA-C2A-C3A | -3.16 | 104.12      | 112.78   |
| 23  | A     | 405  | CLA  | CMA-C3A-C4A | -3.16 | 103.28      | 111.77   |
| 25  | C     | 515  | BCR  | C7-C8-C9    | -3.16 | 121.46      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | C     | 507  | CLA  | C3C-C4C-NC  | 3.16  | 114.11      | 110.57   |
| 23  | C     | 513  | CLA  | C3C-C4C-NC  | 3.16  | 114.11      | 110.57   |
| 39  | F     | 101  | HEM  | C4A-NA-C1A  | 3.16  | 108.44      | 105.35   |
| 23  | C     | 513  | CLA  | C1C-C2C-C3C | -3.15 | 103.64      | 106.96   |
| 36  | C     | 525  | HTG  | C1-O5-C5    | 3.15  | 118.39      | 112.58   |
| 23  | b     | 616  | CLA  | CMC-C2C-C1C | 3.15  | 129.84      | 125.04   |
| 23  | B     | 616  | CLA  | CHD-C1D-ND  | -3.15 | 121.56      | 124.45   |
| 23  | c     | 515  | CLA  | O2D-CGD-O1D | -3.15 | 117.68      | 123.84   |
| 33  | x     | 1301 | PL9  | C20-C19-C21 | 3.15  | 120.57      | 115.27   |
| 23  | a     | 2610 | CLA  | C3C-C4C-NC  | 3.15  | 114.10      | 110.57   |
| 23  | C     | 502  | CLA  | CHD-C1D-ND  | -3.14 | 121.56      | 124.45   |
| 23  | B     | 603  | CLA  | CHD-C4C-C3C | -3.14 | 120.22      | 124.84   |
| 23  | A     | 410  | CLA  | CMA-C3A-C2A | -3.14 | 101.15      | 113.83   |
| 24  | A     | 409  | PHO  | C1A-C2A-C3A | -3.14 | 99.85       | 102.84   |
| 23  | B     | 612  | CLA  | CMC-C2C-C1C | 3.14  | 129.82      | 125.04   |
| 23  | C     | 507  | CLA  | C4-C3-C5    | 3.14  | 120.55      | 115.27   |
| 23  | c     | 509  | CLA  | O2A-CGA-O1A | -3.14 | 115.67      | 123.59   |
| 23  | c     | 511  | CLA  | C1C-C2C-C3C | -3.14 | 103.66      | 106.96   |
| 23  | b     | 620  | CLA  | CAC-C3C-C4C | 3.14  | 128.88      | 124.81   |
| 23  | B     | 607  | CLA  | CHC-C4B-NB  | 3.14  | 127.58      | 124.26   |
| 23  | c     | 512  | CLA  | CMC-C2C-C1C | 3.13  | 129.81      | 125.04   |
| 23  | c     | 508  | CLA  | CHA-C1A-NA  | -3.13 | 119.22      | 126.40   |
| 23  | C     | 514  | CLA  | CMB-C2B-C1B | 3.13  | 130.14      | 125.37   |
| 23  | d     | 408  | CLA  | CHD-C4C-C3C | -3.13 | 120.23      | 124.84   |
| 23  | B     | 606  | CLA  | CMC-C2C-C1C | 3.13  | 129.81      | 125.04   |
| 23  | C     | 508  | CLA  | CMB-C2B-C1B | 3.13  | 130.14      | 125.37   |
| 23  | B     | 608  | CLA  | CHD-C4C-C3C | -3.13 | 120.24      | 124.84   |
| 23  | B     | 604  | CLA  | C1D-CHD-C4C | -3.13 | 119.31      | 126.06   |
| 23  | A     | 405  | CLA  | C1D-CHD-C4C | -3.13 | 119.31      | 126.06   |
| 23  | B     | 607  | CLA  | CHD-C1D-ND  | -3.13 | 121.58      | 124.45   |
| 24  | a     | 2611 | PHO  | C1A-C2A-C3A | -3.12 | 99.87       | 102.84   |
| 23  | B     | 613  | CLA  | O2D-CGD-O1D | -3.12 | 117.73      | 123.84   |
| 23  | C     | 506  | CLA  | CHA-C1A-NA  | -3.12 | 119.24      | 126.40   |
| 23  | B     | 609  | CLA  | C2C-C1C-NC  | 3.12  | 112.90      | 109.97   |
| 27  | A     | 413  | LMG  | C8-O7-C10   | -3.12 | 110.10      | 117.79   |
| 23  | C     | 502  | CLA  | C1D-CHD-C4C | -3.12 | 119.32      | 126.06   |
| 27  | c     | 521  | LMG  | C8-O7-C10   | -3.12 | 110.11      | 117.79   |
| 23  | c     | 506  | CLA  | C4C-C3C-C2C | -3.12 | 102.35      | 106.90   |
| 23  | C     | 513  | CLA  | CMB-C2B-C1B | 3.12  | 130.12      | 125.37   |
| 23  | B     | 603  | CLA  | CBC-CAC-C3C | -3.12 | 103.84      | 112.43   |
| 23  | C     | 513  | CLA  | CBA-CAA-C2A | -3.12 | 104.66      | 113.86   |
| 23  | A     | 410  | CLA  | C3C-C4C-NC  | 3.12  | 114.07      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 33  | d     | 411  | PL9  | C15-C14-C16 | 3.11  | 120.51      | 115.27   |
| 23  | C     | 503  | CLA  | C3C-C4C-NC  | 3.11  | 114.06      | 110.57   |
| 23  | b     | 607  | CLA  | C1D-CHD-C4C | -3.11 | 119.35      | 126.06   |
| 23  | b     | 609  | CLA  | C3D-C4D-ND  | 3.11  | 115.27      | 110.24   |
| 38  | e     | 101  | LHG  | O8-C23-C24  | 3.11  | 121.66      | 111.91   |
| 23  | A     | 406  | CLA  | C3C-C4C-NC  | 3.11  | 114.06      | 110.57   |
| 23  | c     | 512  | CLA  | C4C-C3C-C2C | -3.11 | 102.37      | 106.90   |
| 23  | A     | 405  | CLA  | C4C-C3C-C2C | -3.11 | 102.37      | 106.90   |
| 23  | b     | 607  | CLA  | C1C-C2C-C3C | -3.11 | 103.69      | 106.96   |
| 23  | C     | 504  | CLA  | CBC-CAC-C3C | -3.11 | 103.87      | 112.43   |
| 23  | d     | 408  | CLA  | CMB-C2B-C1B | 3.11  | 130.10      | 125.37   |
| 23  | C     | 509  | CLA  | CAC-C3C-C4C | 3.10  | 128.84      | 124.81   |
| 23  | B     | 613  | CLA  | C1D-CHD-C4C | -3.10 | 119.36      | 126.06   |
| 23  | c     | 510  | CLA  | CBC-CAC-C3C | -3.10 | 103.88      | 112.43   |
| 23  | c     | 506  | CLA  | O2D-CGD-O1D | -3.10 | 117.78      | 123.84   |
| 36  | b     | 604  | HTG  | O5-C5-C4    | 3.10  | 115.32      | 109.69   |
| 42  | V     | 201  | HEC  | CBC-CAC-C3C | 3.10  | 120.97      | 112.43   |
| 23  | a     | 2610 | CLA  | O2A-CGA-O1A | -3.10 | 115.77      | 123.59   |
| 23  | D     | 2303 | CLA  | C1-C2-C3    | -3.10 | 120.69      | 126.04   |
| 23  | A     | 410  | CLA  | C3B-C4B-NB  | 3.10  | 113.39      | 110.52   |
| 23  | B     | 614  | CLA  | C1D-CHD-C4C | -3.10 | 119.38      | 126.06   |
| 23  | C     | 511  | CLA  | C1D-CHD-C4C | -3.09 | 119.38      | 126.06   |
| 23  | B     | 604  | CLA  | O2A-CGA-O1A | -3.09 | 115.78      | 123.59   |
| 23  | b     | 607  | CLA  | C3C-C4C-NC  | 3.09  | 114.04      | 110.57   |
| 23  | B     | 604  | CLA  | O2A-CGA-CBA | 3.09  | 121.60      | 111.91   |
| 23  | B     | 612  | CLA  | C1D-CHD-C4C | -3.09 | 119.40      | 126.06   |
| 23  | B     | 616  | CLA  | C4-C3-C5    | 3.09  | 120.46      | 115.27   |
| 31  | A     | 418  | JOX  | O-C2-C1     | -3.09 | 119.95      | 122.76   |
| 23  | b     | 615  | CLA  | C1-C2-C3    | -3.09 | 120.71      | 126.04   |
| 25  | B     | 618  | BCR  | C24-C23-C22 | -3.08 | 121.58      | 126.23   |
| 37  | H     | 103  | DGD  | O1G-C1A-C2A | 3.08  | 121.58      | 111.91   |
| 23  | c     | 507  | CLA  | C4-C3-C5    | 3.08  | 120.45      | 115.27   |
| 23  | c     | 510  | CLA  | C1D-CHD-C4C | -3.08 | 119.42      | 126.06   |
| 23  | d     | 402  | CLA  | O2A-CGA-O1A | -3.08 | 115.82      | 123.59   |
| 23  | B     | 605  | CLA  | O2A-CGA-O1A | -3.08 | 115.83      | 123.59   |
| 23  | A     | 405  | CLA  | C3B-C4B-NB  | 3.08  | 113.37      | 110.52   |
| 26  | A     | 412  | SQD  | O8-S-C6     | 3.08  | 110.64      | 105.74   |
| 23  | C     | 506  | CLA  | C1C-C2C-C3C | -3.08 | 103.72      | 106.96   |
| 28  | m     | 2804 | LMT  | C1B-C2B-C3B | 3.07  | 116.40      | 110.00   |
| 37  | h     | 102  | DGD  | O1G-C1A-O1A | -3.07 | 115.84      | 123.59   |
| 23  | B     | 610  | CLA  | CHD-C4C-C3C | -3.07 | 120.32      | 124.84   |
| 23  | C     | 511  | CLA  | C3C-C4C-NC  | 3.07  | 114.01      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | C     | 516  | BCR  | C38-C26-C25 | -3.07 | 121.08      | 124.53   |
| 28  | i     | 103  | LMT  | C1'-O5'-C5' | 3.07  | 119.71      | 113.69   |
| 23  | c     | 510  | CLA  | C4-C3-C5    | 3.07  | 120.43      | 115.27   |
| 23  | b     | 613  | CLA  | CBC-CAC-C3C | -3.07 | 103.98      | 112.43   |
| 23  | b     | 616  | CLA  | C1-C2-C3    | -3.07 | 120.74      | 126.04   |
| 23  | C     | 510  | CLA  | C3B-C4B-NB  | 3.06  | 113.36      | 110.52   |
| 23  | B     | 608  | CLA  | CHD-C1D-ND  | -3.06 | 121.64      | 124.45   |
| 23  | C     | 513  | CLA  | C1-C2-C3    | -3.06 | 120.75      | 126.04   |
| 23  | d     | 402  | CLA  | C1-C2-C3    | -3.06 | 120.75      | 126.04   |
| 23  | d     | 408  | CLA  | C4C-C3C-C2C | -3.06 | 102.44      | 106.90   |
| 23  | B     | 616  | CLA  | CMC-C2C-C1C | 3.06  | 129.70      | 125.04   |
| 23  | c     | 509  | CLA  | CAA-C2A-C3A | -3.06 | 104.40      | 112.78   |
| 23  | C     | 507  | CLA  | O2A-CGA-CBA | 3.06  | 121.51      | 111.91   |
| 23  | B     | 614  | CLA  | C3B-C4B-NB  | 3.06  | 113.35      | 110.52   |
| 23  | b     | 608  | CLA  | CHD-C1D-ND  | -3.06 | 121.64      | 124.45   |
| 23  | a     | 2610 | CLA  | C4-C3-C5    | 3.05  | 120.41      | 115.27   |
| 23  | B     | 615  | CLA  | O2A-CGA-O1A | -3.05 | 115.89      | 123.59   |
| 23  | C     | 509  | CLA  | C4C-C3C-C2C | -3.05 | 102.45      | 106.90   |
| 23  | b     | 621  | CLA  | CBC-CAC-C3C | -3.05 | 104.03      | 112.43   |
| 23  | b     | 612  | CLA  | CBC-CAC-C3C | -3.05 | 104.03      | 112.43   |
| 23  | C     | 502  | CLA  | C2C-C1C-NC  | 3.05  | 112.83      | 109.97   |
| 23  | C     | 513  | CLA  | O2D-CGD-O1D | -3.04 | 117.89      | 123.84   |
| 23  | C     | 503  | CLA  | C4C-C3C-C2C | -3.04 | 102.46      | 106.90   |
| 26  | d     | 417  | SQD  | O48-C23-C24 | 3.04  | 121.45      | 111.91   |
| 25  | b     | 623  | BCR  | C38-C26-C25 | -3.04 | 121.11      | 124.53   |
| 33  | x     | 1301 | PL9  | C32-C33-C34 | -3.04 | 120.34      | 127.66   |
| 23  | B     | 604  | CLA  | CHD-C1D-ND  | -3.04 | 121.66      | 124.45   |
| 23  | D     | 2303 | CLA  | C1D-CHD-C4C | -3.03 | 119.51      | 126.06   |
| 27  | A     | 413  | LMG  | C7-O1-C1    | -3.03 | 107.81      | 113.74   |
| 23  | c     | 504  | CLA  | C1D-CHD-C4C | -3.03 | 119.52      | 126.06   |
| 23  | b     | 609  | CLA  | CHA-C1A-NA  | -3.03 | 119.46      | 126.40   |
| 23  | C     | 513  | CLA  | C4C-C3C-C2C | -3.03 | 102.48      | 106.90   |
| 23  | B     | 617  | CLA  | C3C-C4C-NC  | 3.02  | 113.96      | 110.57   |
| 23  | B     | 607  | CLA  | C1C-C2C-C3C | -3.02 | 103.78      | 106.96   |
| 23  | b     | 617  | CLA  | C1-C2-C3    | -3.02 | 120.82      | 126.04   |
| 23  | B     | 605  | CLA  | C3B-C4B-NB  | 3.02  | 113.32      | 110.52   |
| 23  | B     | 605  | CLA  | CHD-C1D-ND  | -3.02 | 121.68      | 124.45   |
| 23  | c     | 504  | CLA  | C3C-C4C-NC  | 3.02  | 113.95      | 110.57   |
| 23  | c     | 512  | CLA  | C3B-C4B-NB  | 3.02  | 113.31      | 110.52   |
| 23  | B     | 617  | CLA  | C4C-C3C-C2C | -3.02 | 102.50      | 106.90   |
| 23  | C     | 514  | CLA  | C2C-C1C-NC  | 3.02  | 112.80      | 109.97   |
| 23  | b     | 613  | CLA  | C1D-CHD-C4C | -3.01 | 119.56      | 126.06   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36  | d     | 407  | HTG  | C1-O5-C5    | 3.01  | 118.13      | 112.58   |
| 23  | A     | 407  | CLA  | O2A-CGA-O1A | -3.01 | 116.00      | 123.59   |
| 23  | B     | 608  | CLA  | C1-O2A-CGA  | 3.01  | 124.33      | 116.44   |
| 23  | C     | 506  | CLA  | C3D-C2D-C1D | -3.01 | 101.73      | 105.83   |
| 23  | B     | 605  | CLA  | C3C-C4C-NC  | 3.00  | 113.94      | 110.57   |
| 23  | B     | 609  | CLA  | C1C-C2C-C3C | -3.00 | 103.80      | 106.96   |
| 23  | a     | 2609 | CLA  | CMC-C2C-C1C | 3.00  | 129.61      | 125.04   |
| 23  | b     | 619  | CLA  | C4C-C3C-C2C | -3.00 | 102.52      | 106.90   |
| 23  | B     | 605  | CLA  | CMC-C2C-C1C | 3.00  | 129.61      | 125.04   |
| 23  | B     | 602  | CLA  | C2C-C1C-NC  | 3.00  | 112.78      | 109.97   |
| 23  | b     | 611  | CLA  | C4C-C3C-C2C | -3.00 | 102.53      | 106.90   |
| 37  | c     | 520  | DGD  | O1G-C1A-C2A | 3.00  | 121.32      | 111.91   |
| 33  | D     | 2306 | PL9  | C25-C24-C26 | 3.00  | 120.31      | 115.27   |
| 23  | c     | 505  | CLA  | C3C-C4C-NC  | 3.00  | 113.93      | 110.57   |
| 23  | b     | 620  | CLA  | C2C-C1C-NC  | 2.99  | 112.78      | 109.97   |
| 23  | c     | 509  | CLA  | C4C-C3C-C2C | -2.99 | 102.53      | 106.90   |
| 23  | b     | 607  | CLA  | CAA-CBA-CGA | -2.99 | 104.50      | 113.25   |
| 23  | b     | 620  | CLA  | C1C-C2C-C3C | -2.99 | 103.81      | 106.96   |
| 23  | c     | 511  | CLA  | C4-C3-C5    | 2.99  | 120.30      | 115.27   |
| 23  | b     | 615  | CLA  | C1C-C2C-C3C | -2.99 | 103.81      | 106.96   |
| 37  | H     | 103  | DGD  | C2G-O2G-C1B | -2.99 | 110.43      | 117.79   |
| 23  | C     | 506  | CLA  | C3C-C4C-NC  | 2.99  | 113.92      | 110.57   |
| 23  | B     | 615  | CLA  | CBC-CAC-C3C | -2.99 | 104.19      | 112.43   |
| 25  | k     | 302  | BCR  | C38-C26-C25 | -2.99 | 121.17      | 124.53   |
| 23  | c     | 505  | CLA  | O2A-CGA-O1A | -2.99 | 116.05      | 123.59   |
| 23  | c     | 509  | CLA  | CHD-C4C-C3C | -2.99 | 120.45      | 124.84   |
| 23  | B     | 606  | CLA  | C2C-C1C-NC  | 2.99  | 112.77      | 109.97   |
| 23  | B     | 607  | CLA  | C4C-C3C-C2C | -2.99 | 102.55      | 106.90   |
| 23  | b     | 606  | CLA  | CHD-C1D-ND  | -2.98 | 121.71      | 124.45   |
| 23  | B     | 605  | CLA  | C4A-NA-C1A  | 2.98  | 108.05      | 106.71   |
| 23  | B     | 602  | CLA  | C1D-CHD-C4C | -2.98 | 119.63      | 126.06   |
| 23  | c     | 507  | CLA  | O2D-CGD-O1D | -2.98 | 118.01      | 123.84   |
| 23  | B     | 603  | CLA  | C3C-C4C-NC  | 2.98  | 113.91      | 110.57   |
| 23  | b     | 617  | CLA  | O2A-CGA-CBA | 2.98  | 121.25      | 111.91   |
| 23  | b     | 610  | CLA  | O2A-CGA-O1A | -2.98 | 116.08      | 123.59   |
| 23  | a     | 2610 | CLA  | O2A-CGA-CBA | 2.98  | 121.25      | 111.91   |
| 23  | B     | 611  | CLA  | CMA-C3A-C4A | -2.98 | 103.78      | 111.77   |
| 36  | C     | 522  | HTG  | O5-C1-C2    | 2.98  | 114.06      | 110.31   |
| 23  | b     | 618  | CLA  | CMB-C2B-C1B | 2.97  | 129.90      | 125.37   |
| 26  | A     | 412  | SQD  | O9-S-C6     | 2.97  | 110.47      | 106.94   |
| 23  | b     | 609  | CLA  | C4A-NA-C1A  | 2.97  | 108.04      | 106.71   |
| 23  | B     | 606  | CLA  | CMB-C2B-C1B | 2.97  | 129.90      | 125.37   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 37  | H     | 103    | DGD  | C3G-O3G-C1D | -2.97 | 107.93      | 113.74   |
| 23  | d     | 408    | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 23  | c     | 516    | CLA  | C3C-C4C-NC  | 2.97  | 113.90      | 110.57   |
| 23  | b     | 620    | CLA  | CED-O2D-CGD | 2.97  | 122.66      | 115.94   |
| 23  | B     | 602    | CLA  | CHD-C4C-C3C | -2.97 | 120.47      | 124.84   |
| 23  | c     | 509    | CLA  | C4-C3-C5    | 2.97  | 120.27      | 115.27   |
| 31  | a     | 2617   | JOX  | C-C1-C2     | -2.97 | 120.80      | 123.18   |
| 25  | T     | 102    | BCR  | C11-C10-C9  | -2.97 | 123.07      | 127.31   |
| 33  | d     | 411    | PL9  | O1-C4-C3    | -2.97 | 117.45      | 120.72   |
| 25  | y     | 101    | BCR  | C16-C17-C18 | -2.97 | 123.08      | 127.31   |
| 23  | c     | 513    | CLA  | C3B-C4B-NB  | 2.97  | 113.27      | 110.52   |
| 23  | c     | 508    | CLA  | O2D-CGD-O1D | -2.96 | 118.04      | 123.84   |
| 23  | C     | 506    | CLA  | CMB-C2B-C1B | 2.96  | 129.88      | 125.37   |
| 23  | b     | 611    | CLA  | CMC-C2C-C1C | 2.96  | 129.55      | 125.04   |
| 26  | A     | 412    | SQD  | C1-C2-C3    | -2.96 | 103.83      | 110.00   |
| 23  | B     | 612    | CLA  | C3C-C4C-NC  | 2.96  | 113.89      | 110.57   |
| 31  | a     | 2617   | JOX  | C-C5-C4     | 2.96  | 123.59      | 117.15   |
| 23  | C     | 508    | CLA  | C3D-C4D-ND  | 2.95  | 115.02      | 110.24   |
| 23  | b     | 616    | CLA  | CAA-C2A-C3A | -2.95 | 104.69      | 112.78   |
| 25  | K     | 101    | BCR  | C7-C8-C9    | -2.95 | 121.78      | 126.23   |
| 23  | B     | 612    | CLA  | CHA-C1A-NA  | -2.95 | 119.64      | 126.40   |
| 23  | C     | 514    | CLA  | C1-C2-C3    | -2.95 | 120.94      | 126.04   |
| 23  | d     | 408    | CLA  | CAA-C2A-C3A | -2.95 | 104.70      | 112.78   |
| 37  | C     | 517    | DGD  | O3G-C3G-C2G | -2.95 | 103.79      | 110.90   |
| 23  | c     | 509    | CLA  | O2A-CGA-CBA | 2.95  | 121.16      | 111.91   |
| 23  | b     | 618    | CLA  | C1D-CHD-C4C | -2.95 | 119.70      | 126.06   |
| 38  | d     | 413    | LHG  | O8-C23-O10  | -2.94 | 116.16      | 123.59   |
| 23  | C     | 512    | CLA  | O2D-CGD-CBD | 2.94  | 116.50      | 111.27   |
| 23  | b     | 615    | CLA  | O2A-CGA-CBA | 2.94  | 121.14      | 111.91   |
| 23  | b     | 619    | CLA  | CBC-CAC-C3C | -2.94 | 104.32      | 112.43   |
| 23  | c     | 512    | CLA  | C4A-NA-C1A  | 2.94  | 108.03      | 106.71   |
| 38  | L     | 101    | LHG  | O8-C23-O10  | -2.94 | 116.17      | 123.59   |
| 23  | b     | 618    | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |
| 23  | D     | 2304   | CLA  | C2C-C1C-NC  | 2.94  | 112.73      | 109.97   |
| 23  | c     | 511    | CLA  | C2C-C1C-NC  | 2.94  | 112.73      | 109.97   |
| 23  | c     | 509    | CLA  | C3C-C4C-NC  | 2.94  | 113.87      | 110.57   |
| 23  | d     | 402    | CLA  | CHC-C1C-C2C | -2.94 | 118.57      | 126.73   |
| 23  | c     | 505    | CLA  | O2A-CGA-CBA | 2.94  | 121.13      | 111.91   |
| 23  | c     | 506    | CLA  | C1-C2-C3    | -2.94 | 120.96      | 126.04   |
| 23  | B     | 617    | CLA  | C3B-C4B-NB  | 2.94  | 113.24      | 110.52   |
| 23  | c     | 505    | CLA  | CMB-C2B-C1B | 2.93  | 129.84      | 125.37   |
| 36  | B     | 624[B] | HTG  | C6-C5-C4    | -2.93 | 106.13      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | A     | 405  | CLA  | O2A-CGA-CBA | 2.93  | 121.11      | 111.91   |
| 23  | d     | 409  | CLA  | CHD-C4C-C3C | -2.93 | 120.53      | 124.84   |
| 23  | b     | 607  | CLA  | C1-C2-C3    | -2.93 | 120.97      | 126.04   |
| 23  | C     | 504  | CLA  | CMB-C2B-C1B | 2.93  | 129.83      | 125.37   |
| 23  | C     | 511  | CLA  | C1-O2A-CGA  | 2.93  | 124.13      | 116.44   |
| 23  | C     | 504  | CLA  | C4C-C3C-C2C | -2.93 | 102.63      | 106.90   |
| 23  | B     | 611  | CLA  | C1-O2A-CGA  | 2.93  | 124.13      | 116.44   |
| 23  | B     | 607  | CLA  | C1-O2A-CGA  | 2.93  | 124.12      | 116.44   |
| 23  | C     | 510  | CLA  | C4C-C3C-C2C | -2.93 | 102.63      | 106.90   |
| 23  | b     | 619  | CLA  | CMB-C2B-C1B | 2.92  | 129.82      | 125.37   |
| 23  | B     | 615  | CLA  | O2A-CGA-CBA | 2.92  | 121.08      | 111.91   |
| 23  | B     | 615  | CLA  | C3B-C4B-NB  | 2.92  | 113.22      | 110.52   |
| 23  | C     | 503  | CLA  | CBC-CAC-C3C | -2.92 | 104.38      | 112.43   |
| 23  | B     | 614  | CLA  | O2A-CGA-CBA | 2.92  | 121.06      | 111.91   |
| 33  | x     | 1301 | PL9  | C37-C38-C39 | -2.91 | 120.64      | 127.66   |
| 23  | a     | 2609 | CLA  | O2A-CGA-CBA | 2.91  | 121.05      | 111.91   |
| 23  | C     | 509  | CLA  | CAA-C2A-C3A | -2.91 | 104.80      | 112.78   |
| 37  | c     | 518  | DGD  | O2G-C1B-O1B | -2.91 | 116.66      | 123.70   |
| 23  | C     | 509  | CLA  | C1D-CHD-C4C | -2.91 | 119.78      | 126.06   |
| 23  | c     | 515  | CLA  | C3C-C4C-NC  | 2.91  | 113.84      | 110.57   |
| 23  | a     | 2609 | CLA  | O2A-CGA-O1A | -2.91 | 116.25      | 123.59   |
| 23  | b     | 618  | CLA  | C3B-C4B-NB  | 2.91  | 113.22      | 110.52   |
| 23  | B     | 613  | CLA  | C4-C3-C5    | 2.91  | 120.16      | 115.27   |
| 23  | b     | 609  | CLA  | CMC-C2C-C1C | 2.91  | 129.47      | 125.04   |
| 23  | C     | 514  | CLA  | C4-C3-C5    | 2.91  | 120.16      | 115.27   |
| 23  | c     | 506  | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.81   |
| 23  | B     | 602  | CLA  | CBC-CAC-C3C | -2.91 | 104.42      | 112.43   |
| 23  | c     | 507  | CLA  | C3C-C4C-NC  | 2.91  | 113.83      | 110.57   |
| 23  | B     | 616  | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.81   |
| 40  | H     | 102  | RRX  | C20-C21-C22 | -2.90 | 123.17      | 127.31   |
| 26  | D     | 2308 | SQD  | O6-C1-C2    | 2.90  | 112.84      | 108.30   |
| 23  | A     | 405  | CLA  | C1-C2-C3    | -2.90 | 121.02      | 126.04   |
| 23  | c     | 516  | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.90   |
| 23  | a     | 2610 | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.90   |
| 23  | a     | 2609 | CLA  | CHD-C1D-ND  | -2.90 | 121.79      | 124.45   |
| 42  | V     | 201  | HEC  | C4C-NC-C1C  | 2.90  | 108.19      | 105.35   |
| 23  | a     | 2609 | CLA  | C4C-C3C-C2C | -2.90 | 102.68      | 106.90   |
| 23  | B     | 604  | CLA  | C4C-C3C-C2C | -2.89 | 102.68      | 106.90   |
| 23  | B     | 604  | CLA  | CBC-CAC-C3C | -2.89 | 104.45      | 112.43   |
| 23  | A     | 410  | CLA  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |
| 23  | b     | 608  | CLA  | C4C-C3C-C2C | -2.89 | 102.68      | 106.90   |
| 23  | b     | 618  | CLA  | C3C-C4C-NC  | 2.89  | 113.81      | 110.57   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 38  | D     | 2311 | LHG  | O8-C23-C24  | 2.89  | 120.98      | 111.91   |
| 23  | C     | 508  | CLA  | C4C-C3C-C2C | -2.89 | 102.69      | 106.90   |
| 31  | A     | 418  | JOX  | C2-C3-CL    | 2.89  | 118.24      | 115.84   |
| 23  | b     | 621  | CLA  | C1-C2-C3    | -2.89 | 121.05      | 126.04   |
| 23  | C     | 504  | CLA  | C2C-C1C-NC  | 2.89  | 112.68      | 109.97   |
| 31  | a     | 2617 | JOX  | O-C2-C1     | -2.89 | 120.13      | 122.76   |
| 23  | b     | 620  | CLA  | C4C-C3C-C2C | -2.89 | 102.69      | 106.90   |
| 26  | A     | 412  | SQD  | O48-C23-C24 | 2.88  | 120.95      | 111.91   |
| 25  | Y     | 302  | BCR  | C35-C13-C14 | -2.88 | 118.89      | 122.92   |
| 28  | J     | 303  | LMT  | C1'-O5'-C5' | 2.88  | 119.34      | 113.69   |
| 37  | h     | 102  | DGD  | O1G-C1A-C2A | 2.88  | 120.94      | 111.91   |
| 23  | b     | 614  | CLA  | O2D-CGD-CBD | 2.88  | 116.38      | 111.27   |
| 23  | d     | 408  | CLA  | O2A-CGA-CBA | 2.88  | 120.94      | 111.91   |
| 23  | A     | 410  | CLA  | CAA-C2A-C3A | -2.88 | 104.90      | 112.78   |
| 23  | c     | 515  | CLA  | CMA-C3A-C4A | -2.88 | 104.04      | 111.77   |
| 23  | b     | 613  | CLA  | C3B-C4B-NB  | 2.87  | 113.18      | 110.52   |
| 23  | B     | 611  | CLA  | CAA-C2A-C3A | -2.87 | 104.91      | 112.78   |
| 23  | b     | 609  | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.90   |
| 23  | B     | 602  | CLA  | C4A-NA-C1A  | 2.87  | 108.00      | 106.71   |
| 23  | c     | 516  | CLA  | CAC-C3C-C4C | 2.87  | 128.54      | 124.81   |
| 23  | b     | 606  | CLA  | C1D-CHD-C4C | -2.87 | 119.87      | 126.06   |
| 23  | D     | 2303 | CLA  | C4C-C3C-C2C | -2.87 | 102.72      | 106.90   |
| 28  | j     | 2701 | LMT  | O1B-C4'-C3' | 2.87  | 114.91      | 107.28   |
| 38  | l     | 103  | LHG  | O7-C7-C8    | 2.87  | 117.68      | 111.50   |
| 42  | v     | 201  | HEC  | CMD-C2D-C1D | 2.87  | 129.40      | 125.04   |
| 23  | b     | 610  | CLA  | CBC-CAC-C3C | -2.87 | 104.53      | 112.43   |
| 26  | a     | 2615 | SQD  | C45-O47-C7  | -2.86 | 110.74      | 117.79   |
| 23  | B     | 608  | CLA  | C3B-C4B-NB  | 2.86  | 113.17      | 110.52   |
| 23  | b     | 609  | CLA  | CHD-C4C-C3C | -2.86 | 120.63      | 124.84   |
| 23  | B     | 616  | CLA  | CMB-C2B-C1B | 2.86  | 129.73      | 125.37   |
| 23  | B     | 609  | CLA  | O2A-CGA-CBA | 2.86  | 120.89      | 111.91   |
| 23  | b     | 610  | CLA  | C3B-C4B-NB  | 2.86  | 113.17      | 110.52   |
| 38  | l     | 103  | LHG  | O8-C23-C24  | 2.86  | 120.89      | 111.91   |
| 26  | b     | 601  | SQD  | C3-C4-C5    | 2.86  | 115.34      | 110.24   |
| 23  | b     | 617  | CLA  | C4-C3-C5    | 2.86  | 120.08      | 115.27   |
| 23  | C     | 510  | CLA  | CHD-C1D-ND  | -2.86 | 121.83      | 124.45   |
| 23  | b     | 621  | CLA  | C1C-C2C-C3C | -2.86 | 103.95      | 106.96   |
| 31  | A     | 419  | JOX  | O1-C5-C     | -2.85 | 117.33      | 121.41   |
| 23  | c     | 514  | CLA  | C3B-C4B-NB  | 2.85  | 113.16      | 110.52   |
| 31  | A     | 418  | JOX  | C-C5-C4     | 2.85  | 123.36      | 117.15   |
| 23  | B     | 616  | CLA  | C4C-C3C-C2C | -2.85 | 102.75      | 106.90   |
| 23  | b     | 621  | CLA  | CAC-C3C-C4C | 2.85  | 128.51      | 124.81   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | a     | 2610 | CLA  | CED-O2D-CGD | 2.85  | 122.38      | 115.94   |
| 23  | C     | 507  | CLA  | C4C-C3C-C2C | -2.85 | 102.75      | 106.90   |
| 23  | C     | 502  | CLA  | CBC-CAC-C3C | -2.85 | 104.58      | 112.43   |
| 23  | C     | 511  | CLA  | C4C-C3C-C2C | -2.85 | 102.75      | 106.90   |
| 23  | b     | 611  | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 33  | A     | 422  | PL9  | C40-C39-C41 | 2.84  | 120.06      | 115.27   |
| 23  | B     | 608  | CLA  | CMB-C2B-C1B | 2.84  | 129.70      | 125.37   |
| 24  | a     | 2611 | PHO  | O2D-CGD-O1D | -2.84 | 118.28      | 123.84   |
| 24  | a     | 2611 | PHO  | C4-C3-C5    | 2.84  | 120.05      | 115.27   |
| 24  | A     | 409  | PHO  | CMB-C2B-C3B | 2.84  | 129.99      | 124.68   |
| 36  | B     | 625  | HTG  | C1-C2-C3    | 2.84  | 116.19      | 110.59   |
| 23  | b     | 613  | CLA  | O2A-CGA-O1A | -2.84 | 116.43      | 123.59   |
| 23  | C     | 512  | CLA  | C3C-C4C-NC  | 2.84  | 113.75      | 110.57   |
| 23  | C     | 512  | CLA  | C4C-C3C-C2C | -2.84 | 102.76      | 106.90   |
| 24  | A     | 408  | PHO  | CMB-C2B-C3B | 2.83  | 129.98      | 124.68   |
| 23  | C     | 505  | CLA  | CMB-C2B-C1B | 2.83  | 129.69      | 125.37   |
| 23  | B     | 615  | CLA  | C4A-NA-C1A  | 2.83  | 107.98      | 106.71   |
| 23  | c     | 507  | CLA  | CMB-C2B-C1B | 2.83  | 129.68      | 125.37   |
| 38  | D     | 2310 | LHG  | O8-C23-O10  | -2.83 | 116.44      | 123.59   |
| 26  | l     | 101  | SQD  | C44-O6-C1   | -2.83 | 108.21      | 113.74   |
| 23  | c     | 513  | CLA  | C3C-C4C-NC  | 2.83  | 113.75      | 110.57   |
| 23  | B     | 617  | CLA  | O2A-CGA-CBA | 2.83  | 120.79      | 111.91   |
| 23  | C     | 512  | CLA  | C4-C3-C5    | 2.83  | 120.03      | 115.27   |
| 23  | b     | 621  | CLA  | CHA-C1A-NA  | -2.83 | 119.92      | 126.40   |
| 25  | B     | 619  | BCR  | C38-C26-C25 | -2.83 | 121.35      | 124.53   |
| 42  | V     | 201  | HEC  | C4B-NB-C1B  | 2.83  | 107.99      | 105.07   |
| 25  | y     | 101  | BCR  | C15-C14-C13 | -2.83 | 123.28      | 127.31   |
| 23  | b     | 618  | CLA  | O2A-CGA-CBA | 2.83  | 120.77      | 111.91   |
| 23  | b     | 620  | CLA  | CHD-C1D-ND  | -2.82 | 121.86      | 124.45   |
| 28  | A     | 414  | LMT  | C1B-O5B-C5B | 2.82  | 119.23      | 113.69   |
| 23  | b     | 615  | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 26  | D     | 2308 | SQD  | O48-C23-C24 | 2.82  | 120.77      | 111.91   |
| 33  | D     | 2306 | PL9  | C10-C9-C11  | 2.82  | 120.01      | 115.27   |
| 23  | c     | 509  | CLA  | CHD-C1D-ND  | -2.82 | 121.86      | 124.45   |
| 23  | B     | 606  | CLA  | C1-C2-C3    | -2.82 | 121.17      | 126.04   |
| 23  | b     | 618  | CLA  | C4C-C3C-C2C | -2.82 | 102.79      | 106.90   |
| 23  | b     | 607  | CLA  | CHD-C4C-C3C | -2.82 | 120.70      | 124.84   |
| 40  | h     | 101  | RRX  | C38-C26-C25 | -2.81 | 121.37      | 124.53   |
| 23  | c     | 507  | CLA  | C3B-C4B-NB  | 2.81  | 113.13      | 110.52   |
| 23  | b     | 615  | CLA  | CMA-C3A-C4A | -2.81 | 104.21      | 111.77   |
| 23  | b     | 608  | CLA  | C6-C7-C8    | -2.81 | 106.83      | 115.92   |
| 23  | D     | 2304 | CLA  | CAA-C2A-C3A | -2.81 | 105.09      | 112.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | B     | 604  | CLA  | CMC-C2C-C1C | 2.81  | 129.31      | 125.04   |
| 26  | D     | 2302 | SQD  | O9-S-C6     | 2.81  | 110.27      | 106.94   |
| 23  | b     | 610  | CLA  | C4C-C3C-C2C | -2.80 | 102.81      | 106.90   |
| 23  | C     | 503  | CLA  | O2A-C1-C2   | 2.80  | 115.99      | 108.64   |
| 36  | i     | 102  | HTG  | O5-C5-C4    | 2.80  | 114.78      | 109.69   |
| 23  | A     | 406  | CLA  | CMC-C2C-C1C | 2.80  | 129.30      | 125.04   |
| 23  | c     | 507  | CLA  | O2A-CGA-O1A | -2.80 | 116.53      | 123.59   |
| 23  | C     | 514  | CLA  | CBC-CAC-C3C | -2.80 | 104.72      | 112.43   |
| 23  | b     | 613  | CLA  | C4C-C3C-C2C | -2.80 | 102.82      | 106.90   |
| 25  | b     | 624  | BCR  | C3-C4-C5    | -2.80 | 109.09      | 114.08   |
| 23  | C     | 513  | CLA  | CHA-C1A-NA  | -2.79 | 120.00      | 126.40   |
| 23  | d     | 409  | CLA  | C3B-C4B-NB  | 2.79  | 113.11      | 110.52   |
| 28  | j     | 2701 | LMT  | C3'-C4'-C5' | -2.79 | 104.52      | 110.93   |
| 23  | a     | 2613 | CLA  | CAA-C2A-C3A | -2.79 | 105.13      | 112.78   |
| 23  | C     | 511  | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 23  | B     | 610  | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 23  | b     | 613  | CLA  | C3C-C4C-NC  | 2.79  | 113.70      | 110.57   |
| 33  | D     | 2306 | PL9  | C37-C38-C39 | -2.79 | 120.94      | 127.66   |
| 23  | b     | 621  | CLA  | O2A-CGA-CBA | 2.79  | 120.66      | 111.91   |
| 23  | D     | 2303 | CLA  | CBC-CAC-C3C | -2.79 | 104.74      | 112.43   |
| 23  | c     | 505  | CLA  | CMC-C2C-C1C | 2.79  | 129.28      | 125.04   |
| 23  | c     | 506  | CLA  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 27  | B     | 622  | LMG  | O8-C28-C29  | 2.79  | 120.65      | 111.91   |
| 23  | c     | 506  | CLA  | CHA-C1A-NA  | -2.78 | 120.02      | 126.40   |
| 23  | C     | 512  | CLA  | CBC-CAC-C3C | -2.78 | 104.76      | 112.43   |
| 23  | B     | 608  | CLA  | C3C-C4C-NC  | 2.78  | 113.69      | 110.57   |
| 23  | a     | 2609 | CLA  | C7-C6-C5    | -2.78 | 105.80      | 113.36   |
| 23  | b     | 614  | CLA  | C4C-C3C-C2C | -2.78 | 102.84      | 106.90   |
| 23  | C     | 508  | CLA  | CHA-C1A-NA  | -2.78 | 120.03      | 126.40   |
| 25  | T     | 102  | BCR  | C7-C6-C5    | -2.78 | 114.73      | 121.46   |
| 23  | c     | 516  | CLA  | O2A-CGA-CBA | 2.78  | 120.63      | 111.91   |
| 23  | B     | 612  | CLA  | C1-O2A-CGA  | 2.78  | 123.73      | 116.44   |
| 23  | b     | 614  | CLA  | CED-O2D-CGD | 2.78  | 122.21      | 115.94   |
| 23  | D     | 2304 | CLA  | CHD-C4C-NC  | 2.77  | 128.57      | 124.20   |
| 25  | k     | 302  | BCR  | C31-C1-C6   | -2.77 | 105.80      | 110.30   |
| 33  | D     | 2306 | PL9  | C42-C43-C44 | -2.77 | 120.98      | 127.66   |
| 23  | B     | 607  | CLA  | C4-C3-C5    | 2.77  | 119.93      | 115.27   |
| 23  | A     | 407  | CLA  | C1-C2-C3    | -2.77 | 121.25      | 126.04   |
| 23  | A     | 410  | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.90   |
| 37  | C     | 518  | DGD  | O1G-C1A-O1A | -2.77 | 116.61      | 123.59   |
| 23  | C     | 513  | CLA  | CHD-C1D-ND  | -2.77 | 121.91      | 124.45   |
| 27  | m     | 2802 | LMG  | O8-C28-C29  | 2.77  | 120.59      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | c     | 511  | CLA  | CAA-C2A-C3A | -2.77 | 105.21      | 112.78   |
| 23  | c     | 515  | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.90   |
| 23  | c     | 510  | CLA  | C3B-C4B-NB  | 2.76  | 113.08      | 110.52   |
| 40  | h     | 101  | RRX  | C10-C11-C12 | -2.76 | 114.59      | 123.22   |
| 38  | d     | 403  | LHG  | O7-C7-C8    | 2.76  | 117.46      | 111.50   |
| 23  | B     | 604  | CLA  | CAA-C2A-C3A | -2.76 | 105.21      | 112.78   |
| 23  | b     | 620  | CLA  | C3C-C4C-NC  | 2.76  | 113.67      | 110.57   |
| 23  | B     | 611  | CLA  | C4-C3-C5    | 2.76  | 119.92      | 115.27   |
| 23  | c     | 514  | CLA  | CMB-C2B-C1B | 2.76  | 129.58      | 125.37   |
| 23  | C     | 508  | CLA  | CBC-CAC-C3C | -2.76 | 104.81      | 112.43   |
| 23  | c     | 504  | CLA  | C1-O2A-CGA  | 2.76  | 123.69      | 116.44   |
| 38  | L     | 101  | LHG  | O7-C7-C8    | 2.76  | 117.45      | 111.50   |
| 23  | b     | 613  | CLA  | CAC-C3C-C4C | 2.76  | 128.39      | 124.81   |
| 23  | D     | 2304 | CLA  | C4C-C3C-C2C | -2.76 | 102.88      | 106.90   |
| 23  | B     | 613  | CLA  | CAC-C3C-C4C | 2.76  | 128.39      | 124.81   |
| 23  | B     | 615  | CLA  | CHC-C1C-C2C | -2.76 | 119.07      | 126.73   |
| 38  | d     | 413  | LHG  | O7-C7-C8    | 2.76  | 117.44      | 111.50   |
| 37  | c     | 518  | DGD  | C2G-O2G-C1B | -2.76 | 111.00      | 117.79   |
| 23  | C     | 504  | CLA  | CHD-C1D-ND  | -2.76 | 121.92      | 124.45   |
| 23  | b     | 611  | CLA  | C4-C3-C5    | 2.76  | 119.91      | 115.27   |
| 23  | C     | 505  | CLA  | CAA-C2A-C3A | -2.75 | 105.23      | 112.78   |
| 23  | A     | 407  | CLA  | C4A-NA-C1A  | -2.75 | 105.47      | 106.71   |
| 23  | b     | 615  | CLA  | CHA-C1A-NA  | -2.75 | 120.09      | 126.40   |
| 23  | c     | 510  | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.90   |
| 23  | b     | 617  | CLA  | CHD-C1D-ND  | -2.75 | 121.93      | 124.45   |
| 39  | e     | 103  | HEM  | C1B-NB-C4B  | 2.75  | 107.91      | 105.07   |
| 23  | D     | 2303 | CLA  | O2A-CGA-O1A | -2.75 | 116.65      | 123.59   |
| 23  | b     | 607  | CLA  | C4-C3-C5    | 2.75  | 119.90      | 115.27   |
| 23  | B     | 616  | CLA  | CHA-C1A-NA  | -2.75 | 120.10      | 126.40   |
| 23  | D     | 2304 | CLA  | C3C-C4C-NC  | 2.75  | 113.65      | 110.57   |
| 23  | b     | 607  | CLA  | C1-O2A-CGA  | 2.75  | 123.65      | 116.44   |
| 23  | C     | 510  | CLA  | O2A-CGA-CBA | 2.74  | 120.52      | 111.91   |
| 23  | b     | 616  | CLA  | CAC-C3C-C4C | 2.74  | 128.37      | 124.81   |
| 23  | d     | 409  | CLA  | C3C-C4C-NC  | 2.74  | 113.65      | 110.57   |
| 25  | C     | 516  | BCR  | C2-C1-C6    | 2.74  | 114.70      | 110.48   |
| 23  | b     | 606  | CLA  | C4C-C3C-C2C | -2.74 | 102.90      | 106.90   |
| 24  | a     | 2612 | PHO  | C4A-C3A-C2A | -2.74 | 100.23      | 102.84   |
| 23  | b     | 606  | CLA  | C1-C2-C3    | -2.74 | 121.31      | 126.04   |
| 23  | C     | 506  | CLA  | O2A-CGA-CBA | 2.74  | 120.50      | 111.91   |
| 23  | B     | 614  | CLA  | CED-O2D-CGD | 2.74  | 122.13      | 115.94   |
| 25  | C     | 516  | BCR  | C15-C14-C13 | -2.74 | 123.40      | 127.31   |
| 40  | h     | 101  | RRX  | C24-C23-C22 | -2.74 | 122.10      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | e     | 103  | HEM  | CBA-CAA-C2A | -2.74 | 105.03      | 112.63   |
| 23  | c     | 513  | CLA  | CHD-C1D-ND  | -2.73 | 121.94      | 124.45   |
| 23  | B     | 615  | CLA  | C3C-C4C-NC  | 2.73  | 113.64      | 110.57   |
| 23  | a     | 2613 | CLA  | CHD-C1D-ND  | -2.73 | 121.94      | 124.45   |
| 23  | a     | 2609 | CLA  | C3B-C4B-NB  | 2.73  | 113.05      | 110.52   |
| 23  | b     | 620  | CLA  | CMB-C2B-C1B | 2.73  | 129.53      | 125.37   |
| 23  | c     | 506  | CLA  | C4A-NA-C1A  | 2.73  | 107.93      | 106.71   |
| 23  | B     | 617  | CLA  | CHC-C4B-NB  | 2.73  | 127.15      | 124.26   |
| 38  | D     | 2311 | LHG  | O7-C7-C8    | 2.73  | 117.39      | 111.50   |
| 23  | c     | 505  | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.90   |
| 23  | C     | 513  | CLA  | C4A-NA-C1A  | 2.73  | 107.93      | 106.71   |
| 23  | B     | 612  | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.90   |
| 23  | c     | 515  | CLA  | C4-C3-C5    | 2.73  | 119.86      | 115.27   |
| 25  | T     | 102  | BCR  | C15-C14-C13 | 2.73  | 131.20      | 127.31   |
| 37  | D     | 2307 | DGD  | O6D-C5D-C4D | 2.73  | 114.65      | 109.69   |
| 23  | C     | 511  | CLA  | CMC-C2C-C1C | 2.73  | 129.19      | 125.04   |
| 26  | B     | 621  | SQD  | O7-S-C6     | 2.73  | 110.18      | 106.94   |
| 23  | b     | 606  | CLA  | C4-C3-C5    | 2.72  | 119.85      | 115.27   |
| 23  | B     | 610  | CLA  | CBC-CAC-C3C | -2.72 | 104.92      | 112.43   |
| 23  | C     | 513  | CLA  | CBC-CAC-C3C | -2.72 | 104.93      | 112.43   |
| 23  | b     | 617  | CLA  | C3B-C4B-NB  | 2.72  | 113.04      | 110.52   |
| 23  | C     | 512  | CLA  | CAC-C3C-C4C | 2.72  | 128.34      | 124.81   |
| 33  | A     | 422  | PL9  | C27-C26-C24 | -2.72 | 104.03      | 112.98   |
| 25  | B     | 633  | BCR  | C35-C13-C12 | 2.72  | 122.36      | 118.08   |
| 38  | d     | 403  | LHG  | O8-C23-C24  | 2.72  | 120.44      | 111.91   |
| 23  | a     | 2609 | CLA  | CAC-C3C-C4C | 2.72  | 128.34      | 124.81   |
| 23  | C     | 502  | CLA  | CHD-C4C-C3C | -2.72 | 120.85      | 124.84   |
| 23  | c     | 511  | CLA  | C1-C2-C3    | -2.72 | 121.35      | 126.04   |
| 23  | b     | 615  | CLA  | CAA-C2A-C3A | -2.71 | 105.34      | 112.78   |
| 25  | k     | 302  | BCR  | C16-C17-C18 | -2.71 | 123.44      | 127.31   |
| 25  | b     | 624  | BCR  | C8-C7-C6    | -2.71 | 119.59      | 127.20   |
| 23  | c     | 504  | CLA  | CMB-C2B-C1B | 2.71  | 129.49      | 125.37   |
| 23  | d     | 409  | CLA  | C1-C2-C3    | -2.71 | 121.36      | 126.04   |
| 23  | b     | 612  | CLA  | C3B-C4B-NB  | 2.71  | 113.03      | 110.52   |
| 31  | a     | 2617 | JOX  | O-C2-C3     | -2.71 | 120.29      | 122.76   |
| 26  | a     | 2615 | SQD  | O48-C23-C24 | 2.71  | 120.40      | 111.91   |
| 23  | b     | 619  | CLA  | O2A-CGA-CBA | 2.71  | 120.40      | 111.91   |
| 23  | c     | 512  | CLA  | CMB-C2B-C1B | 2.70  | 129.49      | 125.37   |
| 23  | d     | 409  | CLA  | C1D-CHD-C4C | -2.70 | 120.22      | 126.06   |
| 23  | B     | 614  | CLA  | C4C-C3C-C2C | -2.70 | 102.96      | 106.90   |
| 28  | j     | 2701 | LMT  | C1'-O5'-C5' | 2.70  | 118.99      | 113.69   |
| 26  | b     | 601  | SQD  | O48-C23-C24 | 2.70  | 120.37      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28  | A     | 414  | LMT  | C3'-C4'-C5' | -2.70 | 104.74      | 110.93   |
| 23  | B     | 603  | CLA  | C4-C3-C5    | 2.70  | 119.81      | 115.27   |
| 23  | c     | 508  | CLA  | O2A-CGA-CBA | 2.69  | 120.36      | 111.91   |
| 23  | c     | 514  | CLA  | O2D-CGD-O1D | -2.69 | 118.57      | 123.84   |
| 37  | c     | 519  | DGD  | C5A-C4A-C3A | -2.69 | 100.75      | 114.42   |
| 23  | a     | 2613 | CLA  | C3C-C4C-NC  | 2.69  | 113.59      | 110.57   |
| 26  | A     | 412  | SQD  | C44-O6-C1   | -2.69 | 108.48      | 113.74   |
| 23  | C     | 514  | CLA  | O2D-CGD-O1D | -2.69 | 118.57      | 123.84   |
| 23  | a     | 2610 | CLA  | CBC-CAC-C3C | -2.69 | 105.02      | 112.43   |
| 23  | b     | 616  | CLA  | C3B-C4B-NB  | 2.69  | 113.01      | 110.52   |
| 38  | D     | 2311 | LHG  | O8-C23-O10  | -2.69 | 116.81      | 123.59   |
| 23  | b     | 616  | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 23  | A     | 407  | CLA  | CHD-C4C-NC  | 2.69  | 128.44      | 124.20   |
| 37  | c     | 519  | DGD  | C3A-C2A-C1A | -2.69 | 103.85      | 113.62   |
| 25  | T     | 102  | BCR  | C3-C4-C5    | -2.68 | 109.29      | 114.08   |
| 23  | d     | 402  | CLA  | CMA-C3A-C2A | -2.68 | 103.02      | 113.83   |
| 37  | C     | 518  | DGD  | O2G-C1B-O1B | -2.68 | 117.23      | 123.70   |
| 25  | A     | 411  | BCR  | C15-C16-C17 | -2.67 | 118.00      | 123.47   |
| 38  | d     | 412  | LHG  | O7-C7-C8    | 2.67  | 117.26      | 111.50   |
| 23  | c     | 508  | CLA  | C3B-C4B-NB  | 2.67  | 112.99      | 110.52   |
| 24  | A     | 409  | PHO  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 23  | b     | 614  | CLA  | C3C-C4C-NC  | 2.67  | 113.57      | 110.57   |
| 23  | C     | 506  | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 23  | B     | 603  | CLA  | C3B-C4B-NB  | 2.67  | 112.99      | 110.52   |
| 36  | B     | 625  | HTG  | C1-O5-C5    | 2.67  | 117.50      | 112.58   |
| 23  | D     | 2304 | CLA  | C1D-CHD-C4C | -2.66 | 120.31      | 126.06   |
| 23  | B     | 612  | CLA  | C4A-NA-C1A  | 2.66  | 107.90      | 106.71   |
| 23  | b     | 611  | CLA  | O2A-CGA-O1A | -2.66 | 116.88      | 123.59   |
| 23  | C     | 503  | CLA  | O2A-CGA-CBA | 2.66  | 120.26      | 111.91   |
| 23  | b     | 614  | CLA  | C1-O2A-CGA  | 2.66  | 123.43      | 116.44   |
| 23  | b     | 616  | CLA  | CMA-C3A-C4A | -2.66 | 104.63      | 111.77   |
| 23  | a     | 2613 | CLA  | O2A-CGA-CBA | 2.66  | 120.25      | 111.91   |
| 25  | k     | 302  | BCR  | C11-C10-C9  | -2.66 | 123.52      | 127.31   |
| 23  | c     | 504  | CLA  | CMC-C2C-C1C | 2.65  | 129.08      | 125.04   |
| 23  | C     | 503  | CLA  | CHA-C1A-NA  | -2.65 | 120.32      | 126.40   |
| 25  | z     | 101  | BCR  | C38-C26-C25 | -2.65 | 121.55      | 124.53   |
| 23  | B     | 609  | CLA  | O2D-CGD-O1D | -2.65 | 118.65      | 123.84   |
| 42  | v     | 201  | HEC  | CHA-C4D-ND  | 2.65  | 127.30      | 124.42   |
| 23  | A     | 406  | CLA  | CMA-C3A-C2A | -2.65 | 103.13      | 113.83   |
| 23  | B     | 609  | CLA  | O2A-CGA-O1A | -2.65 | 116.90      | 123.59   |
| 23  | c     | 515  | CLA  | CHA-C1A-NA  | -2.65 | 120.33      | 126.40   |
| 23  | C     | 512  | CLA  | CHA-C1A-NA  | -2.65 | 120.33      | 126.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | B     | 621  | SQD  | O9-S-C6     | 2.65  | 110.09      | 106.94   |
| 36  | C     | 525  | HTG  | O5-C1-C2    | 2.65  | 113.64      | 110.31   |
| 37  | h     | 102  | DGD  | C2G-O2G-C1B | -2.65 | 111.27      | 117.79   |
| 25  | Y     | 302  | BCR  | C37-C22-C23 | 2.65  | 122.25      | 118.08   |
| 33  | D     | 2306 | PL9  | C17-C18-C19 | -2.65 | 121.29      | 127.66   |
| 23  | b     | 612  | CLA  | C4C-C3C-C2C | -2.65 | 103.04      | 106.90   |
| 23  | B     | 610  | CLA  | CED-O2D-CGD | 2.65  | 121.92      | 115.94   |
| 23  | B     | 611  | CLA  | C1C-C2C-C3C | -2.65 | 104.17      | 106.96   |
| 23  | b     | 618  | CLA  | O2A-CGA-O1A | -2.64 | 116.92      | 123.59   |
| 23  | B     | 614  | CLA  | CMC-C2C-C1C | 2.64  | 129.07      | 125.04   |
| 25  | B     | 633  | BCR  | C1-C6-C7    | 2.64  | 123.26      | 115.78   |
| 33  | D     | 2306 | PL9  | C31-C32-C33 | -2.64 | 103.19      | 111.88   |
| 23  | B     | 603  | CLA  | O2A-CGA-CBA | 2.64  | 120.20      | 111.91   |
| 36  | H     | 101  | HTG  | O5-C5-C4    | 2.64  | 114.85      | 110.77   |
| 23  | b     | 609  | CLA  | C6-C5-C3    | -2.64 | 106.53      | 113.45   |
| 25  | T     | 102  | BCR  | C1-C6-C7    | 2.64  | 123.25      | 115.78   |
| 23  | C     | 514  | CLA  | C4C-C3C-C2C | -2.64 | 103.05      | 106.90   |
| 37  | C     | 517  | DGD  | O1G-C1A-O1A | -2.64 | 116.93      | 123.59   |
| 23  | C     | 510  | CLA  | C4A-NA-C1A  | 2.64  | 107.89      | 106.71   |
| 23  | B     | 615  | CLA  | CHD-C4C-NC  | 2.64  | 128.36      | 124.20   |
| 23  | B     | 603  | CLA  | CAC-C3C-C4C | 2.64  | 128.23      | 124.81   |
| 23  | C     | 505  | CLA  | O2A-CGA-O1A | -2.64 | 116.93      | 123.59   |
| 23  | A     | 405  | CLA  | CAA-CBA-CGA | -2.64 | 105.54      | 113.25   |
| 25  | B     | 633  | BCR  | C3-C4-C5    | -2.64 | 109.37      | 114.08   |
| 23  | B     | 612  | CLA  | C1-C2-C3    | -2.64 | 121.48      | 126.04   |
| 23  | c     | 513  | CLA  | C4C-C3C-C2C | -2.64 | 103.06      | 106.90   |
| 23  | C     | 509  | CLA  | O2A-CGA-CBA | 2.64  | 120.18      | 111.91   |
| 23  | A     | 407  | CLA  | C3C-C4C-NC  | 2.64  | 113.53      | 110.57   |
| 23  | B     | 603  | CLA  | CMC-C2C-C1C | 2.64  | 129.05      | 125.04   |
| 31  | A     | 419  | JOX  | C-C5-C4     | 2.63  | 122.89      | 117.15   |
| 23  | b     | 611  | CLA  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 25  | c     | 517  | BCR  | C21-C20-C19 | -2.63 | 115.00      | 123.22   |
| 26  | D     | 2302 | SQD  | O8-S-C6     | 2.63  | 109.93      | 105.74   |
| 33  | x     | 1301 | PL9  | C15-C14-C16 | 2.63  | 119.70      | 115.27   |
| 23  | a     | 2613 | CLA  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 23  | B     | 602  | CLA  | C4C-C3C-C2C | -2.63 | 103.06      | 106.90   |
| 23  | c     | 513  | CLA  | C1-O2A-CGA  | 2.63  | 123.34      | 116.44   |
| 42  | v     | 201  | HEC  | C3D-C4D-ND  | -2.63 | 107.81      | 110.36   |
| 23  | A     | 405  | CLA  | CMC-C2C-C1C | 2.63  | 129.04      | 125.04   |
| 23  | A     | 405  | CLA  | CAC-C3C-C4C | 2.63  | 128.22      | 124.81   |
| 23  | c     | 505  | CLA  | O2A-C1-C2   | 2.63  | 115.53      | 108.64   |
| 27  | C     | 527  | LMG  | C3-C4-C5    | 2.62  | 114.92      | 110.24   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 606    | CLA  | C1C-C2C-C3C | -2.62 | 104.20      | 106.96   |
| 25  | y     | 101    | BCR  | C24-C23-C22 | -2.62 | 122.27      | 126.23   |
| 23  | c     | 510    | CLA  | CAC-C3C-C4C | 2.62  | 128.21      | 124.81   |
| 23  | c     | 509    | CLA  | C3B-C4B-NB  | 2.62  | 112.95      | 110.52   |
| 26  | A     | 412    | SQD  | O48-C23-O10 | -2.62 | 116.98      | 123.59   |
| 31  | A     | 418    | JOX  | O-C2-C3     | -2.62 | 120.38      | 122.76   |
| 23  | D     | 2304   | CLA  | O2A-CGA-O1A | -2.61 | 117.00      | 123.59   |
| 23  | b     | 611    | CLA  | CBC-CAC-C3C | -2.61 | 105.23      | 112.43   |
| 23  | b     | 607    | CLA  | C3B-C4B-NB  | 2.61  | 112.94      | 110.52   |
| 25  | Y     | 302    | BCR  | C16-C17-C18 | -2.61 | 123.58      | 127.31   |
| 23  | B     | 609    | CLA  | CMA-C3A-C4A | -2.61 | 104.77      | 111.77   |
| 23  | d     | 402    | CLA  | O2A-CGA-CBA | 2.61  | 120.08      | 111.91   |
| 23  | C     | 504    | CLA  | C1-O2A-CGA  | 2.60  | 123.28      | 116.44   |
| 23  | C     | 502    | CLA  | C4C-C3C-C2C | -2.60 | 103.10      | 106.90   |
| 23  | c     | 508    | CLA  | CHD-C1D-ND  | -2.60 | 122.06      | 124.45   |
| 39  | F     | 101    | HEM  | C2A-C1A-NA  | -2.60 | 107.24      | 110.15   |
| 23  | C     | 508    | CLA  | CHD-C1D-ND  | -2.60 | 122.06      | 124.45   |
| 38  | l     | 103    | LHG  | O8-C23-O10  | -2.60 | 117.03      | 123.59   |
| 25  | B     | 633    | BCR  | C7-C6-C5    | -2.60 | 115.16      | 121.46   |
| 23  | c     | 504    | CLA  | C4C-C3C-C2C | -2.60 | 103.11      | 106.90   |
| 36  | H     | 101    | HTG  | C5-C4-C3    | 2.60  | 112.86      | 109.67   |
| 23  | c     | 509    | CLA  | CHA-C1A-NA  | -2.60 | 120.45      | 126.40   |
| 23  | c     | 513    | CLA  | O2A-CGA-CBA | 2.60  | 120.05      | 111.91   |
| 33  | x     | 1301   | PL9  | C35-C34-C36 | 2.59  | 119.64      | 115.27   |
| 23  | C     | 505    | CLA  | C1-O2A-CGA  | 2.59  | 123.25      | 116.44   |
| 23  | C     | 507    | CLA  | CMC-C2C-C1C | 2.59  | 128.99      | 125.04   |
| 23  | b     | 620    | CLA  | C1-C2-C3    | -2.59 | 121.56      | 126.04   |
| 23  | C     | 505    | CLA  | CMC-C2C-C1C | 2.59  | 128.98      | 125.04   |
| 23  | C     | 506    | CLA  | C1-C2-C3    | -2.59 | 121.56      | 126.04   |
| 23  | b     | 621    | CLA  | O2D-CGD-O1D | -2.59 | 118.78      | 123.84   |
| 33  | d     | 411    | PL9  | C53-C6-C1   | 2.59  | 120.28      | 114.99   |
| 23  | B     | 616    | CLA  | CED-O2D-CGD | 2.59  | 121.79      | 115.94   |
| 33  | D     | 2306   | PL9  | C53-C6-C1   | 2.59  | 120.28      | 114.99   |
| 25  | y     | 101    | BCR  | C34-C9-C8   | 2.59  | 122.15      | 118.08   |
| 23  | b     | 619    | CLA  | O2A-CGA-O1A | -2.59 | 117.06      | 123.59   |
| 23  | B     | 617    | CLA  | CHA-C1A-NA  | -2.59 | 120.48      | 126.40   |
| 23  | b     | 616    | CLA  | C4A-NA-C1A  | 2.58  | 107.87      | 106.71   |
| 23  | D     | 2303   | CLA  | CMB-C2B-C1B | 2.58  | 129.30      | 125.37   |
| 36  | B     | 624[A] | HTG  | C1-C2-C3    | 2.58  | 115.69      | 110.59   |
| 23  | c     | 507    | CLA  | CHC-C1C-C2C | -2.58 | 119.56      | 126.73   |
| 23  | B     | 603    | CLA  | CHA-C1A-NA  | -2.58 | 120.49      | 126.40   |
| 23  | c     | 511    | CLA  | CHA-C1A-NA  | -2.58 | 120.49      | 126.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | D     | 2302 | SQD  | O7-S-C6     | 2.58  | 110.00      | 106.94   |
| 25  | C     | 515  | BCR  | C20-C21-C22 | -2.58 | 123.63      | 127.31   |
| 23  | b     | 620  | CLA  | CHA-C1A-NA  | -2.58 | 120.50      | 126.40   |
| 23  | B     | 614  | CLA  | CMA-C3A-C4A | -2.58 | 104.85      | 111.77   |
| 23  | B     | 603  | CLA  | C4C-C3C-C2C | -2.58 | 103.14      | 106.90   |
| 33  | d     | 411  | PL9  | C27-C28-C29 | -2.57 | 121.46      | 127.66   |
| 25  | Y     | 302  | BCR  | C10-C11-C12 | -2.57 | 115.19      | 123.22   |
| 23  | b     | 614  | CLA  | C1D-CHD-C4C | -2.57 | 120.51      | 126.06   |
| 38  | D     | 2309 | LHG  | O7-C7-O9    | -2.57 | 117.49      | 123.70   |
| 23  | B     | 613  | CLA  | O2A-CGA-CBA | 2.57  | 119.98      | 111.91   |
| 23  | C     | 506  | CLA  | CMA-C3A-C4A | -2.57 | 104.86      | 111.77   |
| 24  | A     | 408  | PHO  | CMA-C3A-C4A | -2.57 | 108.75      | 114.38   |
| 23  | b     | 616  | CLA  | C7-C6-C5    | -2.57 | 106.39      | 113.36   |
| 23  | C     | 506  | CLA  | CHD-C4C-C3C | -2.57 | 121.07      | 124.84   |
| 23  | c     | 508  | CLA  | O1D-CGD-CBD | -2.57 | 119.23      | 124.48   |
| 23  | C     | 514  | CLA  | C3C-C4C-NC  | 2.57  | 113.45      | 110.57   |
| 37  | C     | 519  | DGD  | O6E-C1E-O5D | -2.57 | 103.90      | 109.97   |
| 23  | B     | 605  | CLA  | O2A-CGA-CBA | 2.56  | 119.95      | 111.91   |
| 36  | b     | 603  | HTG  | C6-C5-C4    | -2.56 | 107.00      | 113.00   |
| 23  | c     | 510  | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 23  | B     | 611  | CLA  | CAA-CBA-CGA | -2.56 | 105.76      | 113.25   |
| 37  | H     | 103  | DGD  | O1G-C1A-O1A | -2.56 | 117.13      | 123.59   |
| 23  | d     | 409  | CLA  | C4C-C3C-C2C | -2.56 | 103.17      | 106.90   |
| 25  | k     | 302  | BCR  | C33-C5-C6   | -2.56 | 121.65      | 124.53   |
| 25  | z     | 101  | BCR  | C33-C5-C6   | -2.56 | 121.65      | 124.53   |
| 23  | b     | 606  | CLA  | CHD-C4C-C3C | -2.56 | 121.08      | 124.84   |
| 23  | C     | 512  | CLA  | O2A-CGA-CBA | 2.56  | 119.94      | 111.91   |
| 33  | D     | 2306 | PL9  | C51-C49-C50 | 2.56  | 120.25      | 114.60   |
| 28  | M     | 101  | LMT  | C1-O1'-C1'  | -2.56 | 109.60      | 113.84   |
| 23  | b     | 610  | CLA  | CMA-C3A-C4A | -2.56 | 104.90      | 111.77   |
| 23  | b     | 610  | CLA  | CHA-C1A-NA  | -2.56 | 120.54      | 126.40   |
| 23  | b     | 614  | CLA  | CHA-C1A-NA  | -2.56 | 120.55      | 126.40   |
| 38  | D     | 2310 | LHG  | O7-C7-C8    | 2.56  | 117.01      | 111.50   |
| 37  | C     | 517  | DGD  | O2G-C1B-O1B | -2.55 | 117.53      | 123.70   |
| 33  | x     | 1301 | PL9  | C46-C44-C45 | 2.55  | 120.25      | 114.60   |
| 23  | d     | 409  | CLA  | CMC-C2C-C1C | 2.55  | 128.93      | 125.04   |
| 23  | c     | 516  | CLA  | O2D-CGD-O1D | -2.55 | 118.85      | 123.84   |
| 23  | c     | 516  | CLA  | CMC-C2C-C1C | 2.55  | 128.92      | 125.04   |
| 23  | B     | 603  | CLA  | CMA-C3A-C2A | -2.55 | 103.55      | 113.83   |
| 23  | a     | 2610 | CLA  | C11-C10-C8  | -2.55 | 107.68      | 115.92   |
| 33  | d     | 411  | PL9  | C36-C37-C38 | -2.55 | 103.51      | 111.88   |
| 23  | B     | 606  | CLA  | C4-C3-C5    | 2.55  | 119.56      | 115.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | c     | 514  | CLA  | C3C-C4C-NC  | 2.55  | 113.43      | 110.57   |
| 23  | C     | 502  | CLA  | C3C-C4C-NC  | 2.55  | 113.43      | 110.57   |
| 23  | B     | 612  | CLA  | CBC-CAC-C3C | -2.55 | 105.41      | 112.43   |
| 23  | b     | 608  | CLA  | CMC-C2C-C1C | 2.54  | 128.91      | 125.04   |
| 23  | B     | 617  | CLA  | CAC-C3C-C4C | 2.54  | 128.11      | 124.81   |
| 24  | A     | 408  | PHO  | C4-C3-C5    | 2.54  | 119.55      | 115.27   |
| 42  | v     | 201  | HEC  | C2A-C1A-NA  | -2.54 | 107.85      | 110.32   |
| 23  | A     | 405  | CLA  | C4-C3-C5    | 2.54  | 119.54      | 115.27   |
| 23  | A     | 406  | CLA  | O2A-CGA-O1A | -2.54 | 117.18      | 123.59   |
| 40  | h     | 101  | RRX  | C15-C14-C13 | -2.54 | 123.69      | 127.31   |
| 23  | b     | 613  | CLA  | CMC-C2C-C1C | 2.54  | 128.91      | 125.04   |
| 23  | C     | 512  | CLA  | CHC-C1C-C2C | -2.54 | 119.68      | 126.73   |
| 23  | b     | 615  | CLA  | CAC-C3C-C4C | 2.54  | 128.10      | 124.81   |
| 23  | a     | 2609 | CLA  | CMA-C3A-C2A | -2.54 | 103.60      | 113.83   |
| 23  | c     | 514  | CLA  | CMC-C2C-C1C | 2.54  | 128.90      | 125.04   |
| 23  | A     | 407  | CLA  | C3B-C4B-NB  | 2.54  | 112.87      | 110.52   |
| 23  | a     | 2610 | CLA  | C1D-CHD-C4C | -2.53 | 120.59      | 126.06   |
| 27  | c     | 522  | LMG  | O8-C28-C29  | 2.53  | 119.86      | 111.91   |
| 23  | a     | 2610 | CLA  | C1-C2-C3    | -2.53 | 121.66      | 126.04   |
| 23  | B     | 616  | CLA  | CBA-CAA-C2A | -2.53 | 106.38      | 113.86   |
| 23  | C     | 506  | CLA  | C4-C3-C5    | 2.53  | 119.53      | 115.27   |
| 23  | C     | 507  | CLA  | CAA-C2A-C3A | -2.53 | 105.85      | 112.78   |
| 28  | d     | 401  | LMT  | C1B-O1B-C4' | -2.53 | 111.70      | 117.96   |
| 28  | z     | 102  | LMT  | O5B-C5B-C4B | 2.53  | 114.29      | 109.69   |
| 26  | a     | 2615 | SQD  | O47-C7-O49  | -2.53 | 117.59      | 123.70   |
| 23  | A     | 405  | CLA  | O2A-CGA-O1A | -2.53 | 117.22      | 123.59   |
| 23  | b     | 608  | CLA  | C5-C3-C2    | -2.53 | 116.01      | 121.12   |
| 38  | E     | 101  | LHG  | C5-O7-C7    | -2.53 | 111.57      | 117.79   |
| 23  | B     | 608  | CLA  | O2D-CGD-O1D | -2.53 | 118.90      | 123.84   |
| 31  | A     | 419  | JOX  | C4-C3-C2    | -2.52 | 121.16      | 123.18   |
| 25  | B     | 620  | BCR  | C2-C3-C4    | -2.52 | 105.75      | 111.38   |
| 28  | m     | 2804 | LMT  | O5'-C5'-C4' | 2.52  | 115.06      | 109.75   |
| 24  | a     | 2611 | PHO  | CMB-C2B-C3B | 2.52  | 129.39      | 124.68   |
| 23  | A     | 406  | CLA  | O2A-CGA-CBA | 2.52  | 119.81      | 111.91   |
| 23  | C     | 509  | CLA  | C3B-C4B-NB  | 2.52  | 112.85      | 110.52   |
| 23  | b     | 609  | CLA  | O2A-CGA-CBA | 2.51  | 119.80      | 111.91   |
| 23  | B     | 615  | CLA  | C4C-C3C-C2C | -2.51 | 103.23      | 106.90   |
| 23  | B     | 608  | CLA  | C4C-C3C-C2C | -2.51 | 103.23      | 106.90   |
| 23  | A     | 406  | CLA  | CHC-C1C-C2C | -2.51 | 119.75      | 126.73   |
| 23  | C     | 511  | CLA  | CMB-C2B-C1B | 2.51  | 129.20      | 125.37   |
| 25  | B     | 619  | BCR  | C31-C1-C6   | -2.51 | 106.22      | 110.30   |
| 23  | b     | 609  | CLA  | C3B-C4B-NB  | 2.51  | 112.84      | 110.52   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26  | l     | 101    | SQD  | O48-C23-C24 | 2.51  | 119.78      | 111.91   |
| 23  | C     | 503    | CLA  | CMB-C2B-C1B | 2.51  | 129.19      | 125.37   |
| 36  | b     | 604    | HTG  | C3-C4-C5    | 2.51  | 114.71      | 110.24   |
| 23  | b     | 611    | CLA  | CHA-C1A-NA  | -2.50 | 120.66      | 126.40   |
| 23  | D     | 2303   | CLA  | CAA-C2A-C3A | -2.50 | 105.92      | 112.78   |
| 42  | v     | 201    | HEC  | CBC-CAC-C3C | 2.50  | 119.33      | 112.43   |
| 23  | c     | 505    | CLA  | CED-O2D-CGD | 2.50  | 121.60      | 115.94   |
| 26  | B     | 621    | SQD  | O5-C1-C2    | 2.50  | 115.64      | 110.35   |
| 23  | c     | 510    | CLA  | CHA-C1A-NA  | -2.50 | 120.67      | 126.40   |
| 23  | c     | 515    | CLA  | C3B-C4B-NB  | 2.50  | 112.83      | 110.52   |
| 38  | D     | 2310   | LHG  | O8-C23-C24  | 2.50  | 119.75      | 111.91   |
| 23  | c     | 506    | CLA  | O2A-CGA-O1A | -2.50 | 117.28      | 123.59   |
| 33  | A     | 422    | PL9  | C22-C23-C24 | -2.50 | 121.64      | 127.66   |
| 23  | C     | 507    | CLA  | O2A-CGA-O1A | -2.50 | 117.28      | 123.59   |
| 23  | b     | 621    | CLA  | OBD-CAD-C3D | -2.49 | 122.52      | 128.52   |
| 23  | B     | 609    | CLA  | CMA-C3A-C2A | -2.49 | 103.77      | 113.83   |
| 23  | c     | 514    | CLA  | O2A-CGA-O1A | -2.49 | 117.30      | 123.59   |
| 23  | B     | 609    | CLA  | CHD-C1D-ND  | -2.49 | 122.16      | 124.45   |
| 37  | c     | 520    | DGD  | O1G-C1A-O1A | -2.49 | 117.31      | 123.59   |
| 25  | b     | 624    | BCR  | C11-C10-C9  | -2.49 | 123.76      | 127.31   |
| 23  | b     | 620    | CLA  | C6-C5-C3    | -2.49 | 106.93      | 113.45   |
| 23  | a     | 2610   | CLA  | C3B-C4B-NB  | 2.49  | 112.82      | 110.52   |
| 23  | b     | 613    | CLA  | CMA-C3A-C2A | -2.49 | 103.80      | 113.83   |
| 26  | b     | 601    | SQD  | O48-C23-O10 | -2.49 | 117.32      | 123.59   |
| 23  | C     | 510    | CLA  | CAC-C3C-C4C | 2.48  | 128.03      | 124.81   |
| 23  | d     | 402    | CLA  | O2D-CGD-O1D | -2.48 | 118.98      | 123.84   |
| 33  | A     | 422    | PL9  | C37-C38-C39 | -2.48 | 121.68      | 127.66   |
| 23  | b     | 620    | CLA  | C6-C7-C8    | -2.48 | 107.90      | 115.92   |
| 23  | b     | 608    | CLA  | C3B-C4B-NB  | 2.48  | 112.81      | 110.52   |
| 25  | K     | 101    | BCR  | C38-C26-C25 | -2.48 | 121.74      | 124.53   |
| 23  | d     | 408    | CLA  | CBC-CAC-C3C | -2.48 | 105.60      | 112.43   |
| 42  | v     | 201    | HEC  | CBD-CAD-C3D | -2.48 | 105.74      | 112.63   |
| 23  | C     | 505    | CLA  | C3C-C4C-NC  | 2.48  | 113.35      | 110.57   |
| 23  | C     | 503    | CLA  | O2A-CGA-O1A | -2.48 | 117.34      | 123.59   |
| 23  | d     | 409    | CLA  | C6-C7-C8    | -2.48 | 107.91      | 115.92   |
| 36  | B     | 624[A] | HTG  | C1'-S1-C1   | 2.48  | 104.72      | 100.09   |
| 23  | b     | 620    | CLA  | C4-C3-C5    | 2.47  | 119.43      | 115.27   |
| 23  | B     | 603    | CLA  | CMA-C3A-C4A | -2.47 | 105.12      | 111.77   |
| 23  | a     | 2613   | CLA  | CMB-C2B-C1B | 2.47  | 129.14      | 125.37   |
| 26  | D     | 2308   | SQD  | C44-O6-C1   | -2.47 | 108.91      | 113.74   |
| 42  | V     | 201    | HEC  | C4A-NA-C1A  | 2.47  | 107.77      | 105.35   |
| 23  | a     | 2610   | CLA  | CMB-C2B-C1B | 2.47  | 129.13      | 125.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 37  | c     | 519  | DGD  | O1G-C1A-O1A | -2.47 | 117.36      | 123.59   |
| 25  | b     | 623  | BCR  | C8-C7-C6    | -2.47 | 120.26      | 127.20   |
| 23  | b     | 612  | CLA  | O2D-CGD-O1D | -2.47 | 119.01      | 123.84   |
| 23  | c     | 514  | CLA  | O2A-CGA-CBA | 2.47  | 119.66      | 111.91   |
| 36  | I     | 101  | HTG  | O5-C5-C4    | 2.47  | 114.18      | 109.69   |
| 23  | c     | 509  | CLA  | O2A-C1-C2   | 2.46  | 115.11      | 108.64   |
| 23  | B     | 608  | CLA  | CMC-C2C-C1C | 2.46  | 128.79      | 125.04   |
| 37  | D     | 2307 | DGD  | O1G-C1A-O1A | -2.46 | 117.38      | 123.59   |
| 23  | C     | 507  | CLA  | CHA-C1A-NA  | -2.46 | 120.76      | 126.40   |
| 23  | B     | 602  | CLA  | C4-C3-C5    | 2.46  | 119.41      | 115.27   |
| 25  | A     | 411  | BCR  | C3-C4-C5    | -2.46 | 109.68      | 114.08   |
| 23  | C     | 513  | CLA  | C4-C3-C5    | 2.46  | 119.41      | 115.27   |
| 23  | B     | 604  | CLA  | C1-O2A-CGA  | 2.46  | 122.89      | 116.44   |
| 23  | B     | 617  | CLA  | C1-C2-C3    | -2.46 | 121.80      | 126.04   |
| 23  | b     | 607  | CLA  | CMA-C3A-C4A | -2.46 | 105.17      | 111.77   |
| 23  | B     | 614  | CLA  | O2A-CGA-O1A | -2.45 | 117.40      | 123.59   |
| 24  | a     | 2611 | PHO  | CMA-C3A-C4A | -2.45 | 109.00      | 114.38   |
| 25  | y     | 101  | BCR  | C21-C20-C19 | -2.45 | 115.56      | 123.22   |
| 23  | C     | 511  | CLA  | C4A-NA-C1A  | 2.45  | 107.81      | 106.71   |
| 37  | h     | 102  | DGD  | C3G-O3G-C1D | -2.45 | 108.95      | 113.74   |
| 23  | b     | 612  | CLA  | CAA-C2A-C3A | -2.45 | 106.07      | 112.78   |
| 25  | C     | 516  | BCR  | C21-C20-C19 | -2.45 | 115.58      | 123.22   |
| 23  | a     | 2610 | CLA  | CAA-C2A-C3A | -2.45 | 106.07      | 112.78   |
| 33  | d     | 411  | PL9  | C25-C24-C26 | 2.45  | 119.39      | 115.27   |
| 23  | B     | 609  | CLA  | CMB-C2B-C1B | 2.45  | 129.10      | 125.37   |
| 25  | z     | 101  | BCR  | C20-C21-C22 | -2.45 | 123.82      | 127.31   |
| 23  | C     | 508  | CLA  | O2A-CGA-CBA | 2.45  | 119.58      | 111.91   |
| 33  | A     | 422  | PL9  | C20-C19-C21 | 2.45  | 119.39      | 115.27   |
| 33  | d     | 411  | PL9  | C10-C9-C11  | 2.45  | 119.39      | 115.27   |
| 23  | C     | 504  | CLA  | O2A-CGA-CBA | 2.45  | 119.58      | 111.91   |
| 26  | A     | 412  | SQD  | C1-O5-C5    | -2.44 | 108.89      | 113.69   |
| 23  | b     | 607  | CLA  | O2A-CGA-CBA | 2.44  | 119.58      | 111.91   |
| 36  | b     | 625  | HTG  | C1-C2-C3    | 2.44  | 115.42      | 110.59   |
| 23  | d     | 402  | CLA  | CMA-C3A-C4A | -2.44 | 105.20      | 111.77   |
| 37  | C     | 519  | DGD  | O2G-C1B-O1B | -2.44 | 117.80      | 123.70   |
| 27  | C     | 520  | LMG  | O8-C28-O10  | -2.44 | 117.43      | 123.59   |
| 38  | d     | 403  | LHG  | O8-C23-O10  | -2.44 | 117.43      | 123.59   |
| 23  | C     | 504  | CLA  | CHC-C4B-NB  | 2.44  | 126.84      | 124.26   |
| 23  | d     | 408  | CLA  | CMA-C3A-C2A | -2.44 | 103.99      | 113.83   |
| 37  | c     | 519  | DGD  | O2G-C1B-O1B | -2.44 | 117.81      | 123.70   |
| 23  | C     | 508  | CLA  | C4-C3-C5    | 2.43  | 119.36      | 115.27   |
| 23  | b     | 617  | CLA  | O2D-CGD-O1D | -2.43 | 119.08      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | b     | 606  | CLA  | O2A-CGA-CBA | 2.43  | 119.54      | 111.91   |
| 26  | D     | 2308 | SQD  | O9-S-C6     | 2.43  | 109.83      | 106.94   |
| 23  | C     | 502  | CLA  | CHA-C1A-NA  | -2.43 | 120.83      | 126.40   |
| 33  | D     | 2306 | PL9  | C40-C39-C38 | -2.43 | 117.44      | 123.68   |
| 23  | c     | 512  | CLA  | O2A-CGA-CBA | 2.43  | 119.53      | 111.91   |
| 23  | d     | 409  | CLA  | O2A-CGA-O1A | -2.43 | 117.46      | 123.59   |
| 23  | b     | 619  | CLA  | CMC-C2C-C1C | 2.43  | 128.74      | 125.04   |
| 23  | d     | 408  | CLA  | C1D-CHD-C4C | -2.43 | 120.82      | 126.06   |
| 23  | c     | 516  | CLA  | CBC-CAC-C3C | -2.43 | 105.74      | 112.43   |
| 33  | D     | 2306 | PL9  | C15-C14-C16 | 2.43  | 119.36      | 115.27   |
| 23  | c     | 508  | CLA  | CBC-CAC-C3C | -2.43 | 105.74      | 112.43   |
| 25  | T     | 102  | BCR  | C21-C20-C19 | -2.43 | 115.64      | 123.22   |
| 23  | C     | 508  | CLA  | CHB-C1B-C2B | -2.43 | 120.39      | 127.24   |
| 23  | B     | 607  | CLA  | CMC-C2C-C1C | 2.42  | 128.73      | 125.04   |
| 23  | B     | 610  | CLA  | C3B-C4B-NB  | 2.42  | 112.76      | 110.52   |
| 23  | c     | 504  | CLA  | C4-C3-C5    | 2.42  | 119.35      | 115.27   |
| 23  | C     | 506  | CLA  | CMD-C2D-C3D | -2.42 | 122.04      | 127.61   |
| 23  | b     | 607  | CLA  | CHA-C1A-NA  | -2.42 | 120.86      | 126.40   |
| 25  | K     | 101  | BCR  | C15-C14-C13 | -2.42 | 123.86      | 127.31   |
| 25  | k     | 302  | BCR  | C3-C4-C5    | -2.42 | 109.76      | 114.08   |
| 23  | C     | 505  | CLA  | OBD-CAD-C3D | -2.42 | 122.71      | 128.52   |
| 25  | a     | 2614 | BCR  | C11-C10-C9  | -2.41 | 123.86      | 127.31   |
| 23  | b     | 615  | CLA  | CMC-C2C-C1C | 2.41  | 128.71      | 125.04   |
| 23  | c     | 512  | CLA  | CBC-CAC-C3C | -2.41 | 105.78      | 112.43   |
| 23  | A     | 406  | CLA  | CED-O2D-CGD | 2.41  | 121.39      | 115.94   |
| 23  | b     | 616  | CLA  | CHC-C1C-C2C | -2.41 | 120.04      | 126.73   |
| 23  | a     | 2609 | CLA  | O2D-CGD-CBD | 2.41  | 115.55      | 111.27   |
| 39  | e     | 103  | HEM  | C4A-NA-C1A  | 2.41  | 107.71      | 105.35   |
| 23  | d     | 402  | CLA  | C4C-C3C-C2C | -2.41 | 103.39      | 106.90   |
| 23  | b     | 620  | CLA  | O2D-CGD-O1D | -2.41 | 119.14      | 123.84   |
| 23  | A     | 407  | CLA  | CMC-C2C-C1C | 2.40  | 128.70      | 125.04   |
| 25  | B     | 633  | BCR  | C33-C5-C4   | 2.40  | 118.23      | 113.62   |
| 23  | B     | 611  | CLA  | O2A-CGA-CBA | 2.40  | 119.45      | 111.91   |
| 24  | a     | 2611 | PHO  | C1-C2-C3    | -2.40 | 121.89      | 126.04   |
| 36  | c     | 524  | HTG  | C1-O5-C5    | 2.40  | 117.01      | 112.58   |
| 31  | a     | 2617 | JOX  | O1-C5-C4    | -2.40 | 117.97      | 121.41   |
| 23  | b     | 616  | CLA  | C3C-C4C-NC  | 2.40  | 113.27      | 110.57   |
| 25  | k     | 302  | BCR  | C8-C7-C6    | -2.40 | 120.46      | 127.20   |
| 23  | A     | 406  | CLA  | CMA-C3A-C4A | -2.40 | 105.32      | 111.77   |
| 23  | A     | 405  | CLA  | CMA-C3A-C2A | -2.40 | 104.14      | 113.83   |
| 23  | C     | 507  | CLA  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 26  | a     | 2615 | SQD  | C44-O6-C1   | -2.40 | 109.05      | 113.74   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 28  | m     | 2804   | LMT  | C1-O1'-C1'  | -2.40 | 109.86      | 113.84   |
| 23  | d     | 408    | CLA  | CHA-C1A-NA  | -2.40 | 120.91      | 126.40   |
| 23  | b     | 617    | CLA  | O2A-C1-C2   | -2.40 | 102.33      | 108.64   |
| 23  | B     | 609    | CLA  | C4-C3-C5    | 2.40  | 119.30      | 115.27   |
| 23  | C     | 507    | CLA  | CED-O2D-CGD | 2.40  | 121.36      | 115.94   |
| 23  | c     | 506    | CLA  | O2A-CGA-CBA | 2.40  | 119.43      | 111.91   |
| 23  | d     | 409    | CLA  | CHA-C1A-NA  | -2.40 | 120.91      | 126.40   |
| 24  | A     | 409    | PHO  | C4-C3-C2    | -2.40 | 117.53      | 123.68   |
| 23  | c     | 513    | CLA  | CMC-C2C-C1C | 2.40  | 128.69      | 125.04   |
| 23  | b     | 621    | CLA  | C4-C3-C5    | 2.39  | 119.30      | 115.27   |
| 23  | D     | 2304   | CLA  | C4-C3-C5    | 2.39  | 119.30      | 115.27   |
| 23  | D     | 2303   | CLA  | C3B-C4B-NB  | 2.39  | 112.73      | 110.52   |
| 23  | c     | 514    | CLA  | C4C-C3C-C2C | -2.39 | 103.41      | 106.90   |
| 23  | A     | 407    | CLA  | O2A-CGA-CBA | 2.39  | 119.41      | 111.91   |
| 23  | b     | 620    | CLA  | CBC-CAC-C3C | -2.39 | 105.84      | 112.43   |
| 23  | b     | 614    | CLA  | O2A-CGA-O1A | -2.39 | 117.56      | 123.59   |
| 23  | c     | 504    | CLA  | C3B-C4B-NB  | 2.39  | 112.73      | 110.52   |
| 24  | a     | 2611   | PHO  | CBA-CAA-C2A | -2.39 | 106.83      | 113.81   |
| 36  | b     | 604    | HTG  | C1-O5-C5    | 2.39  | 116.99      | 112.58   |
| 23  | B     | 605    | CLA  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 36  | B     | 624[A] | HTG  | O5-C5-C6    | 2.39  | 112.37      | 106.44   |
| 28  | d     | 404    | LMT  | C1'-O5'-C5' | 2.39  | 118.37      | 113.69   |
| 24  | a     | 2612   | PHO  | C4-C3-C2    | -2.39 | 117.56      | 123.68   |
| 23  | B     | 615    | CLA  | CAC-C3C-C4C | 2.38  | 127.90      | 124.81   |
| 23  | B     | 616    | CLA  | O2A-CGA-O1A | -2.38 | 117.57      | 123.59   |
| 23  | b     | 606    | CLA  | CHA-C1A-NA  | -2.38 | 120.94      | 126.40   |
| 23  | b     | 616    | CLA  | CHD-C4C-NC  | 2.38  | 127.96      | 124.20   |
| 27  | C     | 527    | LMG  | O8-C28-O10  | -2.38 | 117.58      | 123.59   |
| 23  | B     | 603    | CLA  | CHC-C1C-C2C | -2.38 | 120.11      | 126.73   |
| 23  | D     | 2303   | CLA  | CAC-C3C-C2C | 2.38  | 131.60      | 127.53   |
| 37  | c     | 520    | DGD  | O3G-C3G-C2G | -2.38 | 105.16      | 110.90   |
| 23  | b     | 619    | CLA  | C3B-C4B-NB  | 2.38  | 112.72      | 110.52   |
| 23  | b     | 618    | CLA  | CMA-C3A-C4A | -2.38 | 105.38      | 111.77   |
| 23  | A     | 405    | CLA  | O2D-CGD-O1D | -2.38 | 119.19      | 123.84   |
| 23  | A     | 410    | CLA  | C7-C6-C5    | -2.38 | 106.90      | 113.36   |
| 38  | D     | 2309   | LHG  | C5-O7-C7    | -2.38 | 111.93      | 117.79   |
| 25  | z     | 101    | BCR  | C11-C10-C9  | -2.38 | 123.92      | 127.31   |
| 26  | D     | 2302   | SQD  | O47-C7-O49  | -2.38 | 117.96      | 123.70   |
| 23  | c     | 514    | CLA  | C4A-NA-C1A  | 2.38  | 107.77      | 106.71   |
| 23  | B     | 616    | CLA  | CHC-C1C-C2C | -2.37 | 120.13      | 126.73   |
| 23  | B     | 612    | CLA  | CHC-C1C-C2C | -2.37 | 120.14      | 126.73   |
| 23  | B     | 611    | CLA  | CMC-C2C-C1C | 2.37  | 128.65      | 125.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42  | v     | 201  | HEC  | C4B-NB-C1B  | 2.37  | 107.52      | 105.07   |
| 38  | E     | 101  | LHG  | O8-C23-C24  | 2.37  | 119.35      | 111.91   |
| 23  | C     | 513  | CLA  | C2C-C1C-NC  | 2.37  | 112.19      | 109.97   |
| 26  | a     | 2603 | SQD  | O48-C23-C24 | 2.37  | 119.35      | 111.91   |
| 23  | C     | 511  | CLA  | CAA-CBA-CGA | -2.37 | 106.33      | 113.25   |
| 33  | x     | 1301 | PL9  | C40-C39-C41 | 2.37  | 119.26      | 115.27   |
| 23  | C     | 505  | CLA  | C3B-C4B-NB  | 2.37  | 112.71      | 110.52   |
| 27  | d     | 414  | LMG  | O7-C10-C11  | 2.37  | 116.60      | 111.50   |
| 23  | b     | 612  | CLA  | C1-C2-C3    | -2.37 | 121.95      | 126.04   |
| 23  | c     | 509  | CLA  | CGD-CBD-CAD | -2.36 | 103.08      | 110.73   |
| 25  | b     | 624  | BCR  | C16-C17-C18 | -2.36 | 123.94      | 127.31   |
| 24  | a     | 2611 | PHO  | O1D-CGD-CBD | -2.36 | 120.80      | 124.74   |
| 42  | v     | 201  | HEC  | C1D-C2D-C3D | -2.36 | 104.47      | 106.96   |
| 23  | C     | 506  | CLA  | O2A-CGA-O1A | -2.36 | 117.63      | 123.59   |
| 25  | K     | 101  | BCR  | C33-C5-C6   | -2.36 | 121.88      | 124.53   |
| 25  | a     | 2614 | BCR  | C38-C26-C25 | -2.36 | 121.88      | 124.53   |
| 27  | D     | 2312 | LMG  | O8-C28-O10  | -2.36 | 117.63      | 123.59   |
| 39  | F     | 101  | HEM  | CBA-CAA-C2A | -2.36 | 106.07      | 112.63   |
| 28  | Z     | 101  | LMT  | C1B-O5B-C5B | 2.36  | 118.32      | 113.69   |
| 23  | C     | 506  | CLA  | C3B-C4B-NB  | 2.36  | 112.70      | 110.52   |
| 28  | T     | 103  | LMT  | C1-O1'-C1'  | -2.36 | 109.93      | 113.84   |
| 33  | D     | 2306 | PL9  | C22-C23-C24 | -2.36 | 121.98      | 127.66   |
| 33  | D     | 2306 | PL9  | C30-C29-C31 | 2.36  | 119.24      | 115.27   |
| 23  | c     | 515  | CLA  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 26  | b     | 601  | SQD  | C45-O47-C7  | -2.36 | 111.99      | 117.79   |
| 23  | B     | 605  | CLA  | CHA-C1A-NA  | -2.35 | 121.01      | 126.40   |
| 23  | b     | 612  | CLA  | O2A-CGA-O1A | -2.35 | 117.65      | 123.59   |
| 23  | b     | 606  | CLA  | CBC-CAC-C3C | -2.35 | 105.94      | 112.43   |
| 26  | A     | 412  | SQD  | O47-C7-O49  | -2.35 | 118.02      | 123.70   |
| 25  | B     | 620  | BCR  | C3-C4-C5    | -2.35 | 109.88      | 114.08   |
| 25  | b     | 624  | BCR  | C21-C20-C19 | -2.35 | 115.88      | 123.22   |
| 23  | b     | 613  | CLA  | CMA-C3A-C4A | -2.35 | 105.45      | 111.77   |
| 23  | C     | 505  | CLA  | CMA-C3A-C4A | -2.35 | 105.45      | 111.77   |
| 23  | B     | 607  | CLA  | CHA-C1A-NA  | -2.35 | 121.02      | 126.40   |
| 23  | b     | 608  | CLA  | CHB-C1B-C2B | -2.35 | 120.60      | 127.24   |
| 25  | k     | 302  | BCR  | C7-C8-C9    | -2.35 | 122.69      | 126.23   |
| 23  | b     | 621  | CLA  | CHC-C1C-C2C | -2.35 | 120.21      | 126.73   |
| 25  | B     | 633  | BCR  | C21-C20-C19 | -2.35 | 115.89      | 123.22   |
| 23  | b     | 621  | CLA  | O1D-CGD-CBD | -2.35 | 119.68      | 124.48   |
| 25  | b     | 622  | BCR  | C38-C26-C25 | -2.35 | 121.89      | 124.53   |
| 23  | B     | 615  | CLA  | CMC-C2C-C1C | 2.35  | 128.61      | 125.04   |
| 26  | a     | 2615 | SQD  | O48-C23-O10 | -2.34 | 117.68      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | b     | 618  | CLA  | CHA-C1A-NA  | -2.34 | 121.03      | 126.40   |
| 23  | c     | 507  | CLA  | C4C-C3C-C2C | -2.34 | 103.49      | 106.90   |
| 23  | b     | 609  | CLA  | O1D-CGD-CBD | -2.34 | 119.70      | 124.48   |
| 23  | C     | 509  | CLA  | CHC-C1C-C2C | -2.34 | 120.24      | 126.73   |
| 23  | c     | 513  | CLA  | CHA-C1A-NA  | -2.34 | 121.05      | 126.40   |
| 25  | b     | 624  | BCR  | C2-C1-C6    | 2.34  | 114.08      | 110.48   |
| 23  | d     | 408  | CLA  | O2A-CGA-O1A | -2.34 | 117.69      | 123.59   |
| 23  | c     | 512  | CLA  | CHA-C1A-NA  | -2.34 | 121.05      | 126.40   |
| 23  | B     | 603  | CLA  | O2A-CGA-O1A | -2.34 | 117.70      | 123.59   |
| 23  | b     | 614  | CLA  | C4-C3-C5    | 2.34  | 119.20      | 115.27   |
| 25  | z     | 101  | BCR  | C35-C13-C14 | -2.33 | 119.65      | 122.92   |
| 23  | c     | 506  | CLA  | CHC-C4B-NB  | 2.33  | 126.73      | 124.26   |
| 27  | A     | 413  | LMG  | O7-C10-O9   | -2.33 | 118.06      | 123.70   |
| 36  | I     | 101  | HTG  | O5-C1-C2    | 2.33  | 113.25      | 110.31   |
| 25  | z     | 101  | BCR  | C8-C7-C6    | -2.33 | 120.65      | 127.20   |
| 23  | b     | 611  | CLA  | CHC-C4B-NB  | 2.33  | 126.72      | 124.26   |
| 25  | K     | 101  | BCR  | C10-C11-C12 | -2.33 | 115.94      | 123.22   |
| 23  | d     | 402  | CLA  | CHB-C4A-NA  | 2.33  | 127.73      | 124.51   |
| 23  | C     | 510  | CLA  | O2A-CGA-O1A | -2.33 | 117.71      | 123.59   |
| 23  | c     | 506  | CLA  | CMC-C2C-C1C | 2.33  | 128.59      | 125.04   |
| 25  | y     | 101  | BCR  | C34-C9-C10  | -2.33 | 119.66      | 122.92   |
| 37  | D     | 2307 | DGD  | C1D-O6D-C5D | 2.33  | 118.26      | 113.69   |
| 23  | A     | 406  | CLA  | C1-O2A-CGA  | 2.33  | 122.55      | 116.44   |
| 23  | c     | 510  | CLA  | O1D-CGD-CBD | -2.33 | 119.72      | 124.48   |
| 23  | c     | 509  | CLA  | CAC-C3C-C4C | 2.33  | 127.83      | 124.81   |
| 23  | c     | 515  | CLA  | C4A-NA-C1A  | 2.33  | 107.75      | 106.71   |
| 23  | B     | 609  | CLA  | CAA-C2A-C3A | -2.32 | 106.42      | 112.78   |
| 23  | B     | 615  | CLA  | OBD-CAD-C3D | -2.32 | 122.93      | 128.52   |
| 25  | Y     | 302  | BCR  | C1-C6-C7    | 2.32  | 122.34      | 115.78   |
| 23  | C     | 511  | CLA  | CMA-C3A-C4A | -2.32 | 105.54      | 111.77   |
| 23  | b     | 608  | CLA  | CMB-C2B-C1B | 2.32  | 128.90      | 125.37   |
| 23  | b     | 616  | CLA  | C4C-C3C-C2C | -2.32 | 103.52      | 106.90   |
| 28  | d     | 404  | LMT  | O5'-C5'-C4' | 2.32  | 114.64      | 109.75   |
| 23  | b     | 613  | CLA  | C11-C12-C13 | -2.32 | 108.43      | 115.92   |
| 28  | Z     | 101  | LMT  | C1-O1'-C1'  | -2.32 | 110.00      | 113.84   |
| 23  | C     | 510  | CLA  | CMC-C2C-C1C | 2.32  | 128.57      | 125.04   |
| 23  | b     | 613  | CLA  | C11-C10-C8  | -2.32 | 108.44      | 115.92   |
| 23  | b     | 618  | CLA  | C4-C3-C5    | 2.31  | 119.16      | 115.27   |
| 25  | b     | 624  | BCR  | C33-C5-C6   | -2.31 | 121.93      | 124.53   |
| 23  | C     | 511  | CLA  | O1D-CGD-CBD | -2.31 | 119.75      | 124.48   |
| 23  | B     | 607  | CLA  | O2A-CGA-O1A | -2.31 | 117.76      | 123.59   |
| 23  | C     | 507  | CLA  | CHB-C1B-C2B | -2.31 | 120.71      | 127.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | C     | 508  | CLA  | O2A-CGA-O1A | -2.31 | 117.76      | 123.59   |
| 23  | B     | 602  | CLA  | CHA-C1A-NA  | -2.31 | 121.11      | 126.40   |
| 23  | A     | 406  | CLA  | C4-C3-C5    | 2.31  | 119.16      | 115.27   |
| 23  | C     | 513  | CLA  | CMC-C2C-C1C | 2.31  | 128.56      | 125.04   |
| 23  | a     | 2613 | CLA  | CMA-C3A-C4A | -2.31 | 105.57      | 111.77   |
| 23  | B     | 605  | CLA  | C4C-C3C-C2C | -2.31 | 103.53      | 106.90   |
| 23  | c     | 508  | CLA  | O2A-CGA-O1A | -2.31 | 117.77      | 123.59   |
| 28  | M     | 101  | LMT  | C1'-C2'-C3' | -2.31 | 105.19      | 110.00   |
| 23  | B     | 607  | CLA  | CHB-C1B-C2B | -2.31 | 120.72      | 127.24   |
| 23  | a     | 2613 | CLA  | C4C-C3C-C2C | -2.31 | 103.54      | 106.90   |
| 23  | b     | 621  | CLA  | CHD-C1D-C2D | -2.31 | 120.64      | 125.48   |
| 23  | C     | 502  | CLA  | O2A-CGA-O1A | -2.30 | 117.78      | 123.59   |
| 23  | a     | 2613 | CLA  | CMC-C2C-C1C | 2.30  | 128.55      | 125.04   |
| 37  | c     | 520  | DGD  | O3G-C1D-C2D | -2.30 | 104.71      | 108.30   |
| 25  | c     | 517  | BCR  | C16-C17-C18 | -2.30 | 124.02      | 127.31   |
| 26  | B     | 621  | SQD  | O47-C7-O49  | -2.30 | 118.14      | 123.70   |
| 23  | B     | 605  | CLA  | CMB-C2B-C1B | 2.30  | 128.88      | 125.37   |
| 28  | T     | 103  | LMT  | O1'-C1'-C2' | 2.30  | 111.90      | 108.30   |
| 25  | B     | 619  | BCR  | C20-C21-C22 | -2.30 | 124.02      | 127.31   |
| 33  | A     | 422  | PL9  | C46-C44-C45 | 2.30  | 119.68      | 114.60   |
| 25  | K     | 101  | BCR  | C3-C4-C5    | -2.30 | 109.98      | 114.08   |
| 23  | b     | 619  | CLA  | CHC-C1C-C2C | -2.29 | 120.36      | 126.73   |
| 33  | d     | 411  | PL9  | C22-C23-C24 | -2.29 | 122.14      | 127.66   |
| 26  | l     | 101  | SQD  | O47-C7-O49  | -2.29 | 118.16      | 123.70   |
| 23  | C     | 511  | CLA  | C4-C3-C2    | -2.29 | 117.80      | 123.68   |
| 23  | A     | 407  | CLA  | C4C-C3C-C2C | -2.29 | 103.56      | 106.90   |
| 25  | B     | 620  | BCR  | C7-C8-C9    | -2.29 | 122.77      | 126.23   |
| 23  | D     | 2304 | CLA  | O2A-CGA-CBA | 2.29  | 119.10      | 111.91   |
| 25  | D     | 2305 | BCR  | C15-C14-C13 | -2.29 | 124.04      | 127.31   |
| 25  | b     | 622  | BCR  | C15-C14-C13 | -2.29 | 124.04      | 127.31   |
| 25  | b     | 624  | BCR  | C10-C11-C12 | -2.29 | 116.07      | 123.22   |
| 25  | z     | 101  | BCR  | C2-C1-C6    | 2.29  | 114.01      | 110.48   |
| 23  | b     | 617  | CLA  | O2A-CGA-O1A | -2.29 | 117.81      | 123.59   |
| 23  | B     | 611  | CLA  | CHA-C1A-NA  | -2.29 | 121.16      | 126.40   |
| 33  | d     | 411  | PL9  | C40-C39-C38 | -2.29 | 117.81      | 123.68   |
| 25  | b     | 624  | BCR  | C32-C1-C6   | -2.29 | 106.59      | 110.30   |
| 25  | c     | 517  | BCR  | C3-C4-C5    | -2.29 | 109.99      | 114.08   |
| 23  | B     | 616  | CLA  | C1-C2-C3    | -2.29 | 122.09      | 126.04   |
| 23  | C     | 503  | CLA  | C4A-NA-C1A  | 2.28  | 107.73      | 106.71   |
| 37  | C     | 518  | DGD  | O1G-C1A-C2A | 2.28  | 119.08      | 111.91   |
| 33  | D     | 2306 | PL9  | C36-C37-C38 | -2.28 | 104.37      | 111.88   |
| 23  | B     | 612  | CLA  | C7-C6-C5    | -2.28 | 107.16      | 113.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | B     | 617  | CLA  | CMA-C3A-C4A | -2.28 | 105.64      | 111.77   |
| 23  | c     | 510  | CLA  | O2A-CGA-O1A | -2.28 | 117.83      | 123.59   |
| 24  | A     | 408  | PHO  | O1D-CGD-CBD | -2.28 | 120.94      | 124.74   |
| 23  | c     | 513  | CLA  | C4-C3-C5    | 2.28  | 119.11      | 115.27   |
| 23  | B     | 612  | CLA  | O2A-CGA-CBA | 2.28  | 119.06      | 111.91   |
| 23  | B     | 607  | CLA  | O2A-CGA-CBA | 2.28  | 119.05      | 111.91   |
| 23  | c     | 514  | CLA  | CHC-C1C-C2C | -2.28 | 120.41      | 126.73   |
| 25  | Y     | 302  | BCR  | C36-C18-C17 | -2.28 | 119.73      | 122.92   |
| 23  | d     | 402  | CLA  | CMB-C2B-C1B | 2.28  | 128.83      | 125.37   |
| 23  | c     | 513  | CLA  | O2A-CGA-O1A | -2.27 | 117.85      | 123.59   |
| 36  | b     | 625  | HTG  | O6-C6-C5    | -2.27 | 103.49      | 111.29   |
| 23  | C     | 510  | CLA  | CHA-C1A-NA  | -2.27 | 121.19      | 126.40   |
| 23  | B     | 614  | CLA  | C1-C2-C3    | -2.27 | 122.11      | 126.04   |
| 23  | a     | 2613 | CLA  | CHC-C1C-C2C | -2.27 | 120.42      | 126.73   |
| 24  | a     | 2611 | PHO  | CBC-CAC-C3C | -2.27 | 109.55      | 112.88   |
| 23  | A     | 407  | CLA  | CHB-C1B-C2B | -2.27 | 120.82      | 127.24   |
| 23  | D     | 2304 | CLA  | CMC-C2C-C1C | 2.27  | 128.50      | 125.04   |
| 23  | B     | 609  | CLA  | CBC-CAC-C3C | -2.27 | 106.17      | 112.43   |
| 42  | v     | 201  | HEC  | C4C-NC-C1C  | 2.27  | 107.57      | 105.35   |
| 23  | C     | 513  | CLA  | CMA-C3A-C4A | -2.27 | 105.67      | 111.77   |
| 33  | A     | 422  | PL9  | C25-C24-C26 | 2.27  | 119.08      | 115.27   |
| 23  | b     | 613  | CLA  | CAA-C2A-C3A | -2.27 | 106.57      | 112.78   |
| 23  | d     | 409  | CLA  | CBC-CAC-C3C | -2.26 | 106.19      | 112.43   |
| 27  | B     | 622  | LMG  | C9-C8-C7    | -2.26 | 106.43      | 111.79   |
| 23  | A     | 410  | CLA  | CMC-C2C-C1C | 2.26  | 128.49      | 125.04   |
| 33  | x     | 1301 | PL9  | C42-C43-C44 | -2.26 | 120.02      | 127.75   |
| 33  | A     | 422  | PL9  | C15-C14-C16 | 2.26  | 119.08      | 115.27   |
| 23  | B     | 617  | CLA  | CHD-C1D-ND  | -2.26 | 122.38      | 124.45   |
| 31  | a     | 2619 | JOX  | C2-C1-CL1   | 2.26  | 117.72      | 115.84   |
| 23  | C     | 502  | CLA  | C4-C3-C5    | 2.26  | 119.07      | 115.27   |
| 25  | c     | 517  | BCR  | C31-C1-C6   | -2.26 | 106.64      | 110.30   |
| 23  | C     | 513  | CLA  | O1D-CGD-CBD | -2.26 | 119.86      | 124.48   |
| 23  | b     | 621  | CLA  | O2A-CGA-O1A | -2.26 | 117.89      | 123.59   |
| 26  | D     | 2302 | SQD  | O48-C23-C24 | 2.26  | 118.99      | 111.91   |
| 23  | b     | 614  | CLA  | O2A-CGA-CBA | 2.26  | 118.98      | 111.91   |
| 23  | B     | 613  | CLA  | CBC-CAC-C3C | -2.26 | 106.21      | 112.43   |
| 23  | c     | 511  | CLA  | C3B-C4B-NB  | 2.26  | 112.61      | 110.52   |
| 23  | d     | 402  | CLA  | CHB-C1B-NB  | -2.25 | 121.87      | 124.26   |
| 33  | x     | 1301 | PL9  | C25-C24-C23 | -2.25 | 117.89      | 123.68   |
| 23  | b     | 613  | CLA  | CHA-C1A-NA  | -2.25 | 121.24      | 126.40   |
| 23  | c     | 509  | CLA  | CHB-C1B-C2B | -2.25 | 120.88      | 127.24   |
| 23  | C     | 502  | CLA  | O2A-CGA-CBA | 2.25  | 118.97      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | b     | 617  | CLA  | CHB-C4A-NA  | 2.25  | 127.62      | 124.51   |
| 23  | A     | 406  | CLA  | O2D-CGD-O1D | -2.25 | 119.44      | 123.84   |
| 23  | c     | 513  | CLA  | CAC-C3C-C4C | 2.25  | 127.73      | 124.81   |
| 42  | v     | 201  | HEC  | CBB-CAB-C3B | 2.25  | 118.63      | 112.43   |
| 23  | B     | 617  | CLA  | O2A-CGA-O1A | -2.25 | 117.92      | 123.59   |
| 25  | b     | 622  | BCR  | C21-C20-C19 | -2.25 | 116.21      | 123.22   |
| 23  | b     | 619  | CLA  | OBD-CAD-C3D | -2.25 | 123.11      | 128.52   |
| 26  | l     | 101  | SQD  | O8-S-C6     | 2.25  | 109.32      | 105.74   |
| 23  | C     | 505  | CLA  | C4C-C3C-C2C | -2.25 | 103.62      | 106.90   |
| 23  | c     | 515  | CLA  | CHC-C1C-C2C | -2.24 | 120.49      | 126.73   |
| 23  | b     | 614  | CLA  | O2D-CGD-O1D | -2.24 | 119.45      | 123.84   |
| 23  | b     | 617  | CLA  | CMA-C3A-C4A | -2.24 | 105.75      | 111.77   |
| 39  | e     | 103  | HEM  | CHC-C1C-NC  | 2.24  | 126.86      | 124.44   |
| 23  | b     | 606  | CLA  | C3C-C4C-NC  | 2.24  | 113.08      | 110.57   |
| 25  | b     | 623  | BCR  | C37-C22-C21 | -2.24 | 119.79      | 122.92   |
| 23  | B     | 610  | CLA  | CHA-C1A-NA  | -2.24 | 121.27      | 126.40   |
| 27  | C     | 520  | LMG  | O7-C10-O9   | -2.24 | 118.29      | 123.70   |
| 23  | B     | 602  | CLA  | CMC-C2C-C1C | 2.24  | 128.44      | 125.04   |
| 29  | b     | 644  | GOL  | C3-C2-C1    | -2.24 | 103.01      | 111.70   |
| 23  | b     | 609  | CLA  | O2D-CGD-O1D | -2.23 | 119.47      | 123.84   |
| 23  | C     | 505  | CLA  | C7-C6-C5    | -2.23 | 107.29      | 113.36   |
| 23  | C     | 511  | CLA  | CHA-C1A-NA  | -2.23 | 121.29      | 126.40   |
| 36  | b     | 602  | HTG  | O5-C1-C2    | 2.23  | 113.12      | 110.31   |
| 25  | B     | 620  | BCR  | C15-C16-C17 | -2.23 | 118.90      | 123.47   |
| 23  | C     | 510  | CLA  | CMB-C2B-C1B | 2.23  | 128.77      | 125.37   |
| 23  | B     | 612  | CLA  | C3B-C4B-NB  | 2.23  | 112.58      | 110.52   |
| 23  | B     | 609  | CLA  | CMC-C2C-C1C | 2.23  | 128.44      | 125.04   |
| 33  | A     | 422  | PL9  | C42-C43-C44 | -2.23 | 120.12      | 127.75   |
| 23  | B     | 615  | CLA  | CMB-C2B-C1B | 2.23  | 128.77      | 125.37   |
| 23  | C     | 504  | CLA  | CHD-C4C-NC  | 2.23  | 127.72      | 124.20   |
| 23  | b     | 609  | CLA  | CHD-C1D-C2D | -2.23 | 120.80      | 125.48   |
| 37  | c     | 518  | DGD  | C6D-O5D-C1E | 2.23  | 118.09      | 113.74   |
| 25  | b     | 622  | BCR  | C3-C4-C5    | -2.23 | 110.10      | 114.08   |
| 23  | b     | 620  | CLA  | C11-C10-C8  | -2.23 | 108.72      | 115.92   |
| 25  | y     | 101  | BCR  | C1-C6-C7    | 2.23  | 122.08      | 115.78   |
| 25  | C     | 515  | BCR  | C8-C7-C6    | -2.23 | 120.94      | 127.20   |
| 33  | D     | 2306 | PL9  | C35-C34-C36 | 2.23  | 119.02      | 115.27   |
| 23  | c     | 516  | CLA  | C3B-C4B-NB  | 2.23  | 112.58      | 110.52   |
| 23  | c     | 516  | CLA  | CHA-C1A-NA  | -2.23 | 121.30      | 126.40   |
| 23  | c     | 511  | CLA  | C6-C7-C8    | -2.22 | 108.73      | 115.92   |
| 26  | B     | 621  | SQD  | O48-C23-C24 | 2.22  | 118.88      | 111.91   |
| 28  | m     | 2804 | LMT  | C1B-O5B-C5B | 2.22  | 118.05      | 113.69   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 33  | d     | 411  | PL9  | C35-C34-C36 | 2.22  | 119.00      | 115.27   |
| 23  | B     | 605  | CLA  | CHC-C1C-C2C | -2.22 | 120.57      | 126.73   |
| 23  | B     | 616  | CLA  | CHD-C4C-NC  | 2.22  | 127.70      | 124.20   |
| 23  | c     | 505  | CLA  | CHA-C1A-NA  | -2.22 | 121.32      | 126.40   |
| 38  | d     | 413  | LHG  | O8-C23-C24  | 2.22  | 118.87      | 111.91   |
| 42  | V     | 201  | HEC  | CMD-C2D-C1D | 2.22  | 128.42      | 125.04   |
| 25  | T     | 102  | BCR  | C33-C5-C4   | 2.22  | 117.88      | 113.62   |
| 27  | c     | 522  | LMG  | C8-O7-C10   | -2.22 | 112.33      | 117.79   |
| 23  | B     | 614  | CLA  | OBD-CAD-C3D | -2.21 | 123.19      | 128.52   |
| 28  | M     | 101  | LMT  | O1B-C1B-C2B | 2.21  | 113.83      | 108.10   |
| 23  | B     | 612  | CLA  | OBD-CAD-C3D | -2.21 | 123.19      | 128.52   |
| 28  | B     | 623  | LMT  | O1B-C4'-C5' | -2.21 | 103.39      | 109.45   |
| 23  | B     | 602  | CLA  | O2A-CGA-O1A | -2.21 | 118.01      | 123.59   |
| 23  | B     | 608  | CLA  | CHA-C1A-NA  | -2.21 | 121.34      | 126.40   |
| 36  | d     | 407  | HTG  | O5-C5-C4    | 2.21  | 113.71      | 109.69   |
| 23  | b     | 610  | CLA  | CHC-C4B-NB  | 2.21  | 126.60      | 124.26   |
| 23  | b     | 610  | CLA  | C1-C2-C3    | -2.21 | 122.22      | 126.04   |
| 25  | k     | 302  | BCR  | C20-C21-C22 | -2.21 | 124.16      | 127.31   |
| 23  | b     | 615  | CLA  | CAA-CBA-CGA | -2.21 | 106.81      | 113.25   |
| 23  | b     | 612  | CLA  | CMB-C2B-C1B | 2.21  | 128.73      | 125.37   |
| 25  | y     | 101  | BCR  | C10-C11-C12 | -2.21 | 116.33      | 123.22   |
| 23  | B     | 610  | CLA  | C7-C6-C5    | -2.20 | 107.37      | 113.36   |
| 25  | D     | 2305 | BCR  | C16-C17-C18 | -2.20 | 124.16      | 127.31   |
| 23  | c     | 514  | CLA  | CHA-C1A-NA  | -2.20 | 121.35      | 126.40   |
| 23  | c     | 513  | CLA  | C1-C2-C3    | -2.20 | 122.23      | 126.04   |
| 23  | b     | 606  | CLA  | CAC-C3C-C4C | 2.20  | 127.67      | 124.81   |
| 25  | C     | 516  | BCR  | C11-C10-C9  | -2.20 | 124.17      | 127.31   |
| 23  | C     | 509  | CLA  | CMB-C2B-C1B | 2.20  | 128.72      | 125.37   |
| 31  | A     | 418  | JOX  | C1-C-C5     | -2.20 | 119.57      | 120.54   |
| 23  | C     | 504  | CLA  | CHA-C1A-NA  | -2.20 | 121.36      | 126.40   |
| 25  | A     | 411  | BCR  | C7-C8-C9    | -2.20 | 122.91      | 126.23   |
| 23  | B     | 614  | CLA  | CBC-CAC-C3C | -2.20 | 106.37      | 112.43   |
| 23  | B     | 609  | CLA  | C1-C2-C3    | -2.20 | 122.24      | 126.04   |
| 23  | B     | 617  | CLA  | CHC-C1C-C2C | -2.20 | 120.62      | 126.73   |
| 23  | a     | 2613 | CLA  | CHD-C4C-NC  | 2.20  | 127.67      | 124.20   |
| 23  | C     | 508  | CLA  | CMC-C2C-C1C | 2.20  | 128.38      | 125.04   |
| 23  | A     | 406  | CLA  | C4C-C3C-C2C | -2.20 | 103.70      | 106.90   |
| 23  | B     | 602  | CLA  | CAC-C3C-C4C | 2.19  | 127.65      | 124.81   |
| 23  | D     | 2303 | CLA  | CMC-C2C-C1C | 2.19  | 128.38      | 125.04   |
| 23  | B     | 608  | CLA  | CHC-C1C-C2C | -2.19 | 120.64      | 126.73   |
| 25  | A     | 411  | BCR  | C31-C1-C6   | -2.19 | 106.75      | 110.30   |
| 23  | b     | 615  | CLA  | O2A-CGA-O1A | -2.19 | 118.06      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | A     | 407  | CLA  | O2D-CGD-O1D | -2.19 | 119.56      | 123.84   |
| 23  | B     | 608  | CLA  | O2A-CGA-CBA | 2.19  | 118.78      | 111.91   |
| 25  | Y     | 302  | BCR  | C35-C13-C12 | 2.19  | 121.52      | 118.08   |
| 23  | b     | 612  | CLA  | CAA-C2A-C1A | -2.19 | 104.81      | 111.97   |
| 37  | C     | 518  | DGD  | O6E-C5E-C6E | 2.19  | 111.87      | 106.44   |
| 23  | A     | 405  | CLA  | CHC-C1C-C2C | -2.19 | 120.66      | 126.73   |
| 23  | c     | 513  | CLA  | C6-C7-C8    | -2.19 | 108.85      | 115.92   |
| 37  | c     | 520  | DGD  | O2G-C1B-C2B | 2.19  | 116.21      | 111.50   |
| 40  | H     | 102  | RRX  | C29-C28-C27 | -2.18 | 107.31      | 110.30   |
| 36  | C     | 522  | HTG  | O5-C5-C4    | 2.18  | 113.66      | 109.69   |
| 23  | B     | 605  | CLA  | CAC-C3C-C4C | 2.18  | 127.64      | 124.81   |
| 23  | a     | 2613 | CLA  | O2A-CGA-O1A | -2.18 | 118.09      | 123.59   |
| 23  | B     | 604  | CLA  | CMA-C3A-C2A | -2.18 | 105.03      | 113.83   |
| 33  | D     | 2306 | PL9  | C12-C13-C14 | -2.18 | 122.41      | 127.66   |
| 23  | B     | 609  | CLA  | CHA-C1A-NA  | -2.18 | 121.41      | 126.40   |
| 23  | b     | 620  | CLA  | CMC-C2C-C1C | 2.18  | 128.36      | 125.04   |
| 25  | A     | 411  | BCR  | C8-C7-C6    | -2.18 | 121.09      | 127.20   |
| 36  | d     | 407  | HTG  | C4-C3-C2    | -2.18 | 107.02      | 110.82   |
| 23  | A     | 407  | CLA  | CHC-C1C-C2C | -2.18 | 120.69      | 126.73   |
| 36  | b     | 603  | HTG  | O5-C5-C4    | 2.17  | 113.64      | 109.69   |
| 23  | C     | 508  | CLA  | O1D-CGD-CBD | -2.17 | 120.04      | 124.48   |
| 26  | D     | 2308 | SQD  | O8-S-C6     | 2.17  | 109.20      | 105.74   |
| 23  | d     | 409  | CLA  | CAC-C3C-C4C | 2.17  | 127.63      | 124.81   |
| 23  | B     | 612  | CLA  | O2A-CGA-O1A | -2.17 | 118.11      | 123.59   |
| 23  | c     | 516  | CLA  | CAA-C2A-C3A | -2.17 | 106.84      | 112.78   |
| 23  | c     | 509  | CLA  | CHC-C1C-C2C | -2.17 | 120.70      | 126.73   |
| 24  | A     | 408  | PHO  | C4D-CHA-CBD | 2.17  | 109.50      | 108.52   |
| 23  | C     | 507  | CLA  | C4-C3-C2    | -2.17 | 118.12      | 123.68   |
| 23  | c     | 513  | CLA  | CHC-C1C-C2C | -2.17 | 120.71      | 126.73   |
| 23  | D     | 2304 | CLA  | CAC-C3C-C2C | 2.16  | 131.23      | 127.53   |
| 40  | h     | 101  | RRX  | C7-C8-C9    | -2.16 | 122.97      | 126.23   |
| 23  | B     | 613  | CLA  | C1-C2-C3    | -2.16 | 122.31      | 126.04   |
| 26  | B     | 621  | SQD  | O8-S-C6     | 2.16  | 109.18      | 105.74   |
| 23  | b     | 614  | CLA  | C4D-CHA-C1A | 2.16  | 123.88      | 121.25   |
| 23  | C     | 509  | CLA  | C11-C12-C13 | -2.16 | 108.94      | 115.92   |
| 23  | B     | 612  | CLA  | CAA-C2A-C3A | -2.16 | 106.87      | 112.78   |
| 23  | a     | 2609 | CLA  | CMA-C3A-C4A | -2.16 | 105.97      | 111.77   |
| 23  | b     | 610  | CLA  | O2A-CGA-CBA | 2.16  | 118.68      | 111.91   |
| 23  | a     | 2610 | CLA  | CMC-C2C-C1C | 2.16  | 128.32      | 125.04   |
| 25  | y     | 101  | BCR  | C32-C1-C6   | -2.16 | 106.80      | 110.30   |
| 23  | A     | 407  | CLA  | CMA-C3A-C2A | -2.16 | 105.13      | 113.83   |
| 25  | a     | 2614 | BCR  | C34-C9-C10  | -2.16 | 119.90      | 122.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | C     | 514  | CLA  | O2A-CGA-CBA | 2.16  | 118.67      | 111.91   |
| 23  | B     | 602  | CLA  | CMB-C2B-C1B | 2.15  | 128.65      | 125.37   |
| 25  | Y     | 302  | BCR  | C34-C9-C8   | 2.15  | 121.47      | 118.08   |
| 27  | c     | 501  | LMG  | C30-C29-C28 | -2.15 | 105.79      | 113.62   |
| 33  | D     | 2306 | PL9  | C47-C48-C49 | -2.15 | 120.39      | 127.75   |
| 23  | C     | 504  | CLA  | O2A-CGA-O1A | -2.15 | 118.16      | 123.59   |
| 36  | c     | 523  | HTG  | C6-C5-C4    | -2.15 | 107.96      | 113.00   |
| 23  | b     | 611  | CLA  | CAC-C3C-C4C | 2.15  | 127.60      | 124.81   |
| 39  | F     | 101  | HEM  | C4C-NC-C1C  | 2.15  | 107.45      | 105.35   |
| 23  | B     | 611  | CLA  | CHC-C1C-C2C | -2.15 | 120.75      | 126.73   |
| 23  | B     | 608  | CLA  | C4A-NA-C1A  | 2.15  | 107.67      | 106.71   |
| 25  | K     | 101  | BCR  | C20-C21-C22 | -2.15 | 124.24      | 127.31   |
| 23  | B     | 611  | CLA  | O2A-C1-C2   | 2.15  | 114.28      | 108.64   |
| 26  | D     | 2302 | SQD  | O5-C1-C2    | 2.15  | 114.90      | 110.35   |
| 27  | D     | 2312 | LMG  | C7-O1-C1    | -2.15 | 109.54      | 113.74   |
| 25  | z     | 101  | BCR  | C37-C22-C23 | 2.15  | 121.46      | 118.08   |
| 23  | B     | 604  | CLA  | CAA-C2A-C1A | -2.15 | 104.94      | 111.97   |
| 23  | D     | 2304 | CLA  | C3B-C4B-NB  | 2.15  | 112.50      | 110.52   |
| 23  | d     | 408  | CLA  | CAC-C3C-C4C | 2.14  | 127.59      | 124.81   |
| 26  | b     | 601  | SQD  | C46-C45-C44 | -2.14 | 106.72      | 111.79   |
| 23  | b     | 607  | CLA  | CAA-C2A-C3A | -2.14 | 106.91      | 112.78   |
| 25  | B     | 618  | BCR  | C21-C20-C19 | -2.14 | 116.53      | 123.22   |
| 24  | A     | 408  | PHO  | C1-O2A-CGA  | 2.14  | 122.06      | 116.44   |
| 25  | T     | 102  | BCR  | C16-C17-C18 | -2.14 | 124.25      | 127.31   |
| 23  | c     | 515  | CLA  | O1D-CGD-CBD | -2.14 | 120.10      | 124.48   |
| 25  | K     | 101  | BCR  | C2-C3-C4    | -2.14 | 106.59      | 111.38   |
| 23  | A     | 410  | CLA  | CHB-C1B-C2B | -2.14 | 121.19      | 127.24   |
| 25  | B     | 619  | BCR  | C29-C28-C27 | -2.14 | 106.60      | 111.38   |
| 23  | B     | 614  | CLA  | CMB-C2B-C1B | 2.14  | 128.62      | 125.37   |
| 36  | d     | 407  | HTG  | C6-C5-C4    | -2.14 | 108.00      | 113.00   |
| 23  | b     | 612  | CLA  | C4A-NA-C1A  | 2.14  | 107.67      | 106.71   |
| 23  | A     | 407  | CLA  | CAA-CBA-CGA | 2.14  | 119.49      | 113.25   |
| 23  | c     | 507  | CLA  | CHD-C4C-NC  | 2.13  | 127.57      | 124.20   |
| 23  | b     | 620  | CLA  | O2A-CGA-O1A | -2.13 | 118.21      | 123.59   |
| 23  | B     | 606  | CLA  | C12-C11-C10 | -2.13 | 103.43      | 113.24   |
| 23  | B     | 602  | CLA  | C3C-C4C-NC  | 2.13  | 112.96      | 110.57   |
| 23  | b     | 618  | CLA  | CBC-CAC-C3C | -2.13 | 106.55      | 112.43   |
| 23  | C     | 503  | CLA  | CHC-C1C-C2C | -2.13 | 120.81      | 126.73   |
| 23  | C     | 510  | CLA  | CHC-C1C-C2C | -2.13 | 120.81      | 126.73   |
| 25  | y     | 101  | BCR  | C23-C24-C25 | -2.13 | 121.21      | 127.20   |
| 23  | B     | 605  | CLA  | CHC-C4B-NB  | 2.13  | 126.51      | 124.26   |
| 28  | A     | 414  | LMT  | C3B-C4B-C5B | 2.13  | 114.04      | 110.24   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 607    | CLA  | CBC-CAC-C3C | -2.13 | 106.56      | 112.43   |
| 23  | C     | 502    | CLA  | C1-C2-C3    | -2.13 | 122.36      | 126.04   |
| 23  | b     | 614    | CLA  | CMC-C2C-C1C | 2.13  | 128.28      | 125.04   |
| 37  | H     | 103    | DGD  | O2G-C1B-O1B | -2.13 | 118.56      | 123.70   |
| 23  | C     | 502    | CLA  | CMD-C2D-C3D | -2.13 | 122.72      | 127.61   |
| 23  | b     | 617    | CLA  | OBD-CAD-C3D | -2.13 | 123.40      | 128.52   |
| 23  | c     | 510    | CLA  | C6-C7-C8    | -2.13 | 109.04      | 115.92   |
| 25  | a     | 2614   | BCR  | C8-C7-C6    | -2.13 | 121.23      | 127.20   |
| 23  | b     | 616    | CLA  | O2A-CGA-O1A | -2.13 | 118.22      | 123.59   |
| 23  | c     | 504    | CLA  | CHD-C4C-NC  | 2.13  | 127.55      | 124.20   |
| 23  | b     | 620    | CLA  | C1-O2A-CGA  | 2.13  | 122.02      | 116.44   |
| 25  | b     | 623    | BCR  | C40-C30-C25 | -2.13 | 106.85      | 110.30   |
| 23  | b     | 606    | CLA  | CAA-C2A-C3A | -2.12 | 106.96      | 112.78   |
| 29  | v     | 203    | GOL  | C3-C2-C1    | -2.12 | 103.45      | 111.70   |
| 25  | k     | 302    | BCR  | C15-C14-C13 | -2.12 | 124.29      | 127.31   |
| 23  | B     | 608    | CLA  | C4-C3-C5    | 2.12  | 118.83      | 115.27   |
| 23  | B     | 615    | CLA  | C4-C3-C5    | 2.12  | 118.83      | 115.27   |
| 23  | C     | 511    | CLA  | C11-C10-C8  | -2.12 | 109.07      | 115.92   |
| 36  | b     | 626    | HTG  | O5-C1-C2    | 2.12  | 112.98      | 110.31   |
| 25  | k     | 302    | BCR  | C21-C20-C19 | -2.12 | 116.61      | 123.22   |
| 23  | D     | 2303   | CLA  | CHD-C4C-NC  | 2.12  | 127.54      | 124.20   |
| 36  | B     | 624[A] | HTG  | O5-C1-C2    | 2.12  | 112.98      | 110.31   |
| 23  | B     | 613    | CLA  | O2A-CGA-O1A | -2.12 | 118.25      | 123.59   |
| 23  | b     | 608    | CLA  | CHA-C1A-NA  | -2.12 | 121.55      | 126.40   |
| 23  | b     | 613    | CLA  | CMB-C2B-C1B | 2.12  | 128.59      | 125.37   |
| 23  | b     | 612    | CLA  | CAA-CBA-CGA | 2.12  | 119.44      | 113.25   |
| 23  | b     | 611    | CLA  | C11-C10-C8  | -2.12 | 109.08      | 115.92   |
| 40  | h     | 101    | RRX  | C20-C21-C22 | -2.12 | 124.29      | 127.31   |
| 25  | z     | 101    | BCR  | C37-C22-C21 | -2.12 | 119.96      | 122.92   |
| 23  | c     | 516    | CLA  | C4-C3-C5    | 2.12  | 118.83      | 115.27   |
| 23  | b     | 619    | CLA  | CAA-C2A-C3A | -2.11 | 106.99      | 112.78   |
| 23  | b     | 610    | CLA  | CHD-C4C-NC  | 2.11  | 127.53      | 124.20   |
| 23  | b     | 614    | CLA  | CAC-C3C-C4C | 2.11  | 127.55      | 124.81   |
| 23  | b     | 606    | CLA  | O1D-CGD-CBD | -2.11 | 120.16      | 124.48   |
| 23  | C     | 505    | CLA  | CHC-C1C-C2C | -2.11 | 120.86      | 126.73   |
| 23  | d     | 409    | CLA  | CMB-C2B-C1B | 2.11  | 128.58      | 125.37   |
| 23  | c     | 514    | CLA  | CHD-C4C-NC  | 2.11  | 127.53      | 124.20   |
| 23  | D     | 2304   | CLA  | CHB-C4A-NA  | 2.11  | 127.43      | 124.51   |
| 26  | l     | 101    | SQD  | O9-S-C6     | 2.11  | 109.44      | 106.94   |
| 25  | T     | 102    | BCR  | C36-C18-C19 | 2.11  | 121.40      | 118.08   |
| 23  | D     | 2304   | CLA  | CMB-C2B-C1B | 2.11  | 128.58      | 125.37   |
| 23  | D     | 2304   | CLA  | C11-C10-C8  | -2.11 | 109.11      | 115.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | C     | 506  | CLA  | O1D-CGD-CBD | -2.11 | 120.17      | 124.48   |
| 37  | H     | 103  | DGD  | C3E-C4E-C5E | -2.11 | 106.48      | 110.24   |
| 23  | C     | 503  | CLA  | C1-O2A-CGA  | 2.11  | 121.97      | 116.44   |
| 23  | C     | 507  | CLA  | C3B-C4B-NB  | 2.10  | 112.47      | 110.52   |
| 23  | A     | 406  | CLA  | CHD-C4C-NC  | 2.10  | 127.52      | 124.20   |
| 23  | B     | 609  | CLA  | CHC-C1C-C2C | -2.10 | 120.89      | 126.73   |
| 23  | C     | 512  | CLA  | CMC-C2C-C1C | 2.10  | 128.24      | 125.04   |
| 23  | b     | 620  | CLA  | CHC-C1C-C2C | -2.10 | 120.89      | 126.73   |
| 23  | A     | 406  | CLA  | CAA-CBA-CGA | 2.10  | 119.39      | 113.25   |
| 42  | V     | 201  | HEC  | C2A-C1A-NA  | -2.10 | 108.28      | 110.32   |
| 25  | B     | 618  | BCR  | C15-C14-C13 | -2.10 | 124.31      | 127.31   |
| 23  | A     | 407  | CLA  | CHA-C1A-NA  | -2.10 | 121.59      | 126.40   |
| 25  | C     | 515  | BCR  | C16-C17-C18 | -2.10 | 124.31      | 127.31   |
| 23  | C     | 509  | CLA  | O2A-CGA-O1A | -2.10 | 118.30      | 123.59   |
| 25  | c     | 517  | BCR  | C33-C5-C4   | 2.10  | 117.65      | 113.62   |
| 23  | b     | 616  | CLA  | CHA-C1A-NA  | -2.10 | 121.59      | 126.40   |
| 23  | B     | 603  | CLA  | CAA-CBA-CGA | -2.10 | 107.13      | 113.25   |
| 23  | B     | 614  | CLA  | CHA-C1A-NA  | -2.10 | 121.60      | 126.40   |
| 26  | D     | 2308 | SQD  | O48-C23-O10 | -2.10 | 118.30      | 123.59   |
| 23  | b     | 606  | CLA  | CMB-C2B-C1B | 2.10  | 128.56      | 125.37   |
| 23  | C     | 504  | CLA  | C4-C3-C5    | 2.09  | 118.80      | 115.27   |
| 23  | c     | 511  | CLA  | CHB-C1B-NB  | -2.09 | 122.04      | 124.26   |
| 25  | D     | 2305 | BCR  | C10-C11-C12 | -2.09 | 116.68      | 123.22   |
| 24  | A     | 409  | PHO  | C4A-C3A-C2A | -2.09 | 100.85      | 102.84   |
| 23  | c     | 510  | CLA  | O2A-CGA-CBA | 2.09  | 118.48      | 111.91   |
| 23  | C     | 506  | CLA  | C4A-NA-C1A  | 2.09  | 107.65      | 106.71   |
| 27  | A     | 413  | LMG  | O8-C28-C29  | 2.09  | 118.47      | 111.91   |
| 23  | c     | 510  | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 23  | B     | 614  | CLA  | CHD-C4C-NC  | 2.09  | 127.50      | 124.20   |
| 23  | b     | 619  | CLA  | CMD-C2D-C3D | -2.09 | 122.80      | 127.61   |
| 23  | B     | 616  | CLA  | C4A-NA-C1A  | 2.09  | 107.65      | 106.71   |
| 23  | b     | 618  | CLA  | CHC-C1C-C2C | -2.09 | 120.92      | 126.73   |
| 23  | b     | 613  | CLA  | OBD-CAD-C3D | -2.09 | 123.49      | 128.52   |
| 25  | z     | 101  | BCR  | C3-C4-C5    | -2.09 | 110.35      | 114.08   |
| 33  | d     | 411  | PL9  | C47-C48-C49 | -2.09 | 120.61      | 127.75   |
| 28  | m     | 2804 | LMT  | O5B-C1B-C2B | 2.09  | 114.77      | 110.35   |
| 38  | L     | 101  | LHG  | O4-P-O5     | 2.09  | 122.56      | 112.24   |
| 23  | b     | 619  | CLA  | CHA-C1A-NA  | -2.09 | 121.62      | 126.40   |
| 28  | z     | 102  | LMT  | C1B-O5B-C5B | 2.09  | 117.78      | 113.69   |
| 23  | B     | 617  | CLA  | OBD-CAD-C3D | -2.09 | 123.50      | 128.52   |
| 23  | C     | 507  | CLA  | CMD-C2D-C3D | -2.08 | 122.82      | 127.61   |
| 23  | b     | 612  | CLA  | C4-C3-C5    | 2.08  | 118.78      | 115.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | a     | 2609 | CLA  | C4-C3-C5    | 2.08  | 118.77      | 115.27   |
| 37  | C     | 519  | DGD  | O1G-C1A-O1A | -2.08 | 118.34      | 123.59   |
| 23  | b     | 621  | CLA  | CMB-C2B-C1B | 2.08  | 128.53      | 125.37   |
| 23  | B     | 611  | CLA  | O2A-CGA-O1A | -2.08 | 118.35      | 123.59   |
| 28  | i     | 103  | LMT  | C3'-C4'-C5' | 2.08  | 113.95      | 110.24   |
| 23  | c     | 515  | CLA  | C1-C2-C3    | -2.08 | 122.45      | 126.04   |
| 31  | a     | 2617 | JOX  | O1-C5-C     | -2.08 | 118.44      | 121.41   |
| 23  | C     | 514  | CLA  | CMC-C2C-C1C | 2.08  | 128.20      | 125.04   |
| 23  | b     | 619  | CLA  | CMA-C3A-C4A | -2.08 | 106.19      | 111.77   |
| 23  | B     | 615  | CLA  | CHC-C1C-NC  | 2.08  | 127.35      | 124.20   |
| 38  | L     | 101  | LHG  | O7-C7-O9    | -2.07 | 118.69      | 123.70   |
| 23  | c     | 507  | CLA  | O2A-CGA-CBA | 2.07  | 118.42      | 111.91   |
| 23  | C     | 512  | CLA  | O2A-CGA-O1A | -2.07 | 118.36      | 123.59   |
| 25  | d     | 410  | BCR  | C21-C20-C19 | -2.07 | 116.75      | 123.22   |
| 26  | D     | 2302 | SQD  | C9-C8-C7    | -2.07 | 106.09      | 113.62   |
| 23  | c     | 511  | CLA  | CHD-C1D-C2D | -2.07 | 121.14      | 125.48   |
| 23  | B     | 604  | CLA  | CHA-C1A-NA  | -2.07 | 121.66      | 126.40   |
| 23  | c     | 516  | CLA  | CMB-C2B-C1B | 2.07  | 128.52      | 125.37   |
| 23  | c     | 513  | CLA  | C11-C10-C8  | -2.07 | 109.23      | 115.92   |
| 23  | B     | 610  | CLA  | CAC-C3C-C4C | 2.07  | 127.49      | 124.81   |
| 23  | c     | 512  | CLA  | O2A-CGA-O1A | -2.07 | 118.37      | 123.59   |
| 38  | e     | 101  | LHG  | O8-C23-O10  | -2.07 | 118.37      | 123.59   |
| 23  | C     | 514  | CLA  | CED-O2D-CGD | 2.07  | 120.61      | 115.94   |
| 36  | b     | 602  | HTG  | C1'-S1-C1   | 2.07  | 103.96      | 100.09   |
| 24  | A     | 408  | PHO  | CBA-CAA-C2A | -2.07 | 107.77      | 113.81   |
| 23  | c     | 510  | CLA  | OBD-CAD-C3D | -2.07 | 123.55      | 128.52   |
| 25  | D     | 2305 | BCR  | C15-C16-C17 | -2.07 | 119.24      | 123.47   |
| 23  | b     | 615  | CLA  | C4-C3-C5    | 2.07  | 118.75      | 115.27   |
| 23  | b     | 612  | CLA  | CAC-C3C-C2C | 2.07  | 131.06      | 127.53   |
| 25  | b     | 623  | BCR  | C29-C28-C27 | -2.06 | 106.76      | 111.38   |
| 23  | a     | 2610 | CLA  | CHA-C1A-NA  | -2.06 | 121.67      | 126.40   |
| 24  | a     | 2611 | PHO  | C1-O2A-CGA  | 2.06  | 121.86      | 116.44   |
| 28  | z     | 102  | LMT  | C1'-O5'-C5' | 2.06  | 117.73      | 113.69   |
| 23  | d     | 408  | CLA  | C4-C3-C5    | 2.06  | 118.74      | 115.27   |
| 40  | h     | 101  | RRX  | C11-C10-C9  | -2.06 | 124.37      | 127.31   |
| 23  | A     | 410  | CLA  | CHC-C1C-C2C | -2.06 | 121.01      | 126.73   |
| 25  | A     | 411  | BCR  | C2-C3-C4    | -2.06 | 106.77      | 111.38   |
| 25  | B     | 620  | BCR  | C38-C26-C25 | -2.06 | 122.22      | 124.53   |
| 40  | H     | 102  | RRX  | C37-C22-C21 | -2.06 | 120.04      | 122.92   |
| 23  | c     | 512  | CLA  | CHD-C1D-ND  | -2.06 | 122.56      | 124.45   |
| 37  | C     | 519  | DGD  | O4D-C4D-C3D | -2.06 | 105.59      | 110.35   |
| 23  | b     | 619  | CLA  | C4-C3-C2    | -2.06 | 118.40      | 123.68   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 36  | V     | 204    | HTG  | O5-C5-C4    | 2.06  | 113.43      | 109.69   |
| 25  | C     | 515    | BCR  | C23-C24-C25 | -2.06 | 121.43      | 127.20   |
| 25  | B     | 620    | BCR  | C10-C11-C12 | -2.06 | 116.80      | 123.22   |
| 24  | a     | 2612   | PHO  | CMA-C3A-C4A | -2.05 | 109.88      | 114.38   |
| 27  | c     | 521    | LMG  | O8-C28-O10  | -2.05 | 118.41      | 123.59   |
| 36  | C     | 525    | HTG  | C4-C3-C2    | -2.05 | 107.24      | 110.82   |
| 28  | A     | 414    | LMT  | O1B-C1B-O5B | -2.05 | 104.94      | 110.67   |
| 26  | A     | 412    | SQD  | C45-O47-C7  | -2.05 | 112.74      | 117.79   |
| 36  | B     | 624[B] | HTG  | O5-C5-C4    | 2.05  | 113.42      | 109.69   |
| 23  | b     | 615    | CLA  | C11-C12-C13 | -2.05 | 109.28      | 115.92   |
| 23  | B     | 610    | CLA  | CHC-C4B-NB  | 2.05  | 126.43      | 124.26   |
| 36  | o     | 301    | HTG  | O5-C5-C6    | 2.05  | 111.54      | 106.44   |
| 26  | b     | 601    | SQD  | O47-C7-O49  | -2.05 | 118.74      | 123.70   |
| 23  | C     | 508    | CLA  | C3B-C4B-NB  | 2.05  | 112.42      | 110.52   |
| 28  | M     | 101    | LMT  | C1B-O1B-C4' | -2.05 | 112.89      | 117.96   |
| 27  | D     | 2312   | LMG  | C9-C8-C7    | -2.05 | 106.94      | 111.79   |
| 23  | B     | 605    | CLA  | CMD-C2D-C3D | -2.05 | 122.90      | 127.61   |
| 23  | c     | 504    | CLA  | CHB-C1B-C2B | -2.05 | 121.45      | 127.24   |
| 23  | b     | 611    | CLA  | C3B-C4B-NB  | 2.05  | 112.42      | 110.52   |
| 23  | b     | 616    | CLA  | CHB-C4A-NA  | 2.05  | 127.34      | 124.51   |
| 25  | b     | 623    | BCR  | C28-C27-C26 | -2.05 | 110.42      | 114.08   |
| 37  | C     | 518    | DGD  | C6D-O5D-C1E | 2.05  | 117.74      | 113.74   |
| 23  | c     | 515    | CLA  | CMC-C2C-C1C | 2.05  | 128.15      | 125.04   |
| 27  | c     | 501    | LMG  | O8-C28-C29  | 2.04  | 118.33      | 111.91   |
| 23  | C     | 514    | CLA  | CMD-C2D-C3D | -2.04 | 122.91      | 127.61   |
| 23  | C     | 509    | CLA  | CMC-C2C-C1C | 2.04  | 128.15      | 125.04   |
| 23  | B     | 610    | CLA  | O2A-CGA-CBA | 2.04  | 118.32      | 111.91   |
| 23  | a     | 2610   | CLA  | CHC-C1C-C2C | -2.04 | 121.06      | 126.73   |
| 27  | c     | 521    | LMG  | O7-C10-O9   | -2.04 | 118.77      | 123.70   |
| 26  | a     | 2615   | SQD  | O5-C1-C2    | -2.04 | 106.03      | 110.35   |
| 36  | H     | 101    | HTG  | O5-C1-C2    | 2.04  | 112.85      | 110.25   |
| 23  | D     | 2303   | CLA  | CHC-C1C-C2C | -2.04 | 121.07      | 126.73   |
| 23  | b     | 606    | CLA  | CHB-C1B-C2B | -2.04 | 121.48      | 127.24   |
| 23  | C     | 513    | CLA  | C1-O2A-CGA  | 2.04  | 121.79      | 116.44   |
| 23  | C     | 503    | CLA  | C3B-C4B-NB  | 2.04  | 112.41      | 110.52   |
| 23  | c     | 507    | CLA  | CMC-C2C-C1C | 2.04  | 128.14      | 125.04   |
| 31  | a     | 2619   | JOX  | C-C5-C4     | 2.04  | 121.58      | 117.15   |
| 23  | b     | 619    | CLA  | CHB-C4A-NA  | 2.03  | 127.33      | 124.51   |
| 23  | b     | 615    | CLA  | CMB-C2B-C1B | 2.03  | 128.47      | 125.37   |
| 23  | b     | 606    | CLA  | C4-C3-C2    | -2.03 | 118.46      | 123.68   |
| 23  | b     | 608    | CLA  | CAA-C2A-C1A | -2.03 | 105.32      | 111.97   |
| 36  | B     | 624[B] | HTG  | C1-C2-C3    | 2.03  | 114.60      | 110.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | C     | 509  | CLA  | CHB-C4A-NA  | 2.03  | 127.32      | 124.51   |
| 36  | B     | 627  | HTG  | C1-O5-C5    | 2.03  | 116.32      | 112.58   |
| 23  | B     | 610  | CLA  | CMA-C3A-C4A | -2.03 | 106.32      | 111.77   |
| 28  | M     | 101  | LMT  | C1B-O5B-C5B | 2.03  | 117.67      | 113.69   |
| 23  | a     | 2610 | CLA  | O2D-CGD-O1D | -2.03 | 119.88      | 123.84   |
| 23  | b     | 613  | CLA  | CHC-C1C-C2C | -2.03 | 121.10      | 126.73   |
| 27  | A     | 413  | LMG  | O6-C5-C4    | 2.03  | 113.37      | 109.69   |
| 31  | A     | 418  | JOX  | C-C1-CL1    | 2.03  | 124.91      | 120.02   |
| 23  | B     | 615  | CLA  | CHB-C1B-NB  | -2.02 | 122.11      | 124.26   |
| 23  | B     | 606  | CLA  | CHA-C1A-NA  | -2.02 | 121.76      | 126.40   |
| 36  | b     | 603  | HTG  | C2'-C1'-S1  | -2.02 | 105.87      | 112.40   |
| 23  | c     | 505  | CLA  | CHD-C4C-NC  | 2.02  | 127.39      | 124.20   |
| 23  | b     | 611  | CLA  | CHC-C1C-C2C | -2.02 | 121.11      | 126.73   |
| 23  | c     | 504  | CLA  | CHC-C1C-C2C | -2.02 | 121.12      | 126.73   |
| 27  | c     | 522  | LMG  | C4-C3-C2    | -2.02 | 107.30      | 110.82   |
| 23  | c     | 509  | CLA  | C1-C2-C3    | -2.02 | 122.55      | 126.04   |
| 23  | c     | 515  | CLA  | CHD-C1D-C2D | -2.02 | 121.25      | 125.48   |
| 23  | B     | 604  | CLA  | CHB-C1B-C2B | -2.02 | 121.54      | 127.24   |
| 23  | C     | 510  | CLA  | OBD-CAD-C3D | -2.02 | 123.67      | 128.52   |
| 25  | b     | 622  | BCR  | C35-C13-C14 | -2.02 | 120.10      | 122.92   |
| 39  | F     | 101  | HEM  | C1B-NB-C4B  | 2.02  | 107.16      | 105.07   |
| 25  | B     | 619  | BCR  | C11-C10-C9  | -2.01 | 124.44      | 127.31   |
| 23  | C     | 512  | CLA  | CMB-C2B-C1B | 2.01  | 128.44      | 125.37   |
| 23  | A     | 410  | CLA  | O2A-CGA-O1A | -2.01 | 118.51      | 123.59   |
| 40  | H     | 102  | RRX  | C21-C20-C19 | -2.01 | 116.94      | 123.22   |
| 23  | B     | 614  | CLA  | C5-C3-C2    | -2.01 | 117.05      | 121.12   |
| 23  | B     | 617  | CLA  | C5-C3-C2    | -2.01 | 117.05      | 121.12   |
| 28  | m     | 2804 | LMT  | C4B-C3B-C2B | 2.01  | 114.33      | 110.82   |
| 23  | d     | 409  | CLA  | O2A-CGA-CBA | 2.01  | 118.22      | 111.91   |
| 25  | a     | 2614 | BCR  | C15-C14-C13 | -2.01 | 124.44      | 127.31   |
| 23  | c     | 511  | CLA  | CHC-C1C-C2C | -2.01 | 121.15      | 126.73   |
| 23  | C     | 513  | CLA  | CAC-C3C-C2C | 2.01  | 130.96      | 127.53   |
| 23  | B     | 613  | CLA  | C2A-C1A-CHA | -2.01 | 120.35      | 123.86   |
| 24  | a     | 2611 | PHO  | C4A-C3A-C2A | -2.00 | 100.93      | 102.84   |
| 25  | b     | 622  | BCR  | C16-C17-C18 | -2.00 | 124.45      | 127.31   |
| 37  | C     | 517  | DGD  | C2G-O2G-C1B | -2.00 | 112.86      | 117.79   |
| 23  | c     | 510  | CLA  | CHC-C1C-C2C | -2.00 | 121.17      | 126.73   |
| 23  | b     | 620  | CLA  | C3B-C4B-NB  | 2.00  | 112.37      | 110.52   |

