



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:35 PM JST

PDB ID : 6JLK / pdb\_00006jlk  
Title : XFEL structure of cyanobacterial photosystem II (1F state, dataset1)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2019-03-06  
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:

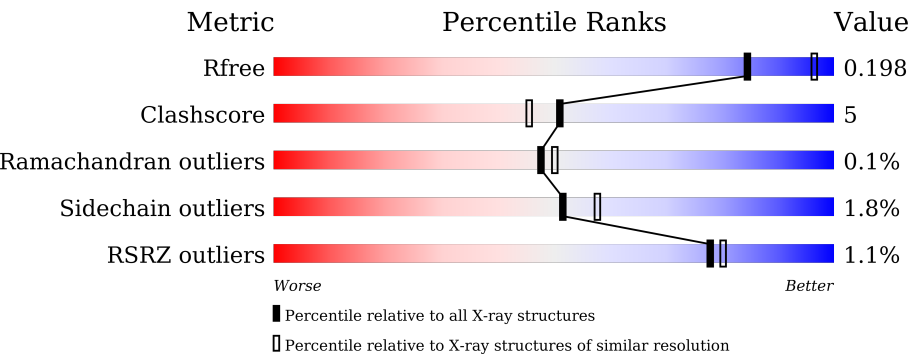
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.015 (Gargrove)  
Density-Fitness : 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)                                      |

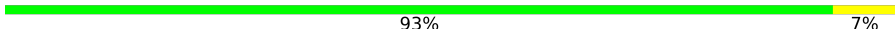
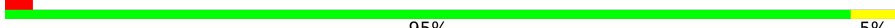
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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>90%7%</div></div>   |
| 1   | a     | 344    | <div><div>%</div><div>88%8%</div></div>  |
| 2   | B     | 505    | <div><div></div><div>91%9%</div></div>   |
| 2   | b     | 505    | <div><div>%</div><div>90%10%</div></div> |
| 3   | C     | 455    | <div><div></div><div>89%10%</div></div>  |
| 3   | c     | 455    | <div><div></div><div>91%8%</div></div>   |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D     | 342    |    |
| 4   | d     | 342    |    |
| 5   | E     | 84     |    |
| 5   | e     | 84     |    |
| 6   | F     | 44     |    |
| 6   | f     | 44     |    |
| 7   | H     | 65     |    |
| 7   | h     | 65     |    |
| 8   | I     | 38     |    |
| 8   | i     | 38     |    |
| 9   | J     | 39     |    |
| 9   | j     | 39     |   |
| 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    |                  |
| 17  | Y     | 30     |                  |
| 17  | y     | 30     |                  |
| 18  | X     | 40     |                  |
| 18  | x     | 40     |                  |
| 19  | Z     | 62     |                  |
| 19  | z     | 62     |                  |
| 20  | R     | 34     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 40  | HEC  | V     | 205 | X         | -        | -       | -                |
| 40  | HEC  | v     | 205 | X         | -        | -       | -                |

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 55631 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       | 53      | 0     |
|     |       |          | 3019  | 1966 | 498 | 537 | 18 |         |         |       |
| 1   | a     | 334      | Total | C    | N   | O   | S  | 0       | 55      | 0     |
|     |       |          | 3027  | 1973 | 498 | 538 | 18 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 504      | Total | C    | N   | O   | S  | 0       | 10      | 0     |
|     |       |          | 4021  | 2639 | 667 | 702 | 13 |         |         |       |
| 2   | b     | 503      | Total | C    | N   | O   | S  | 0       | 12      | 0     |
|     |       |          | 4022  | 2644 | 664 | 701 | 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       | 7       | 0     |
|     |       |          | 3518  | 2300 | 587 | 618 | 13 |         |         |       |
| 3   | c     | 455      | Total | C    | N   | O   | S  | 0       | 13      | 0     |
|     |       |          | 3598  | 2356 | 599 | 629 | 14 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 341      | Total | C    | N   | O   | S  | 0       | 16      | 0     |
|     |       |          | 2849  | 1884 | 469 | 483 | 13 |         |         |       |
| 4   | d     | 341      | Total | C    | N   | O   | S  | 0       | 16      | 0     |
|     |       |          | 2849  | 1884 | 469 | 483 | 13 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5   | E     | 81       | Total | C   | N   | O   | 0       | 2       | 0     |
|     |       |          | 668   | 436 | 107 | 125 |         |         |       |
| 5   | e     | 81       | Total | C   | N   | O   | 0       | 2       | 0     |
|     |       |          | 670   | 439 | 107 | 124 |         |         |       |

- 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     |
|     |       |          | 275   | 187 | 45 | 42 | 1 |         |         |       |
| 6   | f     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 257   | 175 | 43 | 38 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | H     | 65       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 519   | 346 | 85 | 86 | 2 |         |         |       |
| 7   | h     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 511   | 341 | 82 | 86 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | I     | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 314   | 211 | 48 | 54 | 1 |         |         |       |
| 8   | i     | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 314   | 211 | 48 | 54 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | J     | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 272   | 182 | 42 | 47 | 1 |         |         |       |
| 9   | j     | 39       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 280   | 187 | 43 | 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       | 0       | 0     |
|     |       |          | 293   | 204 | 43 | 46 |         |         |       |
| 10  | k     | 37       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 293   | 204 | 43 | 46 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11  | L     | 37       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 309   | 207 | 48 | 53 | 1 |         |         |       |
| 11  | l     | 37       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 309   | 207 | 48 | 53 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | M     | 34       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 274   | 184 | 40 | 49 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | m     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 269   | 179 | 40 | 49 | 1 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | O     | 243      | Total | C    | N   | O   | S | 0       | 8       | 0     |
|     |       |          | 1903  | 1191 | 315 | 392 | 5 |         |         |       |
| 13  | o     | 243      | Total | C    | N   | O   | S | 0       | 5       | 0     |
|     |       |          | 1891  | 1183 | 315 | 388 | 5 |         |         |       |

- 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       | 1       | 0     |
|     |       |          | 264   | 185 | 36 | 41 | 2 |         |         |       |
| 14  | t     | 30       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 264   | 185 | 36 | 41 | 2 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | V     | 137      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1085  | 689 | 181 | 211 | 4 |         |         |       |
| 16  | v     | 137      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1077  | 684 | 178 | 211 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 17  | Y     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 215   | 142 | 37 | 33 | 3 |         |         |       |
| 17  | y     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 215   | 142 | 37 | 33 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18  | X     | 39       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 287   | 191 | 46 | 50 |   |         |         |       |
| 18  | x     | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 281   | 188 | 45 | 48 |   |         |         |       |

- 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     |
|     |       |          | 479   | 328 | 72 | 77 | 2 |         |         |       |
| 19  | z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 479   | 328 | 72 | 77 | 2 |         |         |       |

- Molecule 20 is a protein called Photosystem II protein Y.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 20  | R     | 30       | Total | C   | N  | O  | S | 98      | 0       | 0     |
|     |       |          | 239   | 163 | 41 | 35 |   |         |         |       |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21  | A     | 1        | Total | Fe | 0       | 1       |
|     |       |          | 2     | 2  |         |         |
| 21  | a     | 1        | Total | Fe | 0       | 1       |
|     |       |          | 2     | 2  |         |         |

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

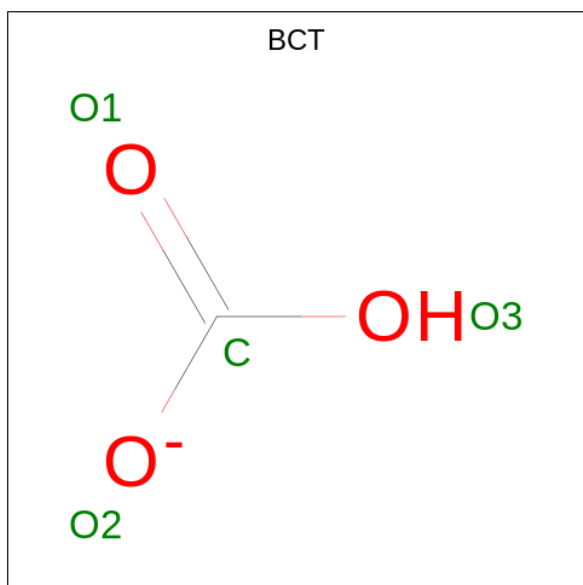
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22  | A     | 2        | Total | Cl | 0       | 2       |
|     |       |          | 4     | 4  |         |         |
| 22  | U     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22  | a     | 2        | Total | Cl | 0       | 2       |
|     |       |          | 4     | 4  |         |         |
| 22  | v     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