All (2) chirality outliers are listed below:

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
|-----|-------|-----|------|------|

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 42  | V     | 201 | HEC  | NA   |
| 42  | v     | 201 | HEC  | NA   |

All (1308) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | B     | 603  | CLA  | CHA-CBD-CGD-O1D |
| 23  | B     | 607  | CLA  | CHA-CBD-CGD-O1D |
| 23  | B     | 607  | CLA  | CHA-CBD-CGD-O2D |
| 23  | B     | 610  | CLA  | C2B-C3B-CAB-CBB |
| 23  | B     | 610  | CLA  | C4B-C3B-CAB-CBB |
| 23  | B     | 611  | CLA  | C14-C13-C15-C16 |
| 23  | B     | 615  | CLA  | CHA-CBD-CGD-O2D |
| 23  | B     | 615  | CLA  | CAD-CBD-CGD-O2D |
| 23  | C     | 504  | CLA  | C2B-C3B-CAB-CBB |
| 23  | C     | 504  | CLA  | C4B-C3B-CAB-CBB |
| 23  | C     | 505  | CLA  | C2B-C3B-CAB-CBB |
| 23  | C     | 505  | CLA  | C4B-C3B-CAB-CBB |
| 23  | C     | 507  | CLA  | C2-C3-C5-C6     |
| 23  | C     | 507  | CLA  | C4-C3-C5-C6     |
| 23  | C     | 514  | CLA  | C2B-C3B-CAB-CBB |
| 23  | C     | 514  | CLA  | C4B-C3B-CAB-CBB |
| 23  | D     | 2304 | CLA  | C2-C3-C5-C6     |
| 23  | D     | 2304 | CLA  | C4-C3-C5-C6     |
| 23  | b     | 607  | CLA  | CHA-CBD-CGD-O1D |
| 23  | b     | 608  | CLA  | C4-C3-C5-C6     |
| 23  | b     | 610  | CLA  | C2-C3-C5-C6     |
| 23  | b     | 610  | CLA  | C4-C3-C5-C6     |
| 23  | b     | 611  | CLA  | CHA-CBD-CGD-O1D |
| 23  | b     | 611  | CLA  | CHA-CBD-CGD-O2D |
| 23  | b     | 614  | CLA  | C2B-C3B-CAB-CBB |
| 23  | b     | 614  | CLA  | C4B-C3B-CAB-CBB |
| 23  | b     | 619  | CLA  | CHA-CBD-CGD-O1D |
| 23  | b     | 619  | CLA  | CHA-CBD-CGD-O2D |
| 23  | b     | 619  | CLA  | CAD-CBD-CGD-O1D |
| 23  | b     | 619  | CLA  | CAD-CBD-CGD-O2D |
| 23  | c     | 505  | CLA  | C2B-C3B-CAB-CBB |
| 23  | c     | 505  | CLA  | C4B-C3B-CAB-CBB |
| 23  | c     | 506  | CLA  | C2B-C3B-CAB-CBB |
| 23  | c     | 506  | CLA  | C4B-C3B-CAB-CBB |
| 23  | c     | 510  | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | c     | 510  | CLA  | C4-C3-C5-C6     |
| 23  | c     | 515  | CLA  | C2B-C3B-CAB-CBB |
| 23  | c     | 515  | CLA  | C4B-C3B-CAB-CBB |
| 25  | B     | 618  | BCR  | C1-C6-C7-C8     |
| 25  | B     | 633  | BCR  | C11-C12-C13-C14 |
| 25  | B     | 633  | BCR  | C11-C12-C13-C35 |
| 25  | B     | 633  | BCR  | C13-C14-C15-C16 |
| 25  | C     | 516  | BCR  | C1-C6-C7-C8     |
| 25  | D     | 2305 | BCR  | C7-C8-C9-C10    |
| 25  | D     | 2305 | BCR  | C7-C8-C9-C34    |
| 25  | D     | 2305 | BCR  | C21-C22-C23-C24 |
| 25  | D     | 2305 | BCR  | C37-C22-C23-C24 |
| 25  | D     | 2305 | BCR  | C23-C24-C25-C30 |
| 25  | T     | 102  | BCR  | C11-C12-C13-C14 |
| 25  | T     | 102  | BCR  | C11-C12-C13-C35 |
| 25  | Y     | 302  | BCR  | C21-C22-C23-C24 |
| 25  | Y     | 302  | BCR  | C37-C22-C23-C24 |
| 25  | b     | 622  | BCR  | C1-C6-C7-C8     |
| 25  | b     | 624  | BCR  | C37-C22-C23-C24 |
| 25  | d     | 410  | BCR  | C7-C8-C9-C10    |
| 25  | d     | 410  | BCR  | C7-C8-C9-C34    |
| 25  | d     | 410  | BCR  | C21-C22-C23-C24 |
| 25  | d     | 410  | BCR  | C37-C22-C23-C24 |
| 25  | y     | 101  | BCR  | C21-C22-C23-C24 |
| 25  | y     | 101  | BCR  | C37-C22-C23-C24 |
| 26  | B     | 621  | SQD  | O5-C1-O6-C44    |
| 26  | B     | 621  | SQD  | O49-C7-O47-C45  |
| 26  | B     | 621  | SQD  | C8-C7-O47-C45   |
| 26  | B     | 621  | SQD  | C5-C6-S-O7      |
| 26  | B     | 621  | SQD  | C5-C6-S-O8      |
| 26  | B     | 621  | SQD  | C5-C6-S-O9      |
| 26  | D     | 2302 | SQD  | O49-C7-O47-C45  |
| 26  | D     | 2308 | SQD  | C8-C7-O47-C45   |
| 26  | D     | 2308 | SQD  | C5-C6-S-O7      |
| 26  | a     | 2603 | SQD  | O6-C44-C45-O47  |
| 26  | a     | 2603 | SQD  | C5-C6-S-O7      |
| 26  | a     | 2603 | SQD  | C5-C6-S-O8      |
| 26  | a     | 2603 | SQD  | C5-C6-S-O9      |
| 26  | b     | 601  | SQD  | C5-C6-S-O7      |
| 26  | b     | 601  | SQD  | C5-C6-S-O8      |
| 26  | b     | 601  | SQD  | C5-C6-S-O9      |
| 26  | d     | 417  | SQD  | C44-C45-O47-C7  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | d     | 417  | SQD  | C46-C45-O47-C7  |
| 26  | d     | 417  | SQD  | O49-C7-O47-C45  |
| 26  | l     | 101  | SQD  | O5-C1-O6-C44    |
| 26  | l     | 101  | SQD  | O49-C7-O47-C45  |
| 26  | l     | 101  | SQD  | C8-C7-O47-C45   |
| 26  | l     | 101  | SQD  | C5-C6-S-O7      |
| 27  | C     | 527  | LMG  | O9-C10-O7-C8    |
| 27  | C     | 527  | LMG  | C11-C10-O7-C8   |
| 27  | c     | 501  | LMG  | O9-C10-O7-C8    |
| 28  | A     | 414  | LMT  | C2'-C1'-O1'-C1  |
| 28  | A     | 414  | LMT  | O5'-C1'-O1'-C1  |
| 28  | A     | 414  | LMT  | C2-C1-O1'-C1'   |
| 28  | A     | 420  | LMT  | O5'-C1'-O1'-C1  |
| 28  | B     | 623  | LMT  | C2-C1-O1'-C1'   |
| 28  | F     | 102  | LMT  | C2'-C1'-O1'-C1  |
| 28  | F     | 102  | LMT  | O5'-C1'-O1'-C1  |
| 28  | J     | 303  | LMT  | C2'-C1'-O1'-C1  |
| 28  | T     | 103  | LMT  | C2'-C1'-O1'-C1  |
| 28  | T     | 103  | LMT  | O5'-C1'-O1'-C1  |
| 28  | Z     | 101  | LMT  | C2-C1-O1'-C1'   |
| 28  | d     | 401  | LMT  | C2'-C1'-O1'-C1  |
| 28  | d     | 401  | LMT  | O5'-C1'-O1'-C1  |
| 28  | d     | 404  | LMT  | C2'-C1'-O1'-C1  |
| 28  | d     | 404  | LMT  | O5'-C1'-O1'-C1  |
| 28  | f     | 101  | LMT  | C2'-C1'-O1'-C1  |
| 28  | f     | 101  | LMT  | O5'-C1'-O1'-C1  |
| 28  | i     | 103  | LMT  | C2'-C1'-O1'-C1  |
| 28  | i     | 103  | LMT  | O5'-C1'-O1'-C1  |
| 28  | z     | 102  | LMT  | C2'-C1'-O1'-C1  |
| 28  | z     | 102  | LMT  | O5'-C1'-O1'-C1  |
| 29  | B     | 632  | GOL  | O1-C1-C2-C3     |
| 29  | C     | 524  | GOL  | O1-C1-C2-O2     |
| 29  | C     | 524  | GOL  | O1-C1-C2-C3     |
| 29  | C     | 526  | GOL  | O1-C1-C2-C3     |
| 29  | J     | 301  | GOL  | O1-C1-C2-C3     |
| 29  | J     | 301  | GOL  | C1-C2-C3-O3     |
| 29  | J     | 301  | GOL  | O2-C2-C3-O3     |
| 29  | O     | 302  | GOL  | C1-C2-C3-O3     |
| 29  | O     | 304  | GOL  | O1-C1-C2-C3     |
| 29  | U     | 502  | GOL  | C1-C2-C3-O3     |
| 29  | b     | 644  | GOL  | O1-C1-C2-C3     |
| 33  | x     | 1301 | PL9  | C18-C19-C21-C22 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 33  | x     | 1301 | PL9  | C20-C19-C21-C22 |
| 36  | C     | 521  | HTG  | C2'-C1'-S1-C1   |
| 36  | I     | 101  | HTG  | C2-C1-S1-C1'    |
| 36  | I     | 101  | HTG  | O5-C1-S1-C1'    |
| 36  | V     | 204  | HTG  | C2-C1-S1-C1'    |
| 36  | V     | 204  | HTG  | O5-C1-S1-C1'    |
| 36  | b     | 602  | HTG  | C2'-C1'-S1-C1   |
| 36  | b     | 625  | HTG  | C2'-C1'-S1-C1   |
| 36  | b     | 626  | HTG  | O5-C1-S1-C1'    |
| 36  | d     | 407  | HTG  | C2-C1-S1-C1'    |
| 36  | d     | 407  | HTG  | O5-C1-S1-C1'    |
| 36  | d     | 407  | HTG  | C2'-C1'-S1-C1   |
| 36  | d     | 415  | HTG  | O5-C1-S1-C1'    |
| 36  | i     | 102  | HTG  | C2-C1-S1-C1'    |
| 36  | i     | 102  | HTG  | O5-C1-S1-C1'    |
| 36  | o     | 301  | HTG  | C2'-C1'-S1-C1   |
| 37  | D     | 2307 | DGD  | C2B-C1B-O2G-C2G |
| 37  | D     | 2307 | DGD  | C2D-C1D-O3G-C3G |
| 37  | D     | 2307 | DGD  | O6D-C1D-O3G-C3G |
| 38  | D     | 2310 | LHG  | C4-O6-P-O4      |
| 38  | E     | 101  | LHG  | C4-O6-P-O5      |
| 38  | L     | 101  | LHG  | C4-O6-P-O4      |
| 38  | d     | 412  | LHG  | O2-C2-C3-O3     |
| 38  | d     | 413  | LHG  | O1-C1-C2-C3     |
| 38  | e     | 101  | LHG  | O10-C23-O8-C6   |
| 38  | e     | 101  | LHG  | C24-C23-O8-C6   |
| 38  | l     | 103  | LHG  | C4-O6-P-O4      |
| 23  | C     | 507  | CLA  | C15-C16-C17-C18 |
| 23  | b     | 611  | CLA  | C10-C11-C12-C13 |
| 26  | D     | 2308 | SQD  | O49-C7-O47-C45  |
| 37  | D     | 2307 | DGD  | O1B-C1B-O2G-C2G |
| 26  | D     | 2308 | SQD  | O10-C23-O48-C46 |
| 26  | D     | 2302 | SQD  | C8-C7-O47-C45   |
| 27  | c     | 501  | LMG  | C11-C10-O7-C8   |
| 42  | v     | 201  | HEC  | C2B-C3B-CAB-CBB |
| 42  | V     | 201  | HEC  | C2B-C3B-CAB-CBB |
| 23  | B     | 606  | CLA  | C4-C3-C5-C6     |
| 23  | B     | 615  | CLA  | C4-C3-C5-C6     |
| 23  | b     | 608  | CLA  | C2-C3-C5-C6     |
| 23  | D     | 2304 | CLA  | C3-C5-C6-C7     |
| 23  | b     | 606  | CLA  | C3-C5-C6-C7     |
| 23  | b     | 621  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | D     | 2308   | SQD  | C24-C23-O48-C46 |
| 36  | I     | 101    | HTG  | S1-C1'-C2'-C3'  |
| 25  | T     | 102    | BCR  | C13-C14-C15-C16 |
| 36  | b     | 626    | HTG  | O5-C5-C6-O6     |
| 23  | B     | 605    | CLA  | C3-C5-C6-C7     |
| 23  | c     | 516    | CLA  | C3-C5-C6-C7     |
| 23  | d     | 409    | CLA  | C3-C5-C6-C7     |
| 38  | E     | 101    | LHG  | C24-C23-O8-C6   |
| 28  | T     | 103    | LMT  | O5'-C5'-C6'-O6' |
| 28  | z     | 102    | LMT  | O5B-C5B-C6B-O6B |
| 28  | A     | 414    | LMT  | C2-C3-C4-C5     |
| 37  | C     | 517    | DGD  | CCB-CDB-CEB-CFB |
| 36  | B     | 624[A] | HTG  | S1-C1'-C2'-C3'  |
| 36  | b     | 602    | HTG  | S1-C1'-C2'-C3'  |
| 38  | E     | 101    | LHG  | O10-C23-O8-C6   |
| 28  | Z     | 101    | LMT  | O5B-C5B-C6B-O6B |
| 23  | b     | 619    | CLA  | C4-C3-C5-C6     |
| 36  | B     | 626    | HTG  | C4-C5-C6-O6     |
| 23  | B     | 606    | CLA  | C2-C3-C5-C6     |
| 23  | B     | 615    | CLA  | C2-C3-C5-C6     |
| 23  | b     | 619    | CLA  | C2-C3-C5-C6     |
| 23  | c     | 510    | CLA  | C2-C3-C5-C6     |
| 28  | B     | 634    | LMT  | O5'-C5'-C6'-O6' |
| 36  | i     | 102    | HTG  | O5-C5-C6-O6     |
| 28  | J     | 303    | LMT  | O5'-C1'-O1'-C1  |
| 33  | A     | 422    | PL9  | C9-C11-C12-C13  |
| 33  | A     | 422    | PL9  | C14-C16-C17-C18 |
| 33  | x     | 1301   | PL9  | C9-C11-C12-C13  |
| 33  | x     | 1301   | PL9  | C14-C16-C17-C18 |
| 37  | C     | 518    | DGD  | C8A-C9A-CAA-CBA |
| 28  | Z     | 101    | LMT  | O5B-C1B-O1B-C4' |
| 37  | c     | 518    | DGD  | C8A-C9A-CAA-CBA |
| 28  | z     | 102    | LMT  | C4B-C5B-C6B-O6B |
| 37  | h     | 102    | DGD  | C9A-CAA-CBA-CCA |
| 28  | B     | 634    | LMT  | C4'-C5'-C6'-O6' |
| 37  | H     | 103    | DGD  | C9A-CAA-CBA-CCA |
| 27  | B     | 622    | LMG  | C15-C16-C17-C18 |
| 23  | a     | 2609   | CLA  | C15-C16-C17-C18 |
| 28  | i     | 103    | LMT  | O5'-C5'-C6'-O6' |
| 23  | B     | 616    | CLA  | C13-C15-C16-C17 |
| 27  | C     | 520    | LMG  | C10-C11-C12-C13 |
| 26  | B     | 621    | SQD  | C2-C1-O6-C44    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 38  | d     | 403  | LHG  | C34-C35-C36-C37 |
| 23  | d     | 409  | CLA  | C4-C3-C5-C6     |
| 23  | A     | 410  | CLA  | C14-C13-C15-C16 |
| 23  | B     | 602  | CLA  | C6-C7-C8-C9     |
| 23  | B     | 616  | CLA  | C11-C10-C8-C9   |
| 23  | C     | 505  | CLA  | C11-C12-C13-C14 |
| 23  | C     | 507  | CLA  | C14-C13-C15-C16 |
| 23  | a     | 2610 | CLA  | C11-C12-C13-C14 |
| 23  | c     | 507  | CLA  | C11-C12-C13-C14 |
| 25  | C     | 515  | BCR  | C37-C22-C23-C24 |
| 36  | d     | 407  | HTG  | O5-C5-C6-O6     |
| 36  | V     | 204  | HTG  | C4-C5-C6-O6     |
| 26  | D     | 2302 | SQD  | C23-C24-C25-C26 |
| 23  | C     | 514  | CLA  | C10-C11-C12-C13 |
| 28  | Z     | 101  | LMT  | C2B-C1B-O1B-C4' |
| 27  | m     | 2802 | LMG  | C30-C31-C32-C33 |
| 28  | J     | 303  | LMT  | O5'-C5'-C6'-O6' |
| 28  | Z     | 101  | LMT  | C4B-C5B-C6B-O6B |
| 36  | i     | 102  | HTG  | C4-C5-C6-O6     |
| 23  | a     | 2613 | CLA  | C5-C6-C7-C8     |
| 23  | b     | 606  | CLA  | C10-C11-C12-C13 |
| 37  | c     | 519  | DGD  | C1B-C2B-C3B-C4B |
| 42  | V     | 201  | HEC  | C2C-C3C-CAC-CBC |
| 23  | B     | 614  | CLA  | C10-C11-C12-C13 |
| 23  | b     | 616  | CLA  | C13-C15-C16-C17 |
| 23  | c     | 515  | CLA  | C10-C11-C12-C13 |
| 23  | c     | 516  | CLA  | C10-C11-C12-C13 |
| 29  | J     | 301  | GOL  | O1-C1-C2-O2     |
| 29  | v     | 202  | GOL  | O2-C2-C3-O3     |
| 37  | C     | 517  | DGD  | C1B-C2B-C3B-C4B |
| 36  | B     | 626  | HTG  | O5-C5-C6-O6     |
| 23  | D     | 2304 | CLA  | C8-C10-C11-C12  |
| 28  | z     | 102  | LMT  | O5'-C5'-C6'-O6' |
| 28  | B     | 623  | LMT  | O1'-C1-C2-C3    |
| 28  | d     | 401  | LMT  | O1'-C1-C2-C3    |
| 23  | d     | 409  | CLA  | C8-C10-C11-C12  |
| 26  | B     | 621  | SQD  | C7-C8-C9-C10    |
| 27  | m     | 2802 | LMG  | C10-C11-C12-C13 |
| 37  | C     | 518  | DGD  | C1B-C2B-C3B-C4B |
| 42  | v     | 201  | HEC  | C2C-C3C-CAC-CBC |
| 23  | A     | 410  | CLA  | C11-C12-C13-C15 |
| 23  | B     | 614  | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | B     | 617  | CLA  | C12-C13-C15-C16 |
| 23  | b     | 611  | CLA  | C12-C13-C15-C16 |
| 23  | b     | 618  | CLA  | C11-C12-C13-C15 |
| 23  | d     | 409  | CLA  | C6-C7-C8-C10    |
| 23  | C     | 508  | CLA  | C15-C16-C17-C18 |
| 33  | A     | 422  | PL9  | C19-C21-C22-C23 |
| 33  | x     | 1301 | PL9  | C24-C26-C27-C28 |
| 33  | x     | 1301 | PL9  | C34-C36-C37-C38 |
| 28  | T     | 103  | LMT  | C4'-C5'-C6'-O6' |
| 23  | B     | 604  | CLA  | C5-C6-C7-C8     |
| 23  | C     | 510  | CLA  | C13-C15-C16-C17 |
| 27  | B     | 622  | LMG  | C10-C11-C12-C13 |
| 36  | b     | 626  | HTG  | C4-C5-C6-O6     |
| 23  | b     | 621  | CLA  | C13-C15-C16-C17 |
| 36  | o     | 301  | HTG  | C4-C5-C6-O6     |
| 23  | B     | 617  | CLA  | C5-C6-C7-C8     |
| 23  | B     | 617  | CLA  | C10-C11-C12-C13 |
| 23  | b     | 621  | CLA  | C5-C6-C7-C8     |
| 38  | E     | 101  | LHG  | C4-O6-P-O3      |
| 38  | l     | 103  | LHG  | C4-O6-P-O3      |
| 23  | B     | 615  | CLA  | C3-C5-C6-C7     |
| 28  | F     | 102  | LMT  | C1-C2-C3-C4     |
| 23  | C     | 504  | CLA  | CBD-CGD-O2D-CED |
| 38  | d     | 412  | LHG  | C1-C2-C3-O3     |
| 23  | d     | 409  | CLA  | C2-C3-C5-C6     |
| 23  | C     | 511  | CLA  | C8-C10-C11-C12  |
| 23  | b     | 620  | CLA  | C10-C11-C12-C13 |
| 23  | B     | 607  | CLA  | C2A-CAA-CBA-CGA |
| 37  | D     | 2307 | DGD  | O6D-C5D-C6D-O5D |
| 28  | B     | 623  | LMT  | O5B-C1B-O1B-C4' |
| 23  | c     | 509  | CLA  | C15-C16-C17-C18 |
| 26  | l     | 101  | SQD  | C31-C32-C33-C34 |
| 38  | l     | 103  | LHG  | C33-C34-C35-C36 |
| 23  | c     | 516  | CLA  | CBD-CGD-O2D-CED |
| 27  | c     | 521  | LMG  | C11-C10-O7-C8   |
| 23  | c     | 512  | CLA  | C8-C10-C11-C12  |
| 26  | D     | 2302 | SQD  | C24-C23-O48-C46 |
| 37  | D     | 2307 | DGD  | C3B-C4B-C5B-C6B |
| 38  | L     | 101  | LHG  | C33-C34-C35-C36 |
| 27  | c     | 521  | LMG  | O9-C10-O7-C8    |
| 37  | c     | 519  | DGD  | C1A-C2A-C3A-C4A |
| 28  | d     | 401  | LMT  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 27  | C     | 520  | LMG  | C16-C17-C18-C19 |
| 28  | j     | 2701 | LMT  | C2'-C1'-O1'-C1  |
| 27  | A     | 413  | LMG  | C30-C31-C32-C33 |
| 37  | C     | 518  | DGD  | C4B-C5B-C6B-C7B |
| 42  | v     | 201  | HEC  | C4B-C3B-CAB-CBB |
| 23  | C     | 502  | CLA  | C16-C17-C18-C19 |
| 23  | C     | 507  | CLA  | C16-C17-C18-C20 |
| 23  | b     | 621  | CLA  | C4-C3-C5-C6     |
| 33  | D     | 2306 | PL9  | C15-C14-C16-C17 |
| 26  | a     | 2603 | SQD  | C34-C35-C36-C37 |
| 36  | H     | 101  | HTG  | C3'-C4'-C5'-C6' |
| 33  | D     | 2306 | PL9  | C13-C14-C16-C17 |
| 23  | B     | 604  | CLA  | C6-C7-C8-C9     |
| 23  | a     | 2610 | CLA  | C6-C7-C8-C9     |
| 23  | c     | 509  | CLA  | C11-C10-C8-C9   |
| 23  | c     | 509  | CLA  | C14-C13-C15-C16 |
| 26  | a     | 2603 | SQD  | C31-C32-C33-C34 |
| 27  | A     | 413  | LMG  | C38-C39-C40-C41 |
| 27  | d     | 414  | LMG  | C19-C20-C21-C22 |
| 28  | z     | 102  | LMT  | C7-C8-C9-C10    |
| 37  | C     | 517  | DGD  | C5B-C6B-C7B-C8B |
| 29  | A     | 415  | GOL  | O1-C1-C2-C3     |
| 29  | A     | 417  | GOL  | C1-C2-C3-O3     |
| 29  | D     | 2301 | GOL  | O1-C1-C2-C3     |
| 29  | a     | 2602 | GOL  | O1-C1-C2-C3     |
| 29  | c     | 530  | GOL  | O1-C1-C2-C3     |
| 29  | c     | 530  | GOL  | C1-C2-C3-O3     |
| 29  | c     | 531  | GOL  | C1-C2-C3-O3     |
| 29  | d     | 416  | GOL  | C1-C2-C3-O3     |
| 29  | v     | 202  | GOL  | C1-C2-C3-O3     |
| 38  | D     | 2310 | LHG  | O1-C1-C2-C3     |
| 38  | D     | 2311 | LHG  | O1-C1-C2-C3     |
| 38  | d     | 412  | LHG  | O1-C1-C2-C3     |
| 27  | d     | 414  | LMG  | O6-C5-C6-O5     |
| 23  | B     | 606  | CLA  | C10-C11-C12-C13 |
| 23  | c     | 513  | CLA  | C8-C10-C11-C12  |
| 26  | D     | 2302 | SQD  | C17-C18-C19-C20 |
| 27  | B     | 622  | LMG  | C37-C38-C39-C40 |
| 27  | C     | 527  | LMG  | C33-C34-C35-C36 |
| 27  | C     | 527  | LMG  | C34-C35-C36-C37 |
| 37  | C     | 518  | DGD  | CBB-CCB-CDB-CEB |
| 37  | c     | 518  | DGD  | C4B-C5B-C6B-C7B |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 37  | c     | 519  | DGD  | C4B-C5B-C6B-C7B |
| 36  | B     | 627  | HTG  | C4-C5-C6-O6     |
| 37  | D     | 2307 | DGD  | C1B-C2B-C3B-C4B |
| 27  | C     | 520  | LMG  | C31-C32-C33-C34 |
| 27  | c     | 521  | LMG  | C36-C37-C38-C39 |
| 27  | C     | 527  | LMG  | O6-C5-C6-O5     |
| 23  | C     | 503  | CLA  | C4B-C3B-CAB-CBB |
| 23  | c     | 504  | CLA  | C4B-C3B-CAB-CBB |
| 26  | l     | 101  | SQD  | C29-C30-C31-C32 |
| 37  | C     | 518  | DGD  | C5A-C6A-C7A-C8A |
| 28  | A     | 420  | LMT  | C1-C2-C3-C4     |
| 37  | c     | 518  | DGD  | CBB-CCB-CDB-CEB |
| 27  | c     | 501  | LMG  | C11-C12-C13-C14 |
| 37  | C     | 518  | DGD  | C3B-C4B-C5B-C6B |
| 38  | D     | 2309 | LHG  | C32-C33-C34-C35 |
| 28  | M     | 101  | LMT  | O5B-C5B-C6B-O6B |
| 23  | B     | 602  | CLA  | CBA-CGA-O2A-C1  |
| 26  | l     | 101  | SQD  | C11-C10-C9-C8   |
| 23  | C     | 513  | CLA  | C3A-C2A-CAA-CBA |
| 23  | C     | 514  | CLA  | C3A-C2A-CAA-CBA |
| 28  | i     | 103  | LMT  | C1-C2-C3-C4     |
| 28  | M     | 101  | LMT  | C2-C1-O1'-C1'   |
| 28  | T     | 103  | LMT  | C6-C7-C8-C9     |
| 37  | C     | 517  | DGD  | C4A-C5A-C6A-C7A |
| 28  | A     | 414  | LMT  | C1-C2-C3-C4     |
| 26  | a     | 2615 | SQD  | C23-C24-C25-C26 |
| 28  | i     | 103  | LMT  | C6-C7-C8-C9     |
| 37  | c     | 519  | DGD  | CCA-CDA-CEA-CFA |
| 23  | C     | 511  | CLA  | C4-C3-C5-C6     |
| 23  | b     | 614  | CLA  | C4-C3-C5-C6     |
| 23  | B     | 612  | CLA  | C2-C3-C5-C6     |
| 23  | C     | 506  | CLA  | C2-C3-C5-C6     |
| 23  | C     | 511  | CLA  | C2-C3-C5-C6     |
| 23  | b     | 614  | CLA  | C2-C3-C5-C6     |
| 33  | d     | 411  | PL9  | C13-C14-C16-C17 |
| 38  | D     | 2309 | LHG  | C24-C25-C26-C27 |
| 29  | A     | 417  | GOL  | O2-C2-C3-O3     |
| 29  | O     | 302  | GOL  | O2-C2-C3-O3     |
| 29  | U     | 502  | GOL  | O2-C2-C3-O3     |
| 29  | b     | 644  | GOL  | O1-C1-C2-O2     |
| 29  | c     | 530  | GOL  | O2-C2-C3-O3     |
| 38  | d     | 413  | LHG  | O1-C1-C2-O2     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | B     | 621  | SQD  | C27-C28-C29-C30 |
| 26  | a     | 2603 | SQD  | C24-C25-C26-C27 |
| 38  | l     | 103  | LHG  | C13-C14-C15-C16 |
| 23  | C     | 503  | CLA  | C2B-C3B-CAB-CBB |
| 23  | b     | 618  | CLA  | C8-C10-C11-C12  |
| 36  | I     | 101  | HTG  | O5-C5-C6-O6     |
| 26  | b     | 601  | SQD  | C24-C25-C26-C27 |
| 38  | L     | 101  | LHG  | C13-C14-C15-C16 |
| 26  | D     | 2302 | SQD  | O10-C23-O48-C46 |
| 28  | B     | 623  | LMT  | C7-C8-C9-C10    |
| 37  | c     | 518  | DGD  | C3B-C4B-C5B-C6B |
| 38  | D     | 2311 | LHG  | C27-C28-C29-C30 |
| 42  | V     | 201  | HEC  | C4B-C3B-CAB-CBB |
| 23  | B     | 602  | CLA  | C2-C1-O2A-CGA   |
| 26  | B     | 621  | SQD  | C28-C29-C30-C31 |
| 27  | B     | 622  | LMG  | C30-C31-C32-C33 |
| 28  | B     | 634  | LMT  | C11-C10-C9-C8   |
| 28  | z     | 102  | LMT  | C6-C7-C8-C9     |
| 23  | B     | 602  | CLA  | O1A-CGA-O2A-C1  |
| 38  | E     | 101  | LHG  | C7-C8-C9-C10    |
| 25  | B     | 618  | BCR  | C5-C6-C7-C8     |
| 25  | C     | 516  | BCR  | C5-C6-C7-C8     |
| 25  | D     | 2305 | BCR  | C23-C24-C25-C26 |
| 25  | Y     | 302  | BCR  | C1-C6-C7-C8     |
| 25  | Y     | 302  | BCR  | C5-C6-C7-C8     |
| 25  | b     | 622  | BCR  | C5-C6-C7-C8     |
| 25  | c     | 517  | BCR  | C1-C6-C7-C8     |
| 25  | c     | 517  | BCR  | C5-C6-C7-C8     |
| 25  | d     | 410  | BCR  | C23-C24-C25-C26 |
| 25  | d     | 410  | BCR  | C23-C24-C25-C30 |
| 25  | y     | 101  | BCR  | C1-C6-C7-C8     |
| 25  | y     | 101  | BCR  | C5-C6-C7-C8     |
| 36  | V     | 204  | HTG  | O5-C5-C6-O6     |
| 26  | l     | 101  | SQD  | C15-C16-C17-C18 |
| 28  | B     | 634  | LMT  | C9-C10-C11-C12  |
| 38  | d     | 403  | LHG  | C32-C33-C34-C35 |
| 27  | D     | 2312 | LMG  | C35-C36-C37-C38 |
| 28  | T     | 103  | LMT  | C9-C10-C11-C12  |
| 37  | D     | 2307 | DGD  | CCB-CDB-CEB-CFB |
| 27  | A     | 413  | LMG  | C35-C36-C37-C38 |
| 36  | V     | 204  | HTG  | C2'-C3'-C4'-C5' |
| 23  | B     | 617  | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 33  | d     | 411  | PL9  | C15-C14-C16-C17 |
| 23  | A     | 410  | CLA  | C12-C13-C15-C16 |
| 23  | B     | 604  | CLA  | C6-C7-C8-C10    |
| 23  | B     | 605  | CLA  | C6-C7-C8-C10    |
| 23  | B     | 617  | CLA  | C2-C3-C5-C6     |
| 23  | C     | 505  | CLA  | C11-C12-C13-C15 |
| 23  | C     | 507  | CLA  | C12-C13-C15-C16 |
| 23  | a     | 2610 | CLA  | C6-C7-C8-C10    |
| 23  | b     | 621  | CLA  | C2-C3-C5-C6     |
| 23  | c     | 507  | CLA  | C11-C12-C13-C15 |
| 23  | c     | 511  | CLA  | C11-C10-C8-C7   |
| 24  | a     | 2611 | PHO  | C2-C3-C5-C6     |
| 23  | A     | 410  | CLA  | C3-C5-C6-C7     |
| 27  | B     | 622  | LMG  | C36-C37-C38-C39 |
| 27  | c     | 501  | LMG  | C36-C37-C38-C39 |
| 28  | Z     | 101  | LMT  | C2-C3-C4-C5     |
| 38  | L     | 101  | LHG  | C30-C31-C32-C33 |
| 42  | V     | 201  | HEC  | C4C-C3C-CAC-CBC |
| 23  | c     | 508  | CLA  | C16-C17-C18-C20 |
| 27  | c     | 521  | LMG  | C10-C11-C12-C13 |
| 23  | b     | 611  | CLA  | C2A-CAA-CBA-CGA |
| 23  | a     | 2613 | CLA  | C10-C11-C12-C13 |
| 26  | l     | 101  | SQD  | C28-C29-C30-C31 |
| 28  | A     | 414  | LMT  | O1'-C1-C2-C3    |
| 26  | D     | 2308 | SQD  | C23-C24-C25-C26 |
| 27  | c     | 522  | LMG  | O6-C5-C6-O5     |
| 28  | M     | 101  | LMT  | C11-C10-C9-C8   |
| 28  | i     | 103  | LMT  | C2-C3-C4-C5     |
| 28  | f     | 101  | LMT  | C1-C2-C3-C4     |
| 26  | D     | 2302 | SQD  | C24-C25-C26-C27 |
| 36  | o     | 301  | HTG  | O5-C5-C6-O6     |
| 37  | D     | 2307 | DGD  | C4D-C5D-C6D-O5D |
| 23  | A     | 407  | CLA  | C16-C17-C18-C20 |
| 23  | b     | 611  | CLA  | C16-C17-C18-C20 |
| 23  | c     | 516  | CLA  | C16-C17-C18-C19 |
| 26  | a     | 2603 | SQD  | O5-C1-O6-C44    |
| 28  | B     | 634  | LMT  | O5'-C1'-O1'-C1  |
| 28  | j     | 2701 | LMT  | O5'-C1'-O1'-C1  |
| 27  | A     | 413  | LMG  | C37-C38-C39-C40 |
| 27  | A     | 413  | LMG  | C11-C10-O7-C8   |
| 27  | m     | 2802 | LMG  | C11-C10-O7-C8   |
| 38  | E     | 101  | LHG  | O6-C4-C5-O7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 38  | d     | 412  | LHG  | C25-C26-C27-C28 |
| 38  | L     | 101  | LHG  | C11-C10-C9-C8   |
| 26  | D     | 2302 | SQD  | C2-C1-O6-C44    |
| 26  | a     | 2603 | SQD  | C2-C1-O6-C44    |
| 28  | B     | 634  | LMT  | C2'-C1'-O1'-C1  |
| 28  | j     | 2701 | LMT  | O5B-C5B-C6B-O6B |
| 37  | h     | 102  | DGD  | C7A-C8A-C9A-CAA |
| 38  | D     | 2309 | LHG  | C25-C26-C27-C28 |
| 27  | D     | 2312 | LMG  | C36-C37-C38-C39 |
| 37  | c     | 520  | DGD  | CBA-CCA-CDA-CEA |
| 38  | D     | 2311 | LHG  | C25-C26-C27-C28 |
| 38  | l     | 103  | LHG  | C30-C31-C32-C33 |
| 23  | c     | 507  | CLA  | C4-C3-C5-C6     |
| 24  | a     | 2611 | PHO  | C4-C3-C5-C6     |
| 26  | b     | 601  | SQD  | C23-C24-C25-C26 |
| 37  | H     | 103  | DGD  | C7A-C8A-C9A-CAA |
| 23  | B     | 614  | CLA  | C11-C12-C13-C14 |
| 23  | C     | 506  | CLA  | C11-C12-C13-C14 |
| 23  | b     | 611  | CLA  | C14-C13-C15-C16 |
| 23  | d     | 409  | CLA  | C6-C7-C8-C9     |
| 27  | A     | 413  | LMG  | C36-C37-C38-C39 |
| 26  | A     | 412  | SQD  | C30-C31-C32-C33 |
| 26  | l     | 101  | SQD  | C32-C33-C34-C35 |
| 37  | c     | 520  | DGD  | C7B-C8B-C9B-CAB |
| 36  | B     | 625  | HTG  | O5-C5-C6-O6     |
| 28  | B     | 623  | LMT  | C4B-C5B-C6B-O6B |
| 37  | C     | 519  | DGD  | C5B-C6B-C7B-C8B |
| 23  | C     | 513  | CLA  | C1A-C2A-CAA-CBA |
| 23  | C     | 514  | CLA  | C1A-C2A-CAA-CBA |
| 23  | b     | 616  | CLA  | C1A-C2A-CAA-CBA |
| 23  | c     | 509  | CLA  | C1A-C2A-CAA-CBA |
| 23  | c     | 511  | CLA  | C1A-C2A-CAA-CBA |
| 23  | C     | 502  | CLA  | C16-C17-C18-C20 |
| 23  | c     | 508  | CLA  | C16-C17-C18-C19 |
| 27  | A     | 413  | LMG  | O9-C10-O7-C8    |
| 27  | B     | 622  | LMG  | C29-C30-C31-C32 |
| 27  | m     | 2802 | LMG  | C13-C14-C15-C16 |
| 38  | d     | 412  | LHG  | C26-C27-C28-C29 |
| 38  | l     | 103  | LHG  | C11-C10-C9-C8   |
| 38  | L     | 101  | LHG  | C4-O6-P-O3      |
| 38  | D     | 2309 | LHG  | C23-C24-C25-C26 |
| 38  | d     | 412  | LHG  | C29-C30-C31-C32 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 37  | c     | 520  | DGD  | C9B-CAB-CBB-CCB |
| 27  | C     | 520  | LMG  | C32-C33-C34-C35 |
| 37  | c     | 518  | DGD  | CDB-CEB-CFB-CGB |
| 23  | c     | 510  | CLA  | C5-C6-C7-C8     |
| 26  | D     | 2302 | SQD  | C34-C35-C36-C37 |
| 37  | C     | 517  | DGD  | O6E-C5E-C6E-O5E |
| 38  | L     | 101  | LHG  | C12-C13-C14-C15 |
| 23  | C     | 506  | CLA  | C4-C3-C5-C6     |
| 26  | d     | 417  | SQD  | C27-C28-C29-C30 |
| 23  | C     | 509  | CLA  | C5-C6-C7-C8     |
| 26  | l     | 101  | SQD  | C12-C13-C14-C15 |
| 38  | d     | 403  | LHG  | C28-C29-C30-C31 |
| 38  | l     | 103  | LHG  | C7-C8-C9-C10    |
| 26  | b     | 601  | SQD  | C11-C12-C13-C14 |
| 27  | A     | 413  | LMG  | C21-C22-C23-C24 |
| 36  | c     | 526  | HTG  | C2'-C3'-C4'-C5' |
| 23  | B     | 611  | CLA  | C2A-CAA-CBA-CGA |
| 23  | C     | 507  | CLA  | C16-C17-C18-C19 |
| 28  | F     | 102  | LMT  | O5'-C5'-C6'-O6' |
| 26  | d     | 417  | SQD  | C44-C45-C46-O48 |
| 26  | l     | 101  | SQD  | C44-C45-C46-O48 |
| 27  | A     | 413  | LMG  | C7-C8-C9-O8     |
| 27  | c     | 521  | LMG  | C7-C8-C9-O8     |
| 37  | c     | 518  | DGD  | C9A-CAA-CBA-CCA |
| 38  | D     | 2309 | LHG  | C11-C10-C9-C8   |
| 23  | A     | 410  | CLA  | C8-C10-C11-C12  |
| 37  | c     | 519  | DGD  | C2G-C3G-O3G-C1D |
| 37  | c     | 519  | DGD  | C5D-C6D-O5D-C1E |
| 27  | c     | 501  | LMG  | C40-C41-C42-C43 |
| 23  | c     | 512  | CLA  | C13-C15-C16-C17 |
| 28  | m     | 2804 | LMT  | C3'-C4'-O1B-C1B |
| 26  | l     | 101  | SQD  | C23-C24-C25-C26 |
| 36  | b     | 625  | HTG  | C4'-C5'-C6'-C7' |
| 28  | B     | 623  | LMT  | C1-C2-C3-C4     |
| 23  | a     | 2610 | CLA  | C8-C10-C11-C12  |
| 29  | a     | 2602 | GOL  | O1-C1-C2-O2     |
| 38  | D     | 2310 | LHG  | O1-C1-C2-O2     |
| 26  | B     | 621  | SQD  | C29-C30-C31-C32 |
| 27  | B     | 622  | LMG  | C32-C33-C34-C35 |
| 38  | E     | 101  | LHG  | C26-C27-C28-C29 |
| 23  | B     | 615  | CLA  | C5-C6-C7-C8     |
| 28  | m     | 2804 | LMT  | O5B-C5B-C6B-O6B |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 37  | c     | 518  | DGD  | O6E-C5E-C6E-O5E |
| 33  | A     | 422  | PL9  | C15-C14-C16-C17 |
| 28  | m     | 2804 | LMT  | C5'-C4'-O1B-C1B |
| 23  | C     | 507  | CLA  | C5-C6-C7-C8     |
| 38  | E     | 101  | LHG  | C13-C14-C15-C16 |
| 26  | B     | 621  | SQD  | C46-C45-O47-C7  |
| 26  | l     | 101  | SQD  | C46-C45-O47-C7  |
| 27  | D     | 2312 | LMG  | O6-C5-C6-O5     |
| 23  | c     | 509  | CLA  | C2-C1-O2A-CGA   |
| 37  | C     | 517  | DGD  | O6D-C5D-C6D-O5D |
| 26  | A     | 412  | SQD  | C11-C12-C13-C14 |
| 23  | c     | 516  | CLA  | CBA-CGA-O2A-C1  |
| 23  | A     | 407  | CLA  | C16-C17-C18-C19 |
| 23  | b     | 611  | CLA  | C16-C17-C18-C19 |
| 26  | b     | 601  | SQD  | C25-C26-C27-C28 |
| 27  | B     | 622  | LMG  | C17-C18-C19-C20 |
| 27  | C     | 520  | LMG  | C39-C40-C41-C42 |
| 36  | b     | 626  | HTG  | C1'-C2'-C3'-C4' |
| 28  | A     | 420  | LMT  | C2'-C1'-O1'-C1  |
| 26  | l     | 101  | SQD  | C27-C28-C29-C30 |
| 27  | m     | 2802 | LMG  | O9-C10-O7-C8    |
| 23  | c     | 516  | CLA  | C16-C17-C18-C20 |
| 26  | a     | 2615 | SQD  | C30-C31-C32-C33 |
| 38  | l     | 103  | LHG  | C12-C13-C14-C15 |
| 26  | D     | 2302 | SQD  | C7-C8-C9-C10    |
| 36  | d     | 407  | HTG  | C3'-C4'-C5'-C6' |
| 37  | D     | 2307 | DGD  | CDB-CEB-CFB-CGB |
| 23  | B     | 611  | CLA  | C12-C13-C15-C16 |
| 23  | B     | 616  | CLA  | C11-C12-C13-C15 |
| 23  | B     | 616  | CLA  | C12-C13-C15-C16 |
| 23  | C     | 506  | CLA  | C11-C12-C13-C15 |
| 23  | A     | 410  | CLA  | C11-C12-C13-C14 |
| 23  | B     | 605  | CLA  | C6-C7-C8-C9     |
| 23  | C     | 508  | CLA  | C11-C10-C8-C9   |
| 23  | C     | 510  | CLA  | C11-C10-C8-C9   |
| 23  | b     | 616  | CLA  | C14-C13-C15-C16 |
| 23  | c     | 508  | CLA  | C11-C12-C13-C14 |
| 23  | c     | 512  | CLA  | C6-C7-C8-C9     |
| 37  | C     | 517  | DGD  | CAA-CBA-CCA-CDA |
| 37  | C     | 517  | DGD  | C2B-C3B-C4B-C5B |
| 38  | e     | 101  | LHG  | C15-C16-C17-C18 |
| 26  | B     | 621  | SQD  | C24-C23-O48-C46 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | b     | 624  | BCR  | C21-C22-C23-C24 |
| 38  | e     | 101  | LHG  | C1-C2-C3-O3     |
| 37  | h     | 102  | DGD  | CDA-CEA-CFA-CGA |
| 23  | a     | 2613 | CLA  | CBA-CGA-O2A-C1  |
| 28  | d     | 401  | LMT  | C9-C10-C11-C12  |
| 36  | d     | 407  | HTG  | C4'-C5'-C6'-C7' |
| 37  | H     | 103  | DGD  | CDA-CEA-CFA-CGA |
| 37  | c     | 519  | DGD  | C8A-C9A-CAA-CBA |
| 38  | D     | 2309 | LHG  | C29-C30-C31-C32 |
| 23  | C     | 513  | CLA  | C4B-C3B-CAB-CBB |
| 23  | b     | 620  | CLA  | C4B-C3B-CAB-CBB |
| 23  | c     | 514  | CLA  | C4B-C3B-CAB-CBB |
| 38  | E     | 101  | LHG  | O6-C4-C5-C6     |
| 38  | e     | 101  | LHG  | O6-C4-C5-C6     |
| 38  | L     | 101  | LHG  | C7-C8-C9-C10    |
| 27  | m     | 2802 | LMG  | C31-C32-C33-C34 |
| 37  | C     | 518  | DGD  | C9A-CAA-CBA-CCA |
| 37  | C     | 519  | DGD  | C6A-C7A-C8A-C9A |
| 38  | D     | 2309 | LHG  | C9-C10-C11-C12  |
| 33  | A     | 422  | PL9  | C13-C14-C16-C17 |
| 37  | c     | 519  | DGD  | C6A-C7A-C8A-C9A |
| 37  | c     | 519  | DGD  | C5B-C6B-C7B-C8B |
| 23  | c     | 516  | CLA  | O1D-CGD-O2D-CED |
| 37  | C     | 518  | DGD  | C6A-C7A-C8A-C9A |
| 37  | c     | 519  | DGD  | CBB-CCB-CDB-CEB |
| 23  | B     | 607  | CLA  | C10-C11-C12-C13 |
| 23  | C     | 512  | CLA  | CBA-CGA-O2A-C1  |
| 37  | c     | 520  | DGD  | C2A-C1A-O1G-C1G |
| 26  | A     | 412  | SQD  | C33-C34-C35-C36 |
| 23  | B     | 610  | CLA  | C3A-C2A-CAA-CBA |
| 23  | C     | 507  | CLA  | C3A-C2A-CAA-CBA |
| 28  | i     | 103  | LMT  | C2-C1-O1'-C1'   |
| 37  | D     | 2307 | DGD  | C4A-C5A-C6A-C7A |
| 38  | D     | 2309 | LHG  | C17-C18-C19-C20 |
| 23  | C     | 513  | CLA  | C10-C11-C12-C13 |
| 27  | C     | 520  | LMG  | C37-C38-C39-C40 |
| 36  | d     | 415  | HTG  | S1-C1'-C2'-C3'  |
| 26  | B     | 621  | SQD  | C44-C45-C46-O48 |
| 26  | a     | 2603 | SQD  | O6-C44-C45-C46  |
| 27  | c     | 501  | LMG  | C7-C8-C9-O8     |
| 23  | d     | 402  | CLA  | C2C-C3C-CAC-CBC |
| 28  | B     | 623  | LMT  | C3'-C4'-O1B-C1B |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | M     | 101  | LMT  | C1-C2-C3-C4     |
| 23  | c     | 516  | CLA  | O1A-CGA-O2A-C1  |
| 23  | B     | 617  | CLA  | C3-C5-C6-C7     |
| 29  | B     | 632  | GOL  | O1-C1-C2-O2     |
| 38  | d     | 412  | LHG  | O1-C1-C2-O2     |
| 36  | B     | 626  | HTG  | C2'-C3'-C4'-C5' |
| 37  | h     | 102  | DGD  | C6B-C7B-C8B-C9B |
| 27  | d     | 414  | LMG  | C36-C37-C38-C39 |
| 28  | F     | 102  | LMT  | O1'-C1-C2-C3    |
| 28  | d     | 404  | LMT  | C6-C7-C8-C9     |
| 23  | C     | 512  | CLA  | O1A-CGA-O2A-C1  |
| 38  | e     | 101  | LHG  | C10-C11-C12-C13 |
| 23  | C     | 513  | CLA  | C2B-C3B-CAB-CBB |
| 23  | b     | 620  | CLA  | C2B-C3B-CAB-CBB |
| 23  | c     | 504  | CLA  | C2B-C3B-CAB-CBB |
| 37  | H     | 103  | DGD  | C7B-C8B-C9B-CAB |
| 37  | C     | 517  | DGD  | C4D-C5D-C6D-O5D |
| 26  | d     | 417  | SQD  | O47-C45-C46-O48 |
| 37  | C     | 518  | DGD  | CDB-CEB-CFB-CGB |
| 28  | Z     | 101  | LMT  | O1'-C1-C2-C3    |
| 37  | H     | 103  | DGD  | C6B-C7B-C8B-C9B |
| 37  | c     | 518  | DGD  | C6B-C7B-C8B-C9B |
| 23  | B     | 614  | CLA  | C13-C15-C16-C17 |
| 23  | b     | 615  | CLA  | C5-C6-C7-C8     |
| 33  | D     | 2306 | PL9  | C39-C41-C42-C43 |
| 33  | d     | 411  | PL9  | C39-C41-C42-C43 |
| 26  | B     | 621  | SQD  | C11-C10-C9-C8   |
| 26  | d     | 417  | SQD  | C26-C27-C28-C29 |
| 27  | m     | 2802 | LMG  | C33-C34-C35-C36 |
| 42  | v     | 201  | HEC  | C4C-C3C-CAC-CBC |
| 23  | B     | 615  | CLA  | C11-C12-C13-C14 |
| 23  | B     | 616  | CLA  | C14-C13-C15-C16 |
| 23  | C     | 505  | CLA  | C6-C7-C8-C9     |
| 23  | c     | 510  | CLA  | C14-C13-C15-C16 |
| 37  | c     | 518  | DGD  | C6A-C7A-C8A-C9A |
| 26  | A     | 412  | SQD  | C34-C35-C36-C37 |
| 28  | B     | 623  | LMT  | C5'-C4'-O1B-C1B |
| 38  | D     | 2311 | LHG  | C2-C3-O3-P      |
| 23  | a     | 2613 | CLA  | O1A-CGA-O2A-C1  |
| 36  | d     | 407  | HTG  | C4-C5-C6-O6     |
| 26  | a     | 2615 | SQD  | C32-C33-C34-C35 |
| 38  | L     | 101  | LHG  | C10-C11-C12-C13 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | b     | 607    | CLA  | C2A-CAA-CBA-CGA |
| 25  | C     | 515    | BCR  | C1-C6-C7-C8     |
| 25  | C     | 515    | BCR  | C5-C6-C7-C8     |
| 25  | C     | 515    | BCR  | C23-C24-C25-C30 |
| 25  | D     | 2305   | BCR  | C1-C6-C7-C8     |
| 25  | D     | 2305   | BCR  | C5-C6-C7-C8     |
| 25  | d     | 410    | BCR  | C1-C6-C7-C8     |
| 23  | B     | 615    | CLA  | C8-C10-C11-C12  |
| 27  | m     | 2802   | LMG  | C20-C21-C22-C23 |
| 37  | h     | 102    | DGD  | O2G-C1B-C2B-C3B |
| 26  | d     | 417    | SQD  | C30-C31-C32-C33 |
| 25  | C     | 515    | BCR  | C21-C22-C23-C24 |
| 38  | D     | 2310   | LHG  | C34-C35-C36-C37 |
| 28  | m     | 2804   | LMT  | C6-C7-C8-C9     |
| 27  | c     | 522    | LMG  | C37-C38-C39-C40 |
| 28  | f     | 101    | LMT  | O1'-C1-C2-C3    |
| 36  | B     | 627    | HTG  | O5-C5-C6-O6     |
| 37  | C     | 517    | DGD  | C2A-C3A-C4A-C5A |
| 38  | e     | 101    | LHG  | O2-C2-C3-O3     |
| 23  | A     | 407    | CLA  | C11-C10-C8-C7   |
| 23  | A     | 410    | CLA  | C6-C7-C8-C10    |
| 23  | B     | 615    | CLA  | C11-C12-C13-C15 |
| 23  | C     | 505    | CLA  | C6-C7-C8-C10    |
| 23  | C     | 508    | CLA  | C11-C10-C8-C7   |
| 23  | C     | 509    | CLA  | C11-C10-C8-C7   |
| 23  | b     | 616    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 621    | CLA  | C11-C10-C8-C7   |
| 23  | c     | 508    | CLA  | C11-C12-C13-C15 |
| 23  | c     | 508    | CLA  | C12-C13-C15-C16 |
| 26  | B     | 621    | SQD  | O10-C23-O48-C46 |
| 23  | b     | 621    | CLA  | CBA-CGA-O2A-C1  |
| 37  | D     | 2307   | DGD  | C6A-C7A-C8A-C9A |
| 26  | d     | 417    | SQD  | C34-C35-C36-C37 |
| 36  | C     | 522    | HTG  | O5-C1-S1-C1'    |
| 36  | b     | 626    | HTG  | C2'-C1'-S1-C1   |
| 36  | B     | 624[B] | HTG  | C1'-C2'-C3'-C4' |
| 23  | c     | 513    | CLA  | CBA-CGA-O2A-C1  |
| 26  | D     | 2308   | SQD  | C33-C34-C35-C36 |
| 23  | B     | 603    | CLA  | C13-C15-C16-C17 |
| 23  | b     | 613    | CLA  | C13-C15-C16-C17 |
| 26  | l     | 101    | SQD  | C34-C35-C36-C37 |
| 28  | d     | 401    | LMT  | C11-C10-C9-C8   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | B     | 611  | CLA  | CAD-CBD-CGD-O2D |
| 23  | B     | 617  | CLA  | CAD-CBD-CGD-O2D |
| 23  | C     | 511  | CLA  | CAD-CBD-CGD-O2D |
| 23  | b     | 621  | CLA  | CAD-CBD-CGD-O2D |
| 23  | c     | 504  | CLA  | CAD-CBD-CGD-O2D |
| 23  | c     | 509  | CLA  | CAD-CBD-CGD-O2D |
| 23  | c     | 515  | CLA  | CAD-CBD-CGD-O2D |
| 24  | A     | 408  | PHO  | CAD-CBD-CGD-O2D |
| 26  | D     | 2308 | SQD  | C46-C45-O47-C7  |
| 26  | B     | 621  | SQD  | C31-C32-C33-C34 |
| 38  | d     | 412  | LHG  | C15-C16-C17-C18 |
| 37  | D     | 2307 | DGD  | C7A-C8A-C9A-CAA |
| 37  | h     | 102  | DGD  | C7B-C8B-C9B-CAB |
| 26  | b     | 601  | SQD  | C28-C29-C30-C31 |
| 23  | a     | 2613 | CLA  | C2-C3-C5-C6     |
| 26  | D     | 2302 | SQD  | O6-C44-C45-C46  |
| 37  | H     | 103  | DGD  | O1G-C1G-C2G-C3G |
| 37  | h     | 102  | DGD  | O1G-C1G-C2G-C3G |
| 38  | d     | 403  | LHG  | C2-C3-O3-P      |
| 37  | C     | 517  | DGD  | C6B-C7B-C8B-C9B |
| 38  | e     | 101  | LHG  | O6-C4-C5-O7     |
| 38  | l     | 103  | LHG  | C11-C12-C13-C14 |
| 36  | c     | 526  | HTG  | S1-C1'-C2'-C3'  |
| 38  | D     | 2309 | LHG  | C33-C34-C35-C36 |
| 37  | c     | 518  | DGD  | C5B-C6B-C7B-C8B |
| 23  | B     | 602  | CLA  | CHA-CBD-CGD-O1D |
| 23  | B     | 602  | CLA  | CHA-CBD-CGD-O2D |
| 23  | B     | 603  | CLA  | CHA-CBD-CGD-O2D |
| 23  | B     | 615  | CLA  | CHA-CBD-CGD-O1D |
| 23  | C     | 503  | CLA  | CHA-CBD-CGD-O1D |
| 23  | C     | 503  | CLA  | CHA-CBD-CGD-O2D |
| 23  | C     | 508  | CLA  | CHA-CBD-CGD-O1D |
| 23  | C     | 508  | CLA  | CHA-CBD-CGD-O2D |
| 23  | C     | 509  | CLA  | CHA-CBD-CGD-O1D |
| 23  | C     | 509  | CLA  | CHA-CBD-CGD-O2D |
| 23  | b     | 606  | CLA  | CHA-CBD-CGD-O1D |
| 23  | b     | 606  | CLA  | CHA-CBD-CGD-O2D |
| 23  | c     | 505  | CLA  | CHA-CBD-CGD-O2D |
| 23  | c     | 510  | CLA  | CHA-CBD-CGD-O1D |
| 23  | c     | 511  | CLA  | CHA-CBD-CGD-O1D |
| 23  | c     | 511  | CLA  | CHA-CBD-CGD-O2D |
| 26  | B     | 621  | SQD  | O47-C45-C46-O48 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | D     | 2302   | SQD  | O6-C44-C45-O47  |
| 26  | D     | 2308   | SQD  | O47-C45-C46-O48 |
| 27  | C     | 527    | LMG  | O7-C8-C9-O8     |
| 37  | D     | 2307   | DGD  | O1G-C1G-C2G-O2G |
| 26  | a     | 2615   | SQD  | C26-C27-C28-C29 |
| 37  | H     | 103    | DGD  | O2G-C1B-C2B-C3B |
| 36  | B     | 624[B] | HTG  | C2'-C3'-C4'-C5' |
| 37  | h     | 102    | DGD  | C8A-C9A-CAA-CBA |
| 29  | A     | 415    | GOL  | O1-C1-C2-O2     |
| 29  | C     | 526    | GOL  | O1-C1-C2-O2     |
| 29  | O     | 305    | GOL  | O2-C2-C3-O3     |
| 29  | a     | 2602   | GOL  | O2-C2-C3-O3     |
| 29  | a     | 2618   | GOL  | O1-C1-C2-O2     |
| 29  | v     | 203    | GOL  | O2-C2-C3-O3     |
| 23  | a     | 2613   | CLA  | C4-C3-C5-C6     |
| 28  | d     | 404    | LMT  | O1'-C1-C2-C3    |
| 23  | c     | 513    | CLA  | O1A-CGA-O2A-C1  |
| 37  | c     | 520    | DGD  | O1A-C1A-O1G-C1G |
| 28  | z     | 102    | LMT  | C2B-C1B-O1B-C4' |
| 38  | d     | 412    | LHG  | C13-C14-C15-C16 |
| 23  | b     | 621    | CLA  | C11-C10-C8-C9   |
| 23  | c     | 508    | CLA  | C14-C13-C15-C16 |
| 27  | A     | 413    | LMG  | C12-C13-C14-C15 |
| 23  | b     | 621    | CLA  | O1A-CGA-O2A-C1  |
| 38  | l     | 103    | LHG  | C10-C11-C12-C13 |
| 26  | D     | 2308   | SQD  | C5-C6-S-O8      |
| 26  | l     | 101    | SQD  | C5-C6-S-O8      |
| 23  | A     | 406    | CLA  | C2C-C3C-CAC-CBC |
| 38  | D     | 2309   | LHG  | O1-C1-C2-C3     |
| 38  | d     | 403    | LHG  | O1-C1-C2-C3     |
| 36  | C     | 521    | HTG  | S1-C1'-C2'-C3'  |
| 36  | b     | 604    | HTG  | O5-C5-C6-O6     |
| 27  | C     | 520    | LMG  | C11-C12-C13-C14 |
| 23  | B     | 605    | CLA  | C1A-C2A-CAA-CBA |
| 27  | A     | 413    | LMG  | C22-C23-C24-C25 |
| 23  | B     | 611    | CLA  | C2-C1-O2A-CGA   |
| 38  | L     | 101    | LHG  | C11-C12-C13-C14 |
| 40  | H     | 102    | RRX  | C9-C10-C11-C12  |
| 40  | h     | 101    | RRX  | C9-C10-C11-C12  |
| 38  | e     | 101    | LHG  | C4-O6-P-O3      |
| 37  | h     | 102    | DGD  | C5B-C6B-C7B-C8B |
| 27  | D     | 2312   | LMG  | C12-C13-C14-C15 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 27  | C     | 527  | LMG  | C31-C32-C33-C34 |
| 27  | d     | 414  | LMG  | C30-C31-C32-C33 |
| 38  | D     | 2309 | LHG  | C26-C27-C28-C29 |
| 23  | B     | 606  | CLA  | C4B-C3B-CAB-CBB |
| 23  | a     | 2610 | CLA  | C4B-C3B-CAB-CBB |
| 23  | b     | 606  | CLA  | C4B-C3B-CAB-CBB |
| 38  | E     | 101  | LHG  | C4-O6-P-O4      |
| 38  | L     | 101  | LHG  | C4-O6-P-O5      |
| 38  | l     | 103  | LHG  | C4-O6-P-O5      |
| 26  | b     | 601  | SQD  | O5-C1-O6-C44    |
| 27  | A     | 413  | LMG  | C29-C28-O8-C9   |
| 28  | z     | 102  | LMT  | C4-C5-C6-C7     |
| 37  | H     | 103  | DGD  | C5B-C6B-C7B-C8B |
| 38  | d     | 412  | LHG  | C30-C31-C32-C33 |
| 26  | a     | 2603 | SQD  | C32-C33-C34-C35 |
| 38  | e     | 101  | LHG  | C13-C14-C15-C16 |
| 37  | H     | 103  | DGD  | C8A-C9A-CAA-CBA |
| 23  | B     | 602  | CLA  | CAD-CBD-CGD-O1D |
| 23  | B     | 606  | CLA  | CAD-CBD-CGD-O1D |
| 23  | B     | 615  | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 503  | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 507  | CLA  | CAD-CBD-CGD-O1D |
| 23  | b     | 606  | CLA  | CAD-CBD-CGD-O1D |
| 23  | b     | 610  | CLA  | CAD-CBD-CGD-O1D |
| 23  | c     | 505  | CLA  | CAD-CBD-CGD-O1D |
| 26  | D     | 2308 | SQD  | C5-C6-S-O9      |
| 26  | a     | 2603 | SQD  | O5-C5-C6-S      |
| 26  | l     | 101  | SQD  | C5-C6-S-O9      |
| 37  | C     | 519  | DGD  | C8A-C9A-CAA-CBA |
| 26  | B     | 621  | SQD  | C23-C24-C25-C26 |
| 26  | a     | 2603 | SQD  | C35-C36-C37-C38 |
| 26  | D     | 2302 | SQD  | C9-C10-C11-C12  |
| 26  | l     | 101  | SQD  | C17-C18-C19-C20 |
| 23  | A     | 410  | CLA  | C11-C10-C8-C7   |
| 23  | B     | 604  | CLA  | C11-C10-C8-C7   |
| 23  | C     | 507  | CLA  | C11-C12-C13-C15 |
| 23  | C     | 514  | CLA  | C12-C13-C15-C16 |
| 23  | a     | 2610 | CLA  | C11-C10-C8-C7   |
| 23  | a     | 2610 | CLA  | C12-C13-C15-C16 |
| 23  | c     | 510  | CLA  | C11-C10-C8-C7   |
| 23  | c     | 515  | CLA  | C12-C13-C15-C16 |
| 36  | C     | 522  | HTG  | C2-C1-S1-C1'    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 36  | c     | 523  | HTG  | C2-C1-S1-C1'    |
| 26  | d     | 417  | SQD  | C32-C33-C34-C35 |
| 37  | c     | 519  | DGD  | C6B-C7B-C8B-C9B |
| 27  | d     | 414  | LMG  | C29-C30-C31-C32 |
| 37  | c     | 518  | DGD  | O6D-C5D-C6D-O5D |
| 23  | b     | 606  | CLA  | CAA-CBA-CGA-O2A |
| 38  | D     | 2310 | LHG  | C32-C33-C34-C35 |
| 38  | e     | 101  | LHG  | C19-C20-C21-C22 |
| 26  | D     | 2308 | SQD  | C44-C45-C46-O48 |
| 26  | b     | 601  | SQD  | C2-C1-O6-C44    |
| 37  | D     | 2307 | DGD  | O1G-C1G-C2G-C3G |
| 26  | A     | 412  | SQD  | O6-C44-C45-O47  |
| 27  | A     | 413  | LMG  | O7-C8-C9-O8     |
| 27  | c     | 521  | LMG  | O7-C8-C9-O8     |
| 37  | H     | 103  | DGD  | O1G-C1G-C2G-O2G |
| 27  | c     | 521  | LMG  | C19-C20-C21-C22 |
| 23  | a     | 2609 | CLA  | C2C-C3C-CAC-CBC |
| 27  | A     | 413  | LMG  | O10-C28-O8-C9   |
| 27  | c     | 521  | LMG  | C31-C32-C33-C34 |
| 27  | d     | 414  | LMG  | C12-C13-C14-C15 |
| 27  | c     | 522  | LMG  | C8-C7-O1-C1     |
| 37  | C     | 518  | DGD  | C2G-C3G-O3G-C1D |
| 37  | C     | 518  | DGD  | C5D-C6D-O5D-C1E |
| 38  | e     | 101  | LHG  | C9-C10-C11-C12  |
| 23  | C     | 505  | CLA  | C15-C16-C17-C18 |
| 23  | b     | 615  | CLA  | C8-C10-C11-C12  |
| 27  | C     | 520  | LMG  | C33-C34-C35-C36 |
| 37  | D     | 2307 | DGD  | C9A-CAA-CBA-CCA |
| 23  | A     | 407  | CLA  | C11-C10-C8-C9   |
| 23  | C     | 507  | CLA  | C11-C12-C13-C14 |
| 23  | C     | 509  | CLA  | C11-C10-C8-C9   |
| 38  | D     | 2311 | LHG  | O10-C23-O8-C6   |
| 26  | a     | 2603 | SQD  | C33-C34-C35-C36 |
| 23  | b     | 617  | CLA  | C8-C10-C11-C12  |
| 27  | c     | 522  | LMG  | C10-C11-C12-C13 |
| 28  | T     | 103  | LMT  | C11-C10-C9-C8   |
| 26  | B     | 621  | SQD  | C26-C27-C28-C29 |
| 28  | J     | 303  | LMT  | C7-C8-C9-C10    |
| 23  | B     | 604  | CLA  | C2B-C3B-CAB-CBB |
| 23  | B     | 606  | CLA  | C2B-C3B-CAB-CBB |
| 23  | b     | 611  | CLA  | C2B-C3B-CAB-CBB |
| 23  | c     | 514  | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 37  | C     | 518    | DGD  | C5B-C6B-C7B-C8B |
| 37  | H     | 103    | DGD  | C9B-CAB-CBB-CCB |
| 23  | a     | 2610   | CLA  | C16-C17-C18-C20 |
| 26  | B     | 621    | SQD  | C12-C13-C14-C15 |
| 36  | b     | 602    | HTG  | C2'-C3'-C4'-C5' |
| 37  | c     | 519    | DGD  | C2A-C3A-C4A-C5A |
| 23  | c     | 506    | CLA  | C15-C16-C17-C18 |
| 37  | c     | 518    | DGD  | C4D-C5D-C6D-O5D |
| 23  | b     | 615    | CLA  | C2A-CAA-CBA-CGA |
| 23  | C     | 510    | CLA  | C2-C1-O2A-CGA   |
| 23  | b     | 619    | CLA  | C2-C1-O2A-CGA   |
| 23  | c     | 510    | CLA  | C2-C1-O2A-CGA   |
| 28  | M     | 101    | LMT  | C7-C8-C9-C10    |
| 37  | c     | 520    | DGD  | C2A-C3A-C4A-C5A |
| 28  | m     | 2803   | LMT  | O5'-C5'-C6'-O6' |
| 36  | I     | 101    | HTG  | C1'-C2'-C3'-C4' |
| 38  | L     | 101    | LHG  | C14-C15-C16-C17 |
| 23  | C     | 507    | CLA  | O1A-CGA-O2A-C1  |
| 26  | l     | 101    | SQD  | C13-C14-C15-C16 |
| 28  | A     | 420    | LMT  | C5-C6-C7-C8     |
| 23  | c     | 506    | CLA  | C10-C11-C12-C13 |
| 25  | C     | 515    | BCR  | C23-C24-C25-C26 |
| 25  | a     | 2614   | BCR  | C1-C6-C7-C8     |
| 25  | d     | 410    | BCR  | C5-C6-C7-C8     |
| 37  | C     | 517    | DGD  | C7A-C8A-C9A-CAA |
| 36  | o     | 301    | HTG  | C2'-C3'-C4'-C5' |
| 37  | C     | 519    | DGD  | C6B-C7B-C8B-C9B |
| 36  | H     | 101    | HTG  | C2'-C3'-C4'-C5' |
| 37  | C     | 519    | DGD  | C2A-C3A-C4A-C5A |
| 38  | e     | 101    | LHG  | C11-C10-C9-C8   |
| 33  | A     | 422    | PL9  | C12-C11-C9-C10  |
| 27  | C     | 520    | LMG  | C11-C10-O7-C8   |
| 28  | m     | 2804   | LMT  | O5'-C1'-O1'-C1  |
| 37  | C     | 517    | DGD  | O6E-C1E-O5D-C6D |
| 37  | C     | 518    | DGD  | O6E-C1E-O5D-C6D |
| 37  | c     | 519    | DGD  | O6E-C1E-O5D-C6D |
| 27  | B     | 622    | LMG  | C28-C29-C30-C31 |
| 23  | c     | 510    | CLA  | C2A-CAA-CBA-CGA |
| 37  | c     | 519    | DGD  | C2E-C1E-O5D-C6D |
| 36  | B     | 624[B] | HTG  | S1-C1'-C2'-C3'  |
| 26  | l     | 101    | SQD  | O47-C45-C46-O48 |
| 27  | c     | 501    | LMG  | O7-C8-C9-O8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 37  | h     | 102  | DGD  | O1G-C1G-C2G-O2G |
| 27  | B     | 622  | LMG  | C16-C17-C18-C19 |
| 27  | m     | 2802 | LMG  | C19-C20-C21-C22 |
| 38  | D     | 2310 | LHG  | C3-O3-P-O6      |
| 38  | d     | 413  | LHG  | C3-O3-P-O6      |
| 27  | C     | 527  | LMG  | C28-C29-C30-C31 |
| 23  | a     | 2609 | CLA  | C16-C17-C18-C20 |
| 28  | m     | 2804 | LMT  | C2B-C1B-O1B-C4' |
| 26  | A     | 412  | SQD  | O6-C44-C45-C46  |
| 27  | C     | 527  | LMG  | C7-C8-C9-O8     |
| 37  | C     | 519  | DGD  | O1G-C1G-C2G-C3G |
| 28  | m     | 2804 | LMT  | C5-C6-C7-C8     |
| 37  | C     | 517  | DGD  | CBA-CCA-CDA-CEA |
| 23  | c     | 513  | CLA  | C2-C3-C5-C6     |
| 24  | A     | 408  | PHO  | C2-C3-C5-C6     |
| 23  | A     | 410  | CLA  | C11-C10-C8-C9   |
| 23  | B     | 617  | CLA  | C14-C13-C15-C16 |
| 23  | b     | 618  | CLA  | C11-C12-C13-C14 |
| 23  | c     | 510  | CLA  | C11-C10-C8-C9   |
| 27  | B     | 622  | LMG  | O6-C5-C6-O5     |
| 23  | c     | 507  | CLA  | C16-C17-C18-C20 |
| 24  | a     | 2612 | PHO  | C2C-C3C-CAC-CBC |
| 38  | E     | 101  | LHG  | C14-C15-C16-C17 |
| 38  | E     | 101  | LHG  | C19-C20-C21-C22 |
| 27  | C     | 520  | LMG  | O9-C10-O7-C8    |
| 24  | A     | 408  | PHO  | C4-C3-C5-C6     |
| 29  | D     | 2301 | GOL  | O1-C1-C2-O2     |
| 29  | c     | 531  | GOL  | O2-C2-C3-O3     |
| 29  | d     | 416  | GOL  | O2-C2-C3-O3     |
| 23  | B     | 602  | CLA  | C2-C3-C5-C6     |
| 38  | D     | 2311 | LHG  | C24-C23-O8-C6   |
| 28  | z     | 102  | LMT  | O5B-C1B-O1B-C4' |
| 23  | B     | 609  | CLA  | C13-C15-C16-C17 |
| 28  | M     | 102  | LMT  | O5'-C5'-C6'-O6' |
| 27  | C     | 527  | LMG  | C39-C40-C41-C42 |
| 37  | C     | 517  | DGD  | CAB-CBB-CCB-CDB |
| 37  | C     | 519  | DGD  | C4B-C5B-C6B-C7B |
| 23  | B     | 604  | CLA  | C4B-C3B-CAB-CBB |
| 23  | B     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 23  | B     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 23  | b     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 23  | b     | 611  | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | a     | 2610   | CLA  | C16-C17-C18-C19 |
| 37  | c     | 518    | DGD  | O6E-C1E-O5D-C6D |
| 23  | b     | 619    | CLA  | C10-C11-C12-C13 |
| 23  | b     | 615    | CLA  | C16-C17-C18-C19 |
| 23  | B     | 602    | CLA  | C4-C3-C5-C6     |
| 23  | c     | 513    | CLA  | C4-C3-C5-C6     |
| 27  | c     | 521    | LMG  | C30-C31-C32-C33 |
| 38  | D     | 2311   | LHG  | C31-C32-C33-C34 |
| 36  | i     | 102    | HTG  | C1'-C2'-C3'-C4' |
| 37  | h     | 102    | DGD  | C9B-CAB-CBB-CCB |
| 23  | b     | 621    | CLA  | C15-C16-C17-C18 |
| 23  | b     | 618    | CLA  | C2-C1-O2A-CGA   |
| 23  | d     | 408    | CLA  | C2-C1-O2A-CGA   |
| 28  | B     | 623    | LMT  | C6-C7-C8-C9     |
| 28  | m     | 2804   | LMT  | O5'-C5'-C6'-O6' |
| 37  | C     | 517    | DGD  | C2E-C1E-O5D-C6D |
| 37  | C     | 518    | DGD  | C2E-C1E-O5D-C6D |
| 23  | c     | 504    | CLA  | C2A-CAA-CBA-CGA |
| 27  | C     | 527    | LMG  | C11-C12-C13-C14 |
| 37  | c     | 519    | DGD  | C9B-CAB-CBB-CCB |
| 36  | B     | 624[A] | HTG  | C2'-C3'-C4'-C5' |
| 38  | d     | 412    | LHG  | C11-C10-C9-C8   |
| 28  | A     | 414    | LMT  | C2B-C1B-O1B-C4' |
| 23  | b     | 614    | CLA  | C3A-C2A-CAA-CBA |
| 23  | a     | 2609   | CLA  | C4C-C3C-CAC-CBC |
| 38  | d     | 413    | LHG  | C34-C35-C36-C37 |
| 26  | A     | 412    | SQD  | C11-C10-C9-C8   |
| 38  | d     | 413    | LHG  | C11-C10-C9-C8   |
| 26  | b     | 601    | SQD  | C16-C17-C18-C19 |
| 27  | A     | 413    | LMG  | C20-C21-C22-C23 |
| 38  | l     | 103    | LHG  | C14-C15-C16-C17 |
| 23  | B     | 612    | CLA  | C4-C3-C5-C6     |
| 33  | x     | 1301   | PL9  | C40-C39-C41-C42 |
| 23  | b     | 611    | CLA  | C11-C10-C8-C9   |
| 23  | b     | 621    | CLA  | C6-C7-C8-C9     |
| 26  | D     | 2308   | SQD  | C25-C26-C27-C28 |
| 39  | F     | 101    | HEM  | CAD-CBD-CGD-O1D |
| 37  | D     | 2307   | DGD  | C2B-C3B-C4B-C5B |
| 23  | b     | 615    | CLA  | C16-C17-C18-C20 |
| 38  | d     | 413    | LHG  | O2-C2-C3-O3     |
| 28  | M     | 102    | LMT  | O5'-C1'-O1'-C1  |
| 28  | m     | 2803   | LMT  | O5'-C1'-O1'-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 38  | d     | 413  | LHG  | C32-C33-C34-C35 |
| 38  | e     | 101  | LHG  | C26-C27-C28-C29 |
| 23  | C     | 513  | CLA  | O1A-CGA-O2A-C1  |
| 28  | A     | 420  | LMT  | C3-C4-C5-C6     |
| 28  | A     | 414  | LMT  | O5B-C1B-O1B-C4' |
| 26  | D     | 2308 | SQD  | C28-C29-C30-C31 |
| 23  | c     | 509  | CLA  | C5-C6-C7-C8     |
| 23  | B     | 614  | CLA  | C11-C12-C13-C15 |
| 23  | b     | 620  | CLA  | C12-C13-C15-C16 |
| 23  | c     | 509  | CLA  | C12-C13-C15-C16 |
| 23  | c     | 514  | CLA  | C11-C12-C13-C15 |
| 37  | C     | 519  | DGD  | C8B-C9B-CAB-CBB |
| 27  | c     | 501  | LMG  | C21-C22-C23-C24 |
| 23  | B     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 27  | A     | 413  | LMG  | C11-C12-C13-C14 |
| 37  | C     | 519  | DGD  | C1A-C2A-C3A-C4A |
| 26  | D     | 2308 | SQD  | C31-C32-C33-C34 |
| 26  | D     | 2308 | SQD  | C34-C35-C36-C37 |
| 26  | a     | 2603 | SQD  | C13-C14-C15-C16 |
| 23  | B     | 608  | CLA  | C16-C17-C18-C19 |
| 23  | D     | 2303 | CLA  | C2B-C3B-CAB-CBB |
| 23  | a     | 2610 | CLA  | C2B-C3B-CAB-CBB |
| 23  | b     | 606  | CLA  | C2B-C3B-CAB-CBB |
| 27  | c     | 521  | LMG  | C14-C15-C16-C17 |
| 23  | C     | 503  | CLA  | C16-C17-C18-C20 |
| 28  | B     | 623  | LMT  | C3-C4-C5-C6     |
| 27  | C     | 527  | LMG  | C30-C31-C32-C33 |
| 24  | A     | 408  | PHO  | C2C-C3C-CAC-CBC |
| 23  | B     | 615  | CLA  | C15-C16-C17-C18 |
| 23  | C     | 504  | CLA  | C10-C11-C12-C13 |
| 38  | d     | 413  | LHG  | C1-C2-C3-O3     |
| 33  | A     | 422  | PL9  | C35-C34-C36-C37 |
| 33  | x     | 1301 | PL9  | C25-C24-C26-C27 |
| 33  | x     | 1301 | PL9  | C38-C39-C41-C42 |
| 27  | C     | 520  | LMG  | O10-C28-O8-C9   |
| 39  | F     | 101  | HEM  | CAA-CBA-CGA-O2A |
| 39  | e     | 103  | HEM  | CAA-CBA-CGA-O2A |
| 36  | i     | 102  | HTG  | C2'-C3'-C4'-C5' |
| 27  | c     | 501  | LMG  | O8-C28-C29-C30  |
| 23  | A     | 410  | CLA  | C6-C7-C8-C9     |
| 36  | I     | 101  | HTG  | C4'-C5'-C6'-C7' |
| 28  | d     | 401  | LMT  | C1-C2-C3-C4     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 37  | C     | 518  | DGD  | CBA-CCA-CDA-CEA |
| 37  | H     | 103  | DGD  | CDB-CEB-CFB-CGB |
| 23  | b     | 609  | CLA  | C13-C15-C16-C17 |
| 23  | C     | 506  | CLA  | C16-C17-C18-C19 |
| 25  | C     | 516  | BCR  | C23-C24-C25-C30 |
| 25  | Y     | 302  | BCR  | C23-C24-C25-C30 |
| 25  | b     | 623  | BCR  | C23-C24-C25-C30 |
| 25  | b     | 624  | BCR  | C23-C24-C25-C30 |
| 25  | y     | 101  | BCR  | C23-C24-C25-C30 |
| 40  | h     | 101  | RRX  | C23-C24-C25-C30 |
| 23  | C     | 509  | CLA  | C10-C11-C12-C13 |
| 23  | B     | 602  | CLA  | CAA-CBA-CGA-O2A |
| 27  | d     | 414  | LMG  | C37-C38-C39-C40 |
| 29  | v     | 204  | GOL  | O1-C1-C2-C3     |
| 27  | d     | 414  | LMG  | C35-C36-C37-C38 |
| 25  | a     | 2614 | BCR  | C19-C20-C21-C22 |
| 23  | C     | 507  | CLA  | CBA-CGA-O2A-C1  |
| 37  | D     | 2307 | DGD  | C5D-C6D-O5D-C1E |
| 26  | l     | 101  | SQD  | C9-C10-C11-C12  |
| 23  | c     | 511  | CLA  | C15-C16-C17-C18 |
| 26  | a     | 2603 | SQD  | C45-C44-O6-C1   |
| 37  | c     | 518  | DGD  | C5D-C6D-O5D-C1E |
| 28  | T     | 103  | LMT  | C4-C5-C6-C7     |
| 37  | D     | 2307 | DGD  | C6B-C7B-C8B-C9B |
| 37  | D     | 2307 | DGD  | O2G-C1B-C2B-C3B |
| 28  | B     | 634  | LMT  | C6-C7-C8-C9     |
| 26  | D     | 2302 | SQD  | C16-C17-C18-C19 |
| 23  | d     | 402  | CLA  | C4C-C3C-CAC-CBC |
| 28  | B     | 634  | LMT  | C4-C5-C6-C7     |
| 23  | D     | 2303 | CLA  | C4B-C3B-CAB-CBB |
| 23  | b     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 23  | d     | 408  | CLA  | C4B-C3B-CAB-CBB |
| 27  | m     | 2802 | LMG  | C18-C19-C20-C21 |
| 37  | h     | 102  | DGD  | CDB-CEB-CFB-CGB |
| 23  | c     | 507  | CLA  | C2-C3-C5-C6     |
| 23  | c     | 509  | CLA  | C11-C12-C13-C15 |
| 23  | c     | 516  | CLA  | C2-C3-C5-C6     |
| 27  | C     | 520  | LMG  | C29-C28-O8-C9   |
| 23  | B     | 612  | CLA  | C15-C16-C17-C18 |
| 37  | D     | 2307 | DGD  | C5A-C6A-C7A-C8A |
| 29  | O     | 304  | GOL  | O1-C1-C2-O2     |
| 23  | C     | 510  | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 37  | C     | 519    | DGD  | O1G-C1A-C2A-C3A |
| 39  | e     | 103    | HEM  | CAD-CBD-CGD-O1D |
| 27  | A     | 413    | LMG  | O1-C7-C8-O7     |
| 26  | b     | 601    | SQD  | O49-C7-O47-C45  |
| 28  | M     | 101    | LMT  | C5-C6-C7-C8     |
| 27  | D     | 2312   | LMG  | C30-C31-C32-C33 |
| 38  | D     | 2311   | LHG  | C30-C31-C32-C33 |
| 39  | e     | 103    | HEM  | CAA-CBA-CGA-O1A |
| 26  | a     | 2615   | SQD  | C28-C29-C30-C31 |
| 27  | C     | 527    | LMG  | C35-C36-C37-C38 |
| 23  | B     | 605    | CLA  | C13-C15-C16-C17 |
| 26  | d     | 417    | SQD  | C5-C6-S-O7      |
| 36  | B     | 624[B] | HTG  | C2'-C1'-S1-C1   |
| 36  | c     | 523    | HTG  | O5-C1-S1-C1'    |
| 23  | B     | 614    | CLA  | C15-C16-C17-C18 |
| 23  | B     | 608    | CLA  | C16-C17-C18-C20 |
| 24  | a     | 2611   | PHO  | C8-C10-C11-C12  |
| 37  | C     | 517    | DGD  | O2G-C1B-C2B-C3B |
| 23  | B     | 604    | CLA  | C11-C10-C8-C9   |
| 23  | C     | 514    | CLA  | C14-C13-C15-C16 |
| 23  | a     | 2610   | CLA  | C11-C10-C8-C9   |
| 23  | a     | 2610   | CLA  | C14-C13-C15-C16 |
| 23  | b     | 614    | CLA  | C11-C10-C8-C9   |
| 23  | b     | 620    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 515    | CLA  | C14-C13-C15-C16 |
| 27  | D     | 2312   | LMG  | C17-C18-C19-C20 |
| 38  | D     | 2309   | LHG  | C30-C31-C32-C33 |
| 23  | c     | 508    | CLA  | C3A-C2A-CAA-CBA |
| 28  | J     | 303    | LMT  | C4'-C5'-C6'-O6' |
| 23  | A     | 405    | CLA  | C2C-C3C-CAC-CBC |
| 39  | F     | 101    | HEM  | CAD-CBD-CGD-O2D |
| 42  | V     | 201    | HEC  | CAD-CBD-CGD-O2D |
| 23  | B     | 605    | CLA  | CAD-CBD-CGD-O2D |
| 23  | B     | 613    | CLA  | CAD-CBD-CGD-O2D |
| 23  | C     | 502    | CLA  | CAD-CBD-CGD-O2D |
| 23  | C     | 506    | CLA  | CAD-CBD-CGD-O2D |
| 23  | b     | 608    | CLA  | CAD-CBD-CGD-O2D |
| 23  | b     | 609    | CLA  | CAD-CBD-CGD-O2D |
| 23  | c     | 512    | CLA  | CAD-CBD-CGD-O2D |
| 23  | c     | 513    | CLA  | CAD-CBD-CGD-O2D |
| 24  | A     | 409    | PHO  | CAD-CBD-CGD-O2D |
| 26  | b     | 601    | SQD  | C14-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | C     | 508  | CLA  | C2A-CAA-CBA-CGA |
| 23  | c     | 509  | CLA  | C13-C15-C16-C17 |
| 23  | D     | 2303 | CLA  | C2-C1-O2A-CGA   |
| 42  | v     | 201  | HEC  | CAD-CBD-CGD-O2D |
| 27  | d     | 414  | LMG  | C13-C14-C15-C16 |
| 36  | b     | 626  | HTG  | C3'-C4'-C5'-C6' |
| 33  | A     | 422  | PL9  | C40-C39-C41-C42 |
| 33  | x     | 1301 | PL9  | C15-C14-C16-C17 |
| 36  | o     | 301  | HTG  | S1-C1'-C2'-C3'  |
| 38  | d     | 413  | LHG  | C31-C32-C33-C34 |
| 26  | b     | 601  | SQD  | C15-C16-C17-C18 |
| 23  | A     | 407  | CLA  | C13-C15-C16-C17 |
| 37  | C     | 518  | DGD  | O2G-C1B-C2B-C3B |
| 28  | M     | 102  | LMT  | C4B-C5B-C6B-O6B |
| 42  | v     | 201  | HEC  | CAD-CBD-CGD-O1D |
| 23  | B     | 614  | CLA  | O2A-C1-C2-C3    |
| 23  | C     | 510  | CLA  | O2A-C1-C2-C3    |
| 23  | C     | 514  | CLA  | O2A-C1-C2-C3    |
| 23  | c     | 515  | CLA  | O2A-C1-C2-C3    |
| 23  | C     | 502  | CLA  | C2A-CAA-CBA-CGA |
| 38  | d     | 412  | LHG  | O8-C23-C24-C25  |
| 28  | T     | 103  | LMT  | C1-C2-C3-C4     |
| 23  | A     | 406  | CLA  | CHA-CBD-CGD-O1D |
| 23  | A     | 406  | CLA  | CHA-CBD-CGD-O2D |
| 23  | B     | 606  | CLA  | CHA-CBD-CGD-O1D |
| 23  | C     | 510  | CLA  | CHA-CBD-CGD-O1D |
| 23  | b     | 607  | CLA  | CHA-CBD-CGD-O2D |
| 23  | c     | 505  | CLA  | CHA-CBD-CGD-O1D |
| 23  | c     | 506  | CLA  | CHA-CBD-CGD-O2D |
| 23  | d     | 402  | CLA  | CHA-CBD-CGD-O1D |
| 23  | d     | 402  | CLA  | CHA-CBD-CGD-O2D |
| 42  | V     | 201  | HEC  | CAD-CBD-CGD-O1D |
| 28  | i     | 103  | LMT  | O1'-C1-C2-C3    |
| 23  | D     | 2304 | CLA  | C16-C17-C18-C19 |
| 37  | D     | 2307 | DGD  | C8B-C9B-CAB-CBB |
| 26  | a     | 2615 | SQD  | O6-C44-C45-O47  |
| 27  | c     | 522  | LMG  | O7-C8-C9-O8     |
| 38  | E     | 101  | LHG  | O7-C5-C6-O8     |
| 23  | A     | 405  | CLA  | C4C-C3C-CAC-CBC |
| 27  | c     | 521  | LMG  | O7-C10-C11-C12  |
| 39  | e     | 103  | HEM  | CAD-CBD-CGD-O2D |
| 24  | A     | 409  | PHO  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 24  | A     | 409  | PHO  | CHA-CBD-CGD-O2D |
| 29  | c     | 530  | GOL  | O1-C1-C2-O2     |
| 26  | B     | 621  | SQD  | C30-C31-C32-C33 |
| 28  | m     | 2804 | LMT  | C2-C3-C4-C5     |
| 36  | B     | 627  | HTG  | C4'-C5'-C6'-C7' |
| 38  | L     | 101  | LHG  | C16-C17-C18-C19 |
| 23  | c     | 513  | CLA  | CAA-CBA-CGA-O2A |
| 23  | C     | 508  | CLA  | C12-C13-C15-C16 |
| 33  | x     | 1301 | PL9  | C13-C14-C16-C17 |
| 23  | C     | 511  | CLA  | CAA-CBA-CGA-O2A |
| 23  | B     | 613  | CLA  | C3-C5-C6-C7     |
| 23  | C     | 508  | CLA  | C14-C13-C15-C16 |
| 23  | c     | 512  | CLA  | C14-C13-C15-C16 |
| 23  | B     | 613  | CLA  | C8-C10-C11-C12  |
| 23  | B     | 607  | CLA  | C2B-C3B-CAB-CBB |
| 23  | B     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 23  | d     | 408  | CLA  | C2B-C3B-CAB-CBB |
| 27  | B     | 622  | LMG  | O8-C28-C29-C30  |
| 37  | c     | 518  | DGD  | O2G-C1B-C2B-C3B |
| 26  | a     | 2615 | SQD  | C5-C6-S-O8      |
| 33  | A     | 422  | PL9  | C12-C11-C9-C8   |
| 23  | c     | 505  | CLA  | C16-C17-C18-C20 |
| 26  | b     | 601  | SQD  | C8-C7-O47-C45   |
| 28  | B     | 623  | LMT  | C5-C6-C7-C8     |
| 28  | A     | 420  | LMT  | C11-C10-C9-C8   |
| 23  | b     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 37  | C     | 519  | DGD  | O1A-C1A-C2A-C3A |
| 23  | a     | 2613 | CLA  | C16-C17-C18-C19 |
| 37  | c     | 520  | DGD  | CAB-CBB-CCB-CDB |
| 29  | B     | 632  | GOL  | C1-C2-C3-O3     |
| 29  | O     | 305  | GOL  | C1-C2-C3-O3     |
| 29  | a     | 2602 | GOL  | C1-C2-C3-O3     |
| 29  | u     | 501  | GOL  | C1-C2-C3-O3     |
| 23  | B     | 613  | CLA  | CAA-CBA-CGA-O2A |
| 23  | C     | 513  | CLA  | CAA-CBA-CGA-O2A |
| 26  | d     | 417  | SQD  | C24-C25-C26-C27 |
| 23  | B     | 610  | CLA  | C1A-C2A-CAA-CBA |
| 26  | l     | 101  | SQD  | C11-C12-C13-C14 |
| 39  | F     | 101  | HEM  | CAA-CBA-CGA-O1A |
| 27  | c     | 501  | LMG  | C30-C31-C32-C33 |
| 23  | B     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 23  | C     | 513  | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 37  | C     | 517  | DGD  | O1B-C1B-C2B-C3B |
| 28  | B     | 623  | LMT  | C2B-C1B-O1B-C4' |
| 27  | A     | 413  | LMG  | O1-C7-C8-C9     |
| 27  | c     | 521  | LMG  | O1-C7-C8-C9     |
| 37  | C     | 519  | DGD  | O6E-C5E-C6E-O5E |
| 23  | C     | 508  | CLA  | C5-C6-C7-C8     |
| 23  | b     | 618  | CLA  | CAA-CBA-CGA-O2A |
| 23  | C     | 513  | CLA  | CAA-CBA-CGA-O1A |
| 37  | c     | 518  | DGD  | C2E-C1E-O5D-C6D |
| 23  | d     | 402  | CLA  | C15-C16-C17-C18 |
| 23  | D     | 2304 | CLA  | C4B-C3B-CAB-CBB |
| 26  | d     | 417  | SQD  | O5-C5-C6-S      |
| 38  | D     | 2310 | LHG  | C4-O6-P-O5      |
| 38  | d     | 413  | LHG  | C3-O3-P-O5      |
| 28  | m     | 2804 | LMT  | O5B-C1B-O1B-C4' |
| 27  | B     | 622  | LMG  | O10-C28-C29-C30 |
| 38  | d     | 412  | LHG  | O10-C23-C24-C25 |
| 28  | z     | 102  | LMT  | C4'-C5'-C6'-O6' |
| 27  | d     | 414  | LMG  | O7-C10-C11-C12  |
| 37  | c     | 520  | DGD  | O1G-C1A-C2A-C3A |
| 25  | a     | 2614 | BCR  | C5-C6-C7-C8     |
| 25  | b     | 624  | BCR  | C23-C24-C25-C26 |
| 25  | y     | 101  | BCR  | C23-C24-C25-C26 |
| 27  | B     | 622  | LMG  | O10-C28-O8-C9   |
| 28  | d     | 401  | LMT  | O5B-C5B-C6B-O6B |
| 38  | L     | 101  | LHG  | O7-C7-C8-C9     |
| 38  | l     | 103  | LHG  | O7-C7-C8-C9     |
| 38  | D     | 2310 | LHG  | C16-C17-C18-C19 |
| 27  | c     | 521  | LMG  | C12-C13-C14-C15 |
| 37  | C     | 519  | DGD  | C9B-CAB-CBB-CCB |
| 37  | C     | 518  | DGD  | O1B-C1B-C2B-C3B |
| 23  | D     | 2304 | CLA  | O1A-CGA-O2A-C1  |
| 38  | L     | 101  | LHG  | C17-C18-C19-C20 |
| 23  | B     | 616  | CLA  | C5-C6-C7-C8     |
| 27  | A     | 413  | LMG  | C29-C30-C31-C32 |
| 23  | B     | 608  | CLA  | CAD-CBD-CGD-O1D |
| 23  | B     | 610  | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 505  | CLA  | CAD-CBD-CGD-O1D |
| 23  | b     | 612  | CLA  | CAD-CBD-CGD-O1D |
| 23  | b     | 614  | CLA  | CAD-CBD-CGD-O1D |
| 23  | b     | 615  | CLA  | CAD-CBD-CGD-O1D |
| 23  | c     | 507  | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | c     | 508  | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 511  | CLA  | CAA-CBA-CGA-O1A |
| 27  | c     | 521  | LMG  | O9-C10-C11-C12  |
| 38  | D     | 2309 | LHG  | C28-C29-C30-C31 |
| 23  | b     | 617  | CLA  | CAA-CBA-CGA-O2A |
| 37  | c     | 520  | DGD  | O6D-C5D-C6D-O5D |
| 23  | A     | 407  | CLA  | C6-C7-C8-C9     |
| 23  | B     | 614  | CLA  | C14-C13-C15-C16 |
| 23  | c     | 509  | CLA  | C11-C12-C13-C14 |
| 29  | A     | 417  | GOL  | O1-C1-C2-O2     |
| 27  | C     | 527  | LMG  | C40-C41-C42-C43 |
| 23  | C     | 506  | CLA  | CAA-CBA-CGA-O2A |
| 23  | c     | 508  | CLA  | CAA-CBA-CGA-O2A |
| 27  | c     | 501  | LMG  | C14-C15-C16-C17 |
| 37  | D     | 2307 | DGD  | C9B-CAB-CBB-CCB |
| 38  | d     | 403  | LHG  | C29-C30-C31-C32 |
| 23  | A     | 406  | CLA  | C15-C16-C17-C18 |
| 37  | c     | 519  | DGD  | C8B-C9B-CAB-CBB |
| 27  | B     | 622  | LMG  | C33-C34-C35-C36 |
| 37  | C     | 519  | DGD  | CBA-CCA-CDA-CEA |
| 36  | o     | 301  | HTG  | C1'-C2'-C3'-C4' |
| 37  | c     | 519  | DGD  | O2G-C1B-C2B-C3B |
| 33  | A     | 422  | PL9  | C16-C17-C18-C19 |
| 23  | c     | 516  | CLA  | C4-C3-C5-C6     |
| 33  | d     | 411  | PL9  | C30-C29-C31-C32 |
| 23  | B     | 616  | CLA  | C11-C10-C8-C7   |
| 23  | a     | 2610 | CLA  | C11-C12-C13-C15 |
| 33  | x     | 1301 | PL9  | C23-C24-C26-C27 |
| 27  | c     | 501  | LMG  | C22-C23-C24-C25 |
| 23  | C     | 504  | CLA  | C15-C16-C17-C18 |
| 23  | b     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 27  | C     | 520  | LMG  | C40-C41-C42-C43 |
| 28  | z     | 102  | LMT  | C11-C10-C9-C8   |
| 26  | A     | 412  | SQD  | C7-C8-C9-C10    |
| 25  | C     | 515  | BCR  | C7-C8-C9-C10    |
| 25  | c     | 517  | BCR  | C7-C8-C9-C10    |
| 23  | C     | 506  | CLA  | CAA-CBA-CGA-O1A |
| 37  | c     | 518  | DGD  | O1B-C1B-C2B-C3B |
| 37  | c     | 519  | DGD  | O1B-C1B-C2B-C3B |
| 28  | M     | 102  | LMT  | C2-C1-O1'-C1'   |
| 28  | m     | 2803 | LMT  | C2-C1-O1'-C1'   |
| 27  | A     | 413  | LMG  | O8-C28-C29-C30  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | B     | 617  | CLA  | C13-C15-C16-C17 |
| 23  | c     | 515  | CLA  | C15-C16-C17-C18 |
| 38  | D     | 2311 | LHG  | O8-C23-C24-C25  |
| 38  | d     | 403  | LHG  | O8-C23-C24-C25  |
| 26  | b     | 601  | SQD  | C26-C27-C28-C29 |
| 23  | b     | 618  | CLA  | CAA-CBA-CGA-O1A |
| 23  | c     | 513  | CLA  | CAA-CBA-CGA-O1A |
| 37  | c     | 520  | DGD  | O1A-C1A-C2A-C3A |
| 27  | B     | 622  | LMG  | C29-C28-O8-C9   |
| 23  | B     | 613  | CLA  | CAA-CBA-CGA-O1A |
| 26  | a     | 2615 | SQD  | C31-C32-C33-C34 |
| 27  | d     | 414  | LMG  | C20-C21-C22-C23 |
| 28  | d     | 404  | LMT  | C3'-C4'-O1B-C1B |

There are no ring outliers.

180 monomers are involved in 316 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 38  | D     | 2311 | LHG  | 2       | 0            |
| 38  | L     | 101  | LHG  | 1       | 0            |
| 23  | a     | 2609 | CLA  | 3       | 0            |
| 25  | b     | 623  | BCR  | 3       | 0            |
| 37  | c     | 519  | DGD  | 1       | 0            |
| 36  | B     | 627  | HTG  | 1       | 0            |
| 34  | O     | 307  | DMS  | 1       | 0            |
| 37  | C     | 518  | DGD  | 2       | 0            |
| 29  | C     | 526  | GOL  | 2       | 0            |
| 38  | D     | 2309 | LHG  | 1       | 0            |
| 23  | b     | 615  | CLA  | 4       | 0            |
| 23  | b     | 616  | CLA  | 1       | 0            |
| 36  | C     | 525  | HTG  | 1       | 0            |
| 23  | B     | 617  | CLA  | 2       | 0            |
| 23  | C     | 504  | CLA  | 6       | 0            |
| 23  | d     | 402  | CLA  | 5       | 0            |
| 26  | d     | 417  | SQD  | 2       | 0            |
| 36  | b     | 604  | HTG  | 1       | 0            |
| 29  | b     | 631  | GOL  | 1       | 0            |
| 23  | a     | 2613 | CLA  | 1       | 0            |
| 26  | a     | 2615 | SQD  | 1       | 0            |
| 40  | H     | 102  | RRX  | 3       | 0            |
| 23  | c     | 506  | CLA  | 7       | 0            |
| 34  | V     | 206  | DMS  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 26  | D     | 2308 | SQD  | 1       | 0            |
| 23  | B     | 602  | CLA  | 1       | 0            |
| 34  | c     | 543  | DMS  | 1       | 0            |
| 25  | c     | 517  | BCR  | 2       | 0            |
| 36  | i     | 102  | HTG  | 1       | 0            |
| 23  | C     | 513  | CLA  | 5       | 0            |
| 28  | M     | 101  | LMT  | 1       | 0            |
| 25  | k     | 302  | BCR  | 1       | 0            |
| 36  | b     | 625  | HTG  | 6       | 0            |
| 25  | d     | 410  | BCR  | 2       | 0            |
| 34  | a     | 2624 | DMS  | 1       | 0            |
| 25  | b     | 624  | BCR  | 2       | 0            |
| 27  | B     | 622  | LMG  | 1       | 0            |
| 23  | b     | 617  | CLA  | 1       | 0            |
| 38  | D     | 2310 | LHG  | 1       | 0            |
| 23  | c     | 516  | CLA  | 2       | 0            |
| 23  | b     | 606  | CLA  | 1       | 0            |
| 27  | d     | 414  | LMG  | 4       | 0            |
| 28  | Z     | 101  | LMT  | 2       | 0            |
| 23  | B     | 614  | CLA  | 3       | 0            |
| 23  | A     | 406  | CLA  | 2       | 0            |
| 23  | b     | 609  | CLA  | 2       | 0            |
| 29  | B     | 632  | GOL  | 2       | 0            |
| 24  | A     | 409  | PHO  | 3       | 0            |
| 23  | A     | 407  | CLA  | 3       | 0            |
| 23  | a     | 2610 | CLA  | 2       | 0            |
| 29  | O     | 302  | GOL  | 1       | 0            |
| 23  | c     | 508  | CLA  | 4       | 0            |
| 23  | b     | 611  | CLA  | 4       | 0            |
| 27  | C     | 527  | LMG  | 2       | 0            |
| 23  | A     | 405  | CLA  | 2       | 0            |
| 23  | D     | 2303 | CLA  | 3       | 0            |
| 23  | c     | 512  | CLA  | 2       | 0            |
| 28  | i     | 103  | LMT  | 1       | 0            |
| 23  | b     | 614  | CLA  | 2       | 0            |
| 25  | y     | 101  | BCR  | 2       | 0            |
| 27  | c     | 522  | LMG  | 4       | 0            |
| 34  | d     | 418  | DMS  | 1       | 0            |
| 23  | C     | 511  | CLA  | 3       | 0            |
| 34  | B     | 642  | DMS  | 1       | 0            |
| 38  | l     | 103  | LHG  | 2       | 0            |
| 28  | z     | 102  | LMT  | 4       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 28  | B     | 634  | LMT  | 1       | 0            |
| 27  | c     | 521  | LMG  | 1       | 0            |
| 36  | b     | 626  | HTG  | 1       | 0            |
| 25  | T     | 102  | BCR  | 3       | 0            |
| 28  | j     | 2701 | LMT  | 1       | 0            |
| 38  | d     | 412  | LHG  | 4       | 0            |
| 34  | C     | 536  | DMS  | 1       | 0            |
| 23  | b     | 621  | CLA  | 3       | 0            |
| 25  | a     | 2614 | BCR  | 2       | 0            |
| 36  | B     | 625  | HTG  | 1       | 0            |
| 34  | B     | 644  | DMS  | 1       | 0            |
| 25  | K     | 101  | BCR  | 1       | 0            |
| 33  | A     | 422  | PL9  | 4       | 0            |
| 34  | U     | 503  | DMS  | 1       | 0            |
| 23  | c     | 507  | CLA  | 2       | 0            |
| 38  | d     | 403  | LHG  | 1       | 0            |
| 26  | D     | 2302 | SQD  | 3       | 0            |
| 34  | B     | 647  | DMS  | 2       | 0            |
| 36  | b     | 602  | HTG  | 2       | 0            |
| 23  | b     | 608  | CLA  | 2       | 0            |
| 25  | Y     | 302  | BCR  | 2       | 0            |
| 25  | C     | 516  | BCR  | 3       | 0            |
| 27  | m     | 2802 | LMG  | 1       | 0            |
| 23  | b     | 618  | CLA  | 4       | 0            |
| 28  | A     | 420  | LMT  | 3       | 0            |
| 25  | D     | 2305 | BCR  | 2       | 0            |
| 28  | d     | 404  | LMT  | 1       | 0            |
| 26  | a     | 2603 | SQD  | 2       | 0            |
| 28  | A     | 414  | LMT  | 6       | 0            |
| 25  | B     | 619  | BCR  | 3       | 0            |
| 25  | B     | 620  | BCR  | 2       | 0            |
| 24  | A     | 408  | PHO  | 1       | 0            |
| 23  | b     | 620  | CLA  | 4       | 0            |
| 36  | o     | 301  | HTG  | 2       | 0            |
| 25  | B     | 618  | BCR  | 1       | 0            |
| 34  | o     | 314  | DMS  | 2       | 0            |
| 25  | B     | 633  | BCR  | 4       | 0            |
| 23  | c     | 515  | CLA  | 2       | 0            |
| 23  | B     | 609  | CLA  | 1       | 0            |
| 29  | c     | 530  | GOL  | 1       | 0            |
| 23  | B     | 611  | CLA  | 4       | 0            |
| 23  | d     | 408  | CLA  | 1       | 0            |

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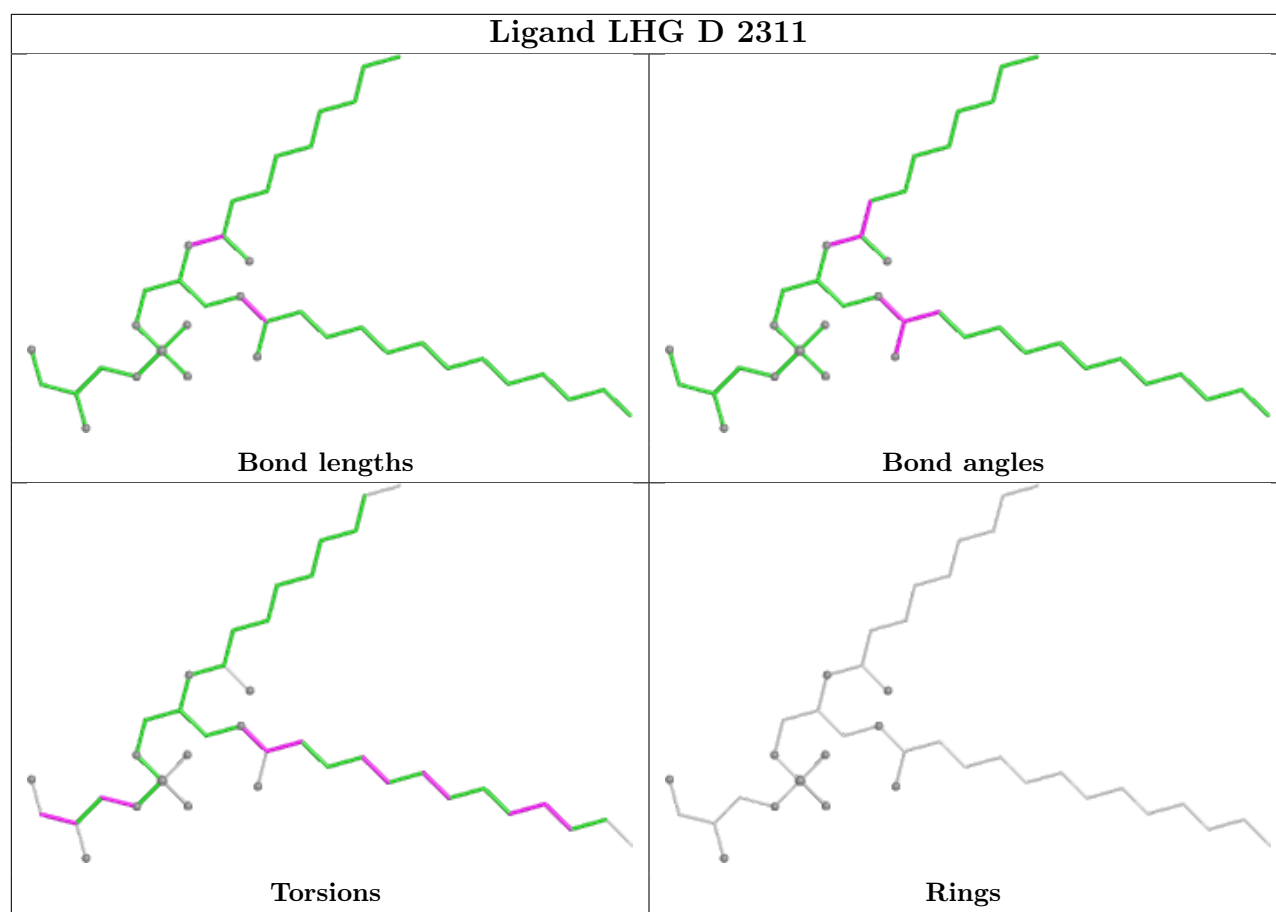
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 36  | C     | 521  | HTG  | 2       | 0            |
| 23  | C     | 502  | CLA  | 5       | 0            |
| 23  | c     | 504  | CLA  | 3       | 0            |
| 26  | l     | 101  | SQD  | 4       | 0            |
| 25  | b     | 622  | BCR  | 2       | 0            |
| 33  | d     | 411  | PL9  | 1       | 0            |
| 23  | C     | 507  | CLA  | 5       | 0            |
| 23  | C     | 510  | CLA  | 3       | 0            |
| 23  | c     | 505  | CLA  | 2       | 0            |
| 27  | c     | 501  | LMG  | 4       | 0            |
| 34  | B     | 637  | DMS  | 1       | 0            |
| 29  | a     | 2602 | GOL  | 1       | 0            |
| 24  | a     | 2612 | PHO  | 2       | 0            |
| 34  | b     | 639  | DMS  | 1       | 0            |
| 36  | b     | 603  | HTG  | 1       | 0            |
| 23  | c     | 514  | CLA  | 5       | 0            |
| 23  | C     | 508  | CLA  | 4       | 0            |
| 34  | o     | 307  | DMS  | 1       | 0            |
| 36  | H     | 101  | HTG  | 2       | 0            |
| 37  | C     | 519  | DGD  | 2       | 0            |
| 28  | d     | 401  | LMT  | 6       | 0            |
| 34  | v     | 209  | DMS  | 1       | 0            |
| 37  | D     | 2307 | DGD  | 3       | 0            |
| 23  | C     | 506  | CLA  | 4       | 0            |
| 39  | e     | 103  | HEM  | 2       | 0            |
| 23  | A     | 410  | CLA  | 4       | 0            |
| 27  | D     | 2312 | LMG  | 2       | 0            |
| 23  | C     | 512  | CLA  | 2       | 0            |
| 40  | h     | 101  | RRX  | 3       | 0            |
| 27  | A     | 413  | LMG  | 3       | 0            |
| 36  | I     | 101  | HTG  | 2       | 0            |
| 25  | z     | 101  | BCR  | 2       | 0            |
| 23  | B     | 613  | CLA  | 2       | 0            |
| 37  | C     | 517  | DGD  | 2       | 0            |
| 36  | d     | 407  | HTG  | 3       | 0            |
| 38  | d     | 413  | LHG  | 1       | 0            |
| 23  | B     | 604  | CLA  | 3       | 0            |
| 34  | c     | 535  | DMS  | 1       | 0            |
| 23  | B     | 605  | CLA  | 1       | 0            |
| 38  | e     | 101  | LHG  | 1       | 0            |
| 29  | b     | 644  | GOL  | 3       | 0            |
| 26  | B     | 621  | SQD  | 2       | 0            |

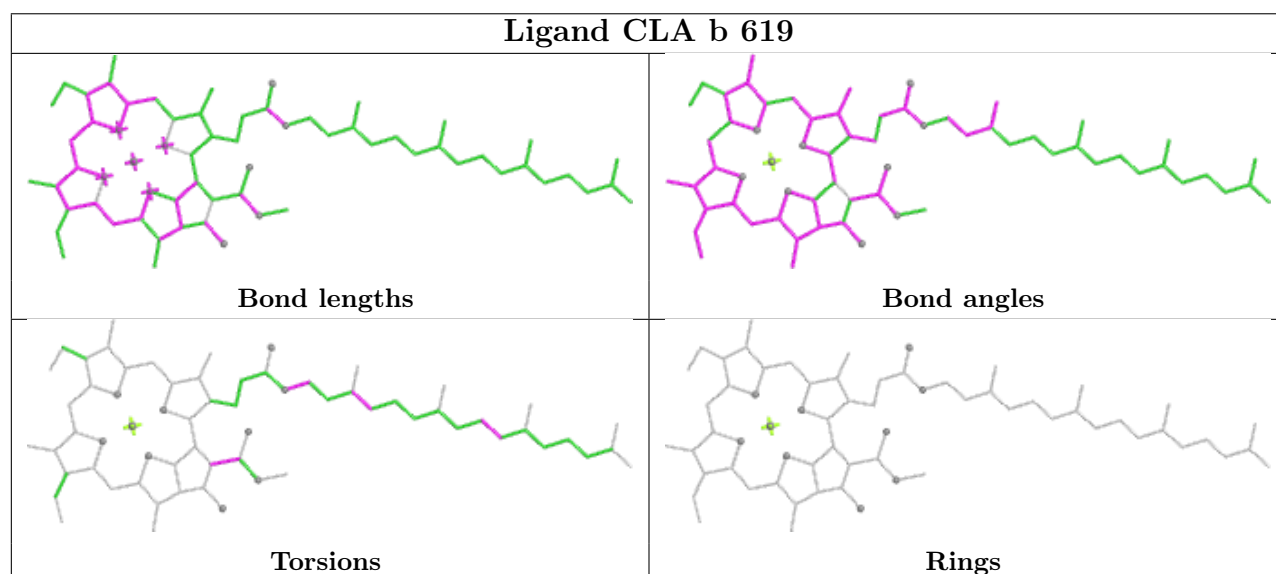
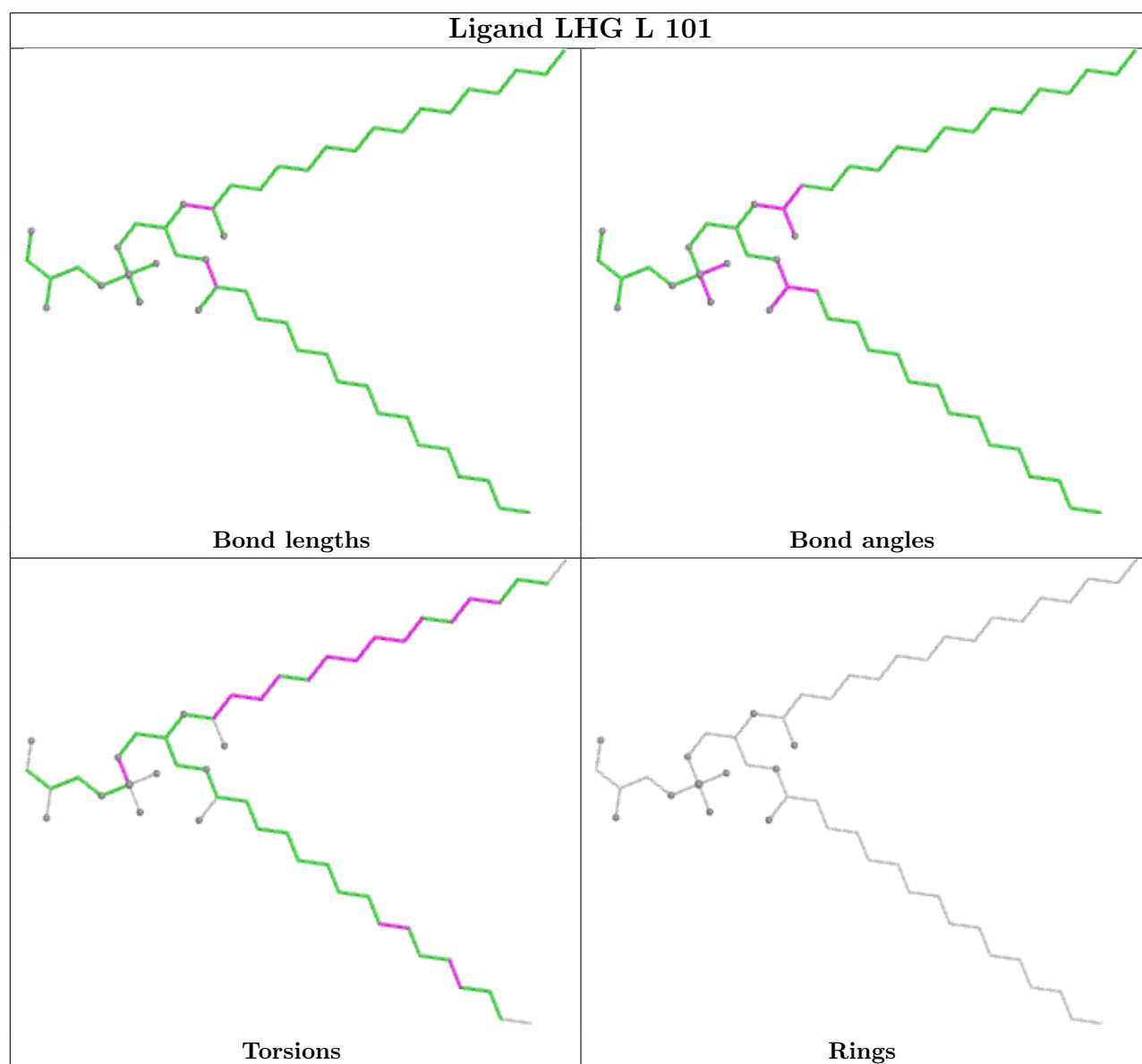
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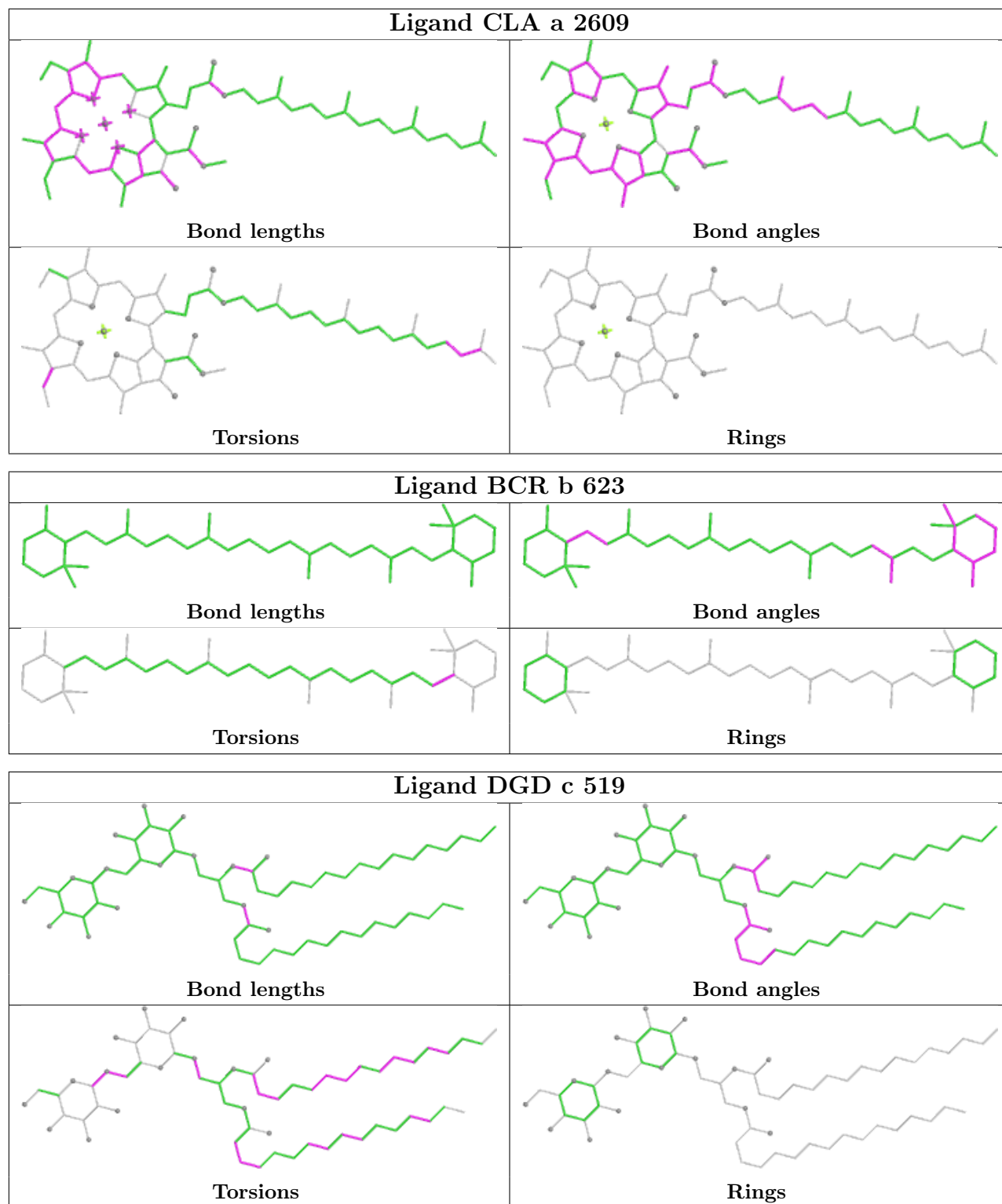
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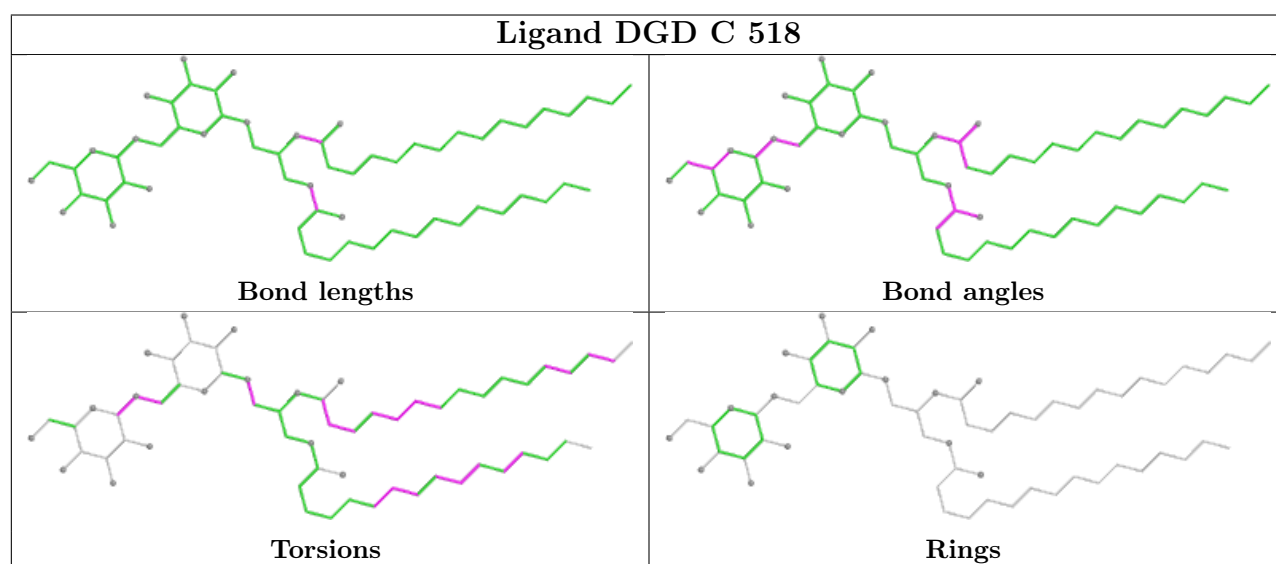
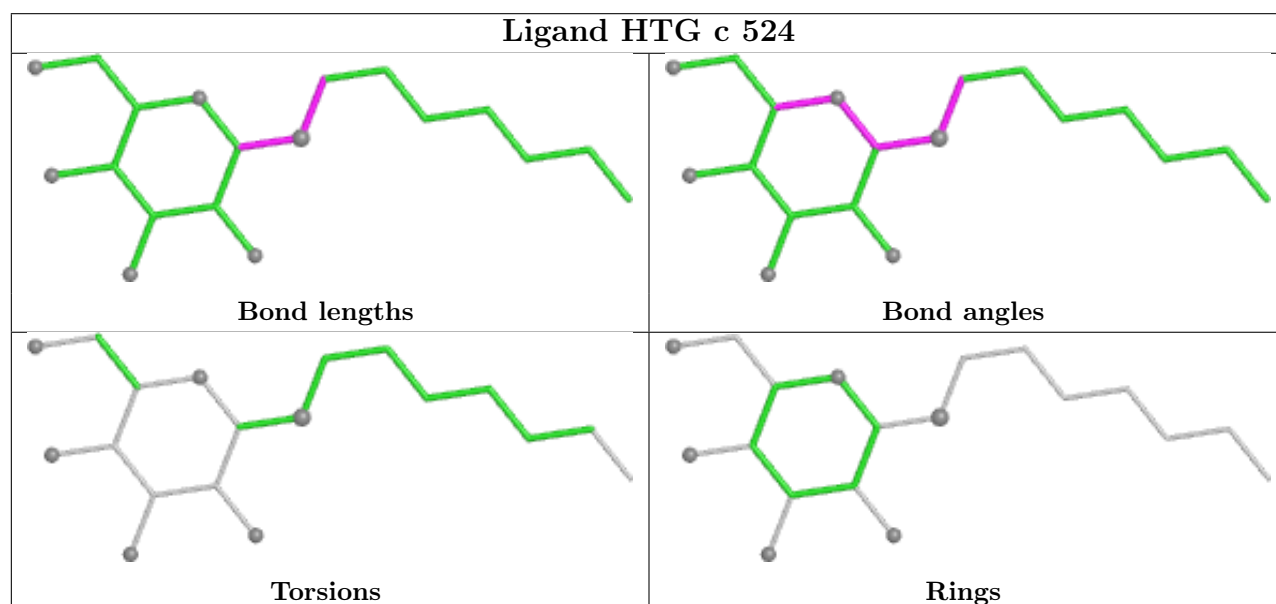
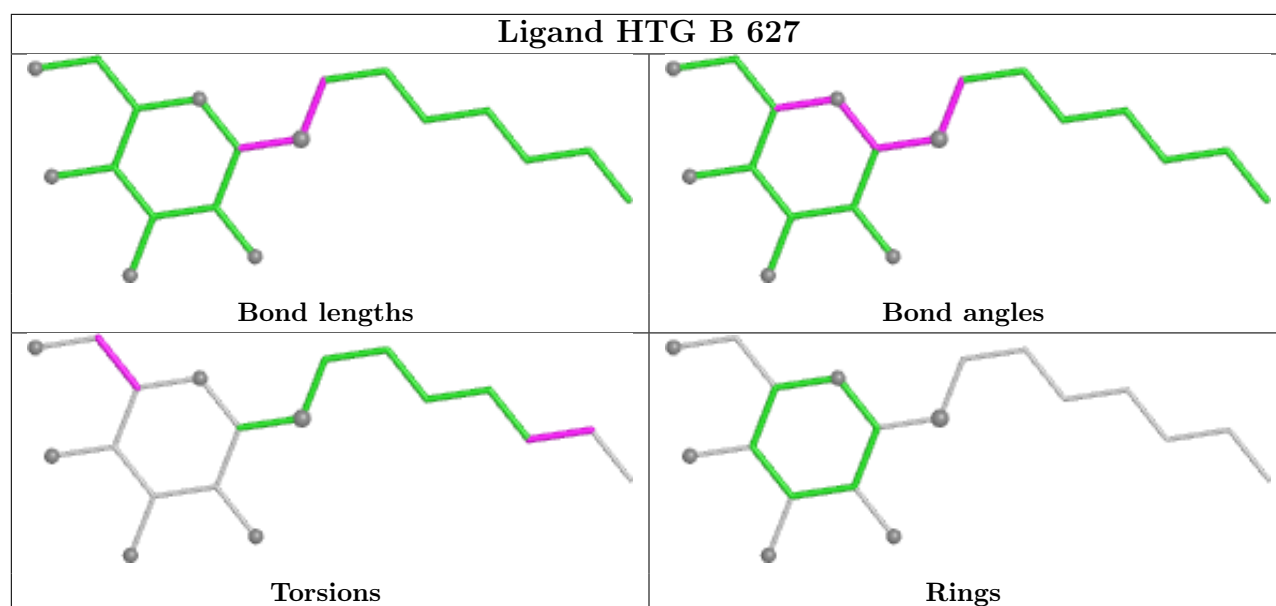
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 33  | x     | 1301   | PL9  | 2       | 0            |
| 23  | b     | 612    | CLA  | 1       | 0            |
| 23  | B     | 606    | CLA  | 4       | 0            |
| 23  | c     | 509    | CLA  | 4       | 0            |
| 25  | C     | 515    | BCR  | 2       | 0            |
| 34  | B     | 638    | DMS  | 1       | 0            |
| 34  | A     | 430    | DMS  | 1       | 0            |
| 34  | c     | 536    | DMS  | 1       | 0            |
| 23  | C     | 505    | CLA  | 2       | 0            |
| 23  | C     | 514    | CLA  | 6       | 0            |
| 28  | m     | 2803   | LMT  | 1       | 0            |
| 23  | B     | 607    | CLA  | 1       | 0            |
| 23  | B     | 610    | CLA  | 1       | 0            |
| 37  | c     | 518    | DGD  | 1       | 0            |
| 34  | D     | 2320   | DMS  | 1       | 0            |
| 23  | B     | 615    | CLA  | 2       | 0            |
| 23  | B     | 616    | CLA  | 2       | 0            |
| 29  | B     | 648    | GOL  | 3       | 0            |
| 34  | V     | 212    | DMS  | 1       | 0            |
| 23  | C     | 503    | CLA  | 4       | 0            |
| 26  | b     | 601    | SQD  | 1       | 0            |
| 28  | B     | 623    | LMT  | 1       | 0            |
| 26  | A     | 412    | SQD  | 2       | 0            |
| 39  | F     | 101    | HEM  | 1       | 0            |
| 36  | B     | 624[B] | HTG  | 2       | 0            |
| 23  | C     | 509    | CLA  | 3       | 0            |
| 23  | c     | 510    | CLA  | 3       | 0            |
| 23  | D     | 2304   | CLA  | 1       | 0            |
| 23  | b     | 607    | CLA  | 1       | 0            |
| 23  | b     | 610    | CLA  | 2       | 0            |

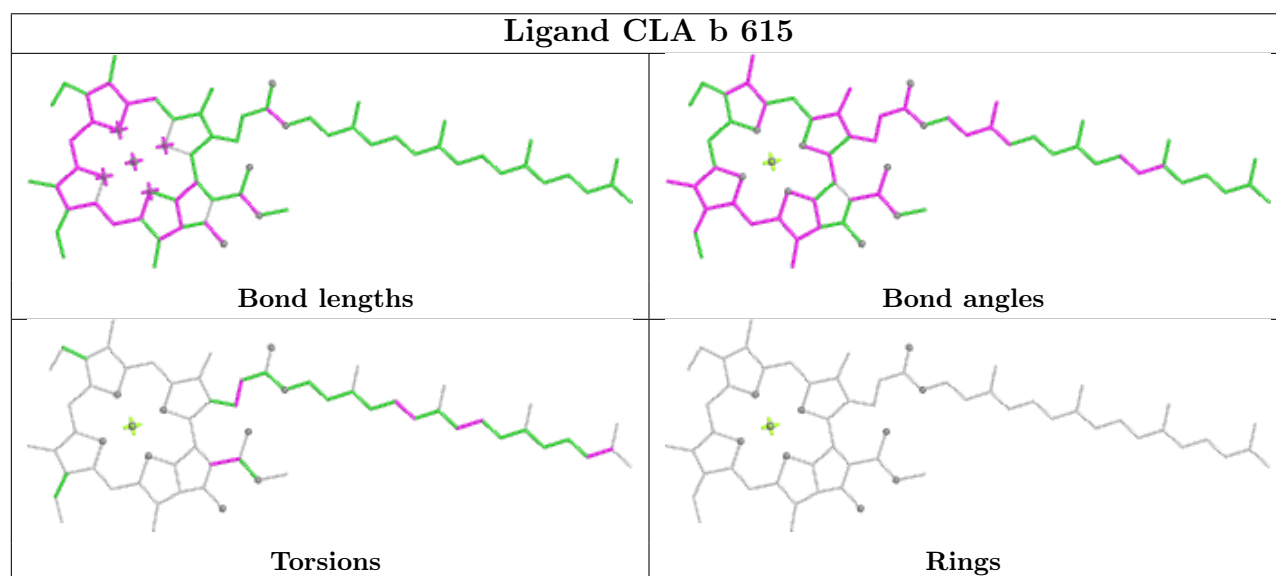
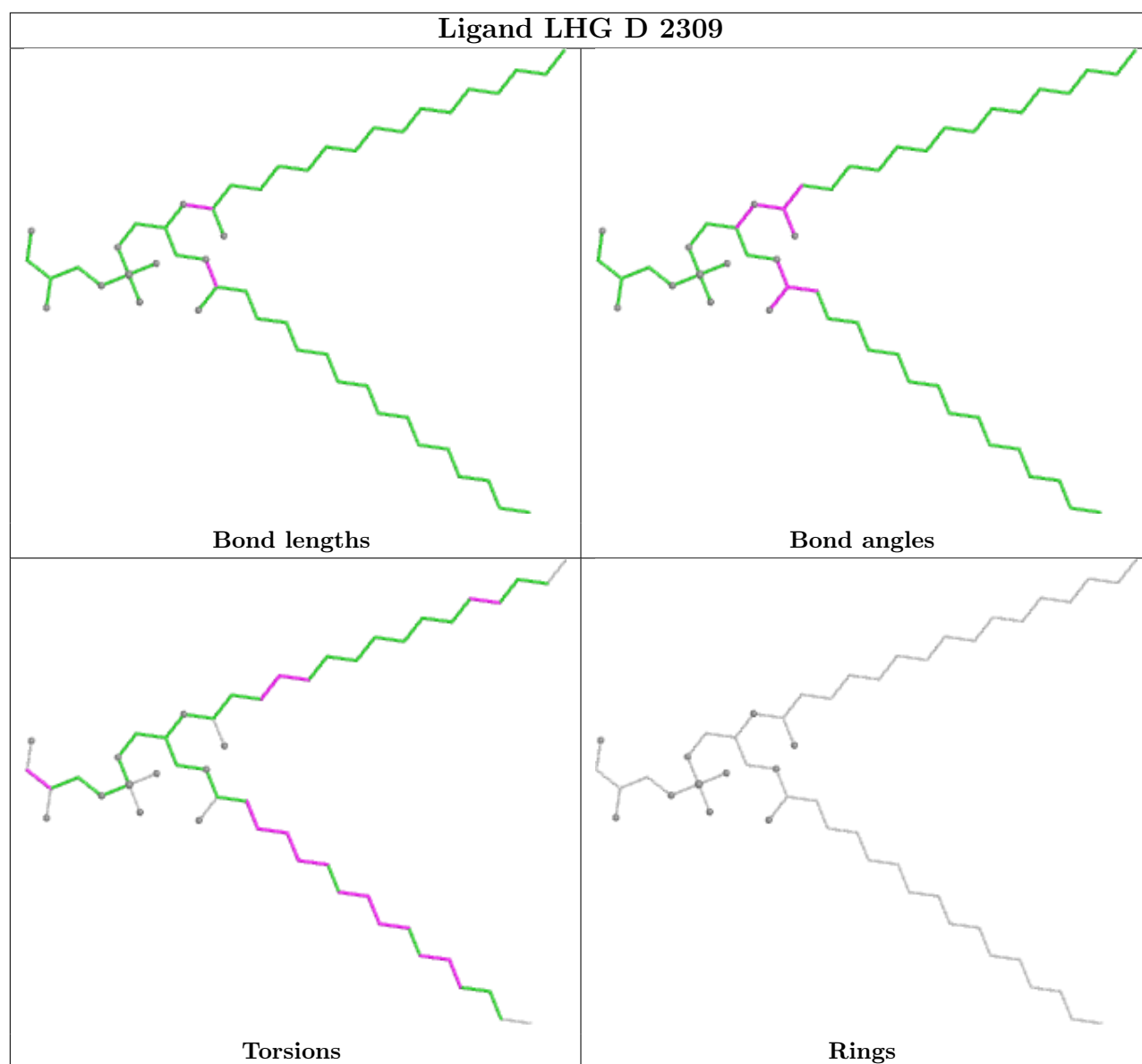
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



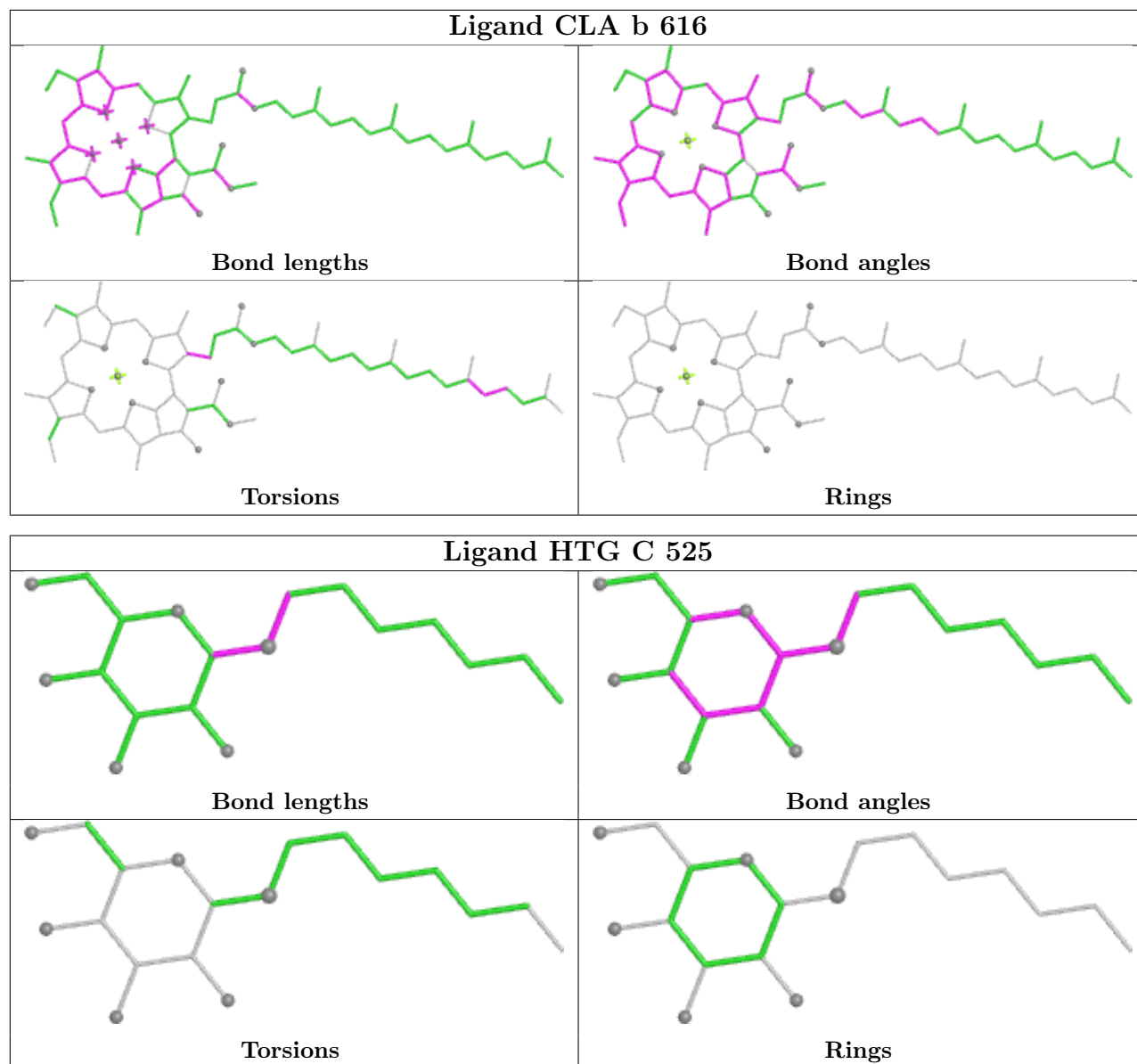




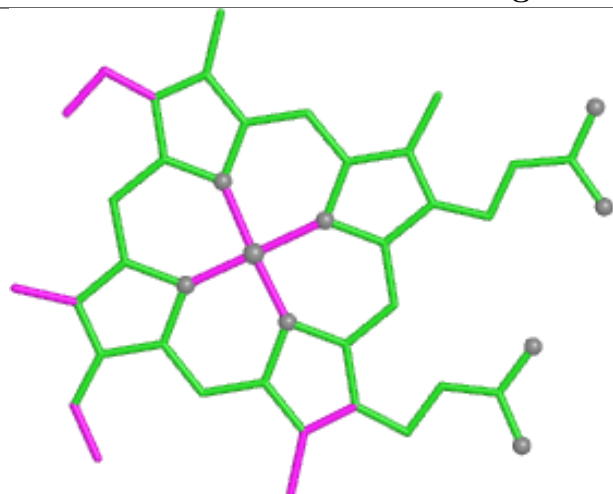




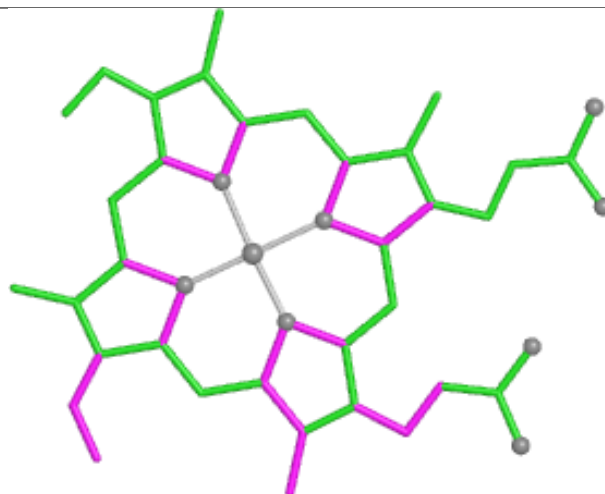




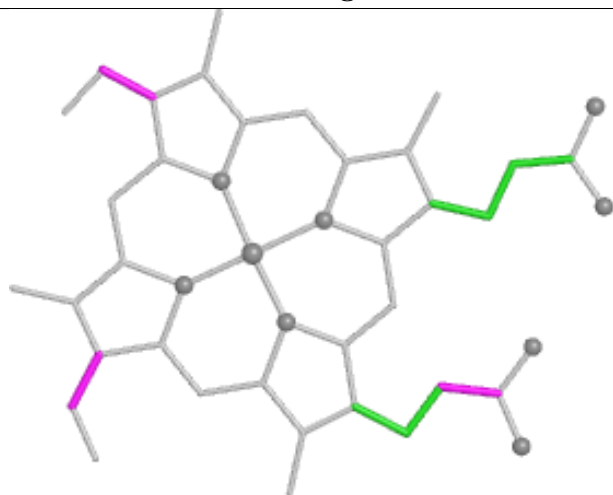
## Ligand HEC V 201



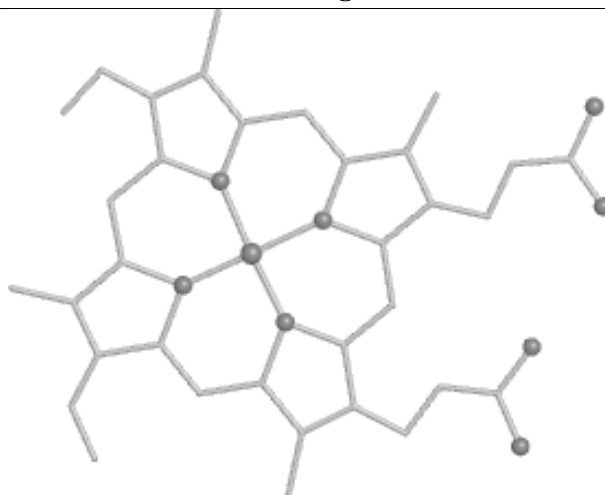
Bond lengths



Bond angles

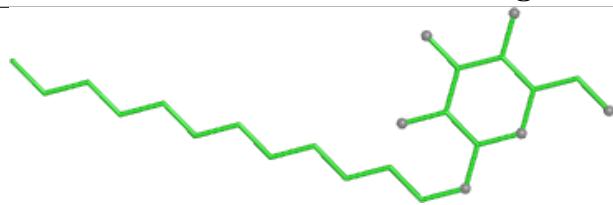


Torsions



Rings

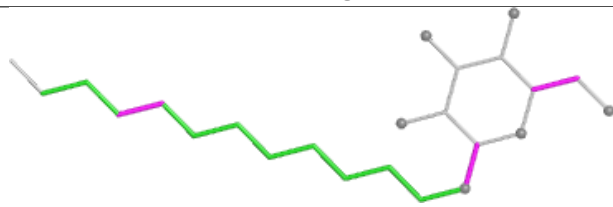
## Ligand LMT J 303



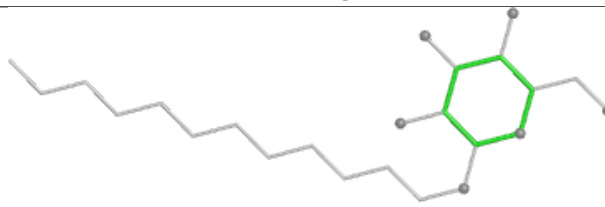
Bond lengths



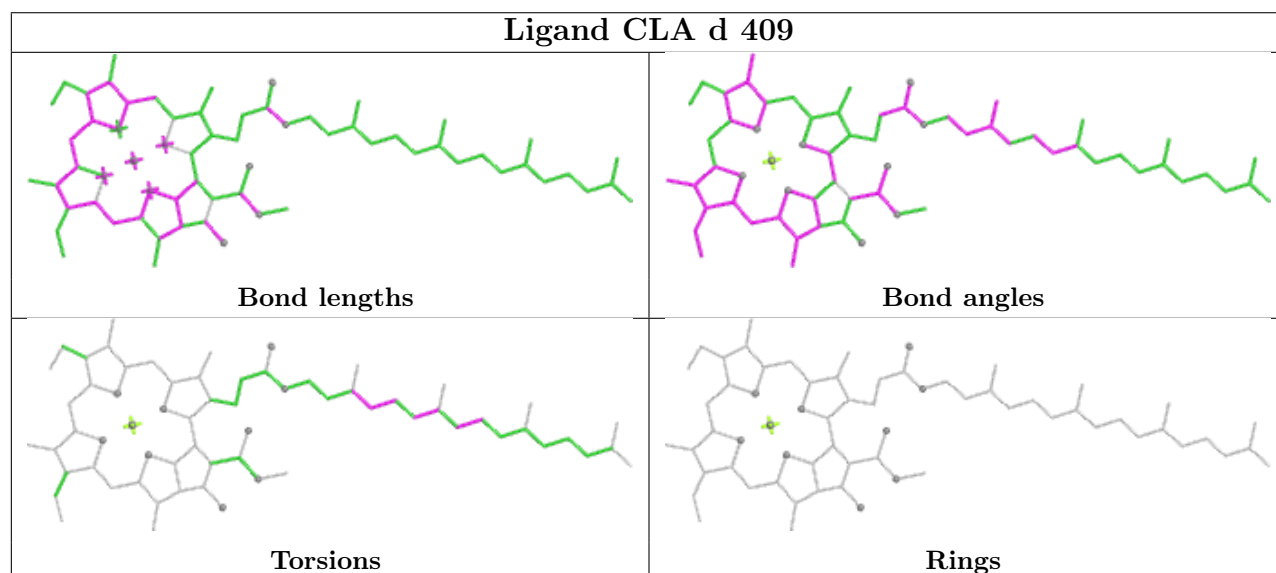
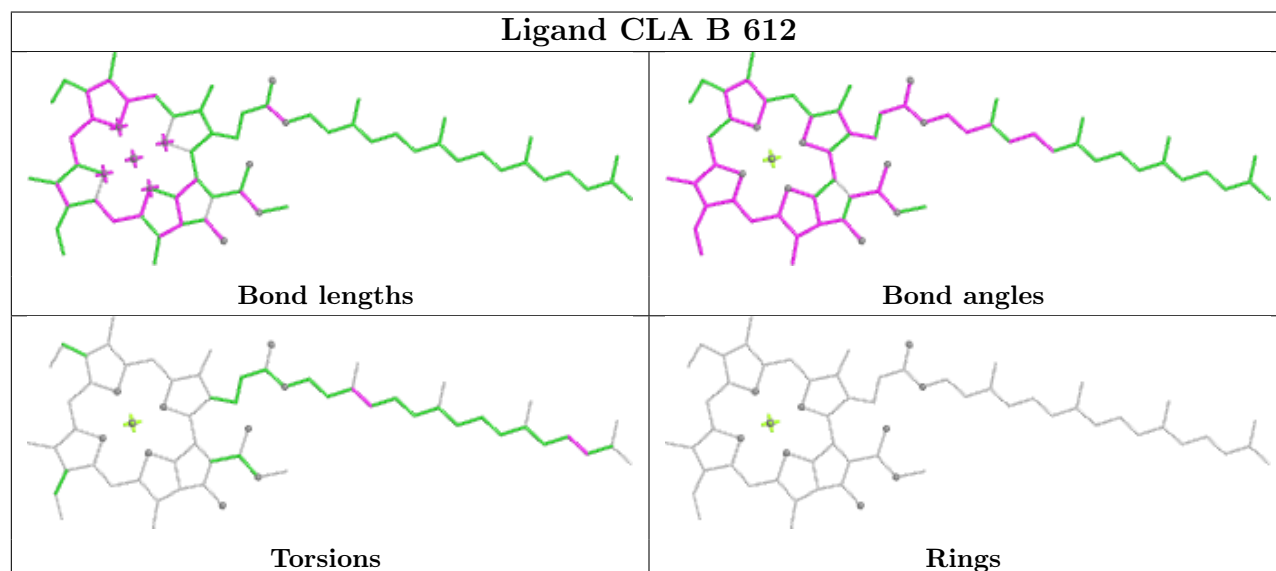
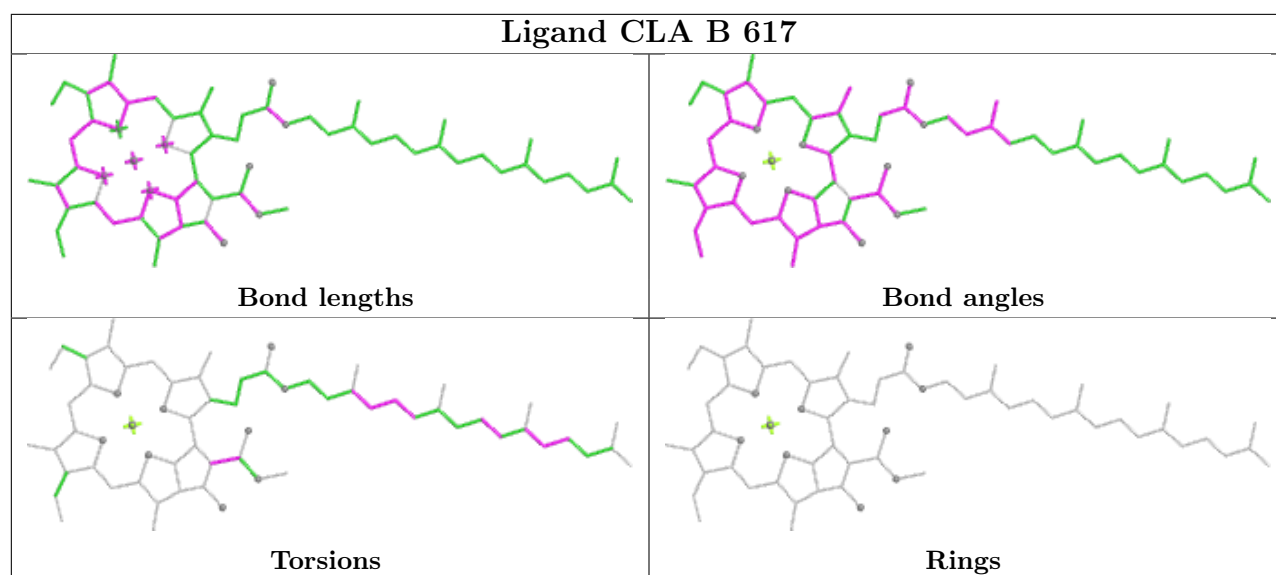
Bond angles

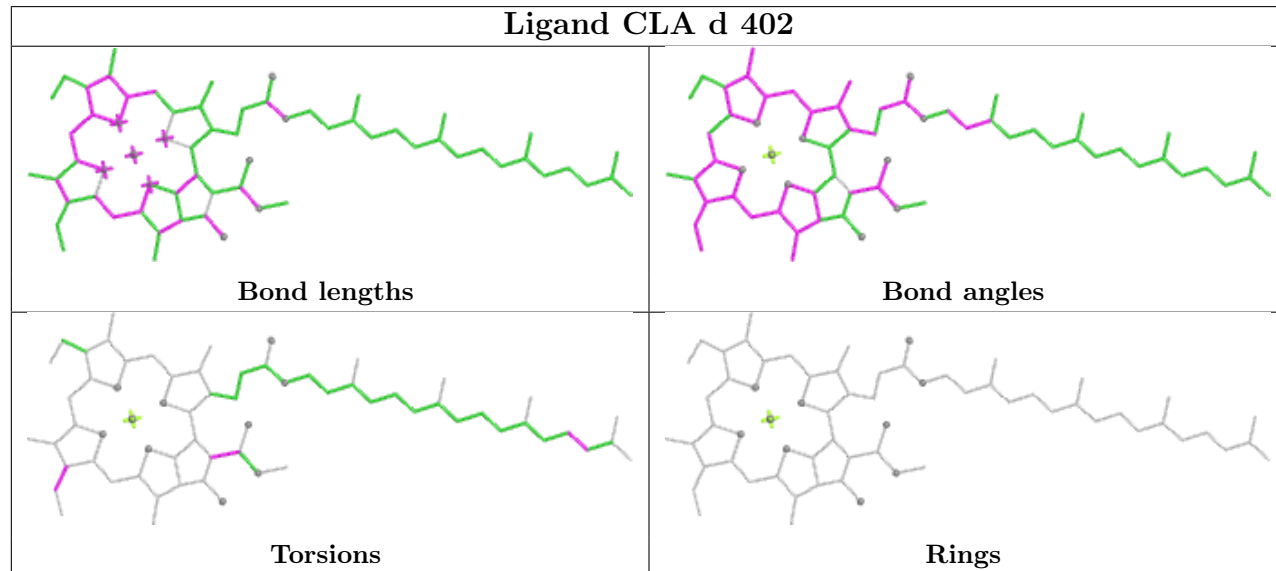
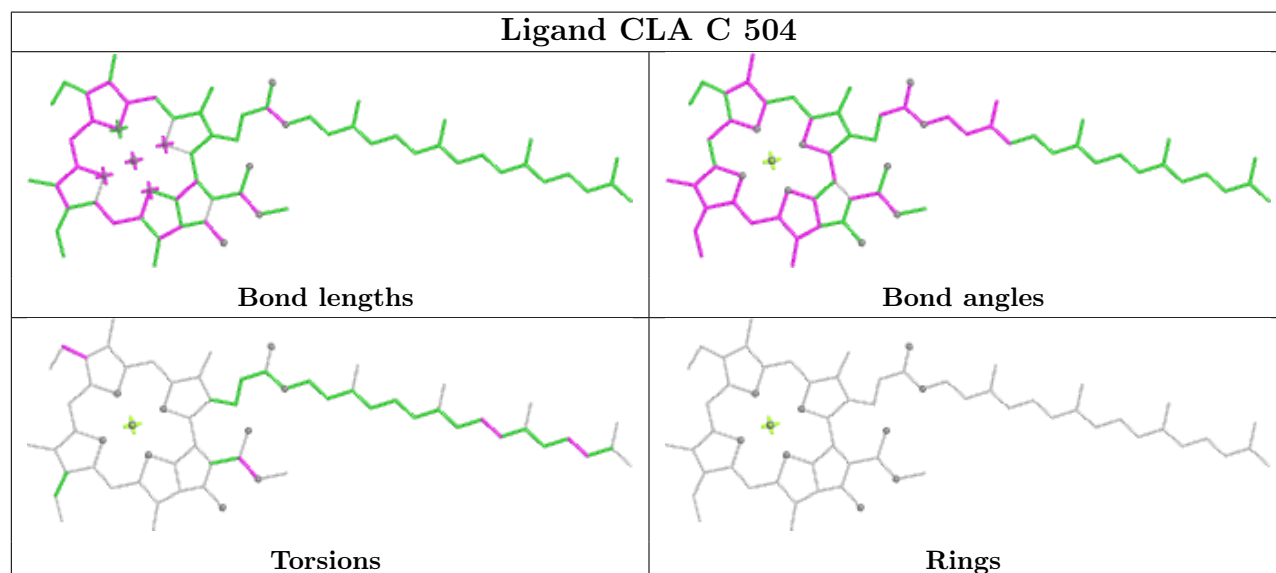
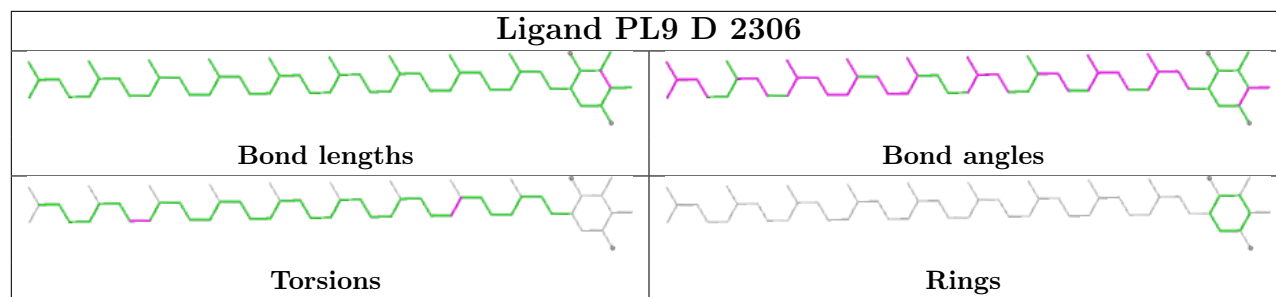


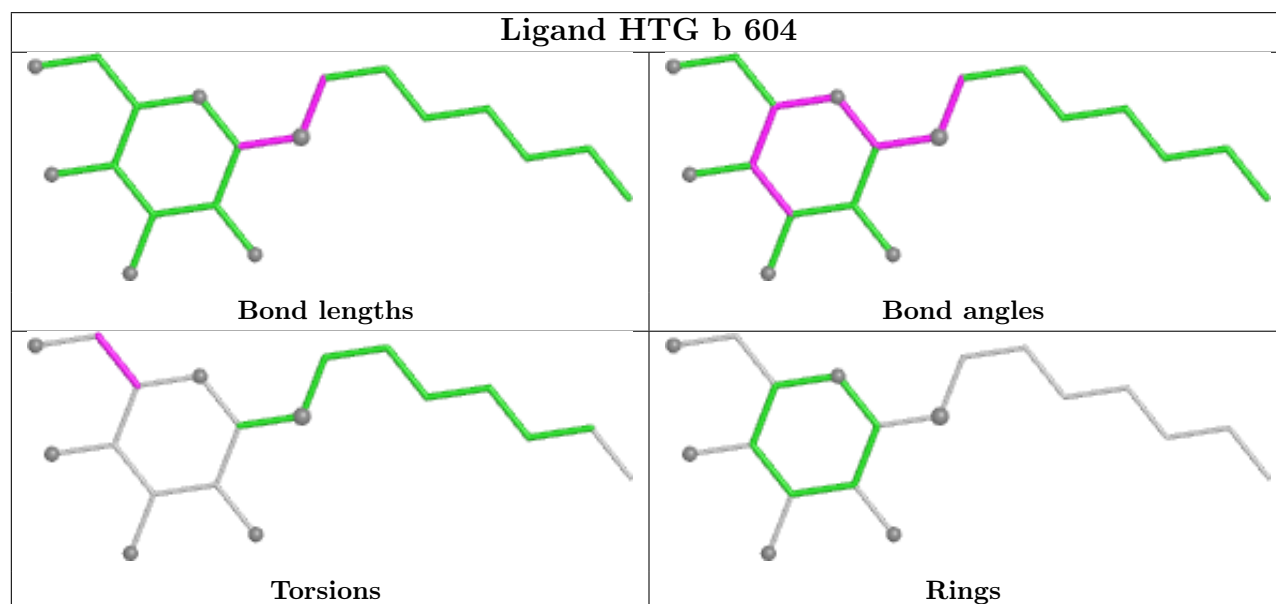
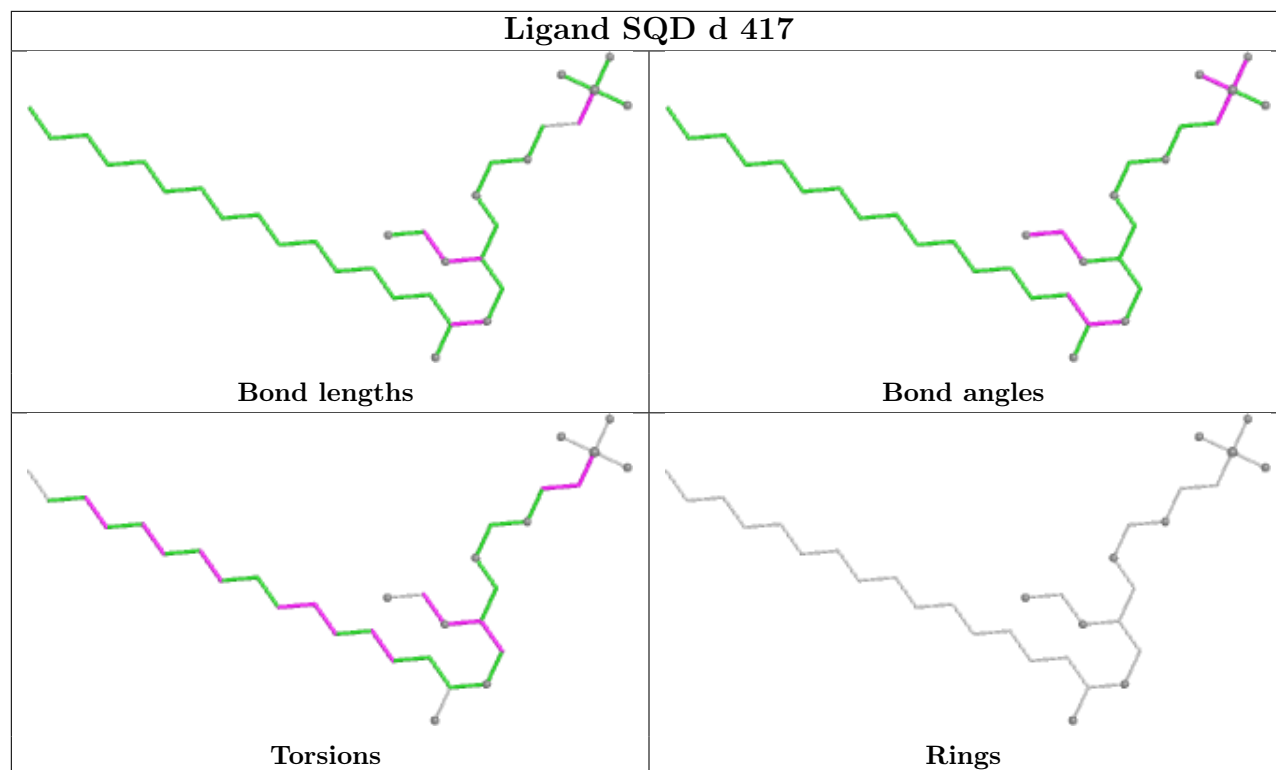
Torsions

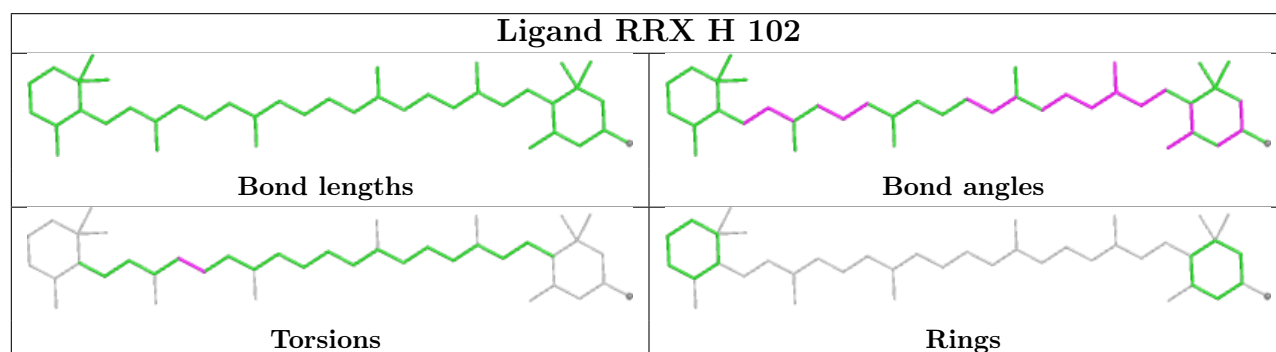
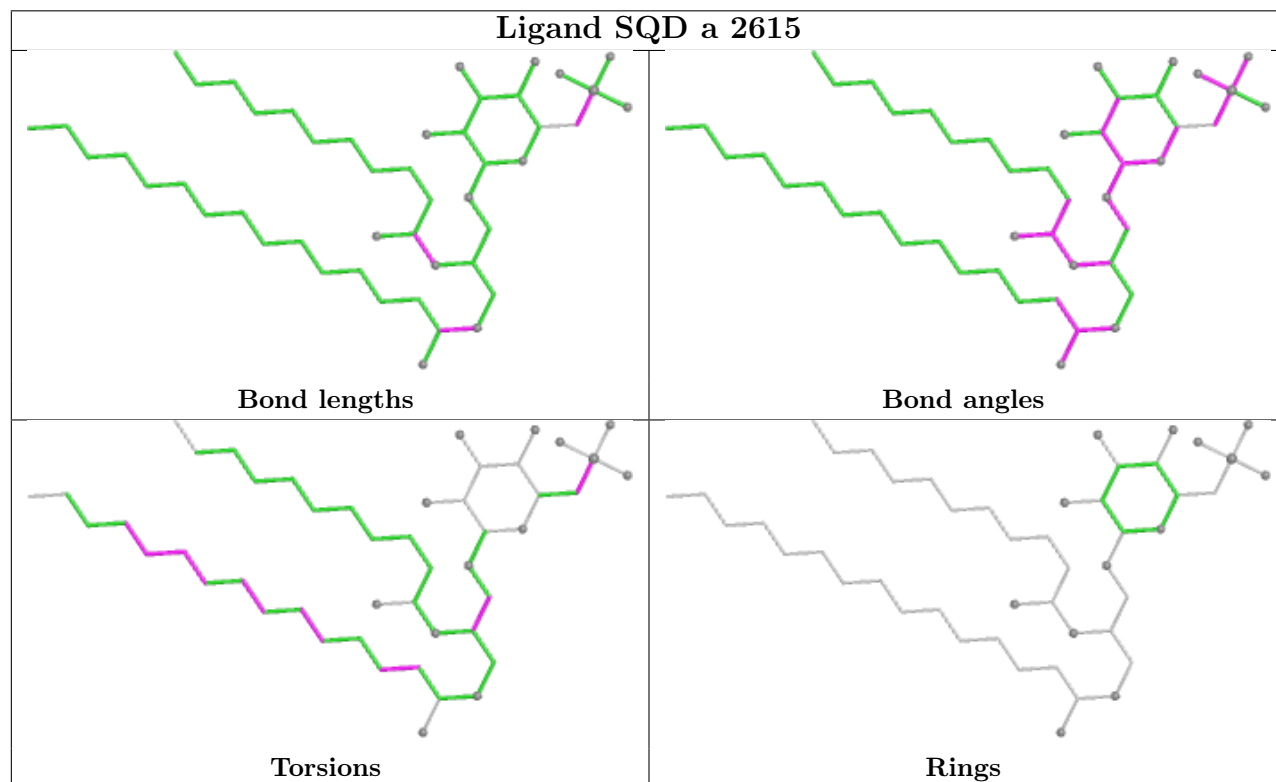
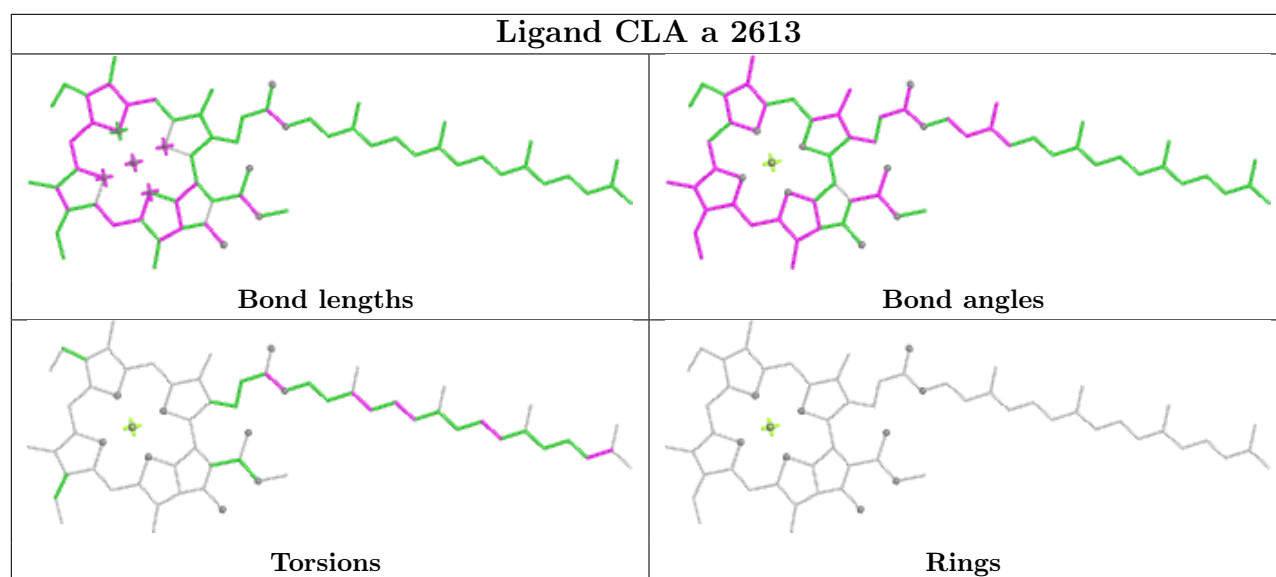


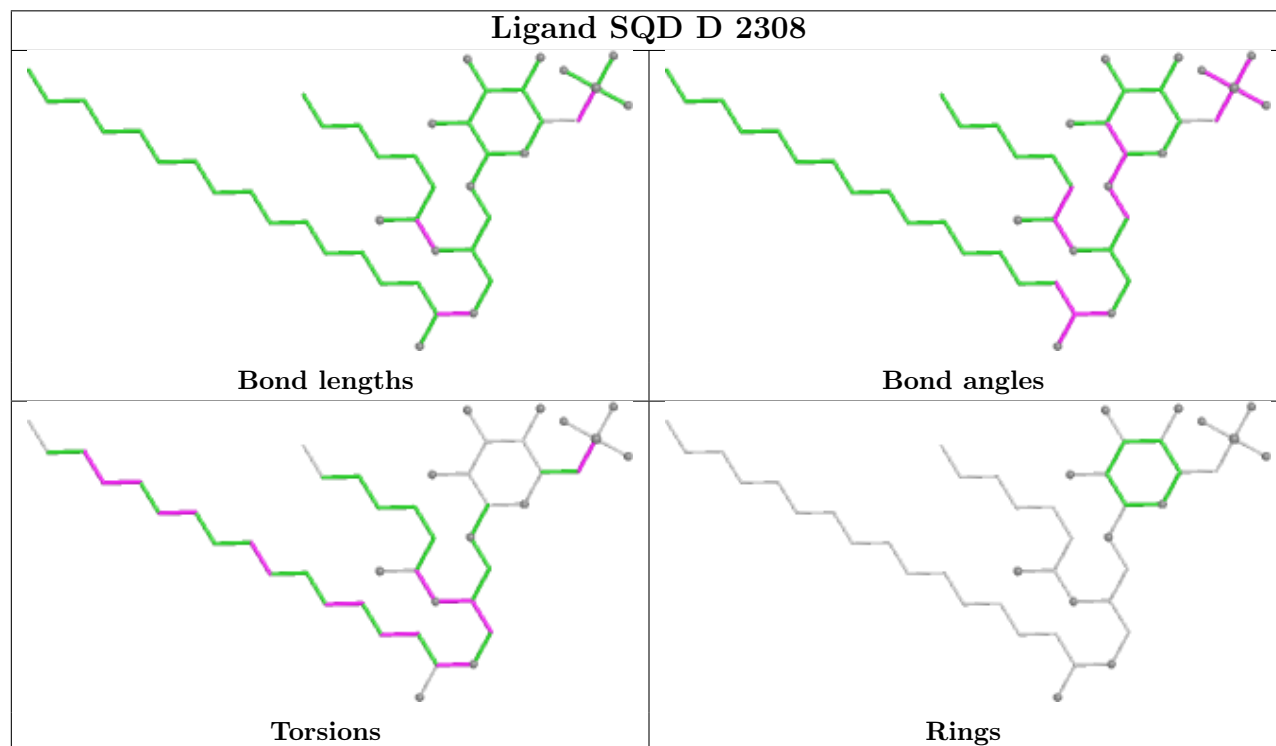
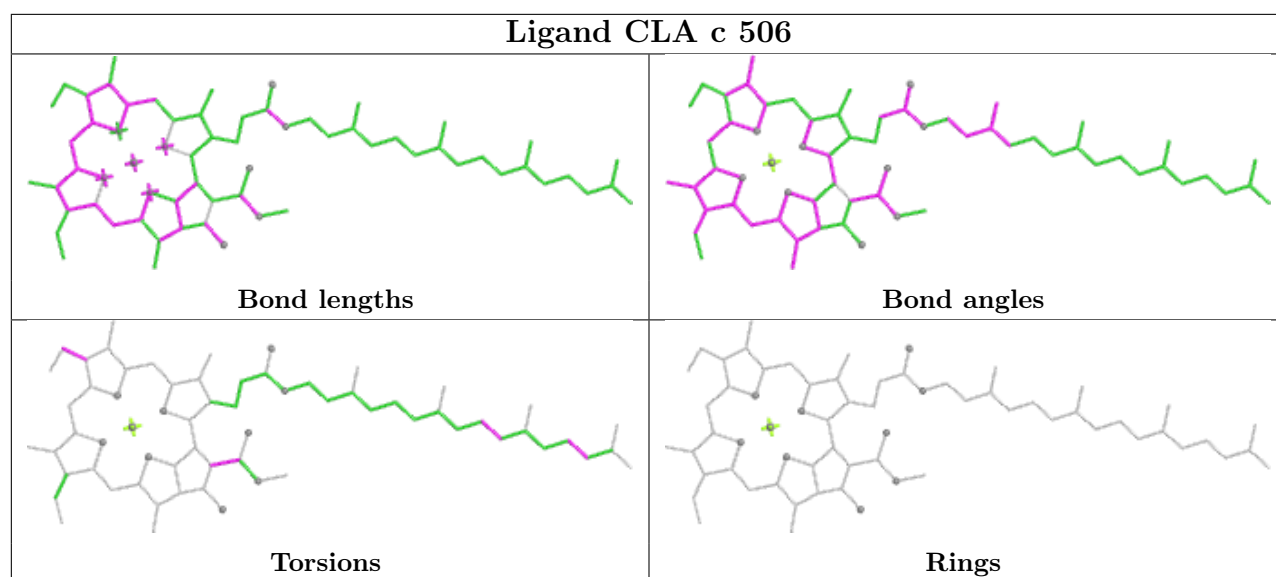
Rings

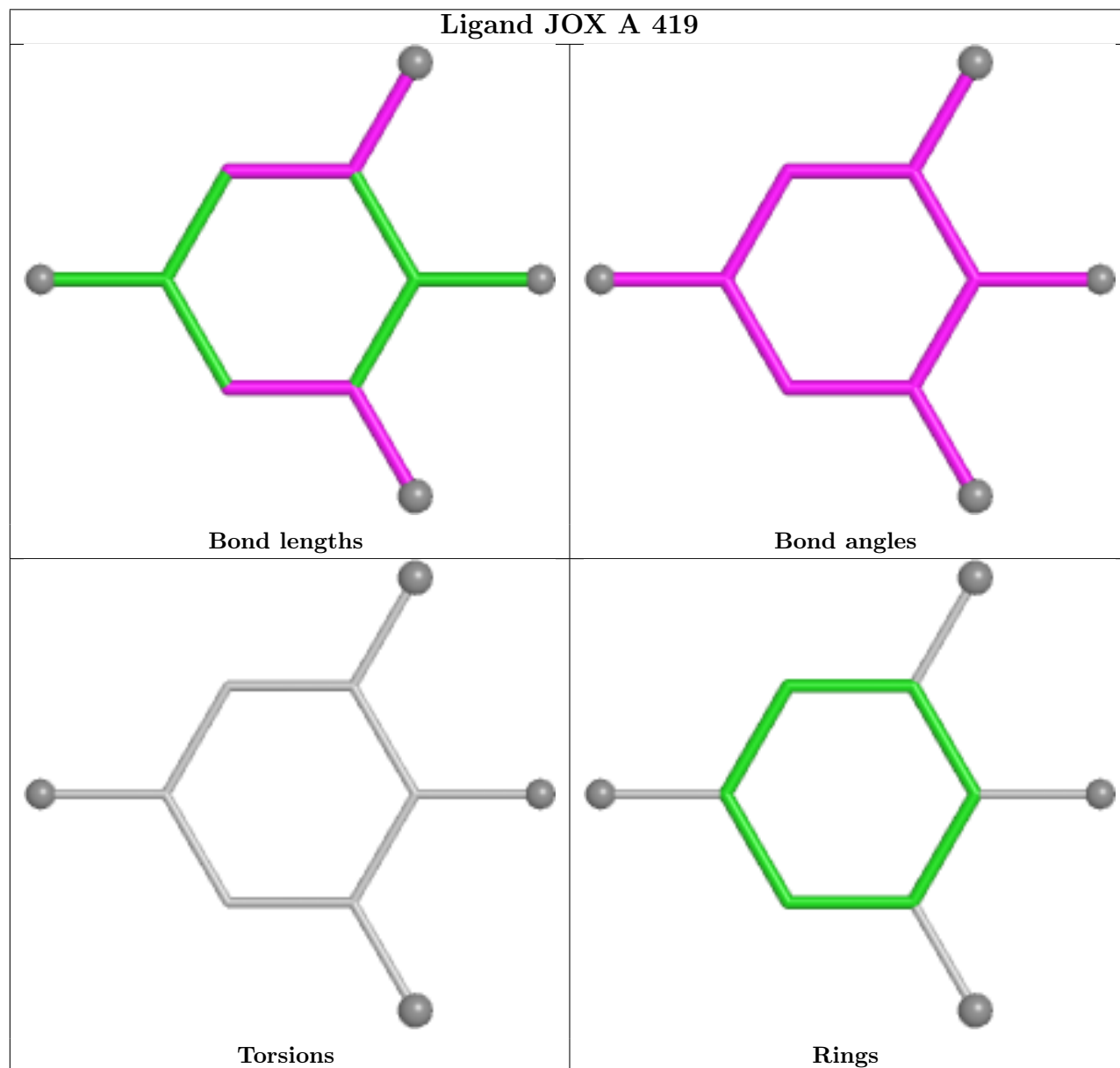
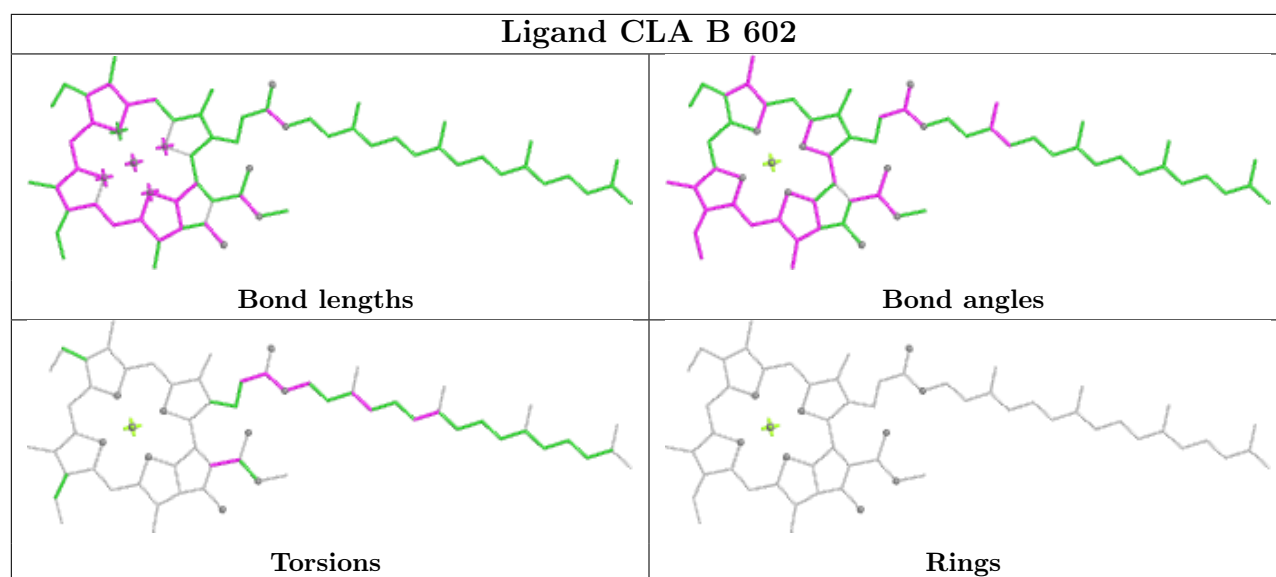




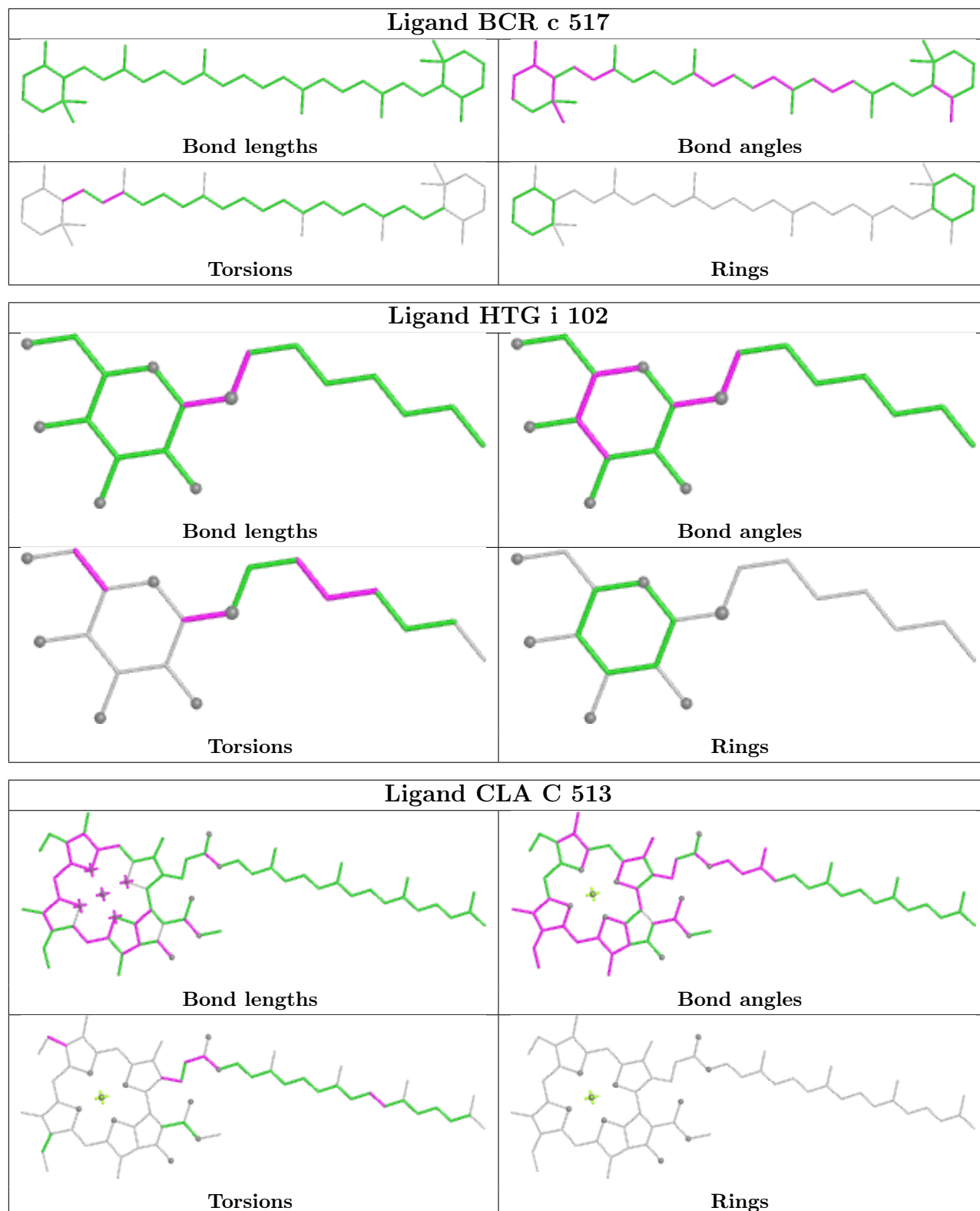


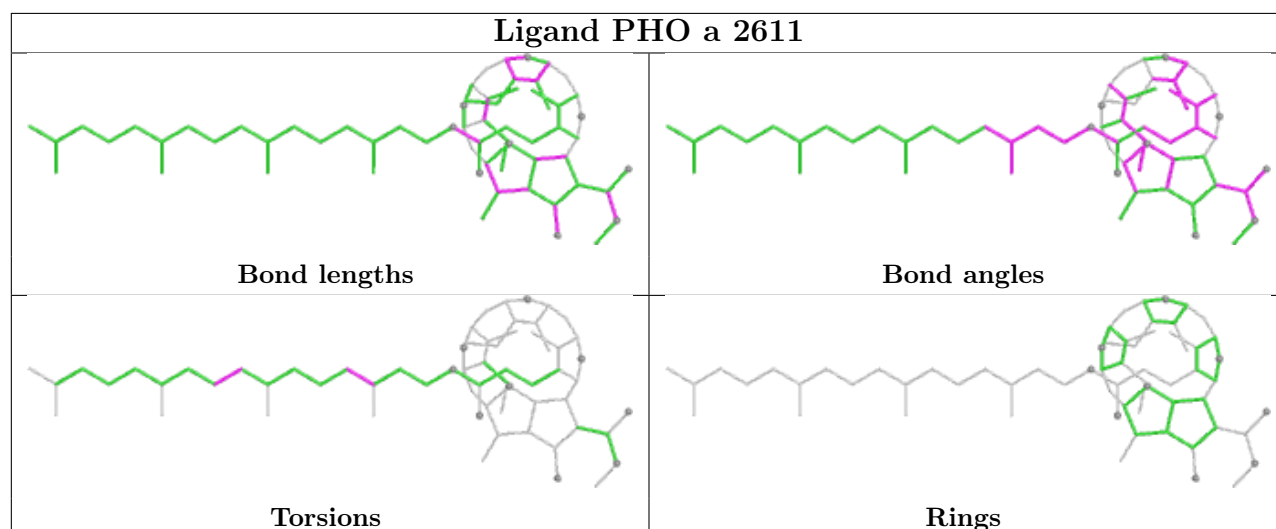
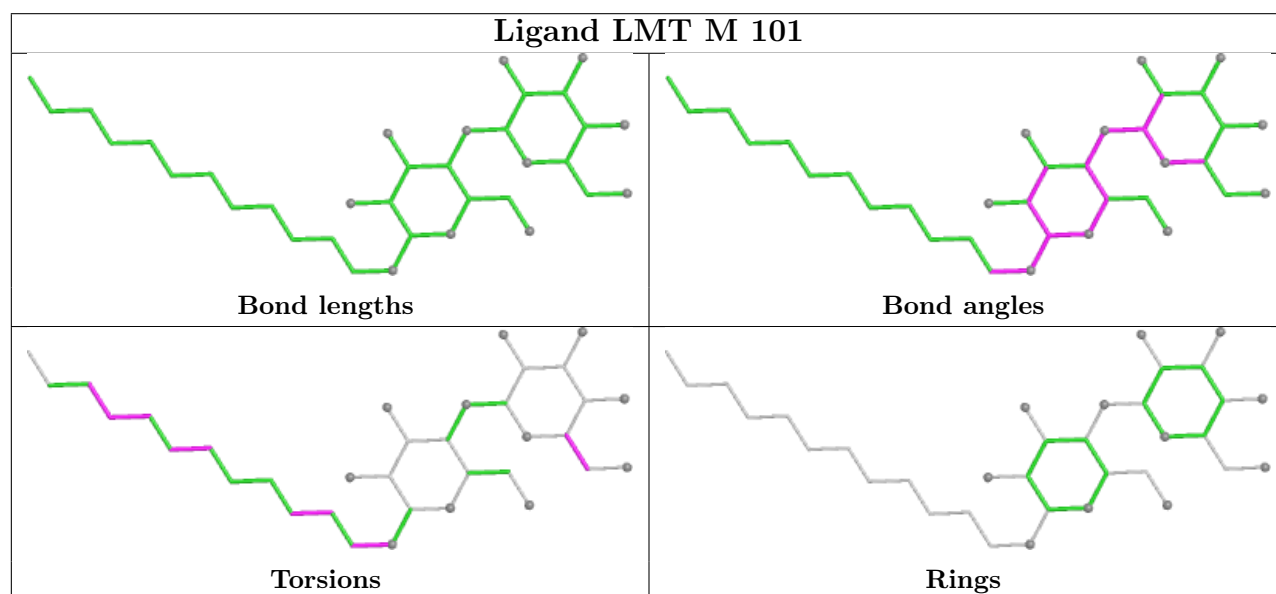
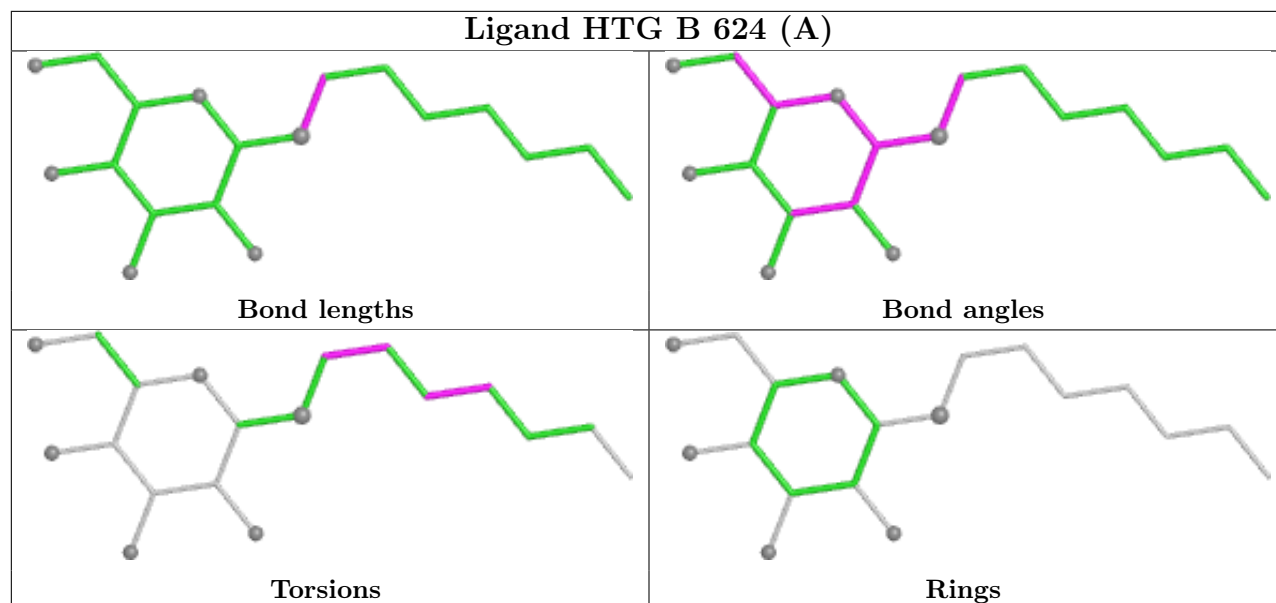


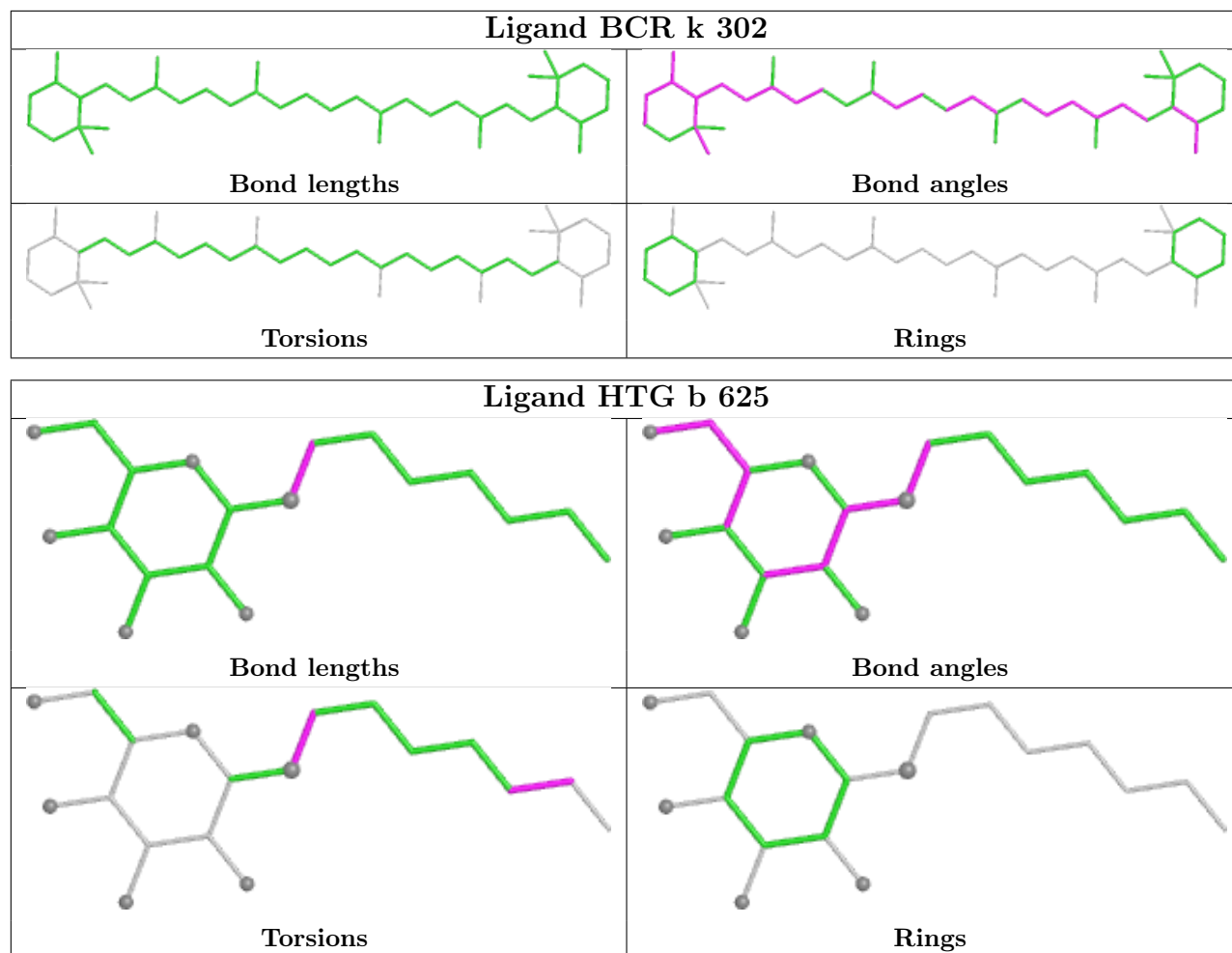


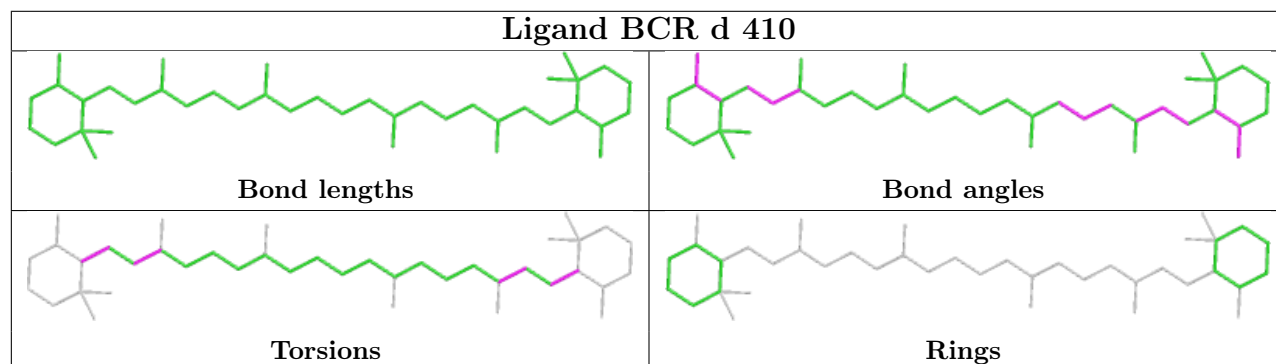
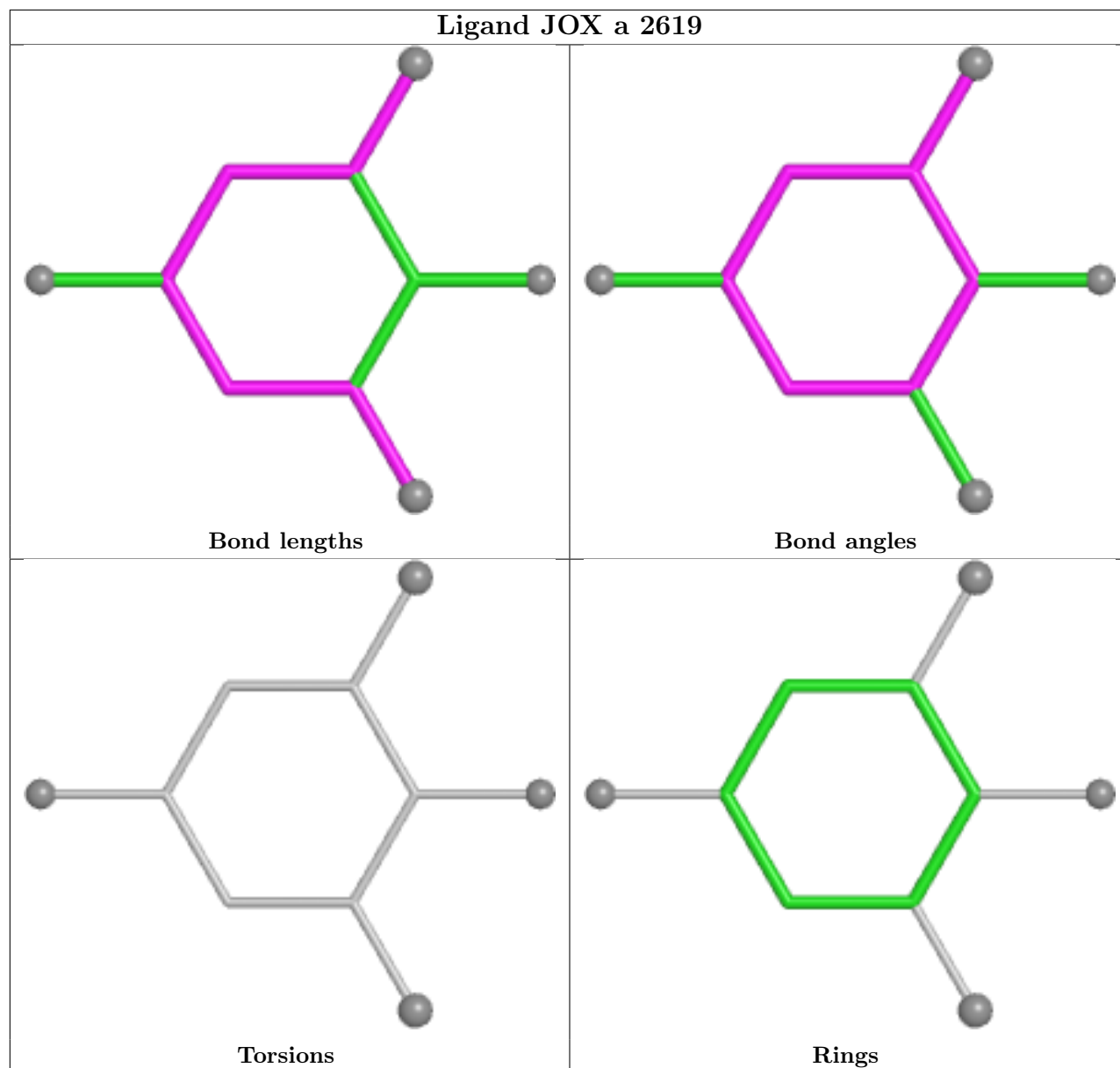


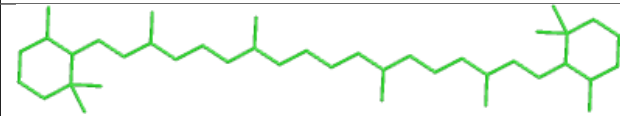
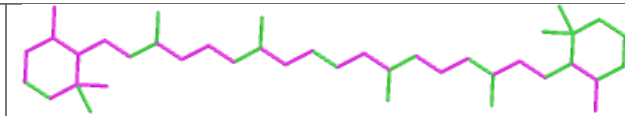
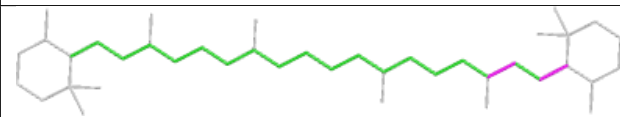
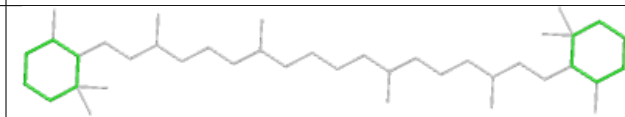


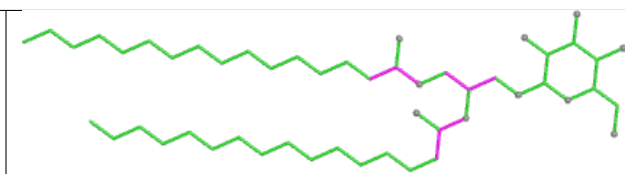
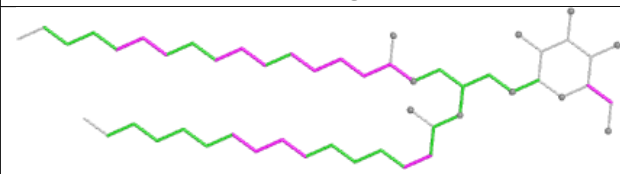
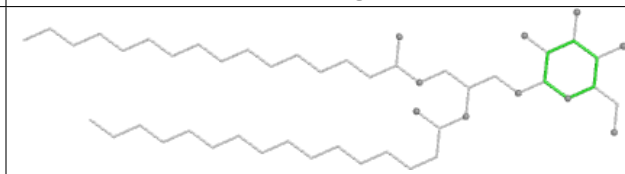


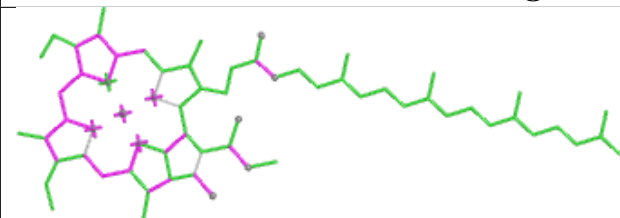
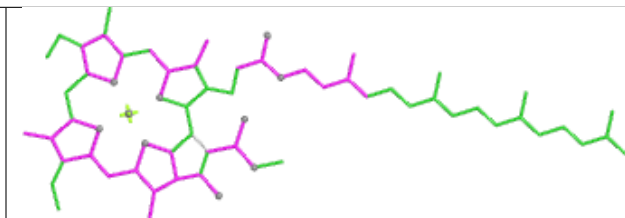
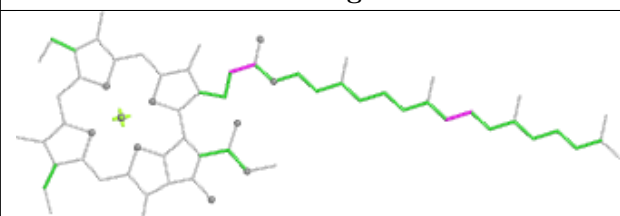
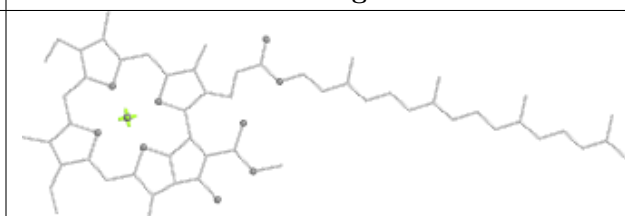


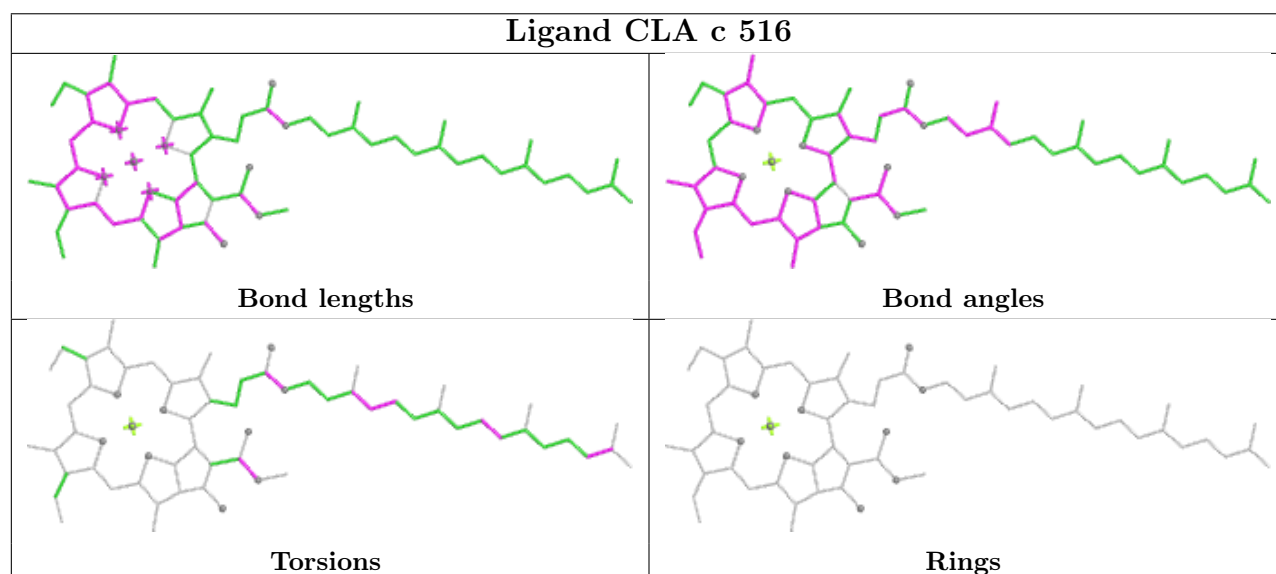
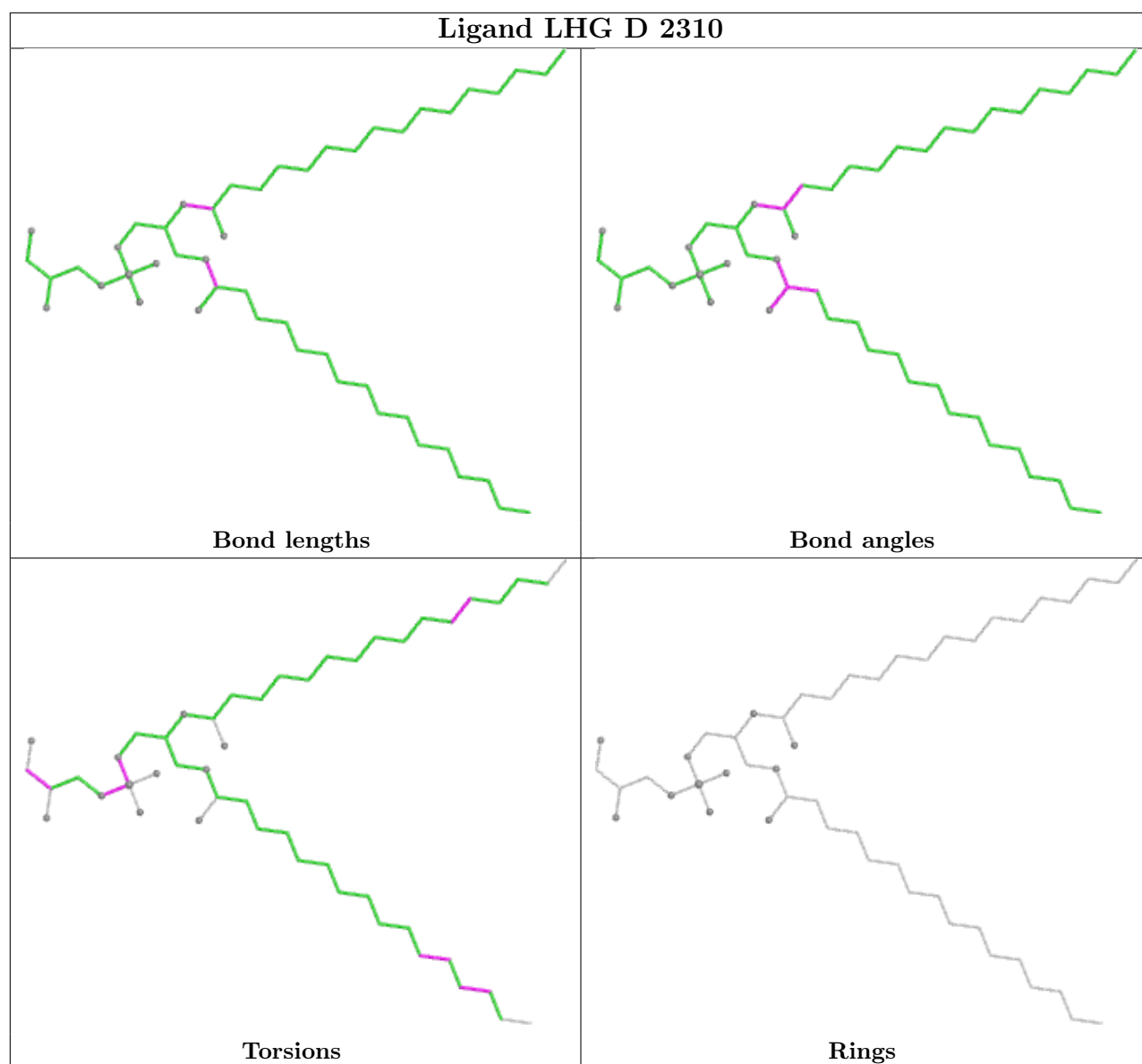


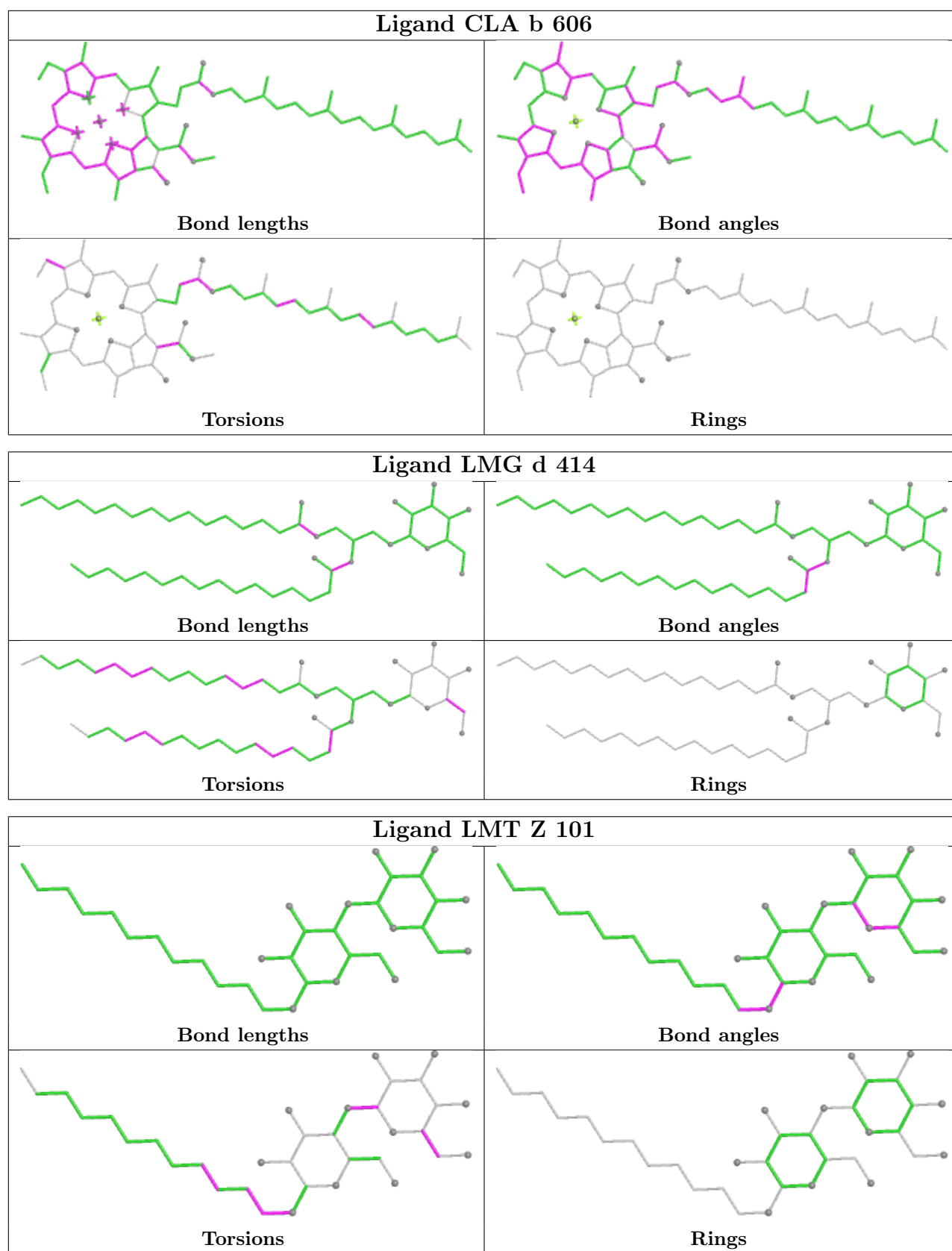


| Ligand BCR b 624                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

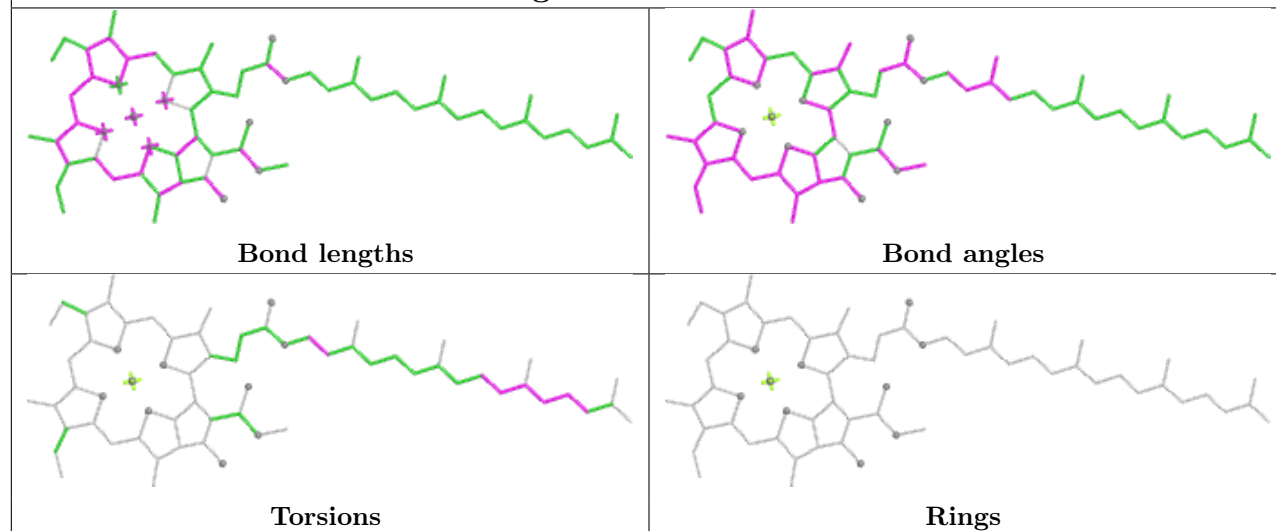
| Ligand LMG B 622                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|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

| Ligand CLA b 617                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