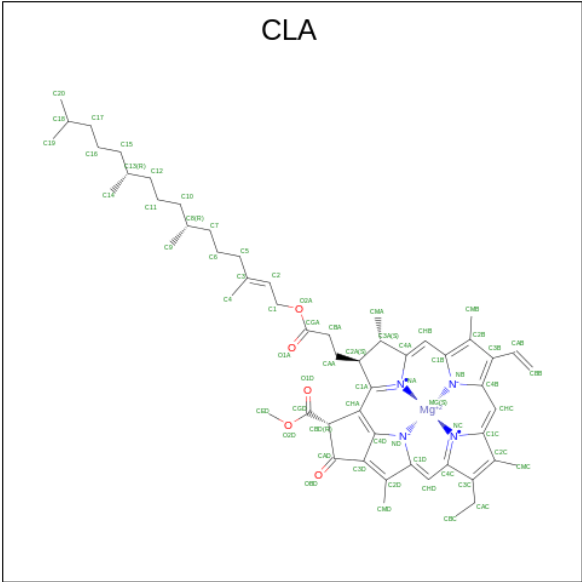
- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3^-$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 23  | A     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 8     | 2 | 6 |         |         |
| 23  | a     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 8     | 2 | 6 |         |         |

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$ ).





| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 24  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 24  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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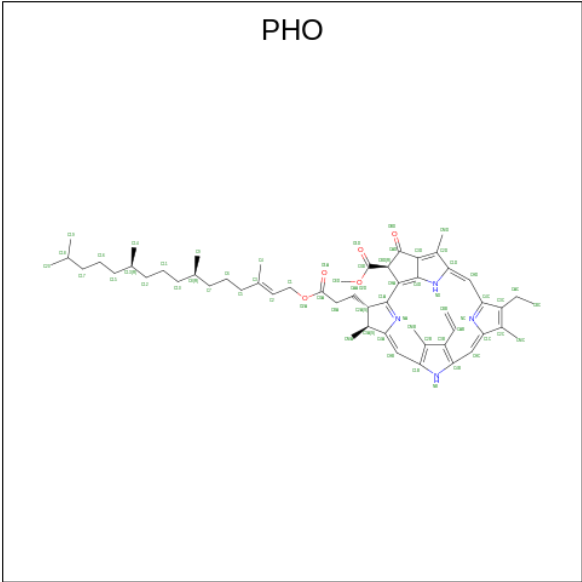
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 24  | a     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | a     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | a     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 24  | c     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

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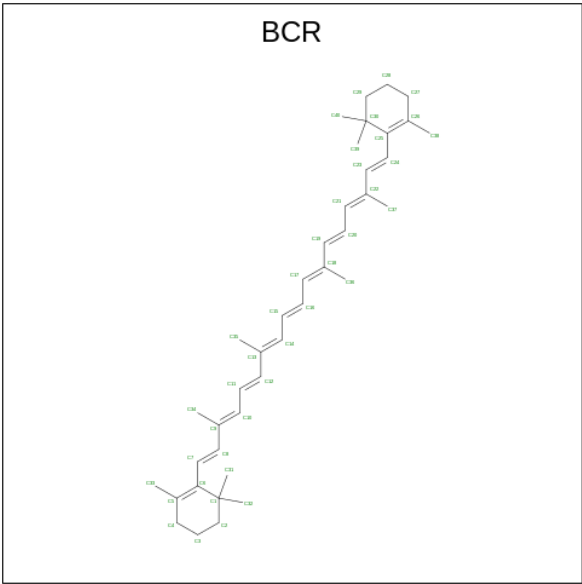
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 24  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



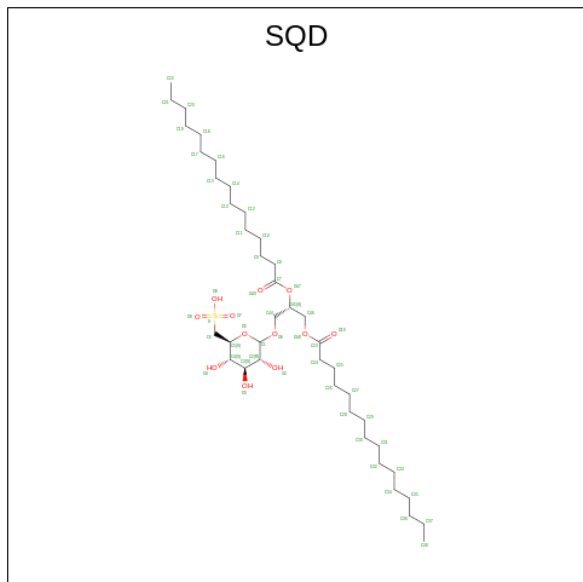
| Mol | Chain | Residues | Atoms |     |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---|----|---------|---------|
| 25  | A     | 1        | Total | C   | N | O  | 0       | 0       |
|     |       |          | 64    | 55  | 4 | 5  |         |         |
| 25  | A     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |
| 25  | a     | 1        | Total | C   | N | O  | 0       | 0       |
|     |       |          | 64    | 55  | 4 | 5  |         |         |
| 25  | a     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



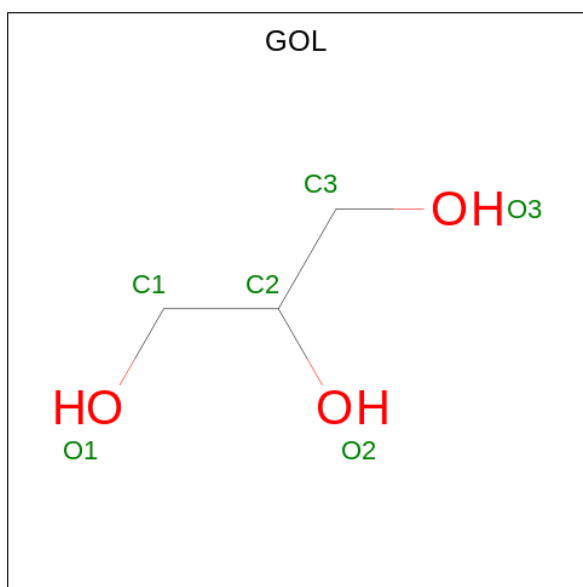
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 26  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | D     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | T     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | a     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | d     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | h     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | k     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | t     | 1        | Total C<br>40 40 | 0       | 0       |
| 26  | y     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 27  | A     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 27  | A     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 27  | B     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 27  | F     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |
| 27  | L     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 27  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 27  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 27  | f     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 28  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |
| 28  | O     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
|     |       |          |       |   |   |         |         |

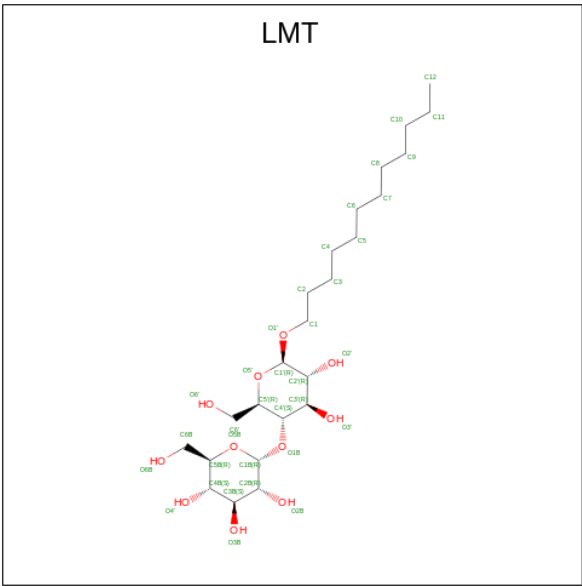
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| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 28  | T     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | T     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | V     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | V     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | V     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | V     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | a     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | a     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | a     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | b     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | b     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | b     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | b     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | b     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | b     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | c     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | c     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | o     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | t     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | v     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | v     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 28  | v     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