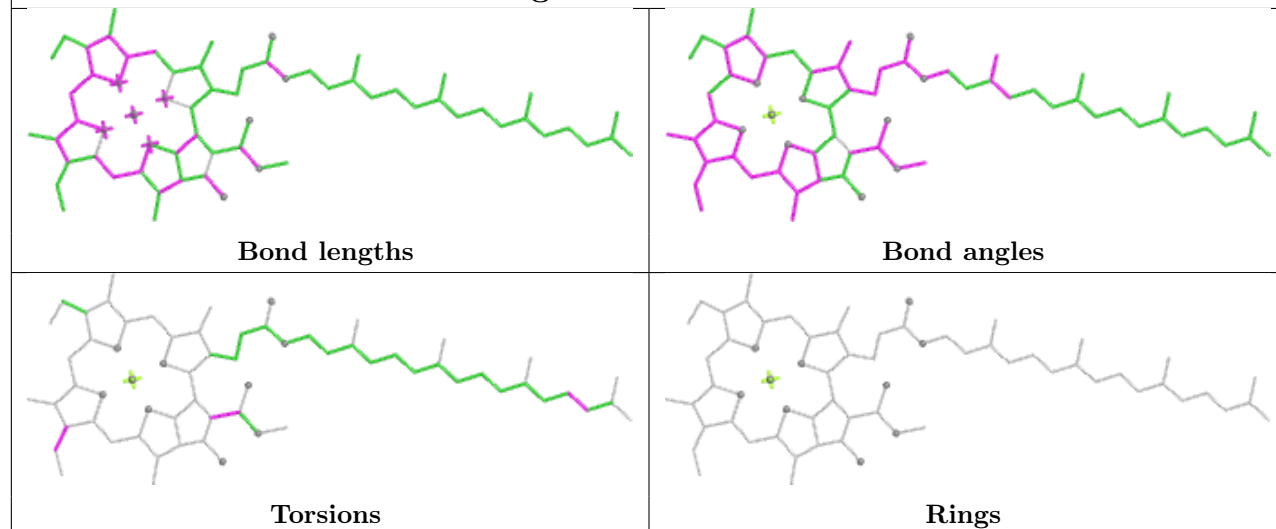




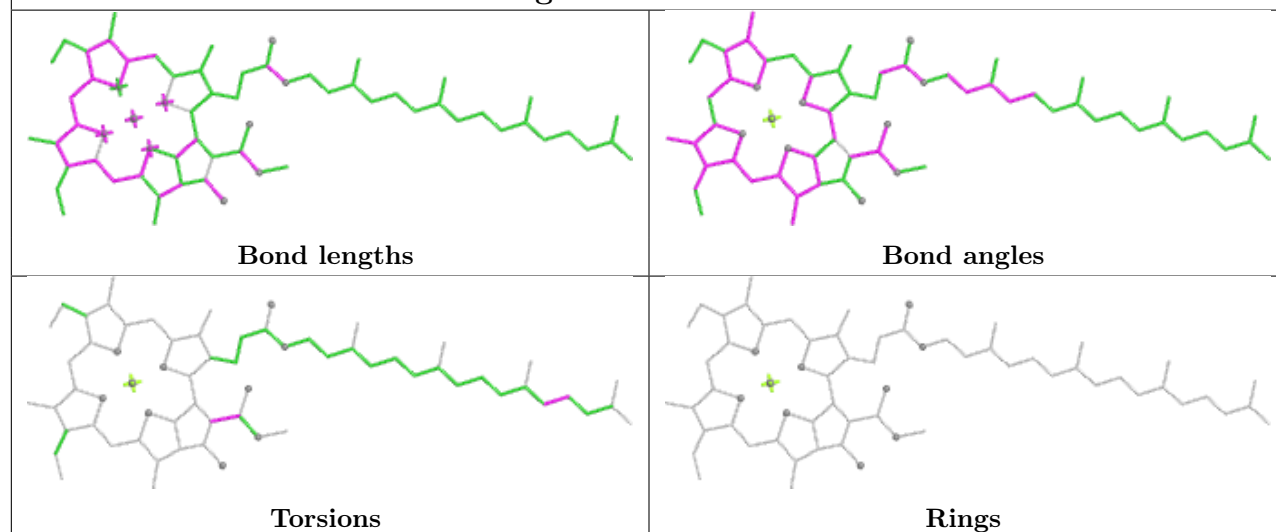
## Ligand CLA B 614



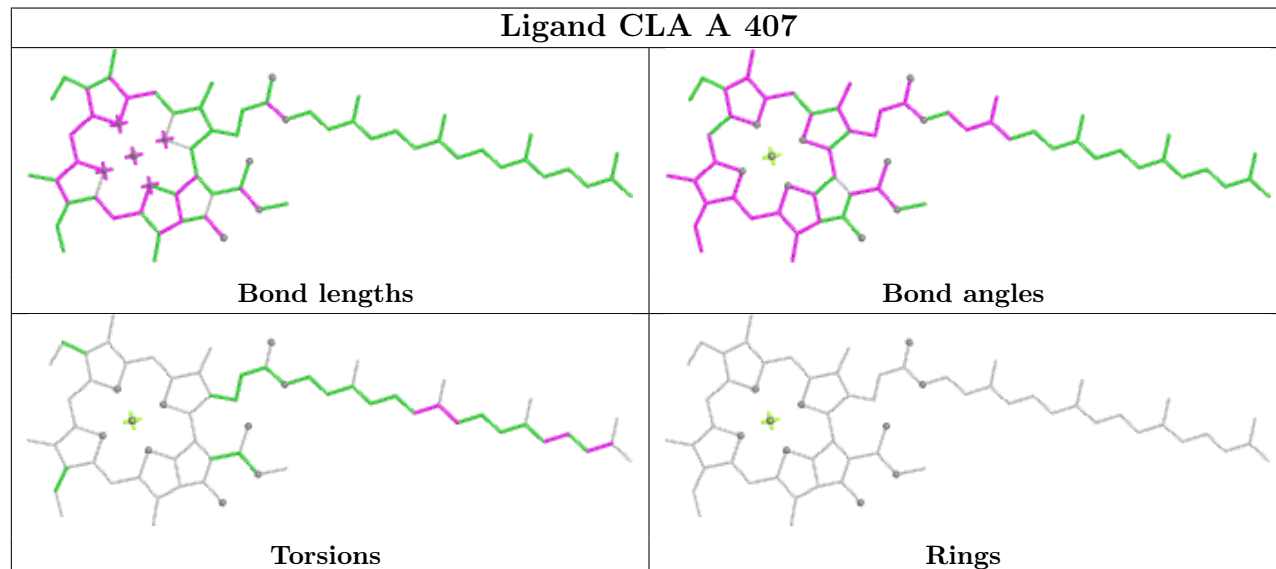
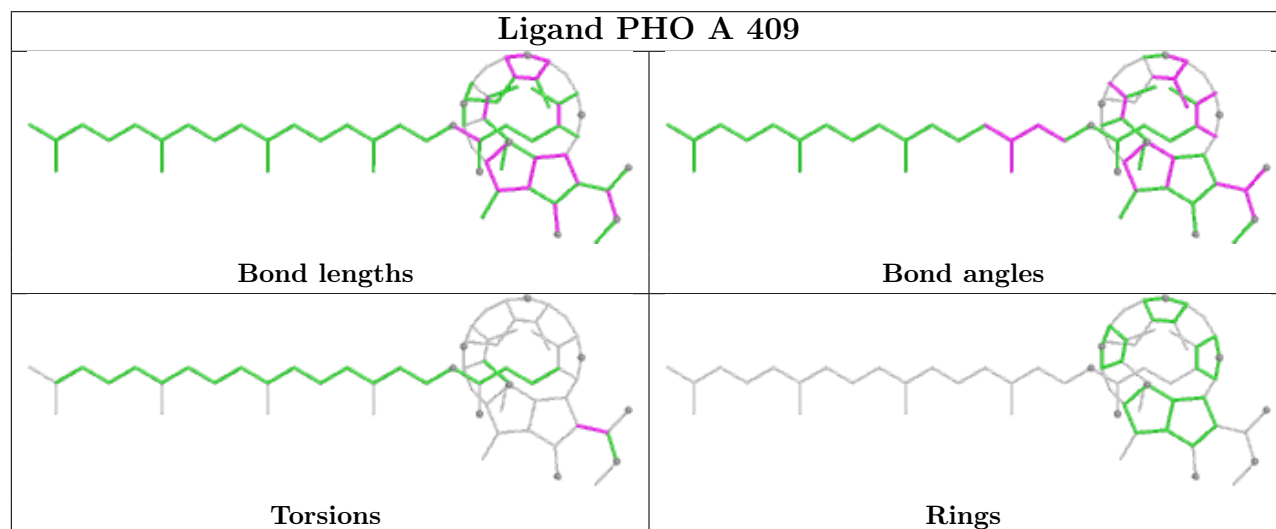
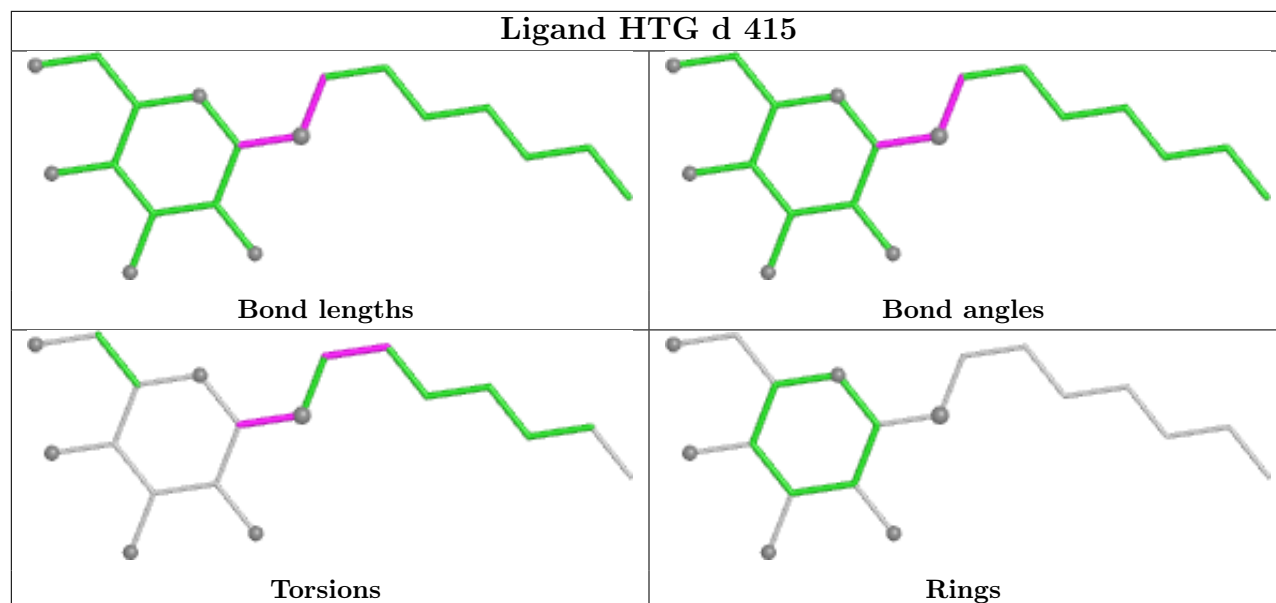
## Ligand CLA A 406



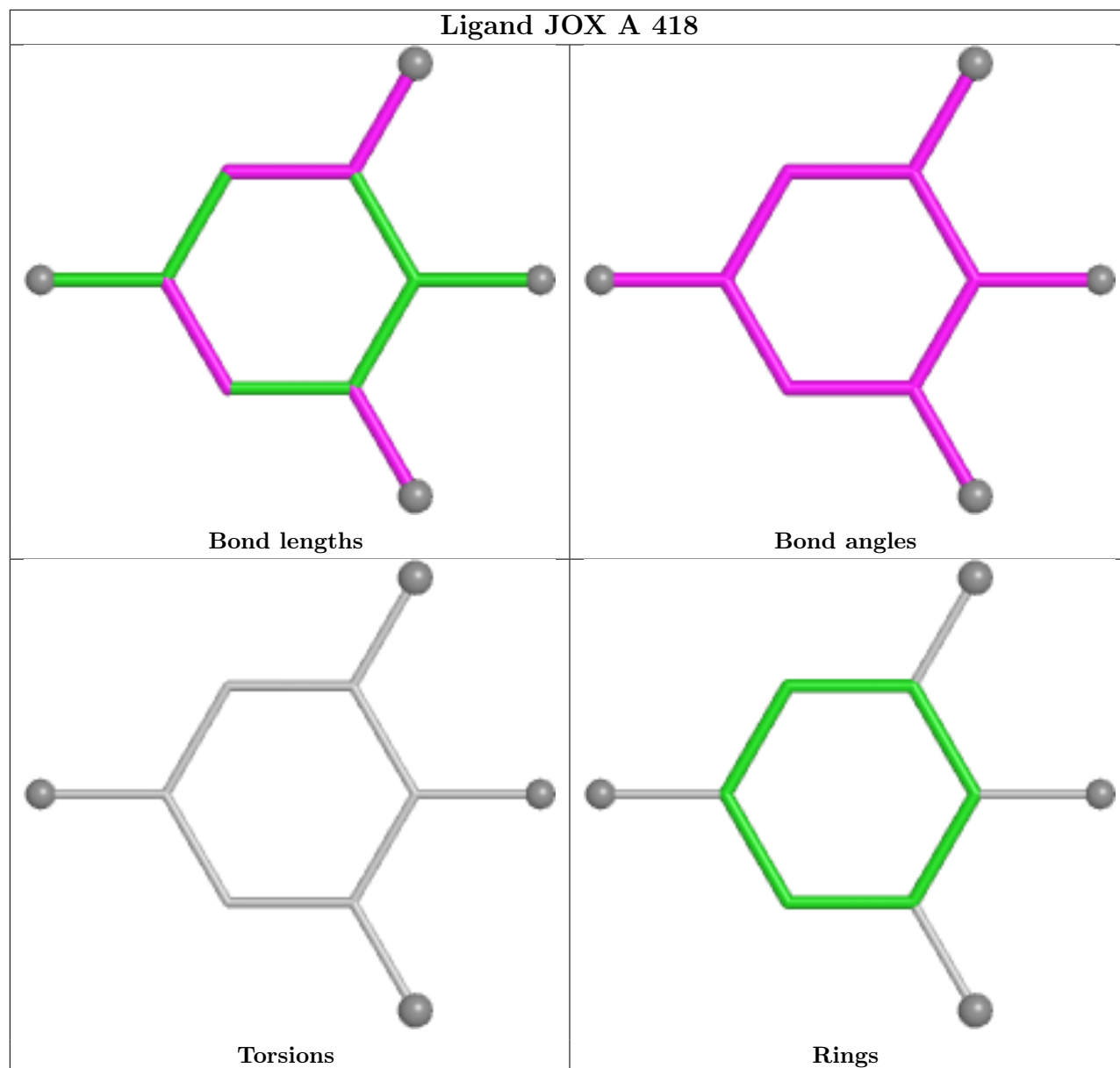
## Ligand CLA b 609



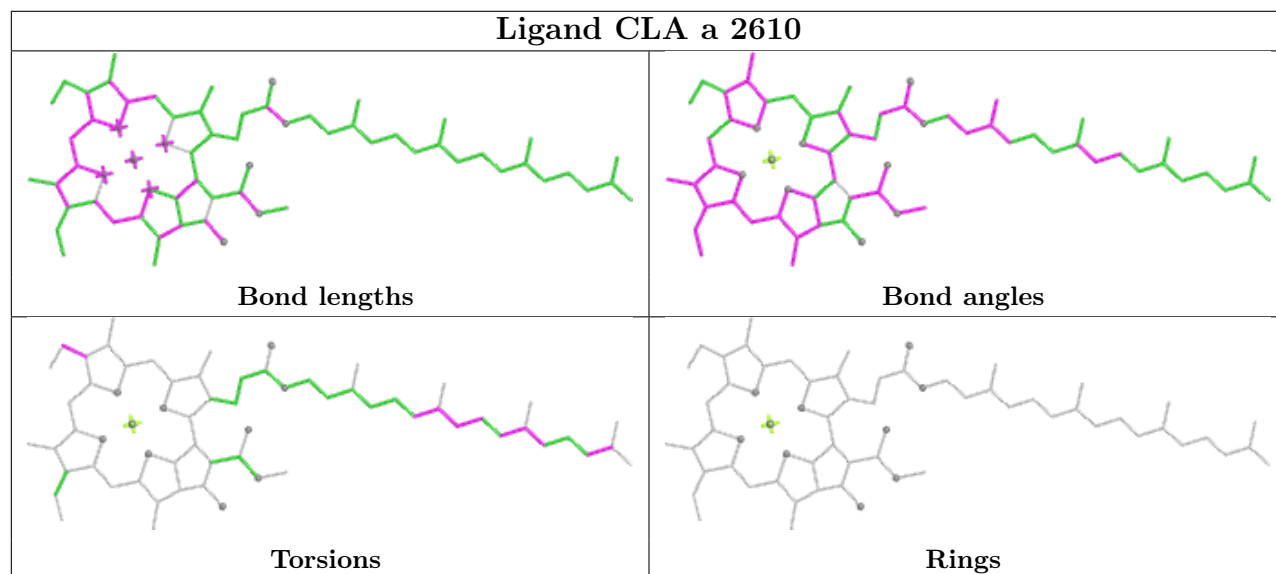


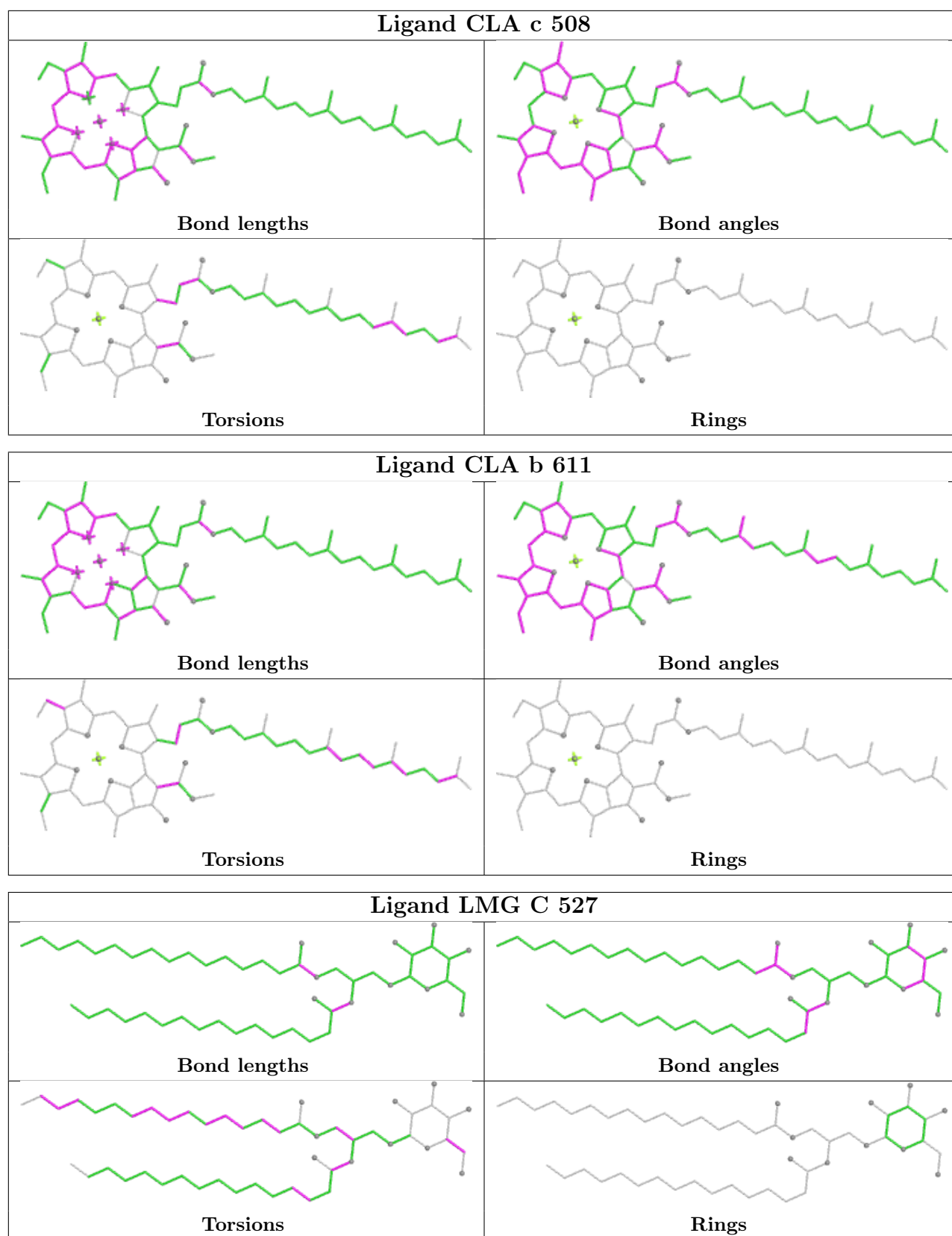


## Ligand JOX A 418

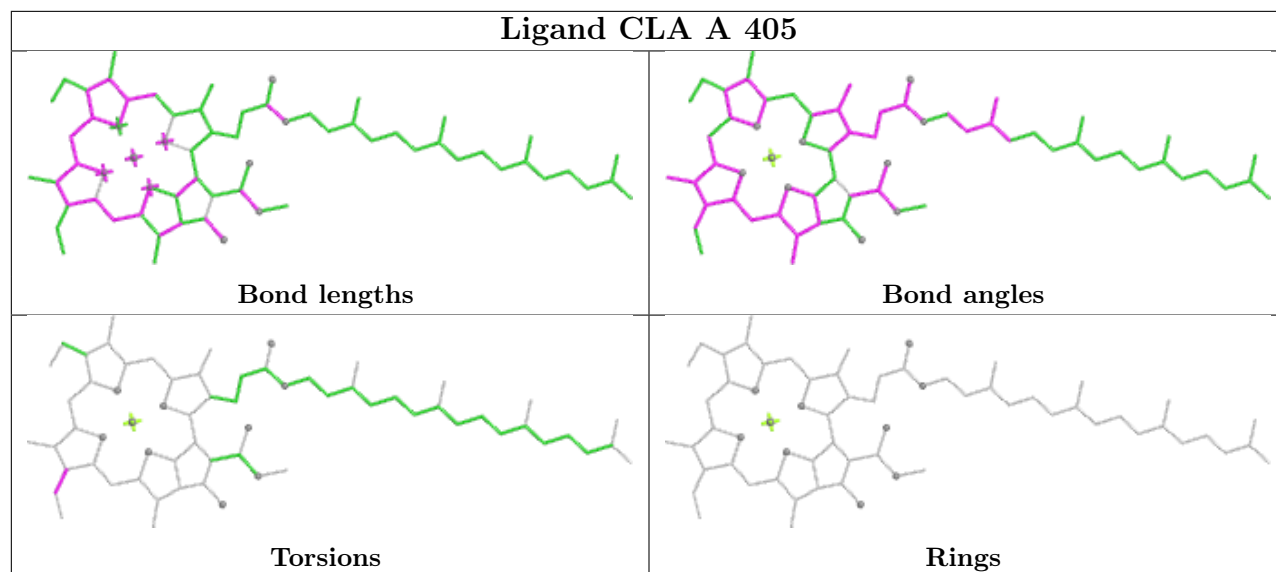


## Ligand CLA a 2610

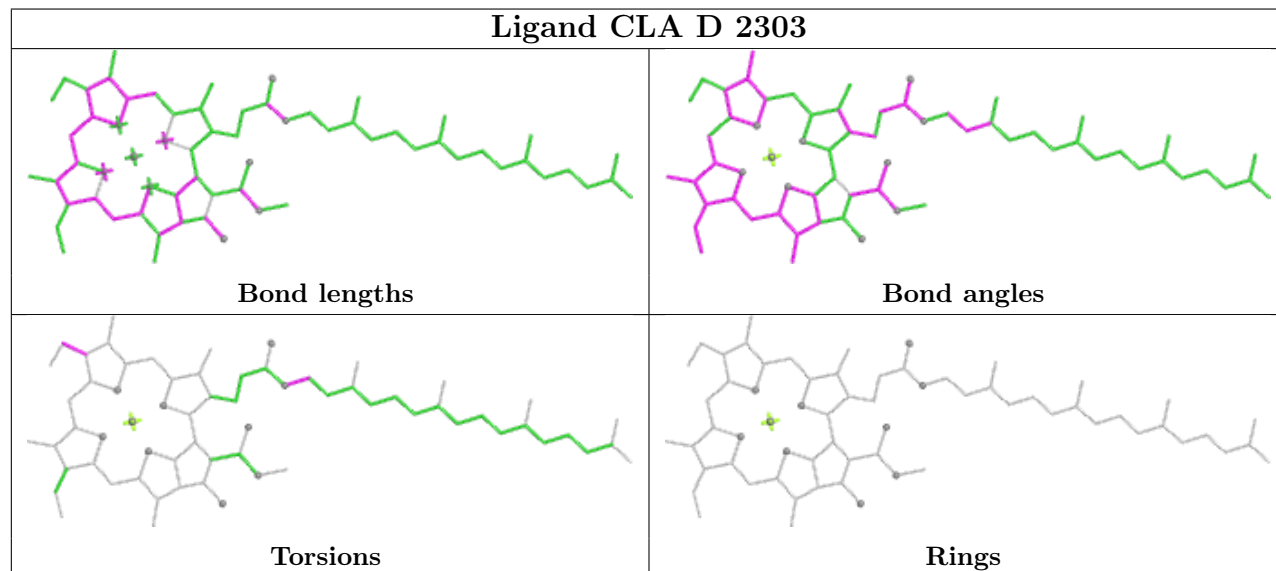




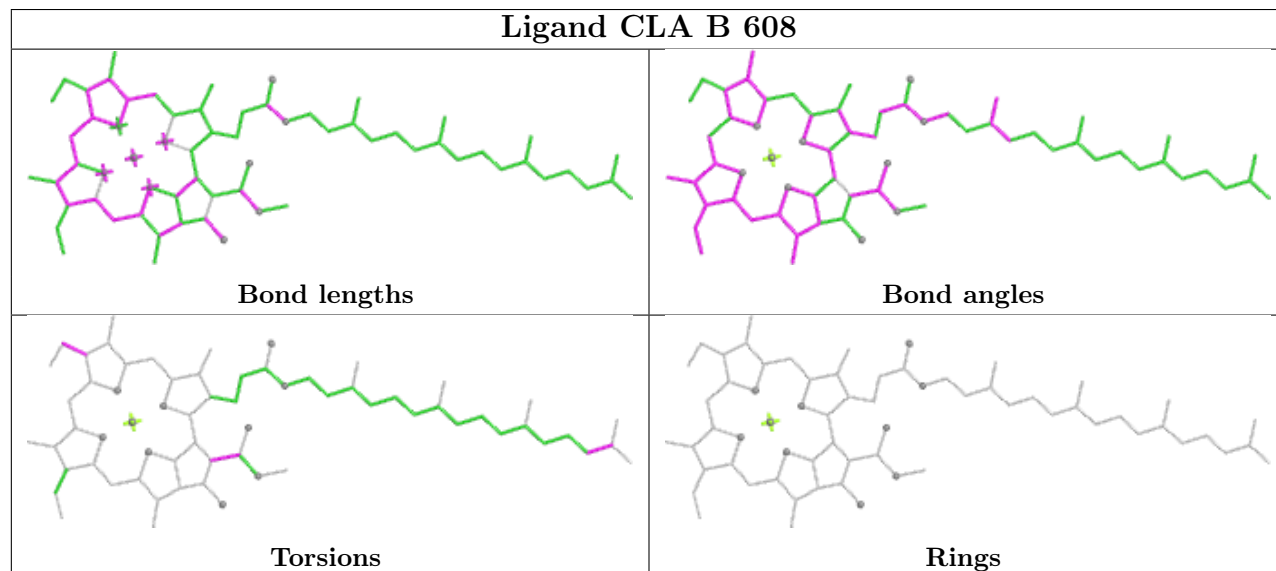
## Ligand CLA A 405



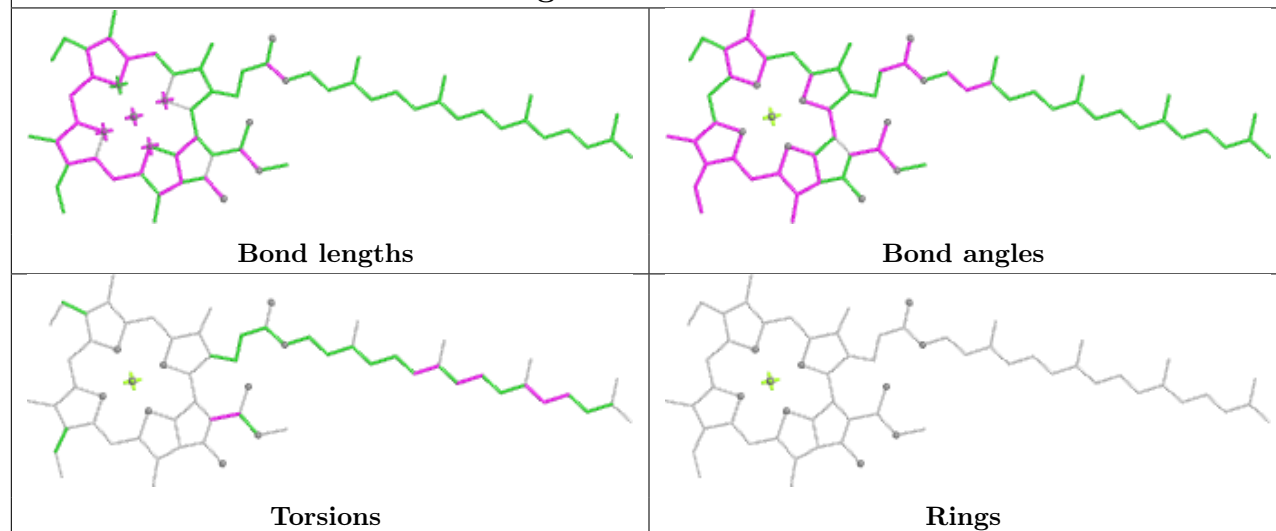
## Ligand CLA D 2303



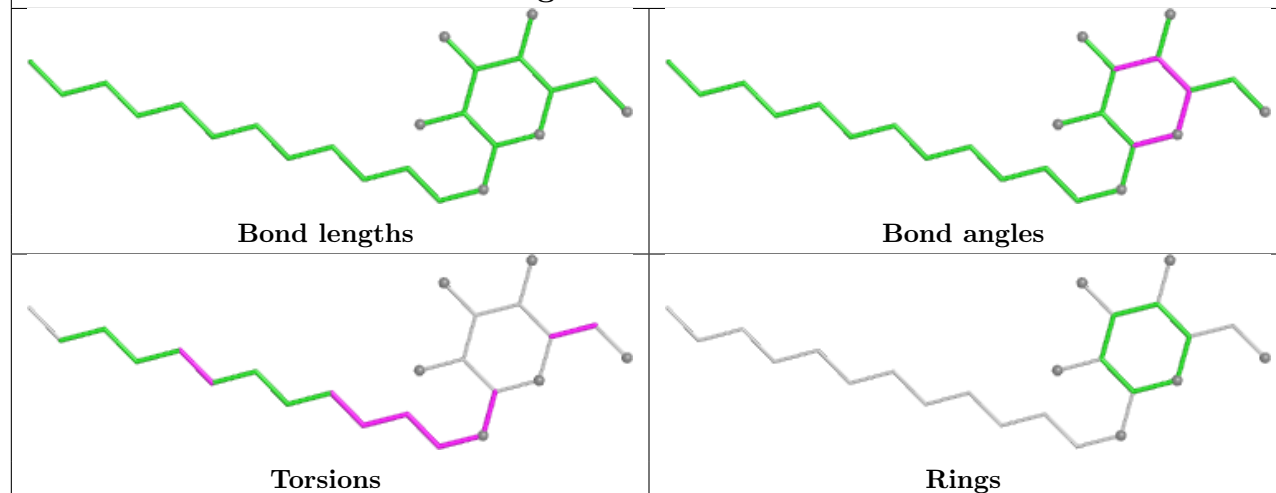
## Ligand CLA B 608



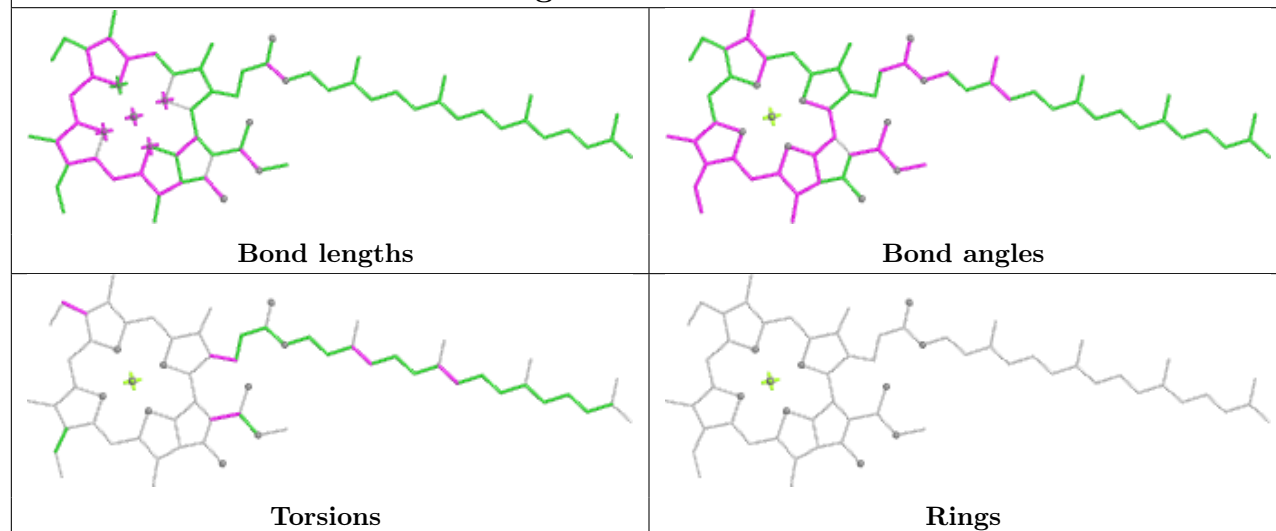
## Ligand CLA c 512

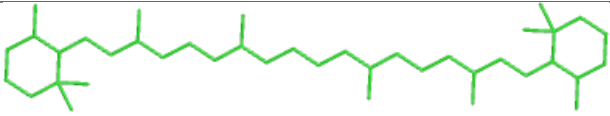
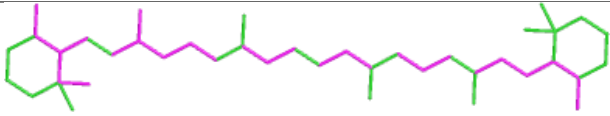
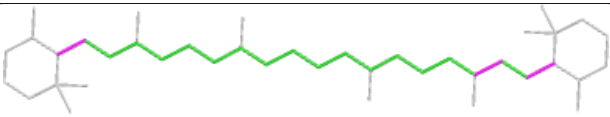
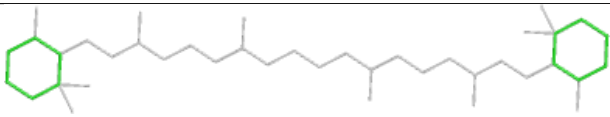
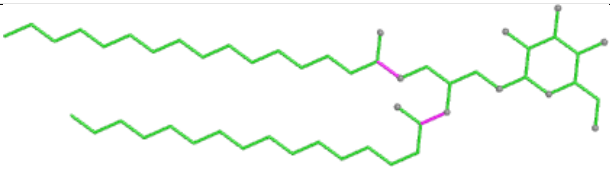
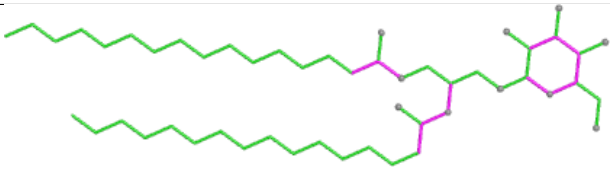
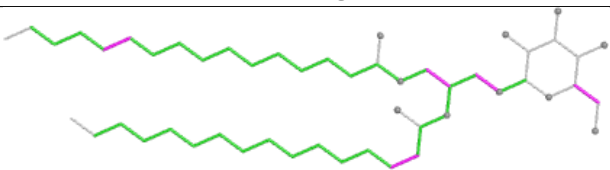
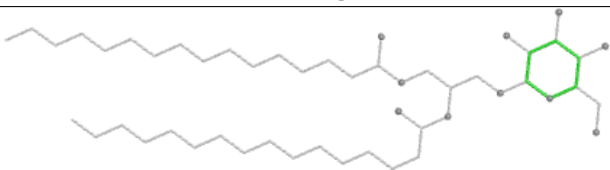
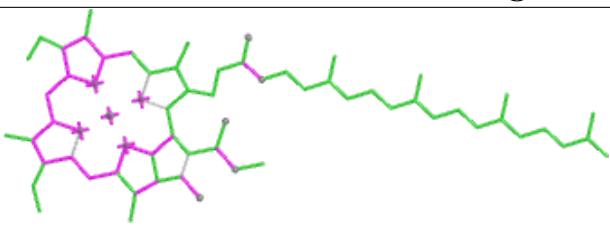
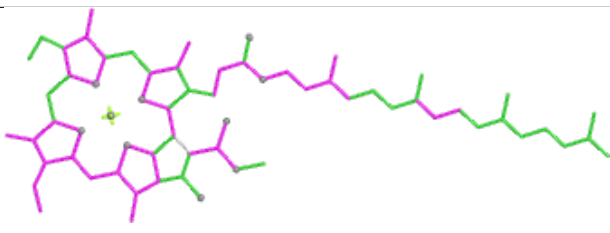
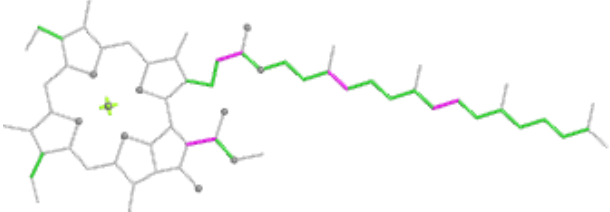
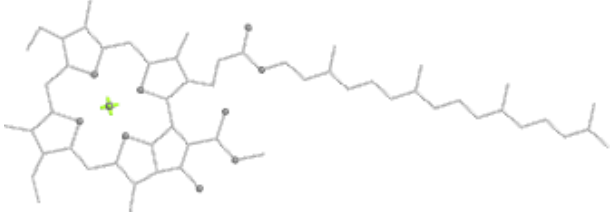


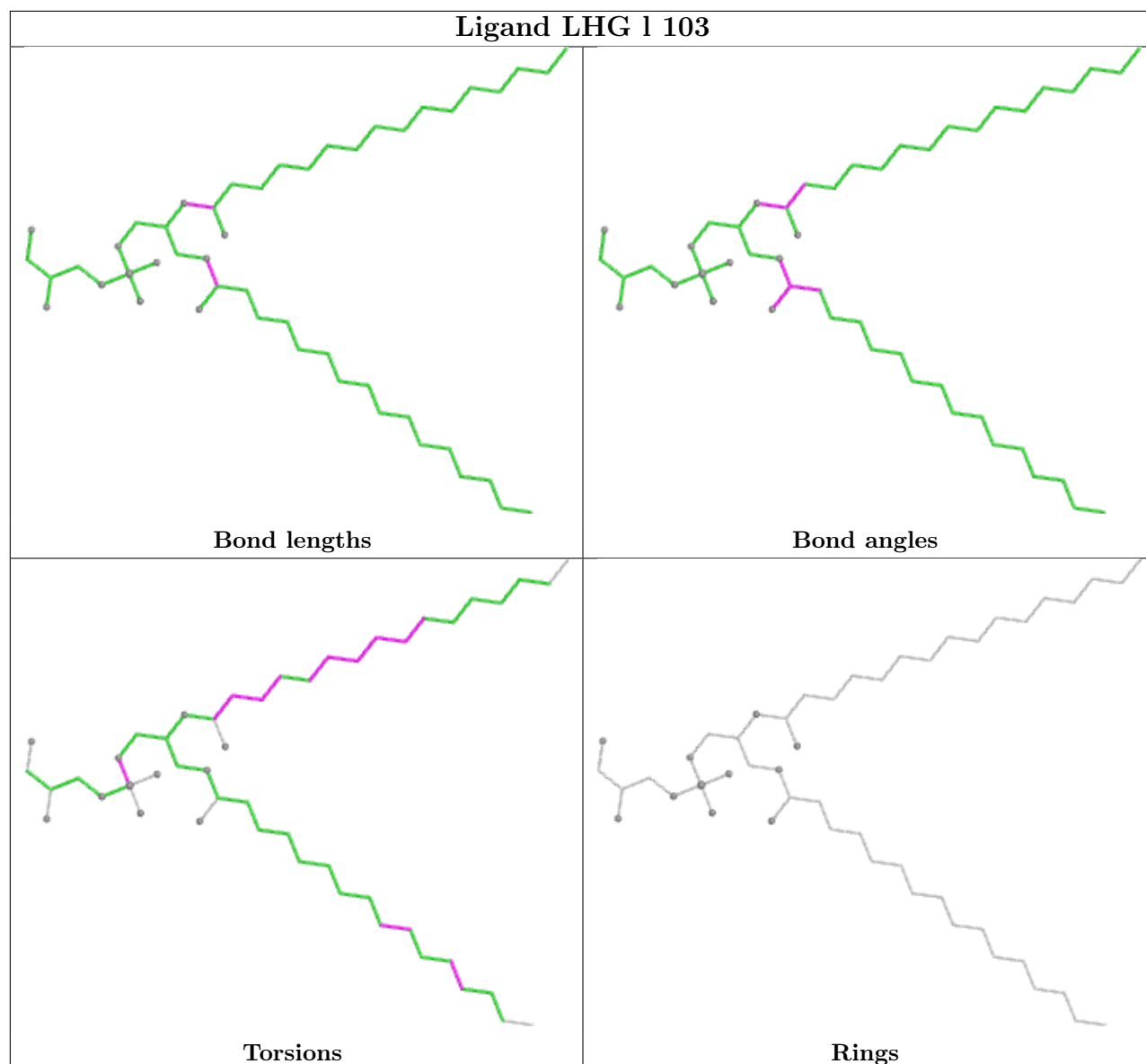
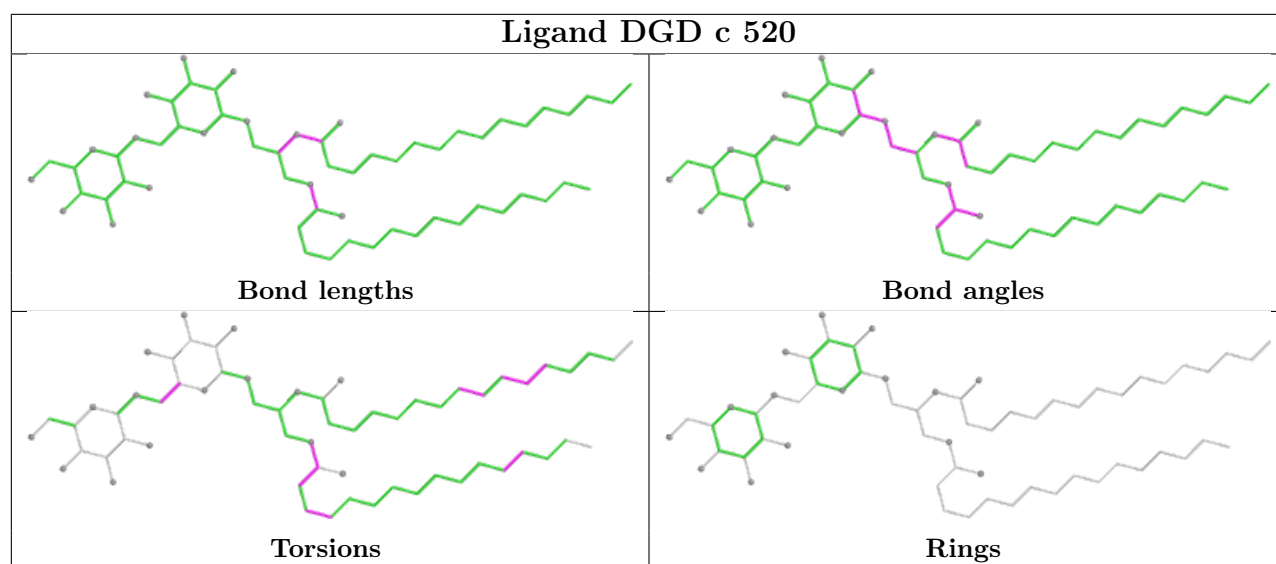
## Ligand LMT i 103

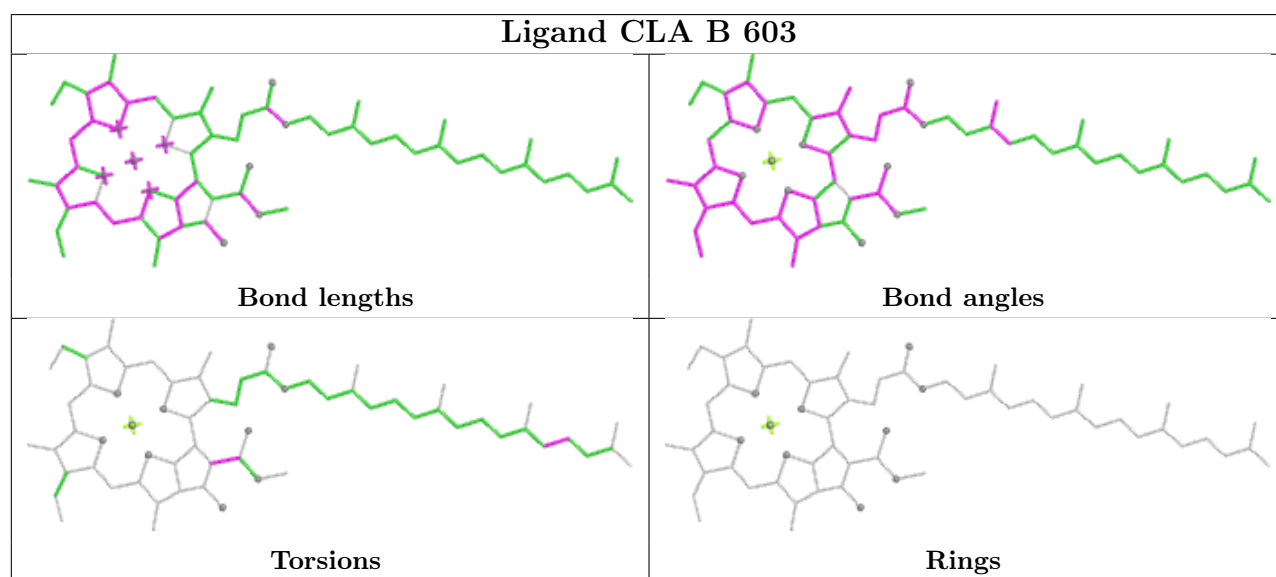
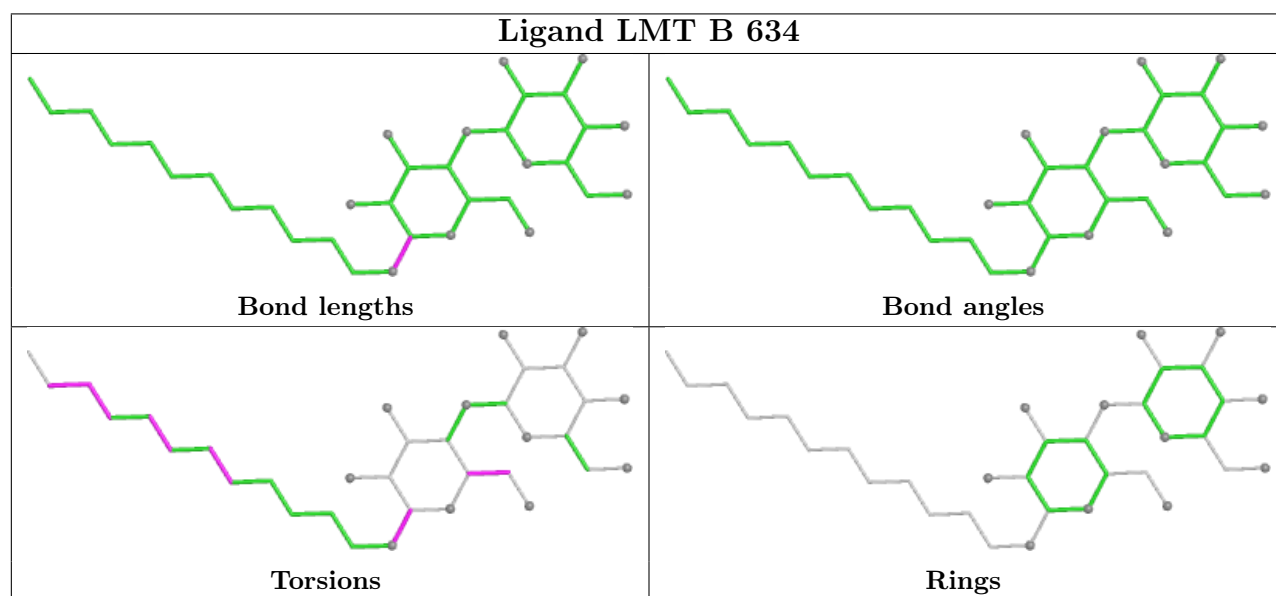
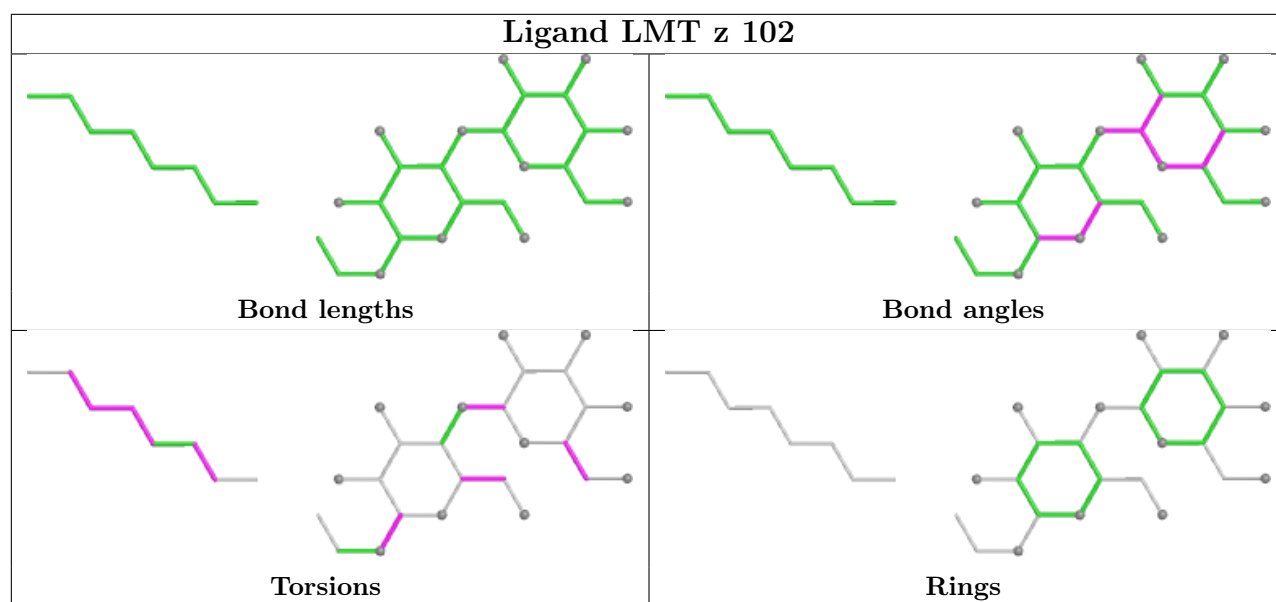


## Ligand CLA b 614

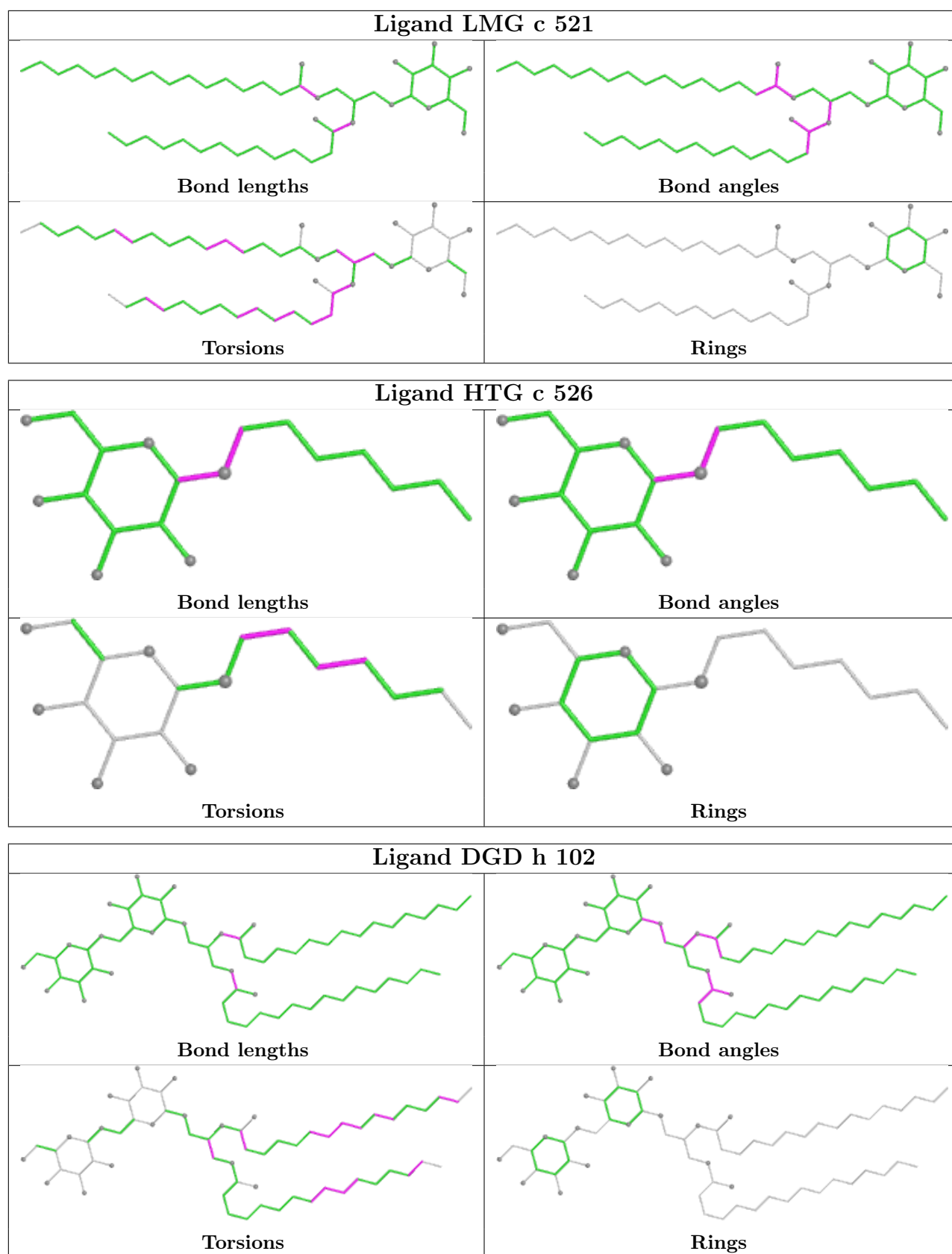


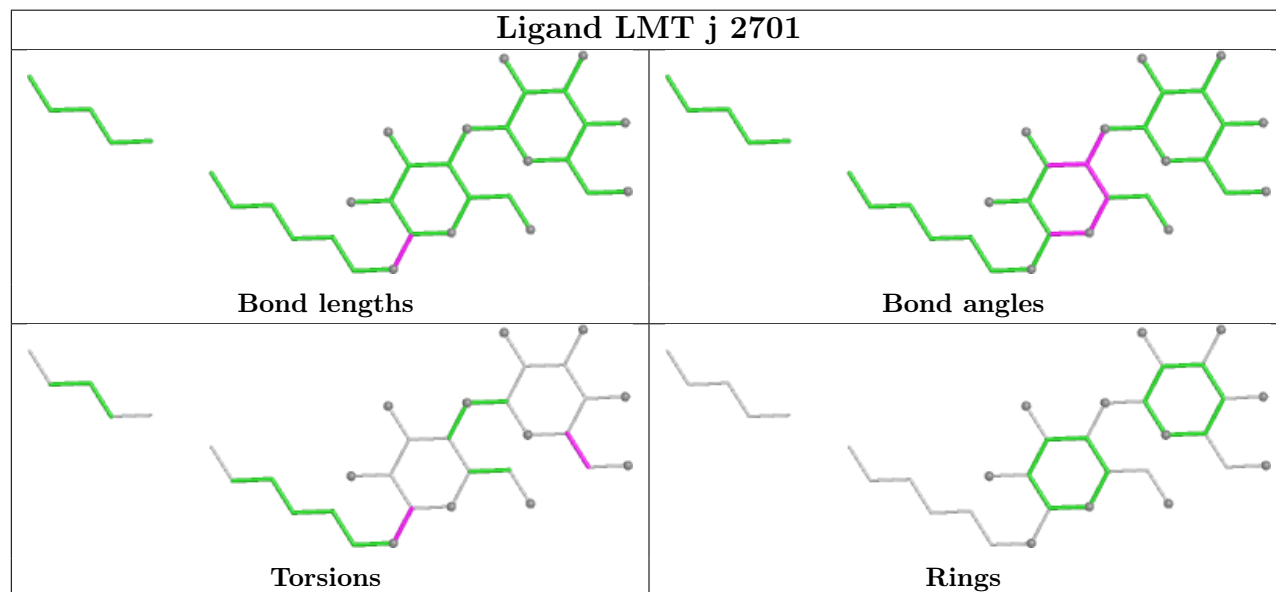
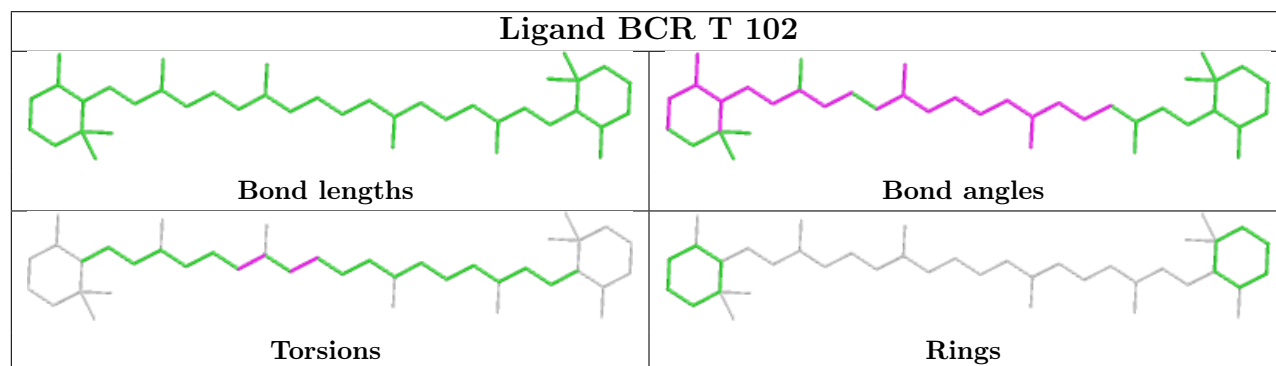
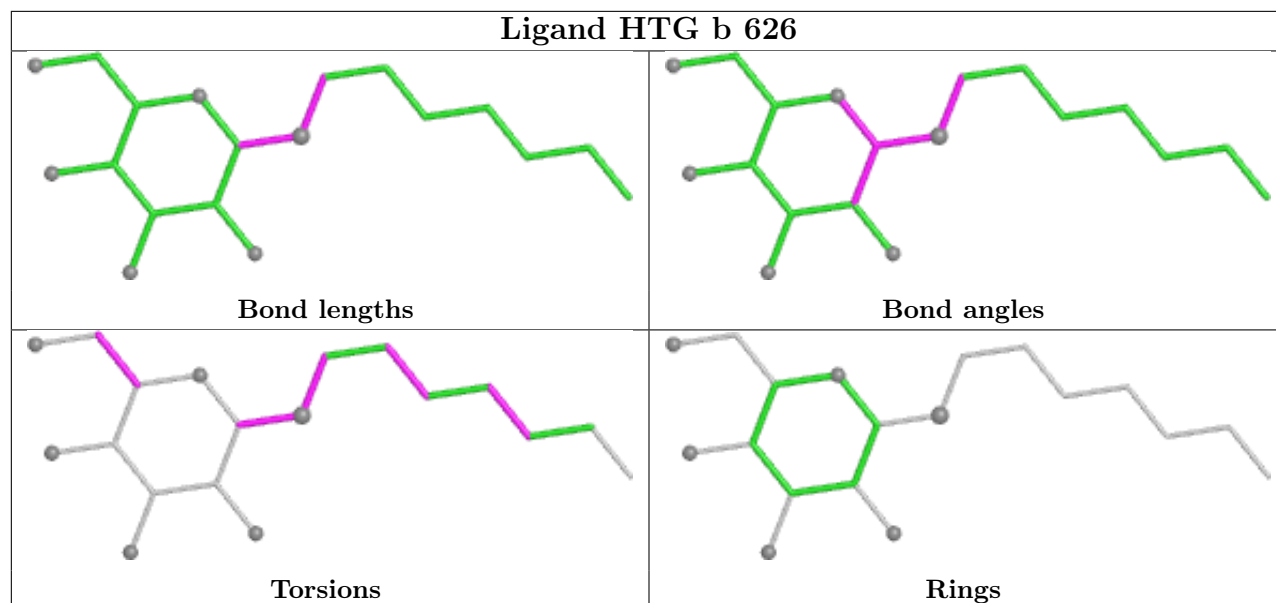
| Ligand BCR y 101                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMG c 522                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand CLA C 511                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

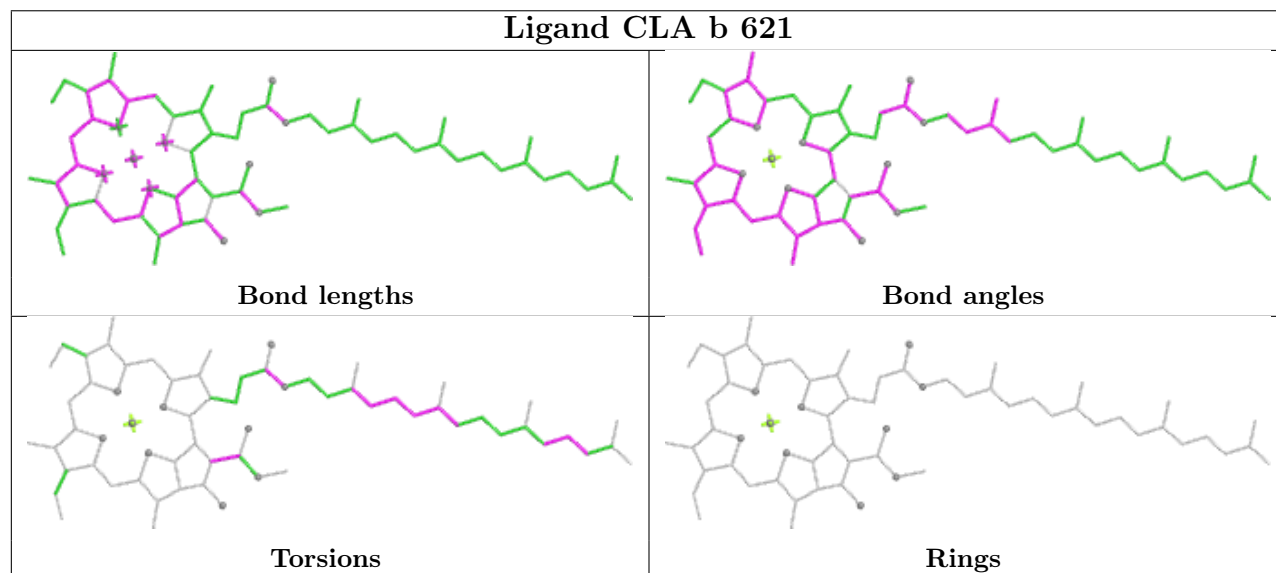
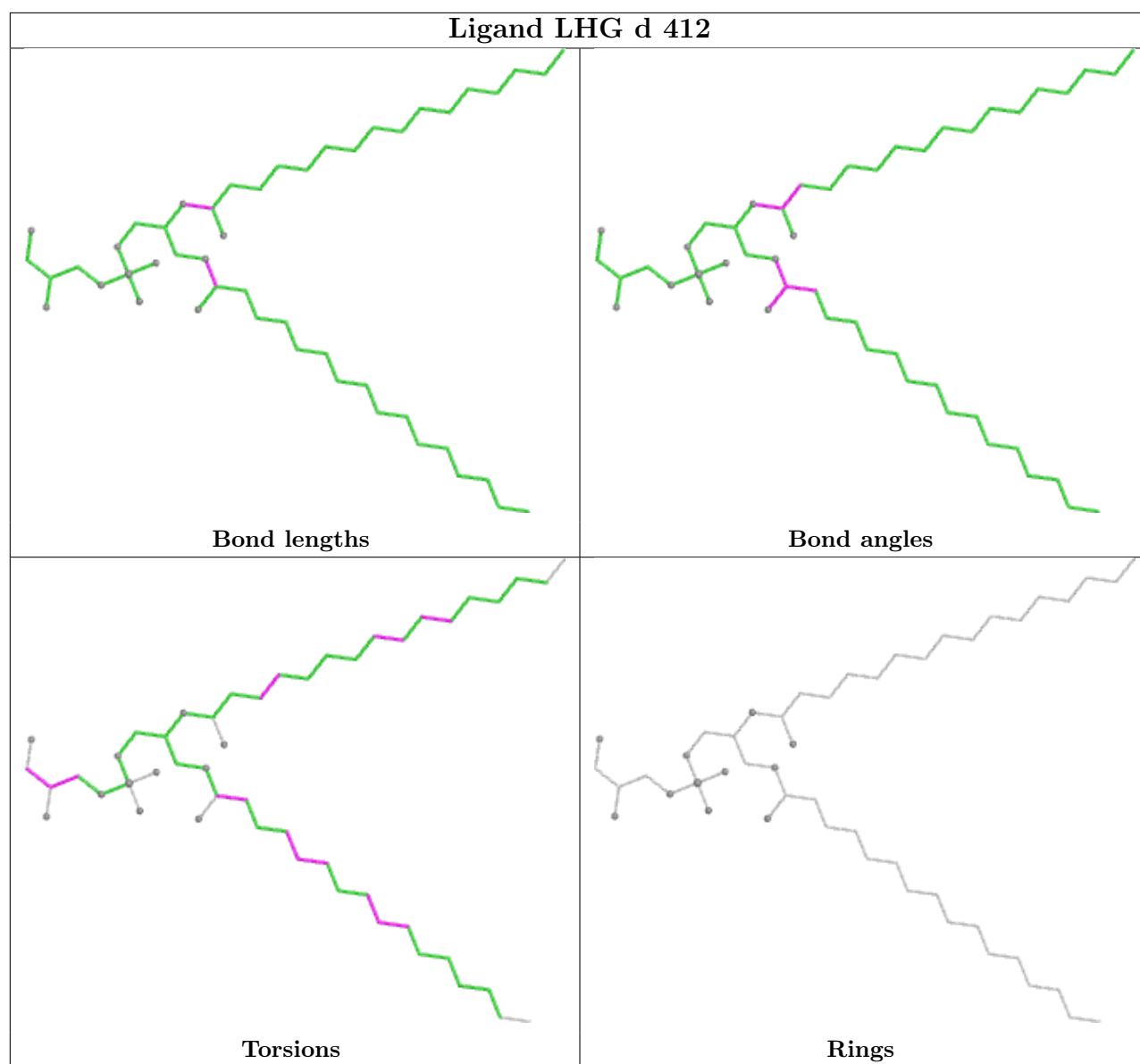


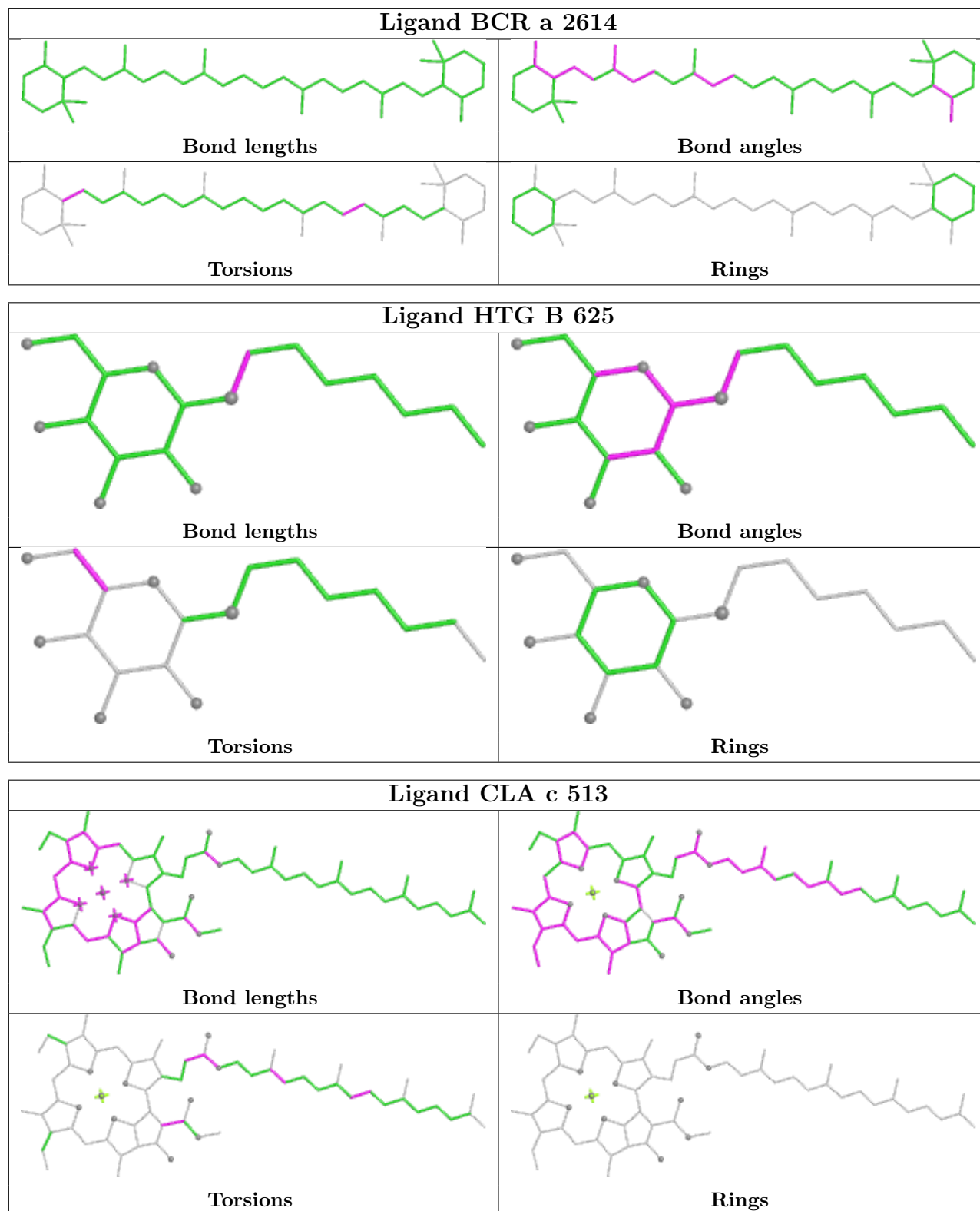


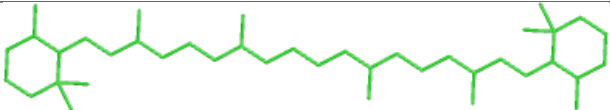
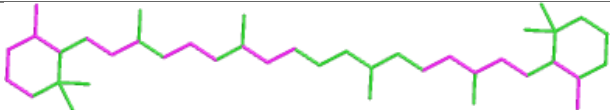
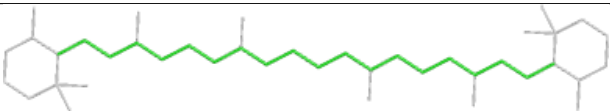
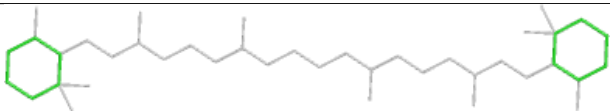
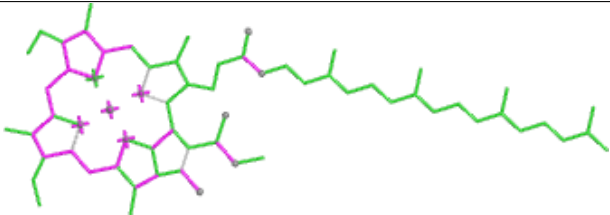
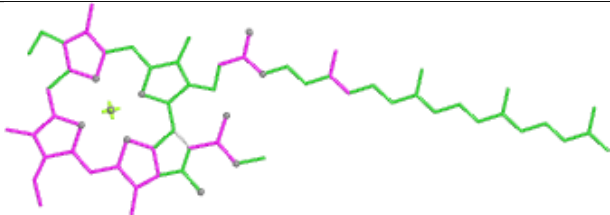
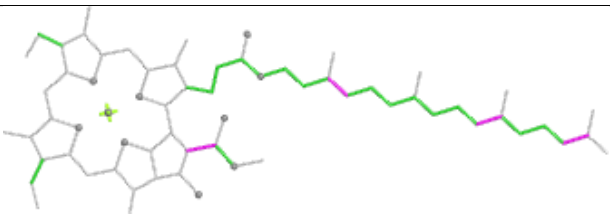
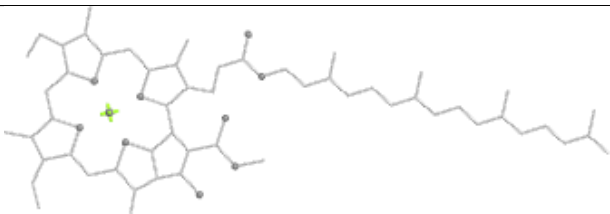


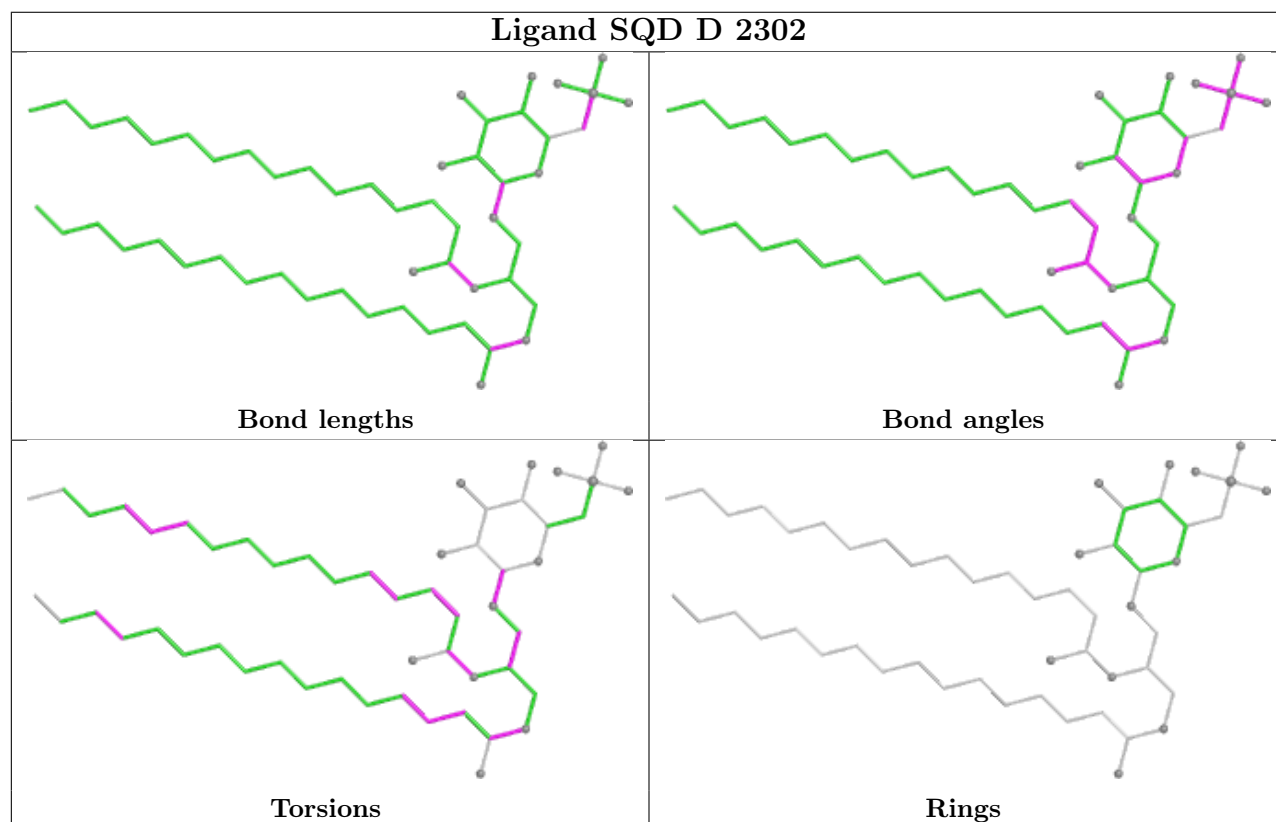
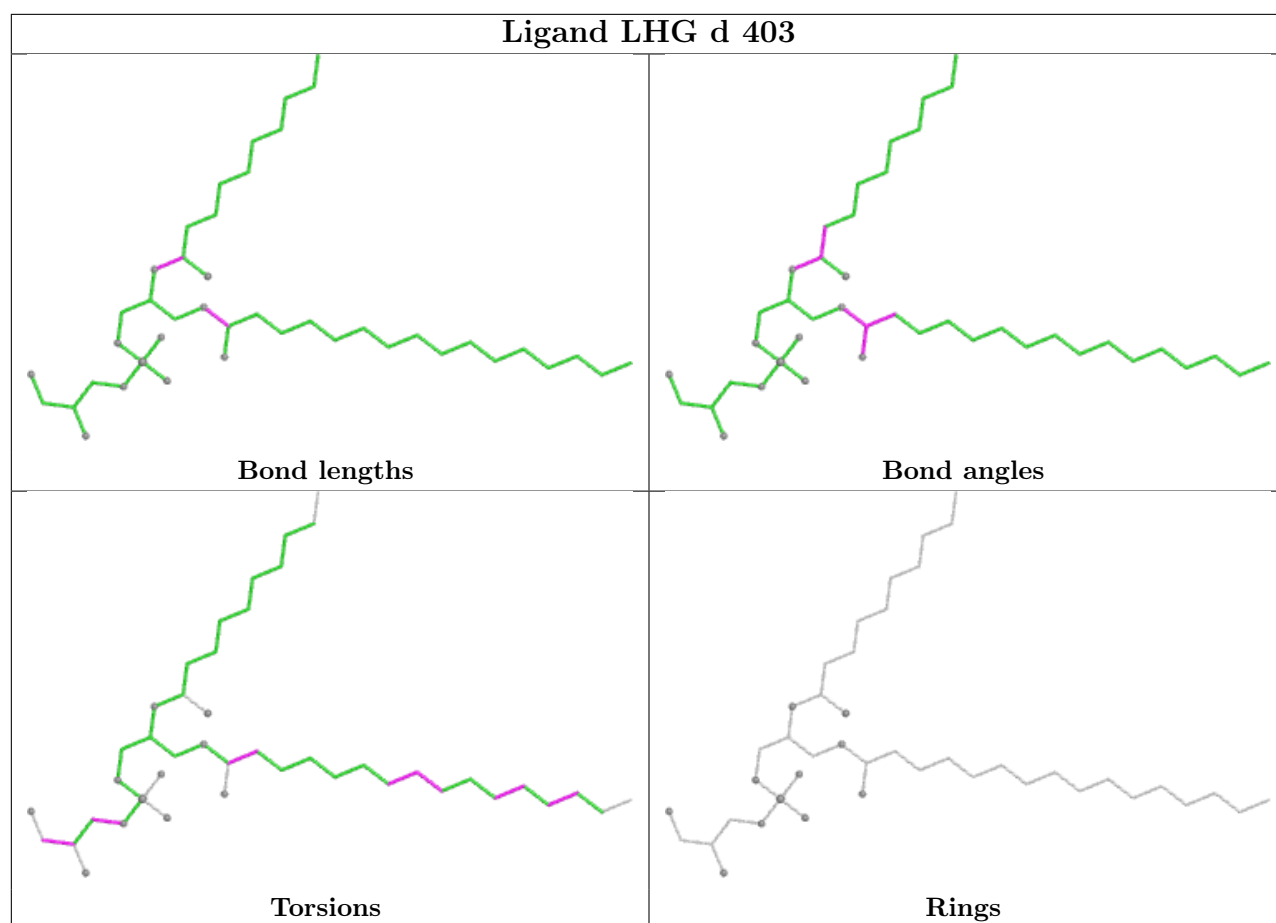


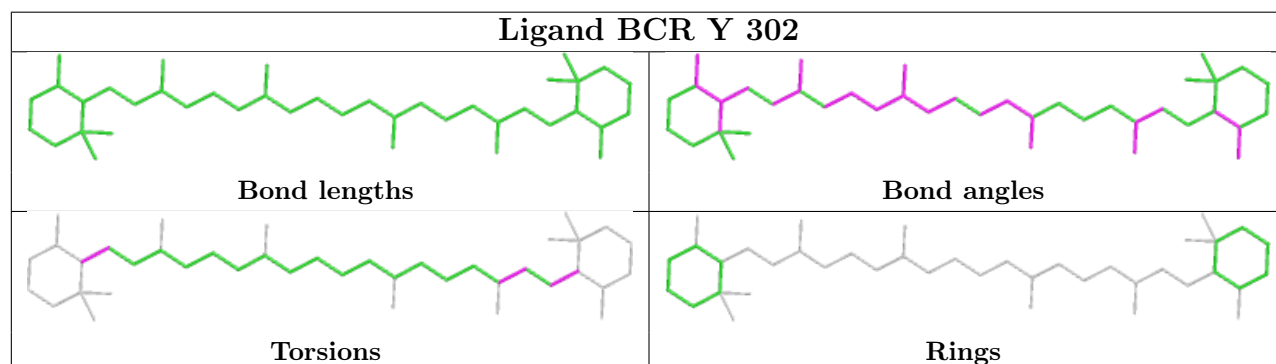
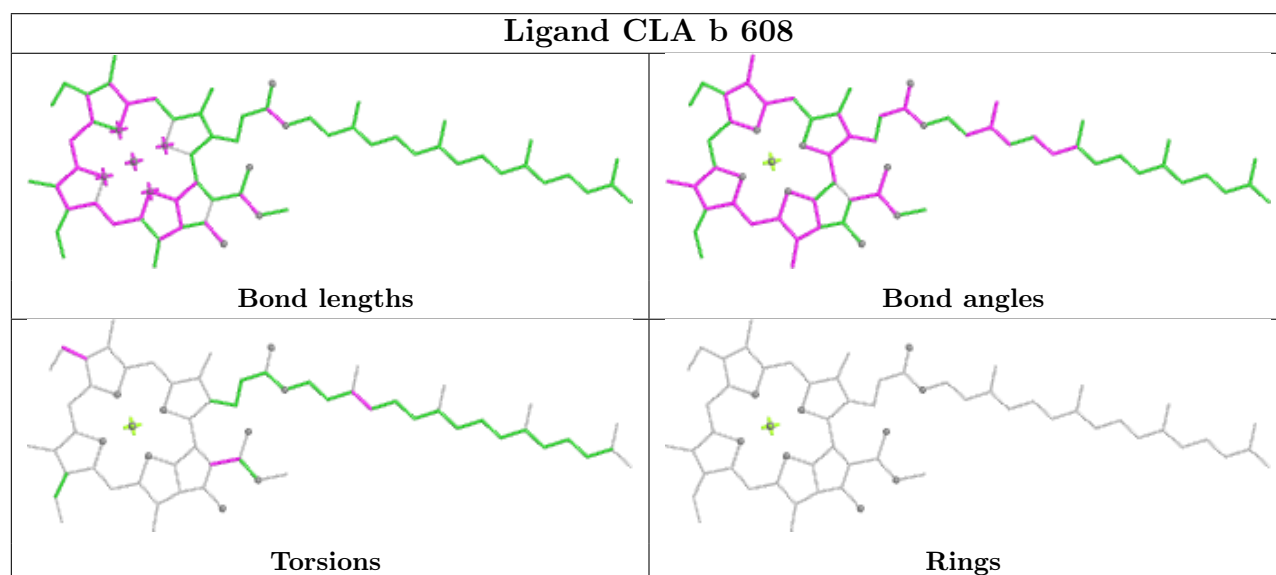
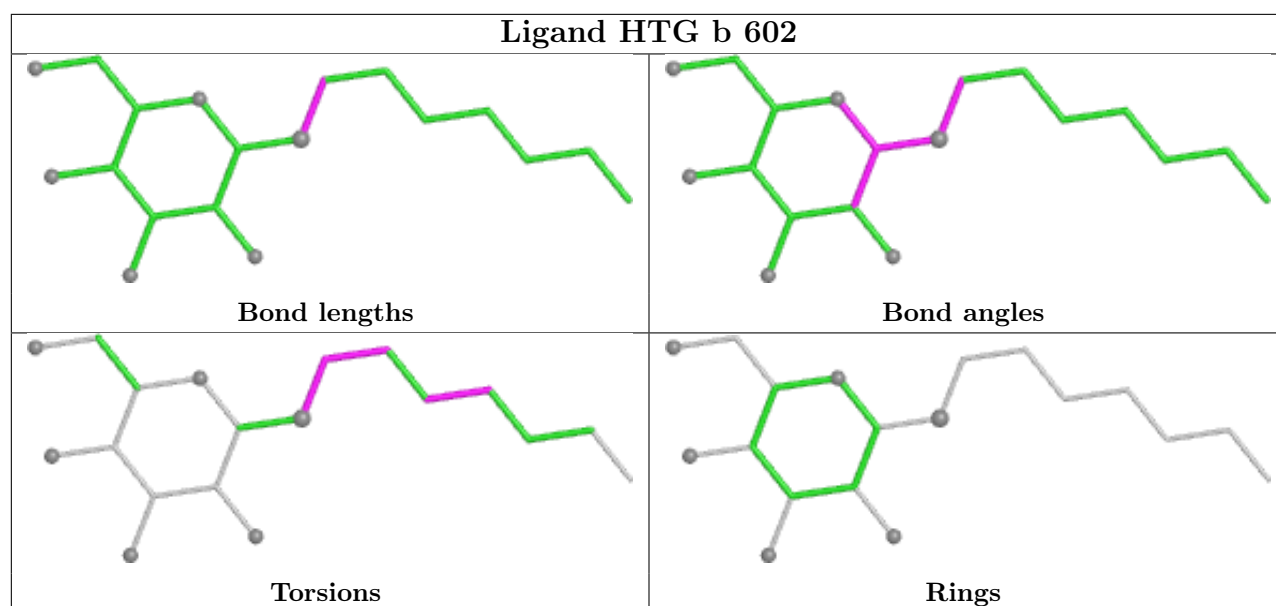


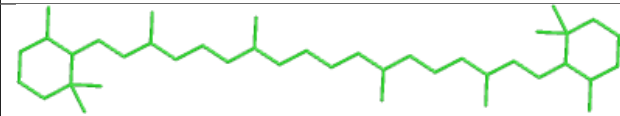
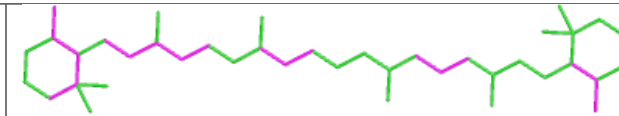
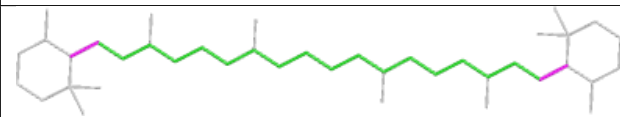
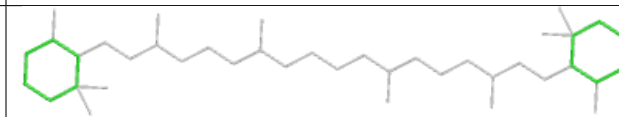


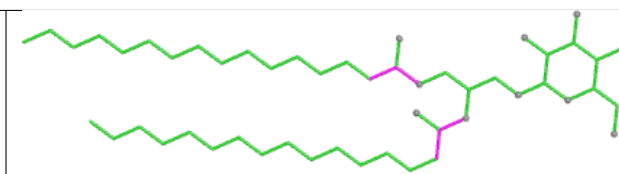
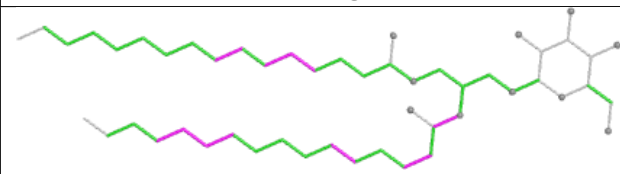
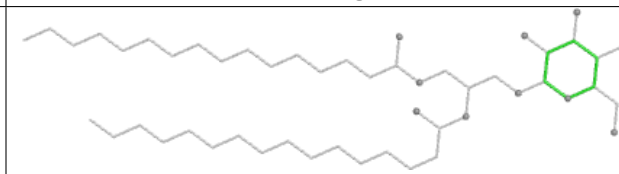


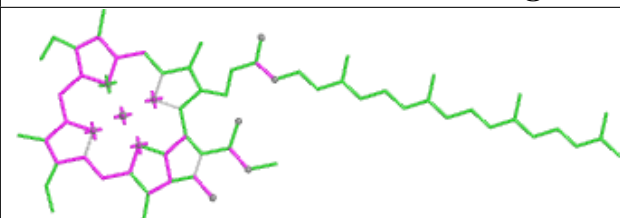
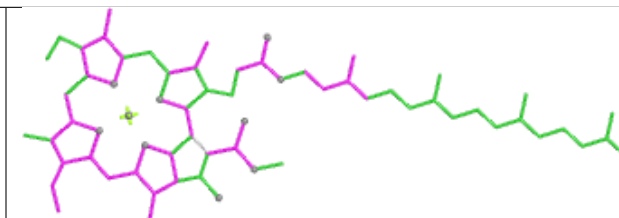
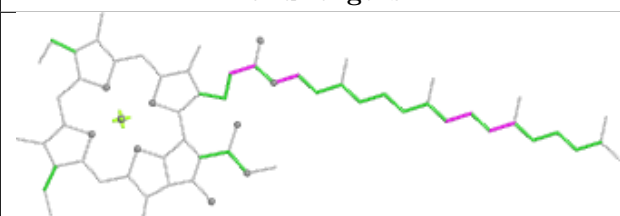
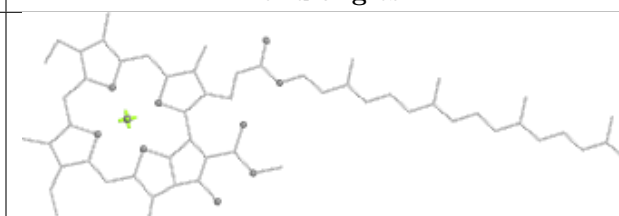
| Ligand BCR K 101                                                                                       |                                                                                                        |
|--------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand PL9 A 422                                                                                       |                                                                                                        |
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand CLA c 507                                                                                       |                                                                                                        |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |



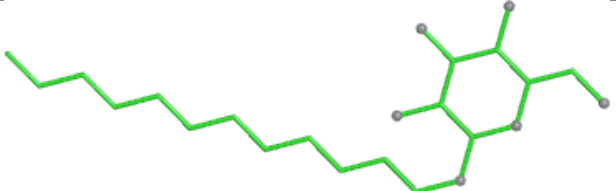
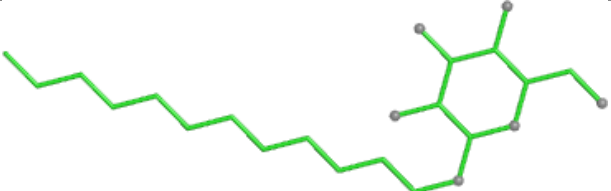
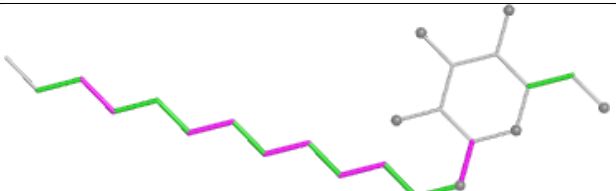
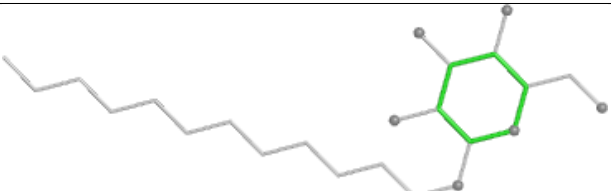


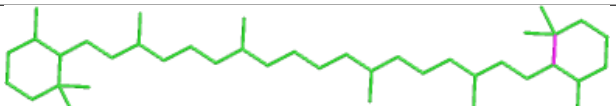
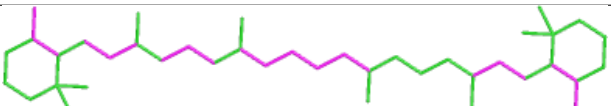
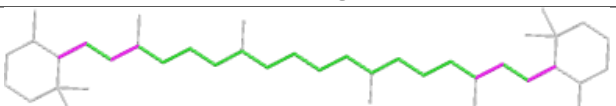
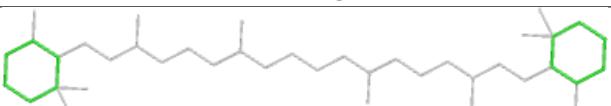
| Ligand BCR C 516                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

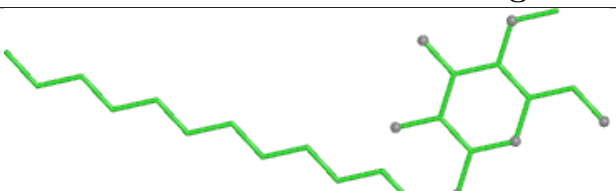
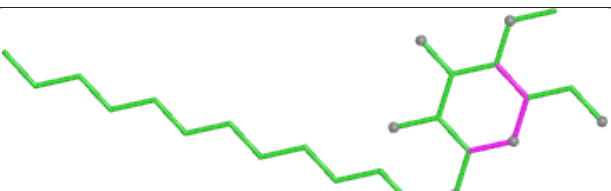
| Ligand LMG m 2802                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

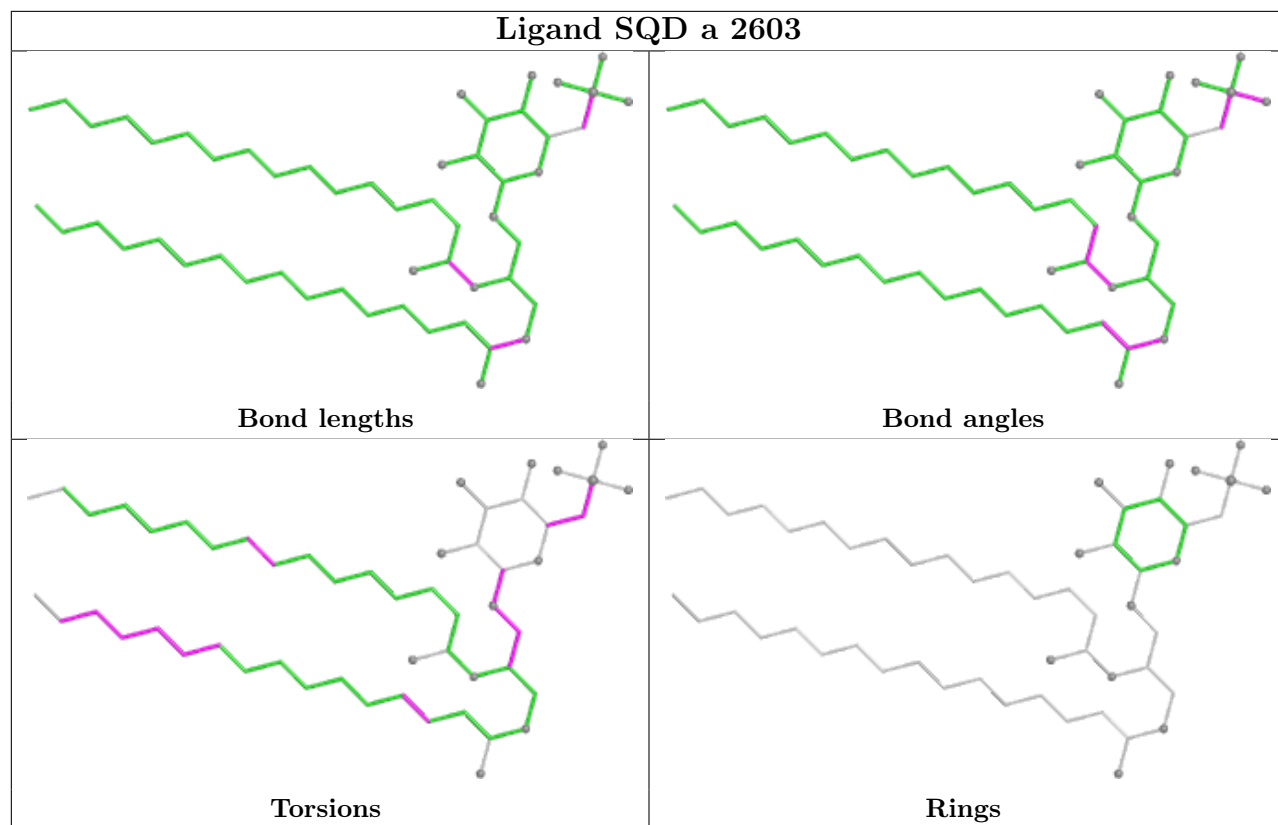
| Ligand CLA b 618                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|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

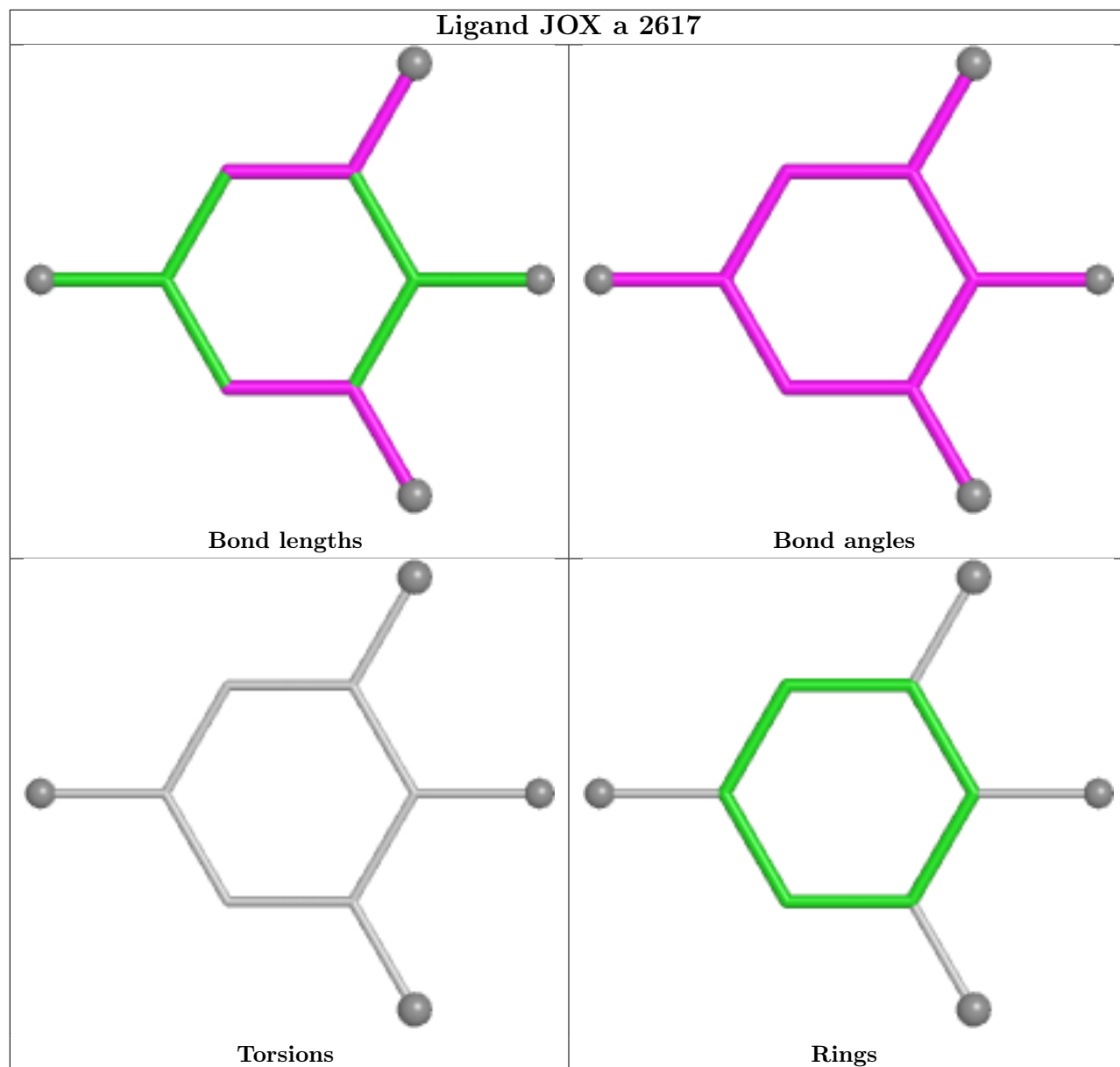


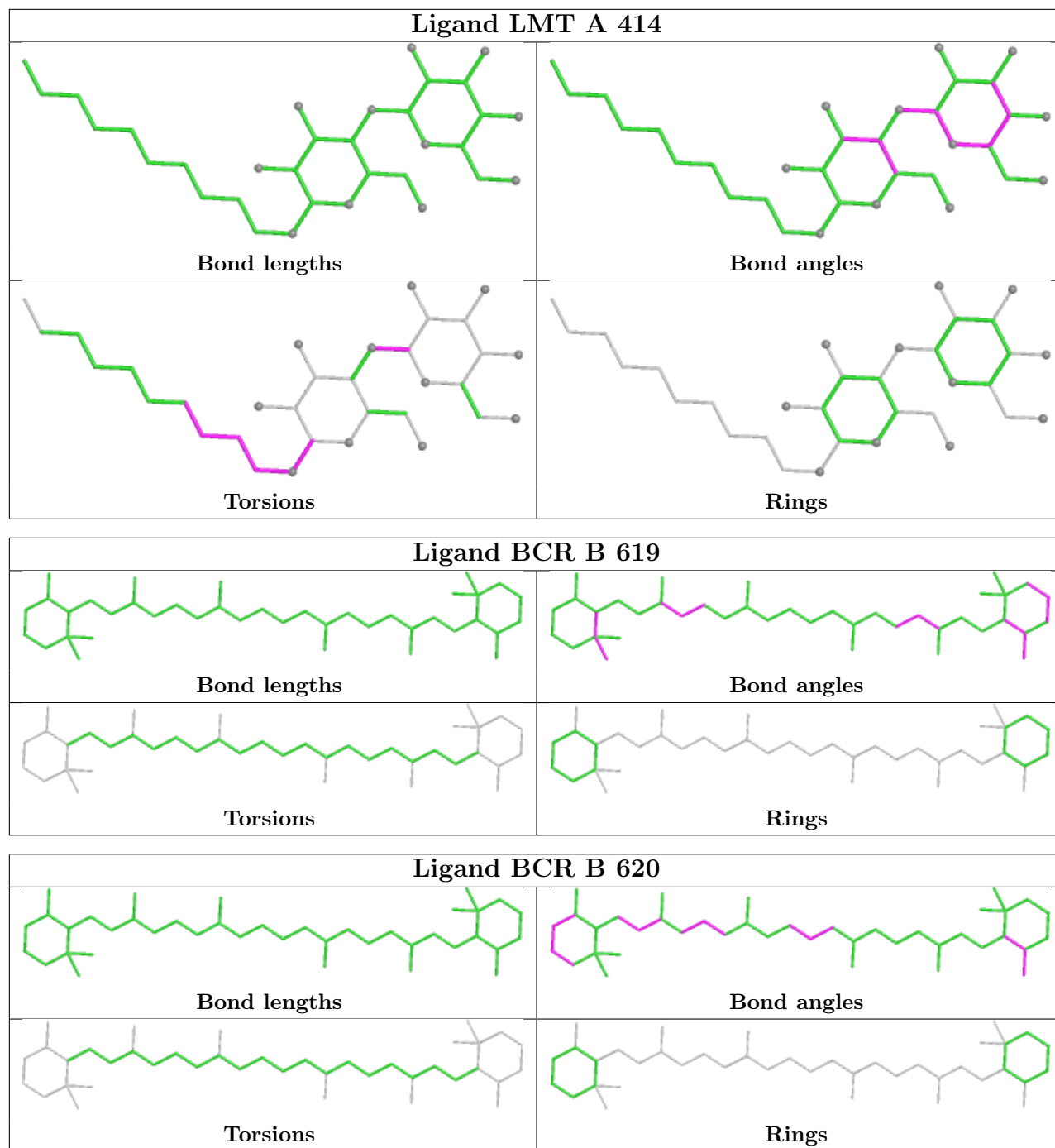
| Ligand LMT A 420                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

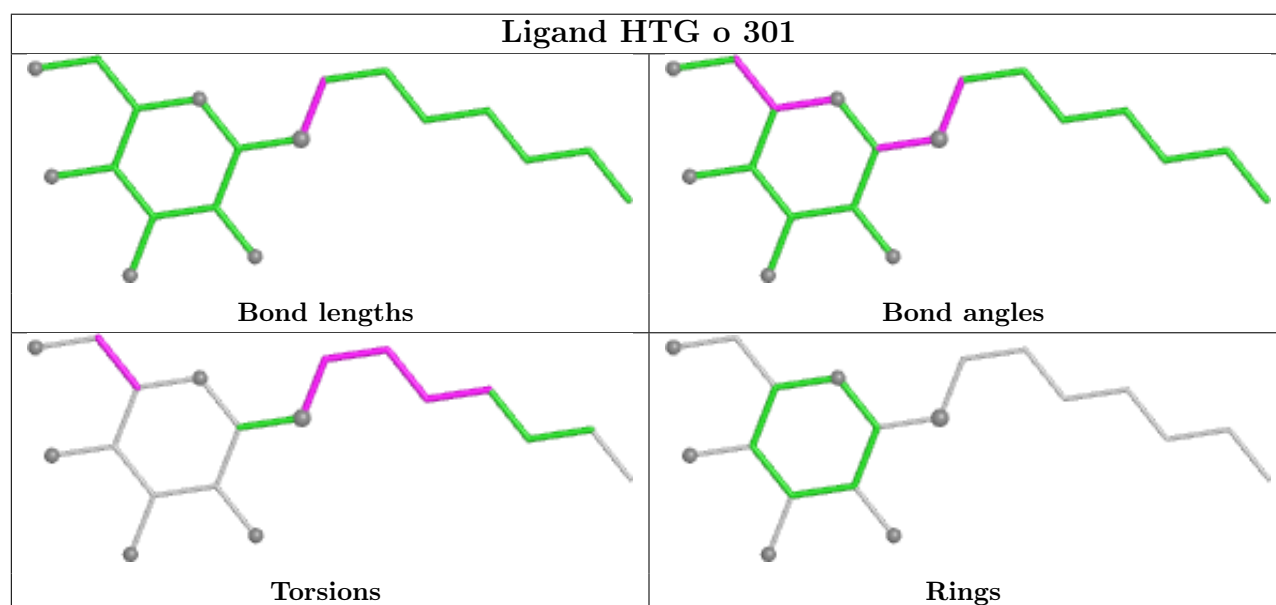
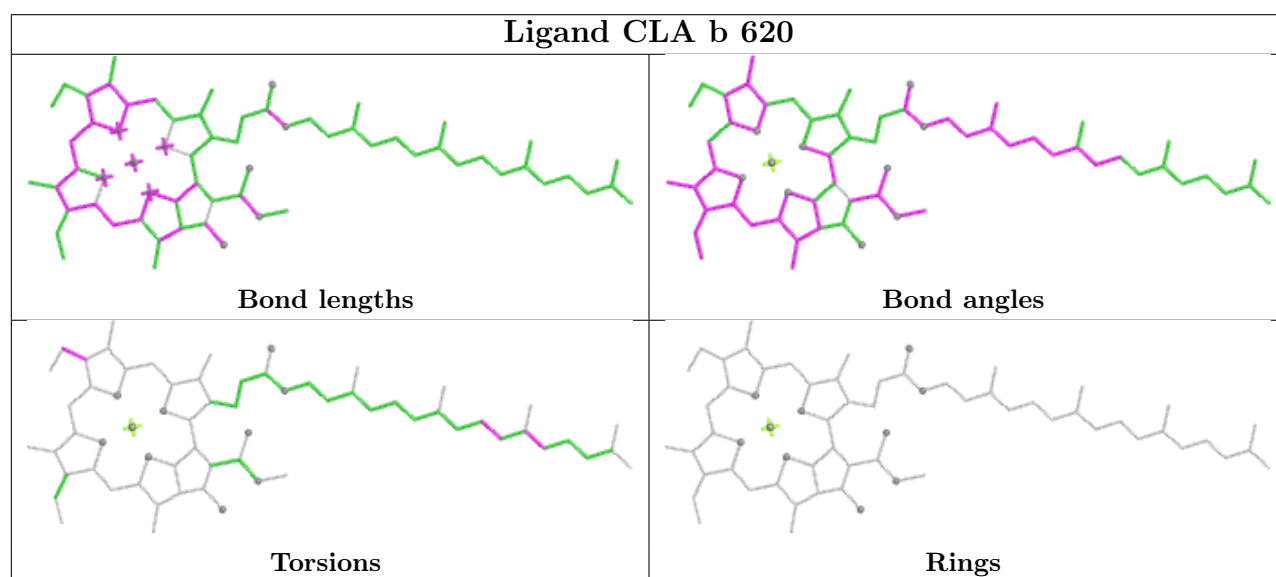
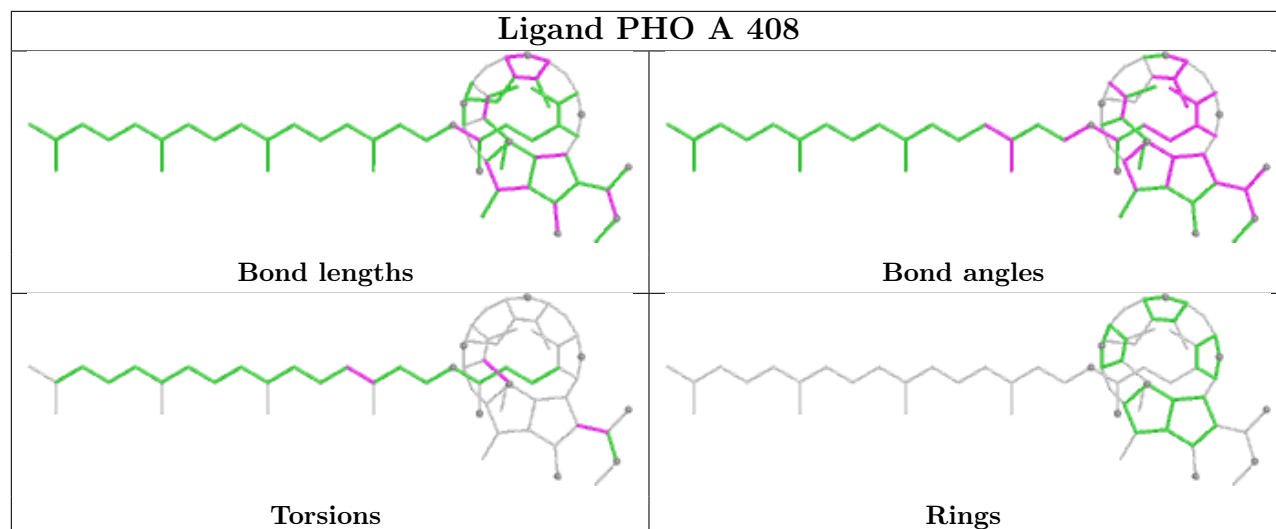
| Ligand BCR D 2305                                                                  |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

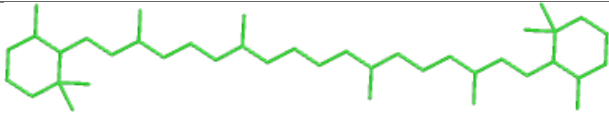
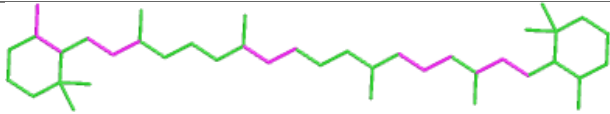
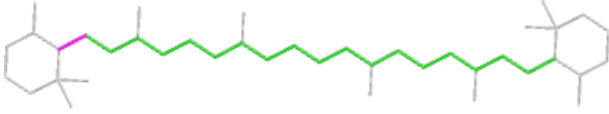
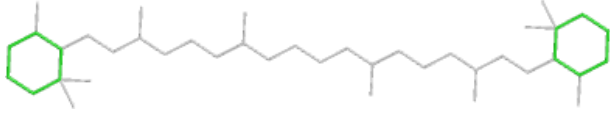
| Ligand LMT d 404                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|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

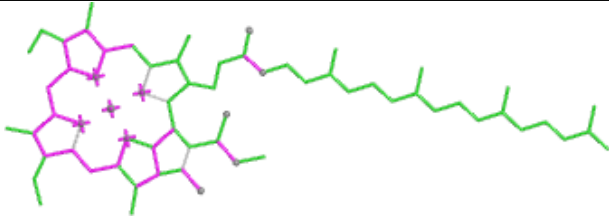
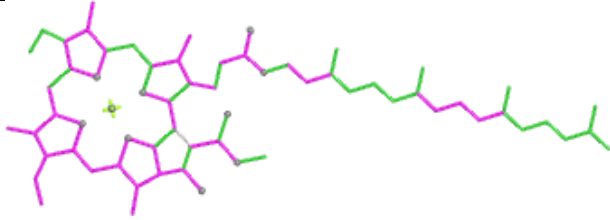
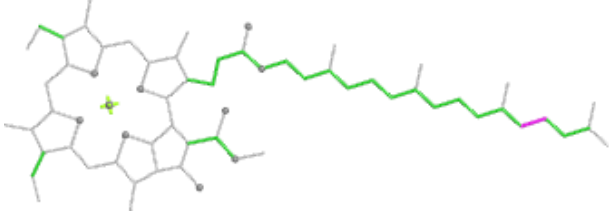
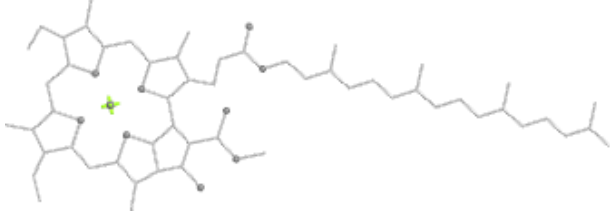


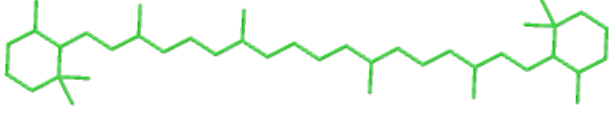
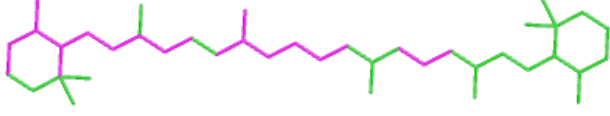
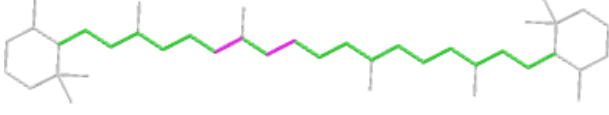
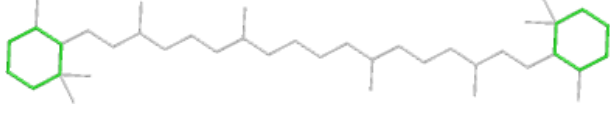




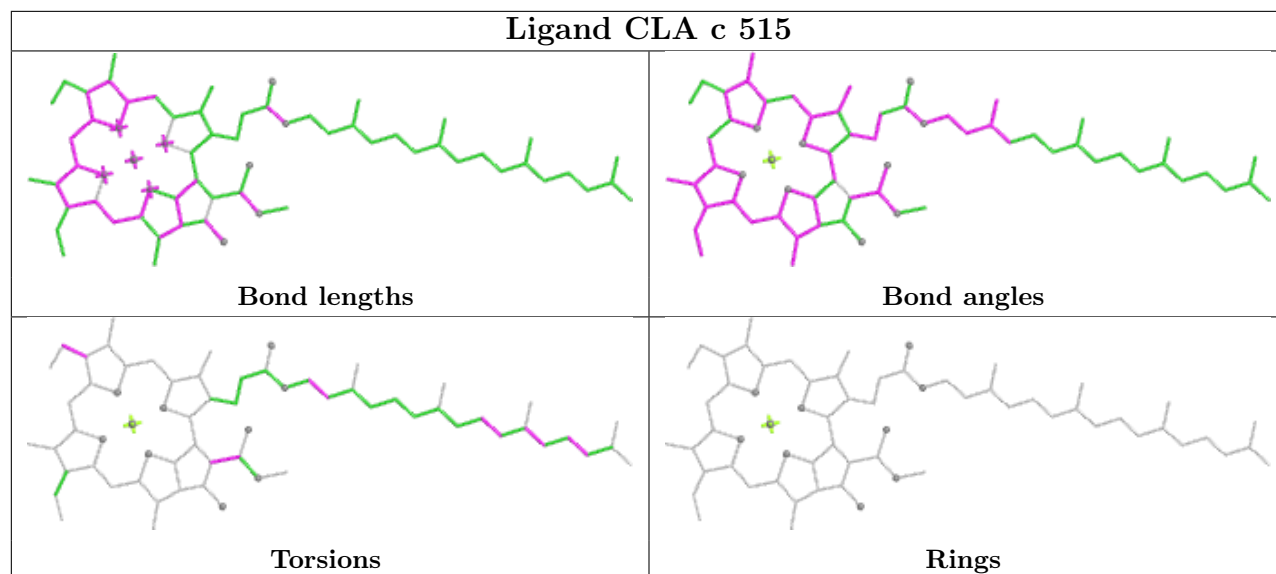


| Ligand BCR B 618                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|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

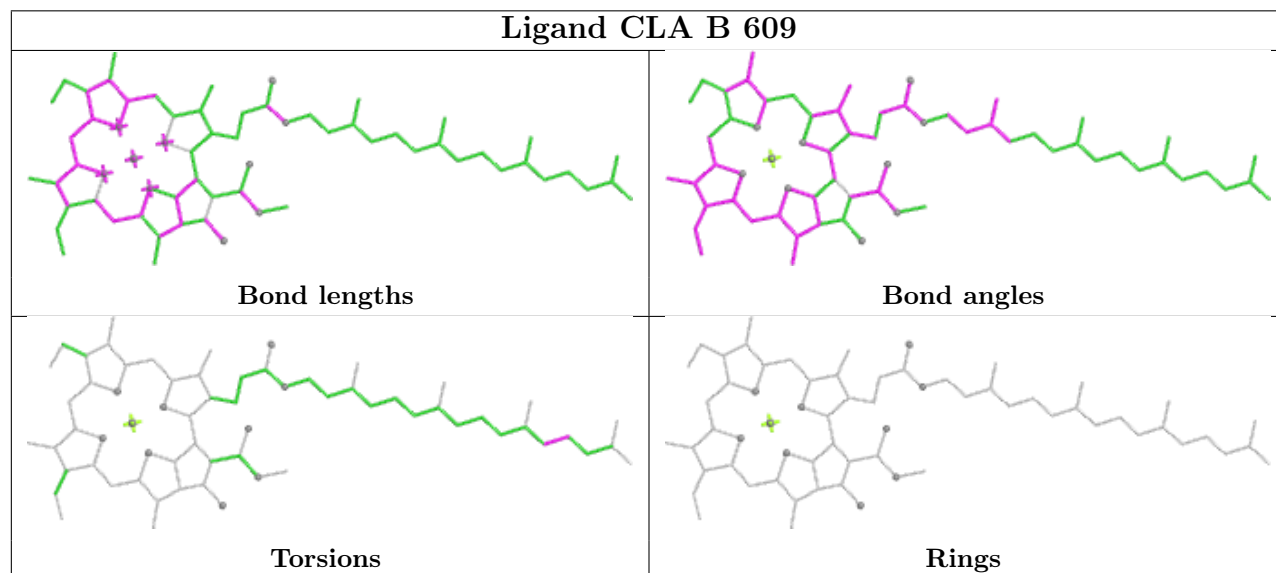
| Ligand CLA b 613                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|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

| Ligand BCR B 633                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