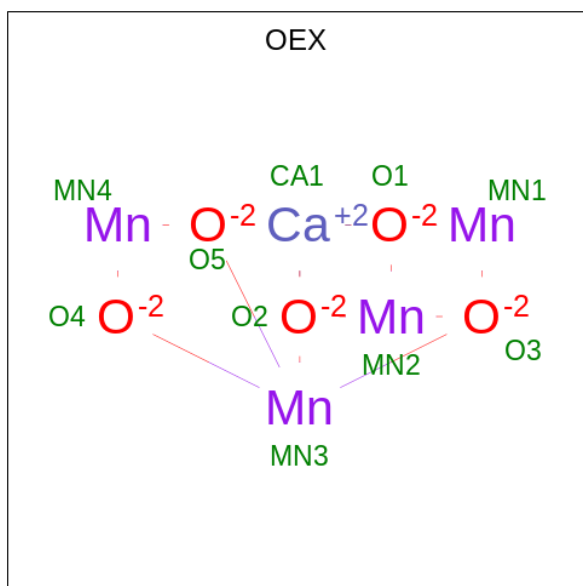
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 29  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 25    | 19 | 6  |         |         |
| 29  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | F     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | T     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 25    | 19 | 6  |         |         |
| 29  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 25    | 19 | 6  |         |         |
| 29  | f     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

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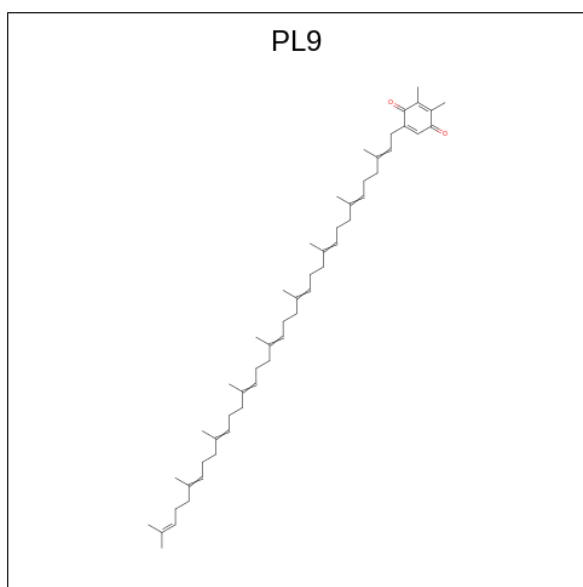
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 29  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 30  | A     | 1        | Total | Ca | Mn | O  | 0       | 1       |
|     |       |          | 20    | 2  | 8  | 10 |         |         |
| 30  | a     | 1        | Total | Ca | Mn | O  | 0       | 1       |
|     |       |          | 20    | 2  | 8  | 10 |         |         |

- Molecule 31 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:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



| Mol | Chain | Residues | Atoms |     |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---|---------|---------|
| 31  | A     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |
| 31  | D     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |
| 31  | a     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |
| 31  | d     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

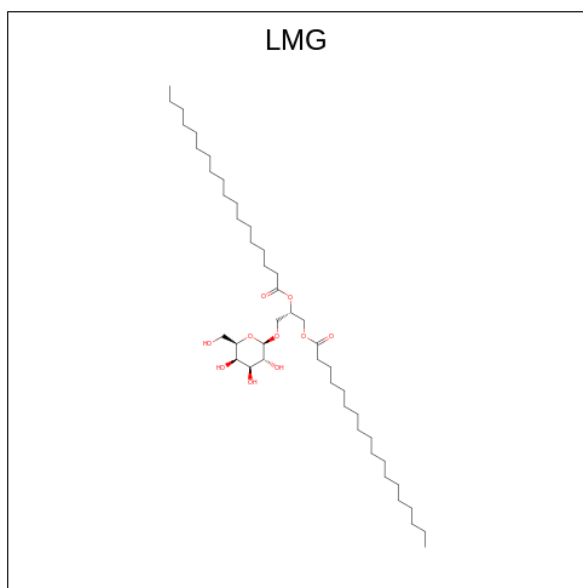
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 32  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 28    | 23 | 5 |         |         |
| 32  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 28 | 5 |         |         |
| 32  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 34    | 29 | 5 |         |         |
| 32  | D     | 2        | Total | C  | O | 0       | 0       |
|     |       |          | 57    | 51 | 6 |         |         |
| 32  | I     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 40    | 35 | 5 |         |         |
| 32  | J     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 10    | 10 |   |         |         |
| 32  | M     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 10    | 10 |   |         |         |
| 32  | X     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 16 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 32  | a     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 30    | 25 | 5 |         |         |
| 32  | b     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 28 | 5 |         |         |
| 32  | c     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 32    | 27 | 5 |         |         |
| 32  | d     | 3        | Total | C  | O | 0       | 0       |
|     |       |          | 71    | 63 | 8 |         |         |
| 32  | i     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 40    | 35 | 5 |         |         |
| 32  | j     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 10    | 10 |   |         |         |
| 32  | m     | 1        | Total | C  |   | 0       | 0       |
|     |       |          | 10    | 10 |   |         |         |

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 33  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 33  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 33  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 33  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |

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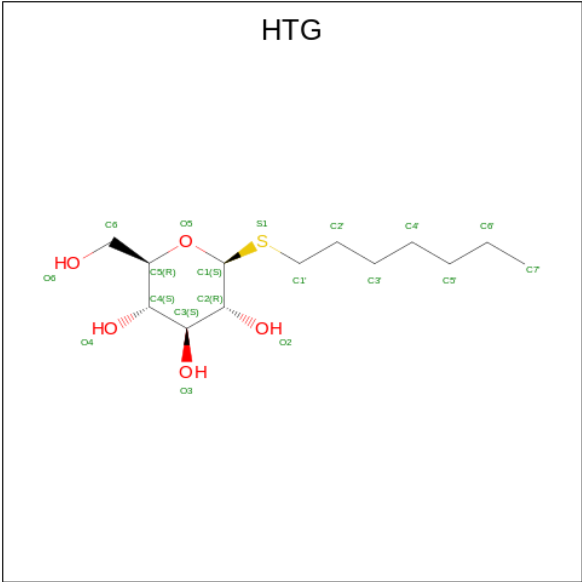
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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 33  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 33  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 37    | 27 | 10 |         |         |
| 33  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 33  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 33  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 33  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 33  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 33  | z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 39    | 29 | 10 |         |         |

- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 34  | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 34  | C     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 34  | F     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 34  | O     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 34  | b     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 34  | c     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 34  | f     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 34  | o     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



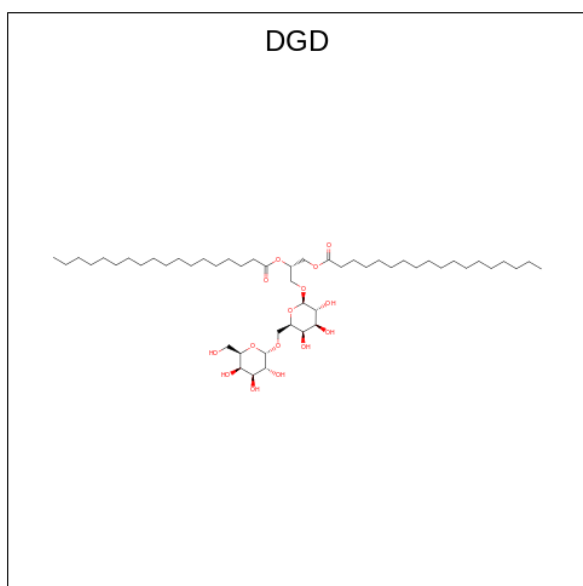
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 35  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | B     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | C     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | C     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | D     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 16    | 10 | 5 | 1 |         |         |
| 35  | V     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 35  | c     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | c     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | d     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 16    | 10 | 5 | 1 |         |         |

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



| Mol | Chain | Residues | Atoms |    |    |  | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|--|---------|---------|
| 36  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 36  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 36  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 36  | D     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 52    | 42 | 10 |  |         |         |
| 36  | H     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 36  | c     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 36  | c     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 36  | c     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |

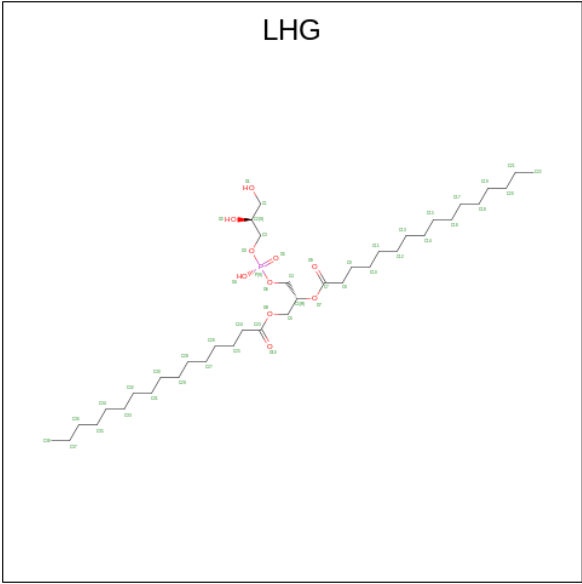
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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 36  | e     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 36  | h     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



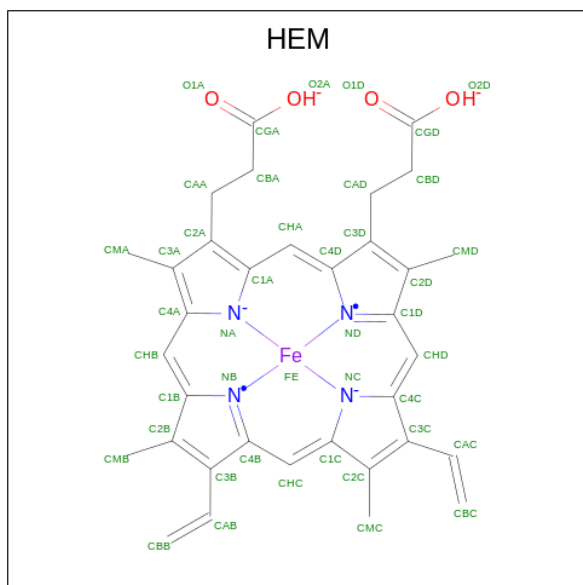
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 37  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 37  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 37  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 37  | E     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |         |
| 37  | L     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 37  | b     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 37  | d     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 37  | d     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 37  | d     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 37  | e     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |         |

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

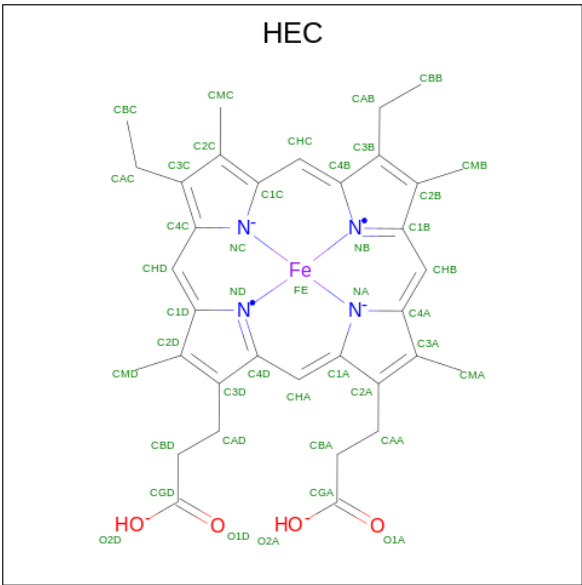


| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 38  | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 38  | e     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula:  $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$ ).



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

- Molecule 41 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 41  | A     | 166      | Total | O   | 0       | 15      |
|     |       |          | 179   | 179 |         |         |
| 41  | B     | 289      | Total | O   | 0       | 4       |
|     |       |          | 293   | 293 |         |         |
| 41  | C     | 229      | Total | O   | 0       | 6       |
|     |       |          | 233   | 233 |         |         |
| 41  | D     | 146      | Total | O   | 0       | 5       |
|     |       |          | 151   | 151 |         |         |
| 41  | E     | 32       | Total | O   | 0       | 1       |
|     |       |          | 33    | 33  |         |         |
| 41  | F     | 8        | Total | O   | 0       | 0       |
|     |       |          | 8     | 8   |         |         |
| 41  | H     | 44       | Total | O   | 0       | 0       |
|     |       |          | 44    | 44  |         |         |
| 41  | I     | 5        | Total | O   | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 41  | J     | 12       | Total | O   | 0       | 0       |
|     |       |          | 12    | 12  |         |         |
| 41  | K     | 8        | Total | O   | 0       | 0       |
|     |       |          | 8     | 8   |         |         |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 41  | L     | 18       | Total O<br>19 19   | 0       | 1       |
| 41  | M     | 19       | Total O<br>19 19   | 0       | 0       |
| 41  | O     | 175      | Total O<br>177 177 | 0       | 2       |
| 41  | T     | 16       | Total O<br>17 17   | 0       | 1       |
| 41  | U     | 82       | Total O<br>82 82   | 0       | 0       |
| 41  | V     | 113      | Total O<br>115 115 | 0       | 2       |
| 41  | Y     | 5        | Total O<br>5 5     | 0       | 0       |
| 41  | X     | 8        | Total O<br>8 8     | 0       | 0       |
| 41  | Z     | 1        | Total O<br>1 1     | 0       | 0       |
| 41  | a     | 155      | Total O<br>167 167 | 0       | 14      |
| 41  | b     | 259      | Total O<br>262 262 | 0       | 3       |
| 41  | c     | 202      | Total O<br>207 207 | 0       | 7       |
| 41  | d     | 134      | Total O<br>137 137 | 0       | 3       |
| 41  | e     | 16       | Total O<br>16 16   | 0       | 0       |
| 41  | f     | 7        | Total O<br>7 7     | 0       | 0       |
| 41  | h     | 42       | Total O<br>42 42   | 0       | 0       |
| 41  | i     | 5        | Total O<br>5 5     | 0       | 0       |
| 41  | j     | 7        | Total O<br>7 7     | 0       | 0       |
| 41  | k     | 7        | Total O<br>7 7     | 0       | 0       |
| 41  | l     | 9        | Total O<br>9 9     | 0       | 0       |
| 41  | m     | 16       | Total O<br>16 16   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 41  | o     | 157      | Total<br>157 | O<br>157 | 0       | 0       |
| 41  | t     | 11       | Total<br>11  | O<br>11  | 0       | 0       |
| 41  | u     | 93       | Total<br>93  | O<br>93  | 0       | 0       |
| 41  | v     | 81       | Total<br>82  | O<br>82  | 0       | 1       |
| 41  | y     | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 41  | x     | 6        | Total<br>6   | O<br>6   | 0       | 0       |

### 3 Residue-property plots

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

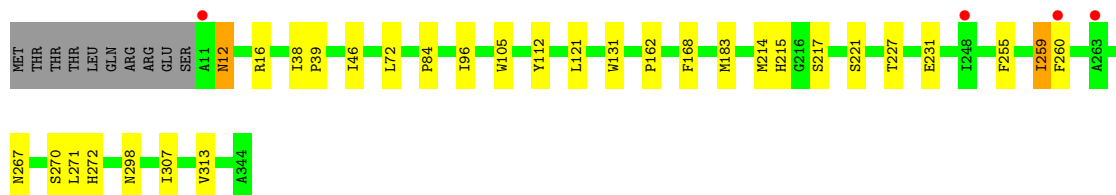
#### • Molecule 1: Photosystem II protein D1

Chain A: 



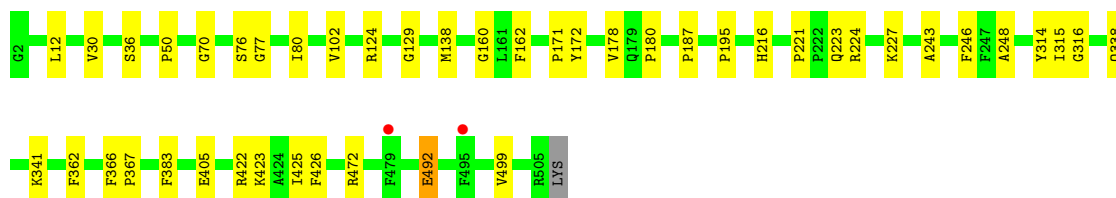
#### • Molecule 1: Photosystem II protein D1