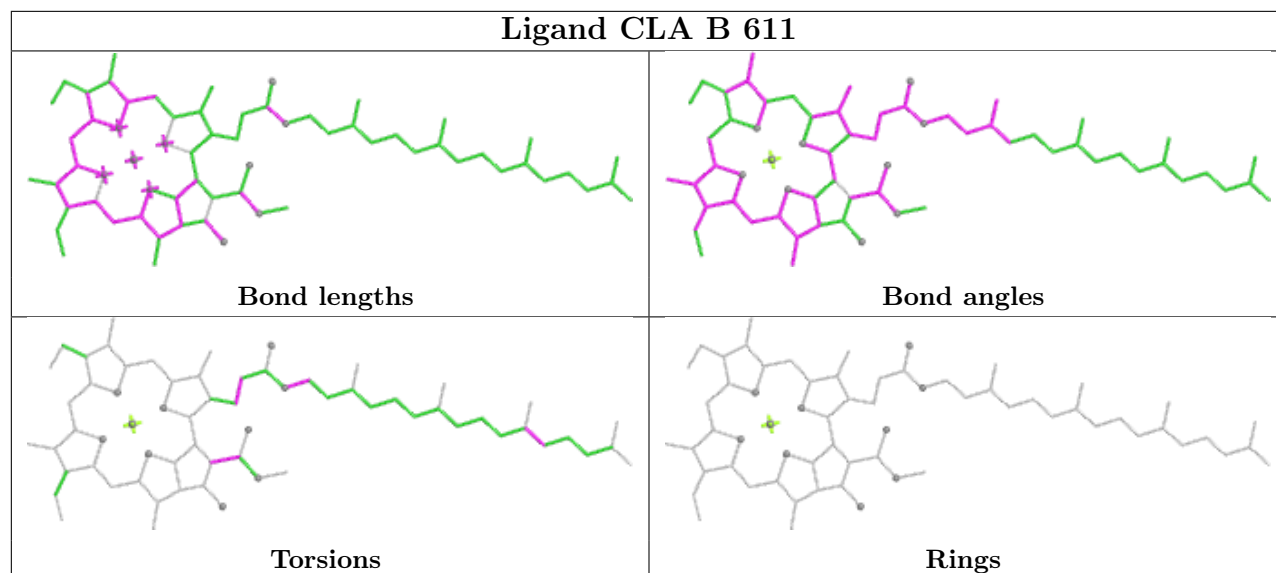
## Ligand CLA c 515



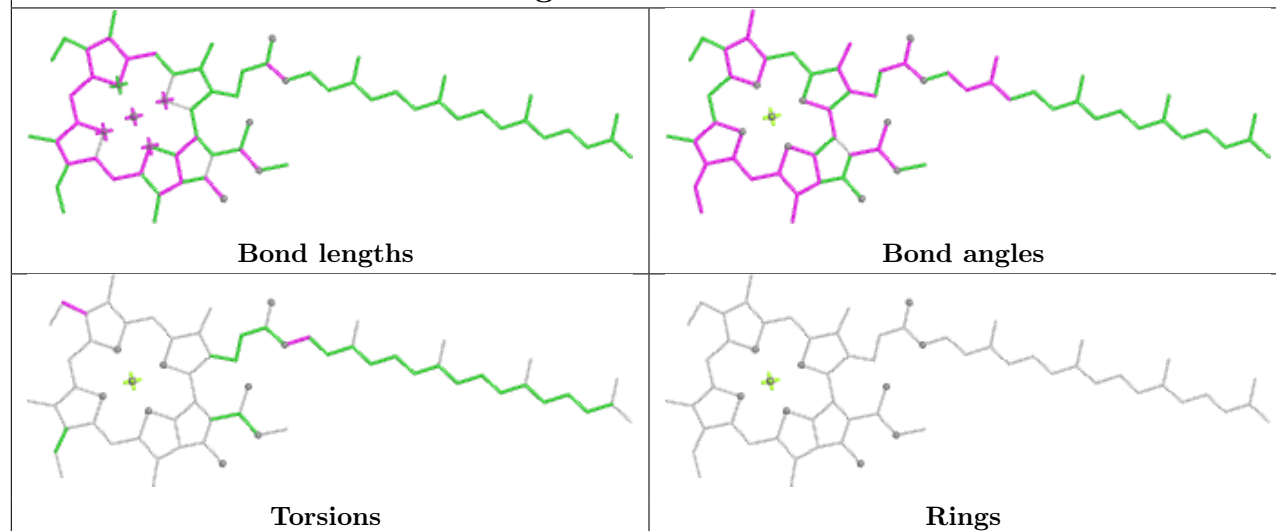
## Ligand CLA B 609



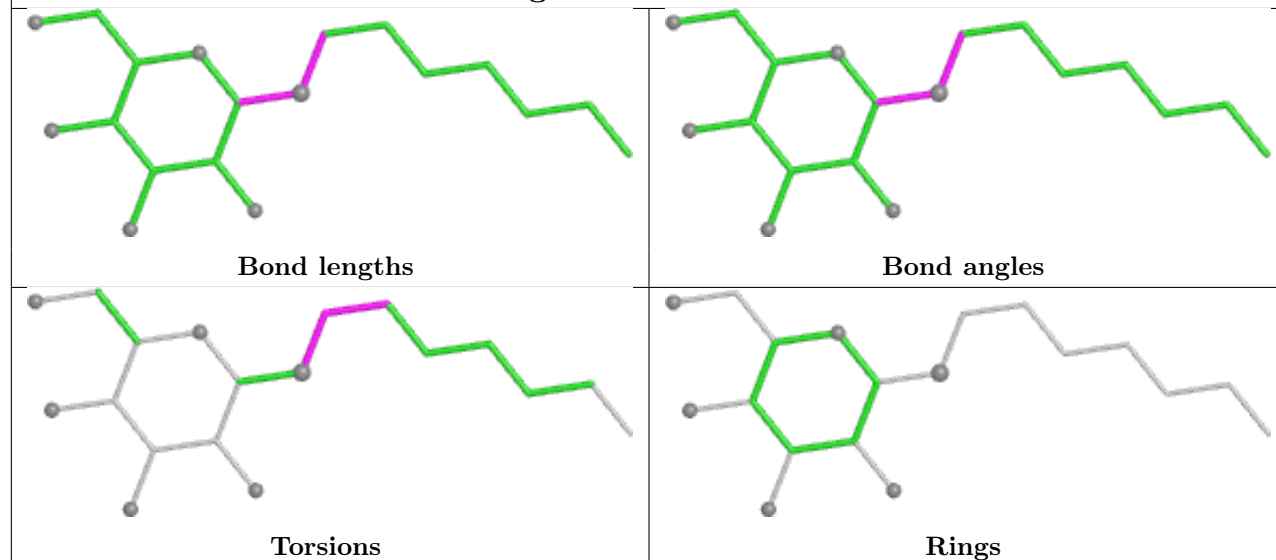
## Ligand CLA B 611



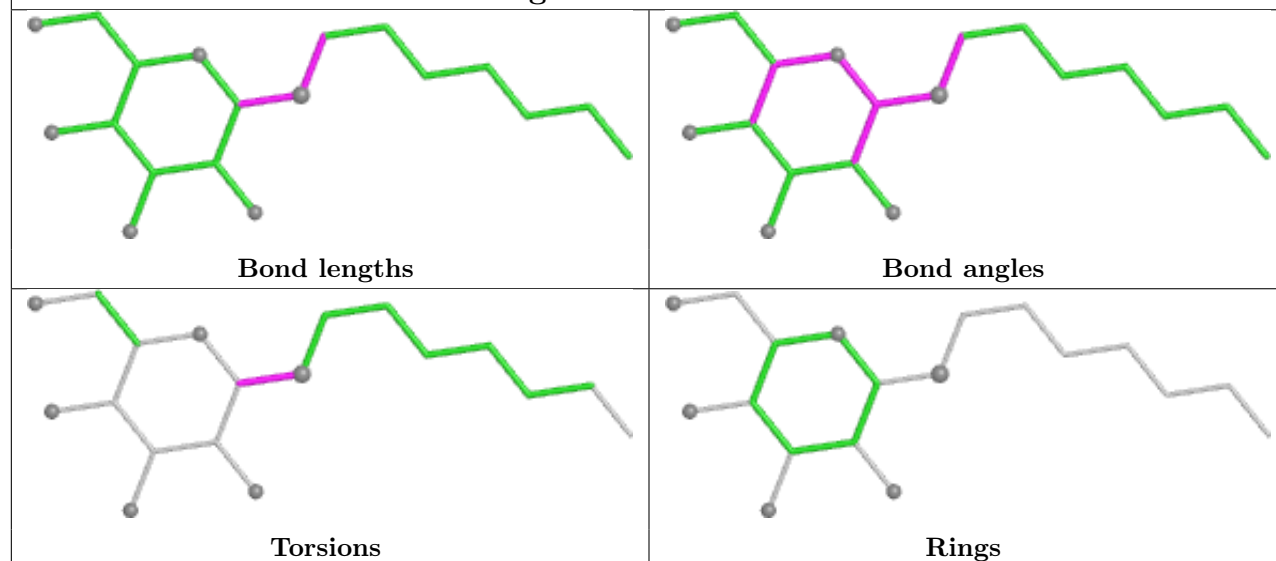
## Ligand CLA d 408



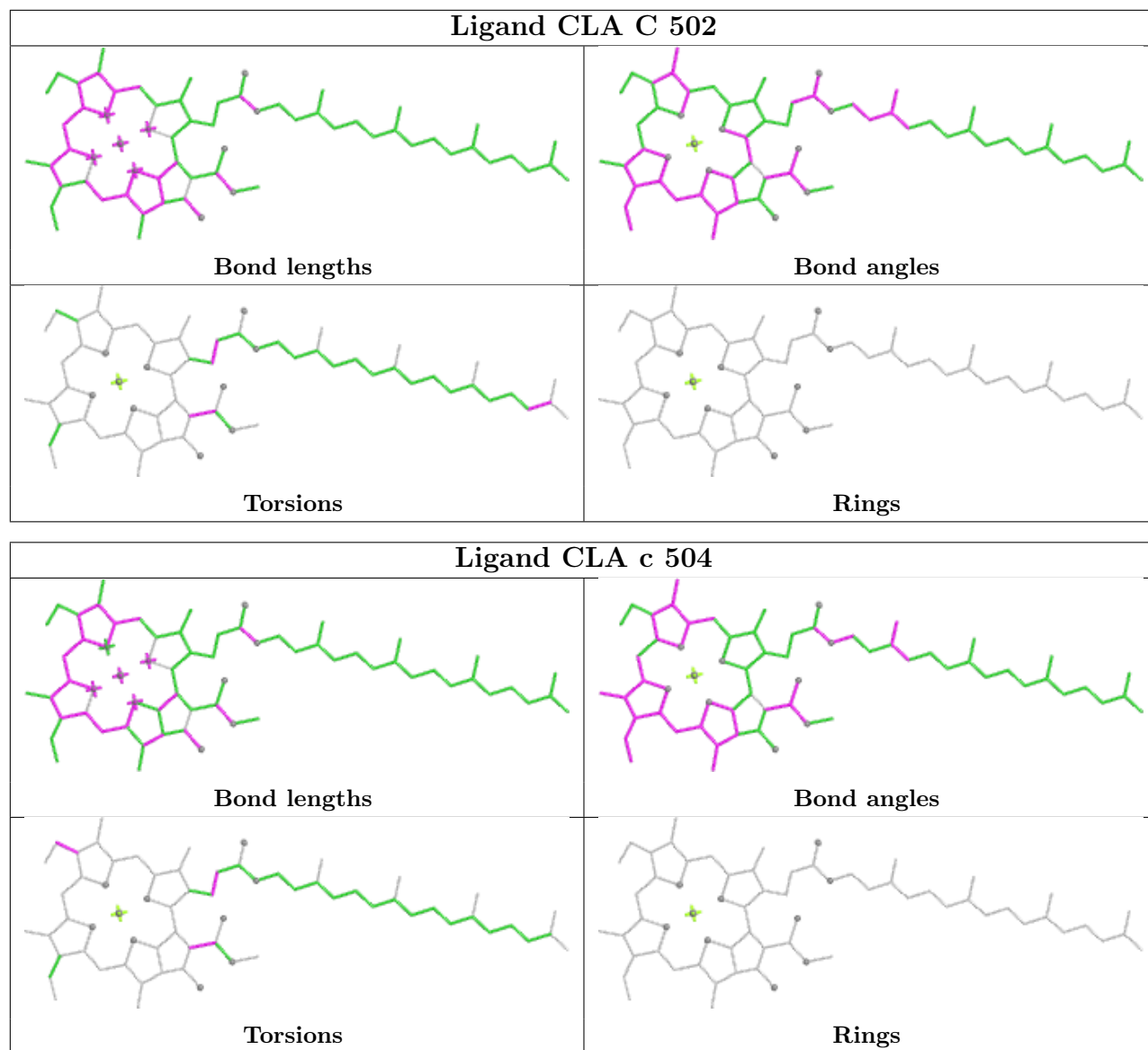
## Ligand HTG C 521

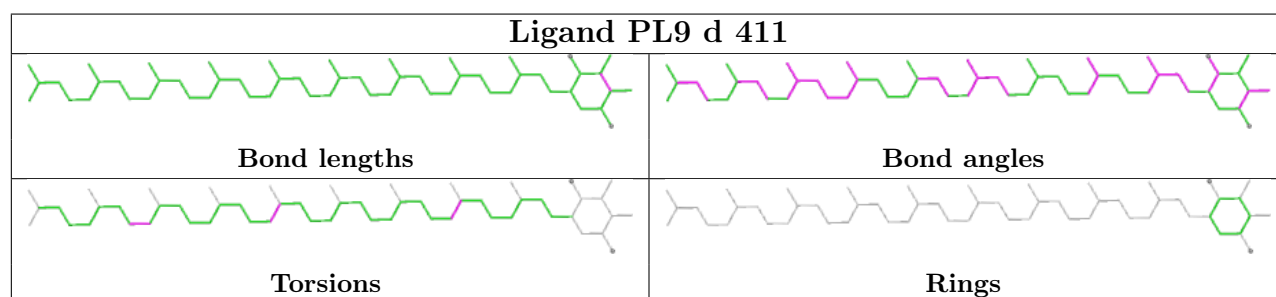
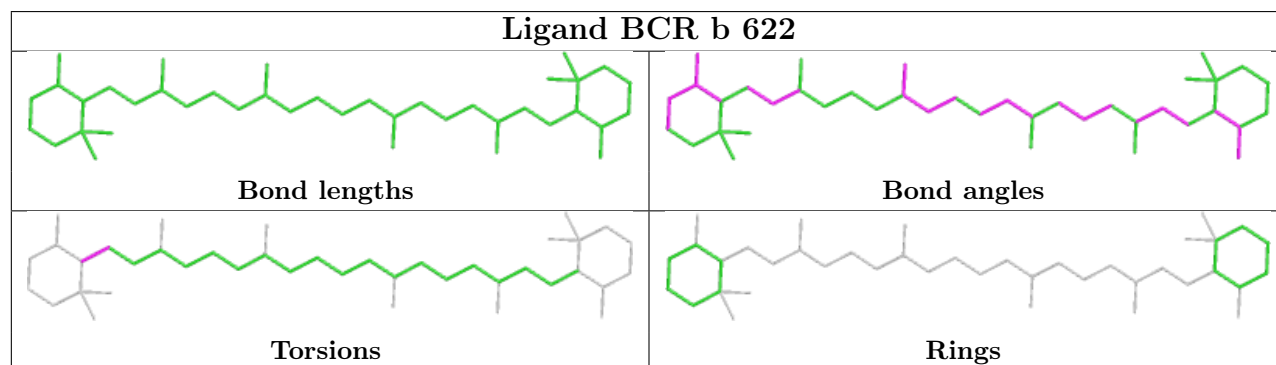
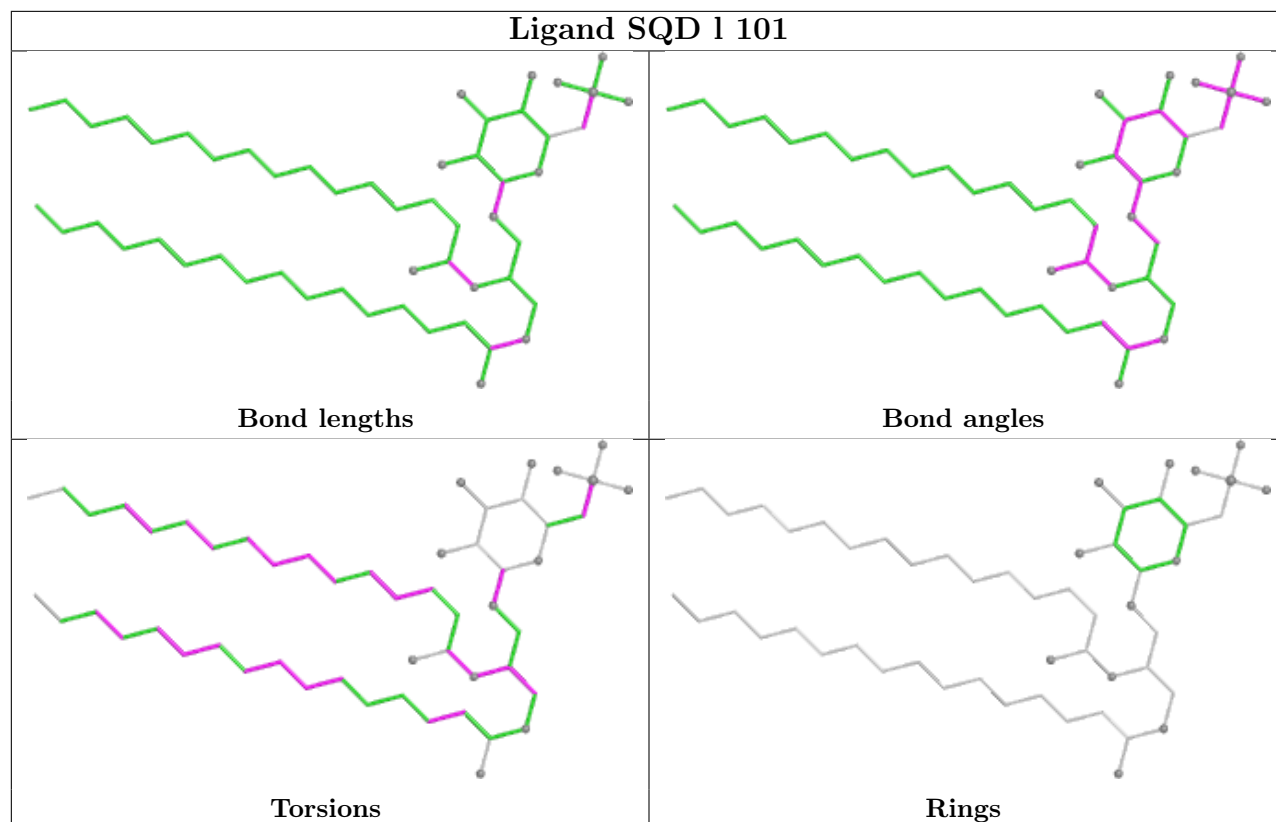


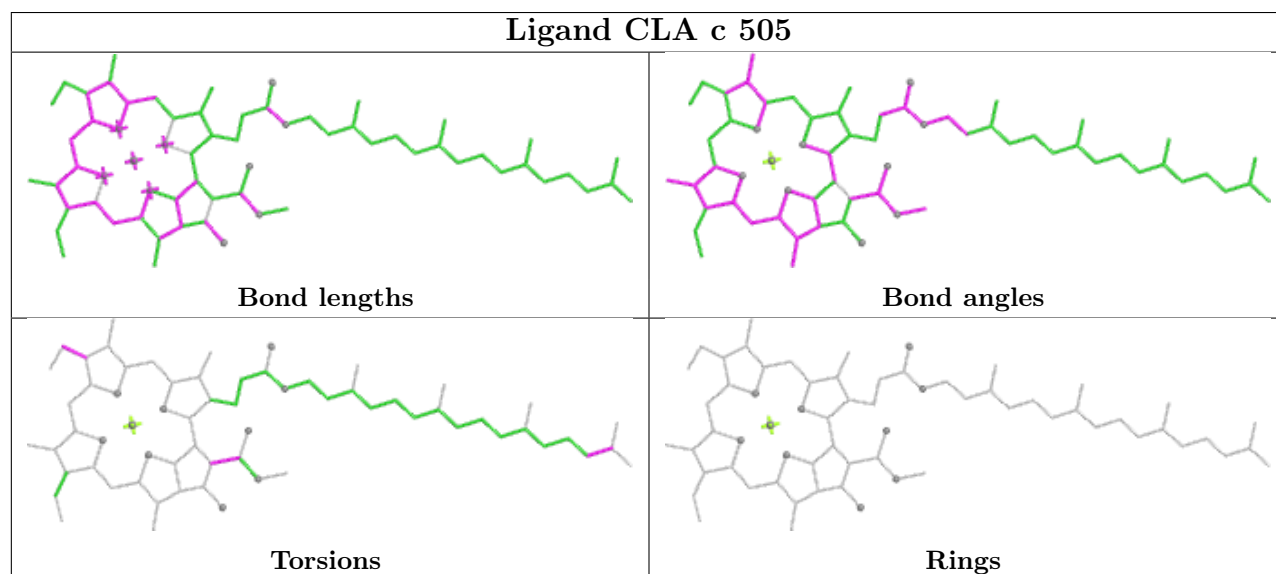
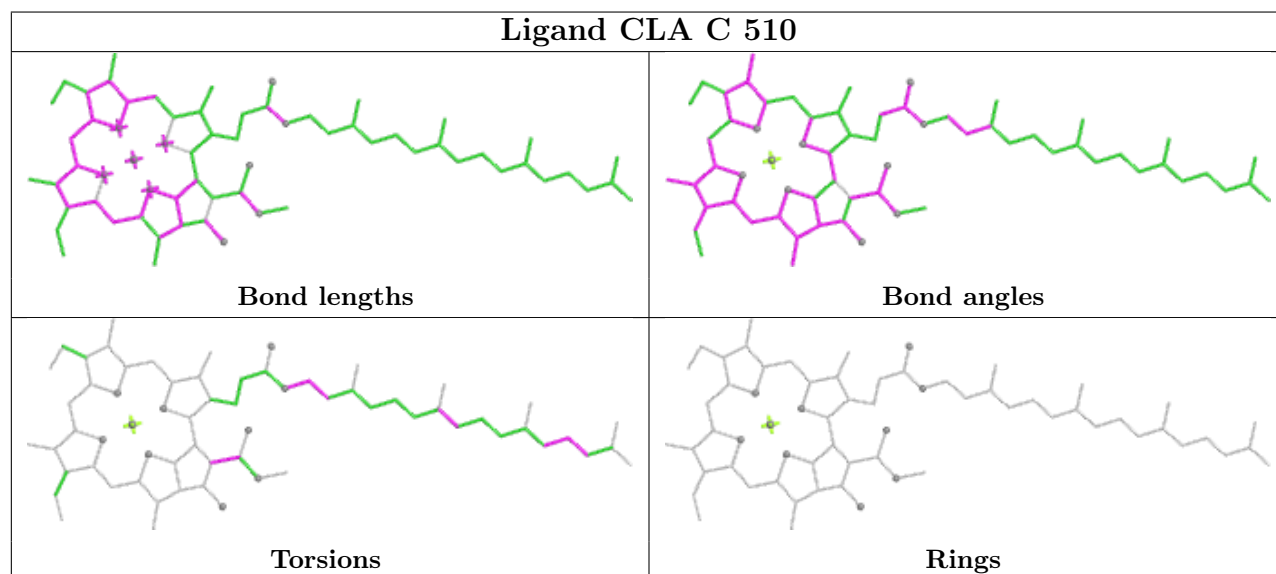
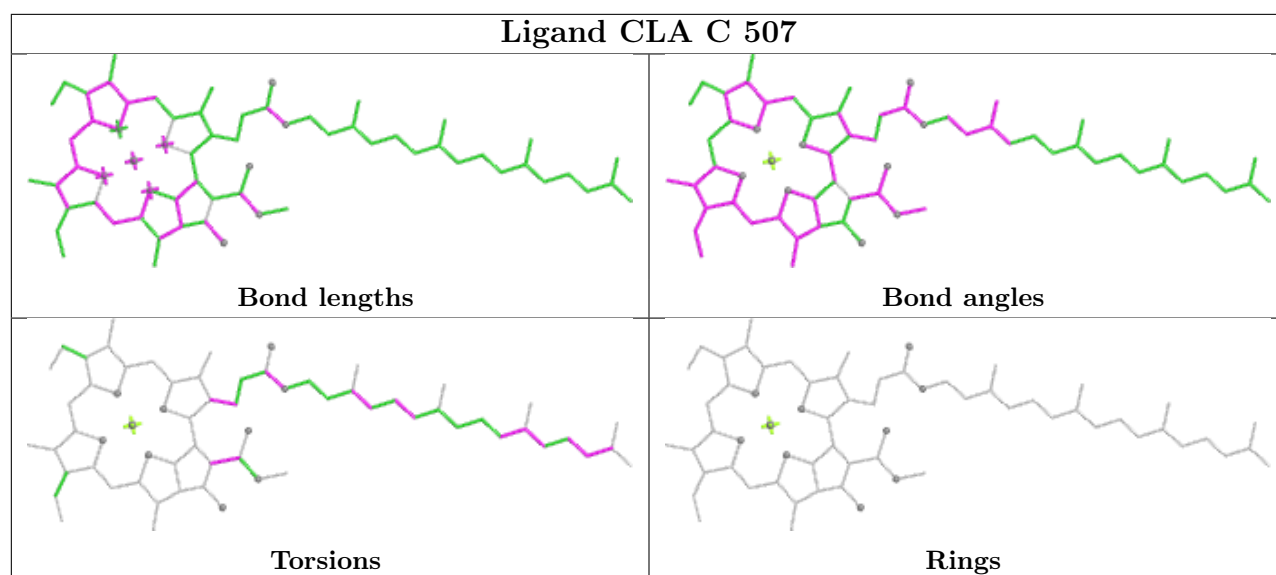
## Ligand HTG C 522



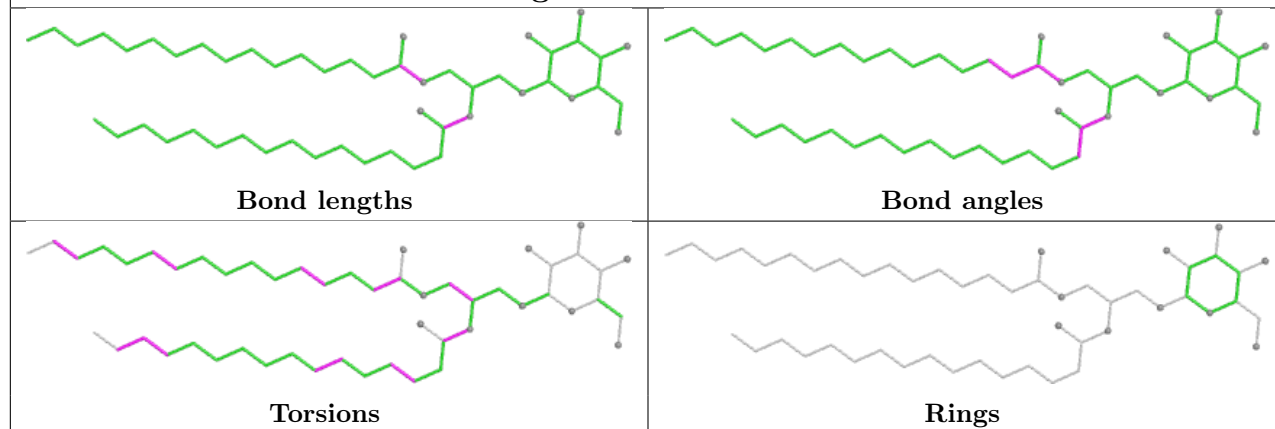




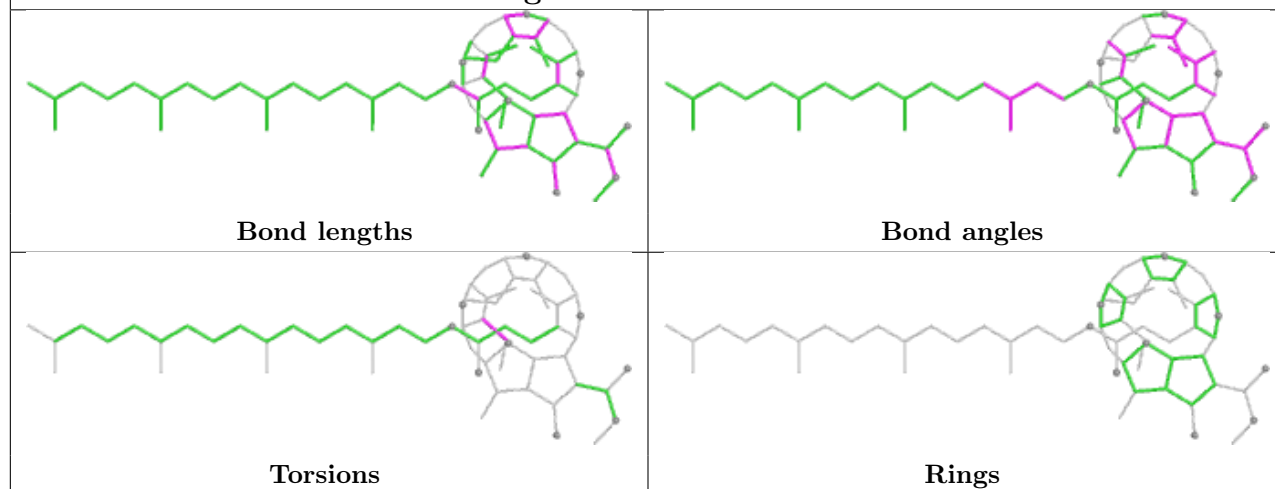




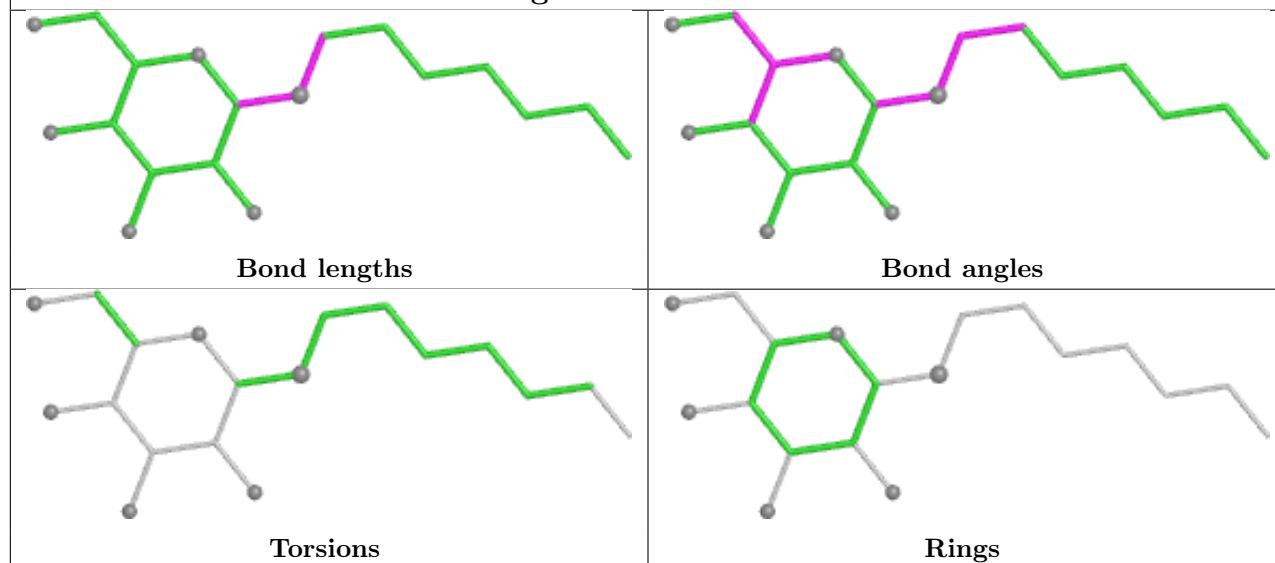
## Ligand LMG c 501



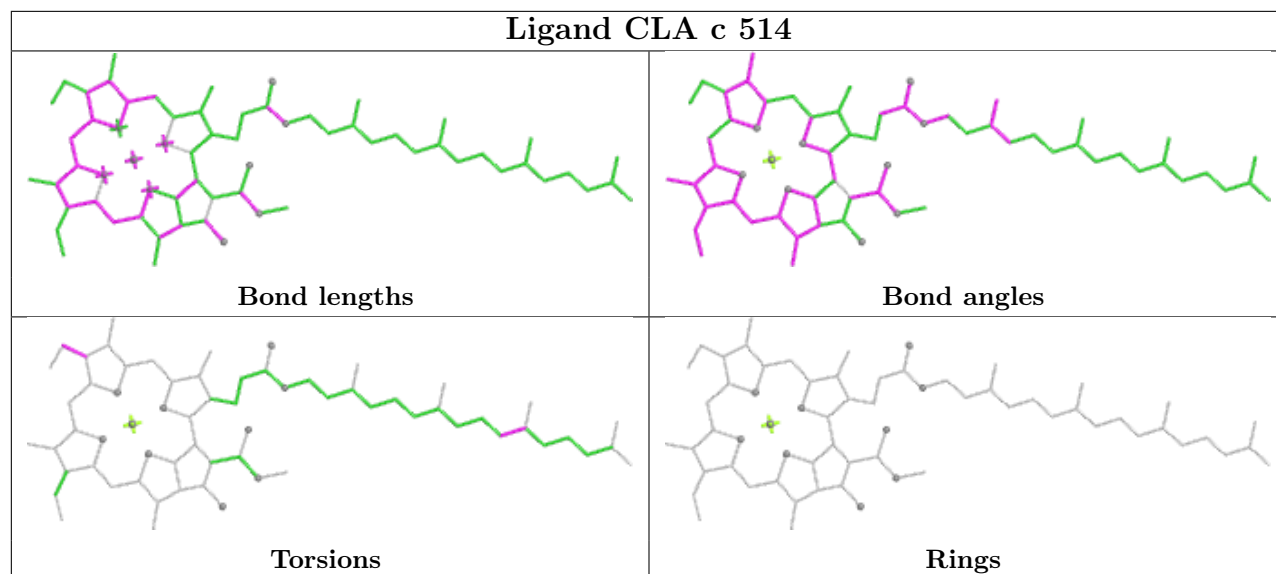
## Ligand PHO a 2612



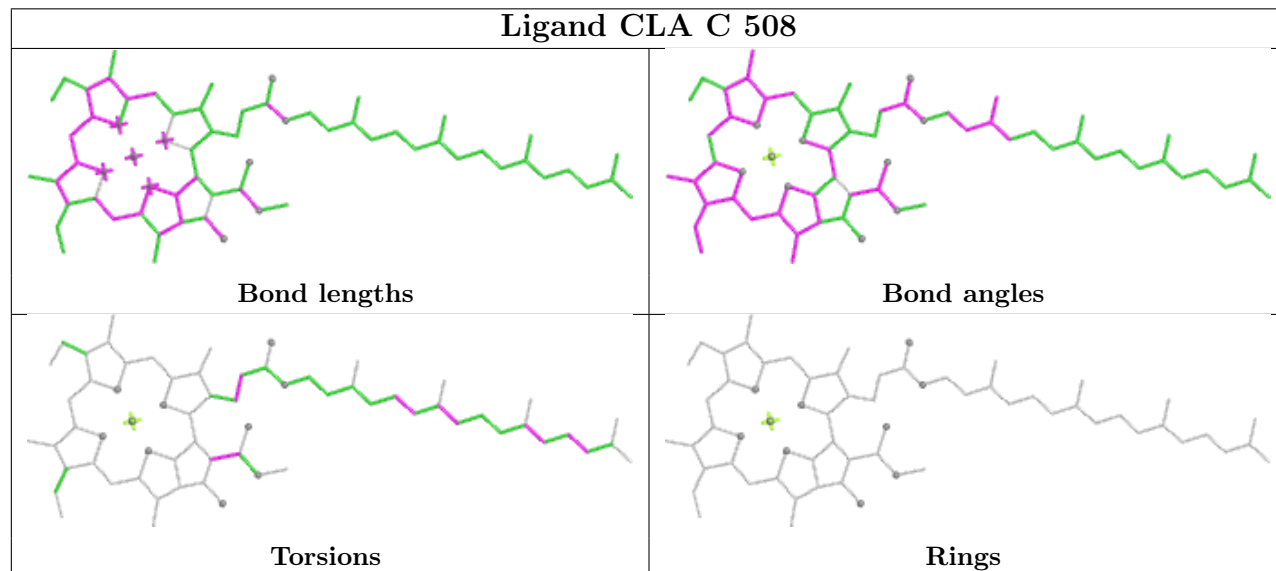
## Ligand HTG b 603



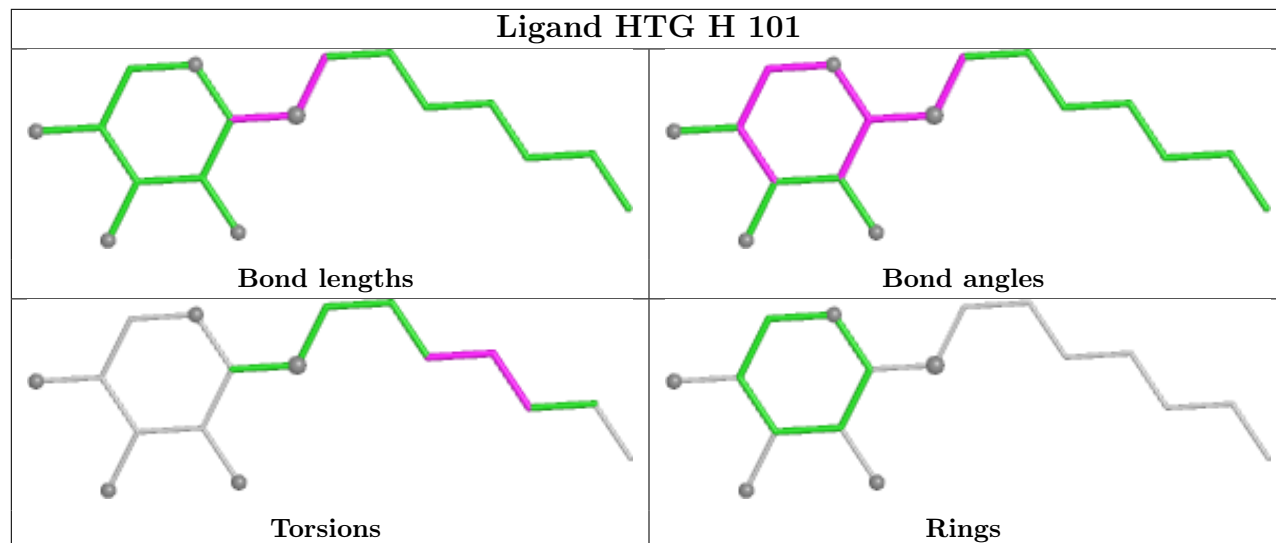
## Ligand CLA c 514

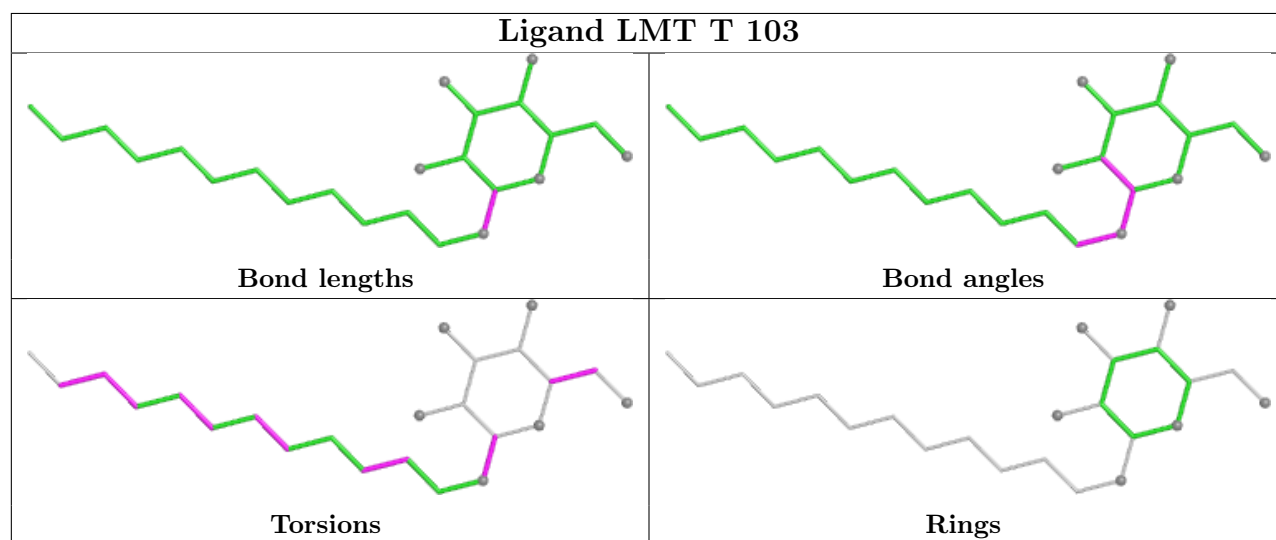
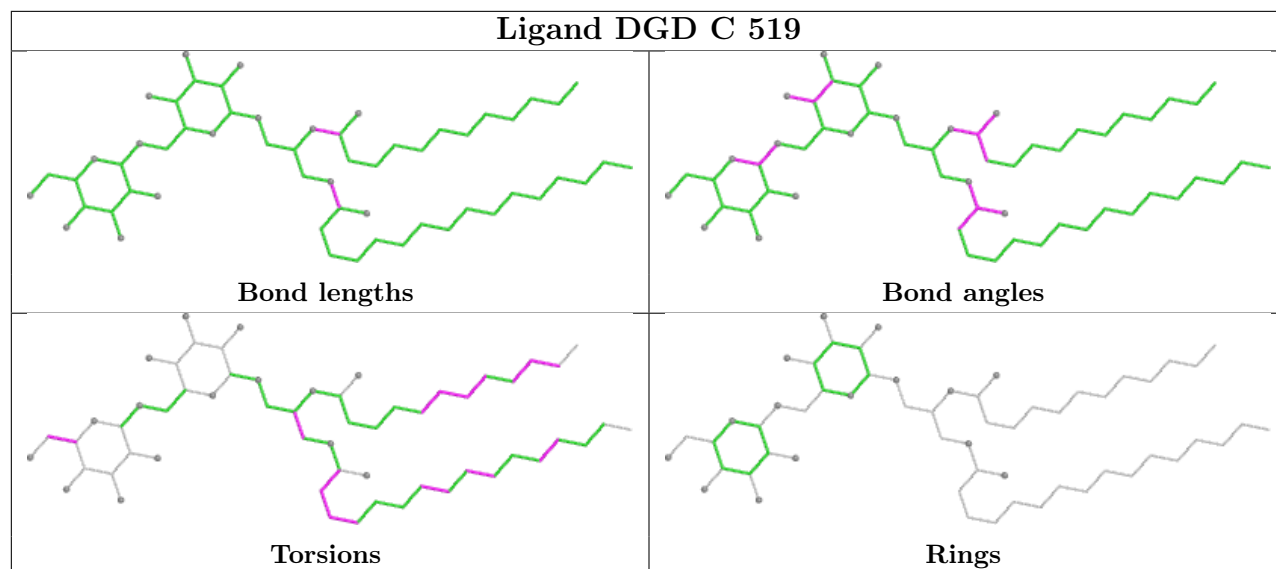


## Ligand CLA C 508

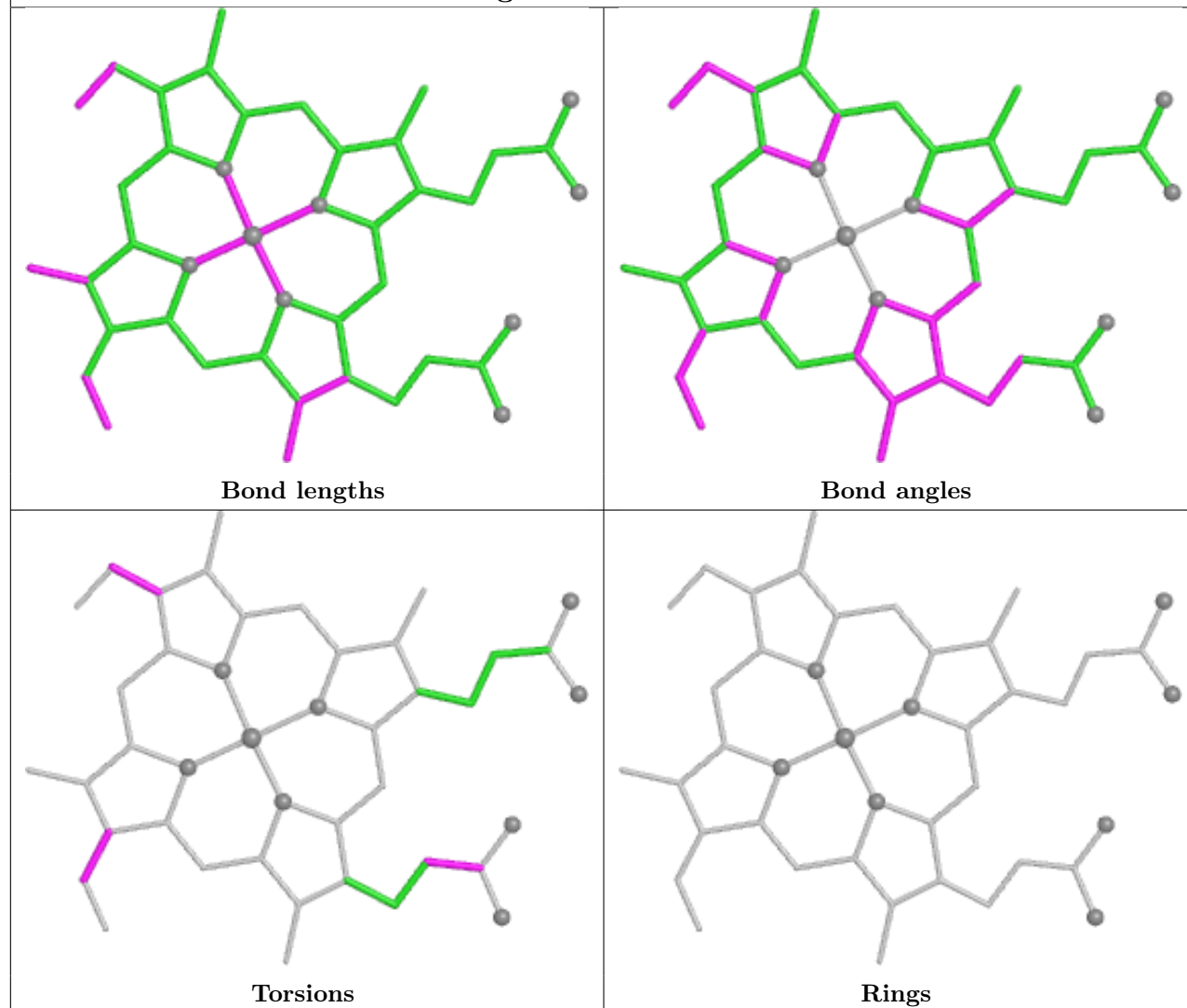


## Ligand HTG H 101

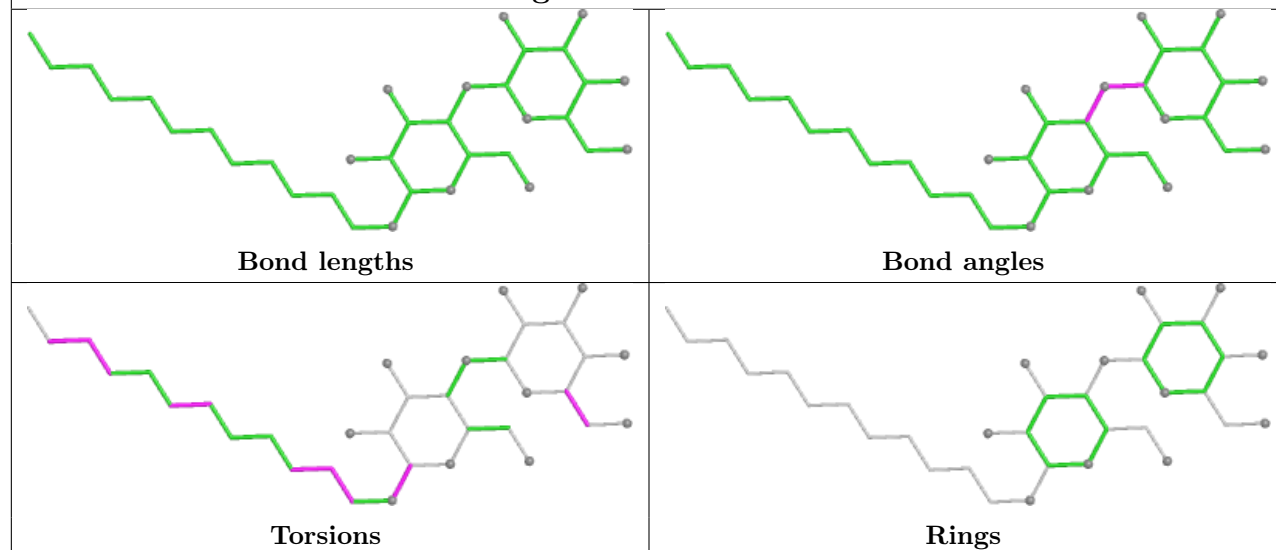


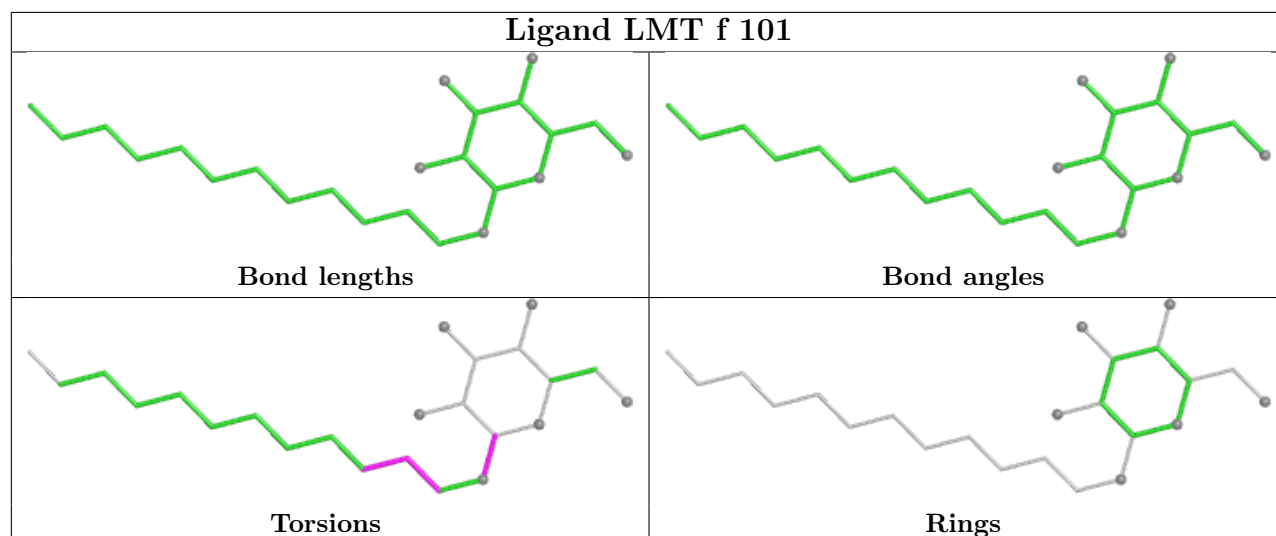
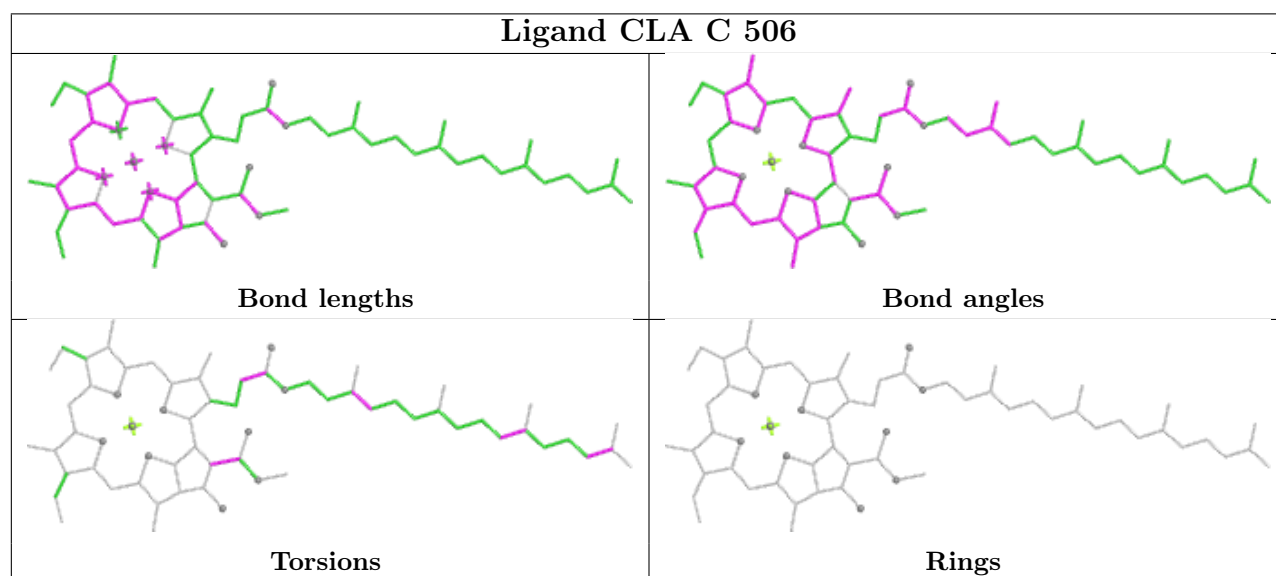
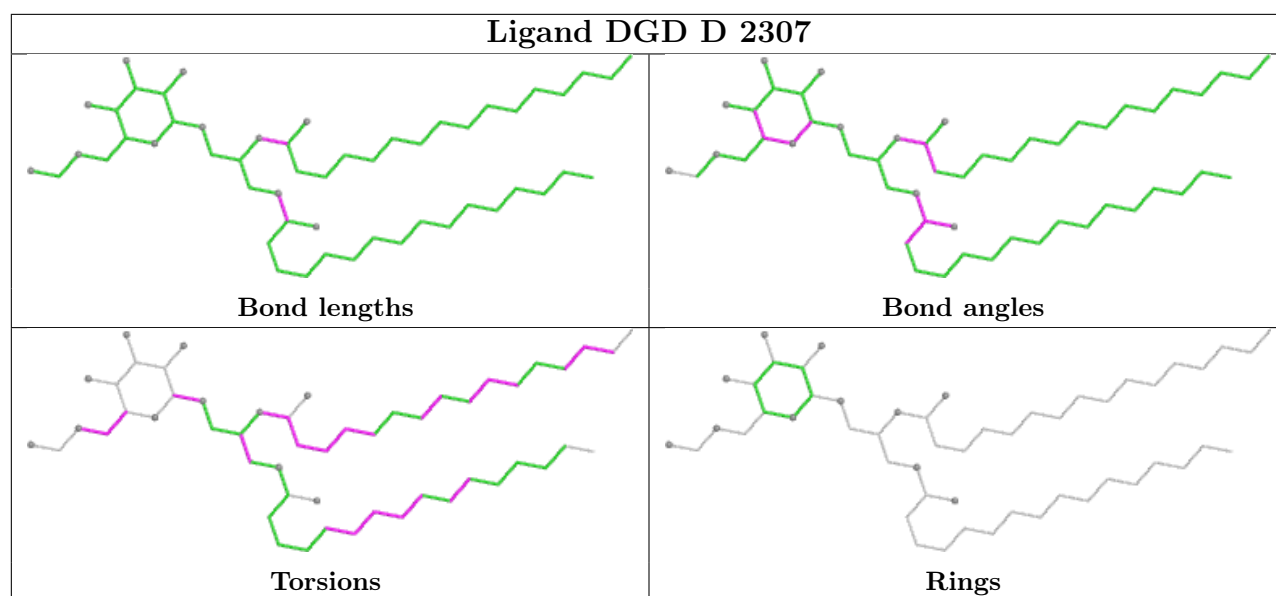


## Ligand HEC v 201



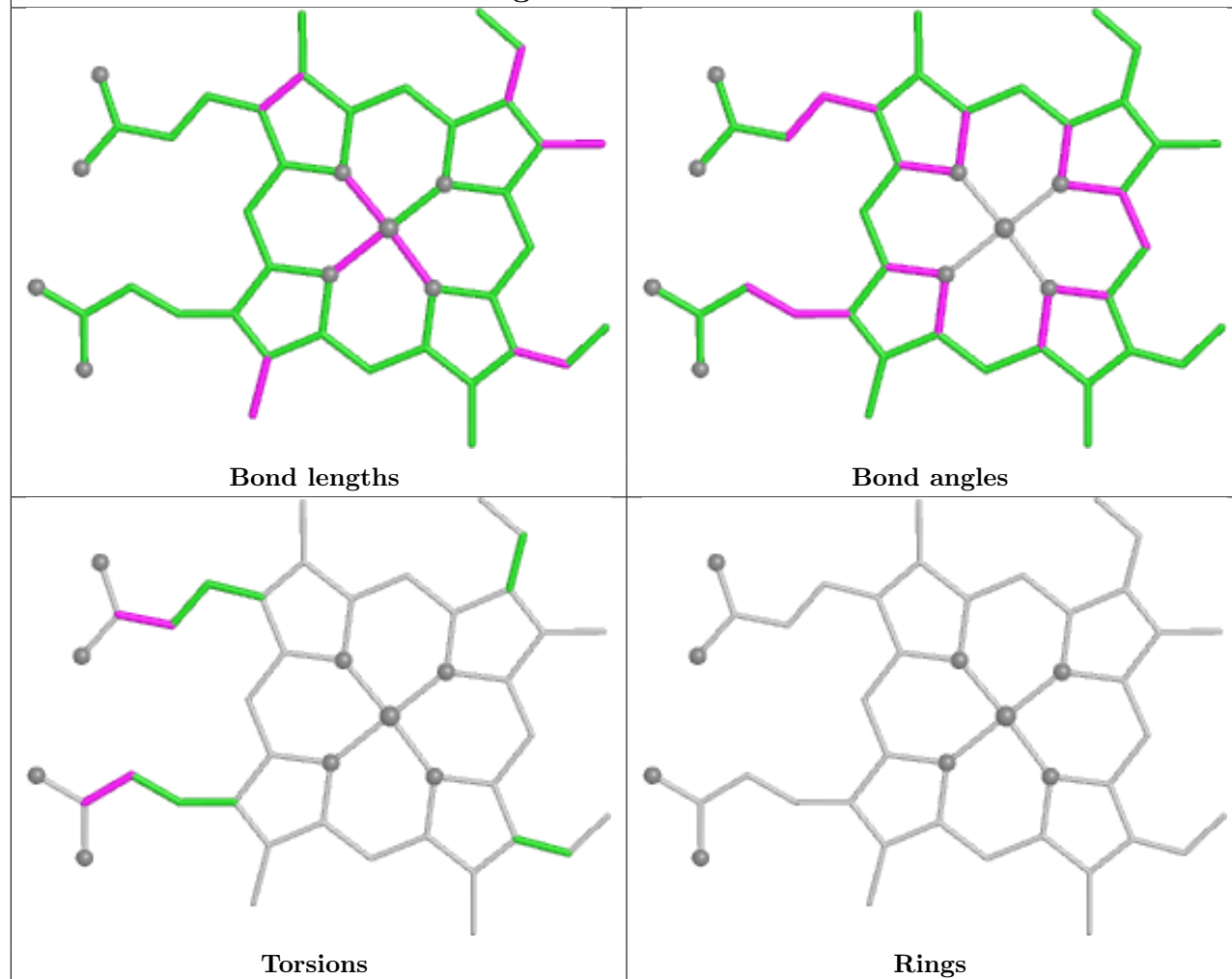
## Ligand LMT d 401



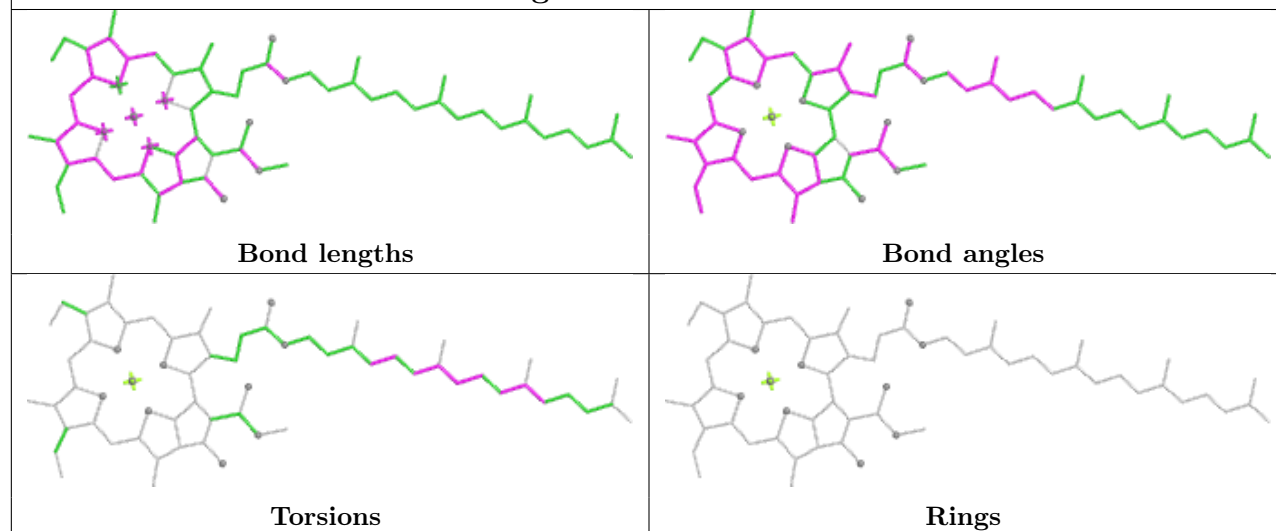


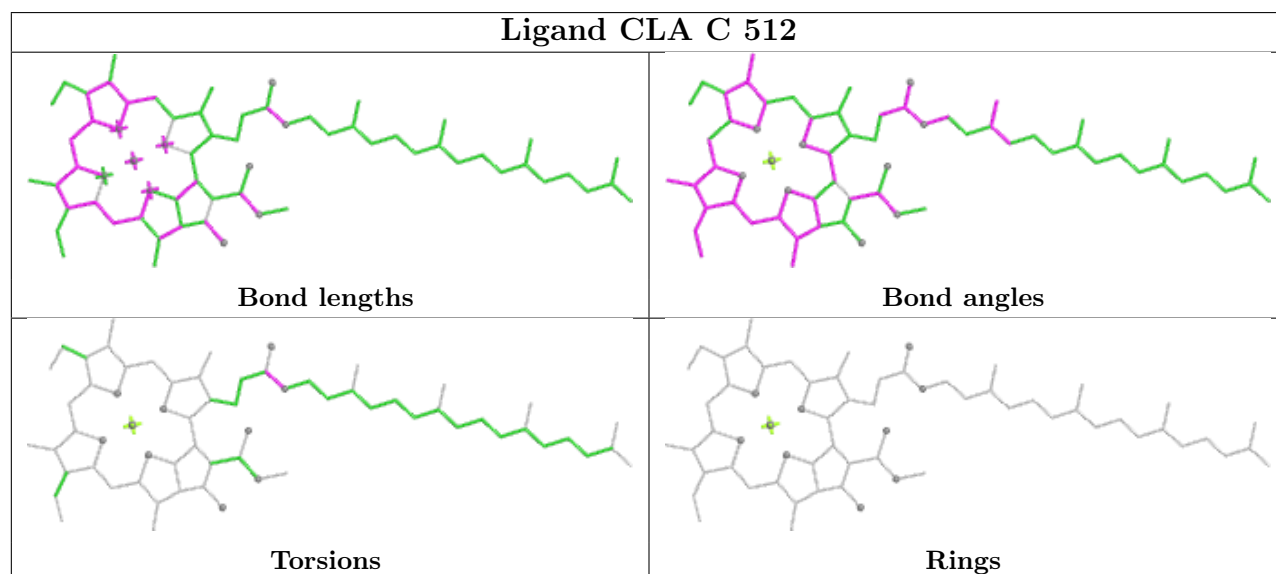
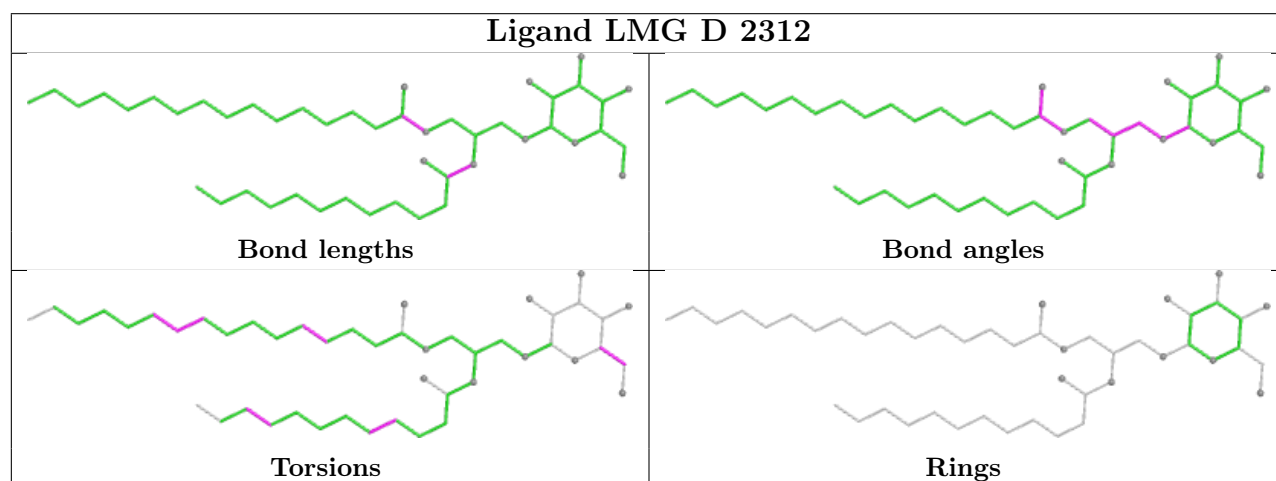
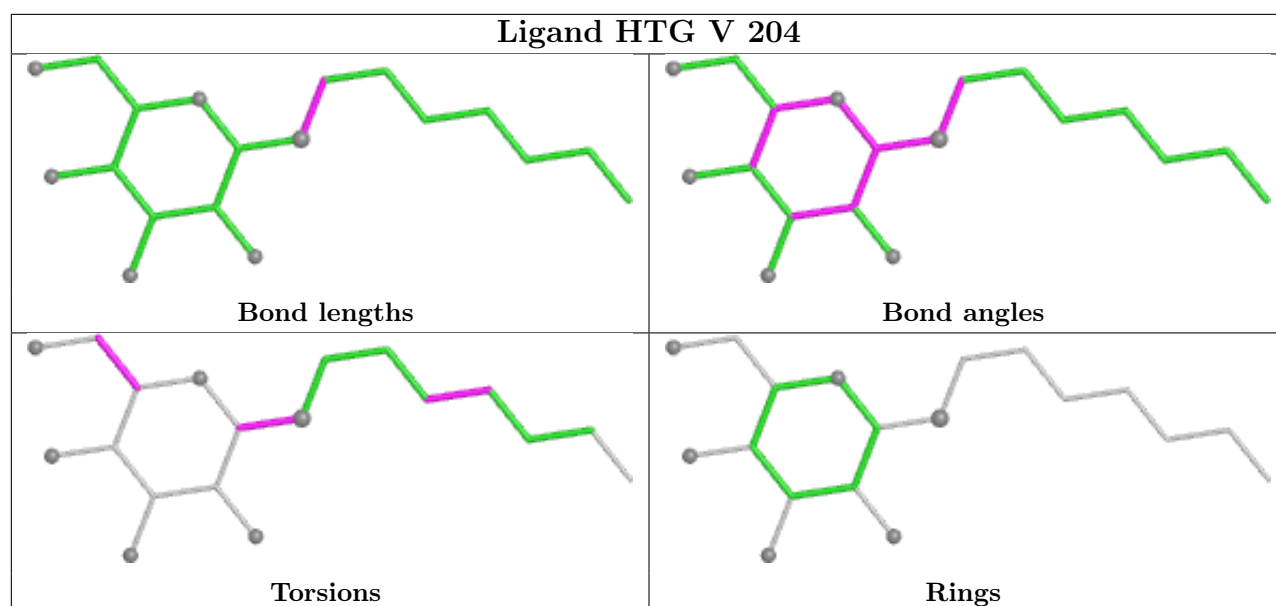


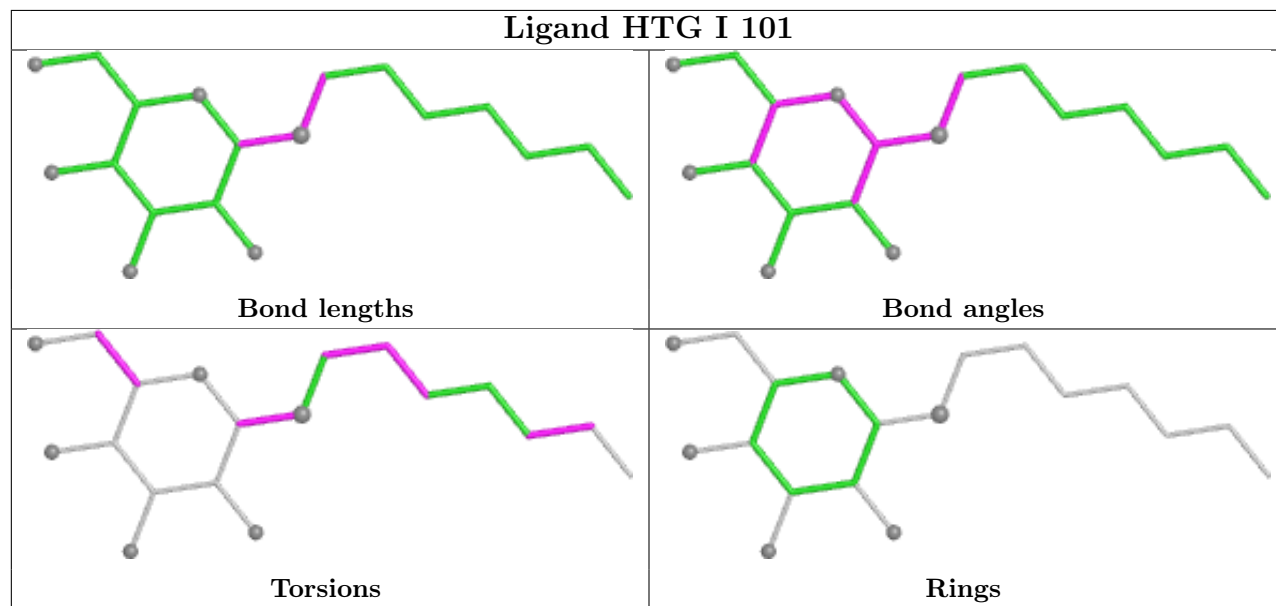
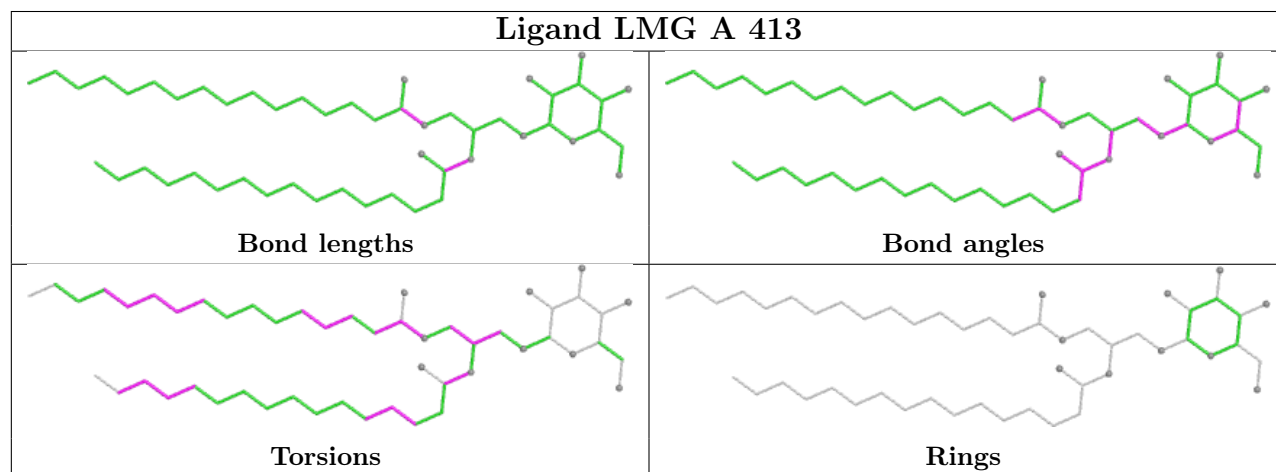
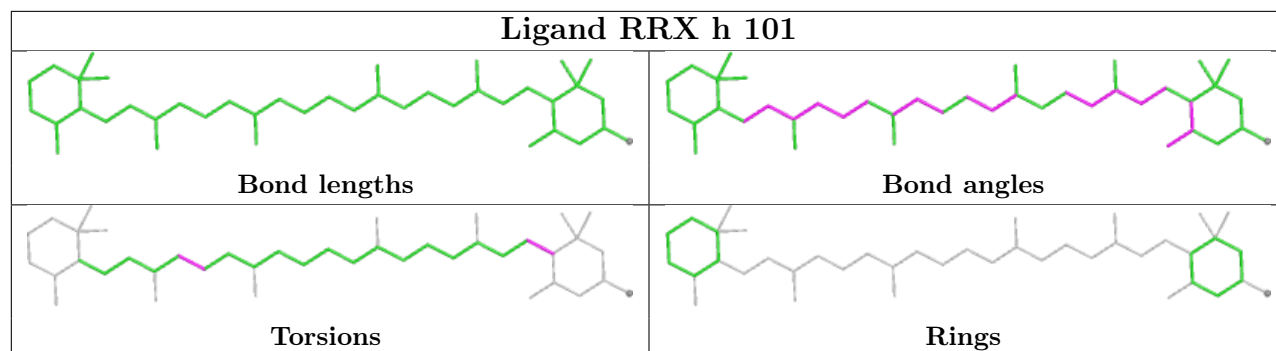
## Ligand HEM e 103



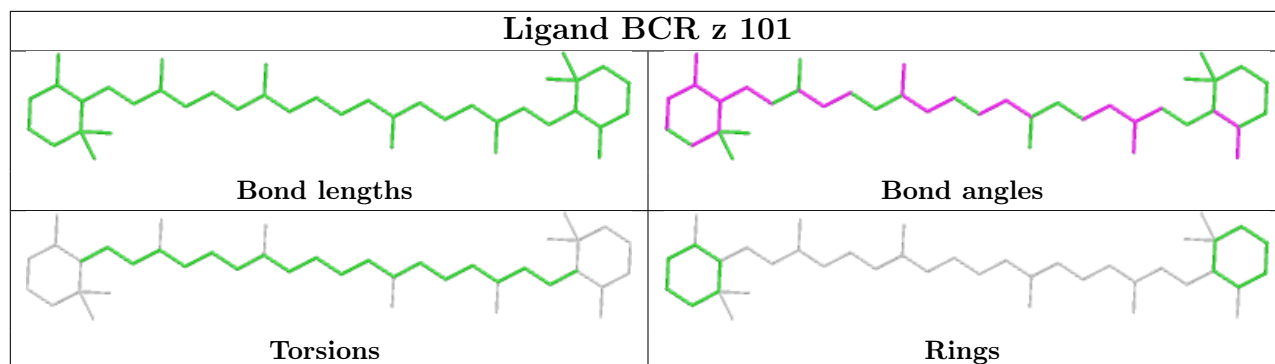
## Ligand CLA A 410



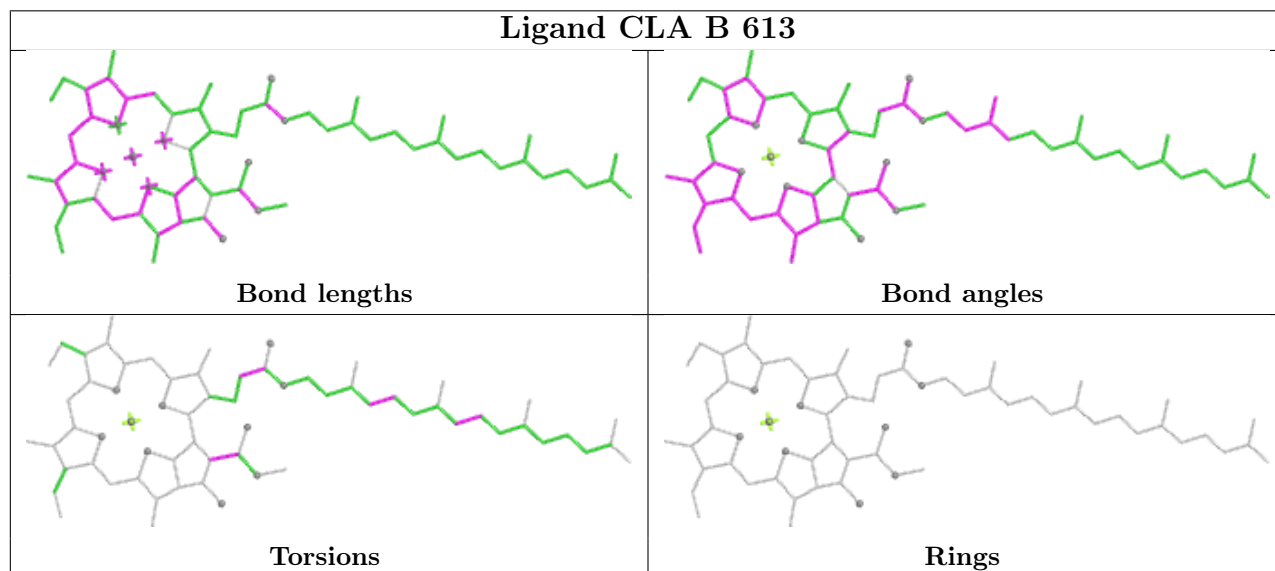




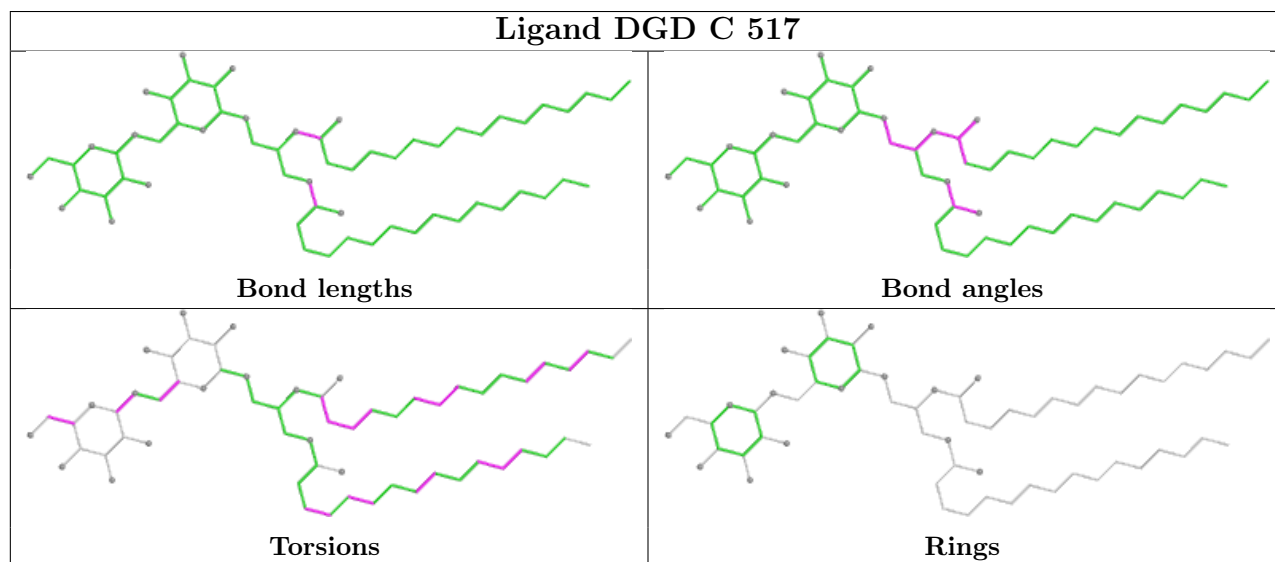
## Ligand BCR z 101

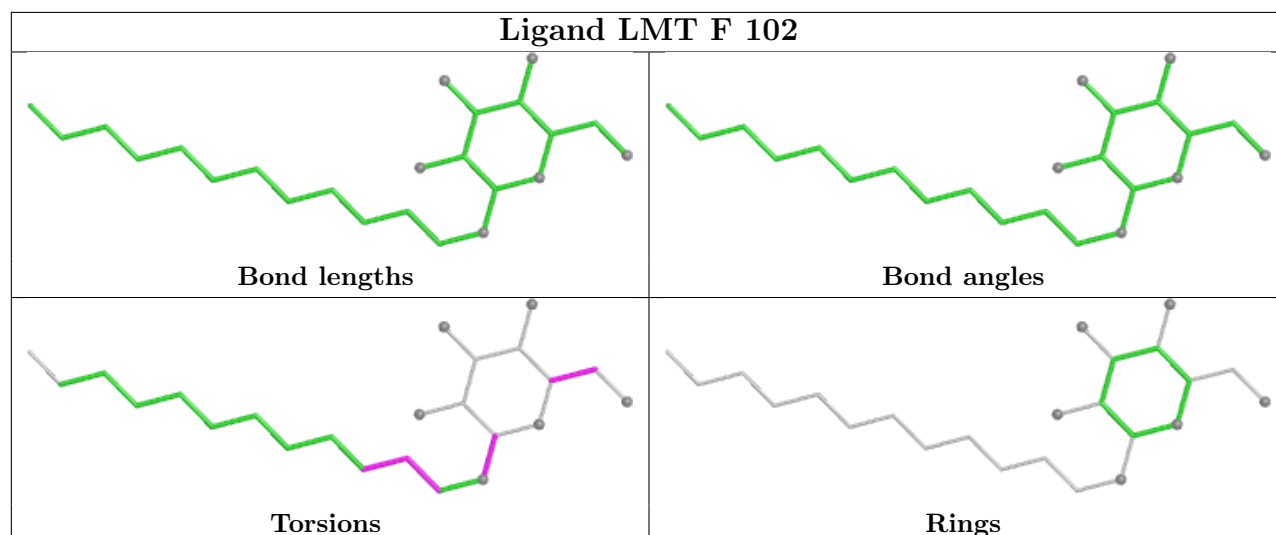
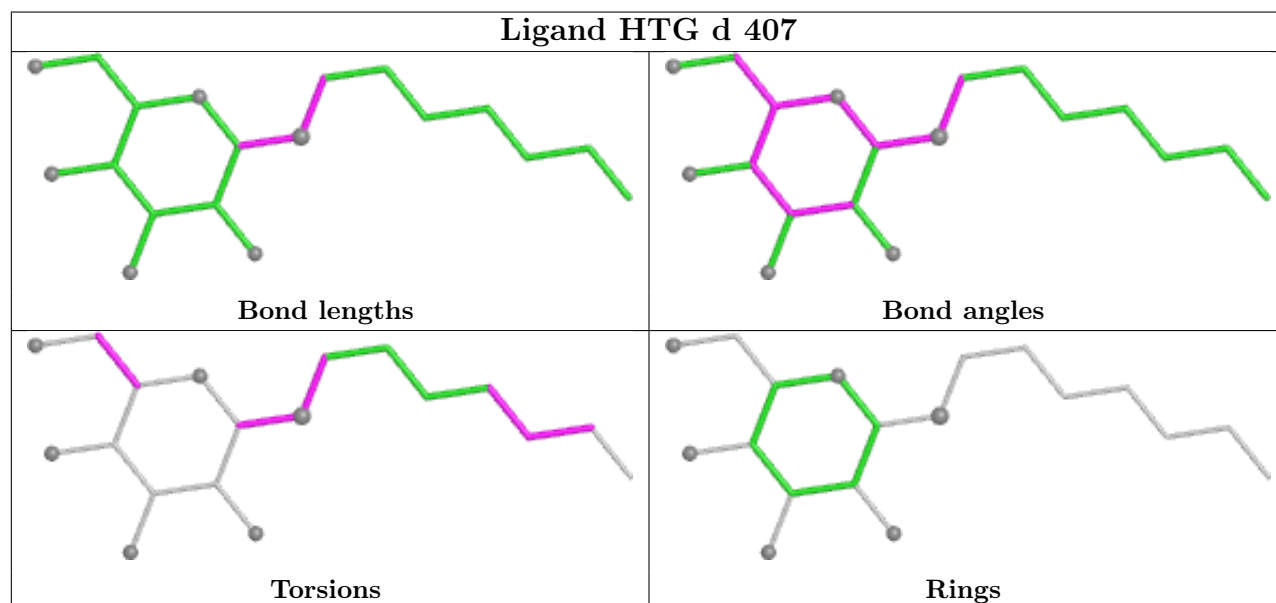
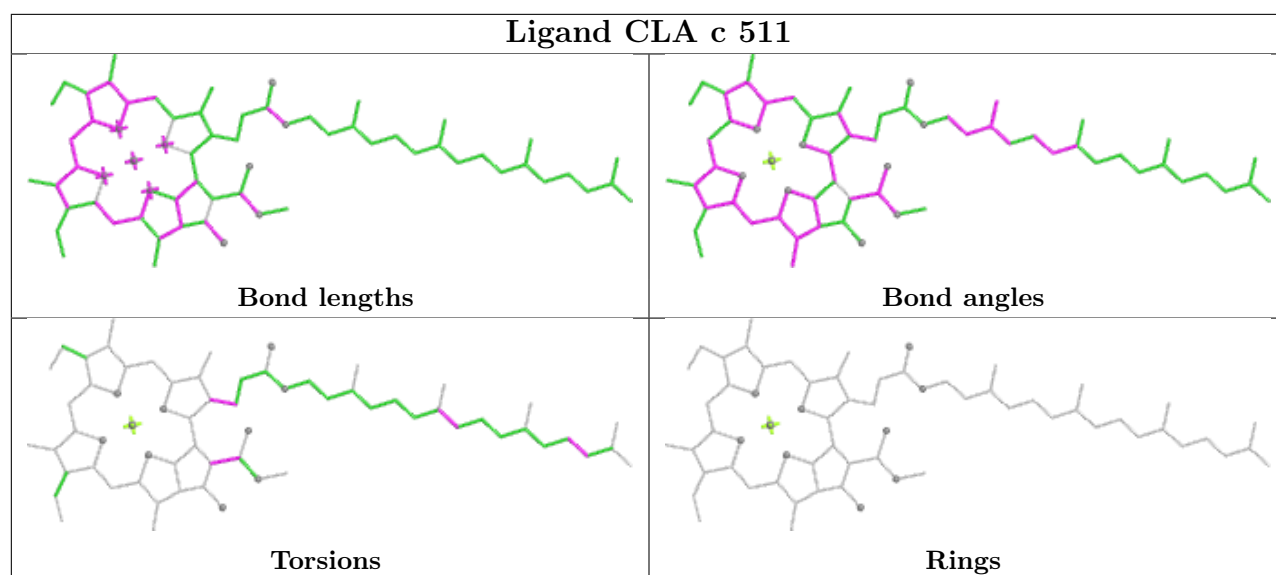


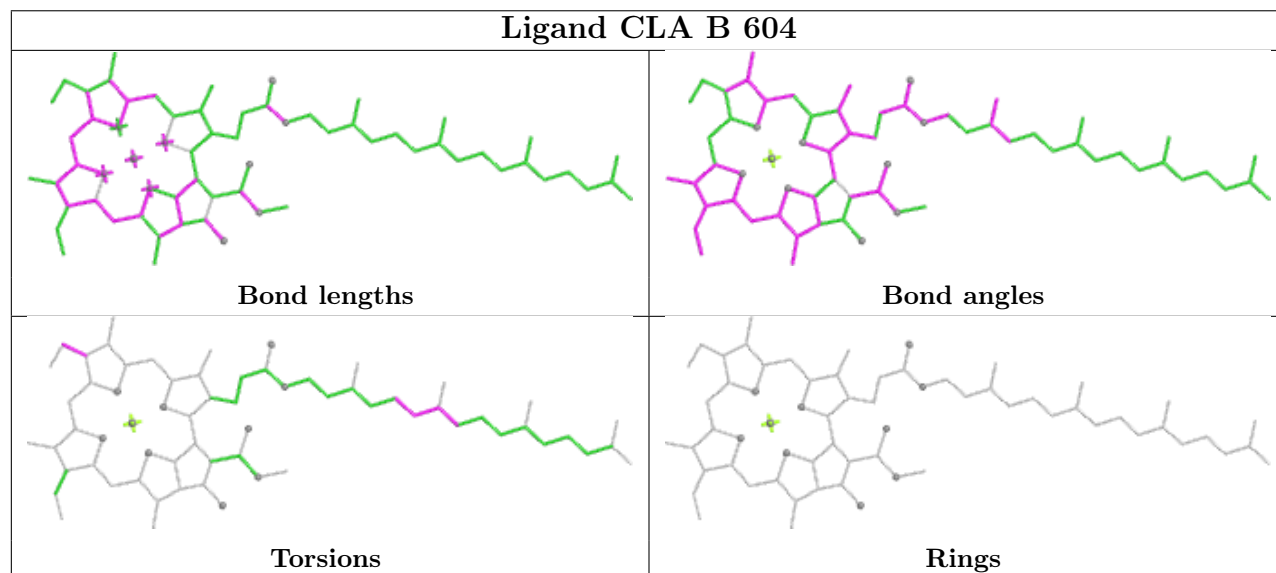
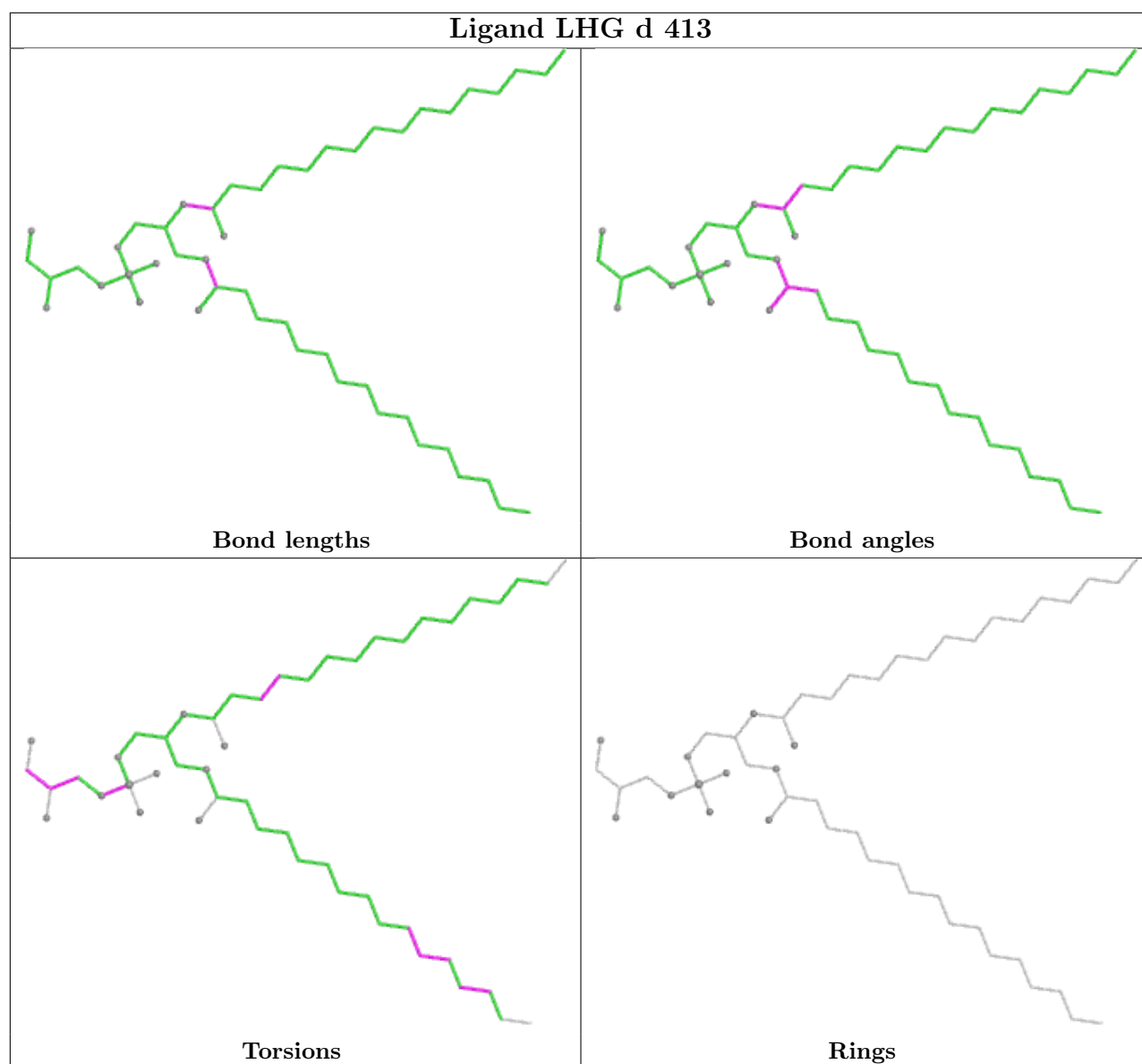
## Ligand CLA B 613



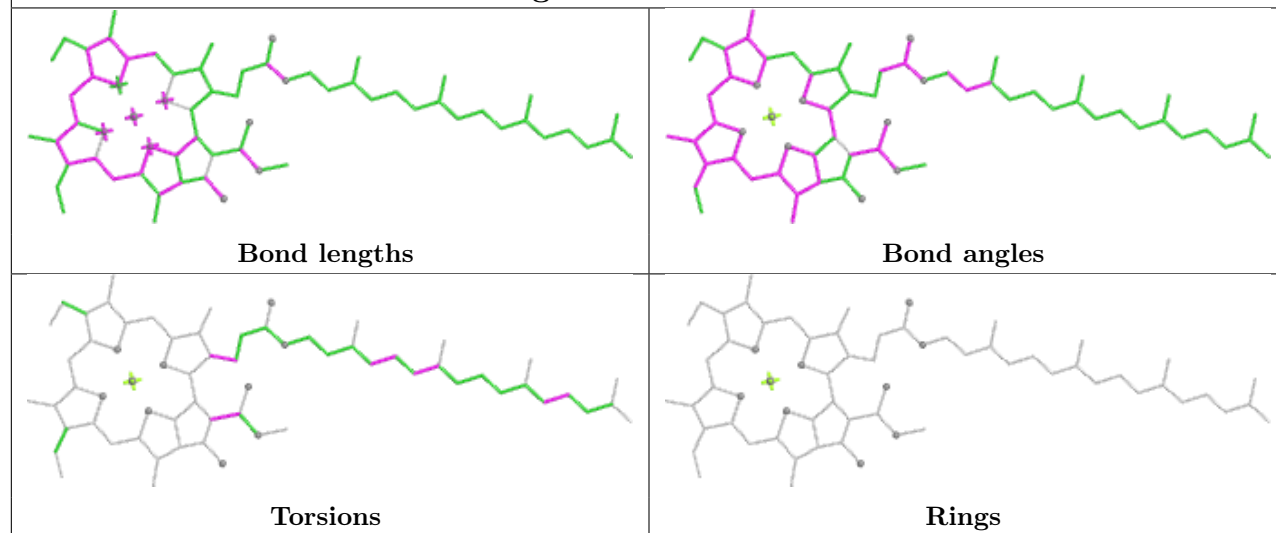
## Ligand DGD C 517



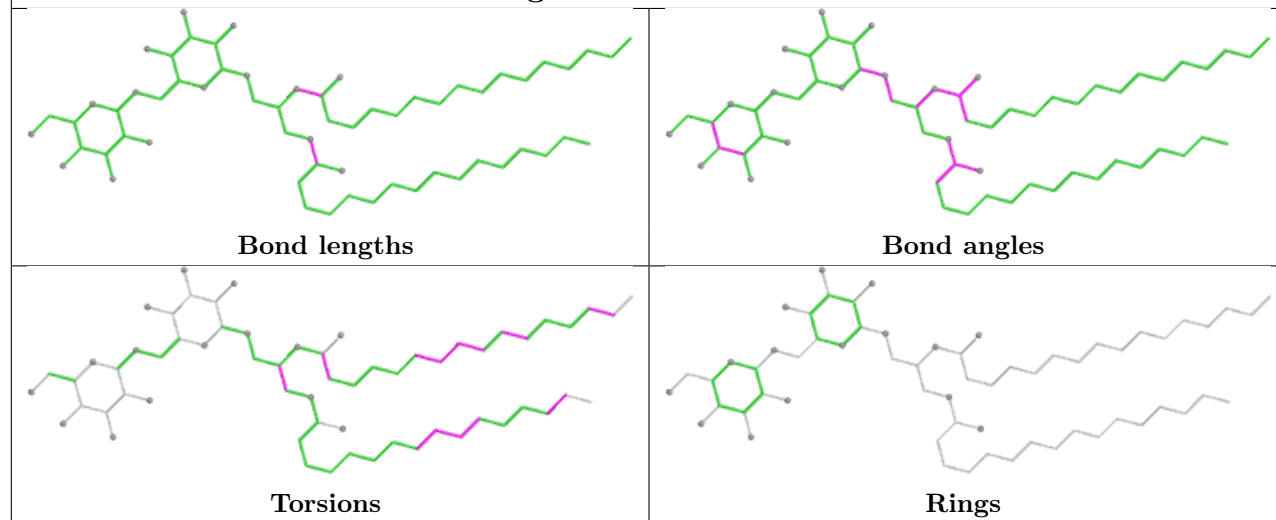


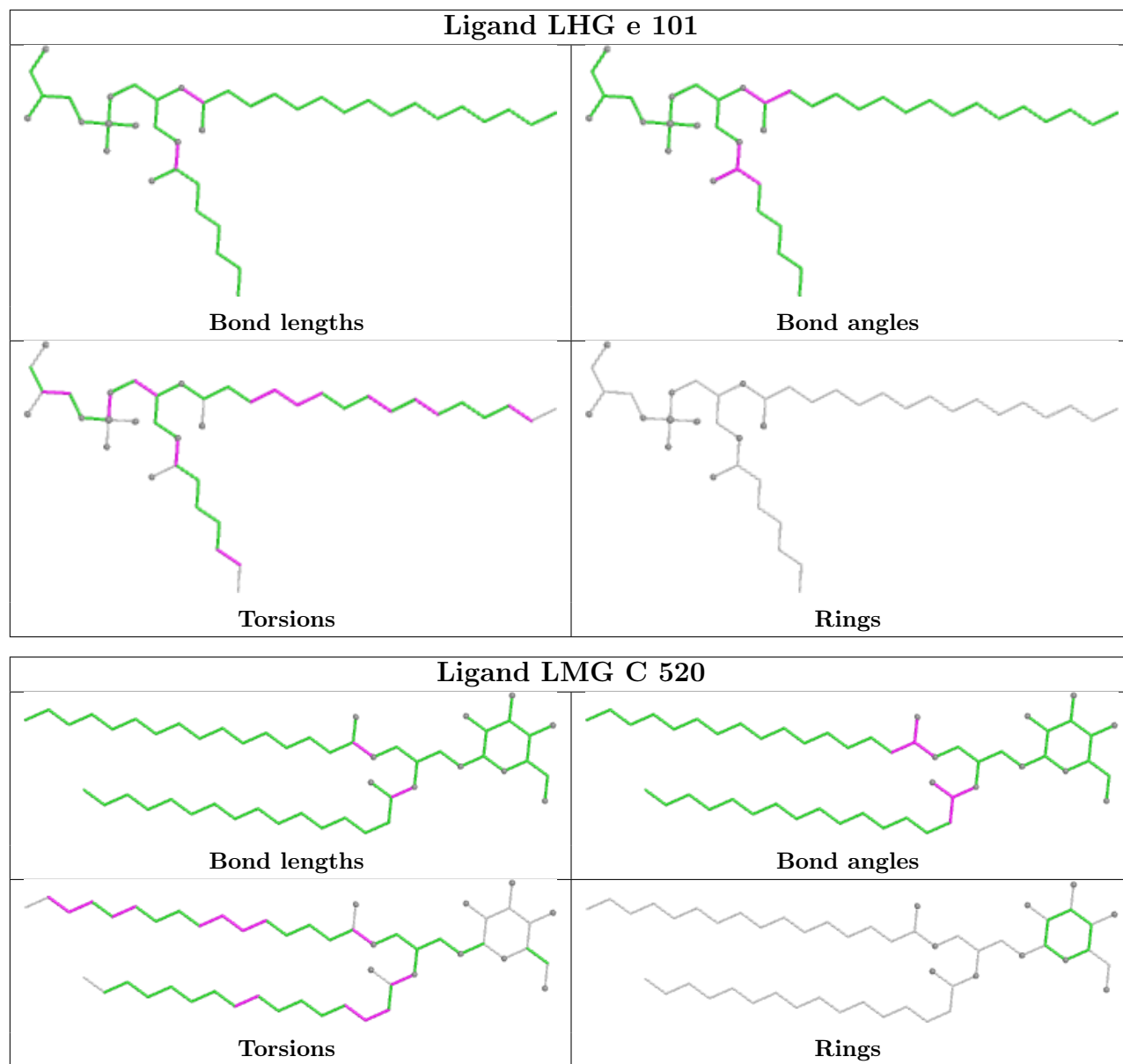


## Ligand CLA B 605

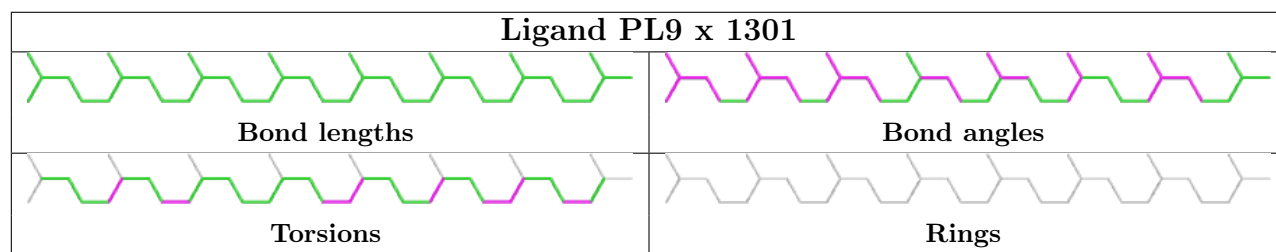
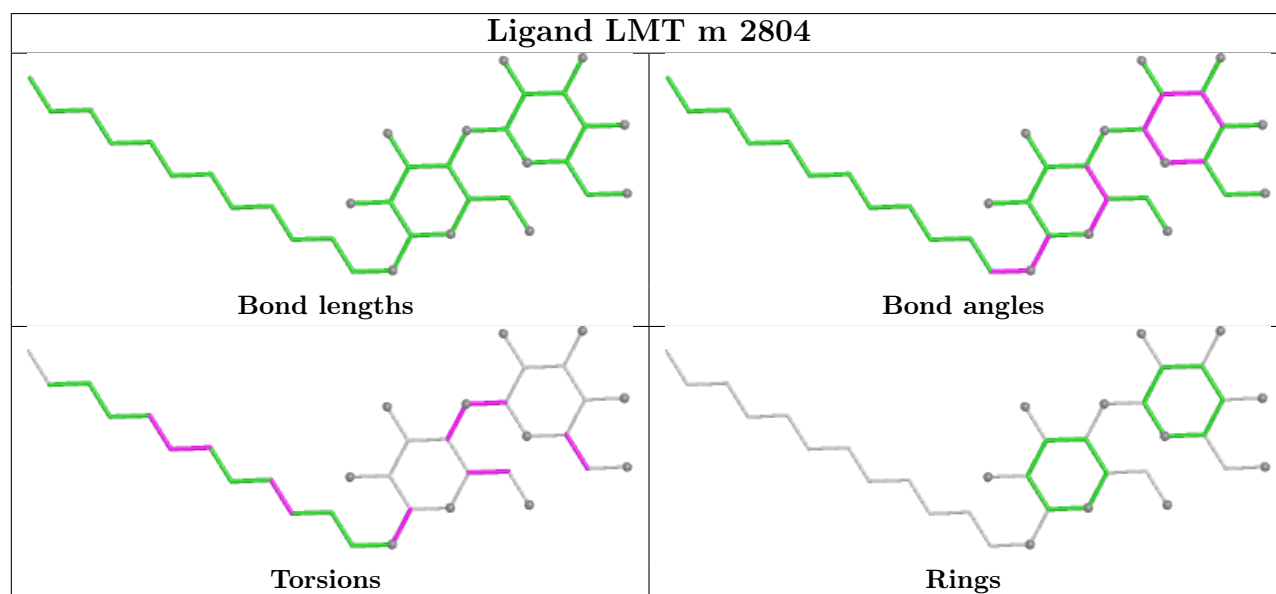
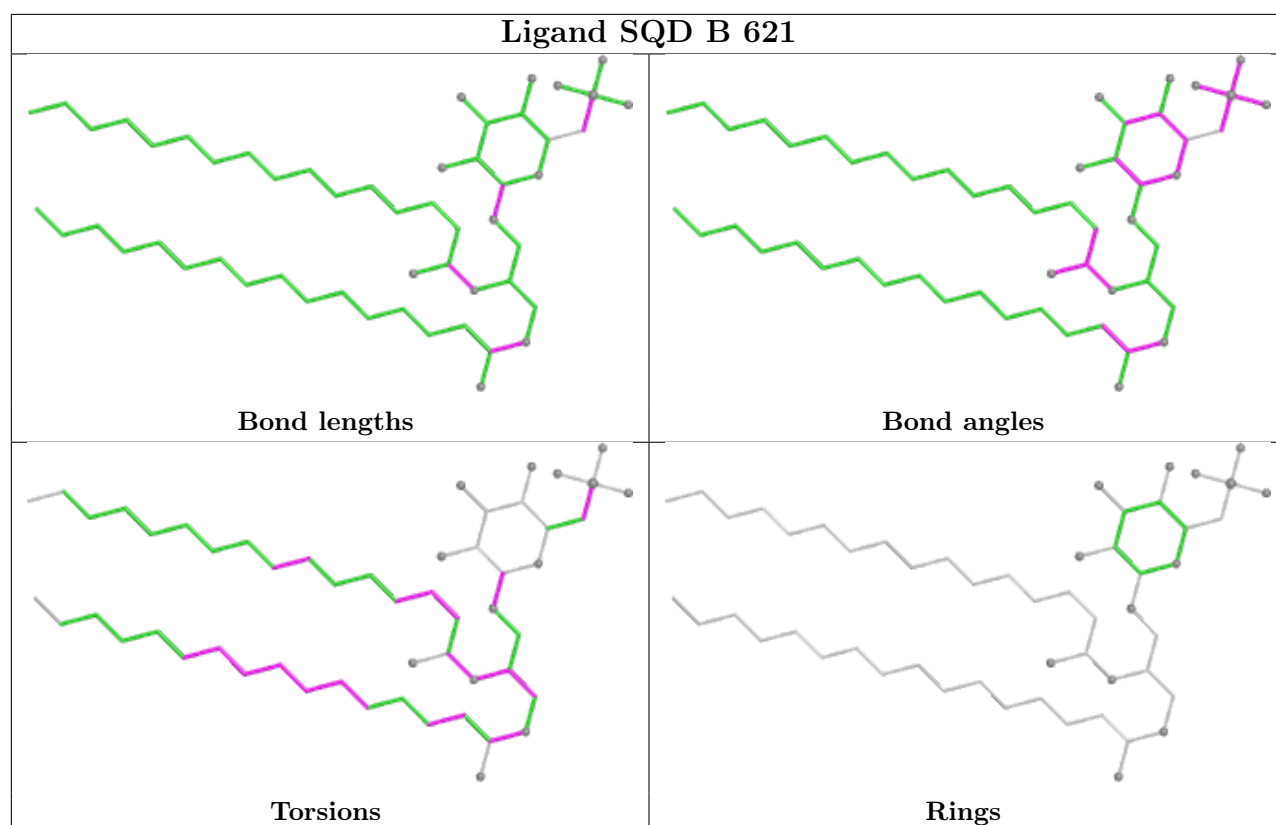


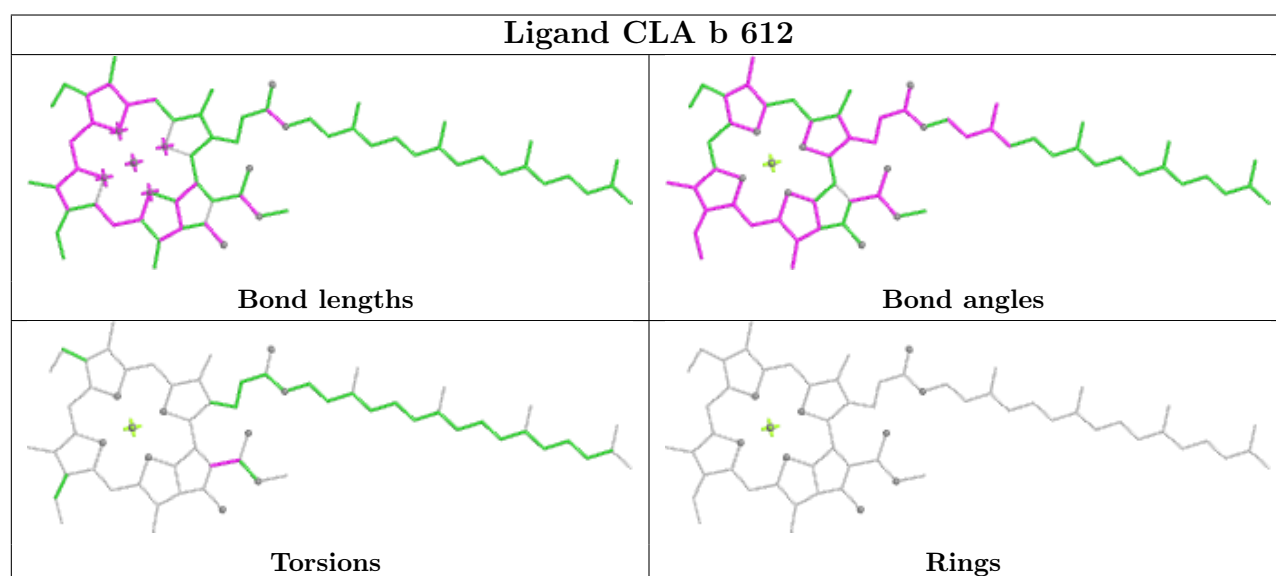
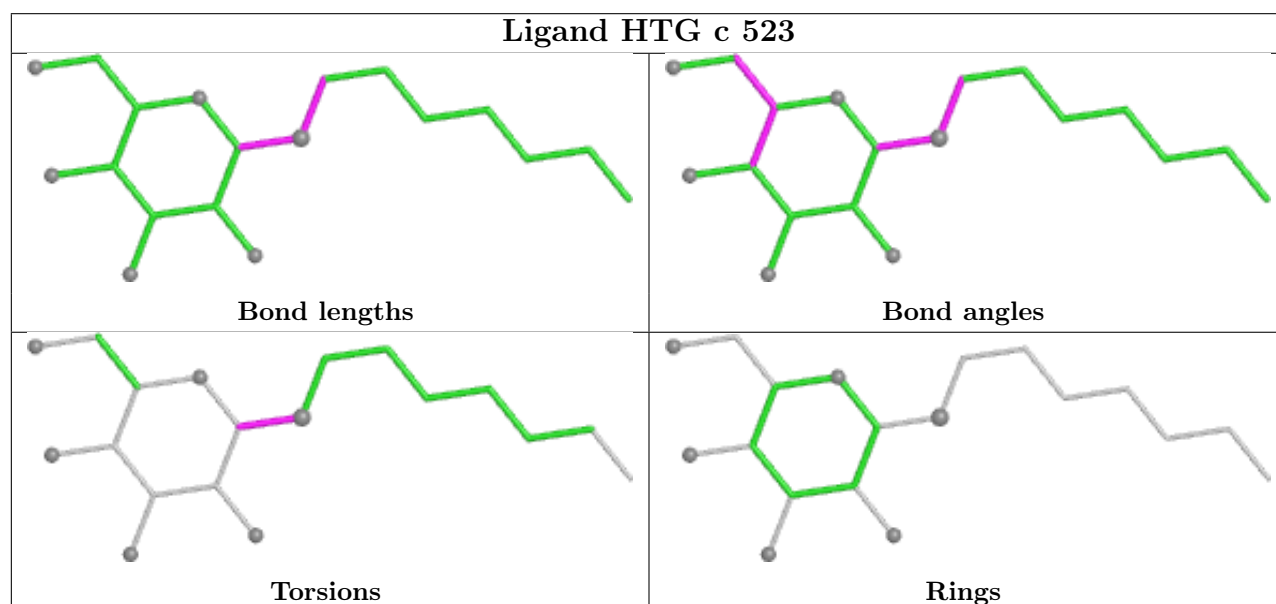
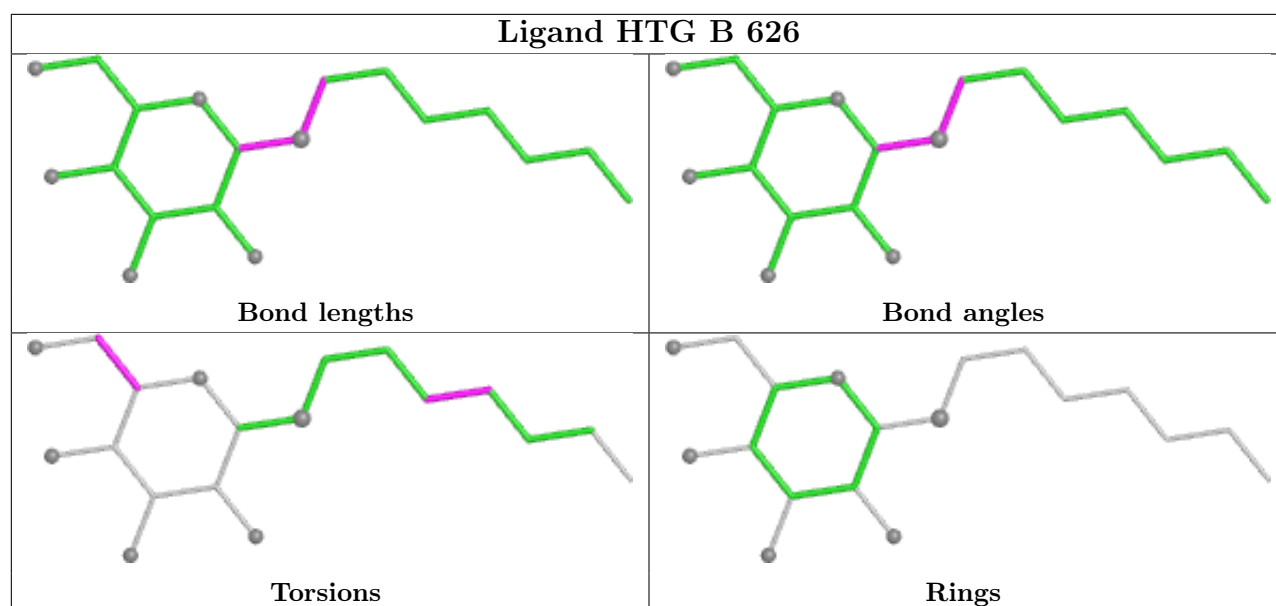
## Ligand DGD H 103

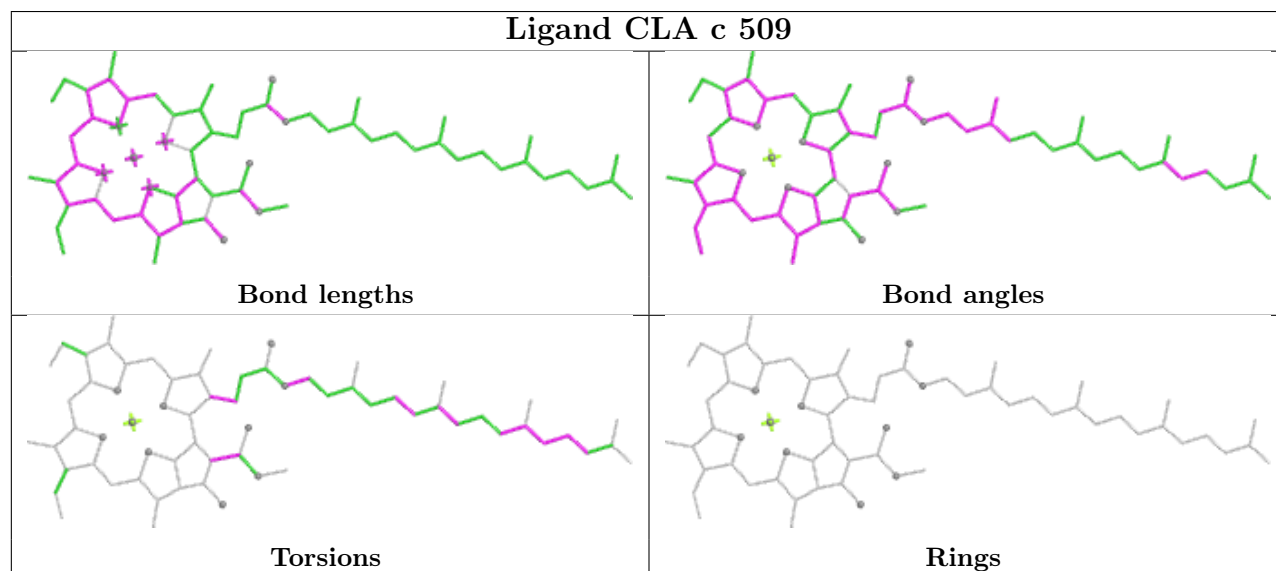
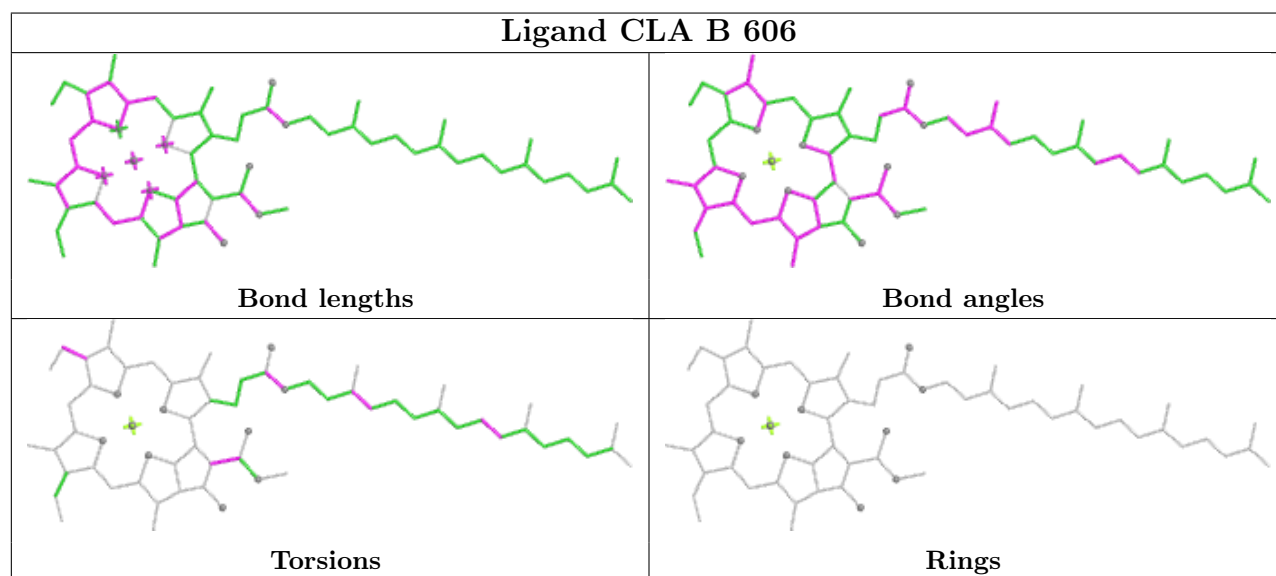
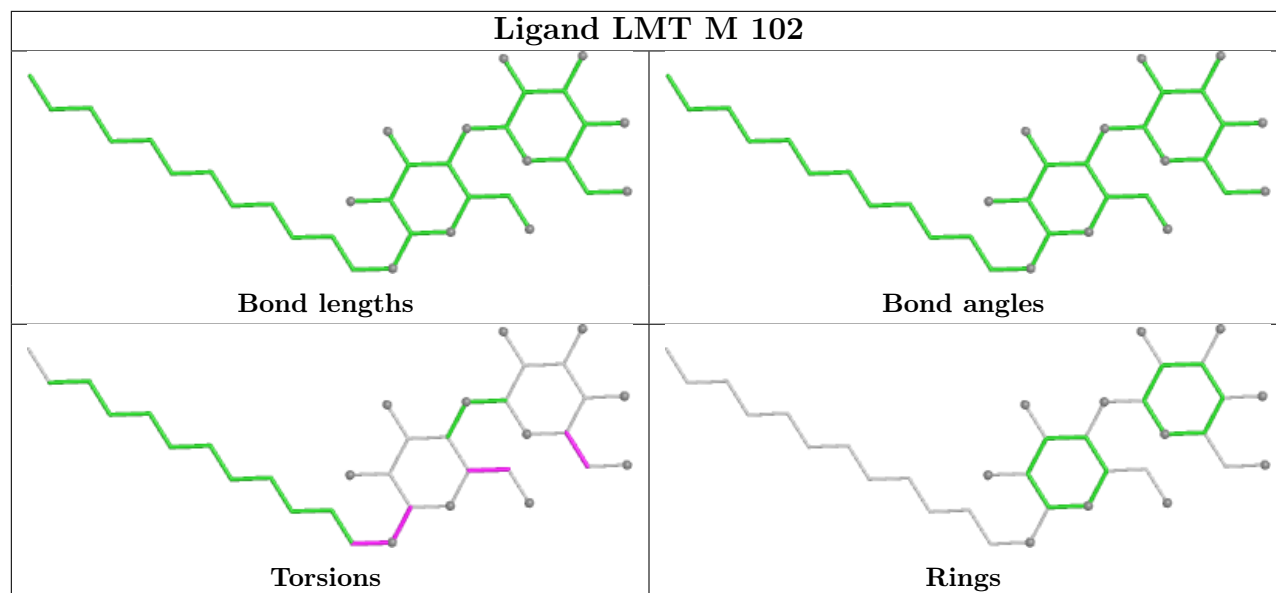


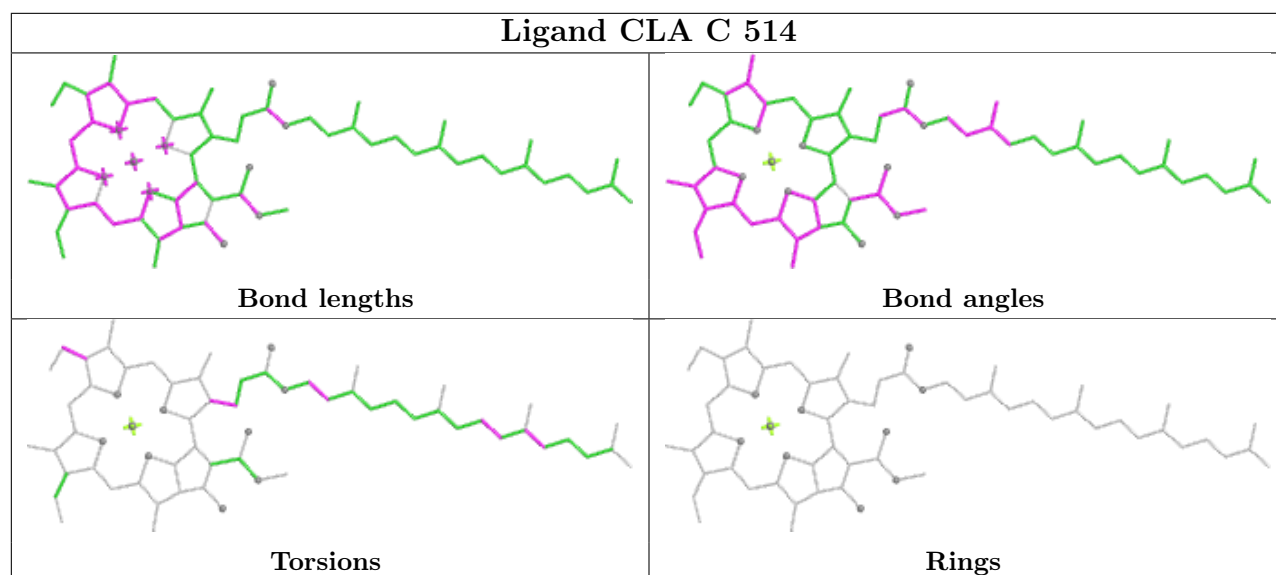
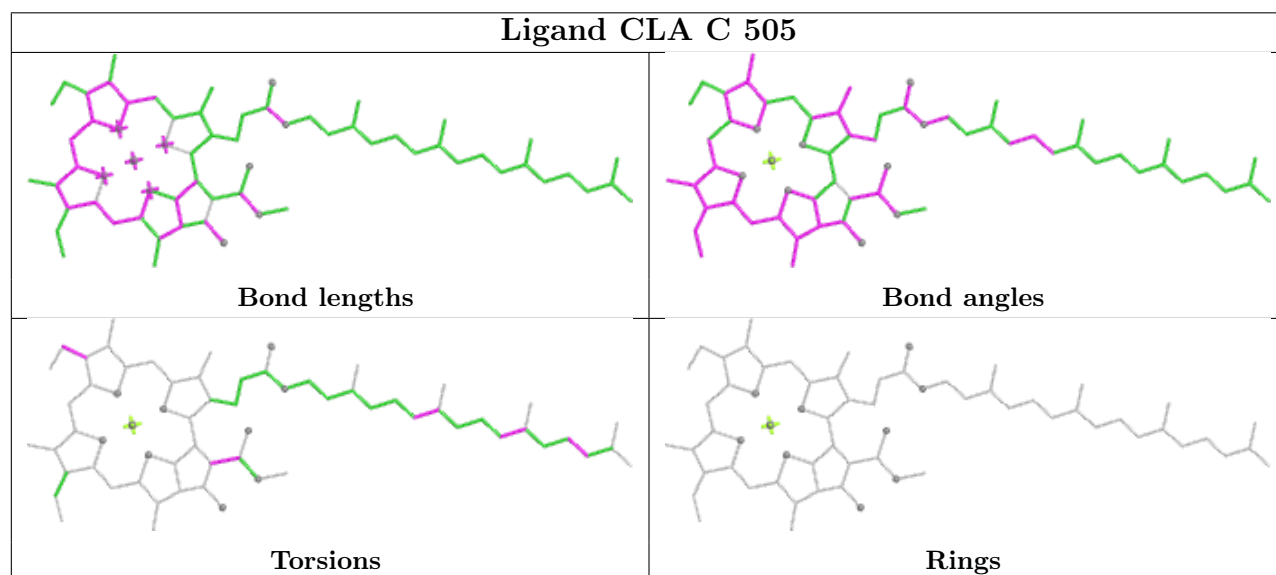
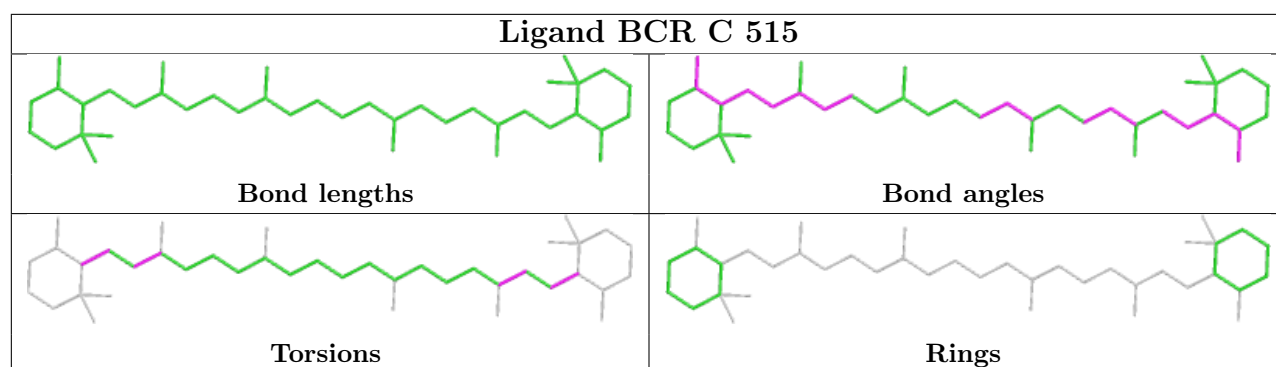


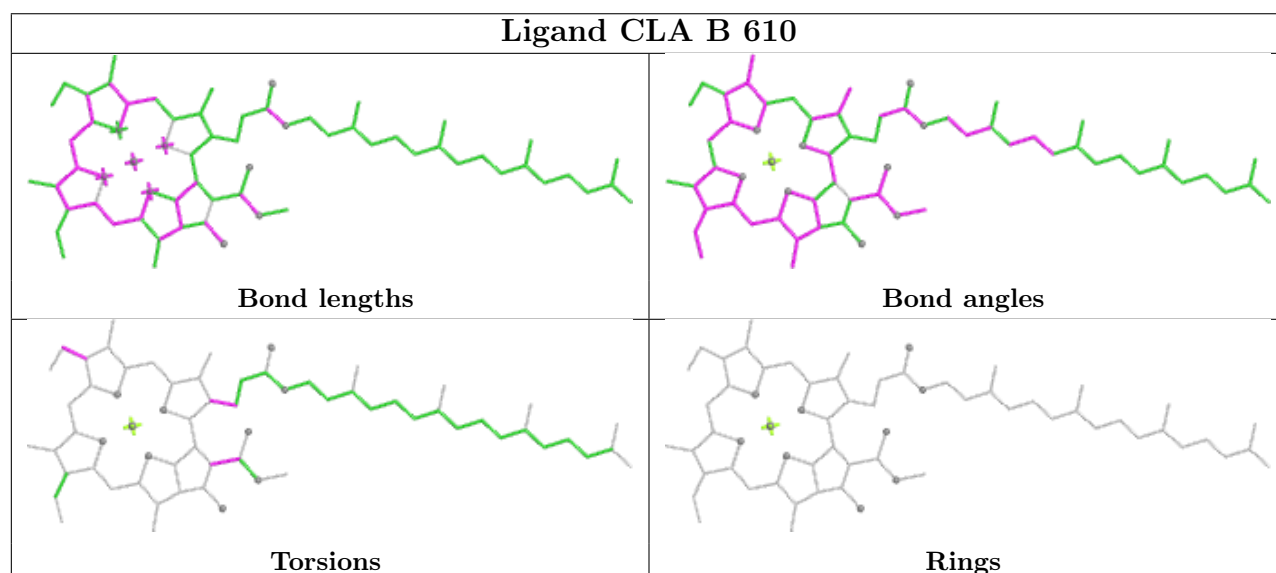
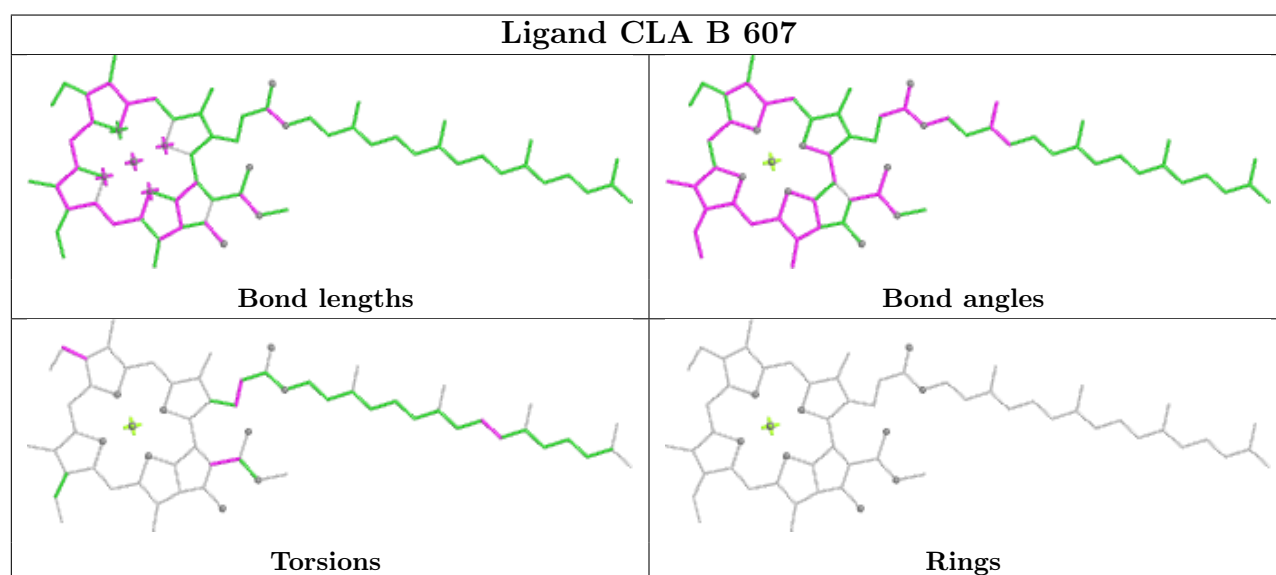
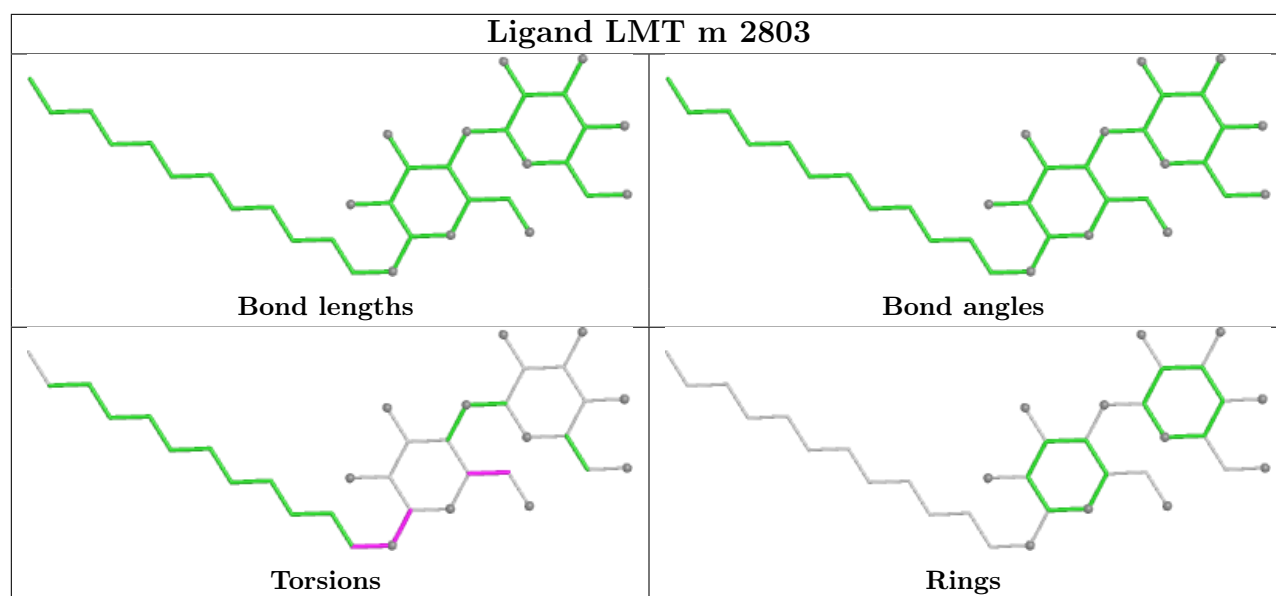


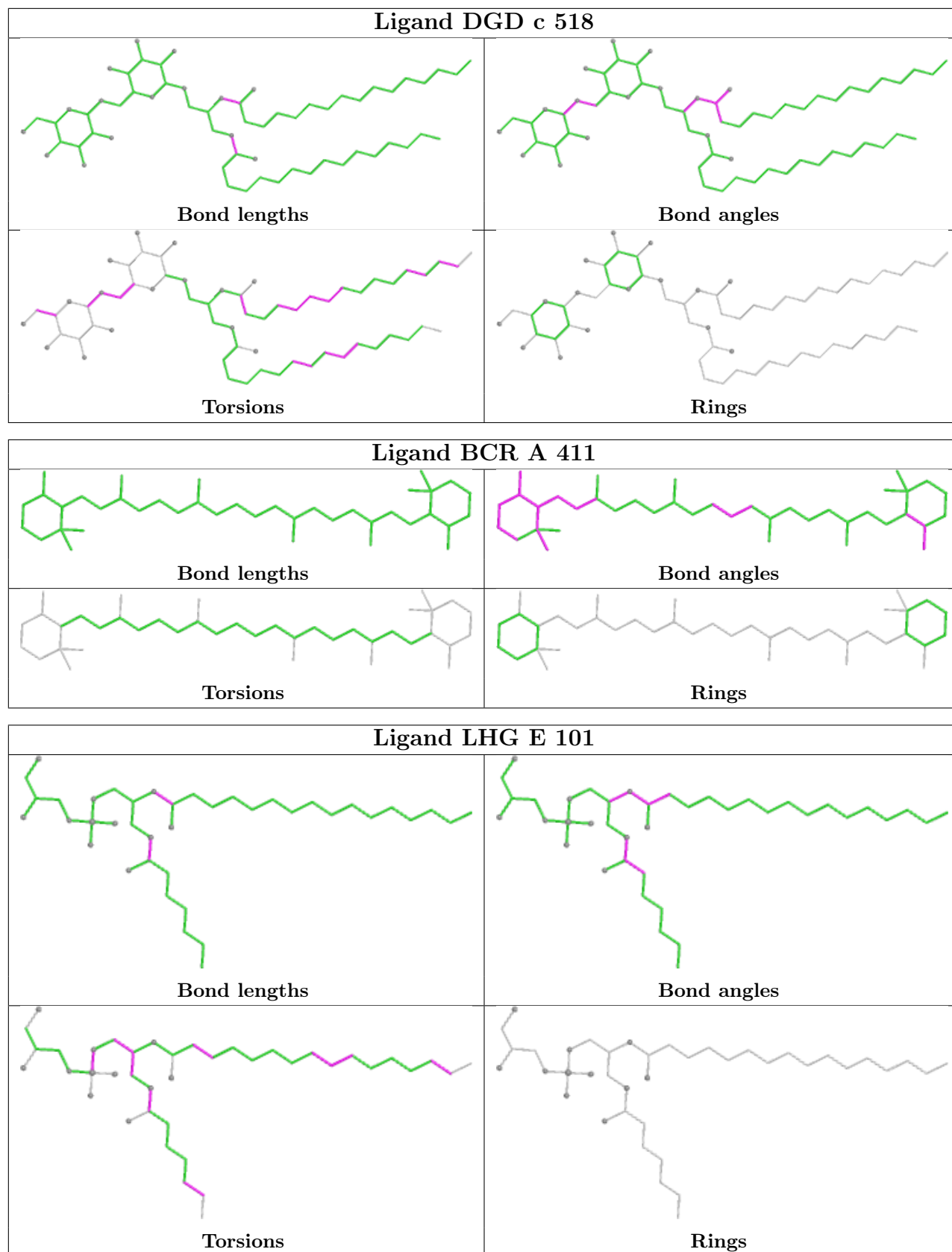




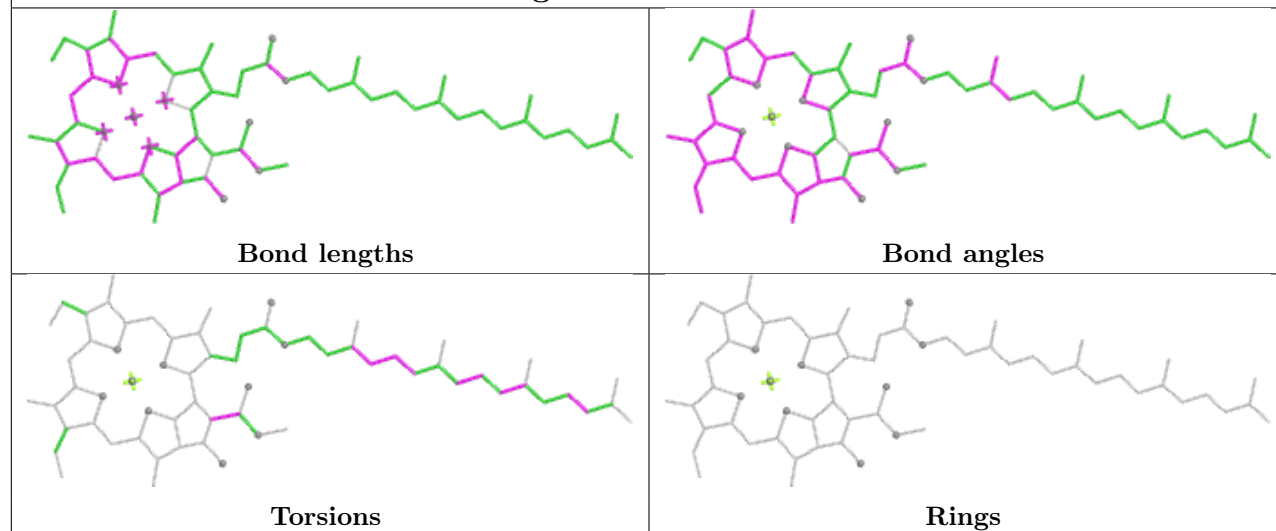




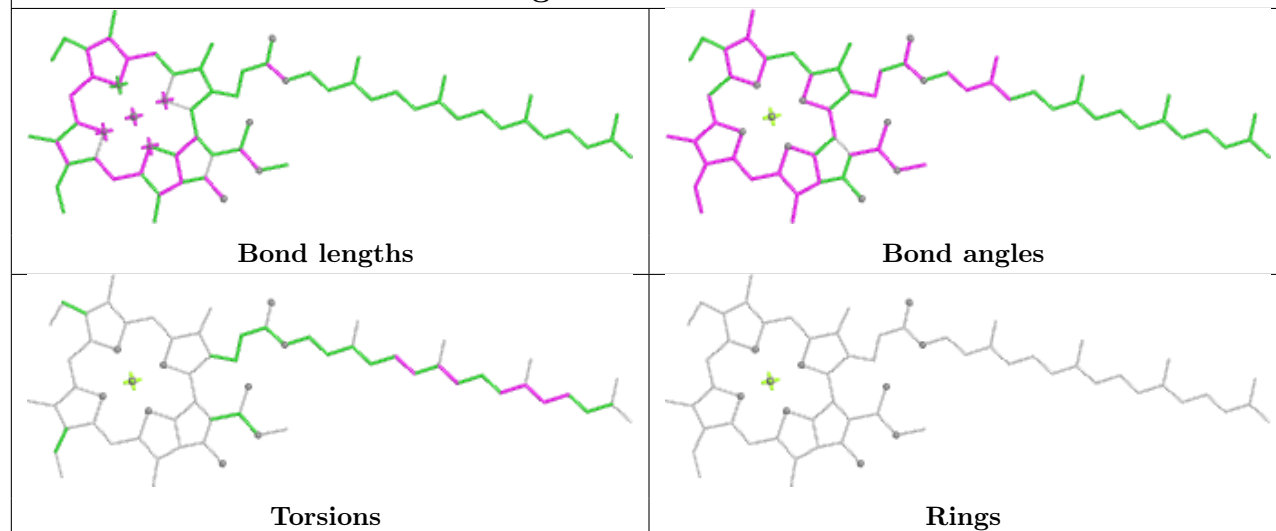




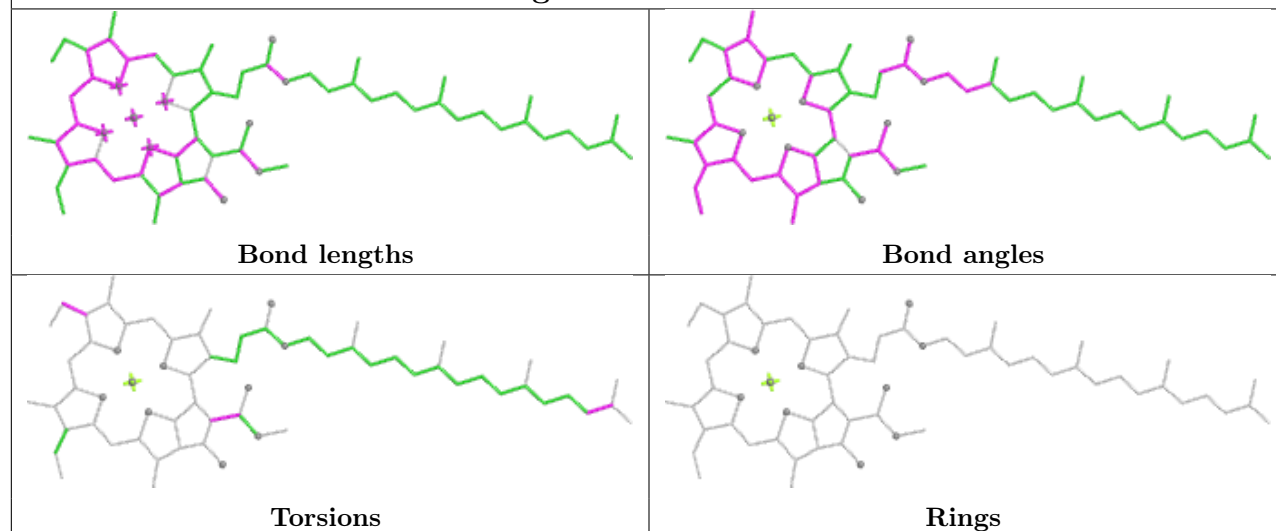
## Ligand CLA B 615

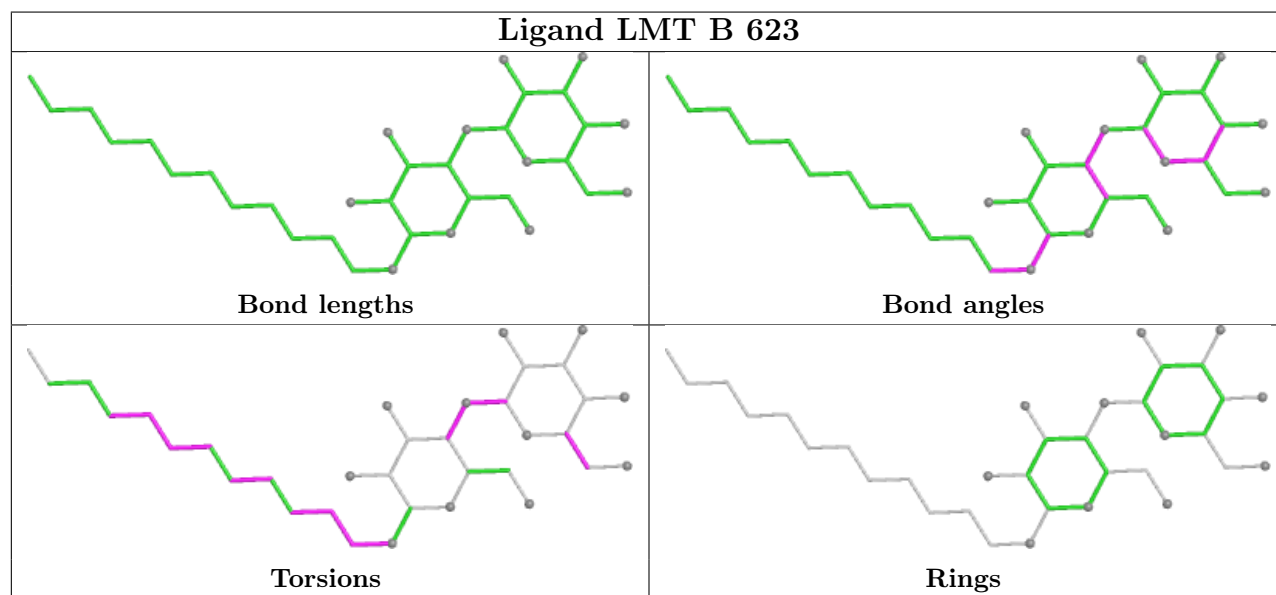
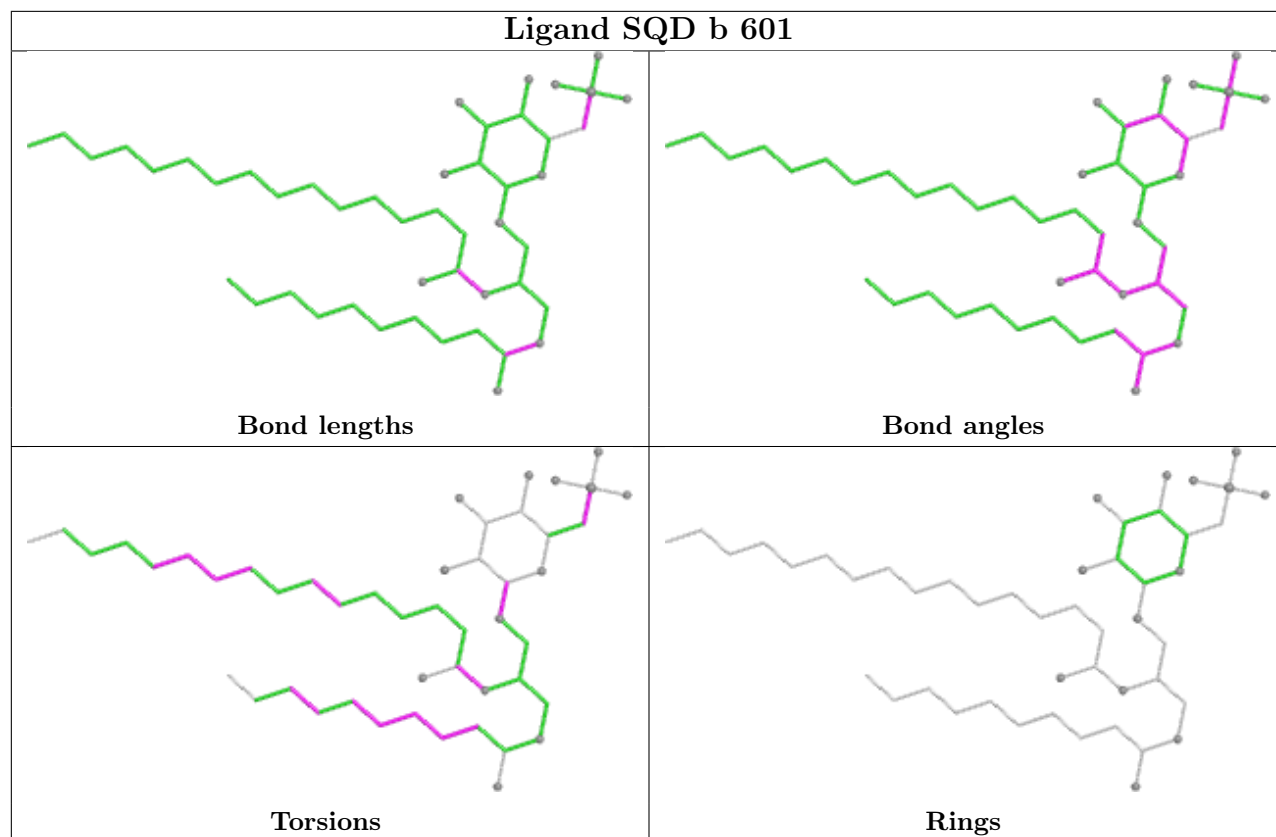


## Ligand CLA B 616

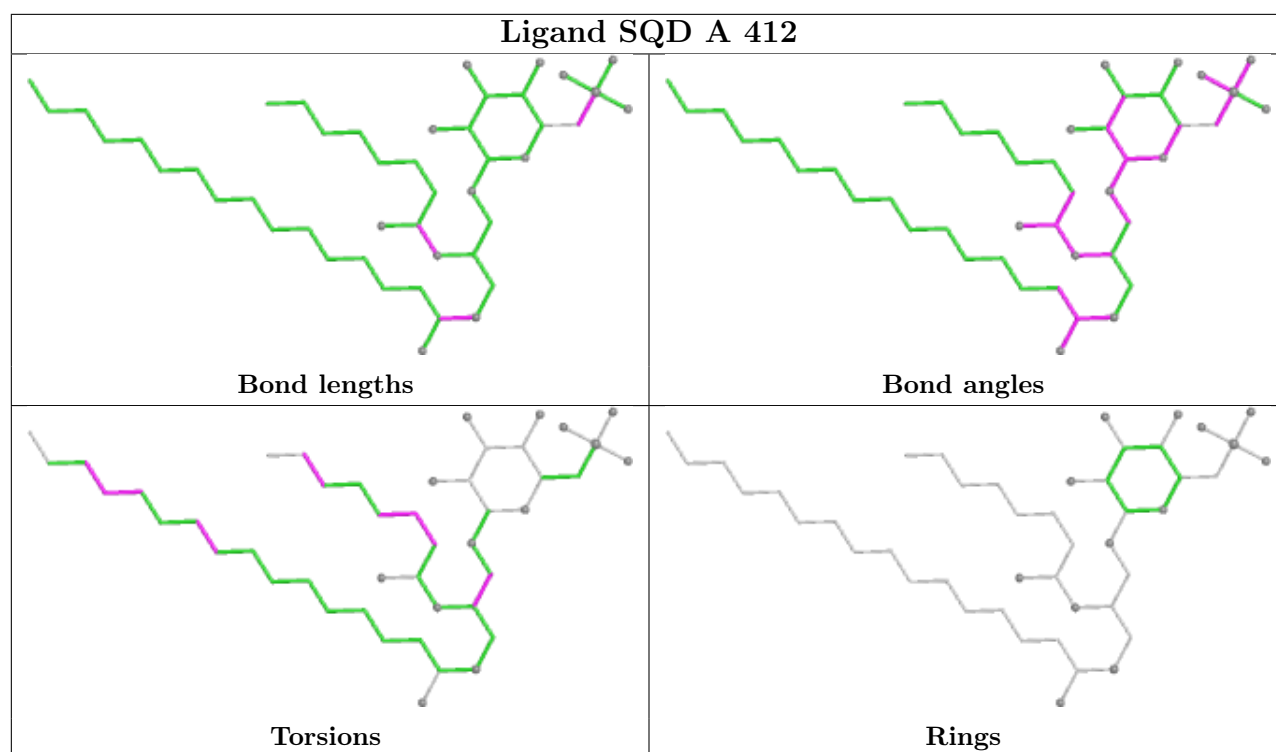


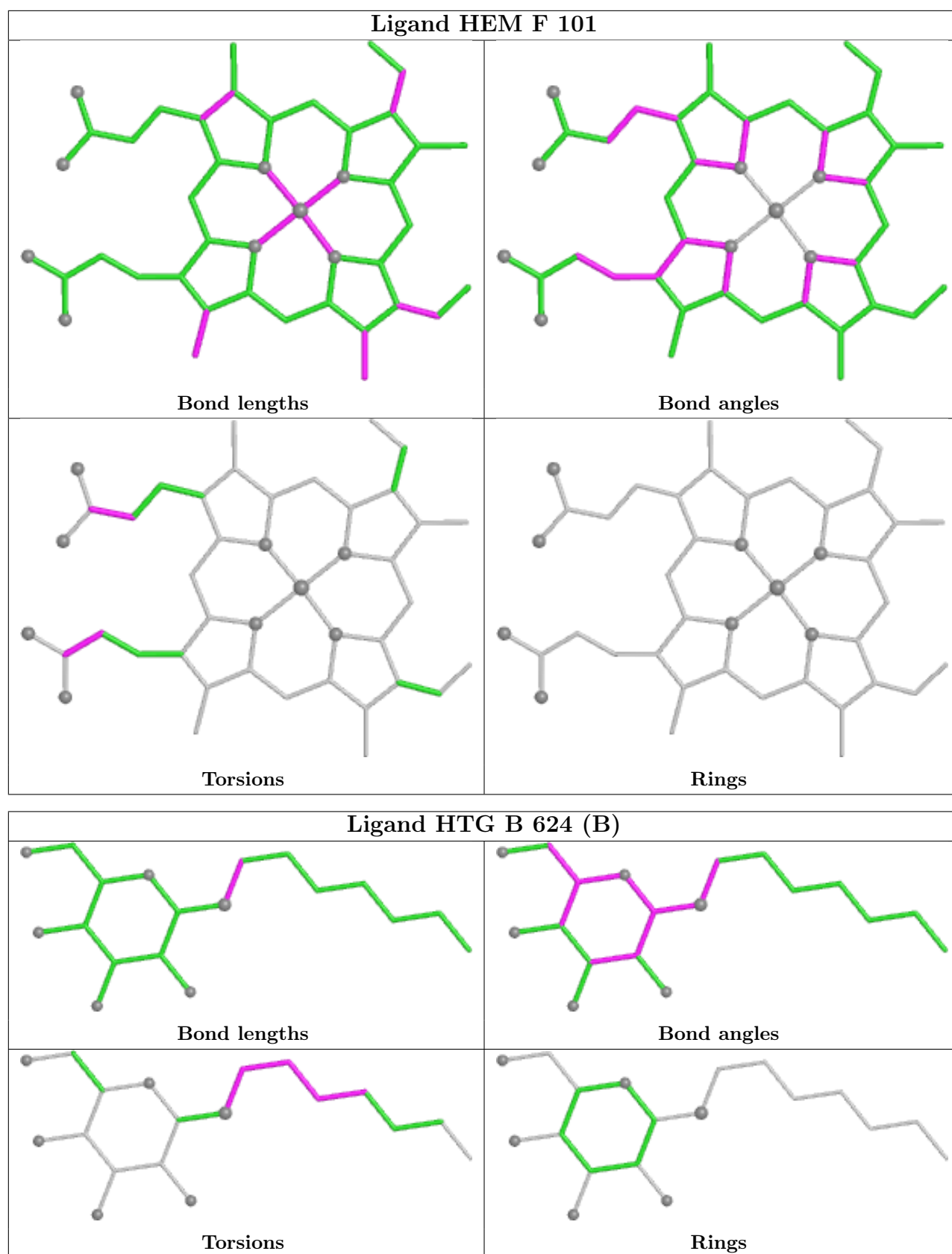
## Ligand CLA C 503



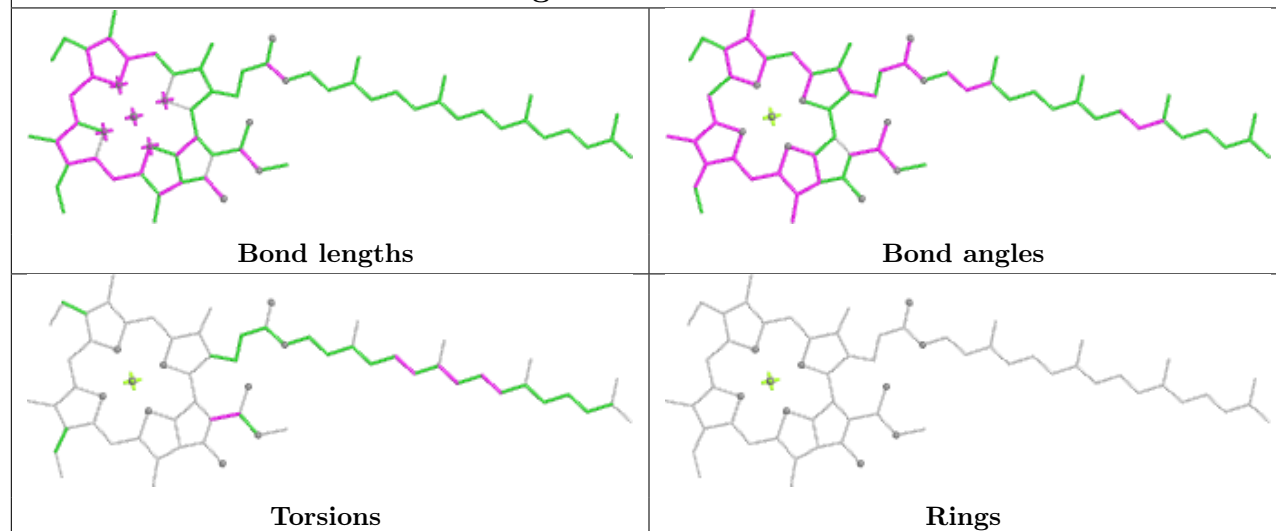




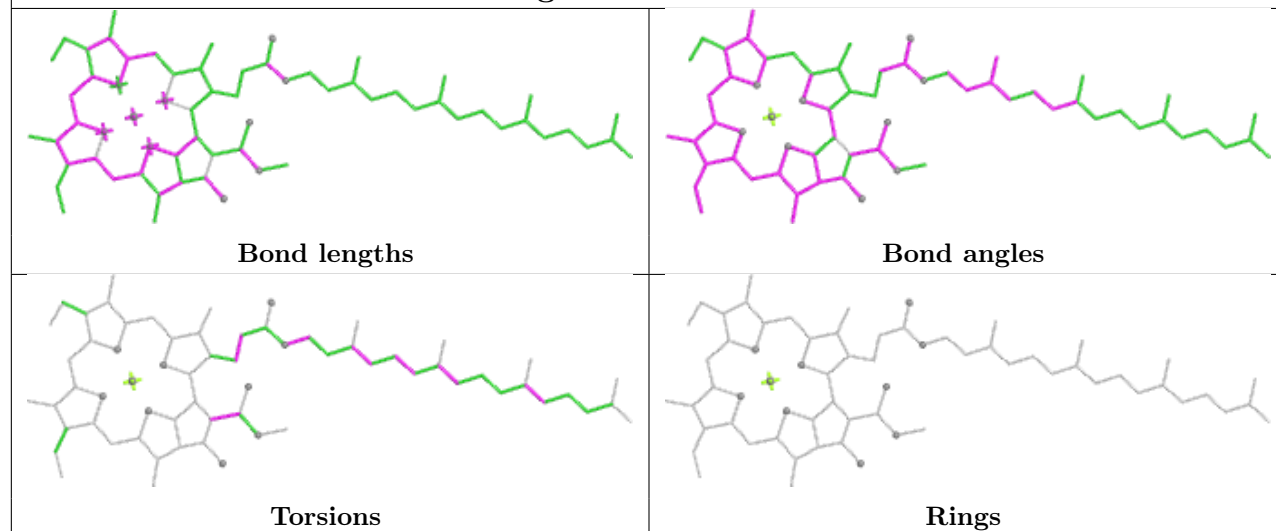




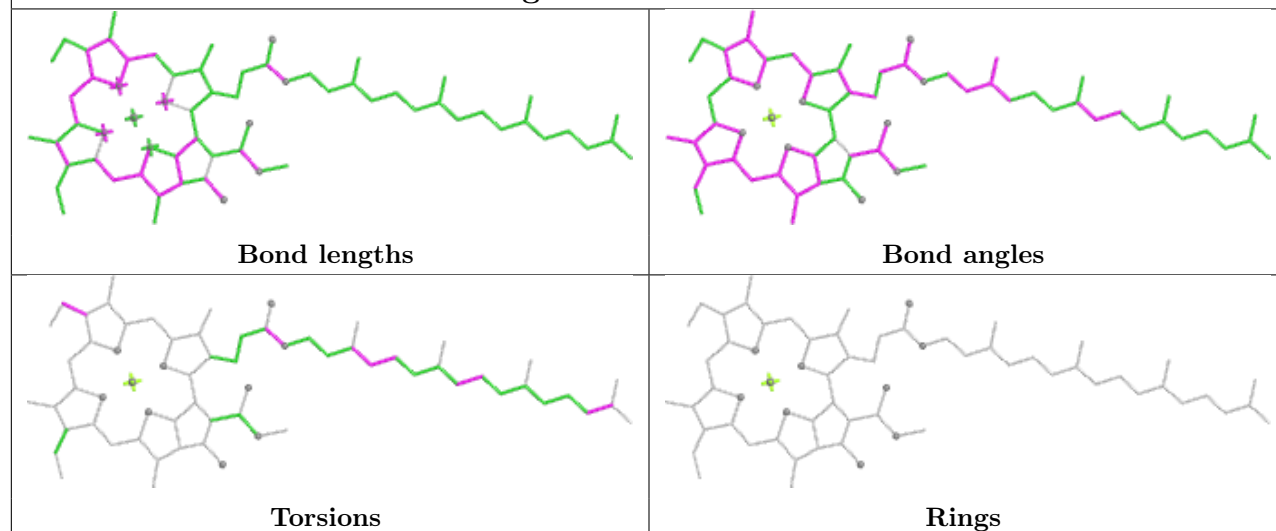
## Ligand CLA C 509

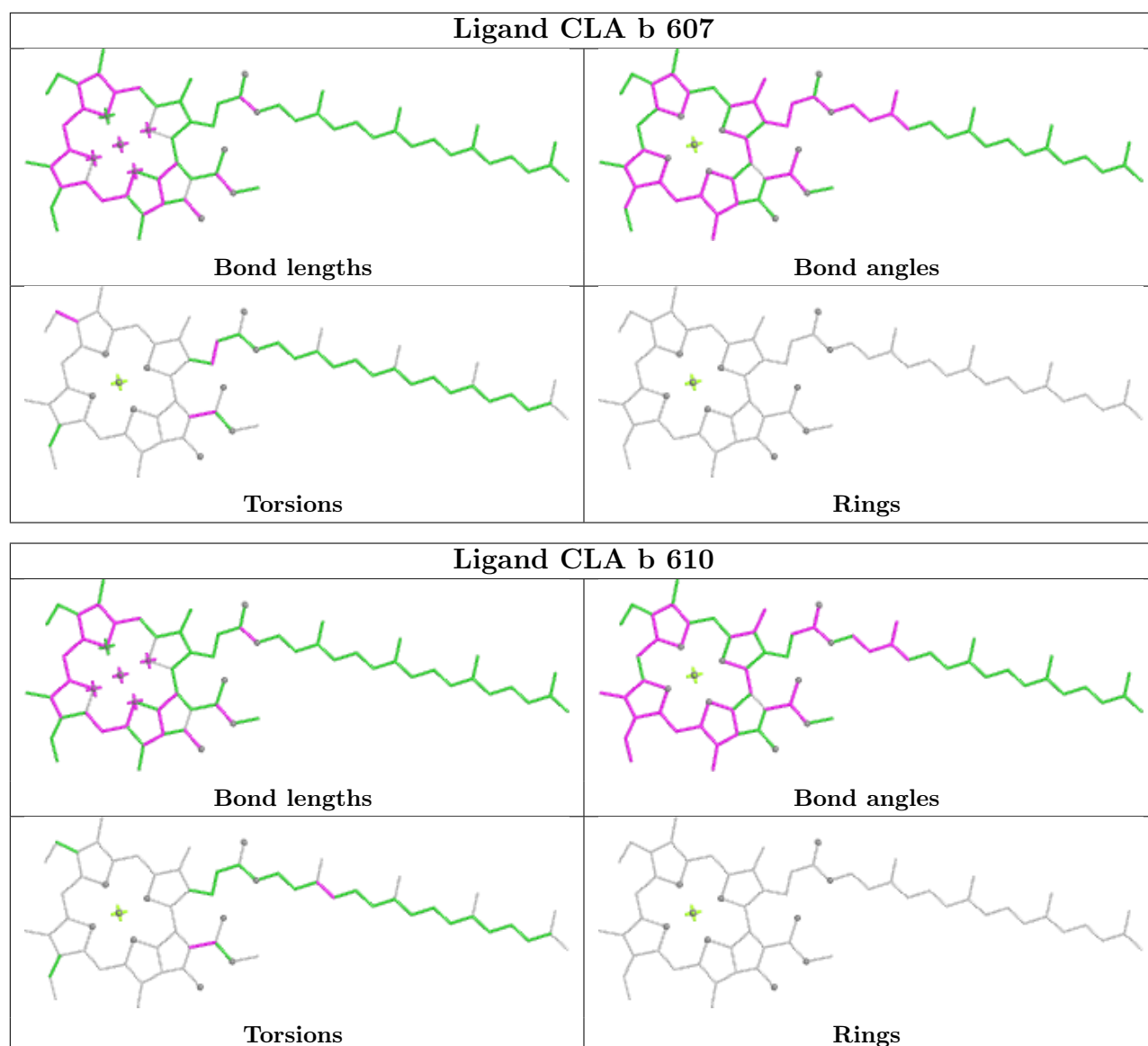


## Ligand CLA c 510



## Ligand CLA D 2304





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|----------------|--------|--------------|-----------------------|--------|
| 1   | A     | 334/344 (97%)  | -0.28  | 5 (1%) 72 76 | 30, 46, 86, 139       | 3 (0%) |
| 1   | a     | 334/344 (97%)  | -0.24  | 9 (2%) 56 60 | 27, 47, 87, 143       | 5 (1%) |
| 2   | B     | 505/505 (100%) | -0.26  | 8 (1%) 70 74 | 28, 52, 92, 138       | 7 (1%) |
| 2   | b     | 483/505 (95%)  | -0.21  | 4 (0%) 82 84 | 33, 53, 83, 143       | 9 (1%) |
| 3   | C     | 451/455 (99%)  | -0.18  | 4 (0%) 81 83 | 39, 59, 83, 164       | 2 (0%) |
| 3   | c     | 455/455 (100%) | -0.16  | 2 (0%) 88 90 | 45, 61, 81, 136       | 0      |
| 4   | D     | 340/342 (99%)  | -0.35  | 2 (0%) 85 87 | 24, 49, 75, 113       | 1 (0%) |
| 4   | d     | 341/342 (99%)  | -0.32  | 1 (0%) 90 91 | 26, 50, 77, 138       | 2 (0%) |
| 5   | E     | 80/83 (96%)    | 0.31   | 7 (8%) 15 17 | 50, 76, 128, 144      | 1 (1%) |
| 5   | e     | 79/83 (95%)    | 0.39   | 5 (6%) 26 29 | 46, 78, 124, 137      | 1 (1%) |
| 6   | F     | 34/44 (77%)    | -0.12  | 2 (5%) 28 32 | 52, 64, 114, 124      | 0      |
| 6   | f     | 32/44 (72%)    | 0.22   | 4 (12%) 8 8  | 53, 66, 119, 132      | 0      |
| 7   | H     | 63/63 (100%)   | 0.12   | 3 (4%) 35 40 | 53, 69, 85, 111       | 0      |
| 7   | h     | 63/63 (100%)   | 0.41   | 1 (1%) 70 74 | 48, 72, 89, 117       | 1 (1%) |
| 8   | I     | 31/38 (81%)    | 0.75   | 6 (19%) 3 4  | 53, 71, 146, 152      | 0      |
| 8   | i     | 31/38 (81%)    | 0.51   | 4 (12%) 7 8  | 51, 67, 129, 137      | 0      |
| 9   | J     | 36/40 (90%)    | -0.07  | 1 (2%) 55 59 | 48, 67, 111, 135      | 0      |
| 9   | j     | 39/40 (97%)    | 0.05   | 1 (2%) 57 61 | 55, 68, 131, 162      | 0      |
| 10  | K     | 37/37 (100%)   | -0.24  | 0 100 100    | 43, 67, 84, 92        | 1 (2%) |
| 10  | k     | 37/37 (100%)   | 0.03   | 0 100 100    | 58, 69, 95, 114       | 0      |
| 11  | L     | 37/37 (100%)   | -0.24  | 1 (2%) 56 60 | 24, 45, 88, 153       | 1 (2%) |
| 11  | l     | 36/37 (97%)    | -0.31  | 0 100 100    | 25, 45, 102, 158      | 2 (5%) |
| 12  | M     | 32/36 (88%)    | -0.41  | 0 100 100    | 27, 47, 66, 106       | 2 (6%) |
| 12  | m     | 33/36 (91%)    | -0.21  | 1 (3%) 52 56 | 27, 49, 100, 129      | 1 (3%) |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 13  | O     | 244/244 (100%)  | -0.15  | 2 (0%) 82 84  | 33, 60, 104, 154      | 3 (1%)  |
| 13  | o     | 243/244 (99%)   | -0.12  | 1 (0%) 88 90  | 31, 60, 108, 162      | 4 (1%)  |
| 14  | T     | 29/32 (90%)     | -0.25  | 1 (3%) 48 52  | 39, 46, 82, 150       | 0       |
| 14  | t     | 29/32 (90%)     | -0.22  | 1 (3%) 48 52  | 40, 46, 80, 129       | 0       |
| 15  | U     | 97/104 (93%)    | -0.23  | 2 (2%) 63 67  | 43, 55, 86, 105       | 1 (1%)  |
| 15  | u     | 97/104 (93%)    | -0.19  | 0 100 100     | 49, 58, 80, 136       | 0       |
| 16  | V     | 137/137 (100%)  | -0.26  | 0 100 100     | 36, 54, 80, 100       | 1 (0%)  |
| 16  | v     | 137/137 (100%)  | -0.17  | 1 (0%) 84 85  | 40, 66, 91, 110       | 1 (0%)  |
| 17  | Y     | 30/30 (100%)    | 0.33   | 1 (3%) 49 53  | 70, 83, 113, 124      | 0       |
| 17  | y     | 30/30 (100%)    | 0.34   | 1 (3%) 49 53  | 75, 88, 105, 136      | 0       |
| 18  | X     | 38/40 (95%)     | 0.22   | 1 (2%) 57 61  | 66, 79, 111, 122      | 0       |
| 18  | x     | 35/40 (87%)     | 0.20   | 2 (5%) 29 33  | 44, 80, 122, 134      | 1 (2%)  |
| 19  | Z     | 61/62 (98%)     | 0.18   | 2 (3%) 49 53  | 66, 81, 124, 140      | 0       |
| 19  | z     | 60/62 (96%)     | 0.49   | 4 (6%) 24 27  | 75, 88, 132, 159      | 0       |
| All | All   | 5210/5346 (97%) | -0.16  | 90 (1%) 69 73 | 24, 56, 97, 164       | 50 (0%) |

All (90) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 19  | z     | 61    | VAL  | 4.2  |
| 2   | B     | 479   | PHE  | 4.1  |
| 8   | I     | 28    | PRO  | 4.1  |
| 8   | i     | 28    | PRO  | 4.0  |
| 5   | e     | 6     | GLY  | 4.0  |
| 18  | x     | 2     | THR  | 3.9  |
| 8   | I     | 32    | PRO  | 3.9  |
| 8   | i     | 29    | ALA  | 3.8  |
| 1   | a     | 246   | TYR  | 3.6  |
| 2   | B     | 84    | THR  | 3.5  |
| 14  | T     | 30    | THR  | 3.5  |
| 5   | e     | 65[A] | LEU  | 3.5  |
| 14  | t     | 30    | THR  | 3.4  |
| 1   | A     | 11    | ALA  | 3.4  |
| 19  | z     | 3     | ILE  | 3.3  |
| 1   | A     | 229   | GLU  | 3.3  |
| 8   | i     | 32    | PRO  | 3.3  |
| 18  | X     | 2     | THR  | 3.2  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | B     | 85     | GLY  | 3.2  |
| 5   | e     | 79     | PHE  | 3.2  |
| 5   | E     | 76     | VAL  | 3.2  |
| 1   | a     | 235    | TYR  | 3.2  |
| 5   | E     | 79     | PHE  | 3.1  |
| 2   | b     | 484    | PRO  | 3.1  |
| 3   | c     | 19     | ASN  | 3.1  |
| 1   | A     | 14     | TRP  | 3.1  |
| 4   | D     | 12     | ARG  | 3.1  |
| 7   | H     | 64     | ALA  | 3.1  |
| 8   | I     | 29     | ALA  | 3.1  |
| 6   | f     | 15     | ILE  | 3.1  |
| 7   | H     | 63     | LYS  | 3.0  |
| 5   | E     | 4      | THR  | 3.0  |
| 1   | a     | 260    | PHE  | 3.0  |
| 2   | b     | 84     | THR  | 3.0  |
| 3   | C     | 24     | THR  | 2.9  |
| 2   | b     | 479    | PHE  | 2.9  |
| 5   | e     | 43     | ALA  | 2.9  |
| 8   | I     | 31     | ASN  | 2.8  |
| 5   | E     | 83     | LEU  | 2.8  |
| 6   | F     | 12     | SER  | 2.8  |
| 1   | a     | 251    | ALA  | 2.8  |
| 11  | L     | 1      | MET  | 2.8  |
| 5   | E     | 72     | ALA  | 2.8  |
| 1   | a     | 224    | ILE  | 2.8  |
| 8   | i     | 30     | ARG  | 2.7  |
| 1   | a     | 222[A] | SER  | 2.7  |
| 19  | z     | 2      | THR  | 2.7  |
| 2   | B     | 487    | SER  | 2.7  |
| 2   | B     | 86     | ILE  | 2.7  |
| 17  | Y     | 18     | VAL  | 2.7  |
| 3   | C     | 23     | ALA  | 2.6  |
| 6   | F     | 15     | ILE  | 2.6  |
| 1   | A     | 230    | THR  | 2.6  |
| 1   | a     | 247    | ASN  | 2.6  |
| 2   | B     | 500    | GLY  | 2.5  |
| 1   | a     | 265    | PHE  | 2.5  |
| 3   | C     | 257    | PHE  | 2.5  |
| 2   | B     | 478    | VAL  | 2.4  |
| 2   | B     | 502    | VAL  | 2.4  |
| 5   | E     | 61     | ARG  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | I     | 26  | GLY  | 2.4  |
| 6   | f     | 42  | PHE  | 2.4  |
| 5   | e     | 76  | VAL  | 2.4  |
| 9   | j     | 2   | MET  | 2.4  |
| 7   | h     | 64  | ALA  | 2.4  |
| 1   | A     | 19  | ASN  | 2.4  |
| 13  | O     | 58  | ASN  | 2.4  |
| 13  | o     | 58  | ASN  | 2.4  |
| 6   | f     | 16  | PHE  | 2.4  |
| 19  | Z     | 60  | PHE  | 2.4  |
| 1   | a     | 14  | TRP  | 2.4  |
| 3   | C     | 143 | TYR  | 2.3  |
| 4   | d     | 135 | LEU  | 2.3  |
| 16  | v     | 26  | TYR  | 2.3  |
| 2   | b     | 482 | ILE  | 2.3  |
| 19  | Z     | 62  | VAL  | 2.2  |
| 8   | I     | 27  | ASP  | 2.2  |
| 17  | y     | 25  | ILE  | 2.2  |
| 7   | H     | 58  | VAL  | 2.2  |
| 3   | c     | 183 | GLY  | 2.2  |
| 15  | U     | 9   | LEU  | 2.2  |
| 13  | O     | 60  | ARG  | 2.2  |
| 15  | U     | 8   | GLU  | 2.1  |
| 12  | m     | 33  | GLN  | 2.1  |
| 5   | E     | 65  | LEU  | 2.1  |
| 19  | z     | 5   | PHE  | 2.1  |
| 18  | x     | 35  | ASP  | 2.0  |
| 6   | f     | 14  | PRO  | 2.0  |
| 4   | D     | 341 | PHE  | 2.0  |
| 9   | J     | 5   | GLY  | 2.0  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 19  | FME  | z     | 1   | 10/11 | 0.84 | 0.11 | 114,129,141,143            | 0     |
| 19  | FME  | Z     | 1   | 10/11 | 0.90 | 0.12 | 96,112,117,118             | 0     |
| 14  | FME  | T     | 1   | 10/11 | 0.94 | 0.09 | 48,54,84,88                | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 4   | HSK  | D     | 336[A] | 10/12 | 0.96 | 0.08 | 49,51,51,51                 | 7     |
| 4   | HSK  | D     | 336[B] | 11/12 | 0.96 | 0.08 | 50,51,51,51                 | 8     |
| 14  | FME  | t     | 1      | 10/11 | 0.96 | 0.08 | 46,51,77,79                 | 0     |
| 12  | FME  | M     | 1      | 10/11 | 0.96 | 0.09 | 48,56,80,81                 | 0     |
| 4   | HSK  | d     | 336[B] | 11/12 | 0.97 | 0.08 | 51,56,59,62                 | 8     |
| 8   | FME  | i     | 1      | 10/11 | 0.97 | 0.06 | 52,60,62,64                 | 0     |
| 12  | FME  | m     | 1      | 10/11 | 0.97 | 0.08 | 43,57,81,84                 | 0     |
| 8   | FME  | I     | 1      | 10/11 | 0.97 | 0.07 | 49,59,63,64                 | 0     |
| 4   | HSK  | d     | 336[A] | 10/12 | 0.97 | 0.08 | 51,56,59,60                 | 7     |

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 29  | GOL  | E     | 104  | 6/6   | 0.56 | 0.13 | 124,126,128,129             | 0     |
| 34  | DMS  | X     | 101  | 4/4   | 0.56 | 0.17 | 172,174,175,175             | 0     |
| 34  | DMS  | A     | 425  | 4/4   | 0.58 | 0.25 | 152,153,153,155             | 0     |
| 34  | DMS  | O     | 308  | 4/4   | 0.61 | 0.21 | 124,127,127,132             | 0     |
| 34  | DMS  | U     | 504  | 4/4   | 0.62 | 0.22 | 119,124,127,129             | 0     |
| 34  | DMS  | C     | 534  | 4/4   | 0.63 | 0.25 | 141,141,143,143             | 0     |
| 34  | DMS  | v     | 210  | 4/4   | 0.64 | 0.22 | 137,140,140,143             | 0     |
| 34  | DMS  | c     | 542  | 4/4   | 0.65 | 0.27 | 148,149,150,151             | 0     |
| 34  | DMS  | o     | 309  | 4/4   | 0.65 | 0.27 | 131,139,139,141             | 0     |
| 34  | DMS  | B     | 645  | 4/4   | 0.65 | 0.17 | 124,125,125,127             | 0     |
| 34  | DMS  | o     | 310  | 4/4   | 0.66 | 0.22 | 144,147,149,149             | 0     |
| 34  | DMS  | c     | 546  | 4/4   | 0.67 | 0.23 | 151,153,154,154             | 0     |
| 34  | DMS  | a     | 2624 | 4/4   | 0.67 | 0.25 | 79,105,106,109              | 0     |
| 34  | DMS  | B     | 642  | 4/4   | 0.68 | 0.24 | 95,106,108,114              | 0     |
| 34  | DMS  | c     | 541  | 4/4   | 0.68 | 0.29 | 121,128,129,132             | 0     |
| 34  | DMS  | c     | 549  | 4/4   | 0.68 | 0.20 | 124,126,128,128             | 0     |
| 34  | DMS  | H     | 104  | 4/4   | 0.69 | 0.17 | 129,131,133,133             | 0     |
| 30  | UNL  | j     | 2702 | 16/-  | 0.69 | 0.23 | 89,96,108,111               | 0     |
| 30  | UNL  | a     | 2616 | 27/-  | 0.70 | 0.19 | 86,103,140,149              | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 29  | GOL  | v     | 202    | 6/6   | 0.70 | 0.12 | 113,114,116,118             | 0     |
| 34  | DMS  | O     | 311    | 4/4   | 0.72 | 0.33 | 130,135,136,138             | 0     |
| 34  | DMS  | C     | 537    | 4/4   | 0.72 | 0.19 | 143,143,144,146             | 0     |
| 34  | DMS  | d     | 420    | 4/4   | 0.72 | 0.16 | 121,122,123,124             | 0     |
| 38  | LHG  | e     | 101    | 40/49 | 0.72 | 0.18 | 93,156,201,202              | 0     |
| 29  | GOL  | O     | 304    | 6/6   | 0.73 | 0.17 | 86,101,103,106              | 0     |
| 34  | DMS  | C     | 535    | 4/4   | 0.73 | 0.22 | 109,109,110,112             | 0     |
| 29  | GOL  | b     | 631    | 6/6   | 0.74 | 0.15 | 84,100,106,106              | 0     |
| 34  | DMS  | l     | 104    | 4/4   | 0.74 | 0.18 | 134,136,139,140             | 0     |
| 37  | DGD  | D     | 2307   | 53/66 | 0.74 | 0.21 | 96,121,171,177              | 0     |
| 30  | UNL  | A     | 416    | 28/-  | 0.74 | 0.18 | 93,104,133,143              | 0     |
| 34  | DMS  | b     | 640    | 4/4   | 0.75 | 0.20 | 110,112,115,117             | 0     |
| 30  | UNL  | E     | 103    | 9/-   | 0.75 | 0.21 | 75,83,107,110               | 0     |
| 30  | UNL  | i     | 101    | 19/-  | 0.76 | 0.14 | 88,112,144,146              | 0     |
| 34  | DMS  | B     | 640    | 4/4   | 0.76 | 0.35 | 154,155,156,157             | 0     |
| 30  | UNL  | c     | 527    | 12/-  | 0.76 | 0.33 | 104,113,125,126             | 0     |
| 34  | DMS  | V     | 211    | 4/4   | 0.76 | 0.19 | 109,112,114,114             | 0     |
| 30  | UNL  | k     | 301    | 16/-  | 0.76 | 0.27 | 89,109,125,126              | 0     |
| 34  | DMS  | v     | 212    | 4/4   | 0.76 | 0.19 | 133,135,138,138             | 0     |
| 34  | DMS  | c     | 547    | 4/4   | 0.76 | 0.23 | 132,138,140,141             | 0     |
| 34  | DMS  | a     | 2620   | 4/4   | 0.76 | 0.19 | 142,146,149,151             | 0     |
| 34  | DMS  | c     | 548    | 4/4   | 0.77 | 0.17 | 123,130,130,130             | 0     |
| 30  | UNL  | b     | 627    | 15/-  | 0.77 | 0.21 | 90,97,113,114               | 0     |
| 30  | UNL  | b     | 629    | 8/-   | 0.77 | 0.22 | 72,94,106,108               | 0     |
| 28  | LMT  | j     | 2701   | 34/35 | 0.77 | 0.15 | 79,145,158,159              | 0     |
| 34  | DMS  | V     | 213    | 4/4   | 0.77 | 0.23 | 115,118,119,120             | 0     |
| 34  | DMS  | B     | 646    | 4/4   | 0.78 | 0.17 | 94,96,102,107               | 0     |
| 34  | DMS  | O     | 319    | 4/4   | 0.78 | 0.18 | 131,134,135,136             | 0     |
| 34  | DMS  | v     | 214    | 4/4   | 0.78 | 0.17 | 131,135,135,136             | 0     |
| 36  | HTG  | B     | 624[A] | 19/19 | 0.78 | 0.19 | 56,72,85,87                 | 19    |
| 36  | HTG  | B     | 624[B] | 19/19 | 0.78 | 0.19 | 57,72,86,88                 | 19    |
| 36  | HTG  | C     | 522    | 19/19 | 0.78 | 0.16 | 88,124,137,140              | 0     |
| 36  | HTG  | i     | 102    | 19/19 | 0.78 | 0.13 | 68,143,157,158              | 0     |
| 34  | DMS  | d     | 422    | 4/4   | 0.78 | 0.19 | 118,121,124,128             | 0     |
| 34  | DMS  | o     | 316    | 4/4   | 0.78 | 0.22 | 85,101,104,108              | 0     |
| 34  | DMS  | B     | 637    | 4/4   | 0.79 | 0.19 | 121,124,125,126             | 0     |
| 34  | DMS  | O     | 307    | 4/4   | 0.79 | 0.21 | 98,107,107,110              | 0     |
| 30  | UNL  | B     | 629    | 15/-  | 0.79 | 0.24 | 90,105,111,112              | 0     |
| 28  | LMT  | F     | 102    | 24/35 | 0.79 | 0.17 | 114,127,159,161             | 0     |
| 36  | HTG  | d     | 407    | 19/19 | 0.79 | 0.15 | 102,133,146,148             | 0     |
| 34  | DMS  | O     | 317    | 4/4   | 0.79 | 0.25 | 114,115,117,120             | 0     |
| 34  | DMS  | O     | 318    | 4/4   | 0.79 | 0.28 | 115,117,119,126             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 34  | DMS  | A     | 427  | 4/4   | 0.79 | 0.21 | 103,106,107,108             | 0     |
| 34  | DMS  | O     | 314  | 4/4   | 0.80 | 0.17 | 117,121,126,133             | 0     |
| 34  | DMS  | B     | 643  | 4/4   | 0.80 | 0.18 | 99,101,107,111              | 0     |
| 36  | HTG  | B     | 627  | 19/19 | 0.80 | 0.16 | 67,130,145,148              | 0     |
| 34  | DMS  | c     | 537  | 4/4   | 0.80 | 0.20 | 116,122,123,125             | 0     |
| 36  | HTG  | V     | 204  | 19/19 | 0.80 | 0.16 | 71,95,125,126               | 0     |
| 34  | DMS  | O     | 309  | 4/4   | 0.80 | 0.19 | 117,118,118,120             | 0     |
| 34  | DMS  | v     | 211  | 4/4   | 0.80 | 0.17 | 120,122,123,123             | 0     |
| 29  | GOL  | V     | 203  | 6/6   | 0.80 | 0.13 | 98,111,118,123              | 0     |
| 34  | DMS  | T     | 104  | 4/4   | 0.80 | 0.25 | 156,160,160,161             | 0     |
| 30  | UNL  | b     | 632  | 10/-  | 0.81 | 0.15 | 83,93,104,105               | 0     |
| 34  | DMS  | C     | 536  | 4/4   | 0.81 | 0.17 | 134,137,138,140             | 0     |
| 34  | DMS  | c     | 543  | 4/4   | 0.81 | 0.15 | 116,121,122,123             | 0     |
| 28  | LMT  | m     | 2804 | 35/35 | 0.81 | 0.18 | 79,146,162,166              | 0     |
| 34  | DMS  | o     | 311  | 4/4   | 0.81 | 0.19 | 86,101,102,104              | 0     |
| 34  | DMS  | o     | 315  | 4/4   | 0.81 | 0.32 | 135,137,138,138             | 0     |
| 30  | UNL  | D     | 2313 | 12/-  | 0.81 | 0.22 | 93,112,114,115              | 0     |
| 34  | DMS  | A     | 429  | 4/4   | 0.81 | 0.25 | 128,129,130,132             | 0     |
| 34  | DMS  | B     | 635  | 4/4   | 0.81 | 0.23 | 130,132,133,133             | 0     |
| 29  | GOL  | O     | 305  | 6/6   | 0.81 | 0.17 | 70,91,97,105                | 0     |
| 30  | UNL  | c     | 525  | 6/-   | 0.82 | 0.26 | 95,97,98,101                | 0     |
| 30  | UNL  | C     | 501  | 40/-  | 0.82 | 0.19 | 102,120,136,139             | 0     |
| 29  | GOL  | c     | 529  | 6/6   | 0.82 | 0.11 | 124,131,132,133             | 0     |
| 29  | GOL  | c     | 530  | 6/6   | 0.82 | 0.11 | 79,107,118,124              | 0     |
| 29  | GOL  | d     | 416  | 6/6   | 0.82 | 0.13 | 129,131,132,133             | 0     |
| 28  | LMT  | A     | 414  | 33/35 | 0.82 | 0.17 | 72,117,128,135              | 0     |
| 29  | GOL  | J     | 301  | 6/6   | 0.82 | 0.14 | 100,103,110,111             | 0     |
| 34  | DMS  | O     | 313  | 4/4   | 0.82 | 0.20 | 103,110,110,111             | 0     |
| 34  | DMS  | A     | 428  | 4/4   | 0.82 | 0.24 | 118,118,118,120             | 0     |
| 34  | DMS  | O     | 316  | 4/4   | 0.82 | 0.16 | 107,108,109,110             | 0     |
| 36  | HTG  | H     | 101  | 17/19 | 0.82 | 0.17 | 109,127,151,151             | 0     |
| 34  | DMS  | o     | 305  | 4/4   | 0.82 | 0.18 | 117,117,119,120             | 0     |
| 36  | HTG  | b     | 625  | 19/19 | 0.82 | 0.17 | 58,83,106,108               | 0     |
| 29  | GOL  | D     | 2301 | 6/6   | 0.82 | 0.14 | 87,93,100,104               | 0     |
| 34  | DMS  | c     | 538  | 4/4   | 0.82 | 0.16 | 136,137,139,141             | 0     |
| 34  | DMS  | c     | 539  | 4/4   | 0.82 | 0.19 | 110,112,114,119             | 0     |
| 34  | DMS  | o     | 313  | 4/4   | 0.82 | 0.19 | 100,102,103,111             | 0     |
| 41  | MG   | K     | 102  | 1/1   | 0.82 | 0.15 | 85,85,85,85                 | 0     |
| 34  | DMS  | C     | 528  | 4/4   | 0.83 | 0.20 | 110,114,115,117             | 0     |
| 30  | UNL  | b     | 628  | 10/-  | 0.83 | 0.23 | 94,111,114,116              | 0     |
| 34  | DMS  | o     | 306  | 4/4   | 0.83 | 0.28 | 118,119,124,125             | 0     |
| 26  | SQD  | D     | 2308 | 45/54 | 0.83 | 0.14 | 92,119,145,154              | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 31  | JOX  | A     | 418  | 10/10 | 0.83 | 0.14 | 65,87,88,94                 | 0     |
| 36  | HTG  | C     | 525  | 19/19 | 0.83 | 0.12 | 91,137,156,156              | 0     |
| 34  | DMS  | O     | 315  | 4/4   | 0.83 | 0.13 | 107,114,115,121             | 0     |
| 28  | LMT  | d     | 401  | 35/35 | 0.83 | 0.18 | 63,106,125,130              | 0     |
| 34  | DMS  | o     | 314  | 4/4   | 0.83 | 0.18 | 112,113,117,118             | 0     |
| 30  | UNL  | I     | 102  | 40/-  | 0.83 | 0.15 | 101,119,151,152             | 0     |
| 34  | DMS  | b     | 637  | 4/4   | 0.83 | 0.15 | 89,107,109,112              | 0     |
| 29  | GOL  | c     | 531  | 6/6   | 0.83 | 0.11 | 116,118,119,120             | 0     |
| 38  | LHG  | E     | 101  | 40/49 | 0.83 | 0.15 | 94,137,163,165              | 0     |
| 34  | DMS  | b     | 642  | 4/4   | 0.83 | 0.15 | 153,154,156,159             | 0     |
| 28  | LMT  | d     | 404  | 25/35 | 0.83 | 0.19 | 91,129,162,164              | 0     |
| 28  | LMT  | f     | 101  | 24/35 | 0.84 | 0.13 | 102,124,156,160             | 0     |
| 30  | UNL  | C     | 523  | 10/-  | 0.84 | 0.21 | 99,101,107,112              | 0     |
| 36  | HTG  | B     | 625  | 19/19 | 0.84 | 0.15 | 77,130,138,140              | 19    |
| 29  | GOL  | u     | 501  | 6/6   | 0.84 | 0.16 | 84,92,98,102                | 0     |
| 34  | DMS  | c     | 540  | 4/4   | 0.84 | 0.18 | 111,115,116,117             | 0     |
| 28  | LMT  | J     | 303  | 24/35 | 0.84 | 0.16 | 80,95,144,147               | 0     |
| 29  | GOL  | v     | 204  | 6/6   | 0.84 | 0.15 | 92,115,115,123              | 0     |
| 34  | DMS  | A     | 430  | 4/4   | 0.84 | 0.20 | 115,127,127,130             | 0     |
| 30  | UNL  | e     | 102  | 15/-  | 0.84 | 0.17 | 74,93,101,101               | 0     |
| 36  | HTG  | c     | 523  | 19/19 | 0.84 | 0.12 | 99,121,130,133              | 0     |
| 30  | UNL  | a     | 2601 | 15/-  | 0.84 | 0.20 | 79,86,93,96                 | 0     |
| 29  | GOL  | U     | 501  | 6/6   | 0.84 | 0.15 | 105,111,113,115             | 0     |
| 28  | LMT  | T     | 103  | 24/35 | 0.84 | 0.17 | 58,91,129,132               | 0     |
| 34  | DMS  | b     | 643  | 4/4   | 0.84 | 0.18 | 125,131,133,136             | 0     |
| 34  | DMS  | c     | 532  | 4/4   | 0.84 | 0.20 | 87,89,96,102                | 0     |
| 34  | DMS  | d     | 423  | 4/4   | 0.84 | 0.16 | 133,137,137,140             | 0     |
| 41  | MG   | k     | 303  | 1/1   | 0.84 | 0.15 | 91,91,91,91                 | 0     |
| 29  | GOL  | B     | 632  | 6/6   | 0.85 | 0.17 | 87,96,98,101                | 0     |
| 30  | UNL  | b     | 630  | 21/-  | 0.85 | 0.14 | 56,79,122,124               | 0     |
| 23  | CLA  | B     | 602  | 65/65 | 0.85 | 0.12 | 58,83,121,131               | 0     |
| 34  | DMS  | V     | 208  | 4/4   | 0.85 | 0.15 | 99,108,109,113              | 0     |
| 27  | LMG  | c     | 522  | 51/55 | 0.85 | 0.14 | 65,117,127,130              | 0     |
| 34  | DMS  | o     | 308  | 4/4   | 0.85 | 0.14 | 127,131,133,135             | 0     |
| 34  | DMS  | V     | 212  | 4/4   | 0.85 | 0.16 | 98,111,112,115              | 0     |
| 34  | DMS  | B     | 647  | 4/4   | 0.85 | 0.20 | 105,106,112,112             | 0     |
| 26  | SQD  | D     | 2302 | 54/54 | 0.85 | 0.17 | 75,106,174,176              | 0     |
| 29  | GOL  | O     | 302  | 6/6   | 0.85 | 0.11 | 78,82,87,91                 | 0     |
| 34  | DMS  | c     | 544  | 4/4   | 0.85 | 0.13 | 105,110,113,115             | 0     |
| 36  | HTG  | c     | 524  | 19/19 | 0.85 | 0.14 | 62,108,119,121              | 19    |
| 36  | HTG  | c     | 526  | 19/19 | 0.85 | 0.14 | 120,165,175,175             | 0     |
| 30  | UNL  | B     | 628  | 18/-  | 0.85 | 0.17 | 85,96,116,117               | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 34  | DMS  | b     | 636  | 4/4   | 0.85 | 0.16 | 101,102,104,106             | 0     |
| 34  | DMS  | t     | 102  | 4/4   | 0.85 | 0.21 | 129,132,137,137             | 0     |
| 34  | DMS  | v     | 208  | 4/4   | 0.85 | 0.17 | 125,126,127,129             | 0     |
| 29  | GOL  | O     | 303  | 6/6   | 0.85 | 0.13 | 96,106,114,114              | 0     |
| 28  | LMT  | B     | 634  | 35/35 | 0.85 | 0.16 | 55,133,160,162              | 0     |
| 34  | DMS  | D     | 2320 | 4/4   | 0.85 | 0.17 | 144,144,144,147             | 0     |
| 34  | DMS  | V     | 207  | 4/4   | 0.86 | 0.17 | 137,139,141,141             | 0     |
| 30  | UNL  | B     | 631  | 32/-  | 0.86 | 0.15 | 66,97,116,117               | 0     |
| 34  | DMS  | o     | 307  | 4/4   | 0.86 | 0.22 | 104,107,109,111             | 0     |
| 30  | UNL  | Y     | 301  | 12/-  | 0.86 | 0.20 | 114,116,120,121             | 0     |
| 34  | DMS  | B     | 641  | 4/4   | 0.86 | 0.12 | 93,102,102,104              | 0     |
| 30  | UNL  | c     | 502  | 36/-  | 0.86 | 0.18 | 91,115,128,130              | 0     |
| 34  | DMS  | D     | 2319 | 4/4   | 0.86 | 0.15 | 104,105,107,118             | 0     |
| 29  | GOL  | B     | 630  | 6/6   | 0.86 | 0.14 | 94,104,109,117              | 0     |
| 28  | LMT  | m     | 2803 | 35/35 | 0.86 | 0.14 | 61,101,118,121              | 0     |
| 36  | HTG  | b     | 626  | 19/19 | 0.86 | 0.14 | 98,151,158,158              | 0     |
| 34  | DMS  | b     | 635  | 4/4   | 0.86 | 0.21 | 98,102,105,109              | 0     |
| 28  | LMT  | z     | 102  | 33/35 | 0.86 | 0.15 | 80,141,156,157              | 0     |
| 30  | UNL  | E     | 102  | 6/-   | 0.86 | 0.16 | 83,87,87,89                 | 0     |
| 34  | DMS  | b     | 638  | 4/4   | 0.86 | 0.24 | 159,163,163,165             | 0     |
| 34  | DMS  | v     | 209  | 4/4   | 0.86 | 0.16 | 82,93,96,102                | 0     |
| 34  | DMS  | T     | 105  | 4/4   | 0.86 | 0.20 | 124,129,130,130             | 0     |
| 29  | GOL  | v     | 203  | 6/6   | 0.86 | 0.14 | 81,87,91,92                 | 0     |
| 34  | DMS  | U     | 505  | 4/4   | 0.86 | 0.18 | 66,72,89,105                | 0     |
| 34  | DMS  | v     | 213  | 4/4   | 0.86 | 0.14 | 119,119,119,123             | 0     |
| 34  | DMS  | V     | 206  | 4/4   | 0.86 | 0.14 | 81,98,100,101               | 0     |
| 25  | BCR  | T     | 102  | 40/40 | 0.87 | 0.11 | 44,56,82,85                 | 0     |
| 29  | GOL  | a     | 2618 | 6/6   | 0.87 | 0.13 | 107,112,115,116             | 0     |
| 26  | SQD  | d     | 417  | 33/54 | 0.87 | 0.14 | 100,120,146,151             | 0     |
| 36  | HTG  | I     | 101  | 19/19 | 0.87 | 0.11 | 83,126,141,145              | 0     |
| 34  | DMS  | u     | 502  | 4/4   | 0.87 | 0.24 | 127,129,129,131             | 0     |
| 36  | HTG  | b     | 604  | 19/19 | 0.87 | 0.13 | 79,131,144,147              | 0     |
| 34  | DMS  | u     | 504  | 4/4   | 0.87 | 0.16 | 74,90,95,98                 | 0     |
| 26  | SQD  | l     | 101  | 54/54 | 0.87 | 0.15 | 59,88,126,130               | 0     |
| 27  | LMG  | C     | 520  | 51/55 | 0.87 | 0.17 | 59,91,107,114               | 0     |
| 34  | DMS  | D     | 2317 | 4/4   | 0.87 | 0.19 | 99,105,106,109              | 0     |
| 30  | UNL  | A     | 423  | 9/-   | 0.87 | 0.20 | 84,89,93,94                 | 0     |
| 31  | JOX  | A     | 419  | 10/10 | 0.87 | 0.13 | 60,69,76,78                 | 0     |
| 33  | PL9  | A     | 422  | 39/55 | 0.87 | 0.21 | 88,101,124,127              | 0     |
| 34  | DMS  | O     | 306  | 4/4   | 0.87 | 0.25 | 146,150,150,153             | 0     |
| 27  | LMG  | C     | 527  | 51/55 | 0.87 | 0.15 | 71,123,148,152              | 0     |
| 30  | UNL  | T     | 101  | 13/-  | 0.87 | 0.23 | 93,100,107,107              | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 28  | LMT  | M     | 101  | 35/35 | 0.87 | 0.16 | 84,157,181,181              | 0     |
| 34  | DMS  | b     | 641  | 4/4   | 0.87 | 0.16 | 75,76,78,84                 | 4     |
| 28  | LMT  | Z     | 101  | 35/35 | 0.88 | 0.14 | 68,142,184,187              | 0     |
| 30  | UNL  | J     | 304  | 5/-   | 0.88 | 0.23 | 97,98,103,104               | 0     |
| 26  | SQD  | b     | 601  | 48/54 | 0.88 | 0.14 | 66,96,152,156               | 0     |
| 34  | DMS  | C     | 531  | 4/4   | 0.88 | 0.17 | 98,102,103,107              | 0     |
| 28  | LMT  | M     | 102  | 35/35 | 0.88 | 0.12 | 59,106,136,139              | 0     |
| 26  | SQD  | a     | 2603 | 54/54 | 0.88 | 0.15 | 55,89,136,138               | 0     |
| 34  | DMS  | U     | 503  | 4/4   | 0.88 | 0.23 | 118,119,119,120             | 0     |
| 36  | HTG  | d     | 415  | 19/19 | 0.88 | 0.18 | 80,117,124,125              | 19    |
| 34  | DMS  | O     | 310  | 4/4   | 0.88 | 0.17 | 103,103,103,108             | 0     |
| 33  | PL9  | x     | 1301 | 39/55 | 0.88 | 0.20 | 94,113,131,132              | 0     |
| 34  | DMS  | v     | 207  | 4/4   | 0.88 | 0.17 | 107,110,111,114             | 0     |
| 29  | GOL  | U     | 502  | 6/6   | 0.88 | 0.14 | 73,82,89,97                 | 0     |
| 28  | LMT  | i     | 103  | 24/35 | 0.88 | 0.15 | 67,119,153,155              | 0     |
| 29  | GOL  | o     | 303  | 6/6   | 0.88 | 0.14 | 71,83,104,109               | 0     |
| 29  | GOL  | b     | 644  | 6/6   | 0.89 | 0.21 | 75,97,105,105               | 0     |
| 28  | LMT  | B     | 623  | 35/35 | 0.89 | 0.12 | 89,122,148,149              | 0     |
| 30  | UNL  | m     | 2801 | 15/-  | 0.89 | 0.18 | 68,85,119,123               | 0     |
| 23  | CLA  | b     | 606  | 65/65 | 0.89 | 0.13 | 66,88,129,133               | 0     |
| 29  | GOL  | a     | 2602 | 6/6   | 0.89 | 0.19 | 64,79,91,91                 | 0     |
| 30  | UNL  | d     | 405  | 37/-  | 0.89 | 0.18 | 74,101,137,137              | 0     |
| 26  | SQD  | B     | 621  | 54/54 | 0.89 | 0.14 | 60,92,128,131               | 0     |
| 29  | GOL  | C     | 524  | 6/6   | 0.89 | 0.11 | 101,110,113,118             | 0     |
| 34  | DMS  | d     | 419  | 4/4   | 0.90 | 0.17 | 92,94,98,106                | 0     |
| 29  | GOL  | A     | 415  | 6/6   | 0.90 | 0.19 | 72,80,92,93                 | 0     |
| 30  | UNL  | l     | 102  | 16/-  | 0.90 | 0.17 | 67,90,115,121               | 0     |
| 25  | BCR  | B     | 633  | 40/40 | 0.90 | 0.11 | 46,62,78,79                 | 0     |
| 34  | DMS  | A     | 426  | 4/4   | 0.90 | 0.18 | 94,103,103,114              | 0     |
| 34  | DMS  | C     | 530  | 4/4   | 0.90 | 0.19 | 115,117,118,123             | 0     |
| 30  | UNL  | t     | 101  | 8/-   | 0.90 | 0.20 | 75,84,103,103               | 0     |
| 34  | DMS  | v     | 206  | 4/4   | 0.90 | 0.16 | 84,102,103,104              | 0     |
| 27  | LMG  | c     | 501  | 51/55 | 0.90 | 0.15 | 67,90,101,105               | 0     |
| 30  | UNL  | c     | 528  | 5/-   | 0.90 | 0.17 | 87,89,97,97                 | 0     |
| 34  | DMS  | a     | 2622 | 4/4   | 0.90 | 0.15 | 105,107,110,115             | 0     |
| 34  | DMS  | c     | 534  | 4/4   | 0.90 | 0.20 | 142,143,143,144             | 0     |
| 34  | DMS  | V     | 202  | 4/4   | 0.90 | 0.20 | 115,124,124,124             | 0     |
| 30  | UNL  | D     | 2314 | 18/-  | 0.91 | 0.13 | 67,79,113,117               | 0     |
| 34  | DMS  | d     | 418  | 4/4   | 0.91 | 0.24 | 98,99,100,111               | 0     |
| 23  | CLA  | C     | 507  | 65/65 | 0.91 | 0.11 | 57,81,109,112               | 0     |
| 34  | DMS  | c     | 535  | 4/4   | 0.91 | 0.20 | 108,108,110,114             | 0     |
| 34  | DMS  | u     | 503  | 4/4   | 0.91 | 0.18 | 81,101,102,103              | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 30  | UNL  | x     | 1302 | 18/-  | 0.91 | 0.13 | 76,86,120,124               | 0     |
| 29  | GOL  | A     | 417  | 6/6   | 0.91 | 0.13 | 110,113,118,126             | 0     |
| 34  | DMS  | O     | 312  | 4/4   | 0.91 | 0.14 | 108,109,110,113             | 0     |
| 40  | RRX  | h     | 101  | 41/41 | 0.91 | 0.13 | 56,81,103,119               | 0     |
| 28  | LMT  | A     | 420  | 24/35 | 0.91 | 0.14 | 63,104,142,148              | 0     |
| 36  | HTG  | B     | 626  | 19/19 | 0.91 | 0.13 | 64,93,111,116               | 0     |
| 27  | LMG  | A     | 413  | 51/55 | 0.92 | 0.13 | 64,82,106,110               | 0     |
| 27  | LMG  | m     | 2802 | 51/55 | 0.92 | 0.14 | 56,81,98,107                | 0     |
| 23  | CLA  | B     | 617  | 65/65 | 0.92 | 0.12 | 49,59,122,126               | 0     |
| 34  | DMS  | a     | 2621 | 4/4   | 0.92 | 0.18 | 115,115,116,118             | 0     |
| 36  | HTG  | C     | 521  | 19/19 | 0.92 | 0.11 | 108,112,121,121             | 0     |
| 34  | DMS  | a     | 2623 | 4/4   | 0.93 | 0.13 | 100,107,108,111             | 0     |
| 34  | DMS  | o     | 312  | 4/4   | 0.93 | 0.13 | 95,98,101,105               | 0     |
| 34  | DMS  | V     | 210  | 4/4   | 0.93 | 0.13 | 101,105,108,111             | 0     |
| 25  | BCR  | b     | 623  | 40/40 | 0.93 | 0.09 | 43,57,74,79                 | 0     |
| 34  | DMS  | c     | 545  | 4/4   | 0.93 | 0.12 | 123,124,125,127             | 0     |
| 27  | LMG  | B     | 622  | 51/55 | 0.93 | 0.12 | 57,81,98,100                | 0     |
| 27  | LMG  | c     | 521  | 49/55 | 0.93 | 0.13 | 60,94,118,121               | 0     |
| 37  | DGD  | h     | 102  | 62/66 | 0.93 | 0.13 | 52,71,117,119               | 0     |
| 38  | LHG  | D     | 2309 | 49/49 | 0.93 | 0.12 | 50,63,78,81                 | 0     |
| 23  | CLA  | b     | 619  | 65/65 | 0.93 | 0.12 | 41,49,109,113               | 0     |
| 38  | LHG  | d     | 412  | 49/49 | 0.93 | 0.12 | 55,66,79,85                 | 0     |
| 36  | HTG  | b     | 603  | 19/19 | 0.93 | 0.12 | 70,89,107,110               | 0     |
| 34  | DMS  | B     | 644  | 4/4   | 0.93 | 0.12 | 82,82,86,88                 | 0     |
| 31  | JOX  | a     | 2617 | 10/10 | 0.93 | 0.09 | 64,69,89,91                 | 0     |
| 34  | DMS  | V     | 209  | 4/4   | 0.93 | 0.13 | 81,89,95,100                | 0     |
| 23  | CLA  | a     | 2613 | 65/65 | 0.94 | 0.11 | 39,48,130,137               | 0     |
| 25  | BCR  | C     | 516  | 40/40 | 0.94 | 0.10 | 54,66,87,91                 | 0     |
| 34  | DMS  | d     | 421  | 4/4   | 0.94 | 0.13 | 75,89,94,98                 | 0     |
| 26  | SQD  | a     | 2615 | 48/54 | 0.94 | 0.12 | 66,86,112,114               | 0     |
| 30  | UNL  | D     | 2315 | 18/-  | 0.94 | 0.15 | 65,90,111,113               | 0     |
| 25  | BCR  | D     | 2305 | 40/40 | 0.94 | 0.10 | 50,60,85,86                 | 0     |
| 23  | CLA  | B     | 615  | 65/65 | 0.94 | 0.11 | 40,49,105,113               | 0     |
| 37  | DGD  | C     | 518  | 62/66 | 0.94 | 0.10 | 48,63,101,111               | 0     |
| 23  | CLA  | C     | 514  | 65/65 | 0.94 | 0.10 | 66,78,111,115               | 0     |
| 37  | DGD  | c     | 518  | 62/66 | 0.94 | 0.12 | 43,57,106,110               | 0     |
| 25  | BCR  | d     | 410  | 40/40 | 0.94 | 0.09 | 54,61,83,86                 | 0     |
| 25  | BCR  | z     | 101  | 40/40 | 0.94 | 0.11 | 68,78,93,97                 | 0     |
| 32  | BCT  | a     | 2608 | 4/4   | 0.94 | 0.14 | 56,61,66,74                 | 0     |
| 26  | SQD  | A     | 412  | 46/54 | 0.94 | 0.11 | 76,88,106,108               | 0     |
| 36  | HTG  | b     | 602  | 19/19 | 0.94 | 0.11 | 56,64,79,79                 | 0     |
| 40  | RRX  | H     | 102  | 41/41 | 0.94 | 0.10 | 48,75,95,100                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 30  | UNL  | d     | 406  | 18/-  | 0.94 | 0.17 | 70,93,104,106               | 0     |
| 23  | CLA  | c     | 509  | 65/65 | 0.94 | 0.11 | 57,76,111,115               | 0     |
| 23  | CLA  | c     | 516  | 65/65 | 0.94 | 0.09 | 61,79,103,108               | 0     |
| 31  | JOX  | a     | 2619 | 10/10 | 0.95 | 0.12 | 46,49,54,56                 | 10    |
| 25  | BCR  | C     | 515  | 40/40 | 0.95 | 0.09 | 55,78,88,89                 | 0     |
| 34  | DMS  | C     | 529  | 4/4   | 0.95 | 0.16 | 94,101,101,102              | 0     |
| 23  | CLA  | B     | 610  | 65/65 | 0.95 | 0.08 | 47,58,69,73                 | 0     |
| 23  | CLA  | b     | 621  | 65/65 | 0.95 | 0.09 | 48,61,128,132               | 0     |
| 23  | CLA  | B     | 607  | 65/65 | 0.95 | 0.08 | 40,52,83,91                 | 0     |
| 25  | BCR  | Y     | 302  | 40/40 | 0.95 | 0.08 | 55,64,70,71                 | 0     |
| 25  | BCR  | a     | 2614 | 40/40 | 0.95 | 0.07 | 38,48,55,57                 | 0     |
| 34  | DMS  | b     | 639  | 4/4   | 0.95 | 0.13 | 93,96,97,98                 | 0     |
| 29  | GOL  | B     | 648  | 6/6   | 0.95 | 0.12 | 54,74,84,89                 | 0     |
| 34  | DMS  | D     | 2316 | 4/4   | 0.95 | 0.11 | 65,77,86,90                 | 0     |
| 23  | CLA  | c     | 515  | 65/65 | 0.95 | 0.10 | 60,71,101,105               | 0     |
| 36  | HTG  | o     | 301  | 19/19 | 0.95 | 0.11 | 62,70,85,87                 | 0     |
| 29  | GOL  | C     | 526  | 6/6   | 0.95 | 0.12 | 65,81,89,93                 | 0     |
| 25  | BCR  | c     | 517  | 40/40 | 0.95 | 0.09 | 52,66,87,89                 | 0     |
| 37  | DGD  | H     | 103  | 62/66 | 0.95 | 0.12 | 51,69,100,104               | 0     |
| 23  | CLA  | C     | 513  | 65/65 | 0.95 | 0.09 | 62,75,115,122               | 0     |
| 37  | DGD  | c     | 519  | 62/66 | 0.95 | 0.11 | 52,65,112,125               | 0     |
| 34  | DMS  | B     | 639  | 4/4   | 0.95 | 0.14 | 84,84,91,92                 | 0     |
| 34  | DMS  | c     | 536  | 4/4   | 0.95 | 0.13 | 64,74,76,78                 | 0     |
| 38  | LHG  | D     | 2310 | 49/49 | 0.95 | 0.10 | 45,52,69,85                 | 0     |
| 25  | BCR  | y     | 101  | 40/40 | 0.95 | 0.08 | 53,65,71,74                 | 0     |
| 38  | LHG  | d     | 403  | 43/49 | 0.95 | 0.11 | 46,59,91,96                 | 0     |
| 27  | LMG  | D     | 2312 | 47/55 | 0.95 | 0.09 | 48,59,97,100                | 0     |
| 23  | CLA  | d     | 409  | 65/65 | 0.95 | 0.09 | 54,61,126,133               | 0     |
| 38  | LHG  | l     | 103  | 49/49 | 0.95 | 0.10 | 46,57,79,86                 | 0     |
| 25  | BCR  | B     | 618  | 40/40 | 0.95 | 0.08 | 43,51,57,60                 | 0     |
| 25  | BCR  | B     | 619  | 40/40 | 0.95 | 0.08 | 45,55,76,79                 | 0     |
| 27  | LMG  | d     | 414  | 51/55 | 0.95 | 0.10 | 54,69,105,109               | 0     |
| 23  | CLA  | b     | 611  | 65/65 | 0.95 | 0.09 | 47,53,90,96                 | 0     |
| 23  | CLA  | D     | 2304 | 65/65 | 0.96 | 0.08 | 49,58,128,136               | 0     |
| 23  | CLA  | C     | 504  | 65/65 | 0.96 | 0.07 | 47,58,66,80                 | 0     |
| 25  | BCR  | B     | 620  | 40/40 | 0.96 | 0.08 | 50,56,67,71                 | 0     |
| 23  | CLA  | C     | 505  | 65/65 | 0.96 | 0.09 | 45,54,89,93                 | 0     |
| 23  | CLA  | B     | 611  | 65/65 | 0.96 | 0.09 | 47,55,67,72                 | 0     |
| 23  | CLA  | b     | 612  | 65/65 | 0.96 | 0.07 | 34,44,63,67                 | 0     |
| 23  | CLA  | b     | 614  | 65/65 | 0.96 | 0.09 | 52,63,74,86                 | 0     |
| 25  | BCR  | K     | 101  | 40/40 | 0.96 | 0.09 | 57,64,69,70                 | 0     |
| 23  | CLA  | b     | 615  | 65/65 | 0.96 | 0.08 | 49,56,63,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | CLA  | b     | 616  | 65/65 | 0.96 | 0.07 | 40,47,68,73                 | 0     |
| 23  | CLA  | C     | 508  | 65/65 | 0.96 | 0.09 | 51,64,83,84                 | 0     |
| 25  | BCR  | b     | 622  | 40/40 | 0.96 | 0.08 | 44,54,66,68                 | 0     |
| 23  | CLA  | b     | 620  | 65/65 | 0.96 | 0.08 | 47,57,88,90                 | 0     |
| 25  | BCR  | b     | 624  | 40/40 | 0.96 | 0.08 | 48,61,76,76                 | 0     |
| 23  | CLA  | C     | 509  | 65/65 | 0.96 | 0.09 | 46,56,115,132               | 0     |
| 37  | DGD  | C     | 517  | 62/66 | 0.96 | 0.11 | 42,55,109,112               | 0     |
| 34  | DMS  | C     | 532  | 4/4   | 0.96 | 0.10 | 67,68,73,74                 | 0     |
| 37  | DGD  | C     | 519  | 58/66 | 0.96 | 0.09 | 43,53,79,93                 | 0     |
| 23  | CLA  | c     | 505  | 65/65 | 0.96 | 0.08 | 45,54,70,78                 | 0     |
| 23  | CLA  | c     | 506  | 65/65 | 0.96 | 0.08 | 47,60,66,82                 | 0     |
| 23  | CLA  | C     | 510  | 65/65 | 0.96 | 0.09 | 53,63,84,88                 | 0     |
| 23  | CLA  | c     | 510  | 65/65 | 0.96 | 0.09 | 48,62,75,83                 | 0     |
| 37  | DGD  | c     | 520  | 62/66 | 0.96 | 0.10 | 47,59,86,95                 | 0     |
| 23  | CLA  | c     | 511  | 65/65 | 0.96 | 0.09 | 46,56,114,137               | 0     |
| 33  | PL9  | D     | 2306 | 55/55 | 0.96 | 0.07 | 38,47,55,64                 | 0     |
| 34  | DMS  | D     | 2318 | 4/4   | 0.96 | 0.12 | 82,85,90,92                 | 0     |
| 38  | LHG  | D     | 2311 | 39/49 | 0.96 | 0.09 | 51,59,92,97                 | 0     |
| 33  | PL9  | d     | 411  | 55/55 | 0.96 | 0.08 | 37,46,56,65                 | 0     |
| 23  | CLA  | c     | 513  | 65/65 | 0.96 | 0.08 | 46,57,68,79                 | 0     |
| 23  | CLA  | c     | 514  | 65/65 | 0.96 | 0.08 | 55,65,73,75                 | 0     |
| 23  | CLA  | C     | 511  | 65/65 | 0.96 | 0.07 | 47,56,68,78                 | 0     |
| 23  | CLA  | A     | 410  | 65/65 | 0.96 | 0.10 | 41,50,123,127               | 0     |
| 39  | HEM  | e     | 103  | 43/43 | 0.96 | 0.09 | 65,76,109,133               | 0     |
| 23  | CLA  | A     | 407  | 65/65 | 0.96 | 0.09 | 36,47,109,115               | 0     |
| 34  | DMS  | b     | 634  | 4/4   | 0.96 | 0.14 | 81,86,88,92                 | 0     |
| 24  | PHO  | A     | 408  | 64/64 | 0.96 | 0.07 | 35,43,49,52                 | 0     |
| 24  | PHO  | A     | 409  | 64/64 | 0.96 | 0.07 | 41,49,58,61                 | 0     |
| 23  | CLA  | B     | 603  | 65/65 | 0.97 | 0.07 | 41,54,70,76                 | 0     |
| 23  | CLA  | C     | 512  | 65/65 | 0.97 | 0.07 | 55,63,74,81                 | 0     |
| 23  | CLA  | c     | 504  | 65/65 | 0.97 | 0.08 | 45,59,72,83                 | 0     |
| 23  | CLA  | B     | 616  | 65/65 | 0.97 | 0.08 | 43,55,83,95                 | 0     |
| 34  | DMS  | c     | 533  | 4/4   | 0.97 | 0.11 | 59,63,63,65                 | 0     |
| 23  | CLA  | B     | 608  | 65/65 | 0.97 | 0.07 | 34,44,61,73                 | 0     |
| 23  | CLA  | c     | 507  | 65/65 | 0.97 | 0.08 | 46,56,91,95                 | 0     |
| 23  | CLA  | c     | 508  | 65/65 | 0.97 | 0.07 | 49,57,80,86                 | 0     |
| 23  | CLA  | C     | 502  | 65/65 | 0.97 | 0.07 | 48,58,75,83                 | 0     |
| 23  | CLA  | a     | 2610 | 65/65 | 0.97 | 0.10 | 38,46,116,121               | 0     |
| 34  | DMS  | V     | 205  | 4/4   | 0.97 | 0.12 | 67,74,74,77                 | 0     |
| 23  | CLA  | C     | 503  | 65/65 | 0.97 | 0.06 | 41,53,70,76                 | 0     |
| 34  | DMS  | v     | 205  | 4/4   | 0.97 | 0.10 | 75,77,83,86                 | 0     |
| 32  | BCT  | A     | 421  | 4/4   | 0.97 | 0.06 | 59,60,65,75                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | CLA  | c     | 512  | 65/65 | 0.97 | 0.08 | 51,59,89,100                | 0     |
| 25  | BCR  | k     | 302  | 40/40 | 0.97 | 0.08 | 53,64,78,79                 | 0     |
| 23  | CLA  | B     | 609  | 65/65 | 0.97 | 0.07 | 45,54,73,79                 | 0     |
| 23  | CLA  | b     | 607  | 65/65 | 0.97 | 0.09 | 48,57,69,76                 | 0     |
| 23  | CLA  | b     | 609  | 65/65 | 0.97 | 0.07 | 37,46,85,92                 | 0     |
| 23  | CLA  | b     | 610  | 65/65 | 0.97 | 0.07 | 39,49,60,63                 | 0     |
| 23  | CLA  | d     | 402  | 65/65 | 0.97 | 0.06 | 35,41,50,62                 | 0     |
| 23  | CLA  | B     | 604  | 65/65 | 0.97 | 0.07 | 42,51,66,72                 | 0     |
| 35  | CA   | b     | 605  | 1/1   | 0.97 | 0.05 | 72,72,72,72                 | 0     |
| 23  | CLA  | C     | 506  | 65/65 | 0.97 | 0.08 | 51,59,80,81                 | 0     |
| 23  | CLA  | b     | 613  | 65/65 | 0.97 | 0.07 | 41,53,72,77                 | 0     |
| 38  | LHG  | L     | 101  | 49/49 | 0.97 | 0.08 | 46,57,73,76                 | 0     |
| 24  | PHO  | a     | 2611 | 64/64 | 0.97 | 0.06 | 38,42,49,57                 | 0     |
| 24  | PHO  | a     | 2612 | 64/64 | 0.97 | 0.06 | 39,49,59,65                 | 0     |
| 38  | LHG  | d     | 413  | 49/49 | 0.97 | 0.07 | 40,49,71,73                 | 0     |
| 25  | BCR  | A     | 411  | 40/40 | 0.97 | 0.06 | 38,48,58,62                 | 0     |
| 34  | DMS  | B     | 638  | 4/4   | 0.97 | 0.09 | 61,68,73,82                 | 0     |
| 23  | CLA  | B     | 606  | 65/65 | 0.97 | 0.07 | 37,47,62,64                 | 0     |
| 23  | CLA  | B     | 612  | 65/65 | 0.97 | 0.06 | 39,47,66,70                 | 0     |
| 23  | CLA  | B     | 613  | 65/65 | 0.97 | 0.07 | 39,46,56,61                 | 0     |
| 23  | CLA  | b     | 618  | 65/65 | 0.97 | 0.07 | 40,46,93,96                 | 0     |
| 23  | CLA  | B     | 614  | 65/65 | 0.97 | 0.07 | 37,45,91,99                 | 0     |
| 34  | DMS  | A     | 424  | 4/4   | 0.98 | 0.09 | 48,50,52,59                 | 0     |
| 23  | CLA  | A     | 406  | 65/65 | 0.98 | 0.06 | 34,41,51,63                 | 0     |
| 23  | CLA  | D     | 2303 | 65/65 | 0.98 | 0.06 | 33,42,62,72                 | 0     |
| 23  | CLA  | A     | 405  | 65/65 | 0.98 | 0.06 | 33,41,55,77                 | 0     |
| 23  | CLA  | b     | 608  | 65/65 | 0.98 | 0.07 | 40,52,71,75                 | 0     |
| 34  | DMS  | C     | 533  | 4/4   | 0.98 | 0.07 | 61,64,65,66                 | 0     |
| 23  | CLA  | d     | 408  | 65/65 | 0.98 | 0.06 | 31,42,60,71                 | 0     |
| 39  | HEM  | F     | 101  | 43/43 | 0.98 | 0.06 | 61,71,100,119               | 0     |
| 23  | CLA  | a     | 2609 | 65/65 | 0.98 | 0.06 | 35,41,55,69                 | 0     |
| 23  | CLA  | B     | 605  | 65/65 | 0.98 | 0.07 | 37,44,85,94                 | 0     |
| 34  | DMS  | o     | 304  | 4/4   | 0.98 | 0.07 | 43,53,55,59                 | 0     |
| 34  | DMS  | B     | 636  | 4/4   | 0.98 | 0.09 | 43,47,47,59                 | 0     |
| 41  | MG   | j     | 2703 | 1/1   | 0.98 | 0.10 | 60,60,60,60                 | 0     |
| 23  | CLA  | b     | 617  | 65/65 | 0.98 | 0.06 | 41,49,56,58                 | 0     |
| 42  | HEC  | v     | 201  | 43/43 | 0.98 | 0.06 | 49,56,62,69                 | 0     |
| 22  | CL   | A     | 403  | 1/1   | 0.99 | 0.05 | 46,46,46,46                 | 0     |
| 35  | CA   | B     | 601  | 1/1   | 0.99 | 0.05 | 68,68,68,68                 | 0     |
| 35  | CA   | O     | 301  | 1/1   | 0.99 | 0.06 | 77,77,77,77                 | 0     |
| 22  | CL   | a     | 2606 | 1/1   | 0.99 | 0.08 | 48,48,48,48                 | 0     |
| 41  | MG   | J     | 302  | 1/1   | 0.99 | 0.09 | 58,58,58,58                 | 0     |

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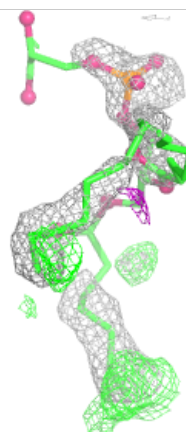
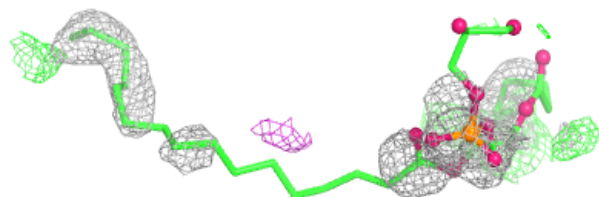
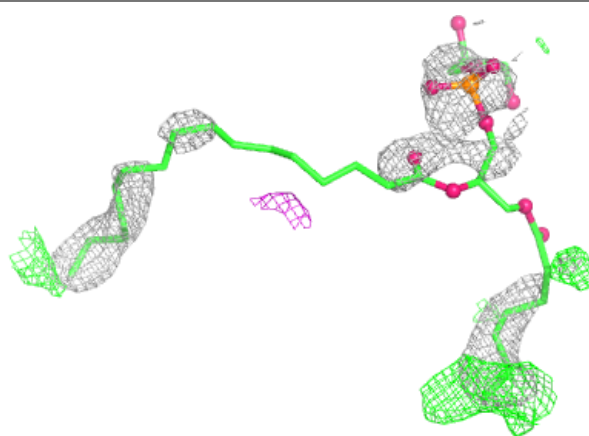
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35  | CA   | c     | 503  | 1/1   | 0.99 | 0.03 | 73,73,73,73                 | 0     |
| 35  | CA   | o     | 302  | 1/1   | 0.99 | 0.03 | 74,74,74,74                 | 0     |
| 34  | DMS  | b     | 633  | 4/4   | 0.99 | 0.06 | 45,50,52,61                 | 0     |
| 42  | HEC  | V     | 201  | 43/43 | 0.99 | 0.06 | 41,46,52,56                 | 0     |
| 20  | OEX  | A     | 401  | 10/10 | 0.99 | 0.03 | 41,46,50,52                 | 0     |
| 22  | CL   | a     | 2607 | 1/1   | 1.00 | 0.03 | 46,46,46,46                 | 0     |
| 21  | FE2  | a     | 2605 | 1/1   | 1.00 | 0.01 | 52,52,52,52                 | 0     |
| 20  | OEX  | a     | 2604 | 10/10 | 1.00 | 0.02 | 41,46,51,52                 | 0     |
| 22  | CL   | A     | 404  | 1/1   | 1.00 | 0.06 | 43,43,43,43                 | 0     |
| 21  | FE2  | A     | 402  | 1/1   | 1.00 | 0.01 | 54,54,54,54                 | 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.

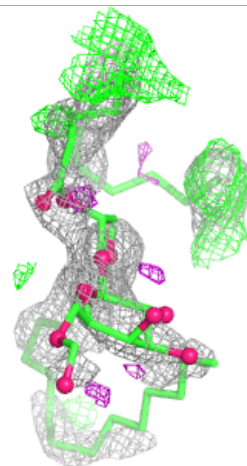
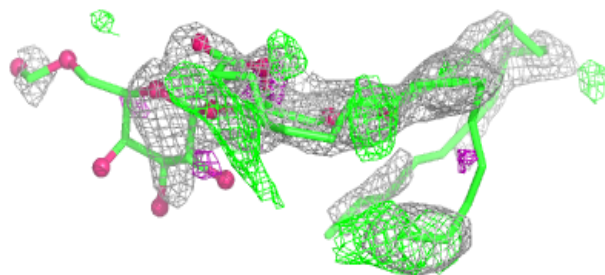
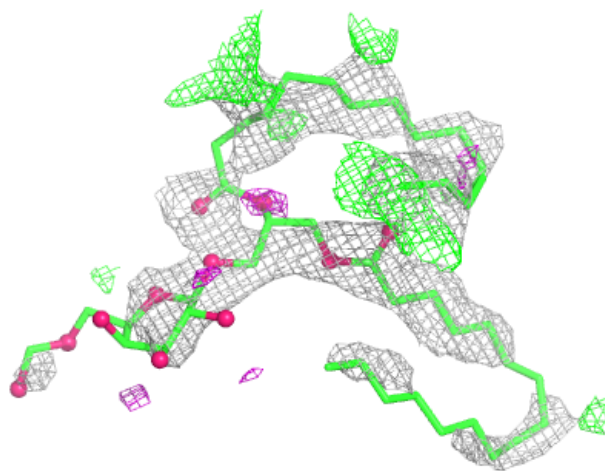
#### Electron density around LHG e 101:

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



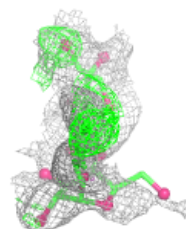
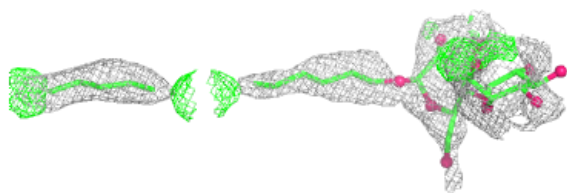
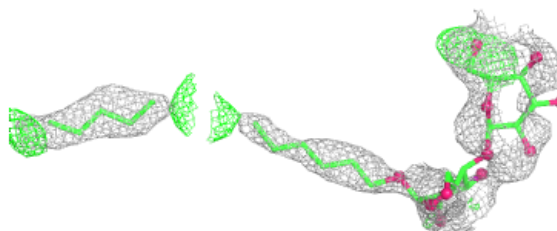
**Electron density around DGD D 2307:**

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



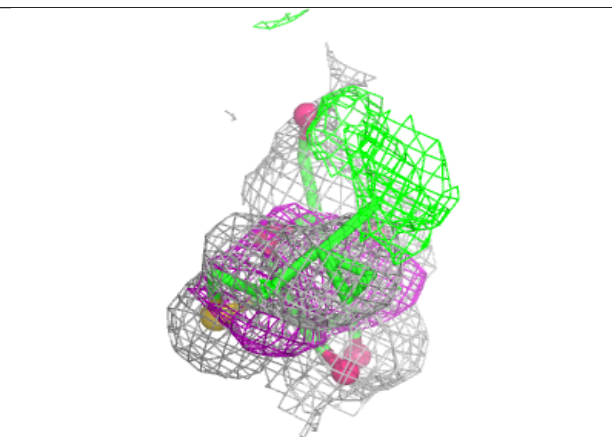
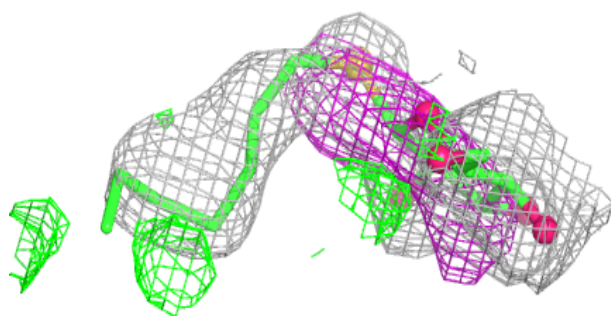
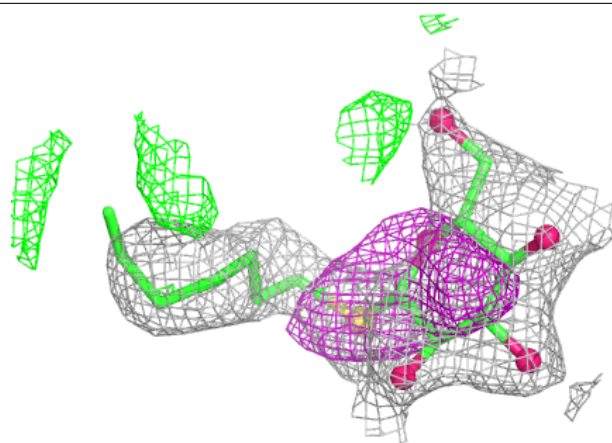
**Electron density around LMT j 2701:**

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

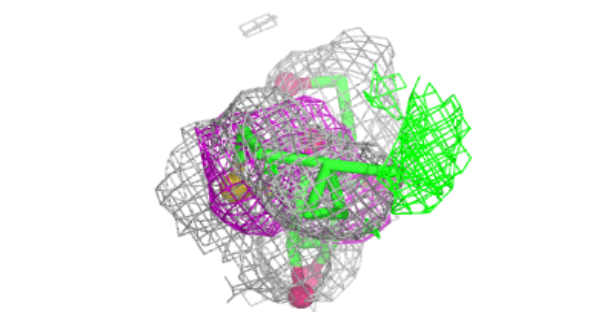
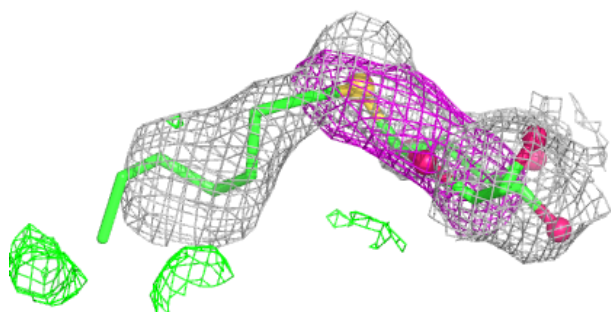
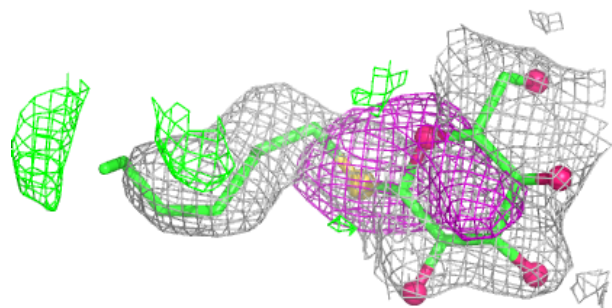


**Electron density around HTG B 624 (A):**

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

**Electron density around HTG B 624 (B):**

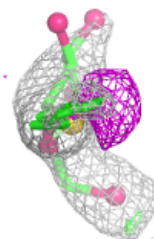
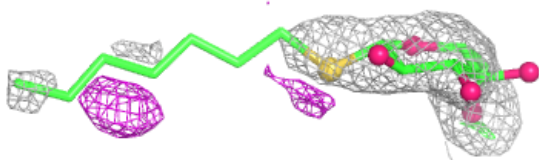
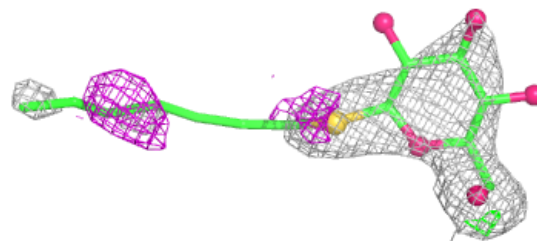
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



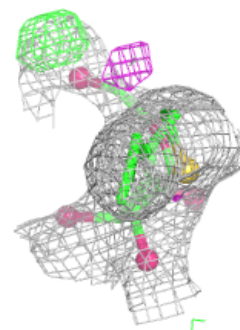
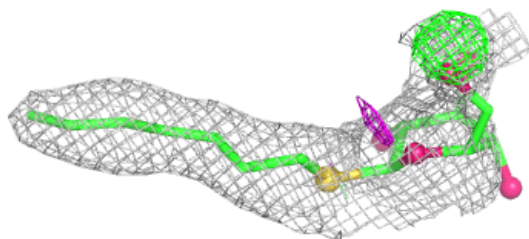
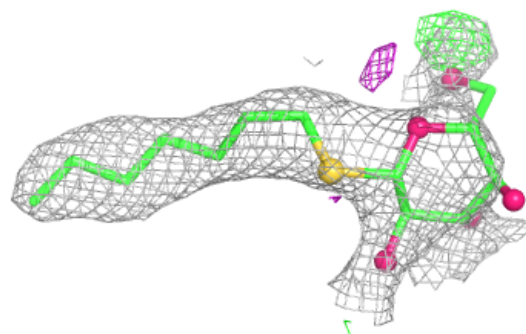


**Electron density around HTG C 522:**

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

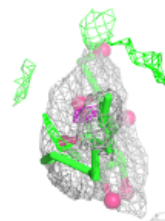
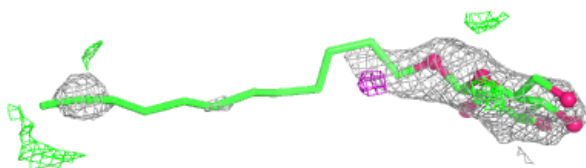
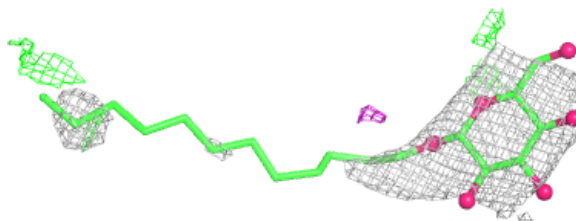
**Electron density around HTG i 102:**

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

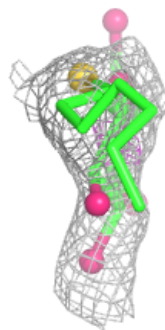
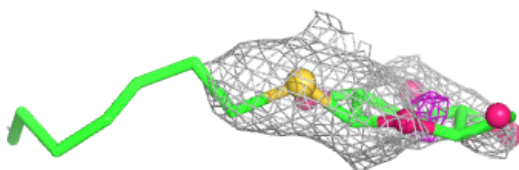
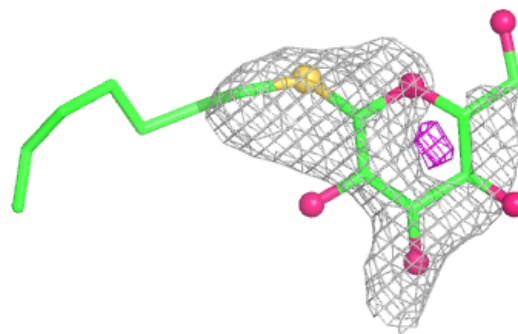


**Electron density around LMT F 102:**

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

**Electron density around HTG d 407:**

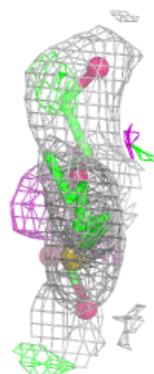
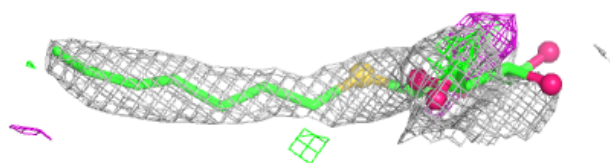
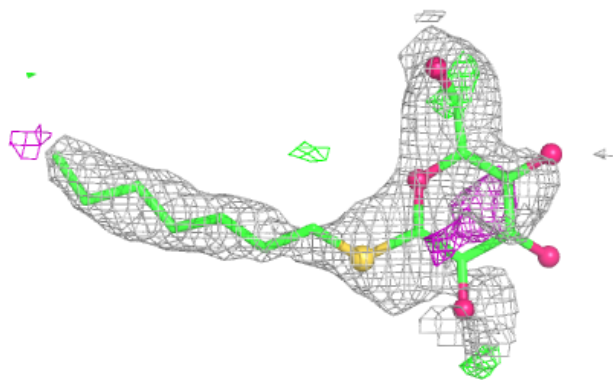
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



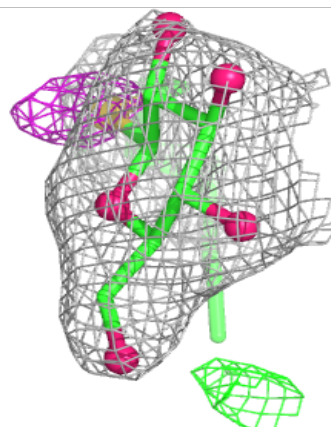
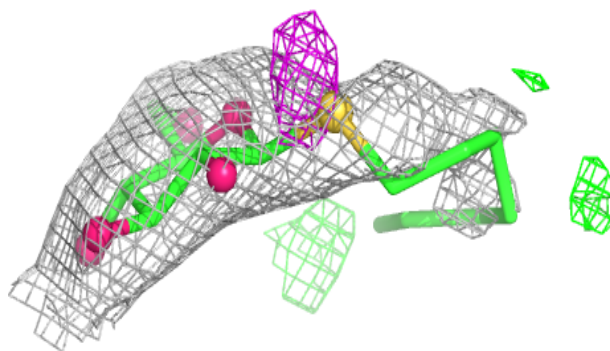
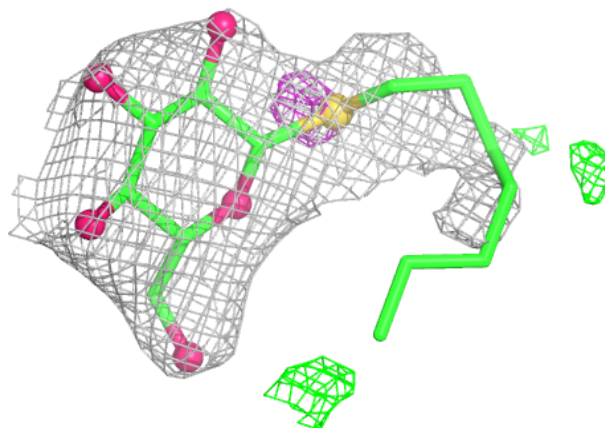


**Electron density around HTG B 627:**

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

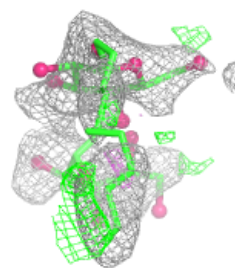
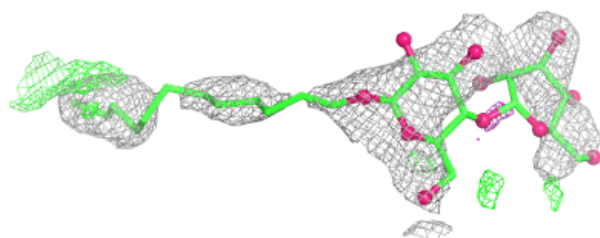
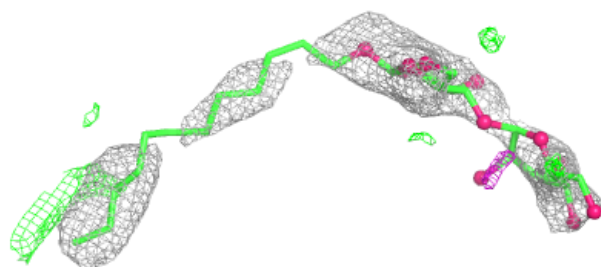
**Electron density around HTG V 204:**

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

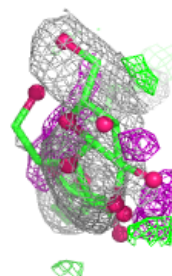
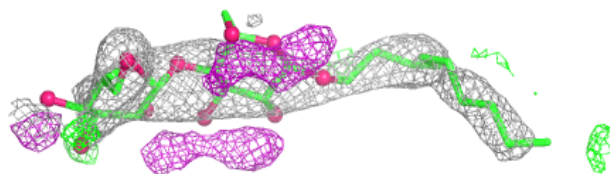
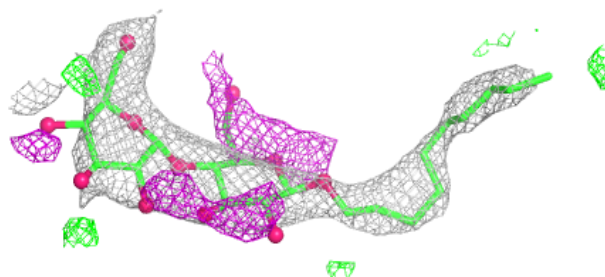


**Electron density around LMT m 2804:**

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

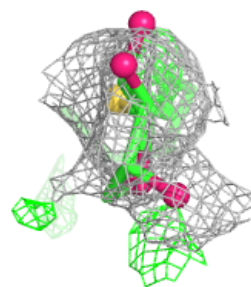
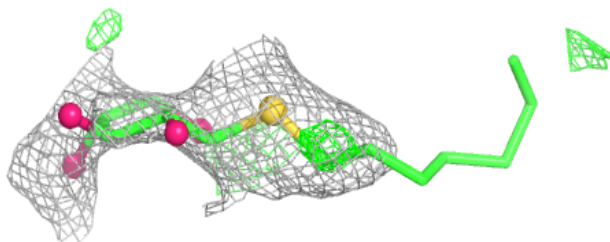
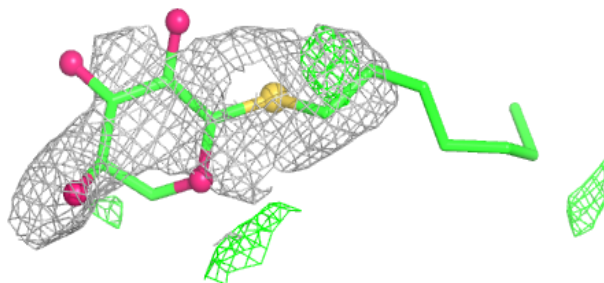
**Electron density around LMT A 414:**

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

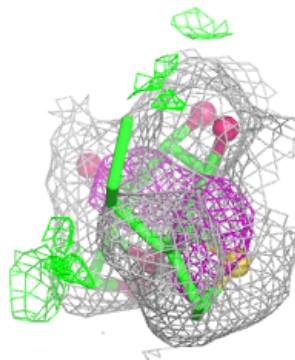
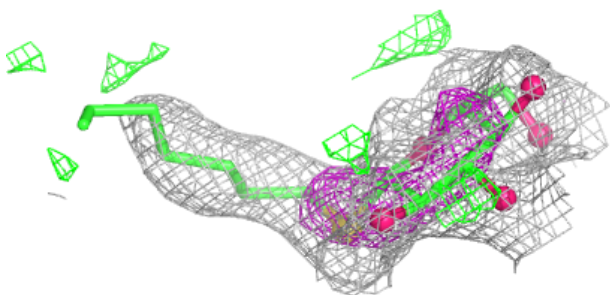
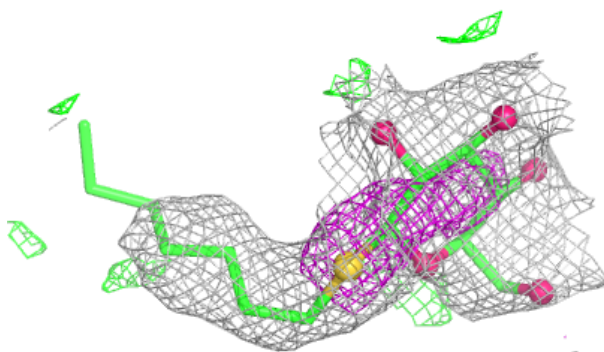


**Electron density around HTG H 101:**

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

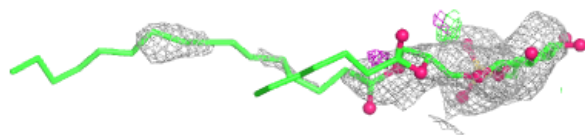
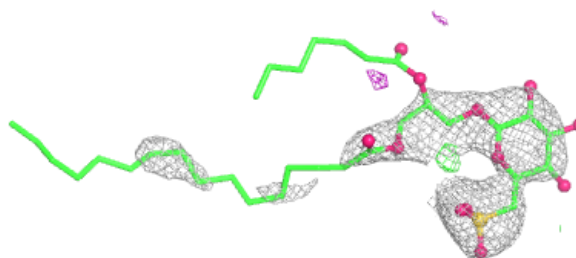
**Electron density around HTG b 625:**

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



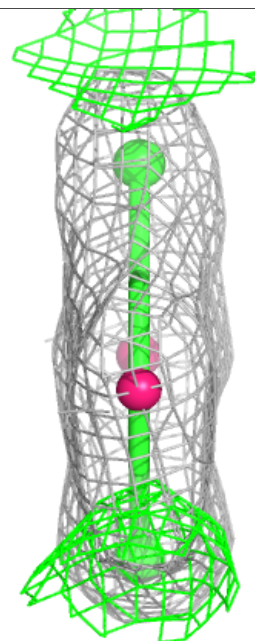
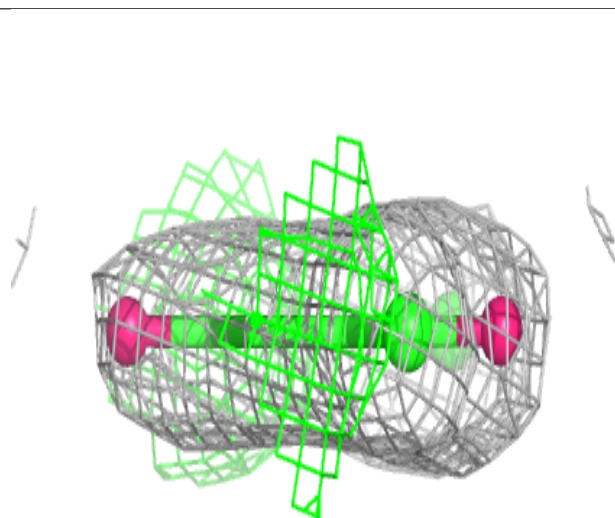
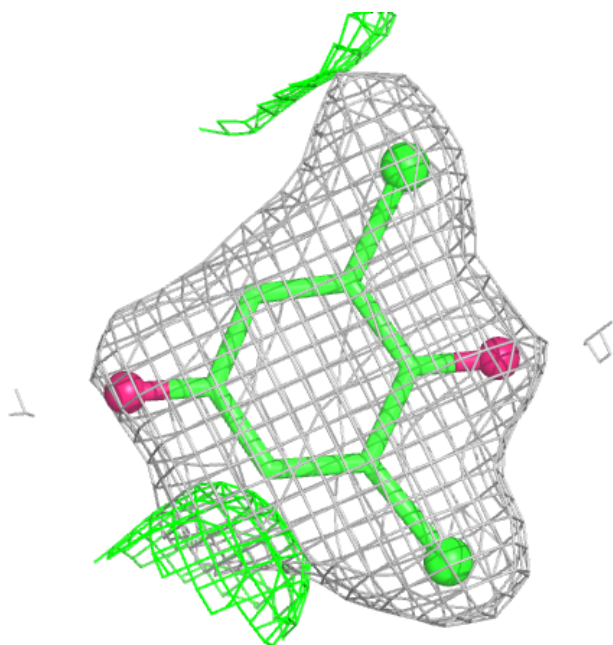
**Electron density around SQD D 2308:**