Chain a: 



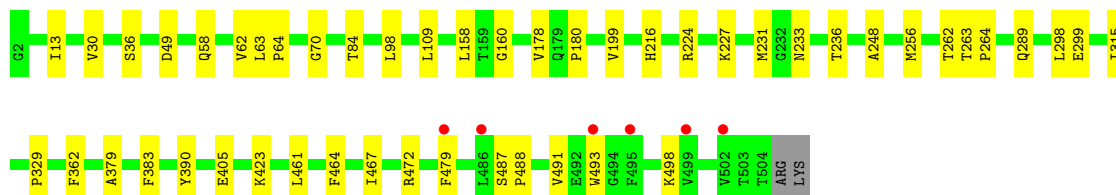
#### • Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

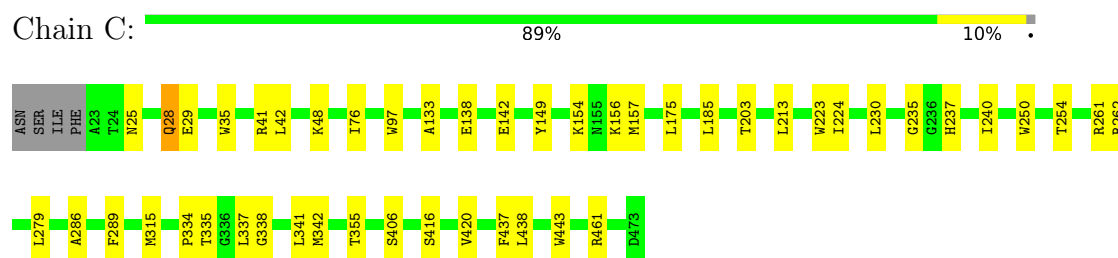


#### • Molecule 2: Photosystem II CP47 reaction center protein

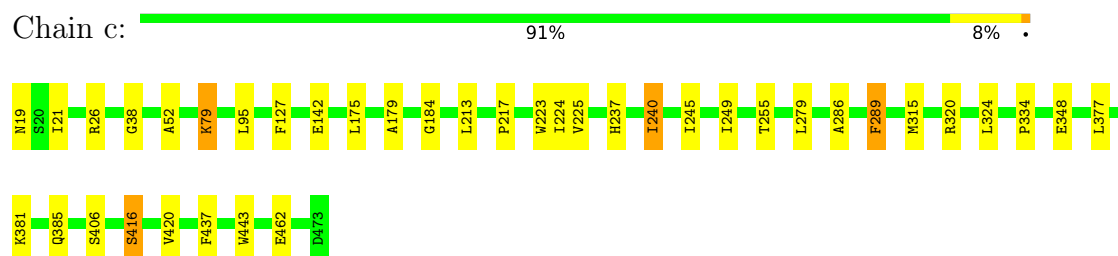
Chain b: 



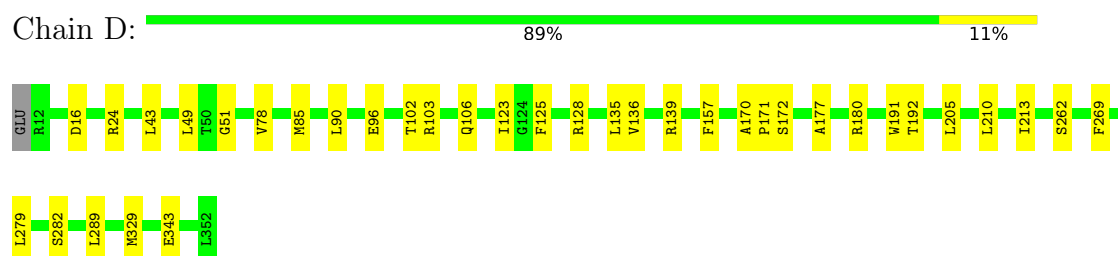
- Molecule 3: Photosystem II CP43 reaction center protein



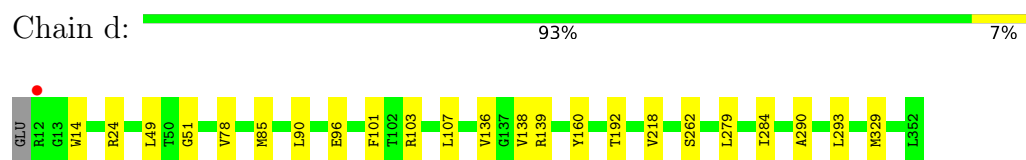
- Molecule 3: Photosystem II CP43 reaction center protein



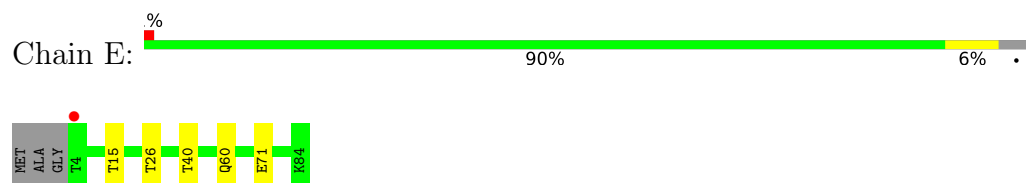
- Molecule 4: Photosystem II D2 protein



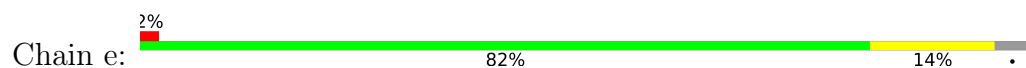
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha

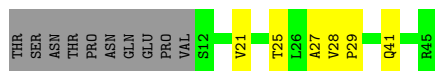


- Molecule 5: Cytochrome b559 subunit alpha

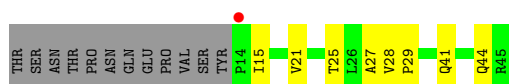




- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



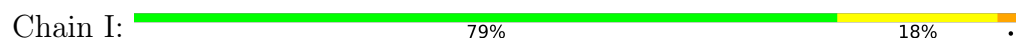
- Molecule 7: Photosystem II reaction center protein H



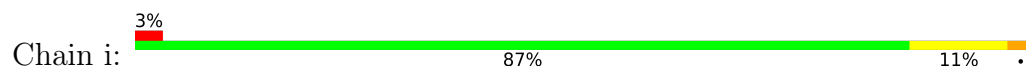
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

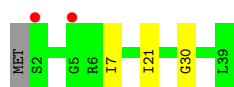
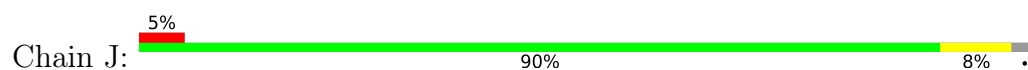


- Molecule 8: Photosystem II reaction center protein I

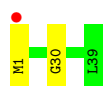
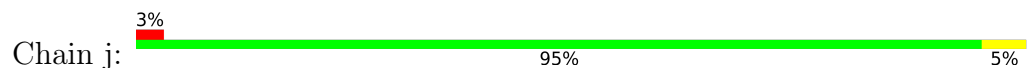


- Molecule 9: Photosystem II reaction center protein J

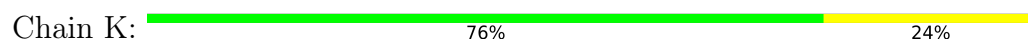




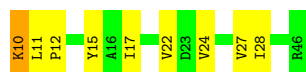
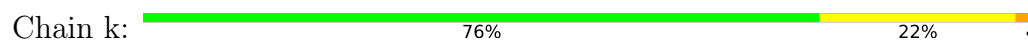
- Molecule 9: Photosystem II reaction center protein J



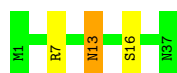
- Molecule 10: Photosystem II reaction center protein K



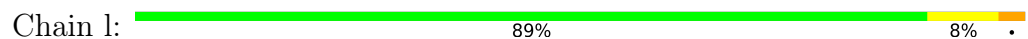
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



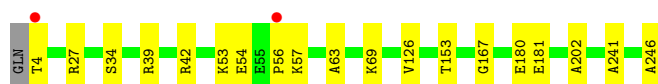
- Molecule 12: Photosystem II reaction center protein M

Chain m:  72% 19% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  92% 8%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  89% 9%



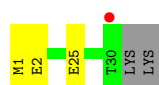
- Molecule 14: Photosystem II reaction center protein T

Chain T:  75% 16% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  84% 9% 6%



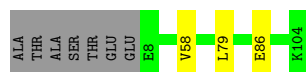
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  87% 7% 7%

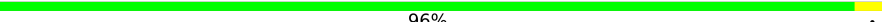


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  90% 7%



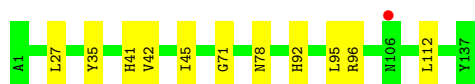
- Molecule 16: Cytochrome c-550

Chain V:  96% .



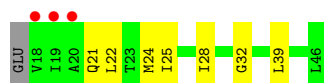
- Molecule 16: Cytochrome c-550

Chain v:  92% 8%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  10% 73% 23% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  10% 70% 23% . .



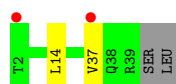
- Molecule 18: Photosystem II reaction center protein X

Chain X:  2% 88% 10% .



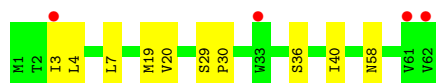
- Molecule 18: Photosystem II reaction center protein X

Chain x:  5% 90% 5% 5%

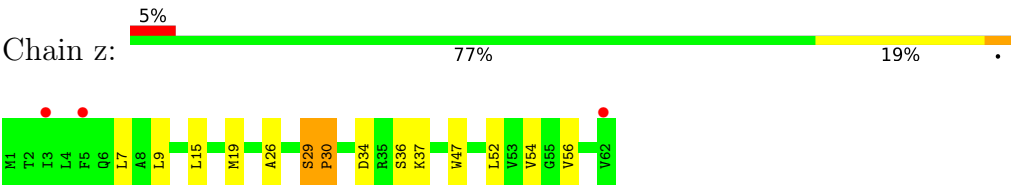


- Molecule 19: Photosystem II reaction center protein Z

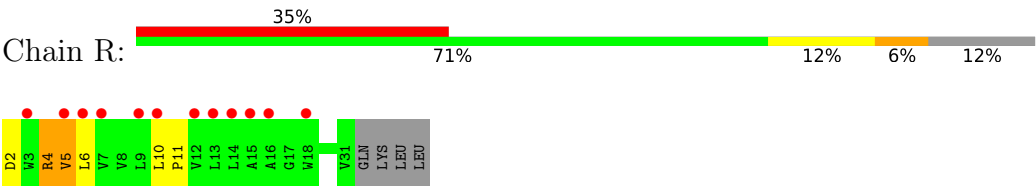
Chain Z:  6% 84% 16%



● Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 121.97Å 228.72Å 286.98Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 19.98 – 2.15<br>19.98 – 2.15                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (19.98-2.15)<br>99.8 (19.98-2.15)                     | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.44 (at 2.00Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.9_1692                                             | Depositor        |
| R, $R_{free}$                                                           | 0.149 , 0.193<br>0.156 , 0.198                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 26831 reflections (5.00%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 35.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.629                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 77.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 55631                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 54.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: UNL, BCR, HEC, GOL, MG, CL, FME, OEX, PHO, DGD, LMG, CLA, LHG, LMT, SQD, BCT, FE2, HTG, HEM, CA, PL9

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     | 0.55         | 0/3121      | 0.82        | 0/4250        |
| 1   | a     | 0.56         | 0/3135      | 0.79        | 0/4269        |
| 2   | B     | 0.55         | 0/4191      | 0.81        | 1/5709 (0.0%) |
| 2   | b     | 0.53         | 0/4198      | 0.81        | 1/5720 (0.0%) |
| 3   | C     | 0.50         | 0/3643      | 0.80        | 4/4958 (0.1%) |
| 3   | c     | 0.48         | 0/3731      | 0.79        | 2/5076 (0.0%) |
| 4   | D     | 0.60         | 0/2952      | 0.80        | 3/4021 (0.1%) |
| 4   | d     | 0.56         | 0/2952      | 0.77        | 1/4021 (0.0%) |
| 5   | E     | 0.46         | 0/693       | 0.78        | 0/944         |
| 5   | e     | 0.44         | 0/695       | 0.80        | 0/948         |
| 6   | F     | 0.57         | 0/284       | 0.79        | 0/387         |
| 6   | f     | 0.54         | 0/265       | 0.77        | 0/360         |
| 7   | H     | 0.44         | 0/535       | 0.87        | 0/728         |
| 7   | h     | 0.43         | 0/524       | 0.76        | 0/713         |
| 8   | I     | 0.43         | 0/311       | 0.74        | 0/419         |
| 8   | i     | 0.47         | 0/311       | 0.81        | 0/419         |
| 9   | J     | 0.46         | 0/278       | 0.76        | 0/376         |
| 9   | j     | 0.44         | 0/286       | 0.76        | 0/386         |
| 10  | K     | 0.47         | 0/303       | 0.79        | 0/416         |
| 10  | k     | 0.53         | 0/303       | 0.86        | 0/416         |
| 11  | L     | 0.58         | 0/319       | 0.69        | 0/433         |
| 11  | l     | 0.50         | 0/319       | 0.74        | 0/433         |
| 12  | M     | 0.60         | 0/270       | 0.84        | 0/368         |
| 12  | m     | 0.57         | 0/262       | 0.84        | 0/357         |
| 13  | O     | 0.46         | 0/1958      | 0.78        | 0/2654        |
| 13  | o     | 0.44         | 0/1937      | 0.79        | 0/2625        |
| 14  | T     | 0.57         | 0/266       | 0.72        | 0/362         |
| 14  | t     | 0.57         | 0/266       | 0.74        | 0/362         |
| 15  | U     | 0.49         | 0/785       | 0.74        | 0/1064        |
| 15  | u     | 0.47         | 0/785       | 0.70        | 0/1064        |
| 16  | V     | 0.51         | 0/1109      | 0.75        | 0/1502        |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 16  | v     | 0.46         | 0/1098  | 0.80        | 2/1488 (0.1%)   |
| 17  | Y     | 0.49         | 0/216   | 0.85        | 0/289           |
| 17  | y     | 0.42         | 0/216   | 0.75        | 0/289           |
| 18  | X     | 0.41         | 0/290   | 0.79        | 0/392           |
| 18  | x     | 0.41         | 0/284   | 0.75        | 0/384           |
| 19  | Z     | 0.38         | 0/490   | 0.76        | 0/669           |
| 19  | z     | 0.34         | 0/490   | 0.80        | 0/669           |
| 20  | R     | 0.35         | 0/245   | 0.67        | 0/338           |
| All | All   | 0.51         | 0/44316 | 0.79        | 14/60278 (0.0%) |

There are no bond length outliers.