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



**Electron density around JOX A 418:**

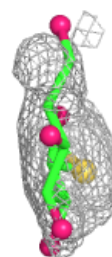
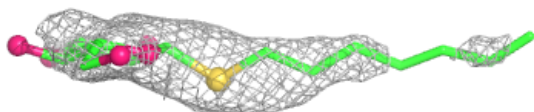
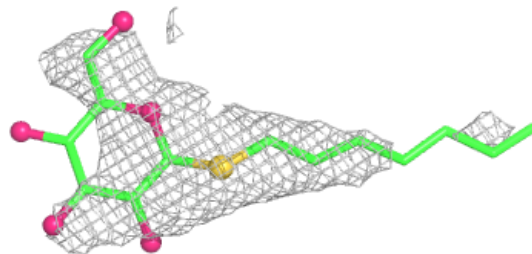
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



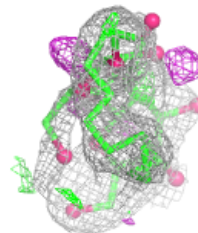
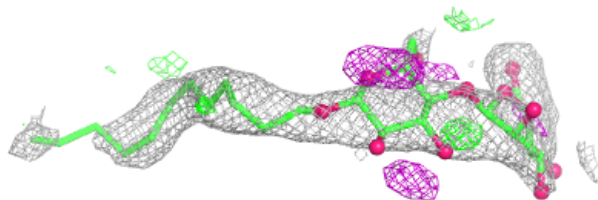
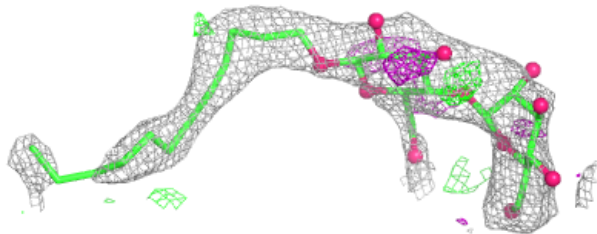


**Electron density around HTG C 525:**

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

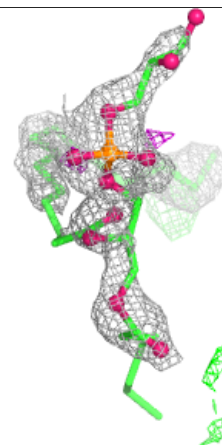
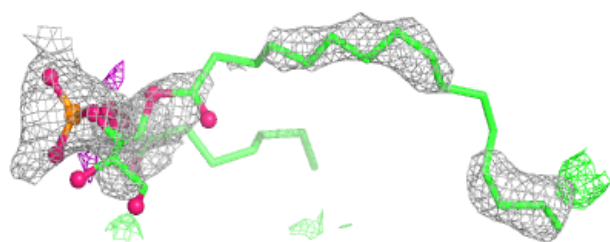
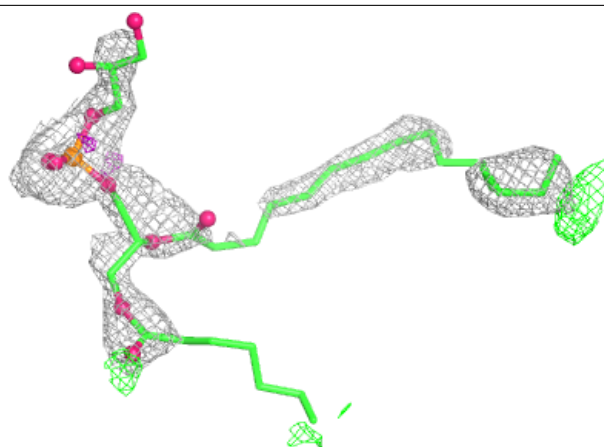
**Electron density around LMT d 401:**

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

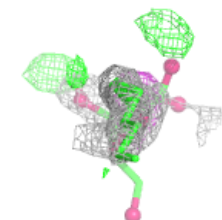
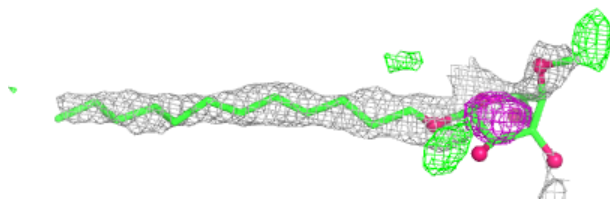
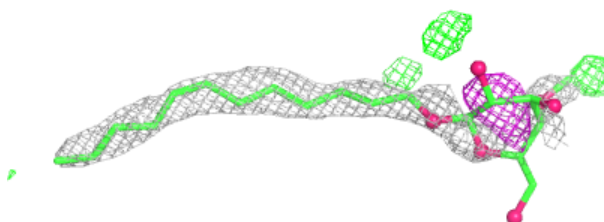


**Electron density around LHG E 101:**

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

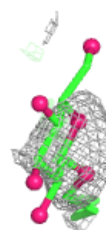
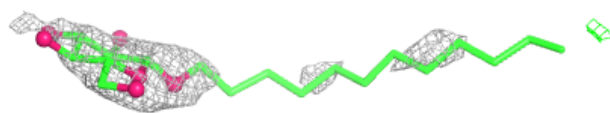
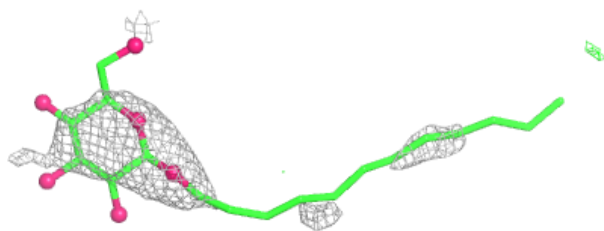
**Electron density around LMT d 404:**

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

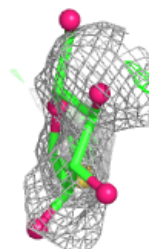
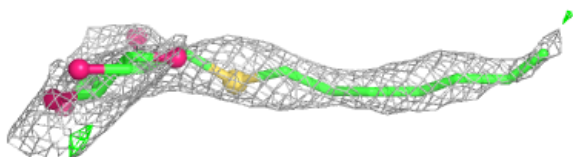
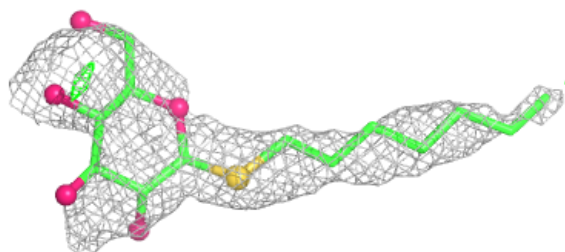


**Electron density around LMT f 101:**

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

**Electron density around HTG B 625:**

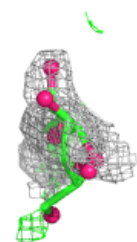
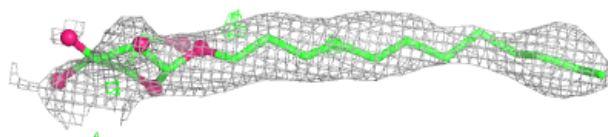
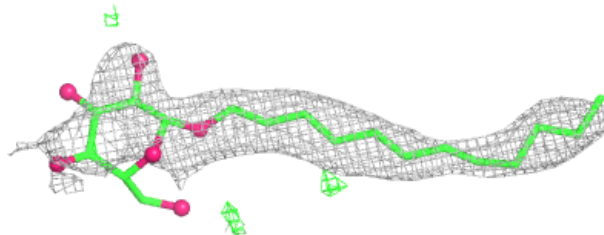
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



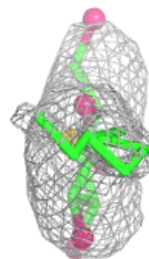
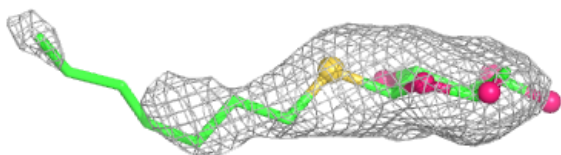
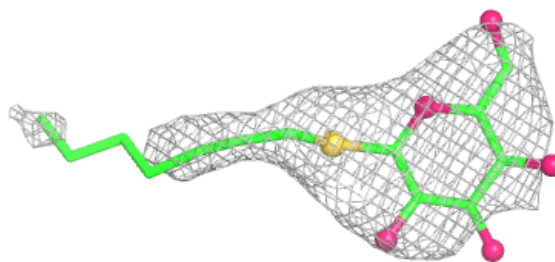


**Electron density around LMT J 303:**

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

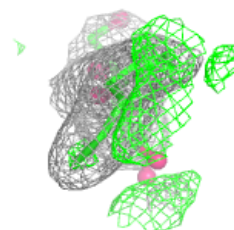
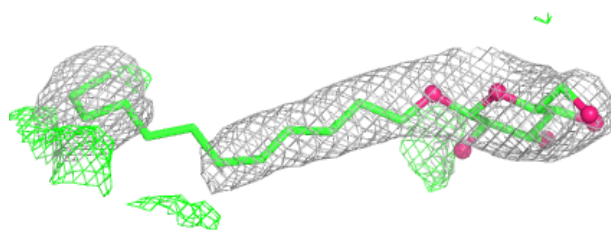
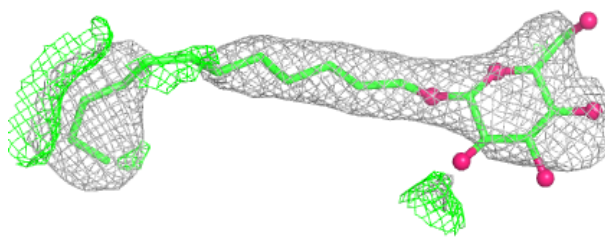
**Electron density around HTG c 523:**

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



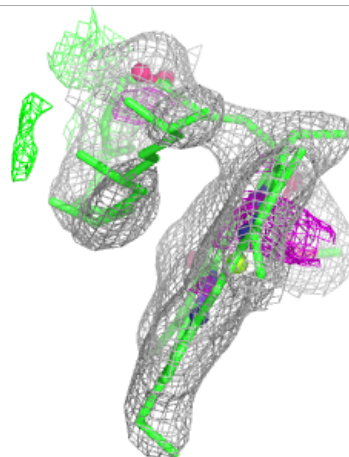
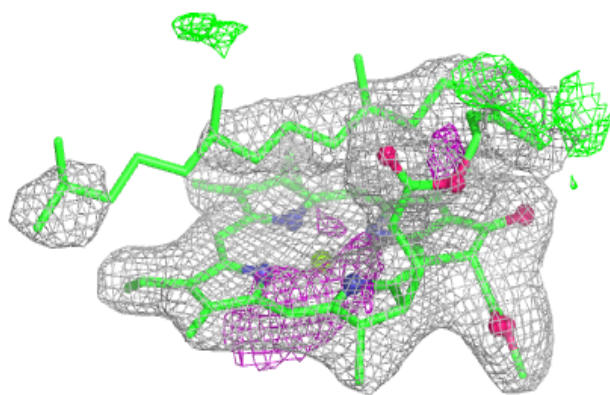
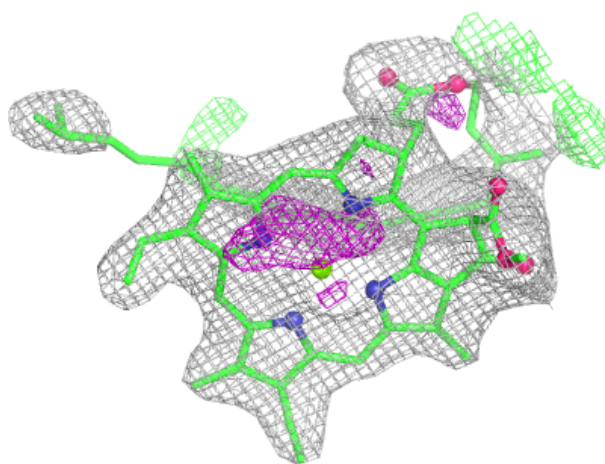
**Electron density around LMT T 103:**

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



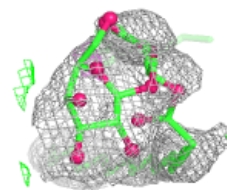
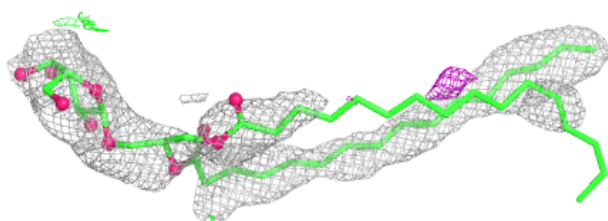
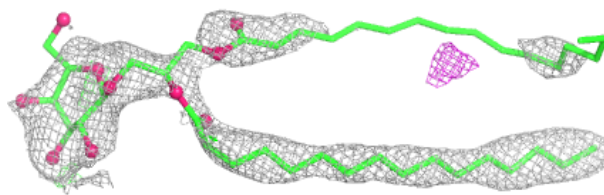
**Electron density around CLA B 602:**

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

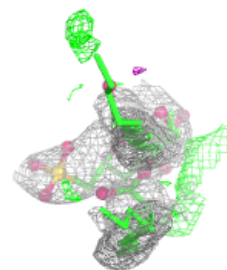
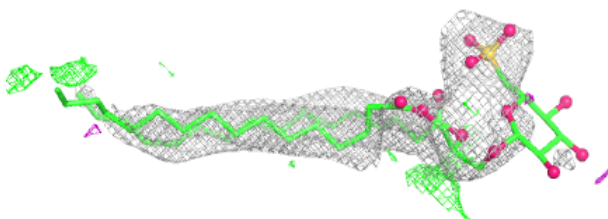
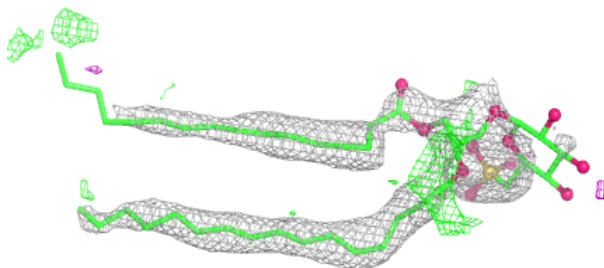


**Electron density around LMG c 522:**

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

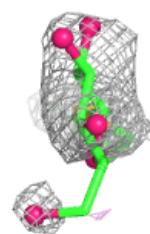
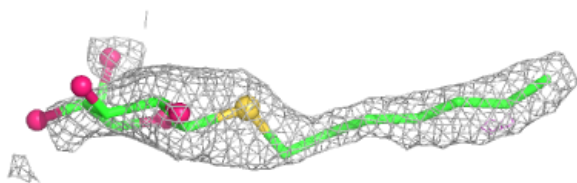
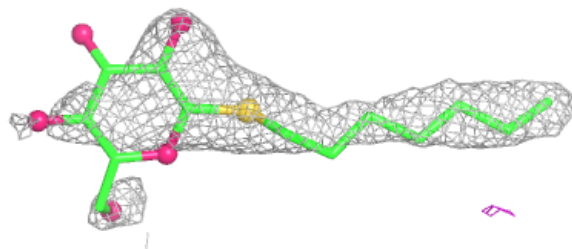
**Electron density around SQD D 2302:**

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

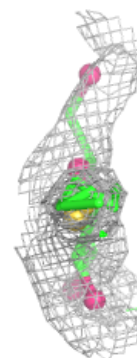
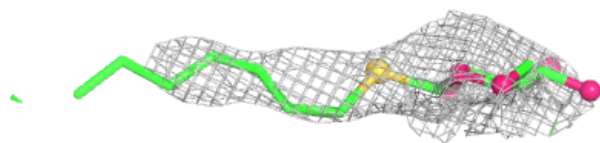
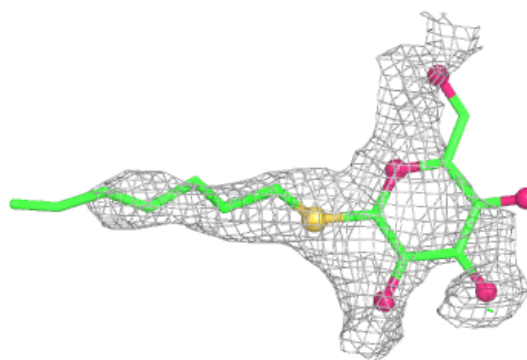


**Electron density around HTG c 524:**

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

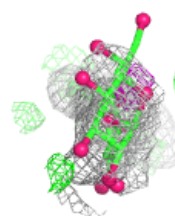
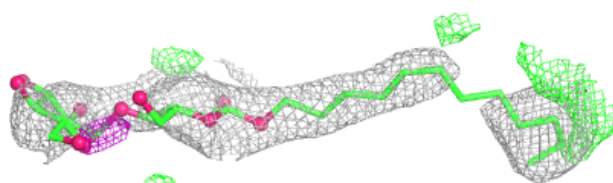
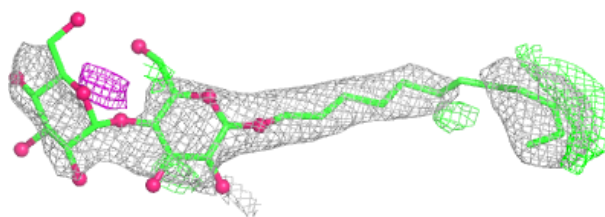
**Electron density around HTG c 526:**

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

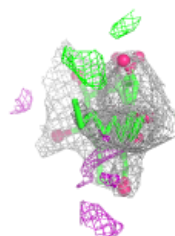
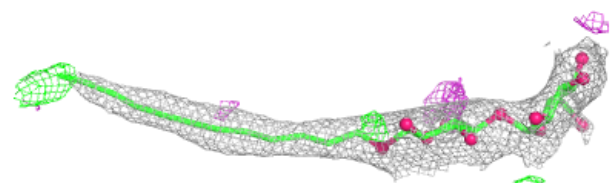
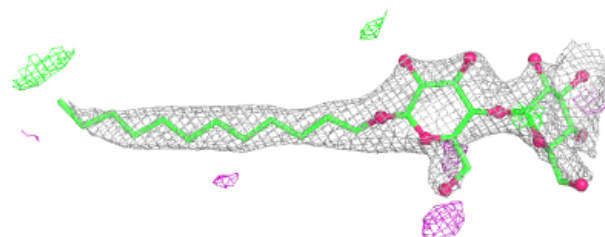


**Electron density around LMT B 634:**

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

**Electron density around LMT m 2803:**

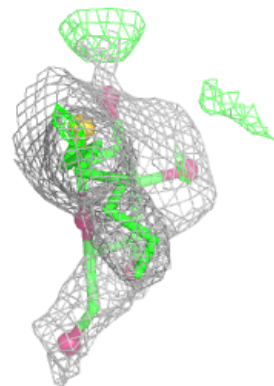
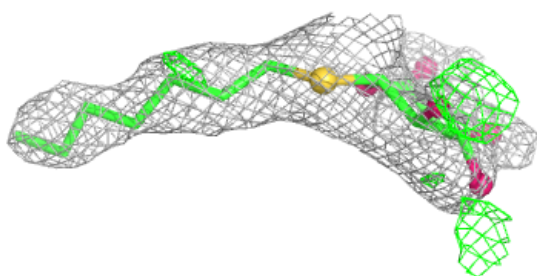
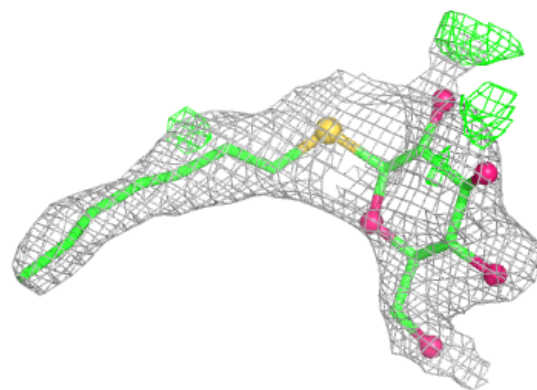
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



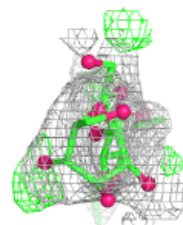
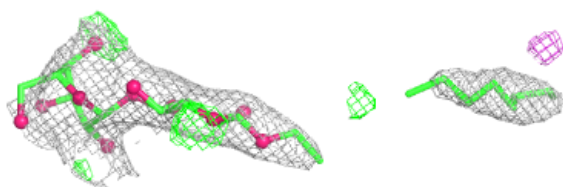
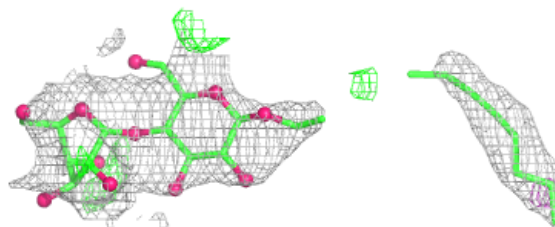


**Electron density around HTG b 626:**

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

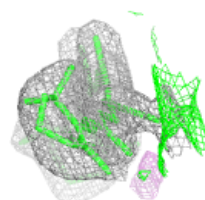
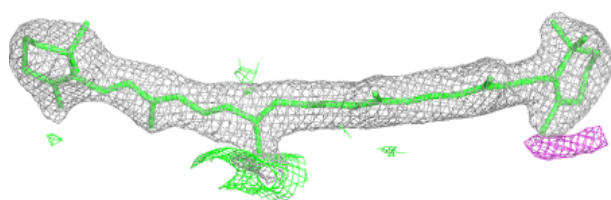
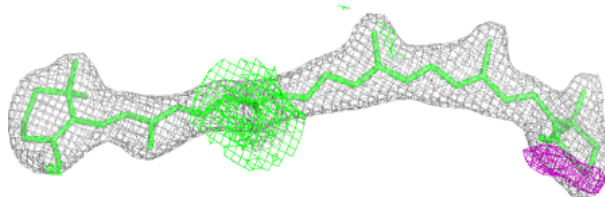
**Electron density around LMT z 102:**

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

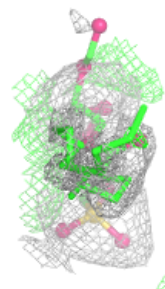
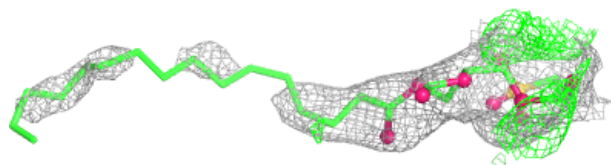
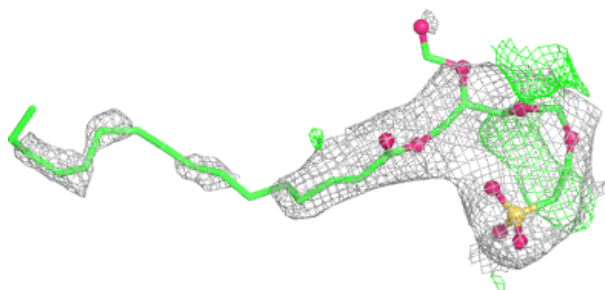


**Electron density around BCR T 102:**

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

**Electron density around SQD d 417:**

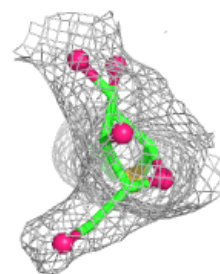
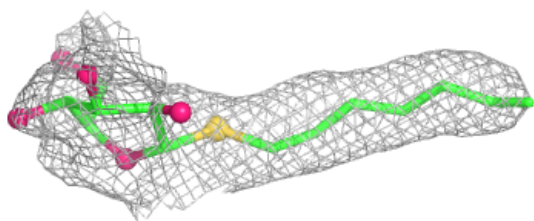
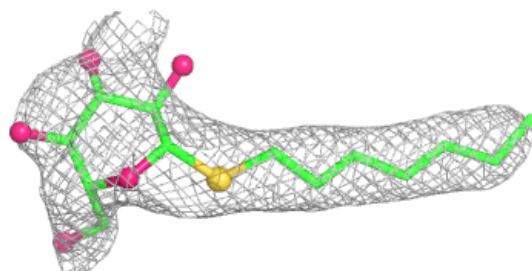
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



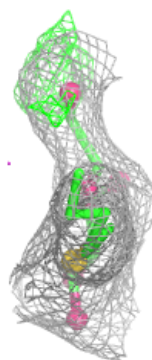
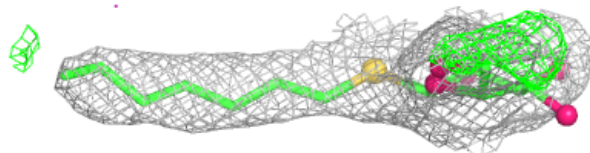
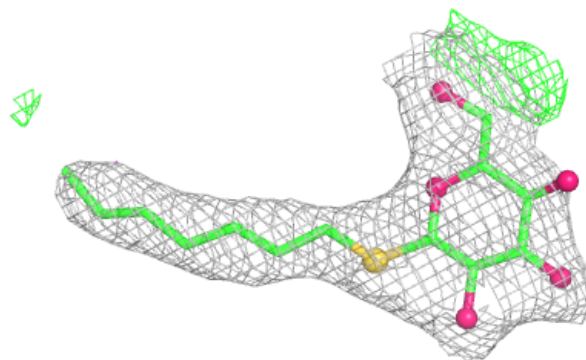


**Electron density around HTG I 101:**

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

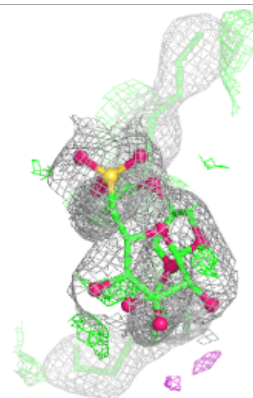
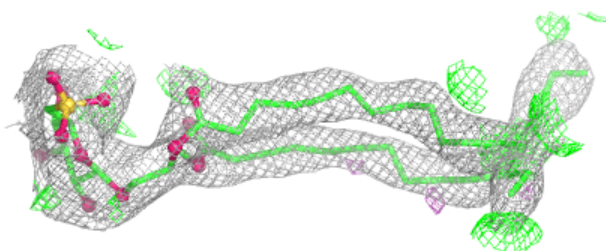
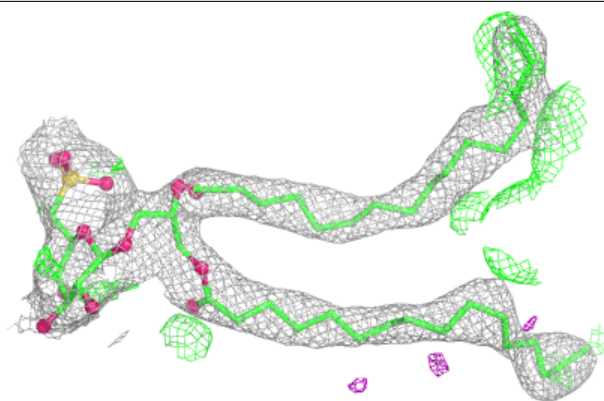
**Electron density around HTG b 604:**

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

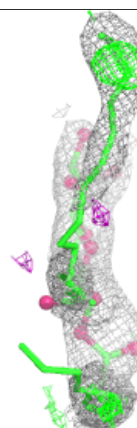
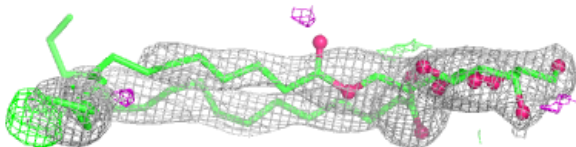
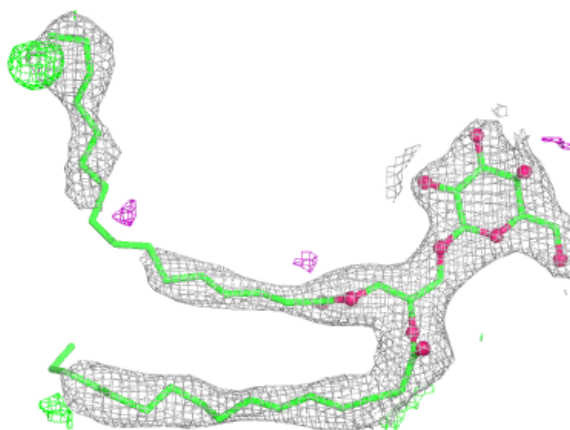


**Electron density around SQD 1 101:**

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

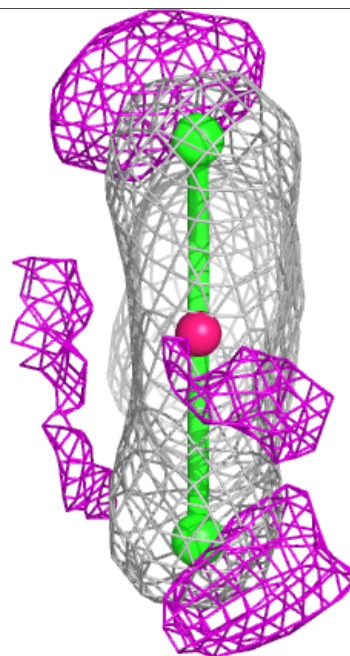
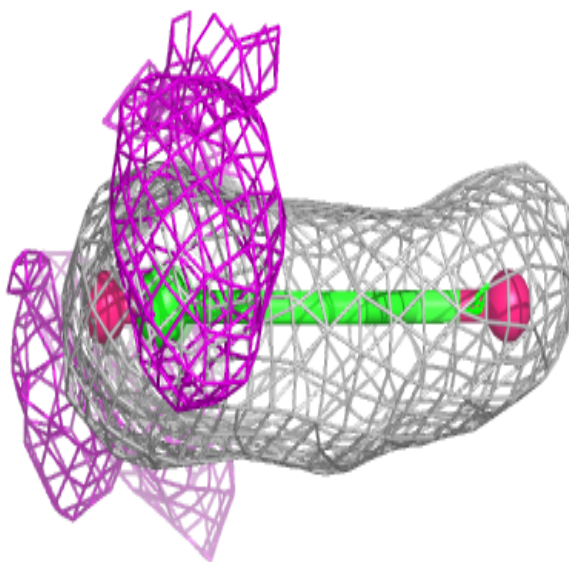
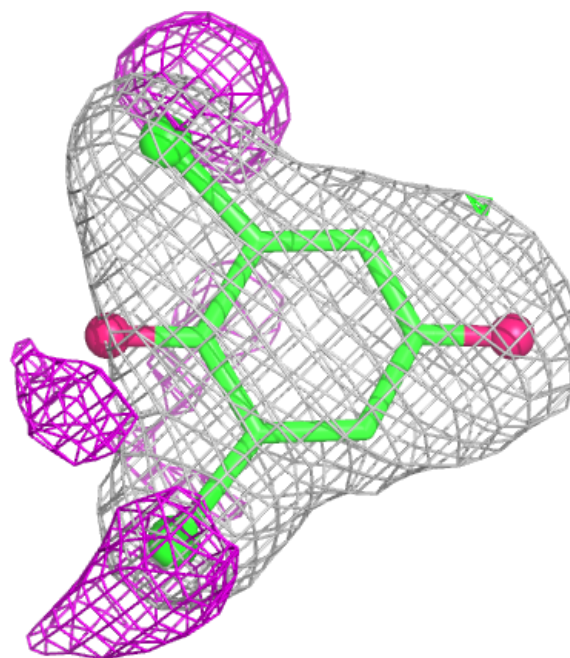
**Electron density around LMG C 520:**

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



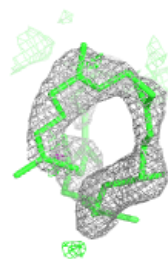
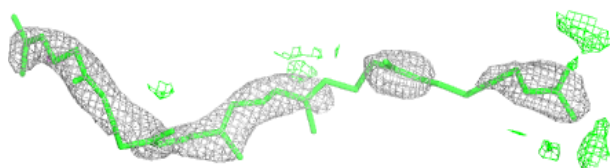
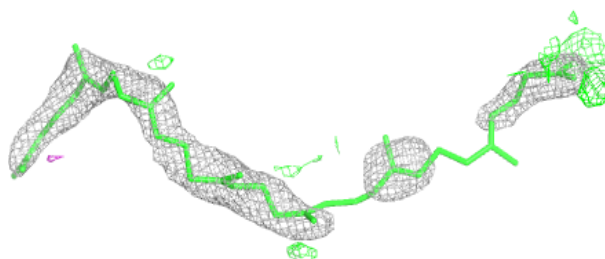
**Electron density around JOX A 419:**

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

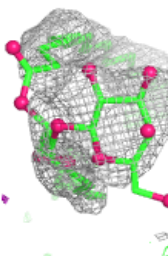
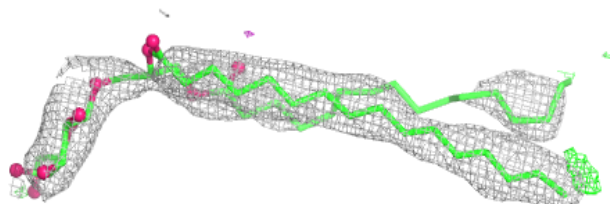
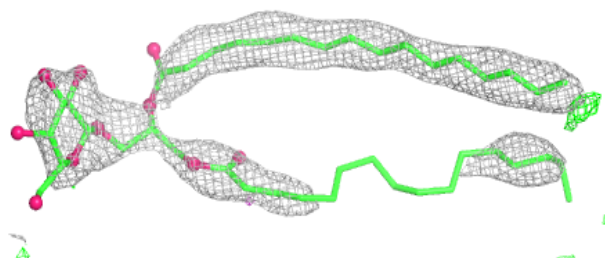


**Electron density around PL9 A 422:**

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

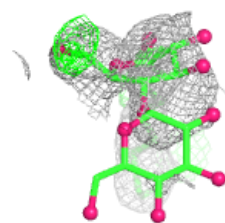
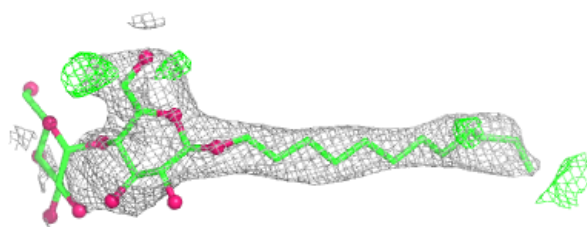
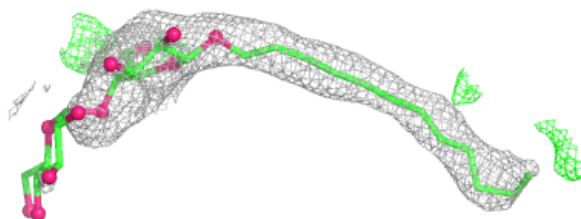
**Electron density around LMG C 527:**

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

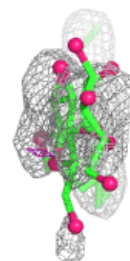
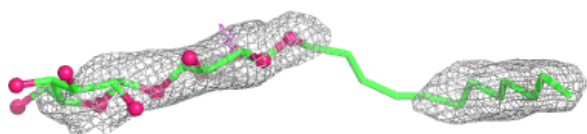
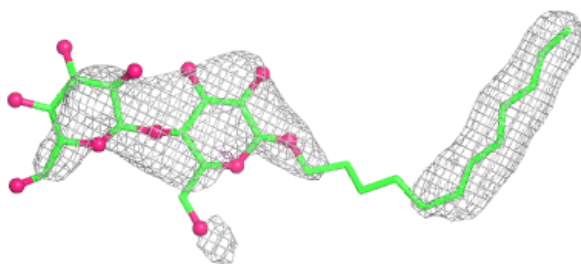


**Electron density around LMT M 101:**

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

**Electron density around LMT Z 101:**

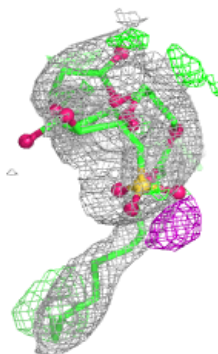
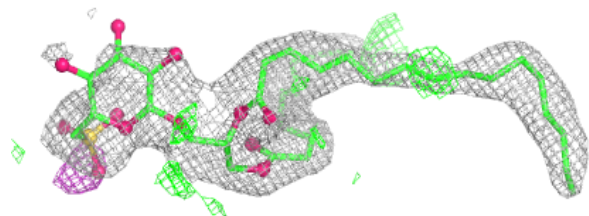
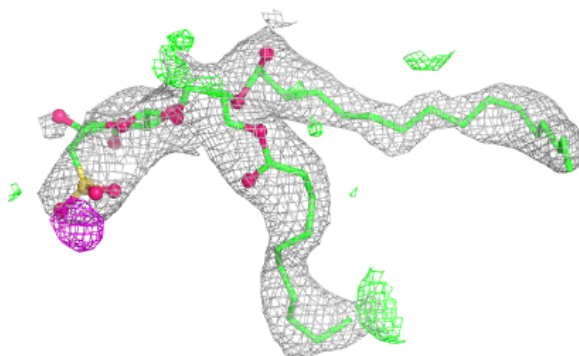
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



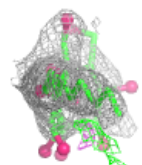
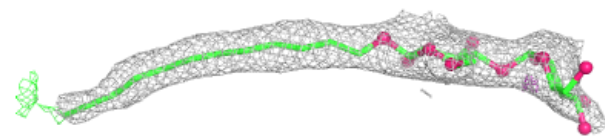
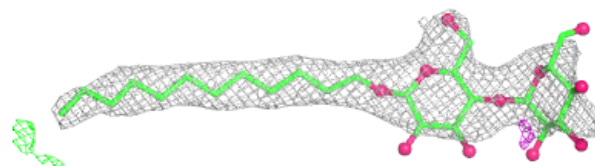


**Electron density around SQD b 601:**

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

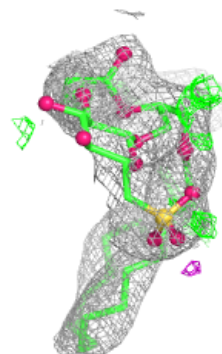
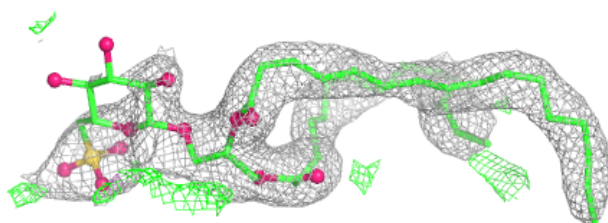
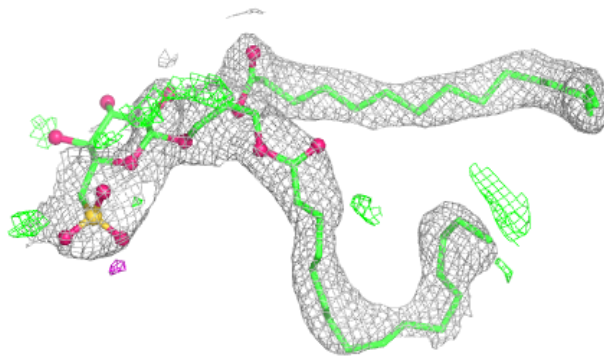
**Electron density around LMT M 102:**

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

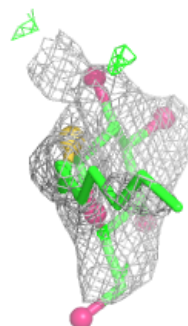
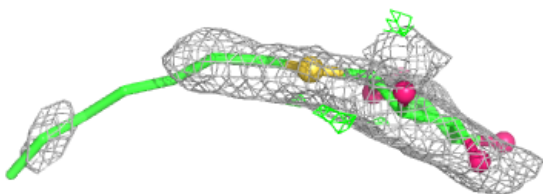
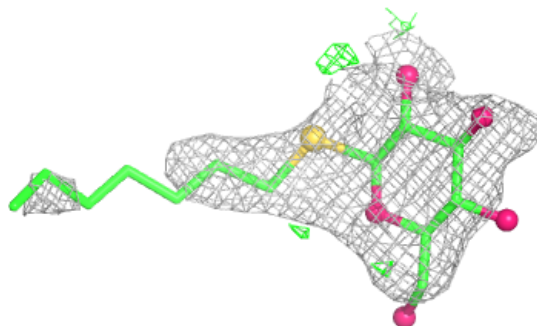


**Electron density around SQD a 2603:**

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

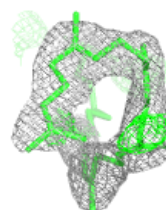
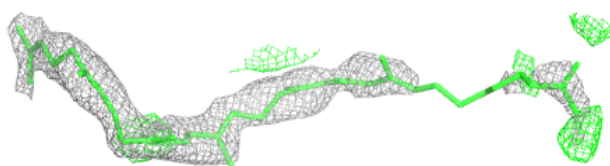
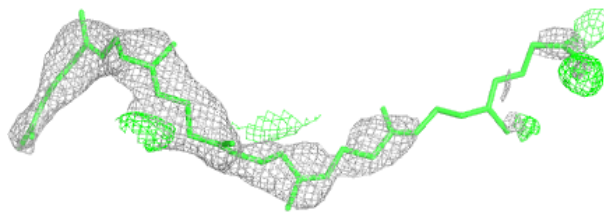
**Electron density around HTG d 415:**

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

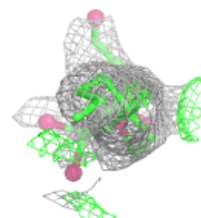
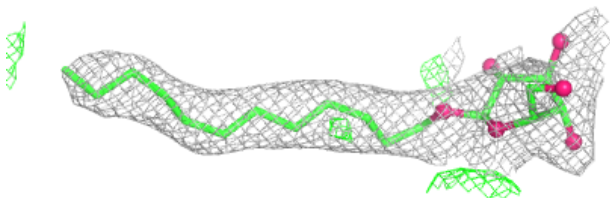
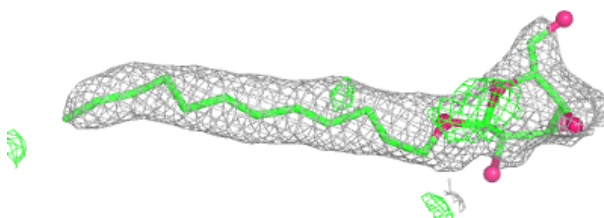


**Electron density around PL9 x 1301:**

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

**Electron density around LMT i 103:**

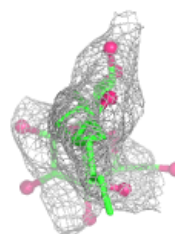
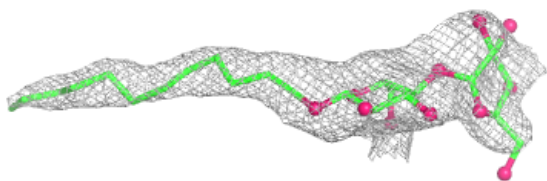
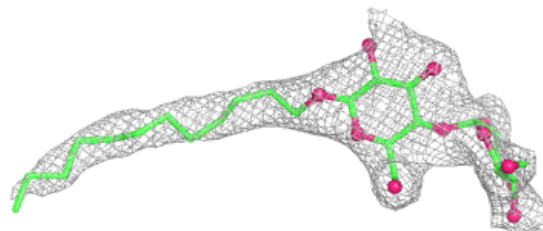
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



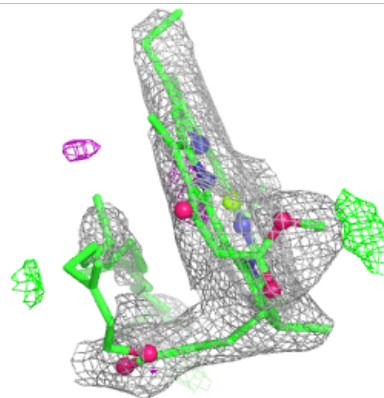
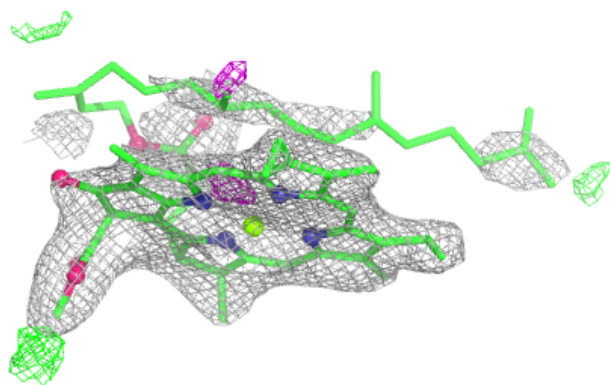
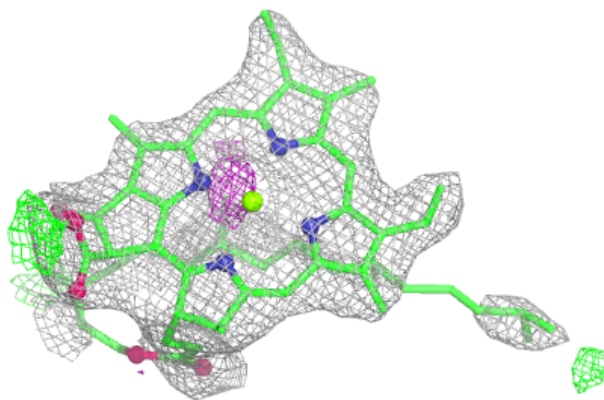


**Electron density around LMT B 623:**

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

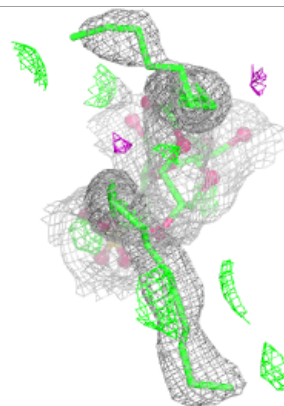
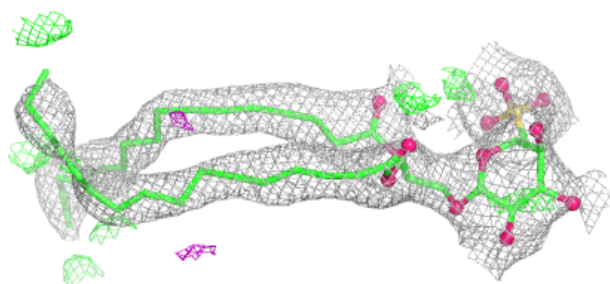
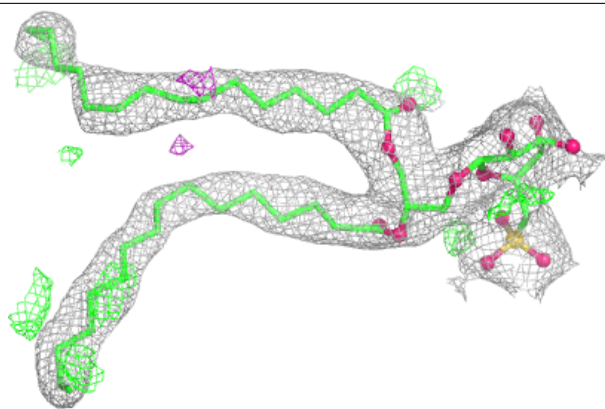
**Electron density around CLA b 606:**

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

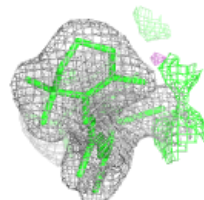
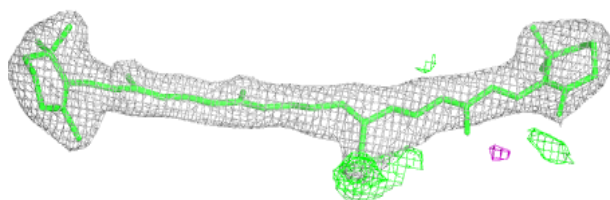
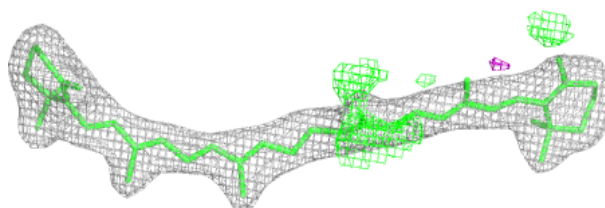


**Electron density around SQD B 621:**

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

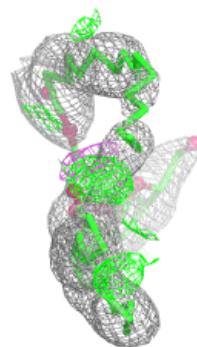
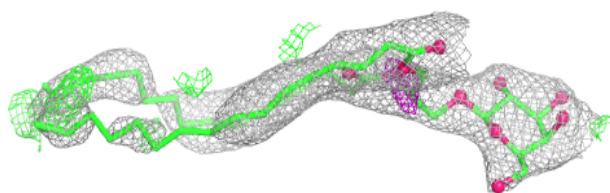
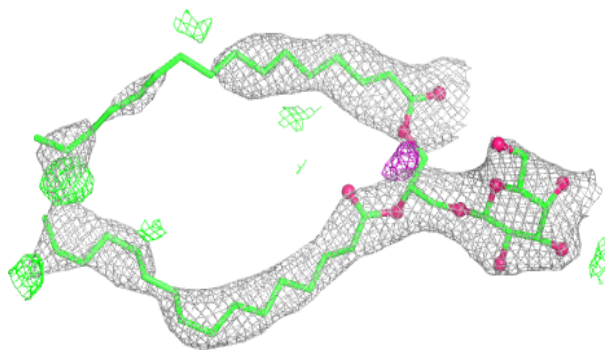
**Electron density around BCR B 633:**

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

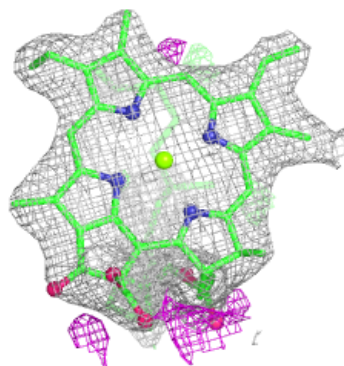
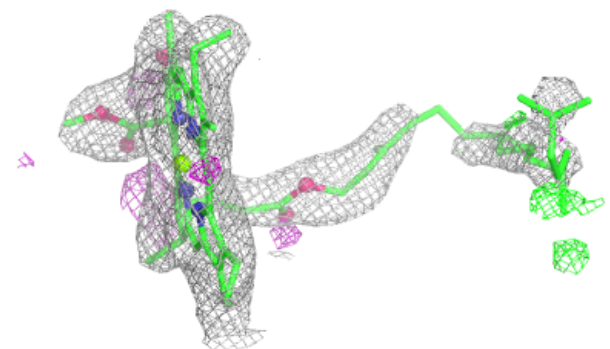
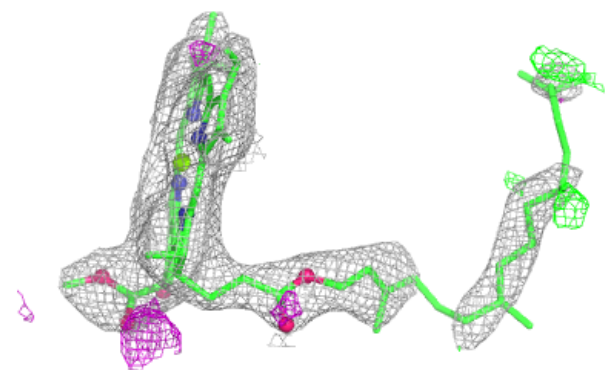


**Electron density around LMG c 501:**

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

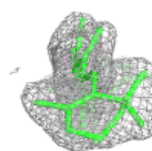
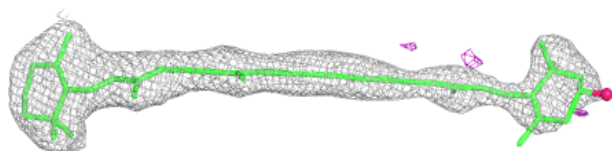
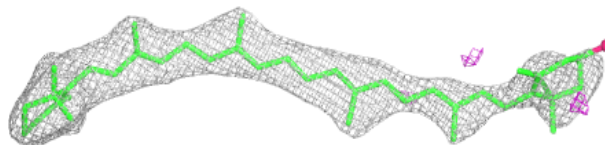
**Electron density around CLA C 507:**

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

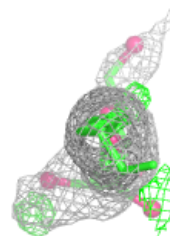
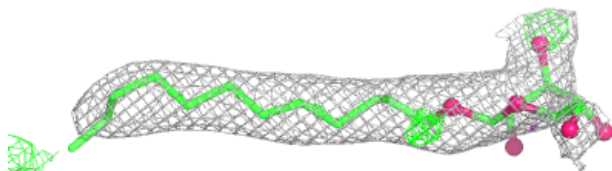
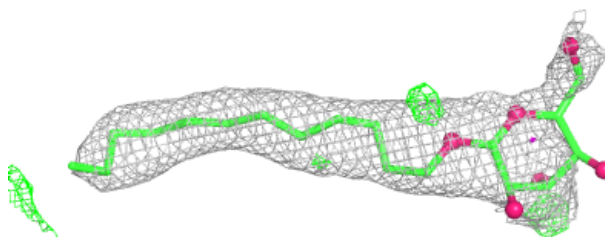


**Electron density around RRX h 101:**

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

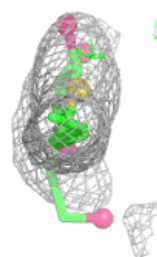
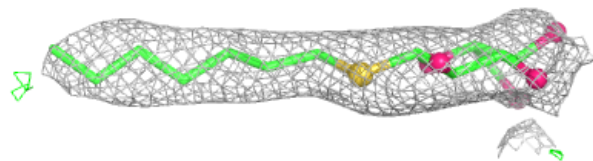
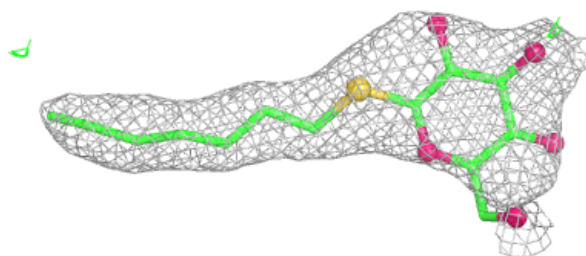
**Electron density around LMT A 420:**

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

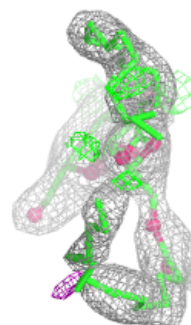
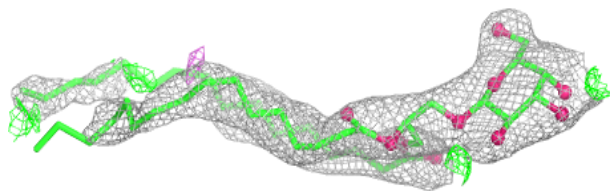
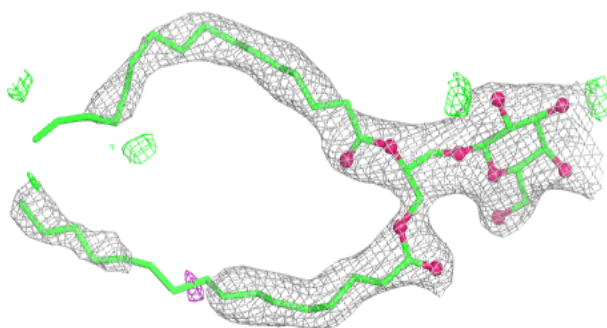


**Electron density around HTG B 626:**

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

**Electron density around LMG A 413:**

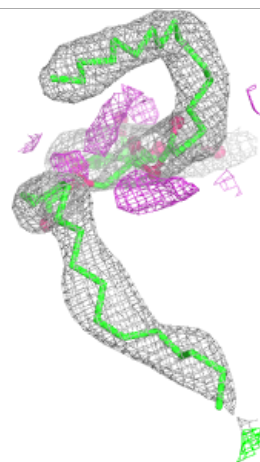
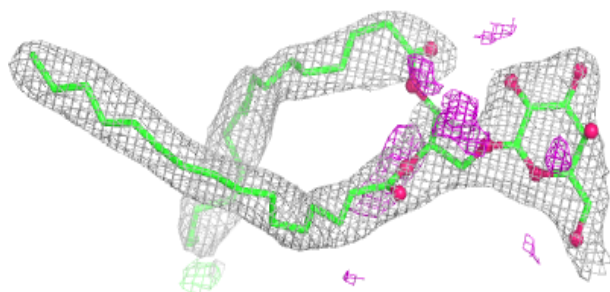
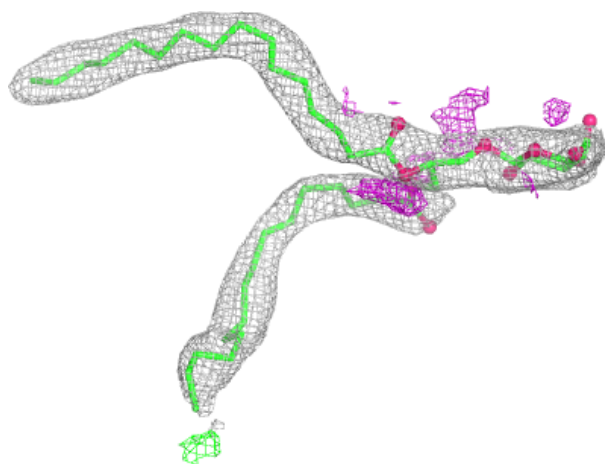
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





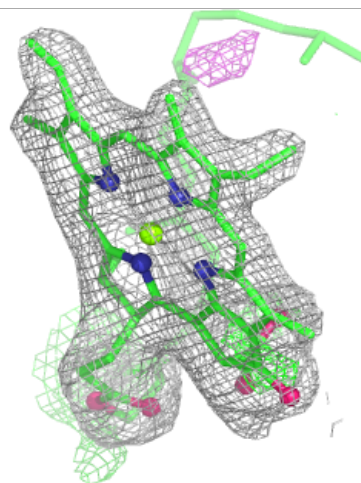
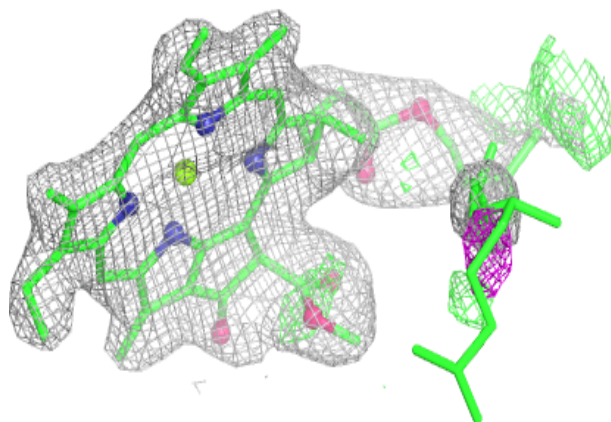
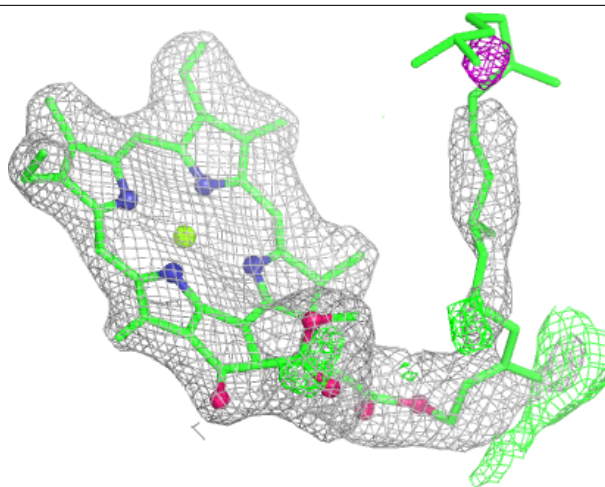
**Electron density around LMG m 2802:**

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



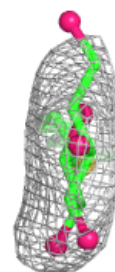
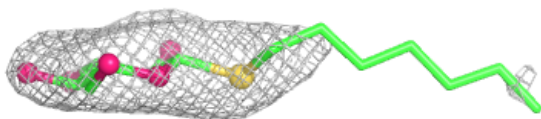
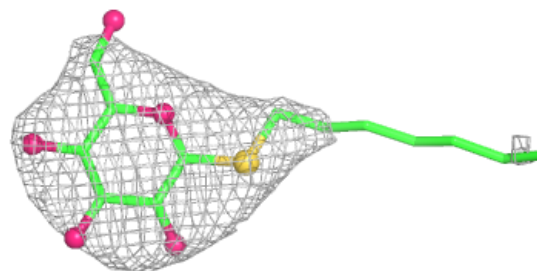
**Electron density around CLA B 617:**

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

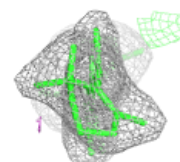
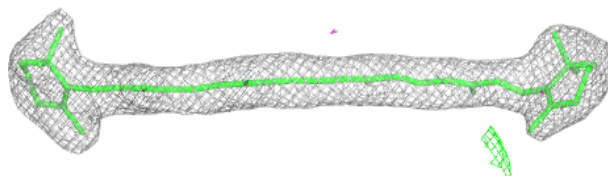
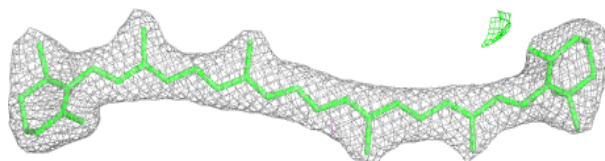


**Electron density around HTG C 521:**

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

**Electron density around BCR b 623:**

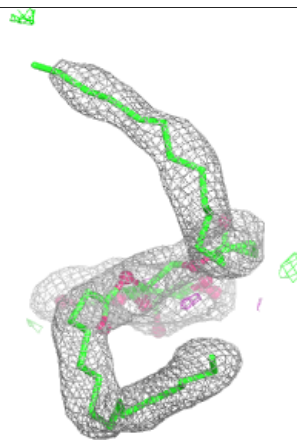
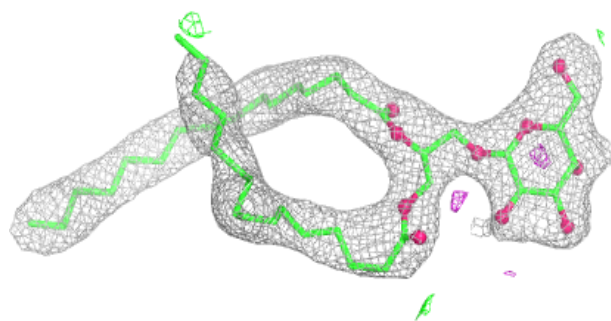
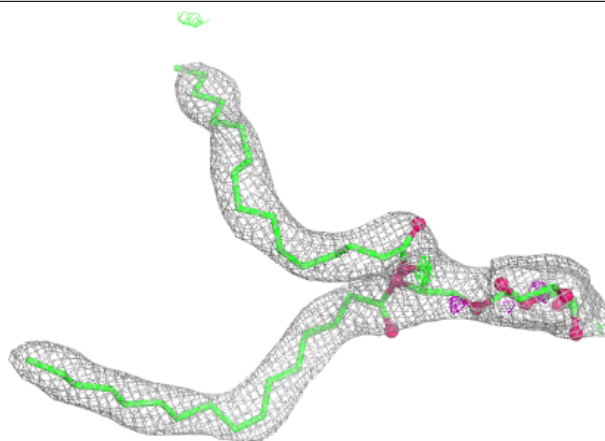
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





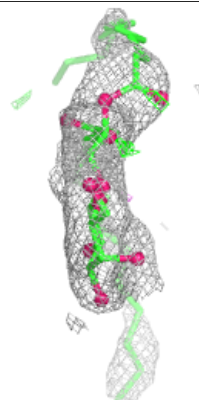
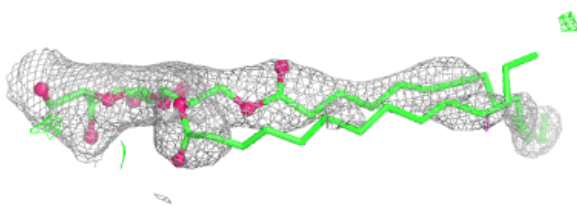
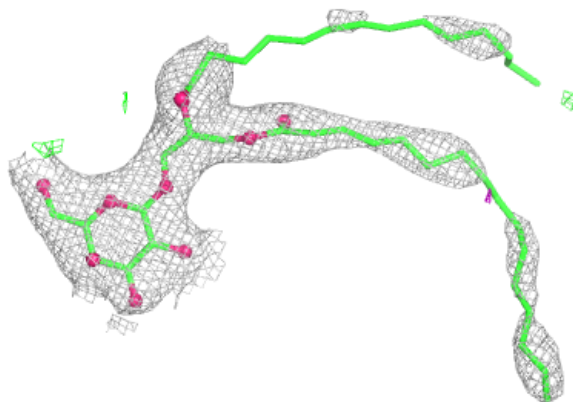
**Electron density around LMG B 622:**

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

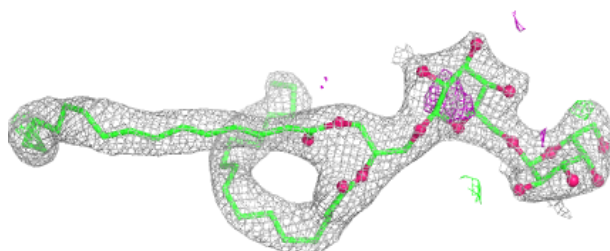
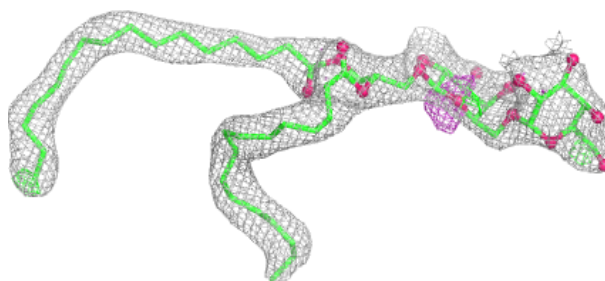


**Electron density around LMG c 521:**

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

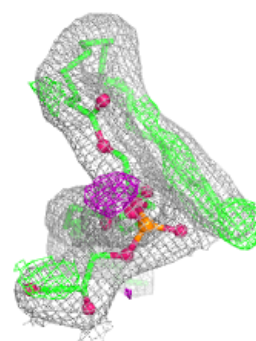
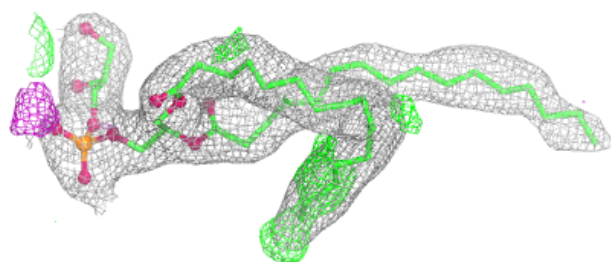
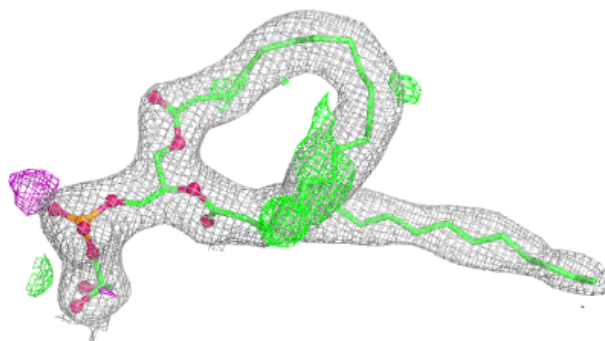
**Electron density around DGD h 102:**

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

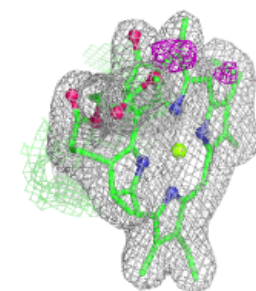
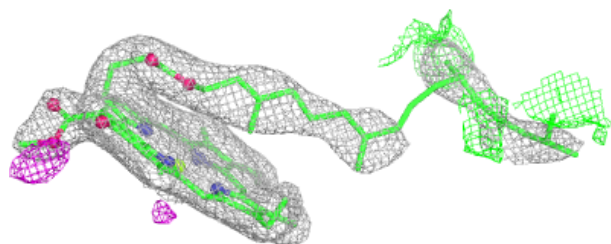
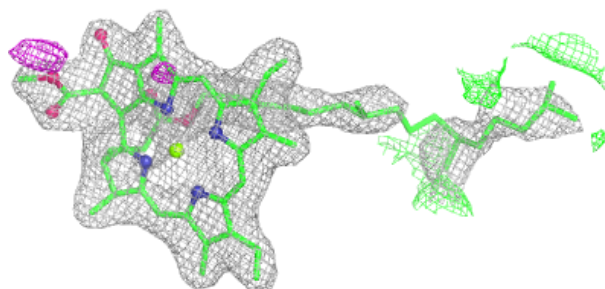


**Electron density around LHG D 2309:**

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

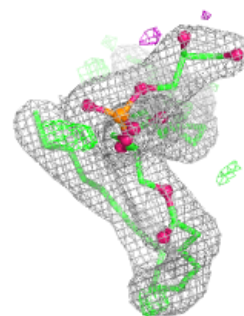
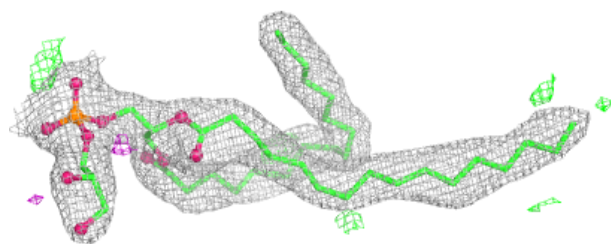
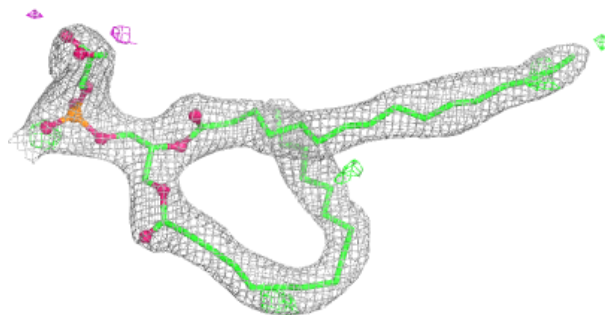
**Electron density around CLA b 619:**

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

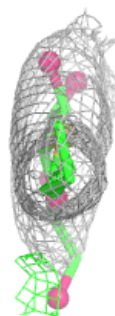
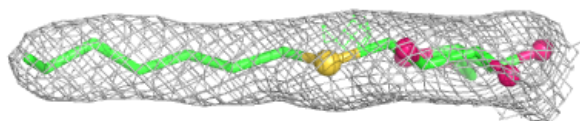
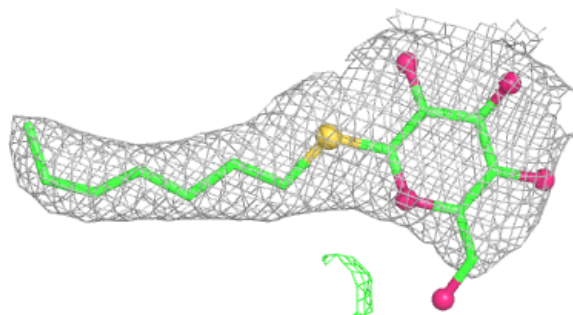


**Electron density around LHG d 412:**

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

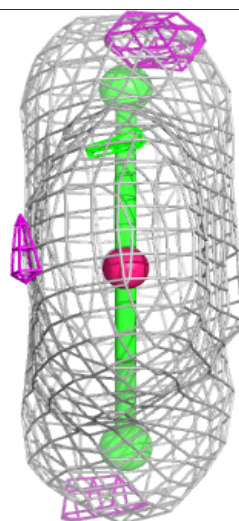
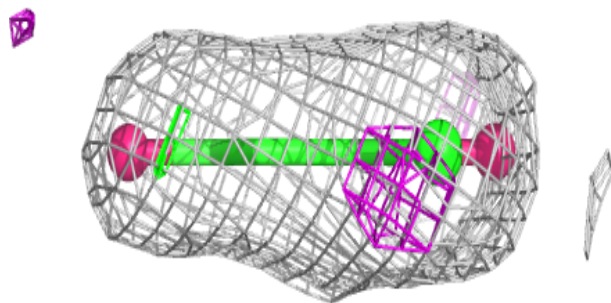
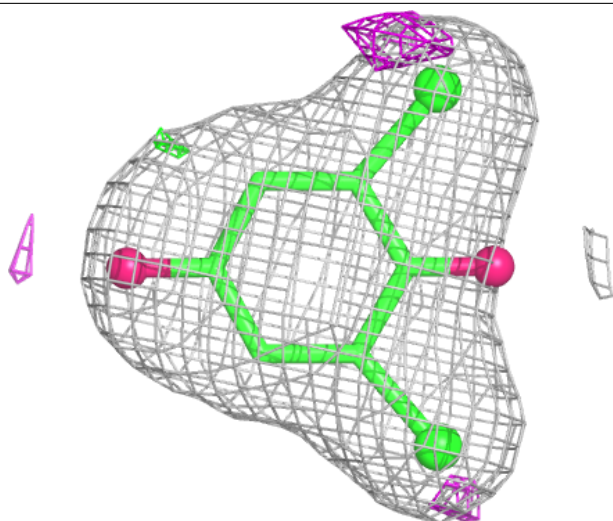
**Electron density around HTG b 603:**

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



**Electron density around JOX a 2617:**

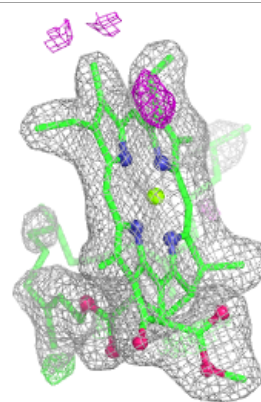
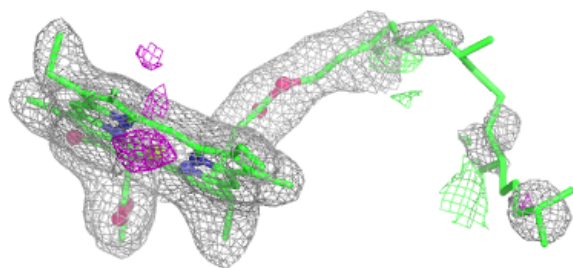
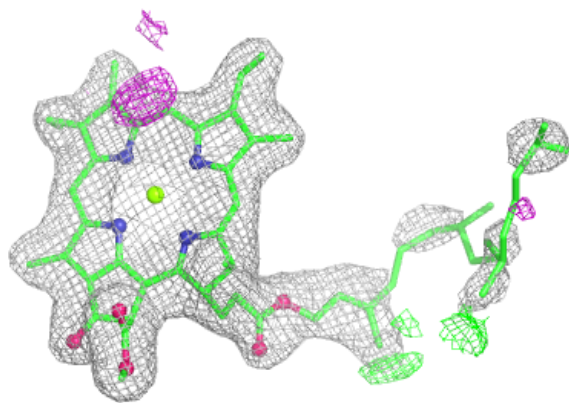
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



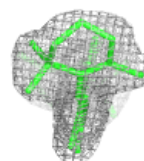
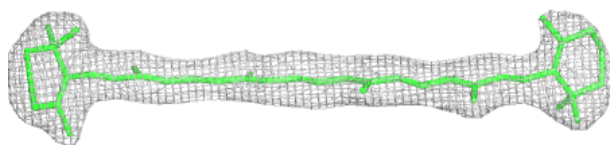
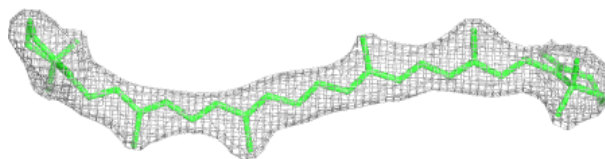


**Electron density around CLA a 2613:**

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

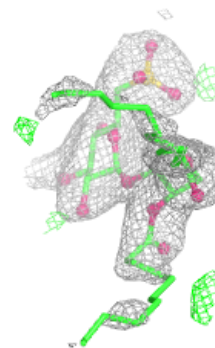
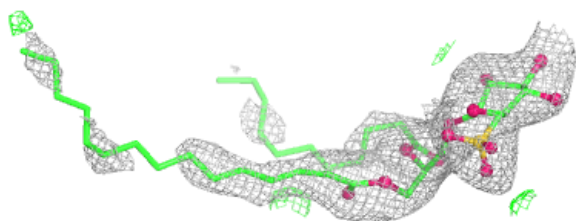
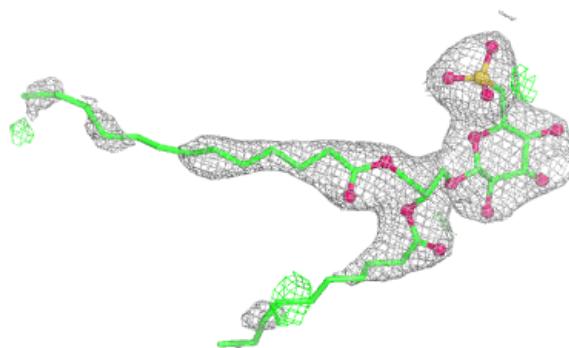
**Electron density around BCR C 516:**

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

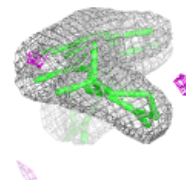
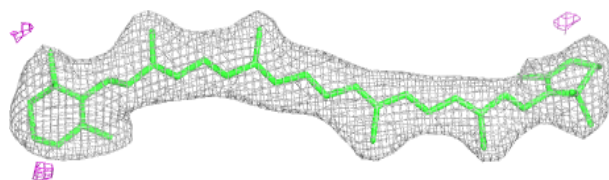
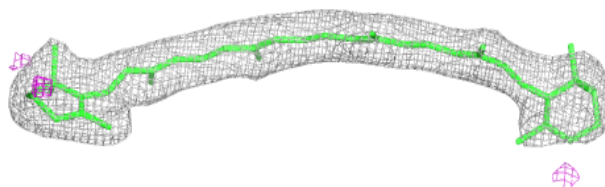


**Electron density around SQD a 2615:**

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

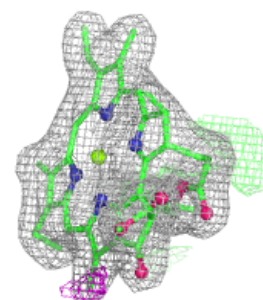
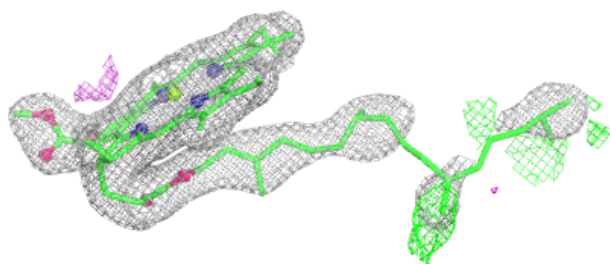
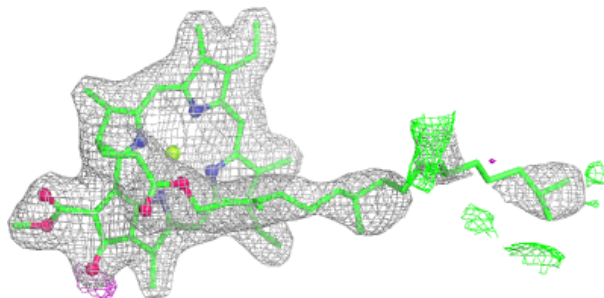
**Electron density around BCR D 2305:**

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

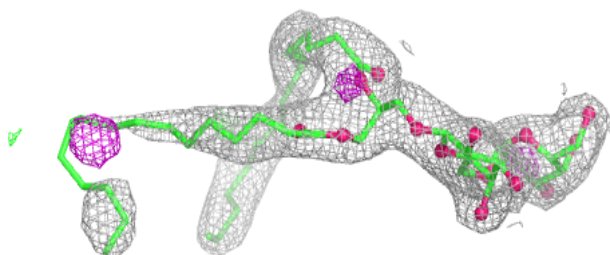
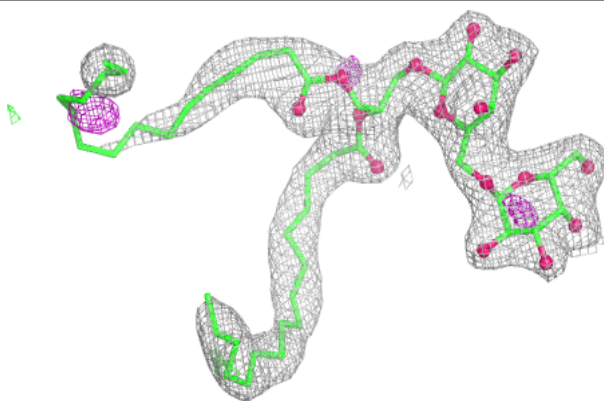


**Electron density around CLA B 615:**

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

**Electron density around DGD C 518:**

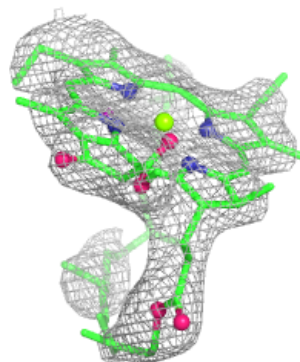
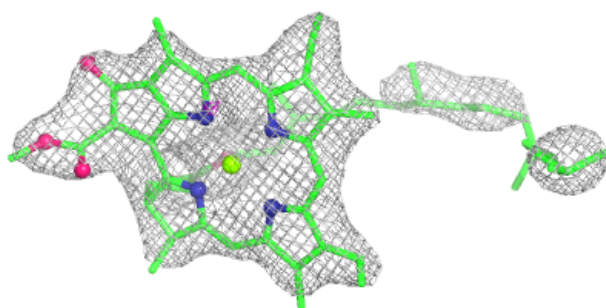
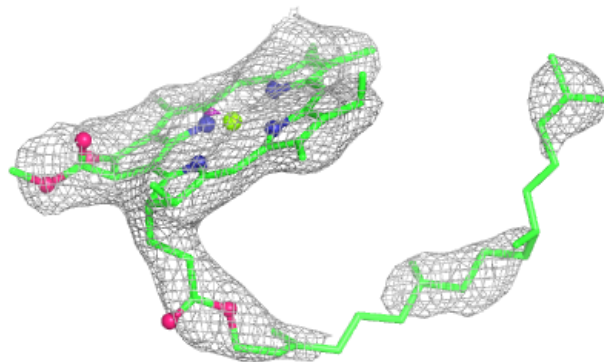
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



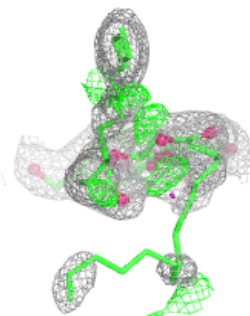
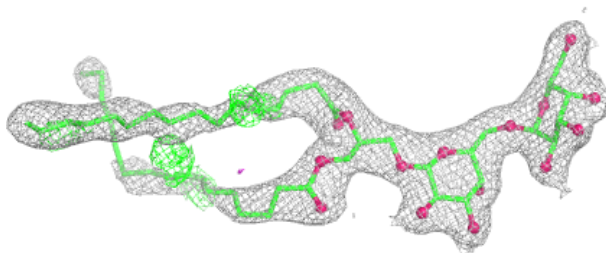
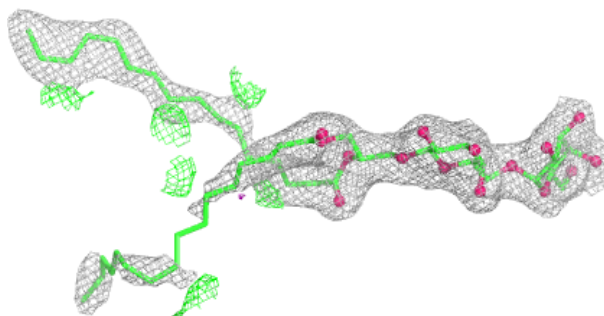


**Electron density around CLA C 514:**

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

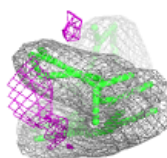
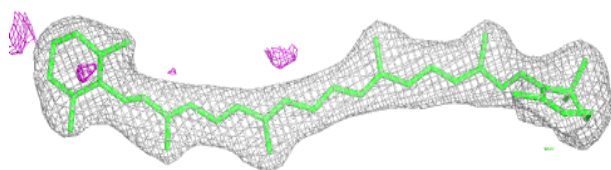
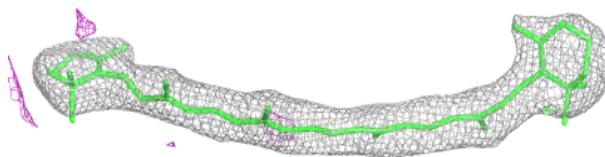
**Electron density around DGD c 518:**

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

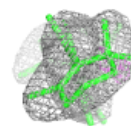
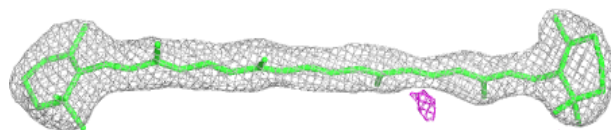
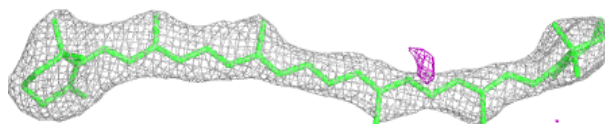


**Electron density around BCR d 410:**

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

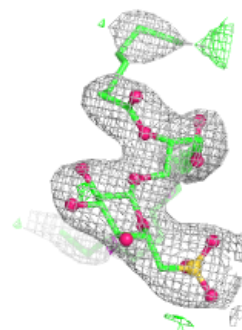
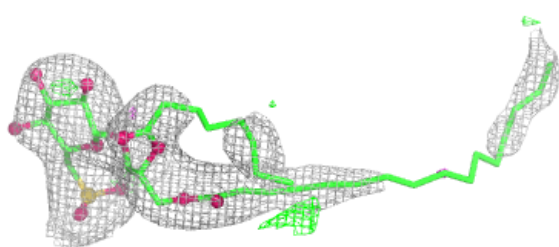
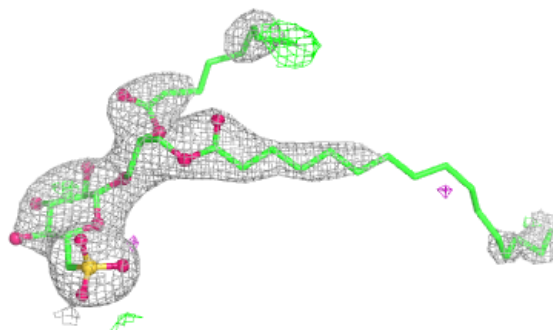
**Electron density around BCR z 101:**

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

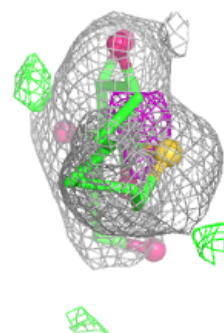
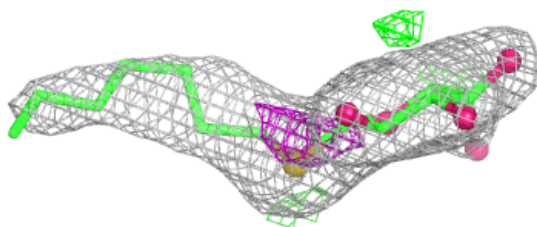
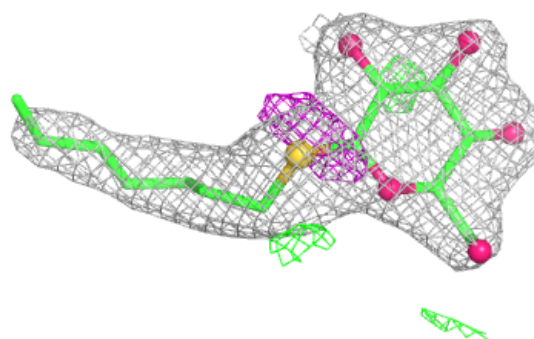


**Electron density around SQD A 412:**

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

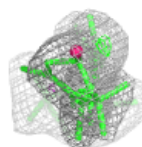
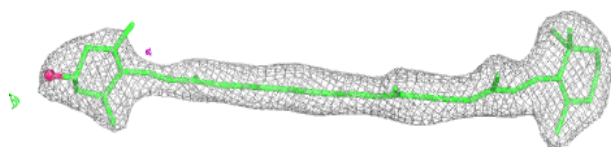
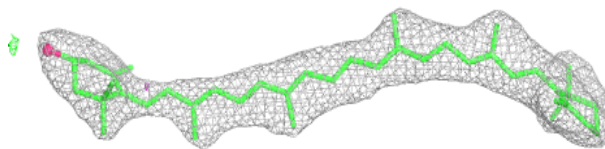
**Electron density around HTG b 602:**

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

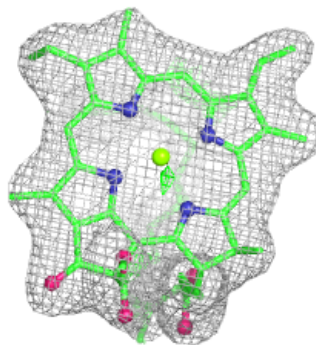
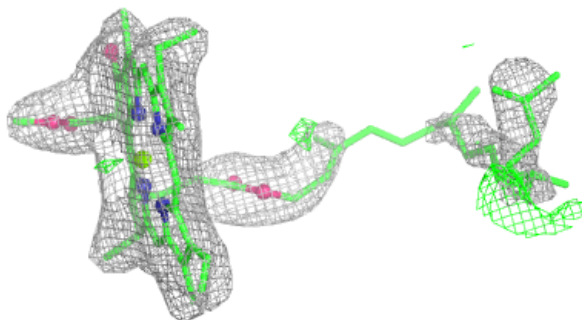
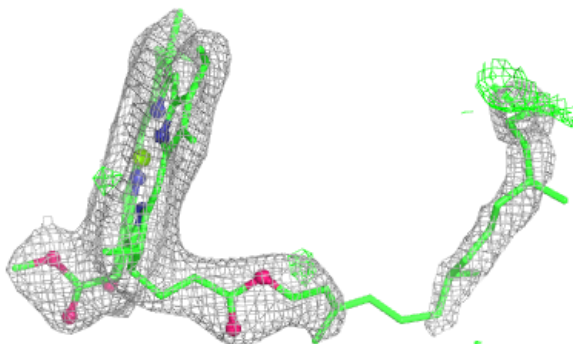


**Electron density around RRX H 102:**

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

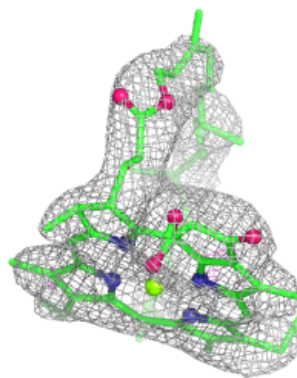
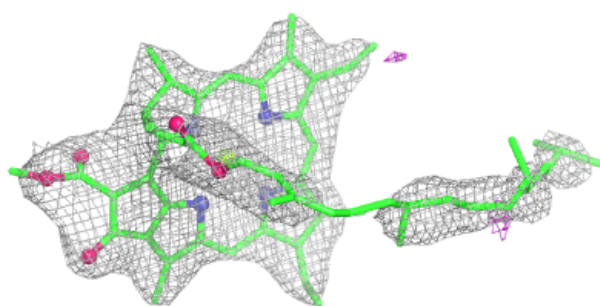
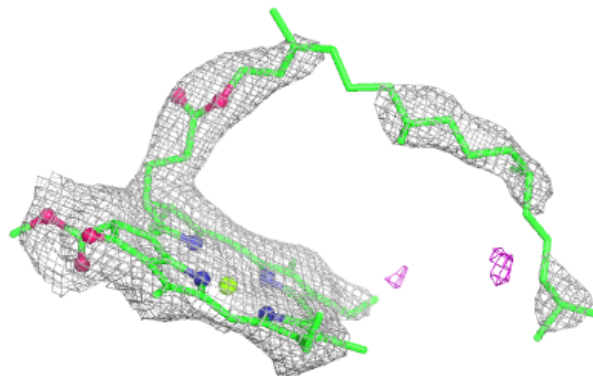
**Electron density around CLA c 509:**

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



**Electron density around CLA c 516:**

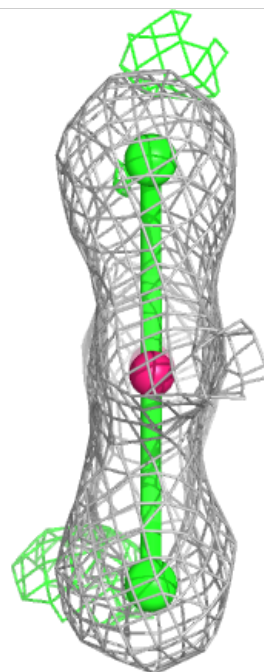
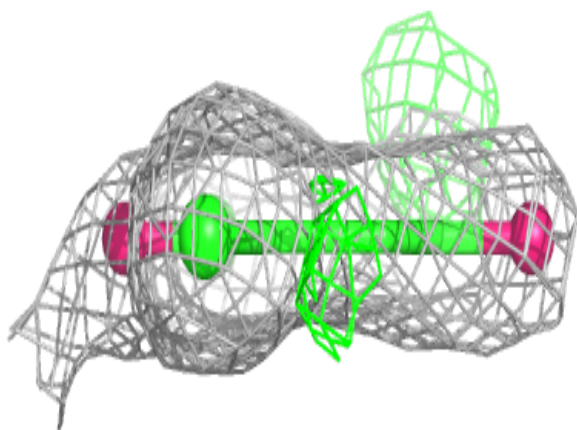
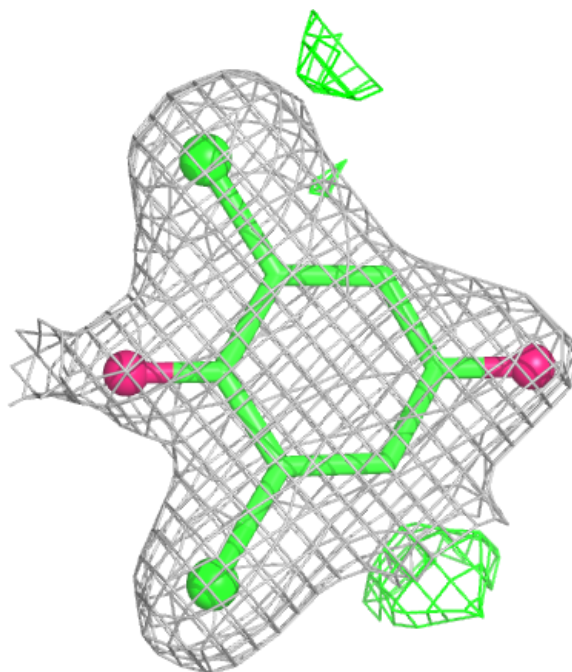
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





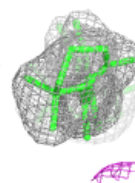
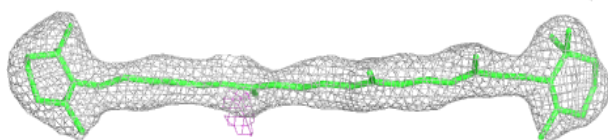
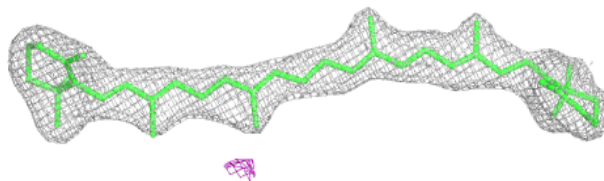
**Electron density around JOX a 2619:**

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

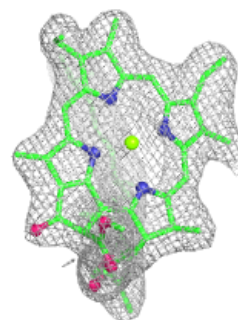
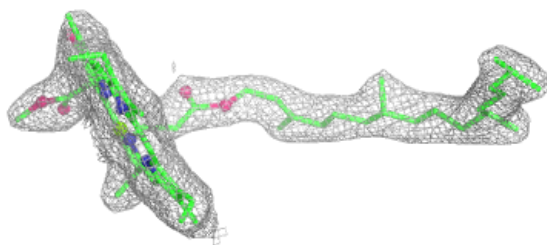
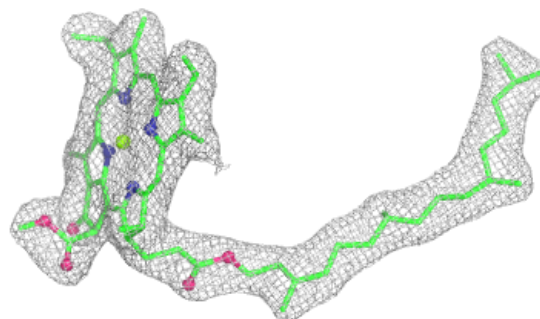


**Electron density around BCR C 515:**

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

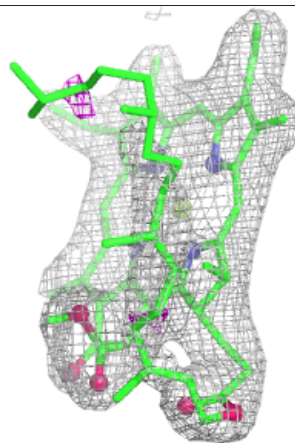
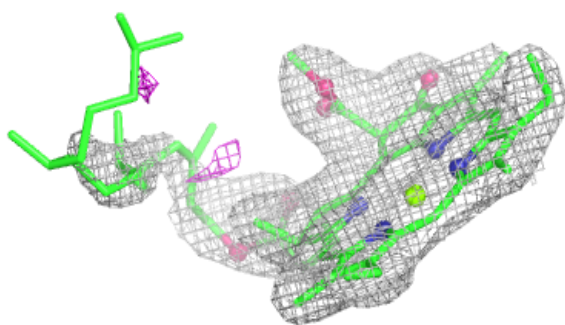
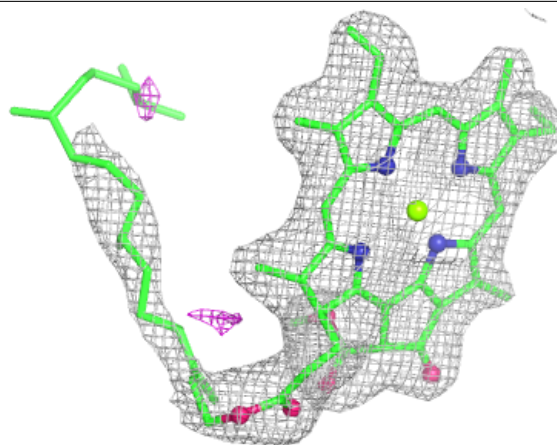
**Electron density around CLA B 610:**

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



**Electron density around CLA b 621:**

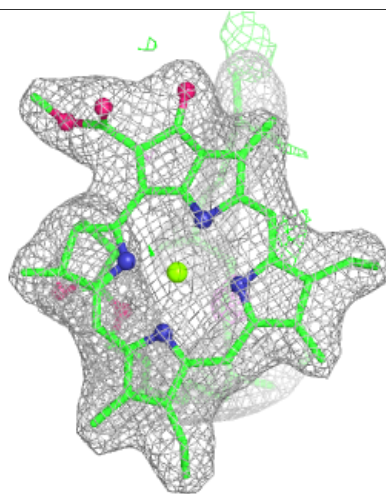
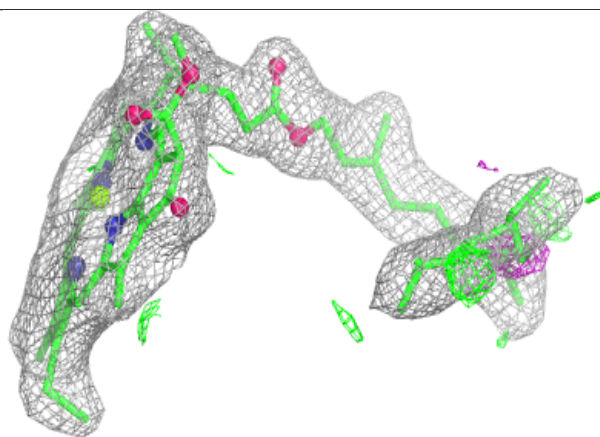
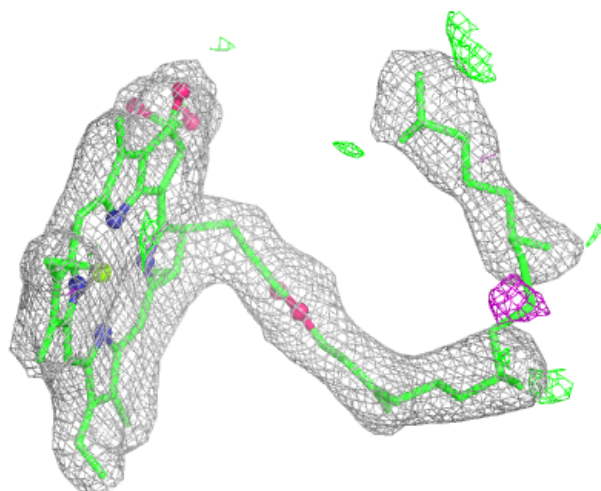
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





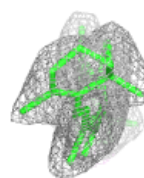
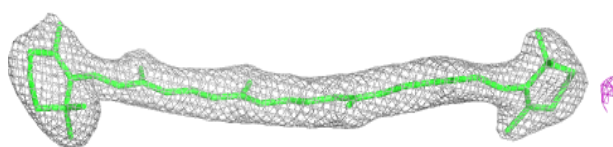
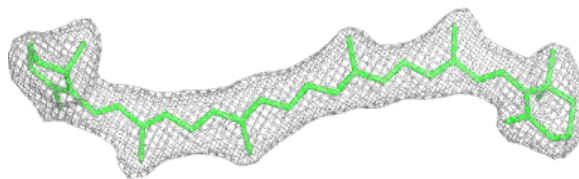
**Electron density around CLA B 607:**

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

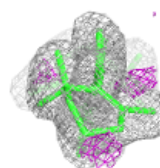
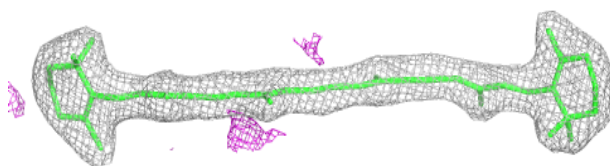
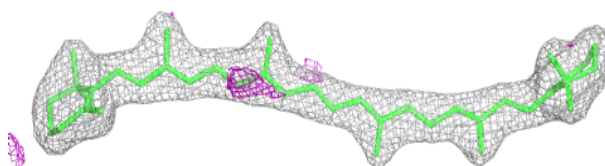


**Electron density around BCR Y 302:**

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

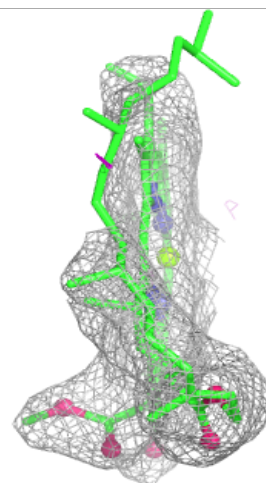
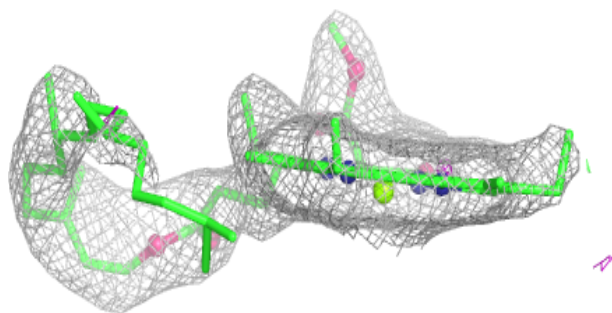
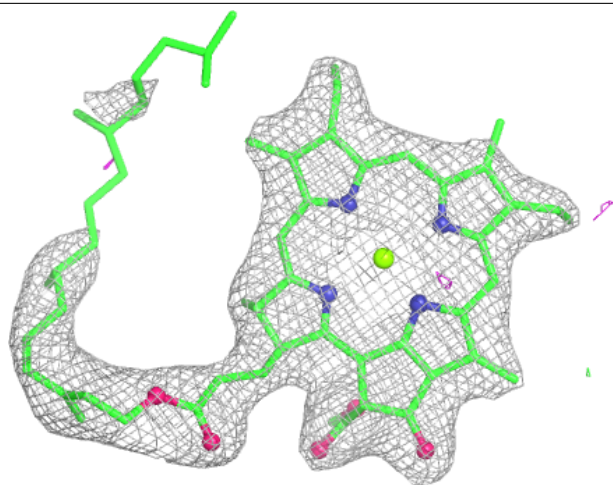
**Electron density around BCR a 2614:**

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



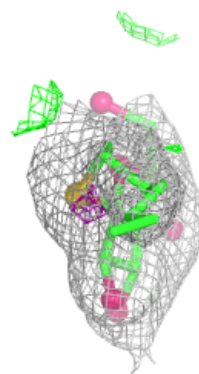
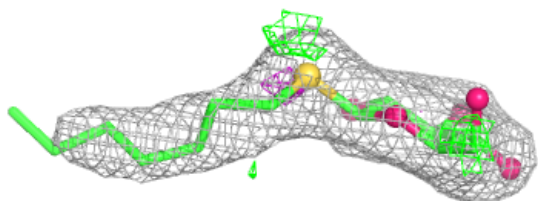
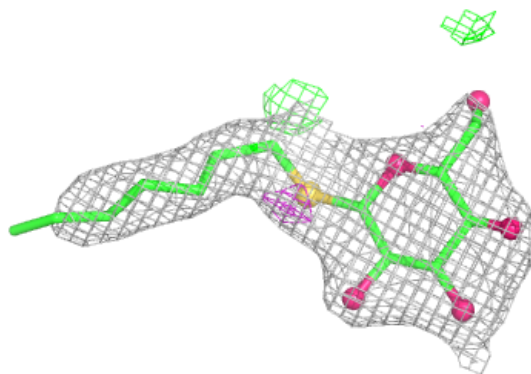
**Electron density around CLA c 515:**

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

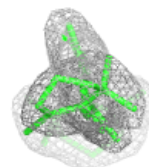
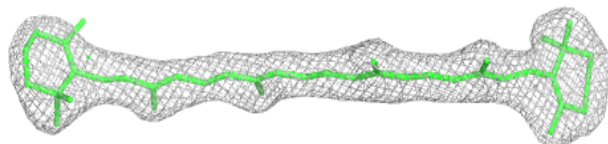
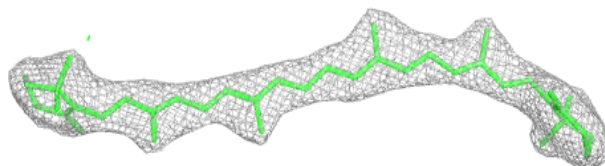


**Electron density around HTG o 301:**

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

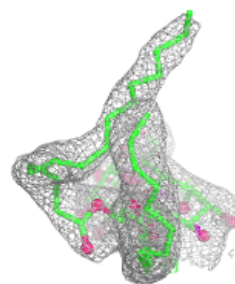
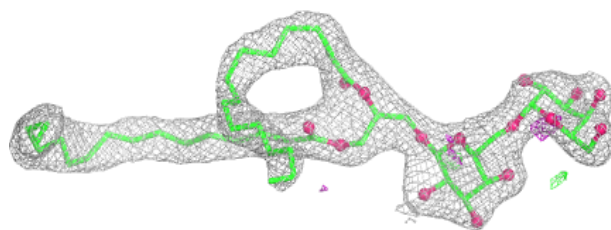
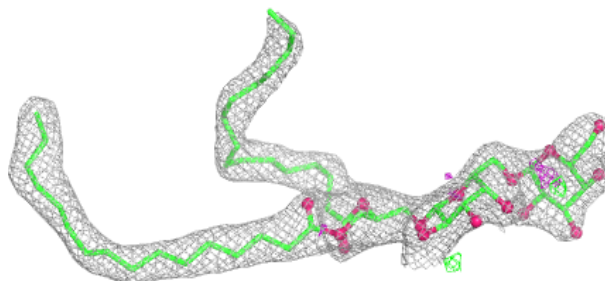
**Electron density around BCR c 517:**

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



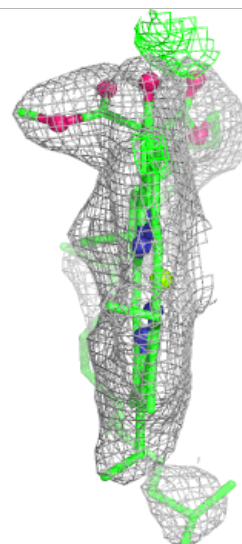
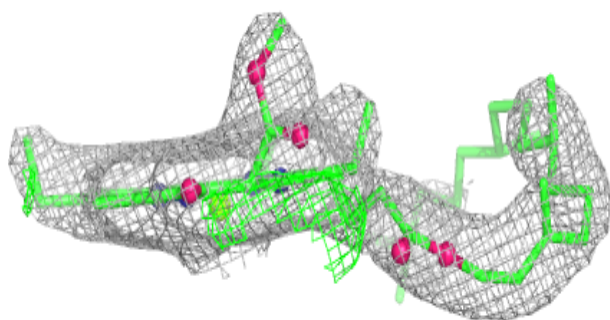
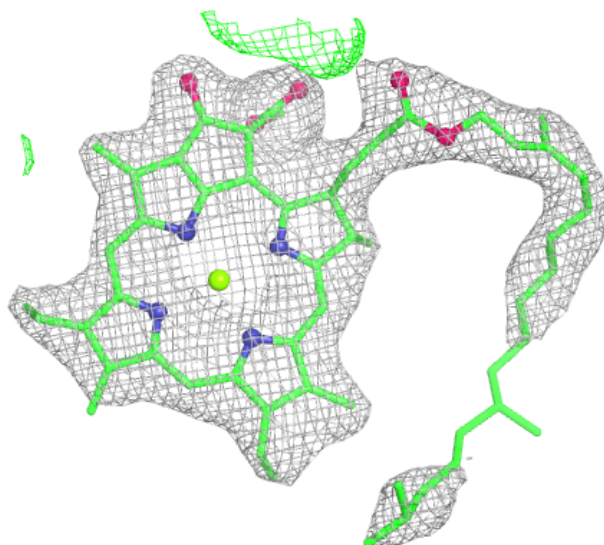
**Electron density around DGD H 103:**

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



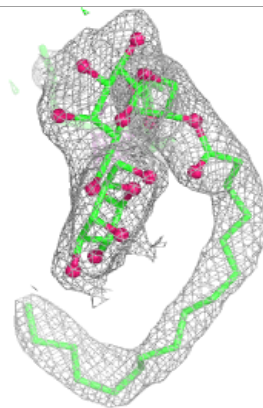
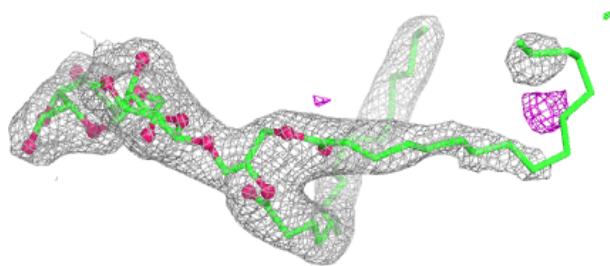
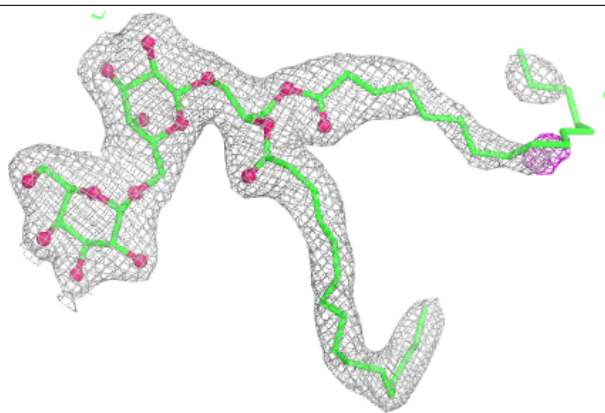
**Electron density around CLA C 513:**

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



**Electron density around DGD c 519:**

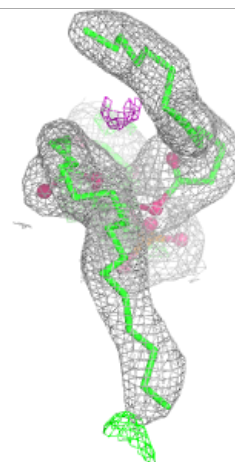
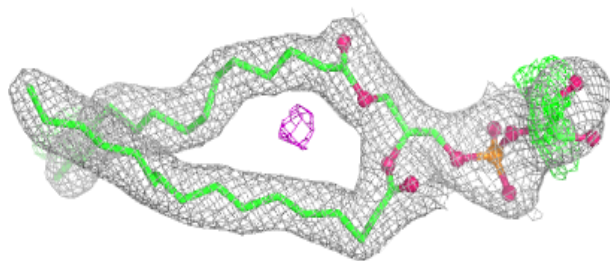
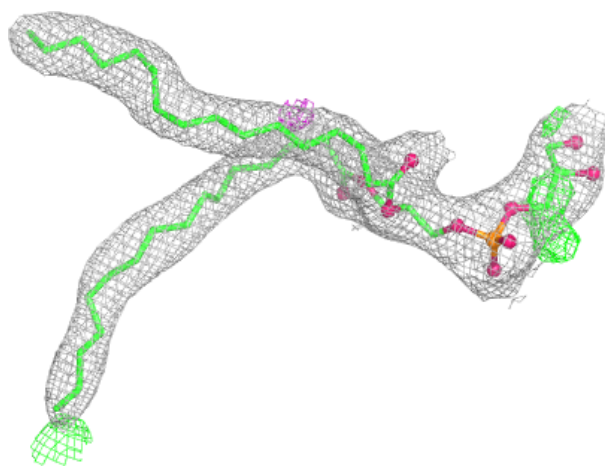
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around LHG D 2310:**

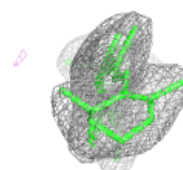
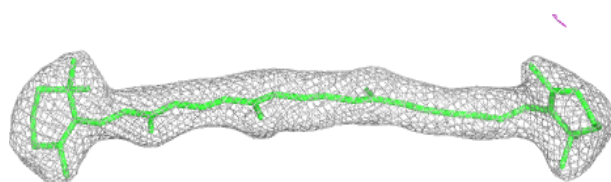
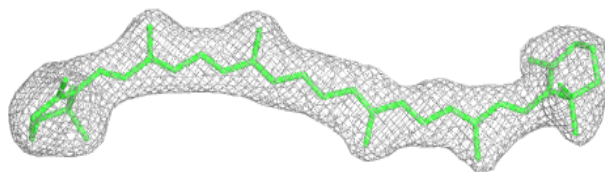
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



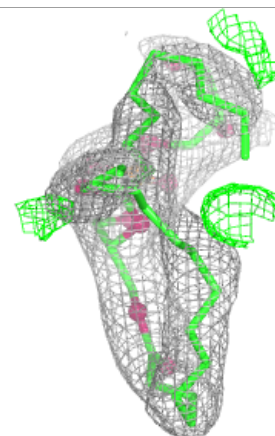
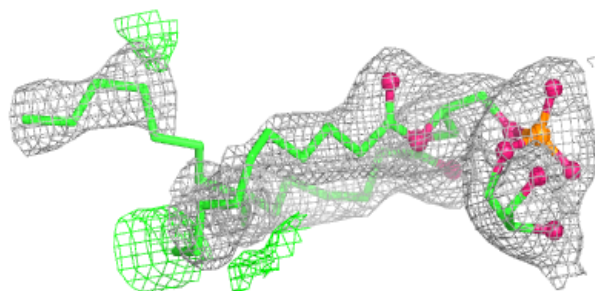
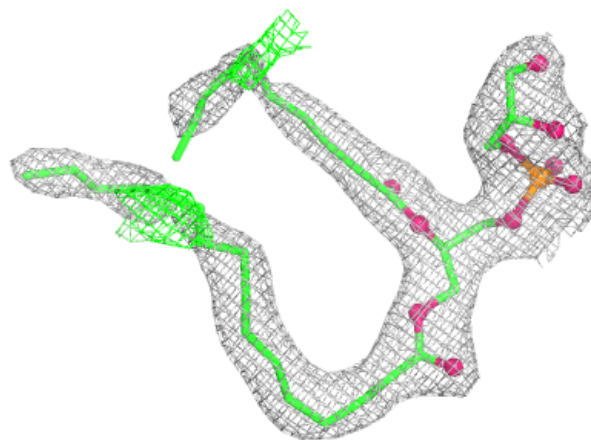


**Electron density around BCR y 101:**

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

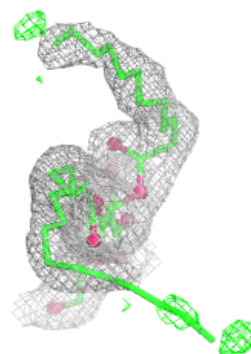
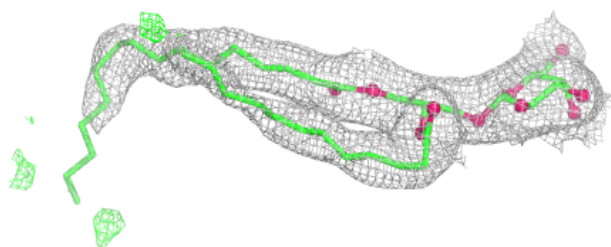
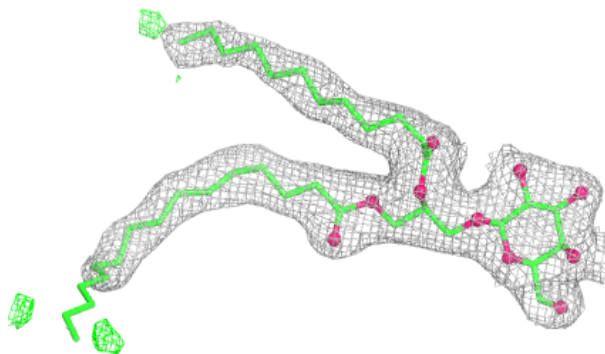
**Electron density around LHG d 403:**

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

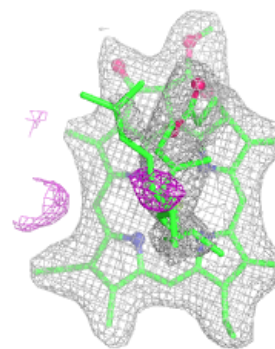
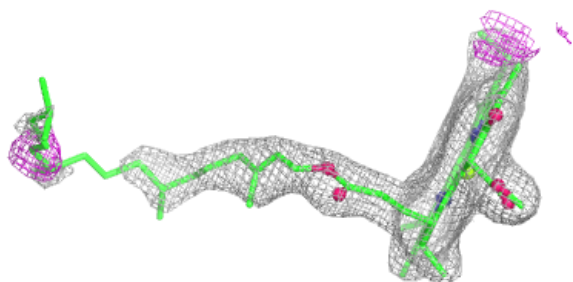
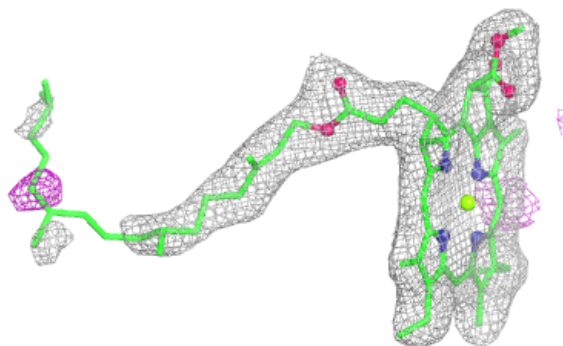


**Electron density around LMG D 2312:**

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

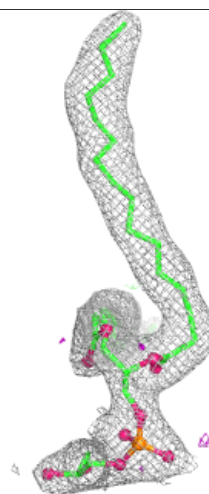
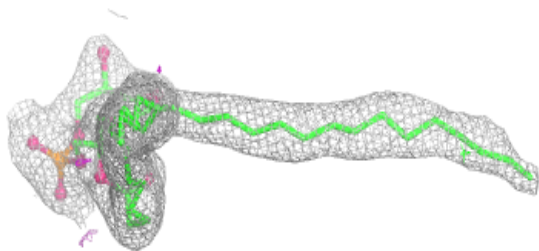
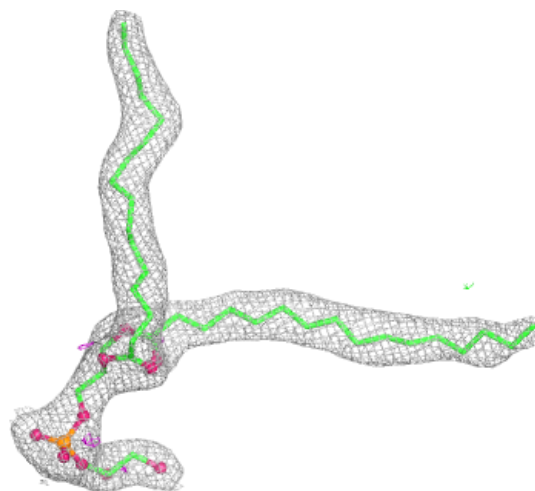
**Electron density around CLA d 409:**

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



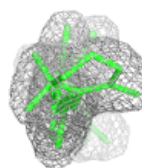
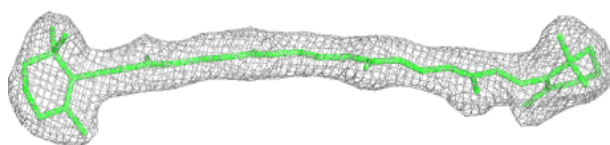
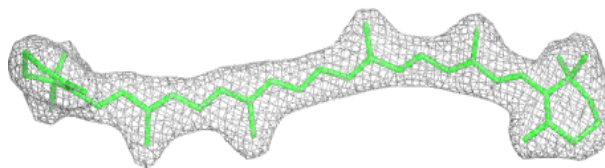
**Electron density around LHG 1 103:**

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

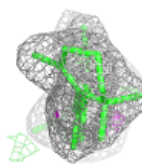
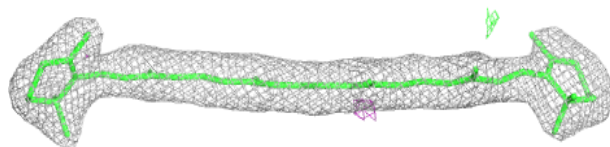
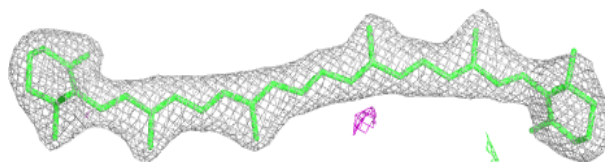


**Electron density around BCR B 618:**

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

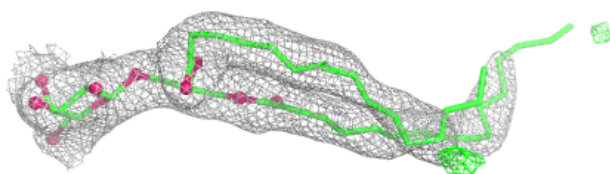
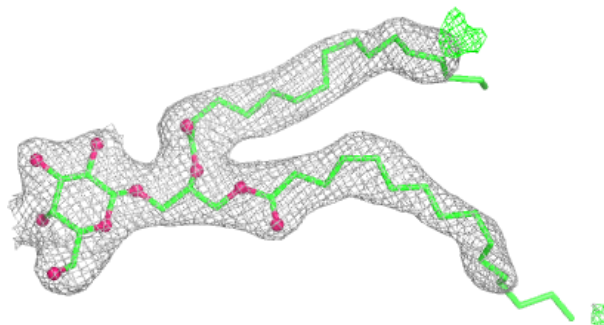
**Electron density around BCR B 619:**

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



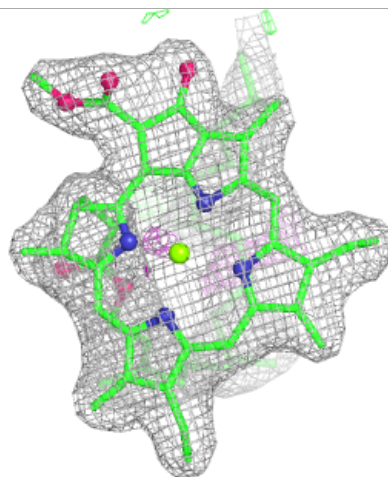
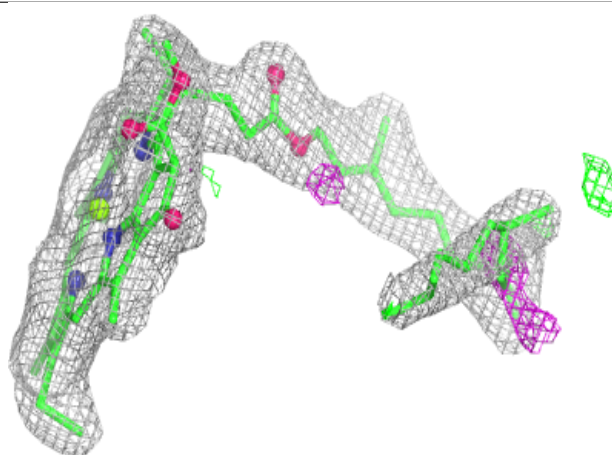
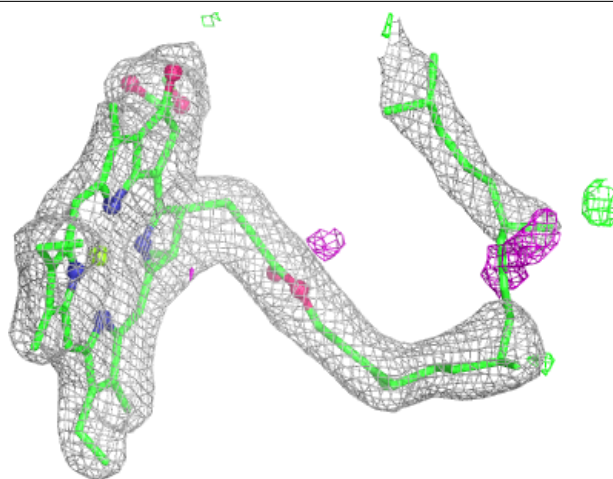
**Electron density around LMG d 414:**

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



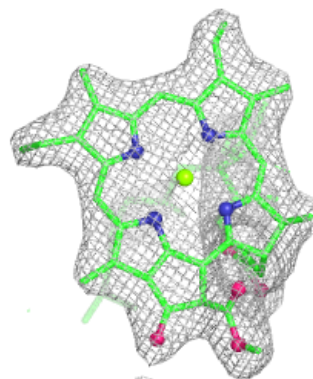
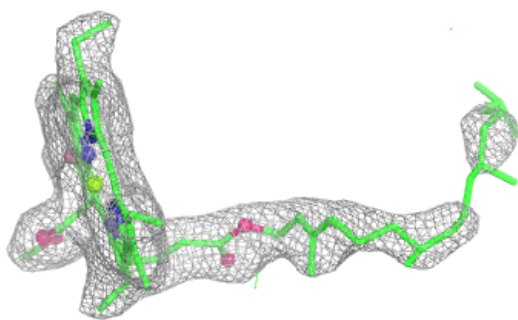
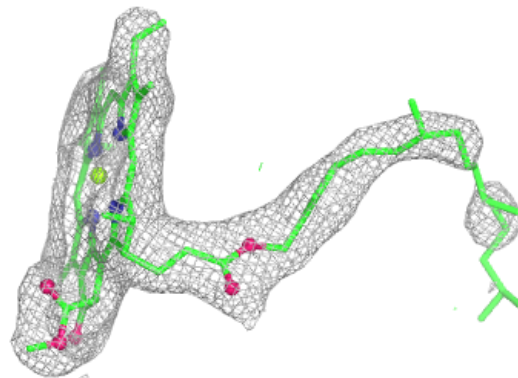
**Electron density around CLA b 611:**

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



**Electron density around CLA D 2304:**

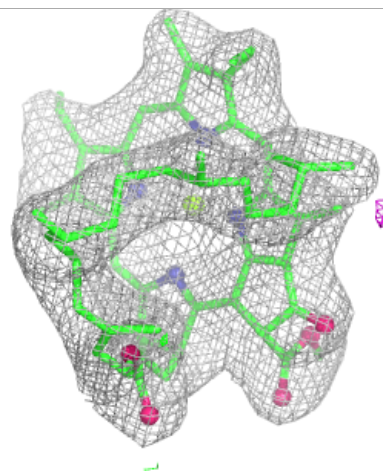
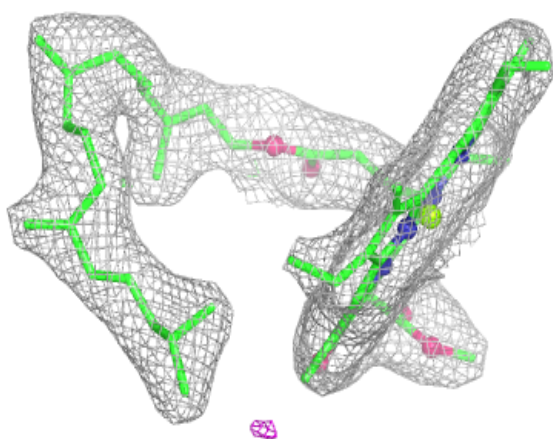
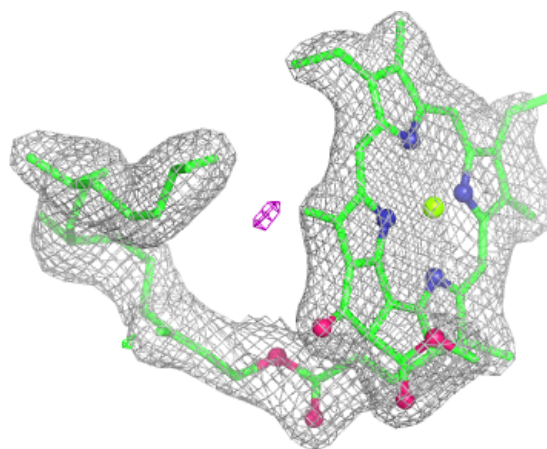
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA C 504:**

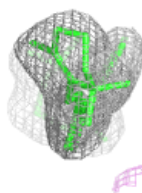
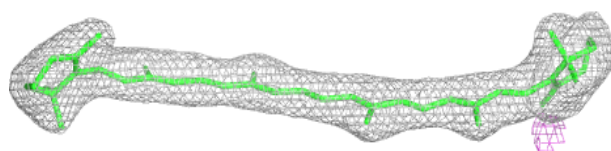
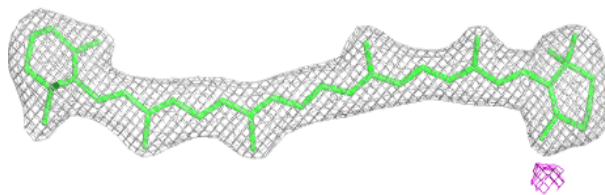
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



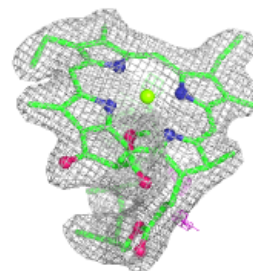
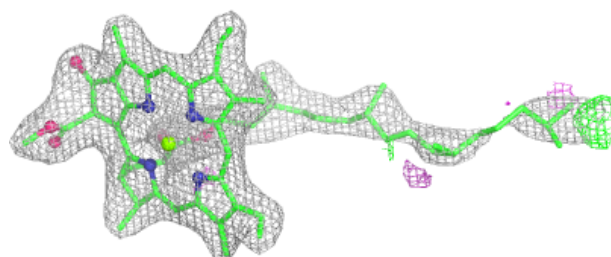
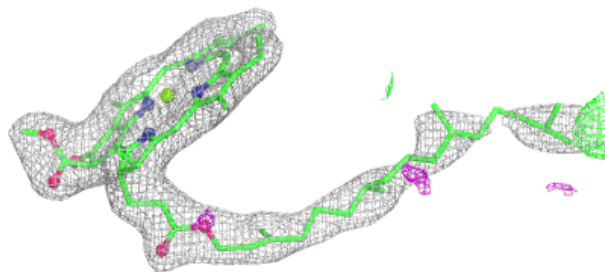


**Electron density around BCR B 620:**

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

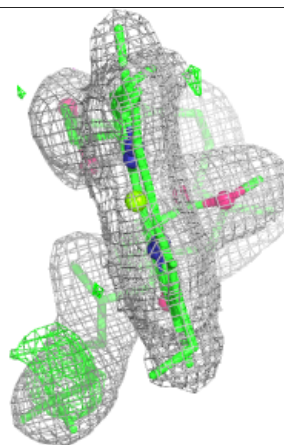
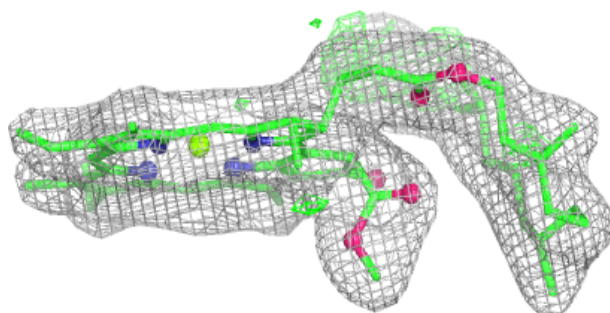
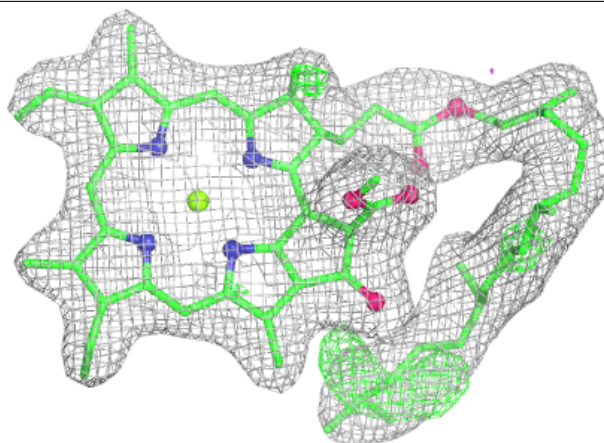
**Electron density around CLA C 505:**

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



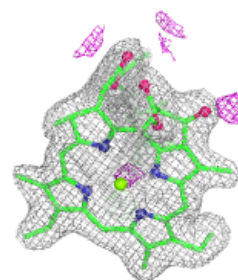
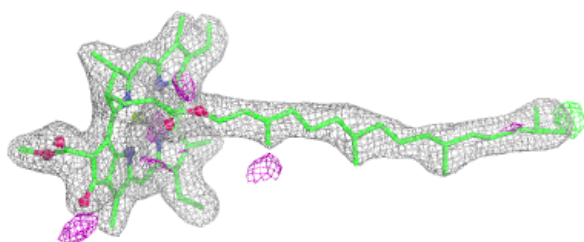
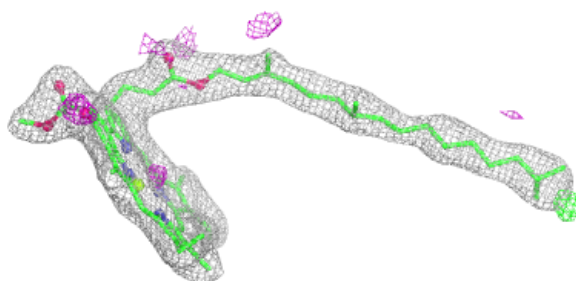
**Electron density around CLA B 611:**

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

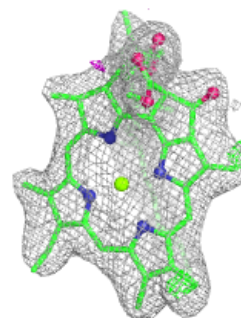
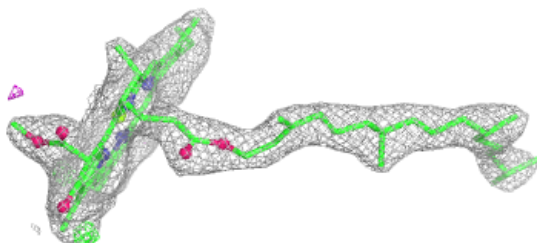
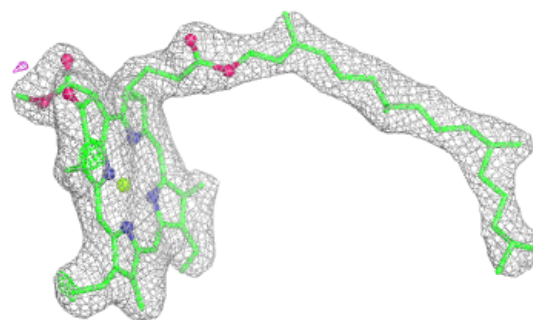


**Electron density around CLA b 612:**

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

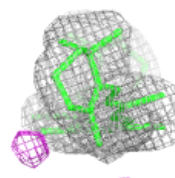
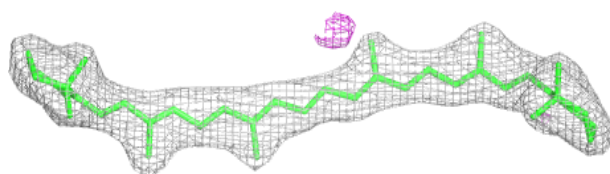
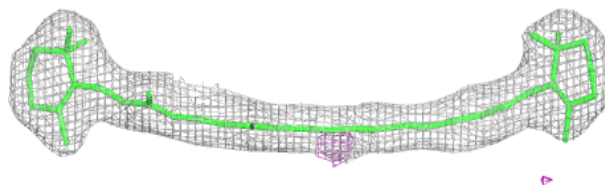
**Electron density around CLA b 614:**

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

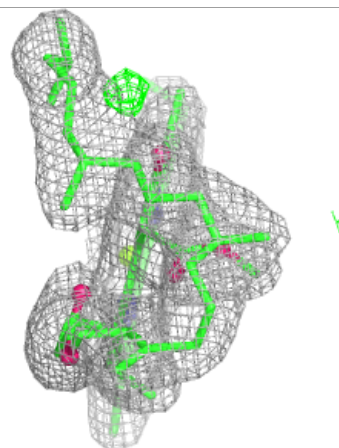
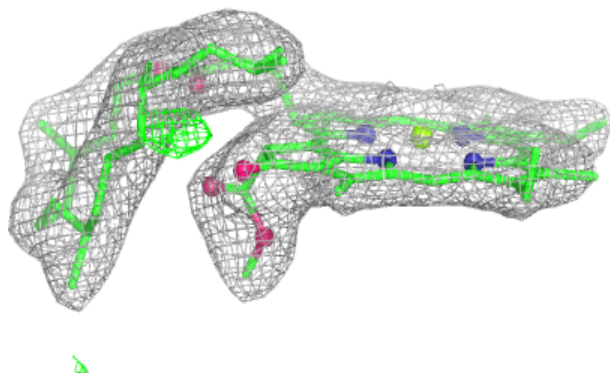
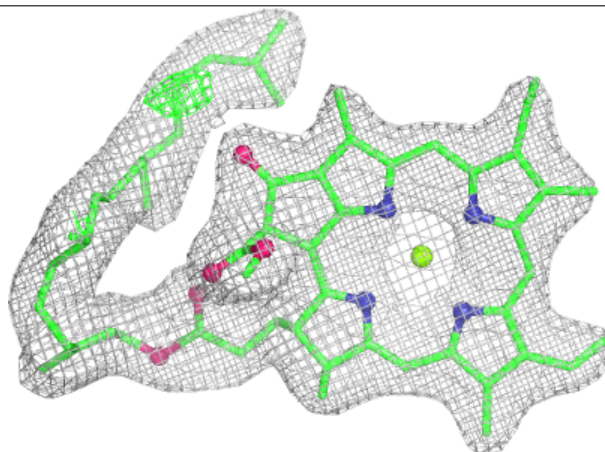


**Electron density around BCR K 101:**

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

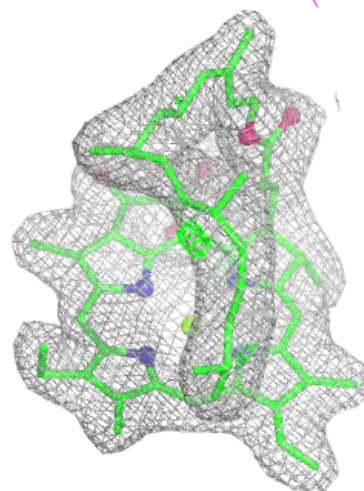
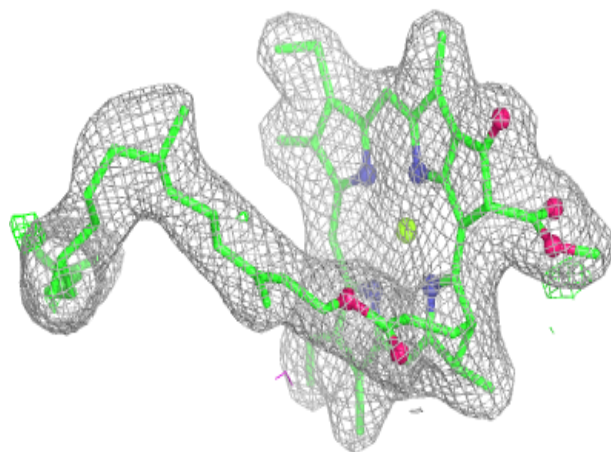
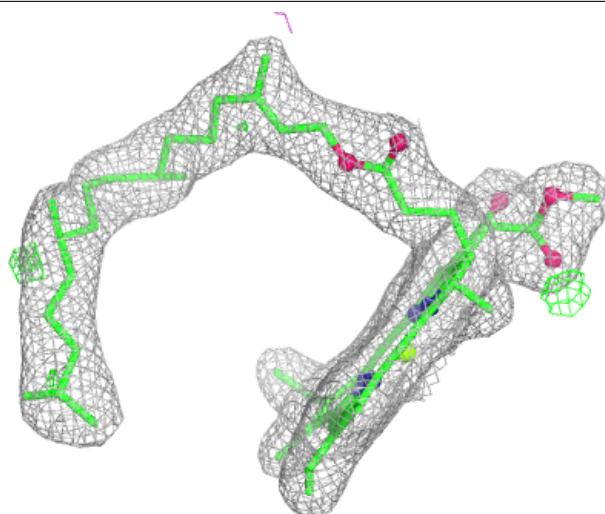
**Electron density around CLA b 615:**

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



**Electron density around CLA b 616:**

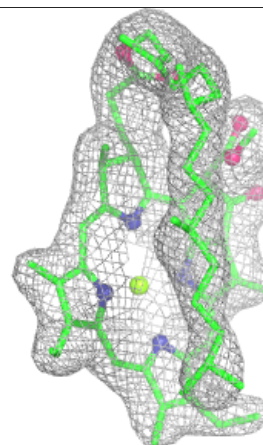
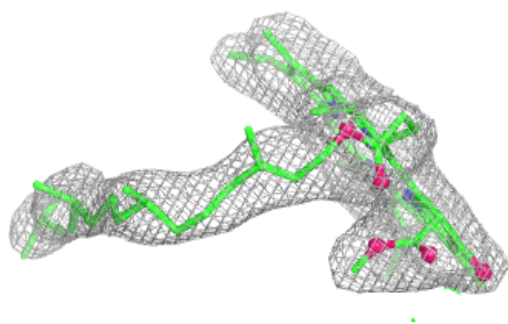
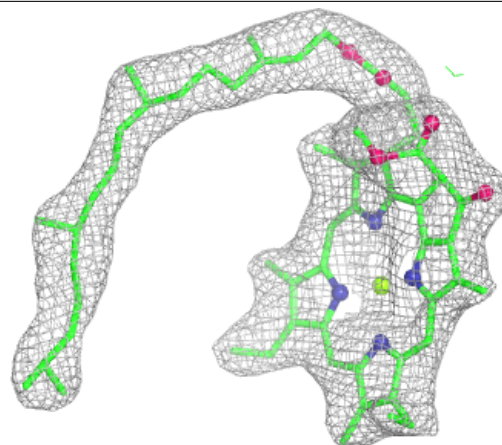
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



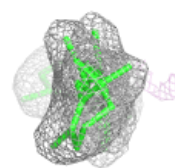
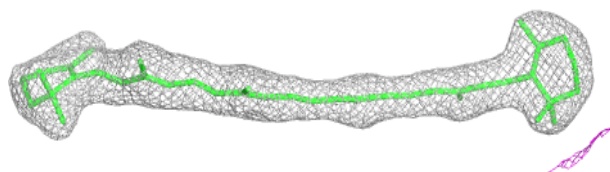
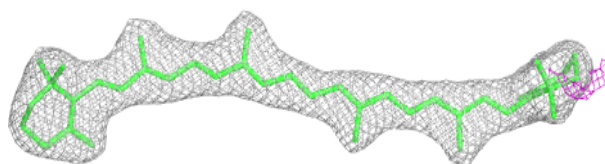


**Electron density around CLA C 508:**

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

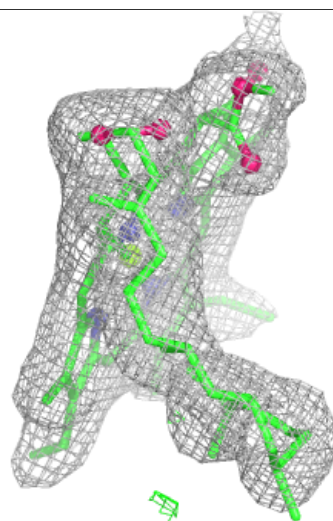
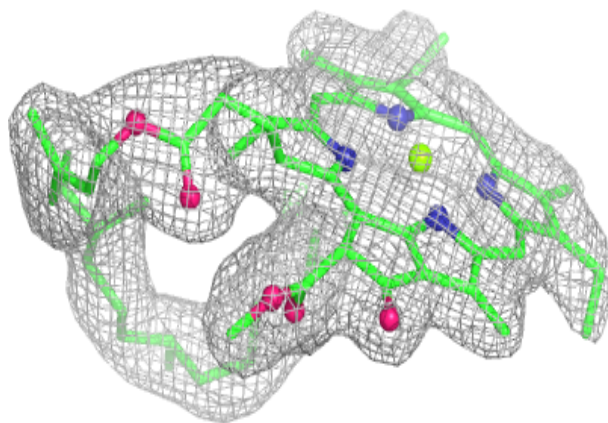
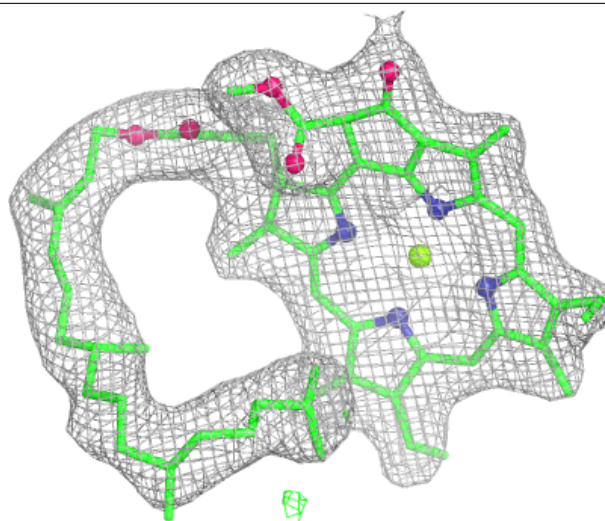
**Electron density around BCR b 622:**

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



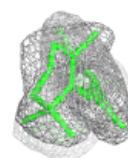
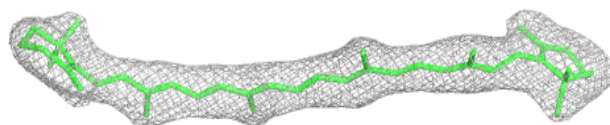
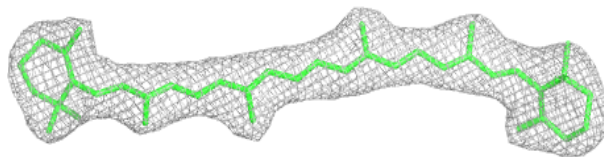
**Electron density around CLA b 620:**

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

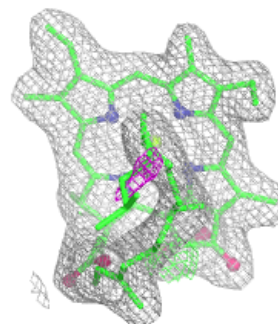
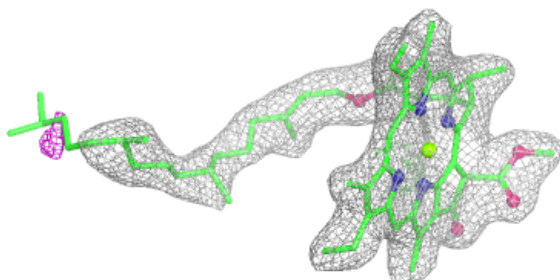
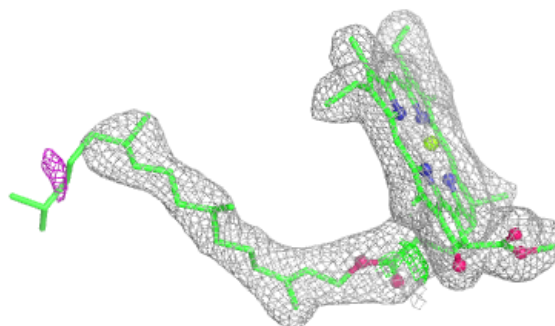


**Electron density around BCR b 624:**

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

**Electron density around CLA C 509:**

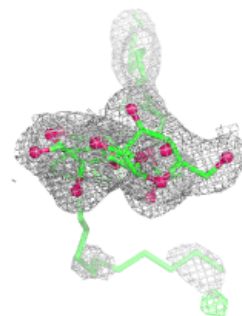
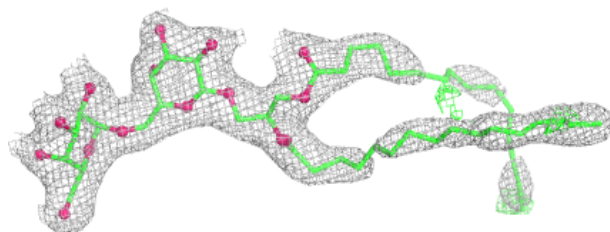
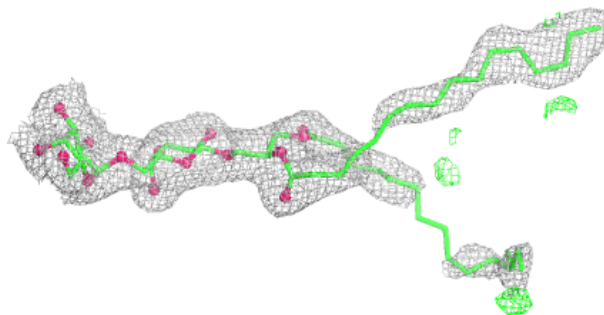
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



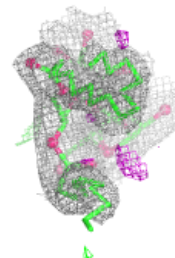
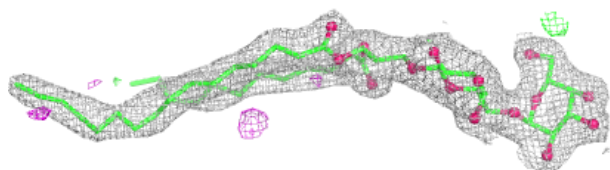
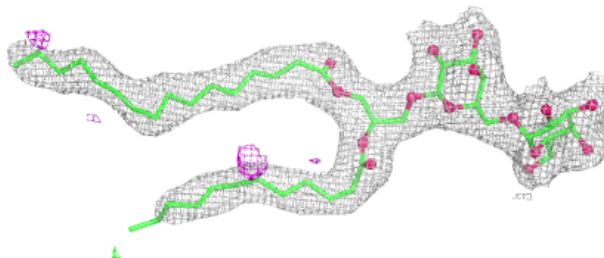


**Electron density around DGD C 517:**

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

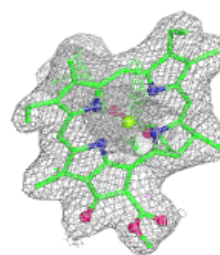
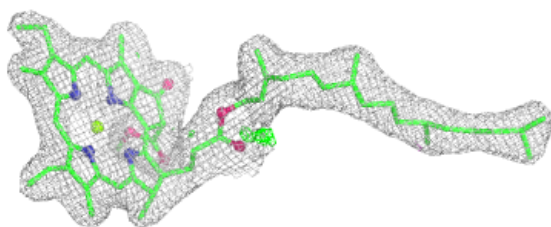
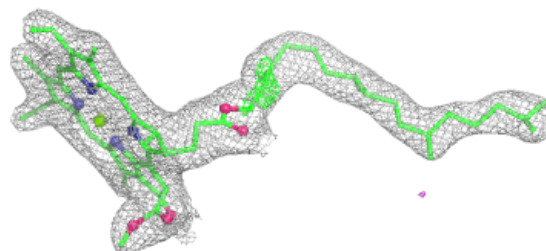
**Electron density around DGD C 519:**

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



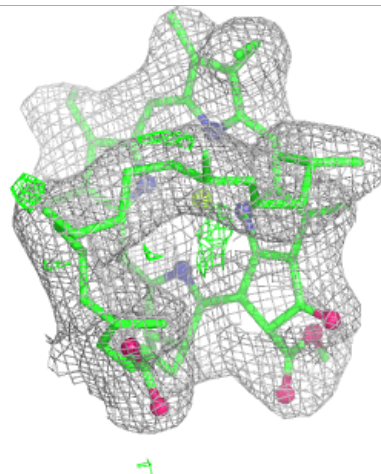
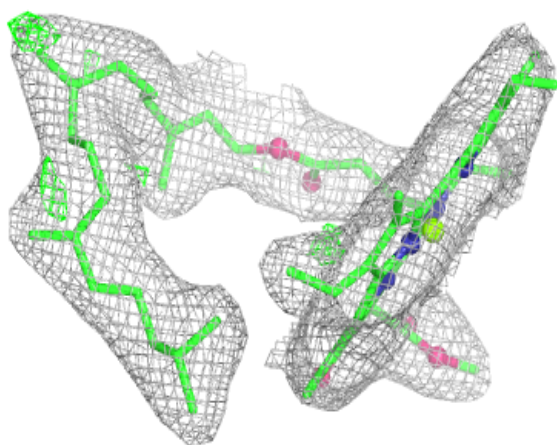
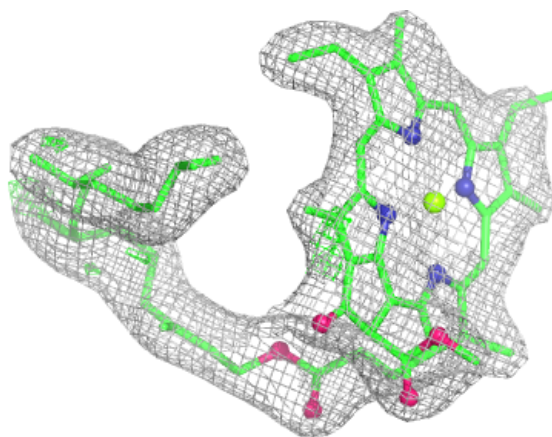
**Electron density around CLA c 505:**

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



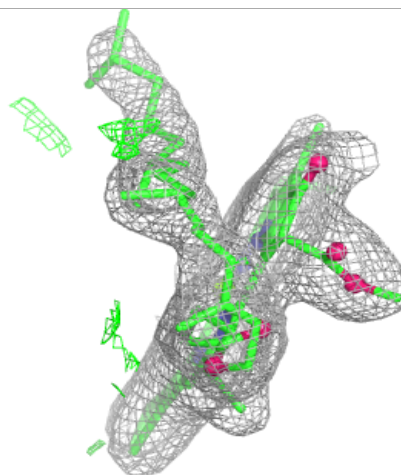
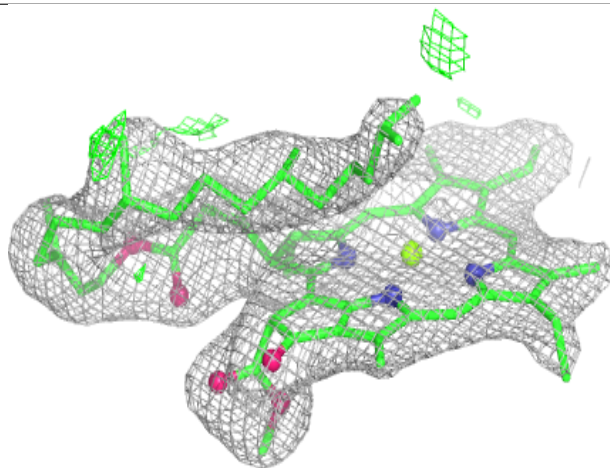
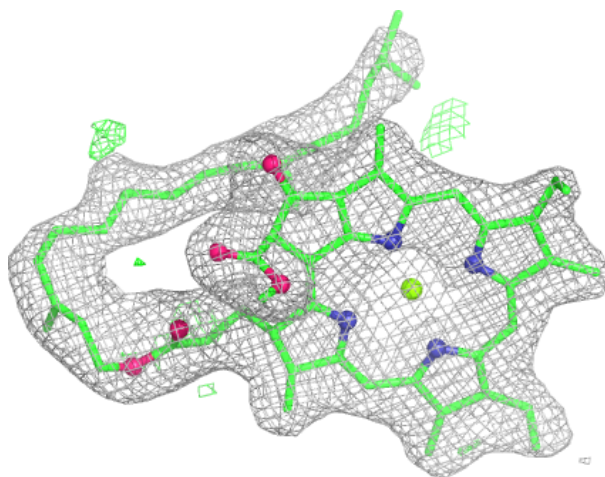
**Electron density around CLA c 506:**

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



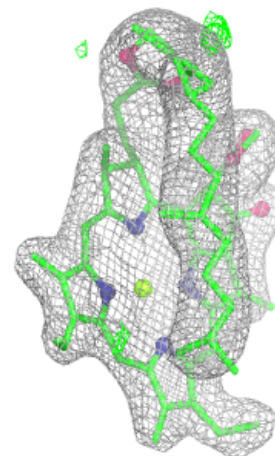
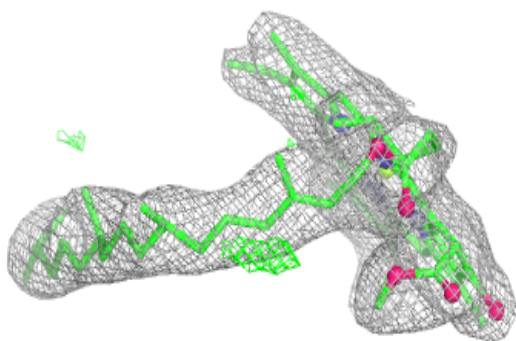
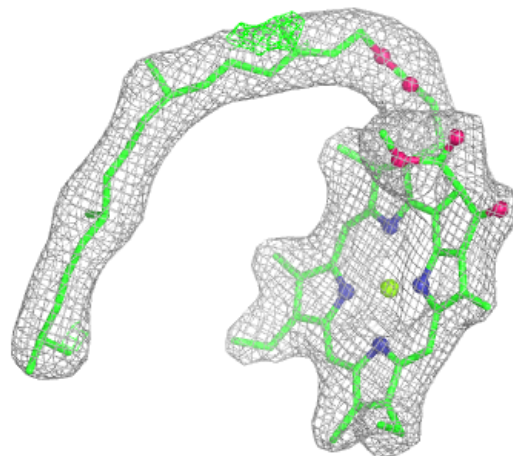
**Electron density around CLA C 510:**

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



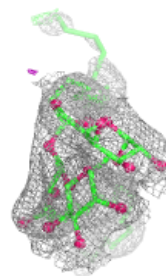
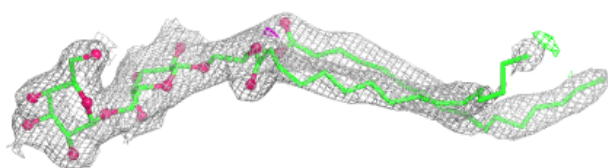
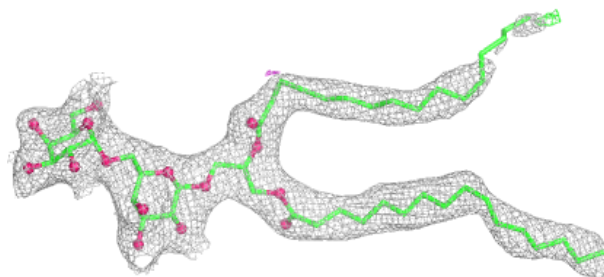
**Electron density around CLA c 510:**

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

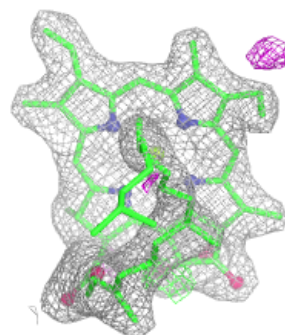
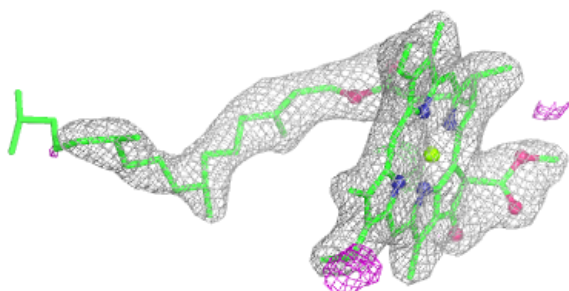


**Electron density around DGD c 520:**

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

**Electron density around CLA c 511:**

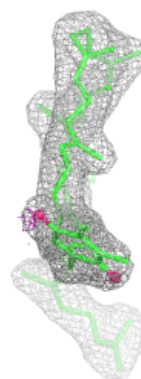
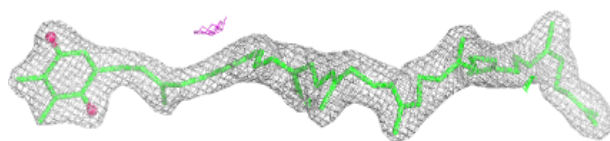
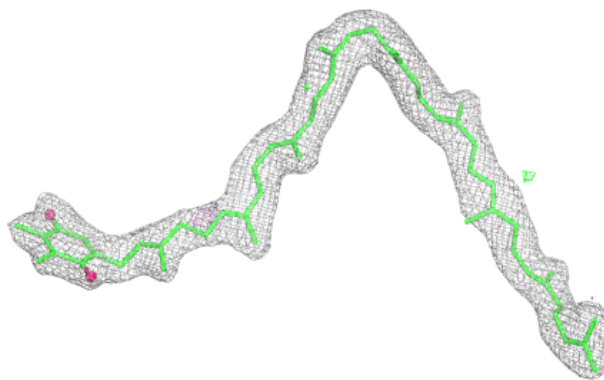
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





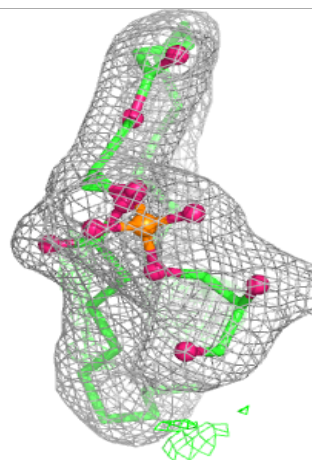
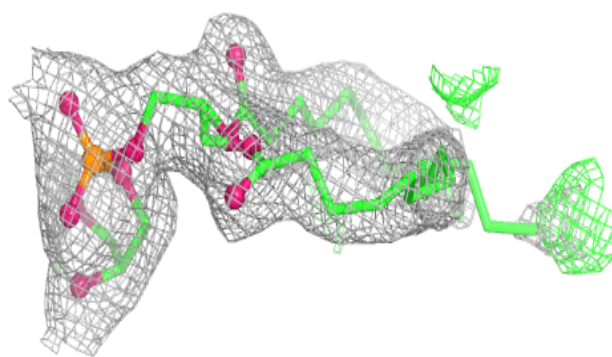
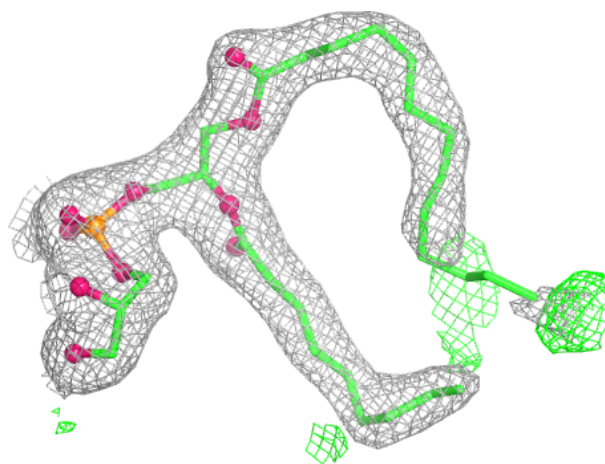
**Electron density around PL9 D 2306:**

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



**Electron density around LHG D 2311:**

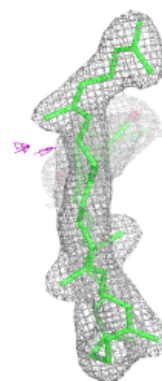
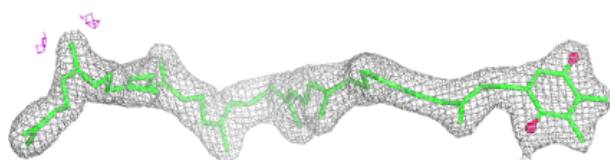
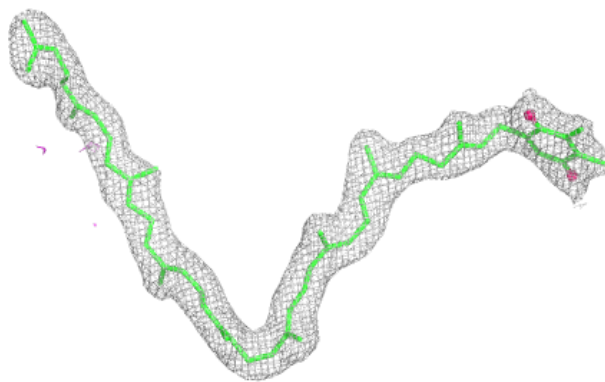
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





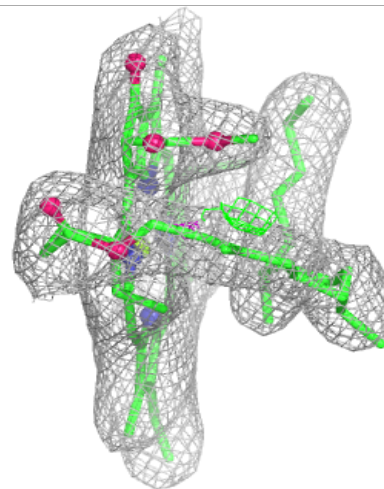
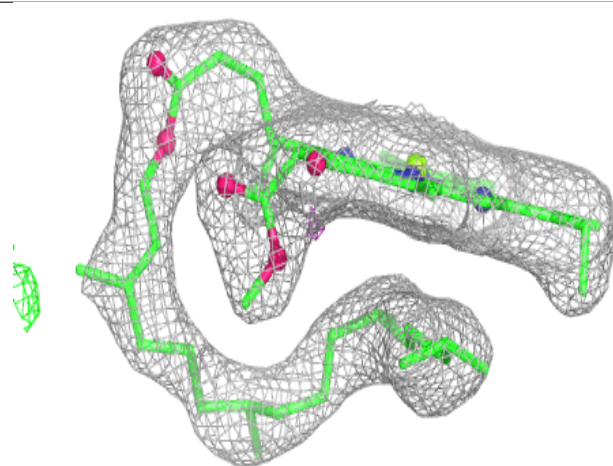
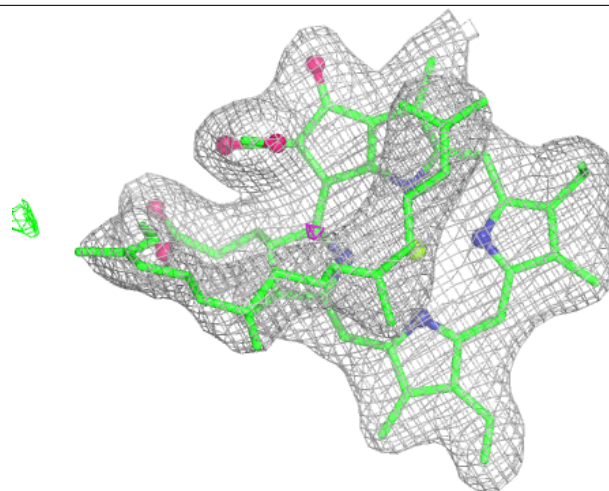
**Electron density around PL9 d 411:**

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



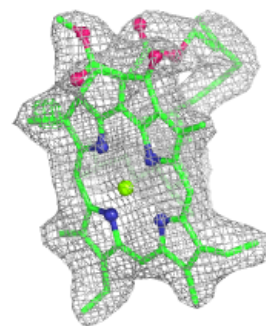
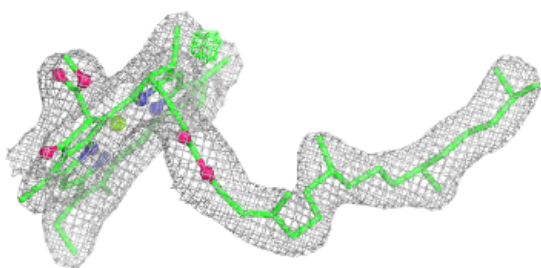
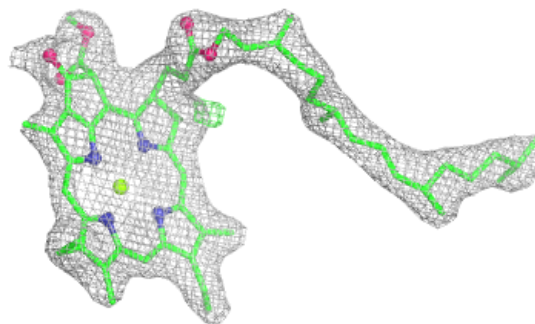
**Electron density around CLA c 513:**

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



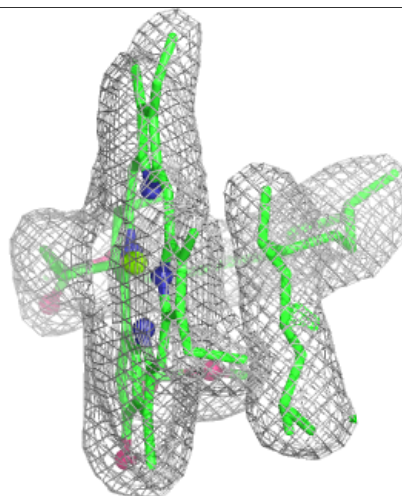
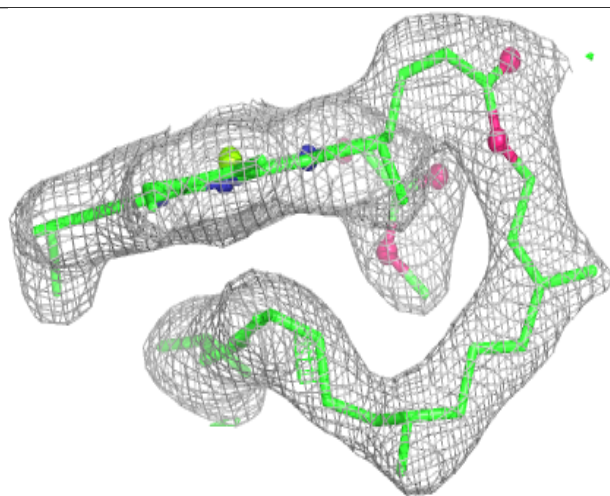
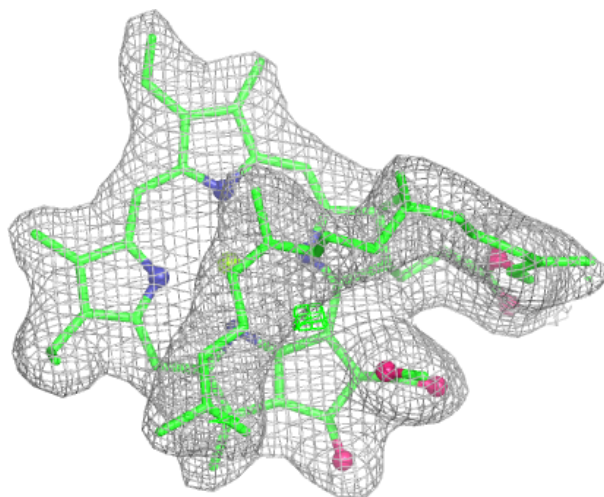
**Electron density around CLA c 514:**

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



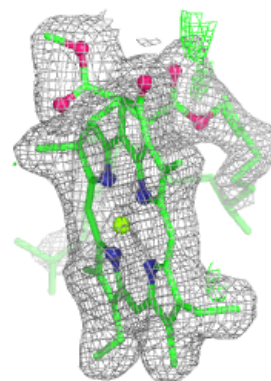
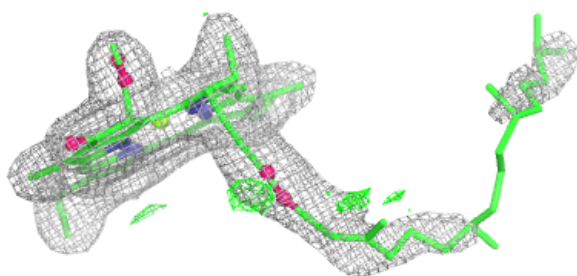
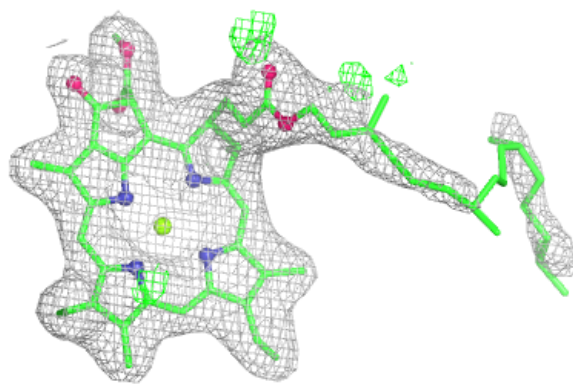
**Electron density around CLA C 511:**

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



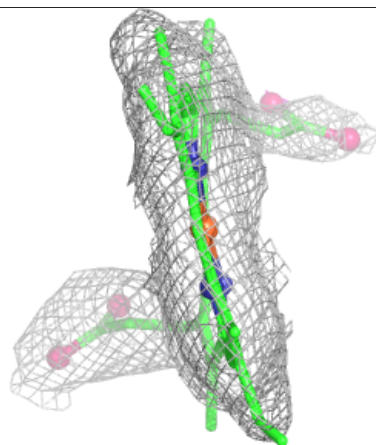
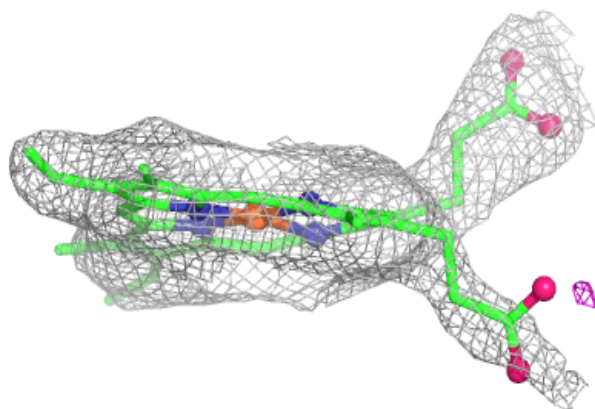
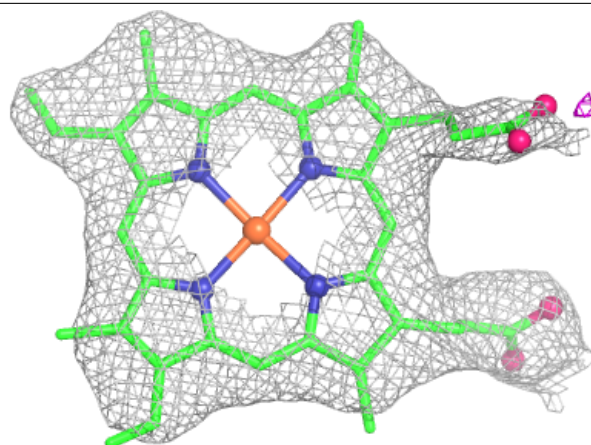
**Electron density around CLA A 410:**

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



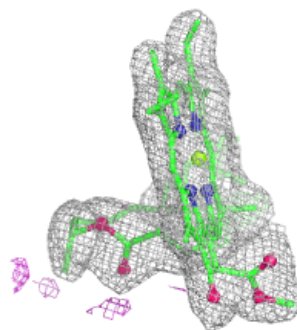
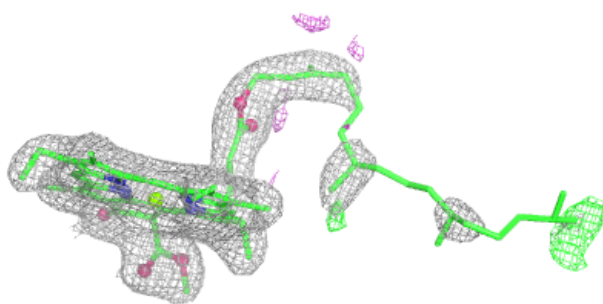
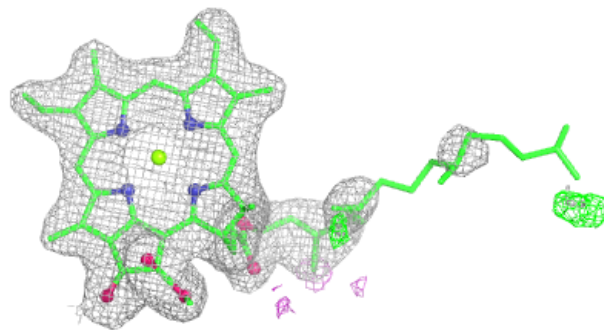
**Electron density around HEM e 103:**

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



**Electron density around CLA A 407:**

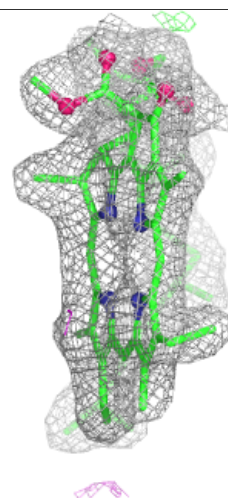
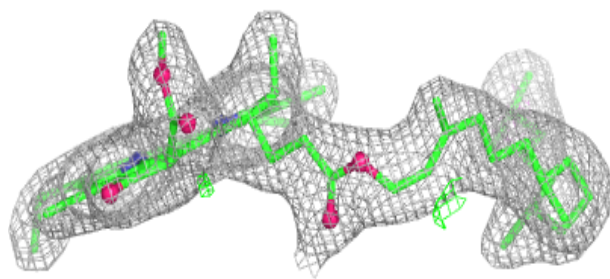
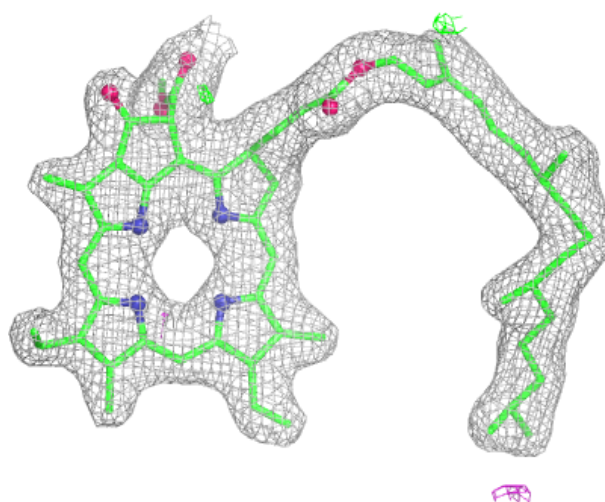
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PHO A 408:**

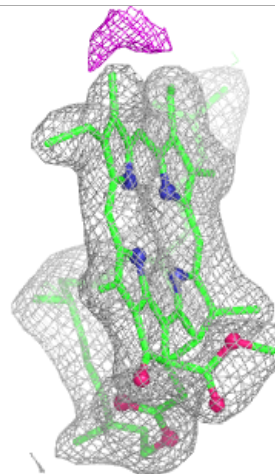
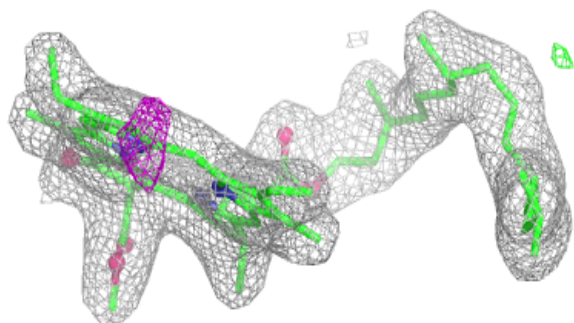
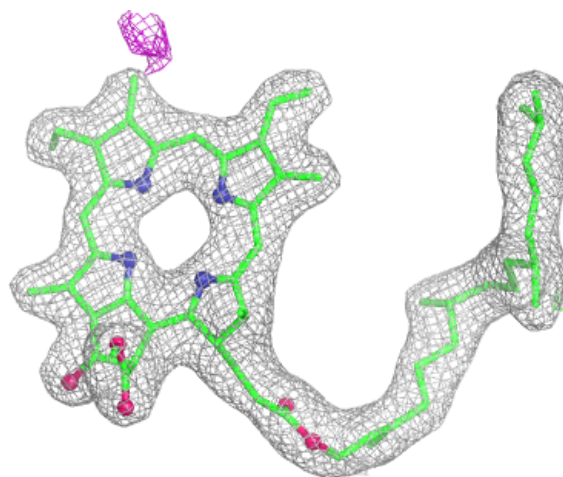
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





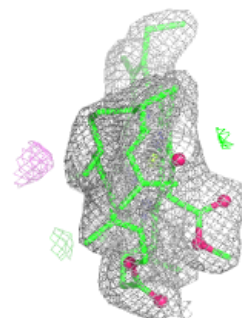
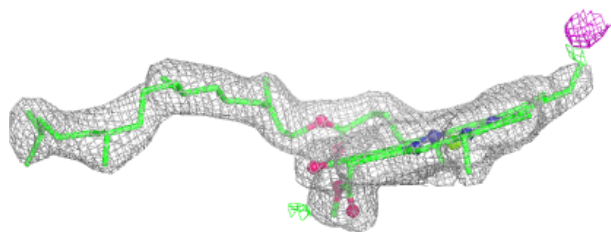
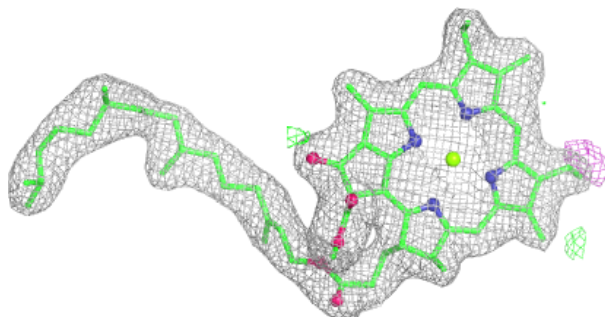
**Electron density around PHO A 409:**

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

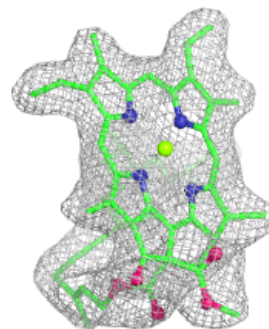
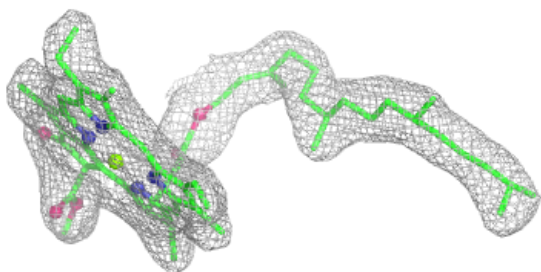
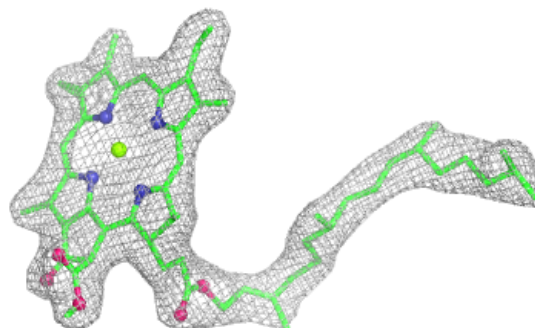


**Electron density around CLA B 603:**

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

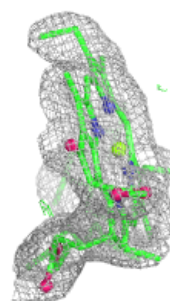
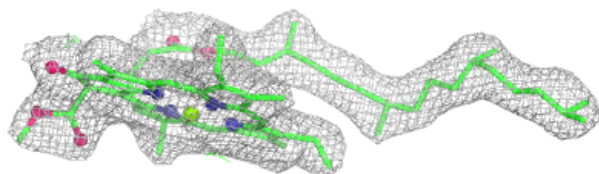
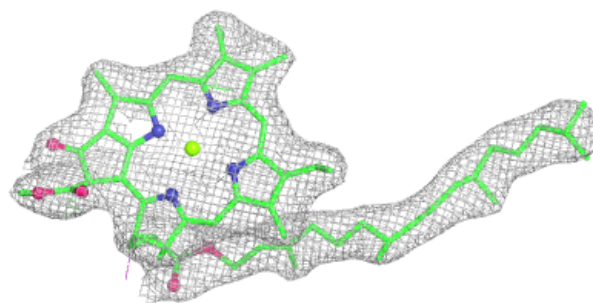
**Electron density around CLA C 512:**

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



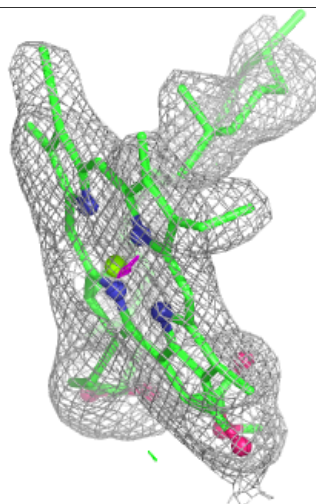
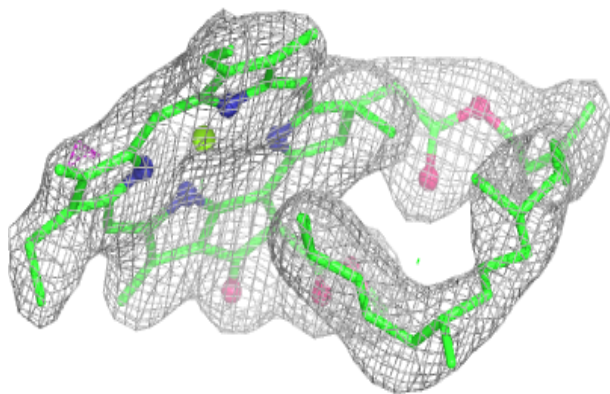
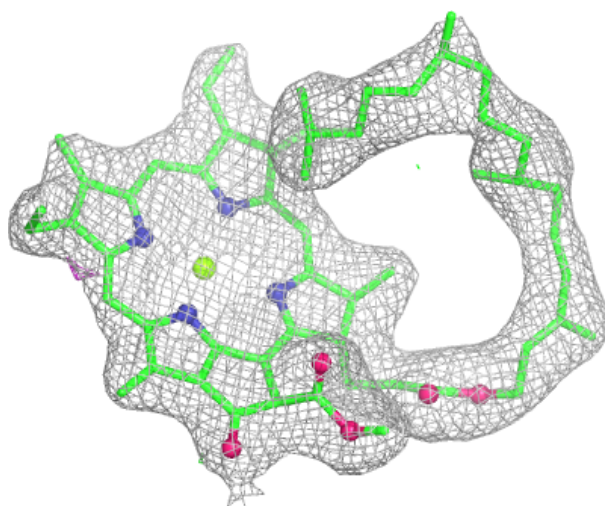
**Electron density around CLA c 504:**

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



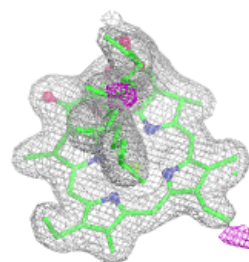
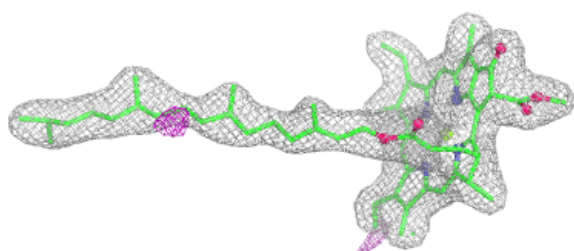
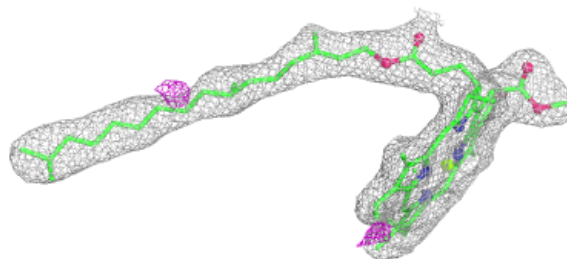
**Electron density around CLA B 616:**

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

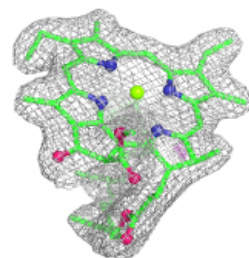
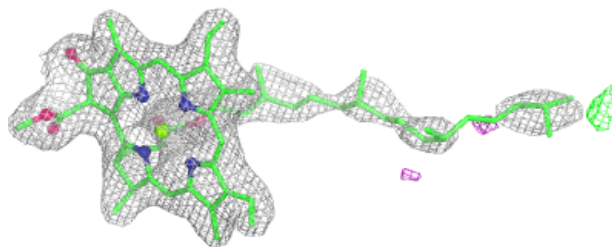
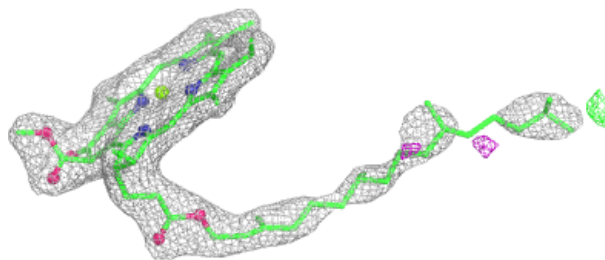


**Electron density around CLA B 608:**

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

**Electron density around CLA c 507:**

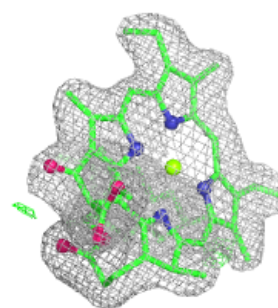
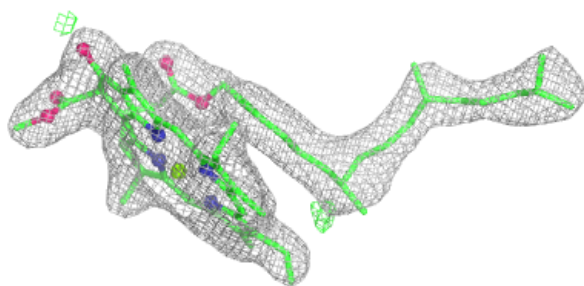
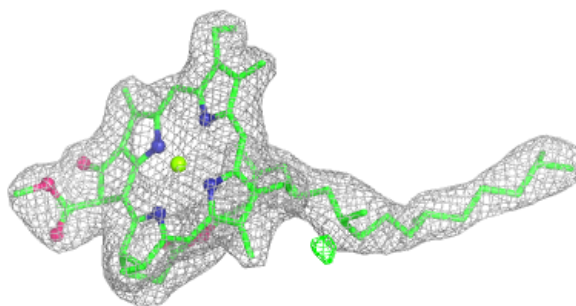
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



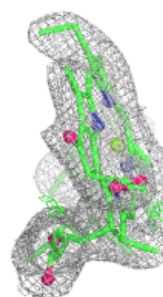
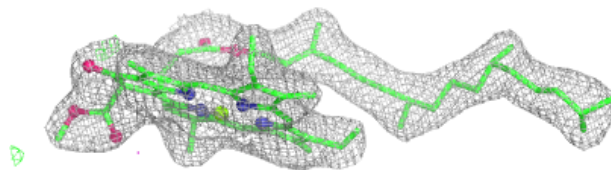
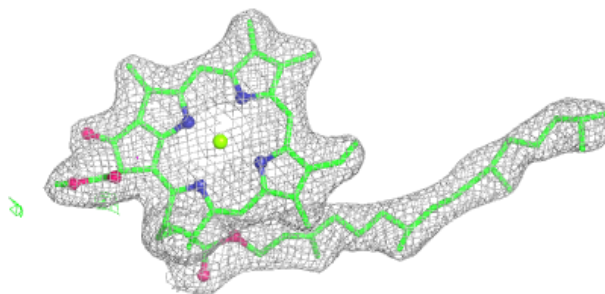


**Electron density around CLA c 508:**

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

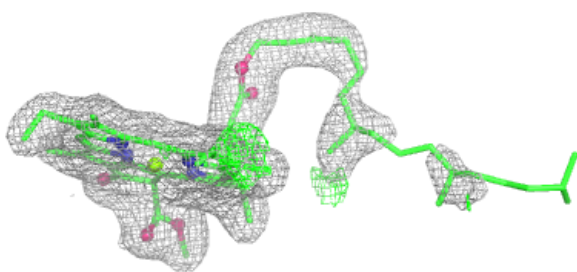
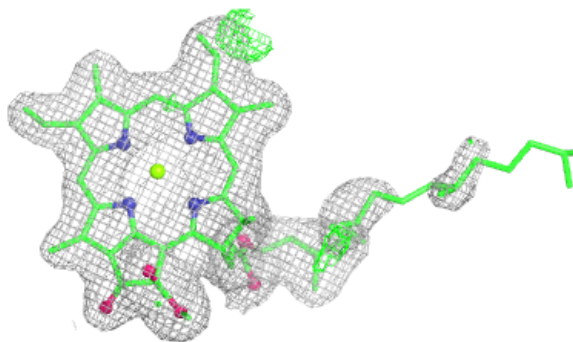
**Electron density around CLA C 502:**

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

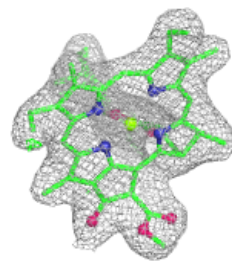
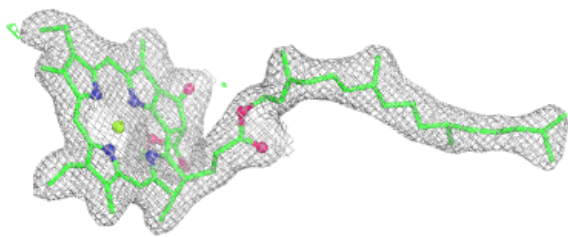
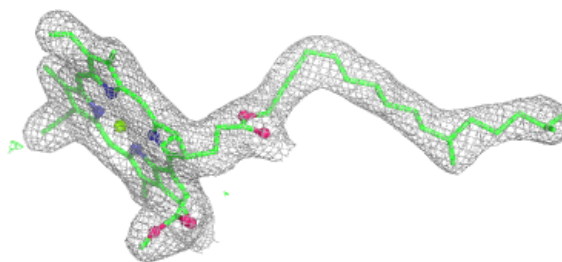


**Electron density around CLA a 2610:**

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

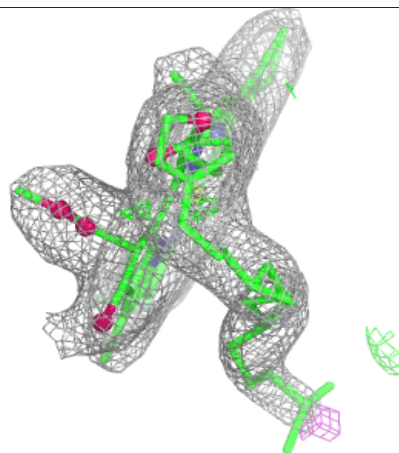
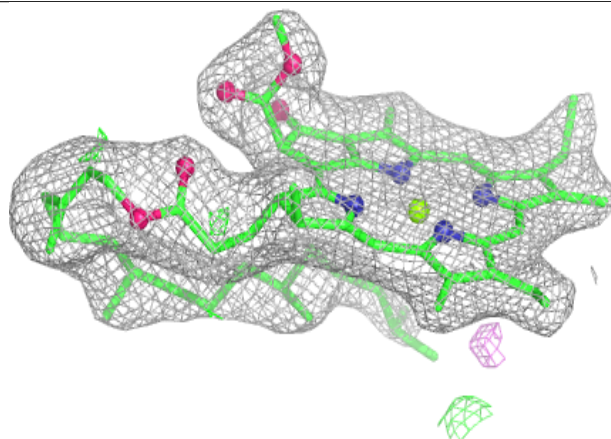
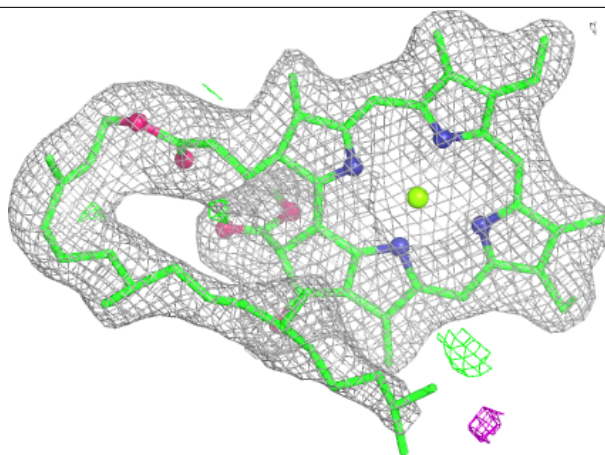
**Electron density around CLA C 503:**

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

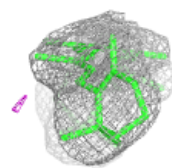
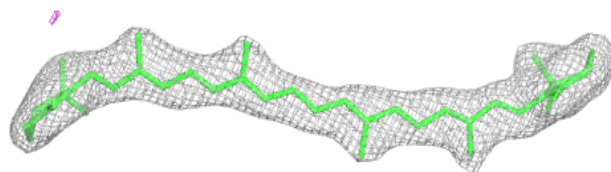
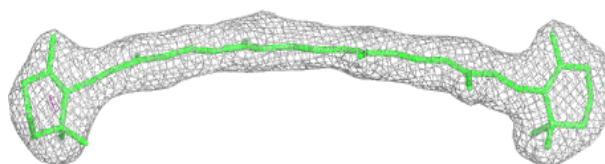


**Electron density around CLA c 512:**

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

**Electron density around BCR k 302:**

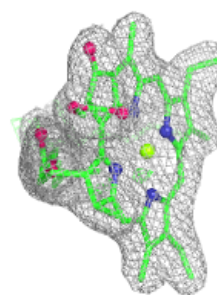
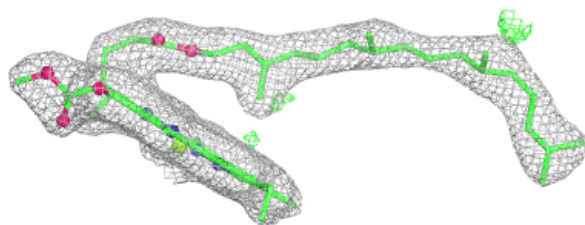
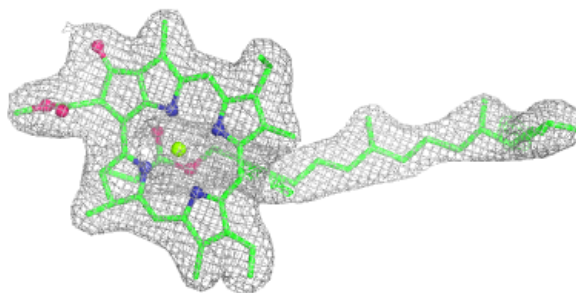
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



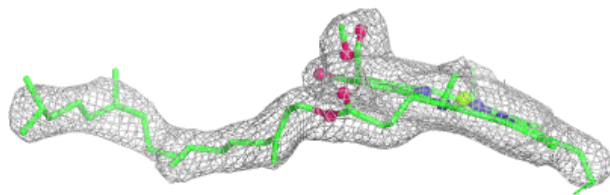
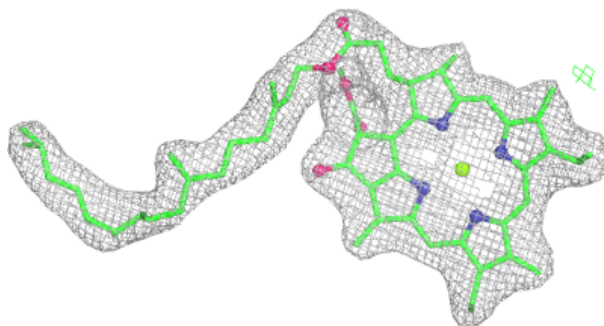


**Electron density around CLA B 609:**

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

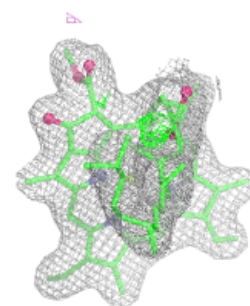
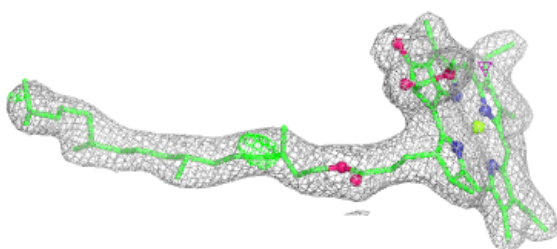
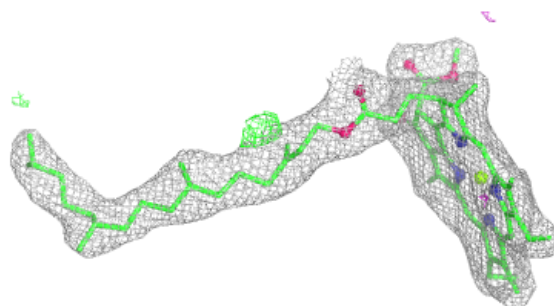
**Electron density around CLA b 607:**

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

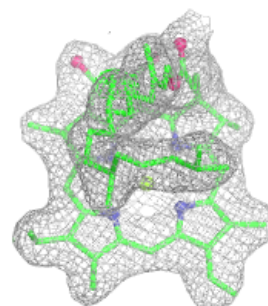
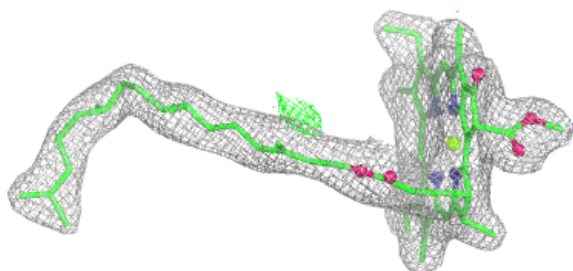
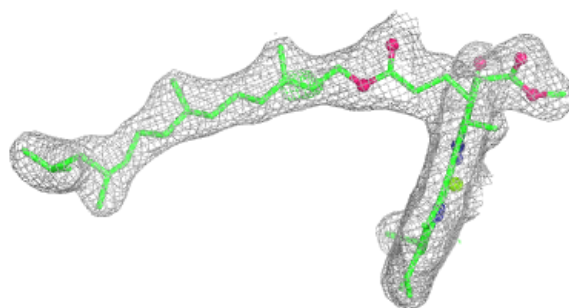


**Electron density around CLA b 609:**

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

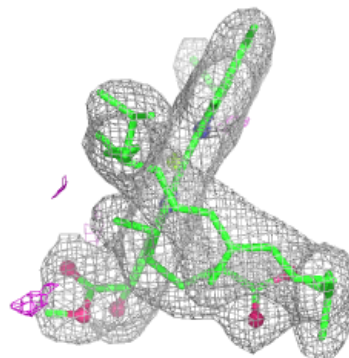
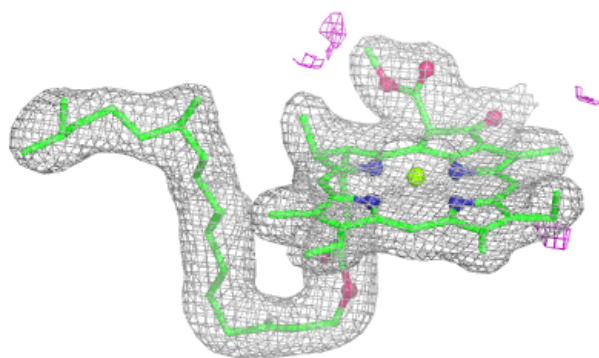
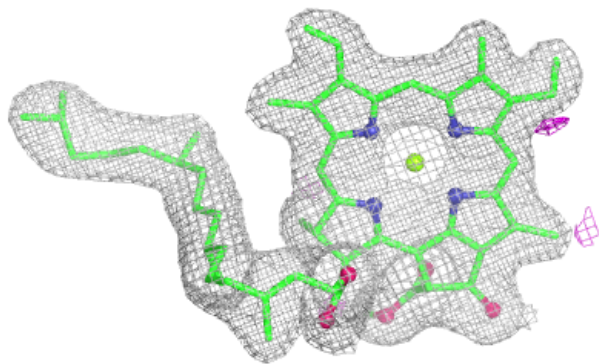
**Electron density around CLA b 610:**

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

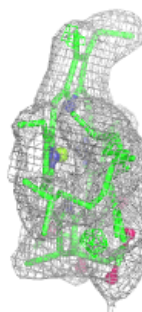
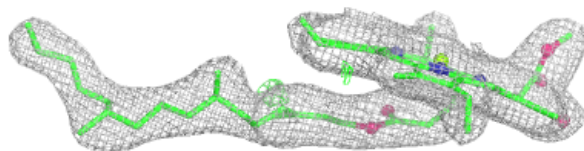
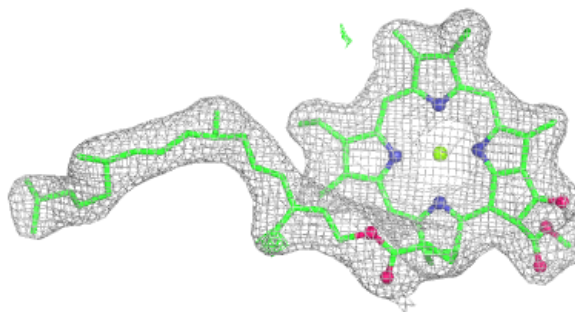


**Electron density around CLA d 402:**

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

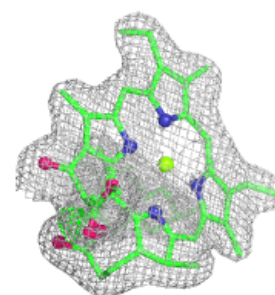
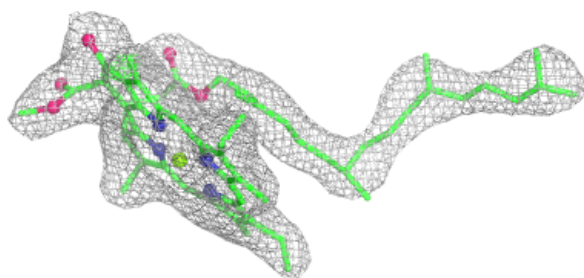
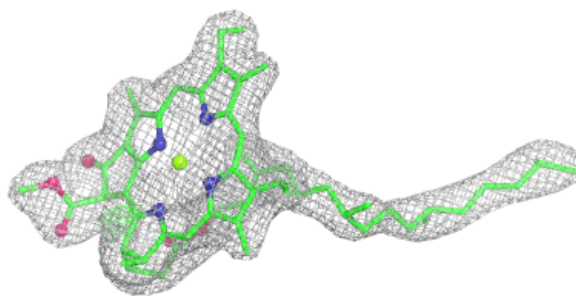
**Electron density around CLA B 604:**

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

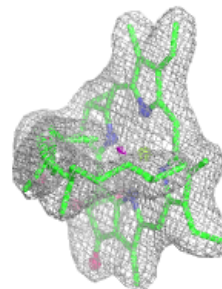
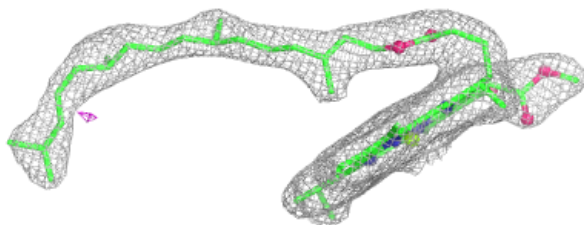
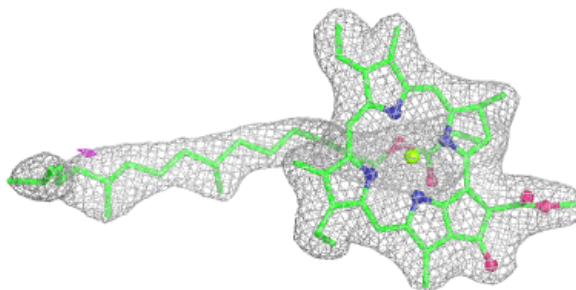


**Electron density around CLA C 506:**

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

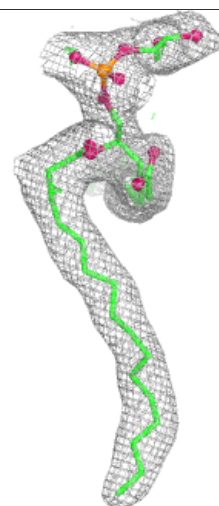
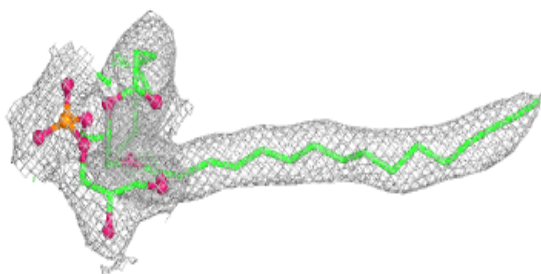
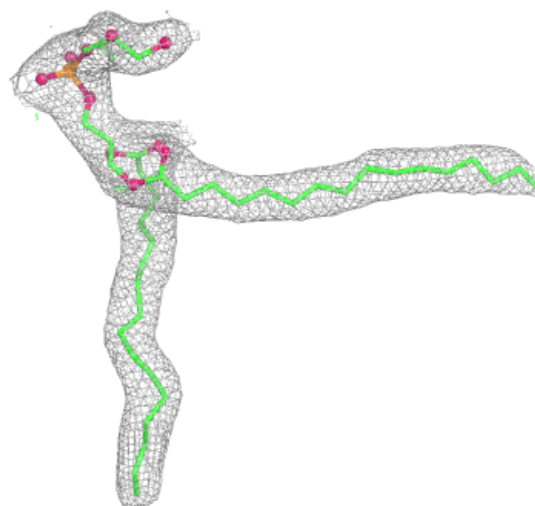
**Electron density around CLA b 613:**

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



**Electron density around LHG L 101:**

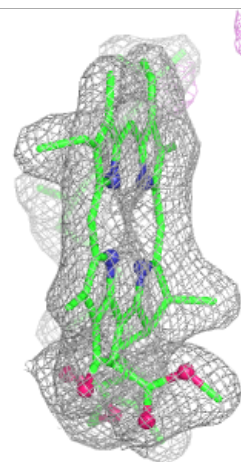
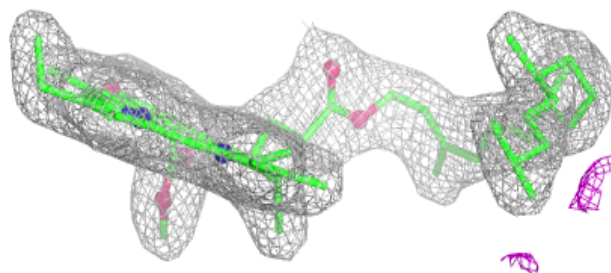
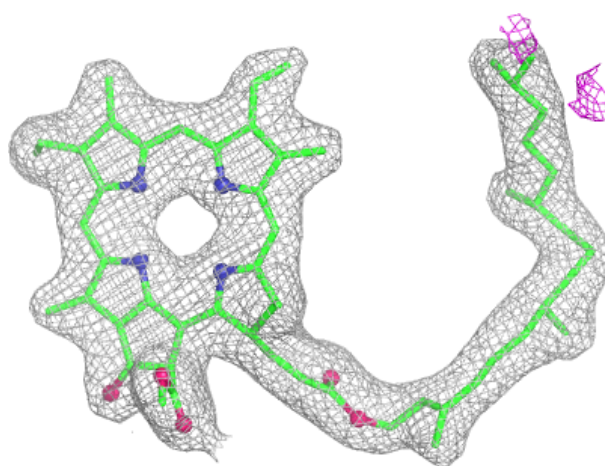
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





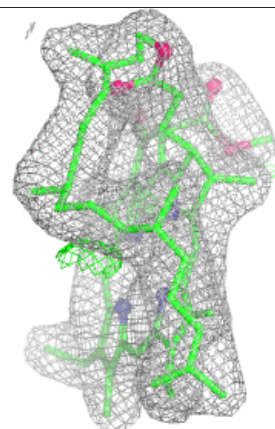
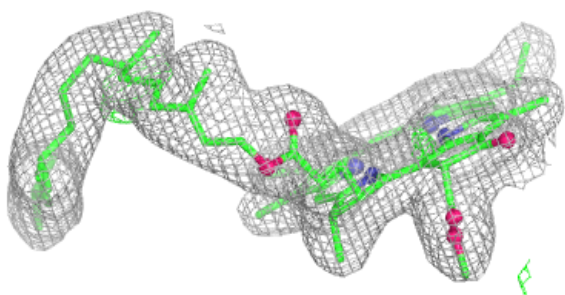
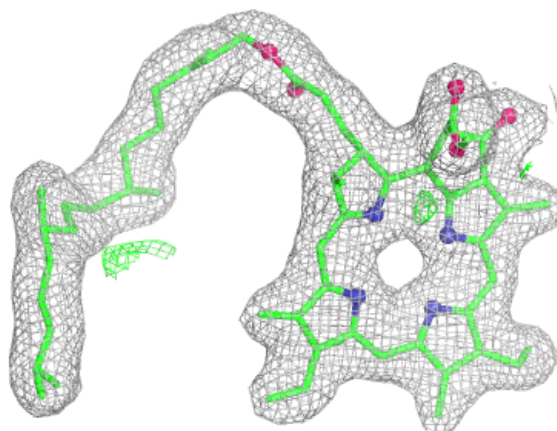
**Electron density around PHO a 2611:**

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



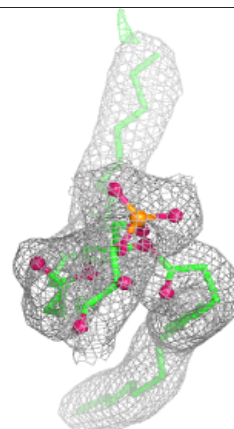
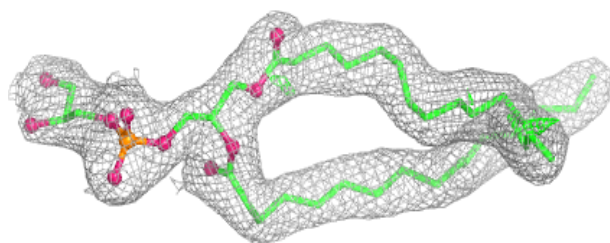
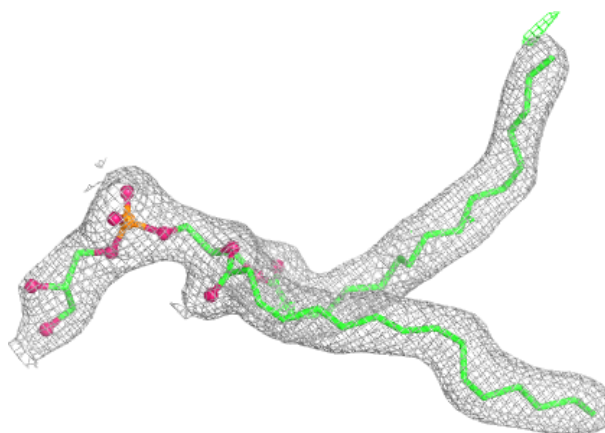
**Electron density around PHO a 2612:**

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

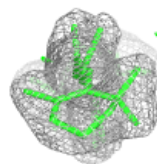
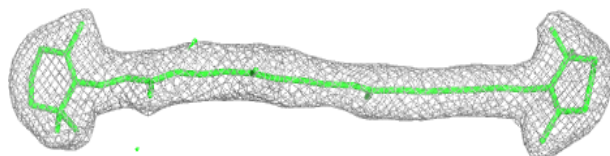
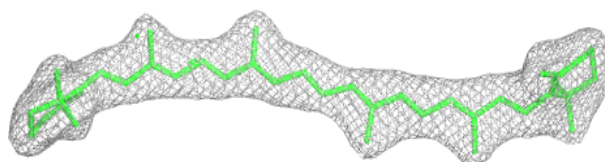


**Electron density around LHG d 413:**

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

**Electron density around BCR A 411:**

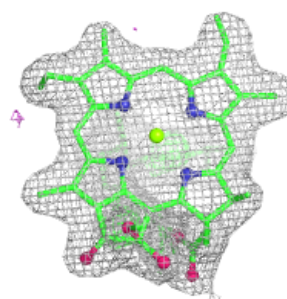
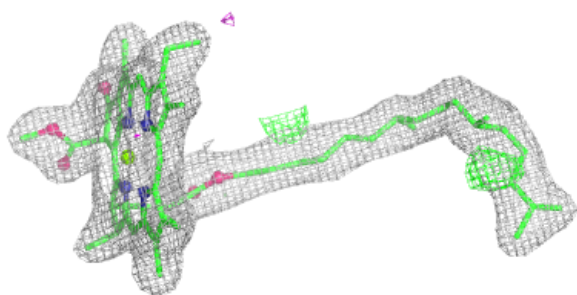
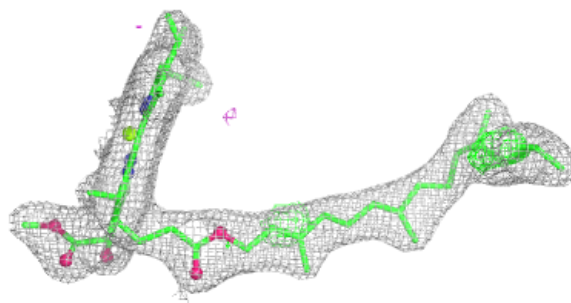
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





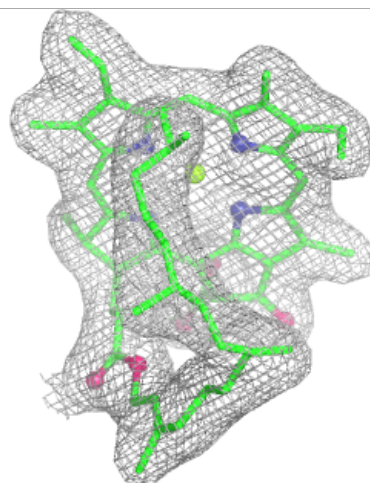
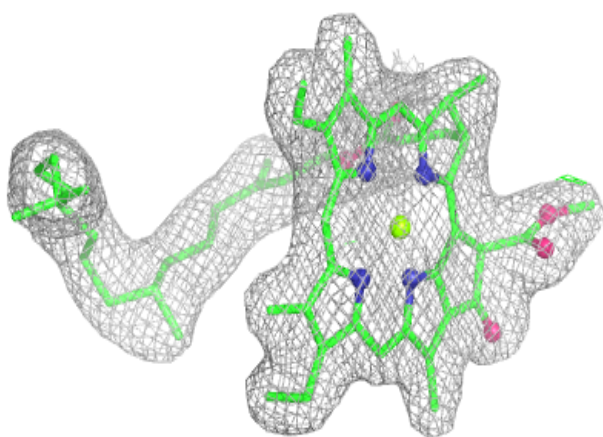
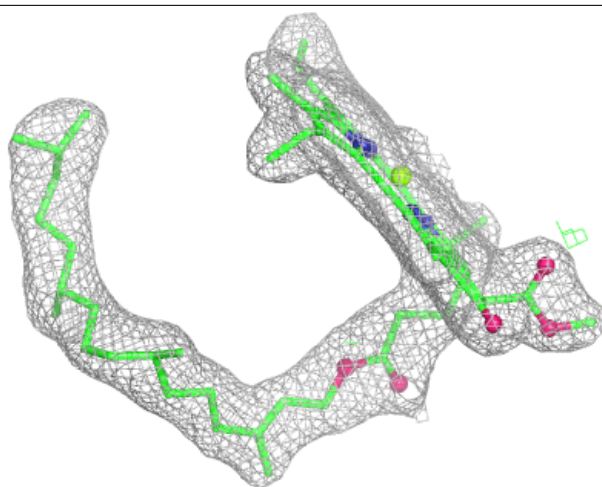
**Electron density around CLA B 606:**

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



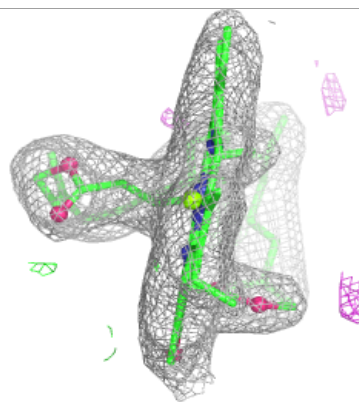
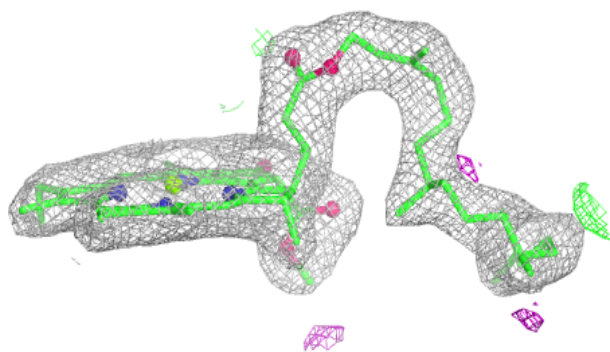
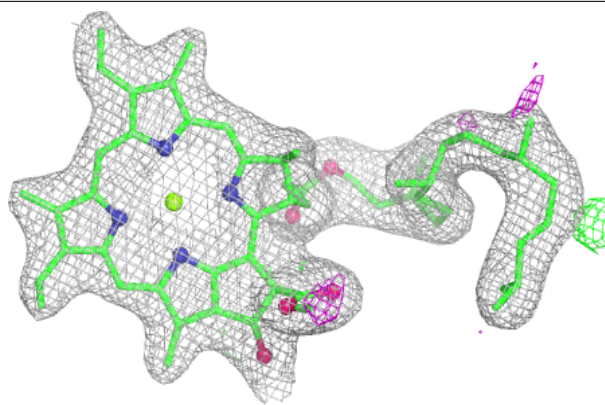
**Electron density around CLA B 612:**

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



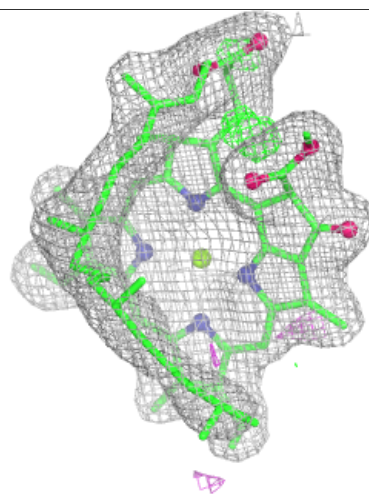
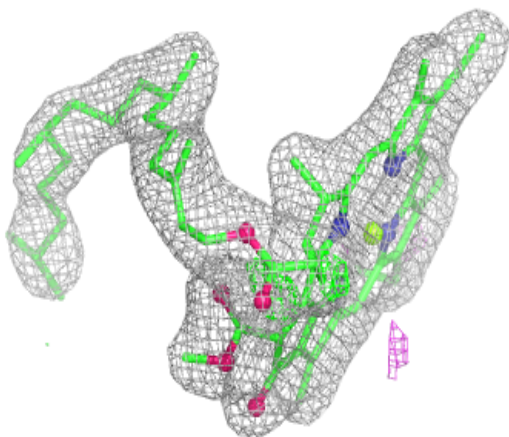
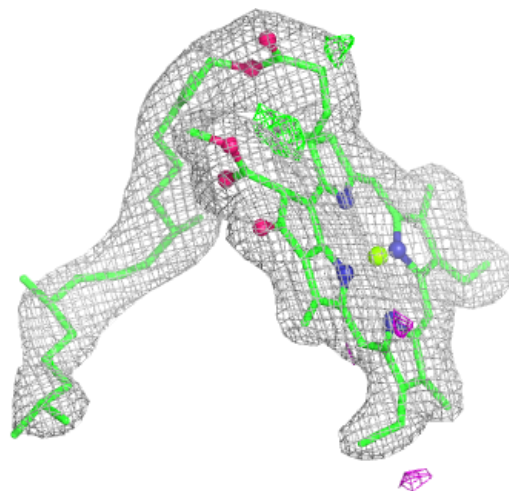
**Electron density around CLA B 613:**

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



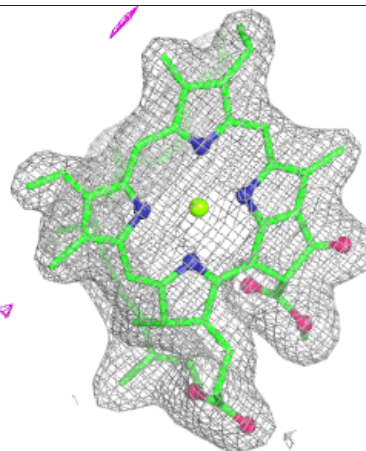
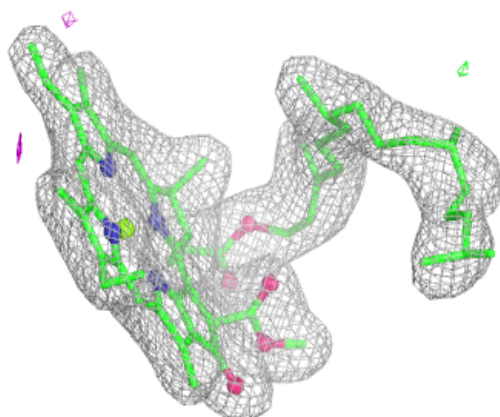
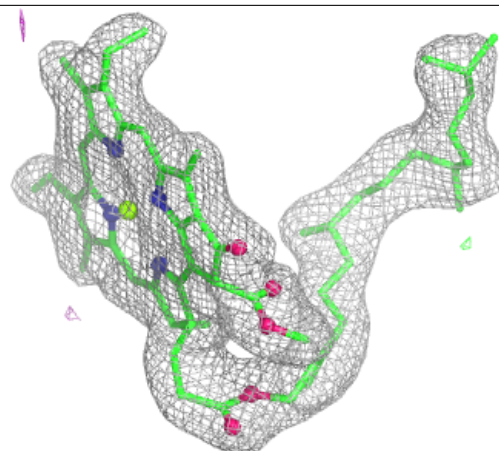
**Electron density around CLA b 618:**

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

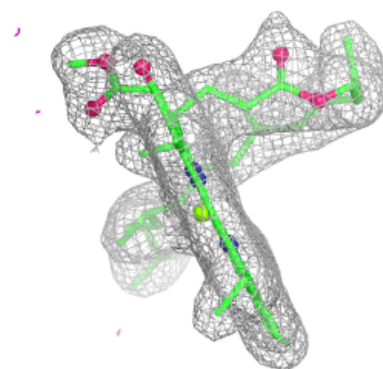
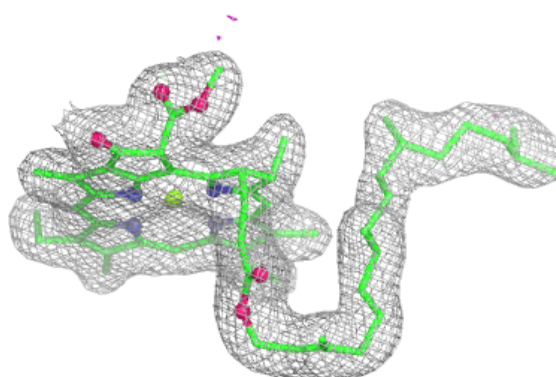
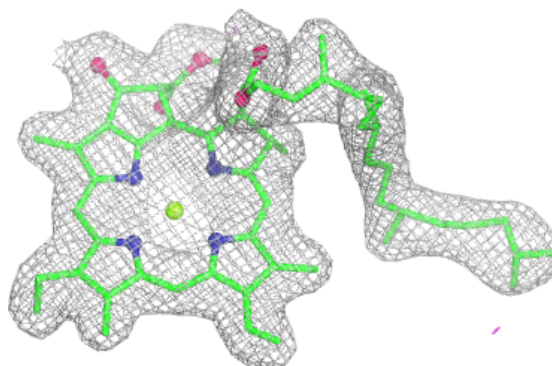


**Electron density around CLA B 614:**

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

**Electron density around CLA A 406:**

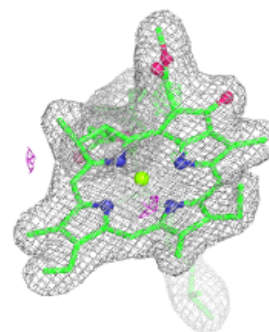
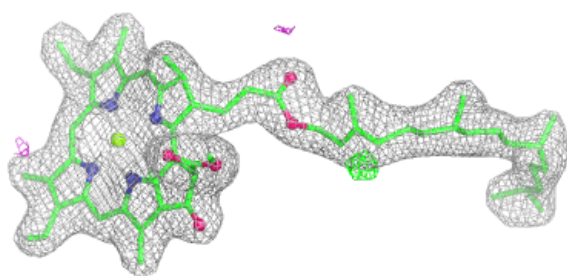
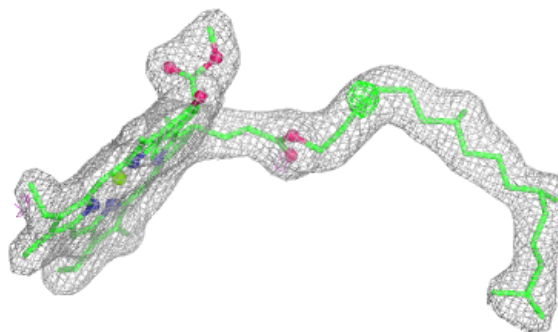
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



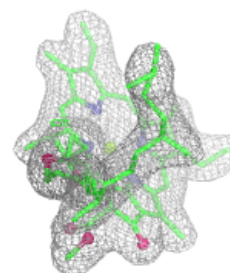
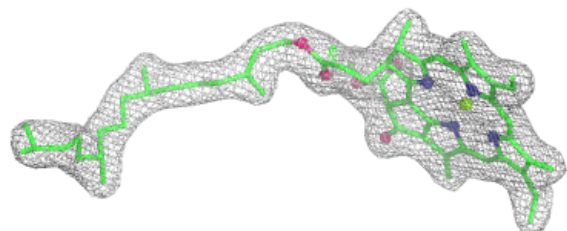
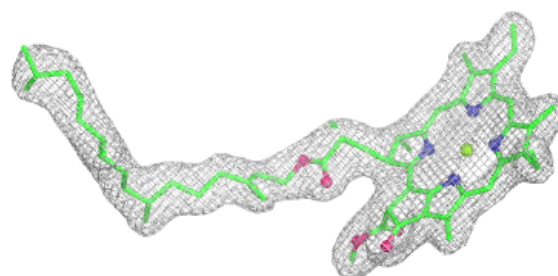


**Electron density around CLA D 2303:**

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

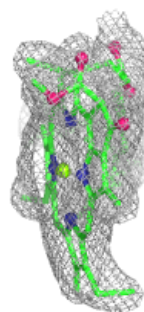
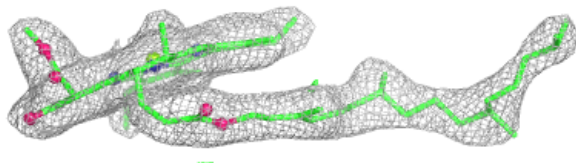
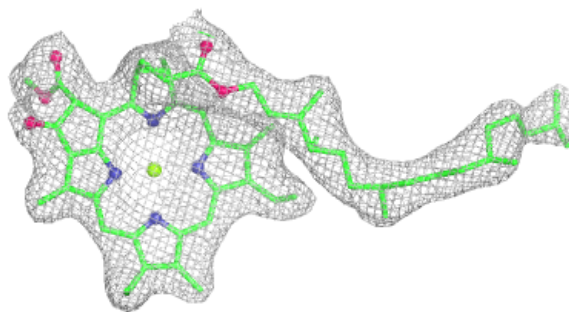
**Electron density around CLA A 405:**

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

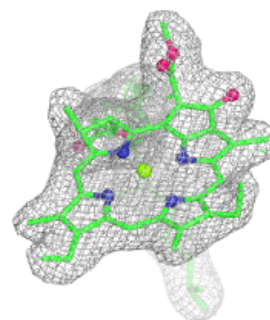
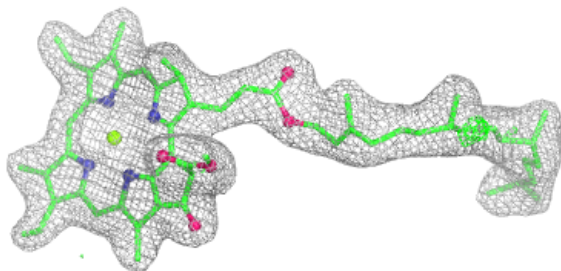
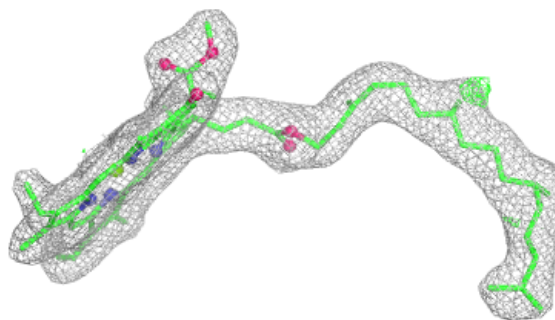


**Electron density around CLA b 608:**

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

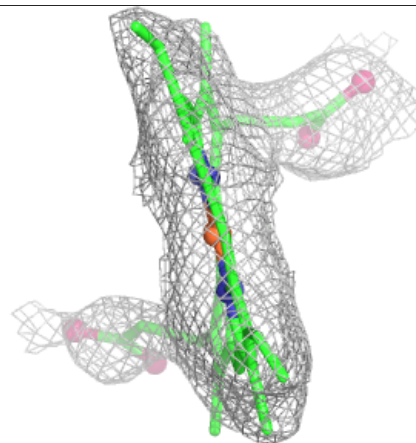
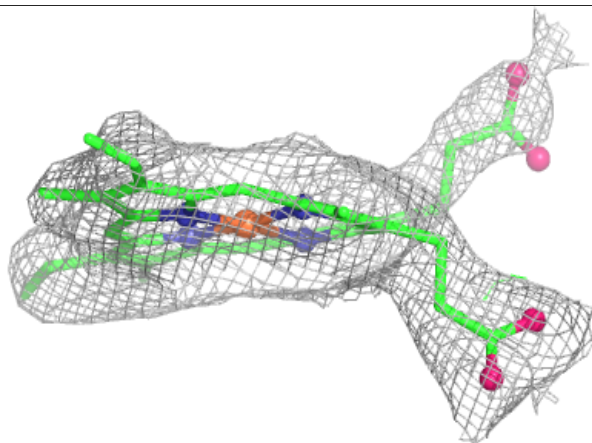
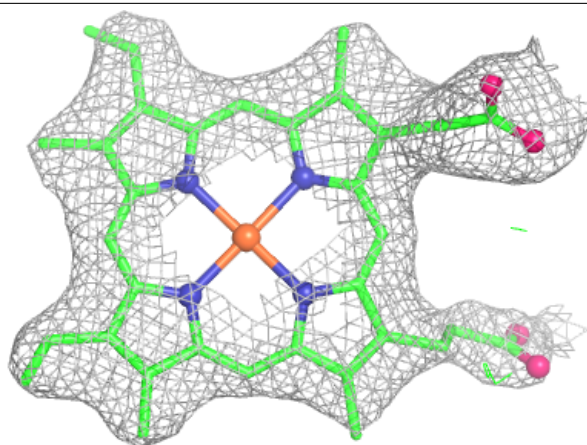
**Electron density around CLA d 408:**

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



**Electron density around HEM F 101:**

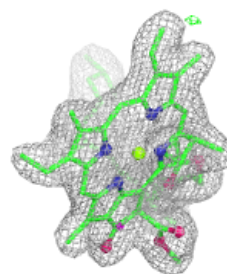
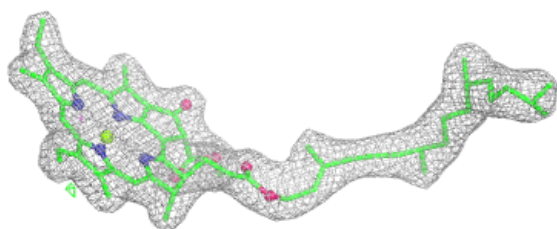
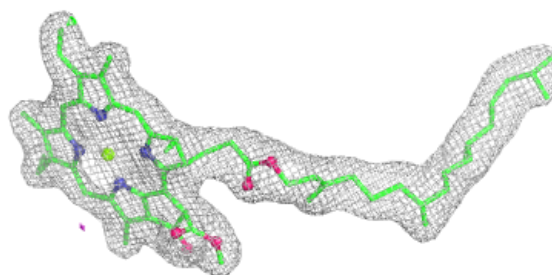
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



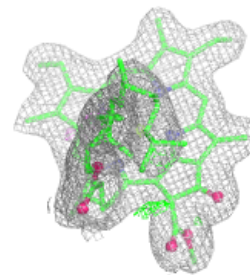
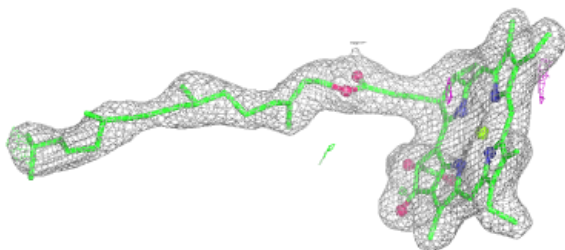
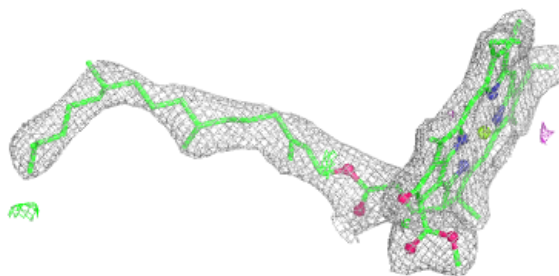


**Electron density around CLA a 2609:**

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

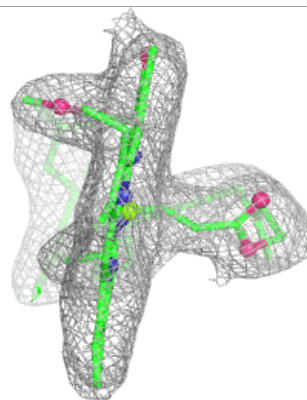
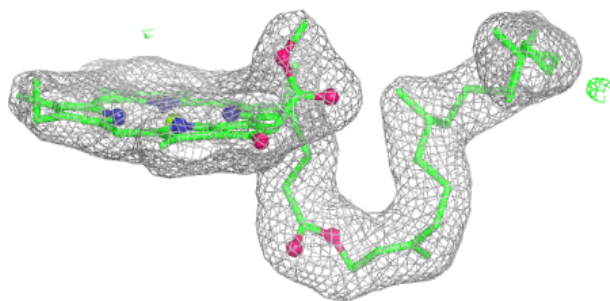
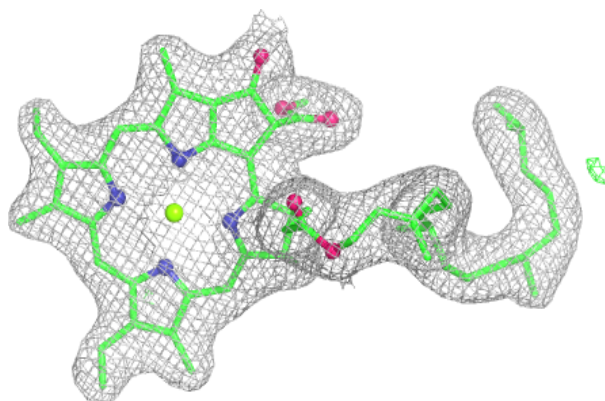
**Electron density around CLA B 605:**

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



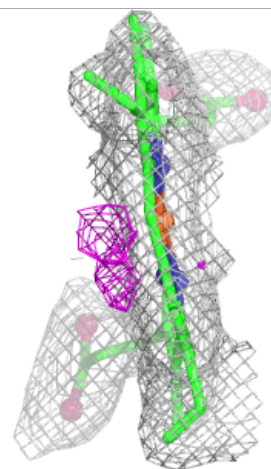
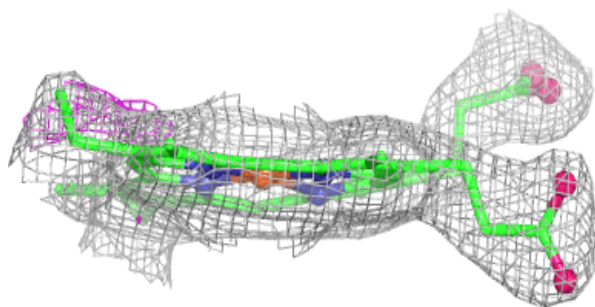
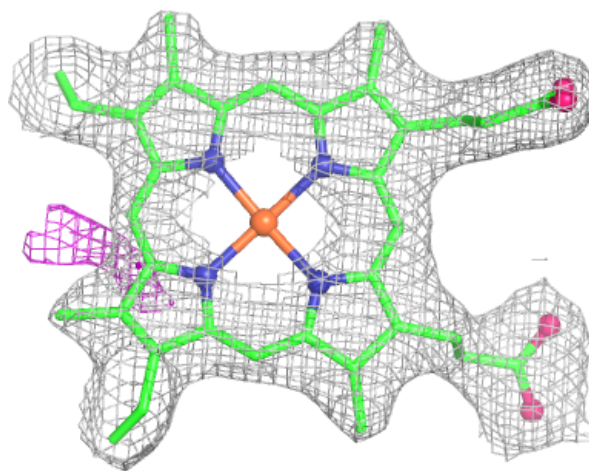
**Electron density around CLA b 617:**

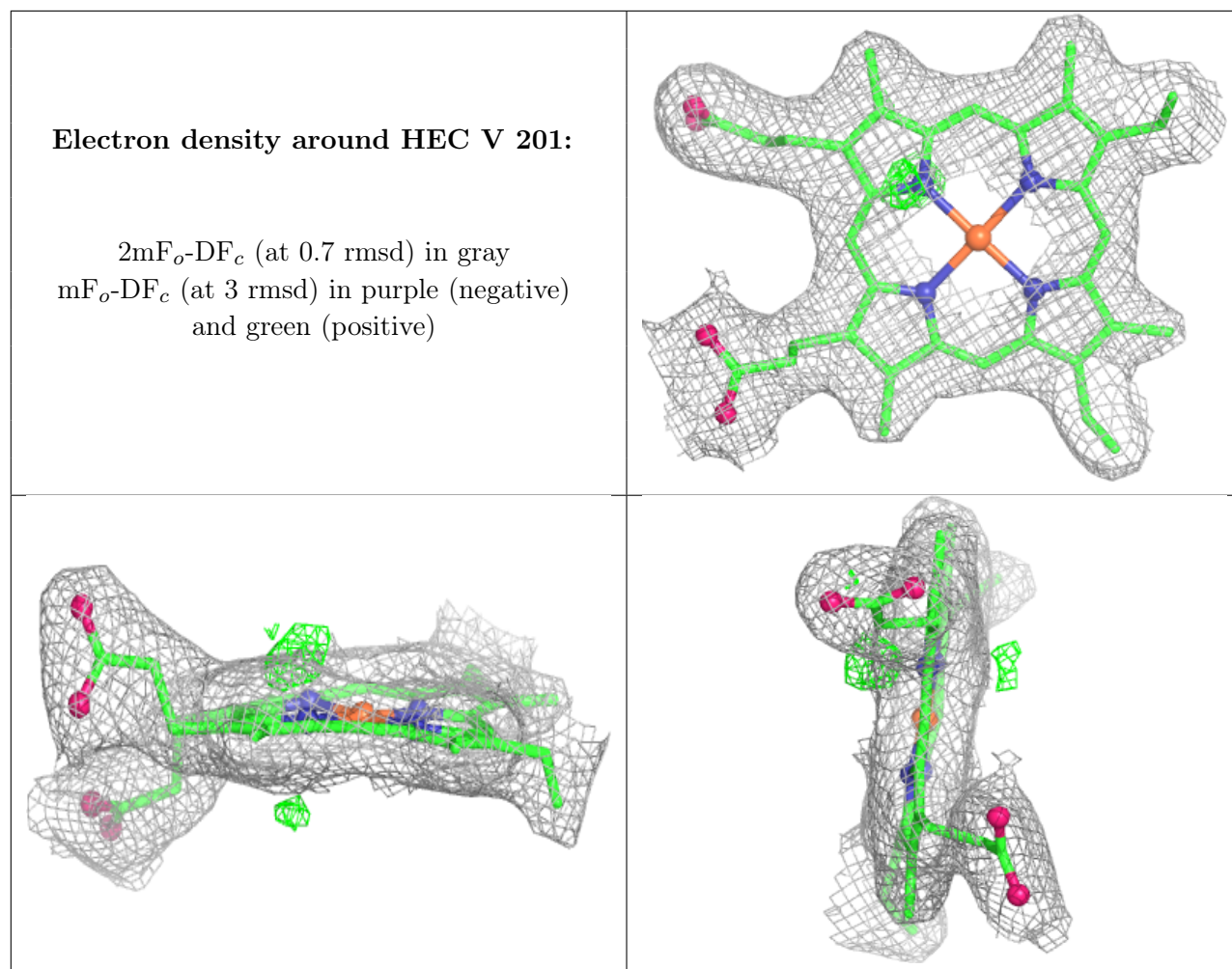
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC v 201:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.