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | C     | 76  | ILE  | CA-C-N | 6.94  | 127.52      | 119.47   |
| 3   | C     | 76  | ILE  | C-N-CA | 6.94  | 127.52      | 119.47   |
| 4   | D     | 170 | ALA  | CA-C-N | -6.39 | 113.37      | 119.76   |
| 4   | D     | 170 | ALA  | C-N-CA | -6.39 | 113.37      | 119.76   |
| 3   | C     | 133 | ALA  | CA-C-N | -5.38 | 116.12      | 122.36   |
| 3   | C     | 133 | ALA  | C-N-CA | -5.38 | 116.12      | 122.36   |
| 3   | c     | 385 | GLN  | CA-C-N | 5.23  | 124.68      | 119.24   |
| 3   | c     | 385 | GLN  | C-N-CA | 5.23  | 124.68      | 119.24   |
| 4   | D     | 262 | SER  | N-CA-C | -5.19 | 107.97      | 114.56   |
| 2   | B     | 77  | GLY  | N-CA-C | 5.07  | 121.52      | 114.92   |
| 16  | v     | 92  | HIS  | CA-C-N | 5.03  | 125.31      | 119.93   |
| 16  | v     | 92  | HIS  | C-N-CA | 5.03  | 125.31      | 119.93   |
| 4   | d     | 262 | SER  | N-CA-C | -5.03 | 108.18      | 114.56   |
| 2   | b     | 13  | ILE  | N-CA-C | 5.01  | 115.73      | 110.62   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3019  | 0        | 2872     | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | a     | 3027  | 0        | 2888     | 28      | 0            |
| 2   | B     | 4021  | 0        | 3898     | 38      | 0            |
| 2   | b     | 4022  | 0        | 3908     | 36      | 0            |
| 3   | C     | 3518  | 0        | 3439     | 30      | 0            |
| 3   | c     | 3598  | 0        | 3529     | 26      | 0            |
| 4   | D     | 2849  | 0        | 2741     | 27      | 0            |
| 4   | d     | 2849  | 0        | 2741     | 18      | 0            |
| 5   | E     | 668   | 0        | 658      | 4       | 0            |
| 5   | e     | 670   | 0        | 664      | 10      | 0            |
| 6   | F     | 275   | 0        | 282      | 4       | 0            |
| 6   | f     | 257   | 0        | 269      | 4       | 0            |
| 7   | H     | 519   | 0        | 545      | 9       | 0            |
| 7   | h     | 511   | 0        | 532      | 8       | 0            |
| 8   | I     | 314   | 0        | 328      | 5       | 0            |
| 8   | i     | 314   | 0        | 328      | 3       | 0            |
| 9   | J     | 272   | 0        | 279      | 3       | 0            |
| 9   | j     | 280   | 0        | 291      | 1       | 0            |
| 10  | K     | 293   | 0        | 305      | 7       | 0            |
| 10  | k     | 293   | 0        | 305      | 6       | 0            |
| 11  | L     | 309   | 0        | 327      | 4       | 0            |
| 11  | l     | 309   | 0        | 327      | 5       | 0            |
| 12  | M     | 274   | 0        | 299      | 8       | 0            |
| 12  | m     | 269   | 0        | 288      | 8       | 0            |
| 13  | O     | 1903  | 0        | 1886     | 10      | 0            |
| 13  | o     | 1891  | 0        | 1870     | 16      | 0            |
| 14  | T     | 264   | 0        | 267      | 4       | 0            |
| 14  | t     | 264   | 0        | 267      | 2       | 0            |
| 15  | U     | 774   | 0        | 773      | 3       | 1            |
| 15  | u     | 774   | 0        | 773      | 1       | 0            |
| 16  | V     | 1085  | 0        | 1095     | 4       | 0            |
| 16  | v     | 1077  | 0        | 1082     | 8       | 0            |
| 17  | Y     | 215   | 0        | 246      | 5       | 0            |
| 17  | y     | 215   | 0        | 246      | 5       | 0            |
| 18  | X     | 287   | 0        | 317      | 3       | 0            |
| 18  | x     | 281   | 0        | 312      | 2       | 0            |
| 19  | Z     | 479   | 0        | 516      | 5       | 0            |
| 19  | z     | 479   | 0        | 516      | 8       | 0            |
| 20  | R     | 239   | 0        | 262      | 4       | 0            |
| 21  | A     | 2     | 0        | 0        | 0       | 0            |
| 21  | a     | 2     | 0        | 0        | 0       | 0            |
| 22  | A     | 4     | 0        | 0        | 0       | 0            |
| 22  | U     | 1     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | a     | 4     | 0        | 0        | 0       | 0            |
| 22  | v     | 1     | 0        | 0        | 1       | 0            |
| 23  | A     | 8     | 0        | 0        | 0       | 0            |
| 23  | a     | 8     | 0        | 0        | 0       | 0            |
| 24  | A     | 260   | 0        | 288      | 11      | 0            |
| 24  | B     | 1040  | 0        | 1152     | 36      | 0            |
| 24  | C     | 845   | 0        | 936      | 30      | 0            |
| 24  | D     | 130   | 0        | 144      | 4       | 0            |
| 24  | a     | 195   | 0        | 216      | 9       | 0            |
| 24  | b     | 1040  | 0        | 1152     | 28      | 0            |
| 24  | c     | 845   | 0        | 936      | 35      | 0            |
| 24  | d     | 195   | 0        | 216      | 9       | 0            |
| 25  | A     | 192   | 0        | 222      | 6       | 0            |
| 25  | a     | 192   | 0        | 222      | 3       | 0            |
| 26  | A     | 40    | 0        | 56       | 1       | 0            |
| 26  | B     | 120   | 0        | 168      | 11      | 0            |
| 26  | C     | 80    | 0        | 112      | 11      | 0            |
| 26  | D     | 40    | 0        | 56       | 1       | 0            |
| 26  | H     | 40    | 0        | 56       | 3       | 0            |
| 26  | K     | 40    | 0        | 56       | 0       | 0            |
| 26  | T     | 40    | 0        | 56       | 5       | 0            |
| 26  | Y     | 40    | 0        | 56       | 4       | 0            |
| 26  | a     | 40    | 0        | 56       | 1       | 0            |
| 26  | b     | 120   | 0        | 168      | 10      | 0            |
| 26  | c     | 80    | 0        | 112      | 5       | 0            |
| 26  | d     | 40    | 0        | 56       | 3       | 0            |
| 26  | h     | 40    | 0        | 56       | 4       | 0            |
| 26  | k     | 40    | 0        | 56       | 1       | 0            |
| 26  | t     | 40    | 0        | 56       | 5       | 0            |
| 26  | y     | 40    | 0        | 56       | 2       | 0            |
| 27  | A     | 108   | 0        | 156      | 7       | 0            |
| 27  | B     | 54    | 0        | 78       | 3       | 0            |
| 27  | F     | 43    | 0        | 53       | 2       | 0            |
| 27  | L     | 54    | 0        | 78       | 3       | 0            |
| 27  | a     | 108   | 0        | 156      | 3       | 0            |
| 27  | f     | 43    | 0        | 53       | 1       | 1            |
| 28  | A     | 24    | 0        | 32       | 1       | 0            |
| 28  | B     | 42    | 0        | 56       | 1       | 0            |
| 28  | C     | 12    | 0        | 16       | 0       | 0            |
| 28  | O     | 6     | 0        | 8        | 0       | 0            |
| 28  | T     | 12    | 0        | 16       | 3       | 0            |
| 28  | V     | 24    | 0        | 32       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | a     | 18    | 0        | 23       | 2       | 0            |
| 28  | b     | 30    | 0        | 40       | 0       | 0            |
| 28  | c     | 12    | 0        | 16       | 2       | 0            |
| 28  | o     | 6     | 0        | 8        | 0       | 0            |
| 28  | t     | 6     | 0        | 8        | 1       | 0            |
| 28  | v     | 18    | 0        | 24       | 1       | 0            |
| 29  | A     | 35    | 0        | 46       | 2       | 0            |
| 29  | B     | 25    | 0        | 35       | 0       | 0            |
| 29  | C     | 35    | 0        | 46       | 1       | 0            |
| 29  | D     | 35    | 0        | 46       | 1       | 0            |
| 29  | F     | 35    | 0        | 46       | 0       | 0            |
| 29  | M     | 70    | 0        | 92       | 4       | 0            |
| 29  | T     | 25    | 0        | 35       | 0       | 0            |
| 29  | a     | 70    | 0        | 92       | 2       | 0            |
| 29  | b     | 25    | 0        | 35       | 3       | 0            |
| 29  | f     | 35    | 0        | 46       | 1       | 0            |
| 29  | m     | 70    | 0        | 92       | 3       | 0            |
| 30  | A     | 20    | 0        | 0        | 0       | 0            |
| 30  | a     | 20    | 0        | 0        | 0       | 0            |
| 31  | A     | 110   | 0        | 160      | 9       | 0            |
| 31  | D     | 110   | 0        | 160      | 1       | 0            |
| 31  | a     | 110   | 0        | 160      | 14      | 0            |
| 31  | d     | 110   | 0        | 160      | 0       | 0            |
| 32  | A     | 28    | 0        | 0        | 0       | 0            |
| 32  | B     | 33    | 0        | 0        | 0       | 0            |
| 32  | C     | 34    | 0        | 0        | 0       | 0            |
| 32  | D     | 57    | 0        | 0        | 0       | 0            |
| 32  | I     | 40    | 0        | 0        | 0       | 0            |
| 32  | J     | 10    | 0        | 0        | 0       | 0            |
| 32  | M     | 10    | 0        | 0        | 0       | 0            |
| 32  | X     | 18    | 0        | 0        | 0       | 0            |
| 32  | a     | 30    | 0        | 0        | 0       | 0            |
| 32  | b     | 33    | 0        | 0        | 0       | 0            |
| 32  | c     | 32    | 0        | 0        | 0       | 0            |
| 32  | d     | 71    | 0        | 0        | 0       | 0            |
| 32  | i     | 40    | 0        | 0        | 0       | 0            |
| 32  | j     | 10    | 0        | 0        | 0       | 0            |
| 32  | m     | 10    | 0        | 0        | 0       | 0            |
| 33  | A     | 51    | 0        | 72       | 4       | 0            |
| 33  | B     | 51    | 0        | 72       | 1       | 0            |
| 33  | C     | 102   | 0        | 144      | 7       | 0            |
| 33  | D     | 51    | 0        | 72       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33  | Z     | 37    | 0        | 44       | 1       | 0            |
| 33  | b     | 51    | 0        | 72       | 3       | 0            |
| 33  | c     | 153   | 0        | 216      | 7       | 0            |
| 33  | d     | 51    | 0        | 72       | 2       | 0            |
| 33  | z     | 39    | 0        | 48       | 5       | 0            |
| 34  | B     | 1     | 0        | 0        | 0       | 0            |
| 34  | C     | 1     | 0        | 0        | 0       | 0            |
| 34  | F     | 1     | 0        | 0        | 0       | 0            |
| 34  | O     | 1     | 0        | 0        | 0       | 0            |
| 34  | b     | 1     | 0        | 0        | 0       | 0            |
| 34  | c     | 2     | 0        | 0        | 0       | 0            |
| 34  | f     | 1     | 0        | 0        | 0       | 0            |
| 34  | o     | 1     | 0        | 0        | 0       | 0            |
| 35  | B     | 95    | 0        | 130      | 1       | 0            |
| 35  | C     | 38    | 0        | 52       | 0       | 0            |
| 35  | D     | 16    | 0        | 17       | 2       | 0            |
| 35  | V     | 19    | 0        | 26       | 1       | 0            |
| 35  | b     | 95    | 0        | 130      | 1       | 0            |
| 35  | c     | 38    | 0        | 52       | 1       | 0            |
| 35  | d     | 16    | 0        | 17       | 3       | 0            |
| 36  | C     | 186   | 0        | 246      | 4       | 0            |
| 36  | D     | 52    | 0        | 71       | 2       | 0            |
| 36  | H     | 62    | 0        | 82       | 0       | 0            |
| 36  | c     | 186   | 0        | 246      | 2       | 0            |
| 36  | e     | 62    | 0        | 82       | 7       | 0            |
| 36  | h     | 62    | 0        | 82       | 0       | 0            |
| 37  | D     | 147   | 0        | 222      | 11      | 0            |
| 37  | E     | 42    | 0        | 57       | 2       | 0            |
| 37  | L     | 49    | 0        | 74       | 0       | 0            |
| 37  | b     | 49    | 0        | 74       | 3       | 0            |
| 37  | d     | 147   | 0        | 222      | 9       | 0            |
| 37  | e     | 42    | 0        | 57       | 4       | 0            |
| 38  | F     | 43    | 0        | 30       | 2       | 0            |
| 38  | e     | 43    | 0        | 30       | 5       | 0            |
| 39  | J     | 1     | 0        | 0        | 0       | 0            |
| 39  | j     | 1     | 0        | 0        | 0       | 0            |
| 40  | V     | 43    | 0        | 30       | 0       | 0            |
| 40  | v     | 43    | 0        | 30       | 0       | 0            |
| 41  | A     | 179   | 0        | 0        | 1       | 0            |
| 41  | B     | 293   | 0        | 0        | 2       | 0            |
| 41  | C     | 233   | 0        | 0        | 3       | 0            |
| 41  | D     | 151   | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41  | E     | 33    | 0        | 0        | 0       | 0            |
| 41  | F     | 8     | 0        | 0        | 0       | 0            |
| 41  | H     | 44    | 0        | 0        | 0       | 0            |
| 41  | I     | 5     | 0        | 0        | 1       | 0            |
| 41  | J     | 12    | 0        | 0        | 0       | 0            |
| 41  | K     | 8     | 0        | 0        | 1       | 0            |
| 41  | L     | 19    | 0        | 0        | 0       | 0            |
| 41  | M     | 19    | 0        | 0        | 0       | 0            |
| 41  | O     | 177   | 0        | 0        | 2       | 0            |
| 41  | T     | 17    | 0        | 0        | 1       | 0            |
| 41  | U     | 82    | 0        | 0        | 2       | 0            |
| 41  | V     | 115   | 0        | 0        | 1       | 0            |
| 41  | X     | 8     | 0        | 0        | 0       | 0            |
| 41  | Y     | 5     | 0        | 0        | 0       | 0            |
| 41  | Z     | 1     | 0        | 0        | 0       | 0            |
| 41  | a     | 167   | 0        | 0        | 2       | 0            |
| 41  | b     | 262   | 0        | 0        | 4       | 0            |
| 41  | c     | 207   | 0        | 0        | 1       | 0            |
| 41  | d     | 137   | 0        | 0        | 2       | 0            |
| 41  | e     | 16    | 0        | 0        | 0       | 0            |
| 41  | f     | 7     | 0        | 0        | 0       | 0            |
| 41  | h     | 42    | 0        | 0        | 0       | 0            |
| 41  | i     | 5     | 0        | 0        | 0       | 0            |
| 41  | j     | 7     | 0        | 0        | 0       | 0            |
| 41  | k     | 7     | 0        | 0        | 0       | 0            |
| 41  | l     | 9     | 0        | 0        | 1       | 0            |
| 41  | m     | 16    | 0        | 0        | 0       | 0            |
| 41  | o     | 157   | 0        | 0        | 2       | 0            |
| 41  | t     | 11    | 0        | 0        | 0       | 0            |
| 41  | u     | 93    | 0        | 0        | 0       | 0            |
| 41  | v     | 82    | 0        | 0        | 1       | 0            |
| 41  | x     | 6     | 0        | 0        | 0       | 0            |
| 41  | y     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 55631 | 0        | 54162    | 559     | 1            |

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 5.

All (559) 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) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:A:214[B]:MET:HG2   | 31:A:419[B]:PL9:H102 | 1.48                     | 0.93              |
| 1:A:214[A]:MET:HG2   | 31:A:419[A]:PL9:H102 | 1.50                     | 0.93              |
| 24:B:616:CLA:H71     | 24:B:617:CLA:H192    | 1.52                     | 0.92              |
| 24:c:518:CLA:HHC     | 24:c:518:CLA:HBB1    | 1.56                     | 0.87              |
| 24:c:506:CLA:H202    | 24:c:512:CLA:HBB1    | 1.61                     | 0.82              |
| 24:C:503:CLA:HBB1    | 24:C:512:CLA:H41     | 1.62                     | 0.81              |
| 41:B:954:HOH:O       | 22:U:201:CL:CL       | 2.34                     | 0.81              |
| 4:d:192:THR:HG23     | 24:d:402:CLA:HBC2    | 1.67                     | 0.77              |
| 2:b:491:VAL:HG12     | 4:d:136:VAL:HG13     | 1.67                     | 0.76              |
| 24:D:403:CLA:H171    | 18:X:15:LEU:HD13     | 1.68                     | 0.75              |
| 33:b:629:LMG:H421    | 37:b:634:LHG:H371    | 1.69                     | 0.75              |
| 1:a:298:ASN:ND2      | 41:a:501[A]:HOH:O    | 2.19                     | 0.74              |
| 16:v:71:GLY:HA2      | 28:v:201:GOL:H31     | 1.68                     | 0.74              |
| 24:C:505:CLA:CMD     | 24:C:507:CLA:HAB     | 2.18                     | 0.74              |
| 24:b:624:CLA:HHC     | 24:b:624:CLA:HBB1    | 1.68                     | 0.73              |
| 1:a:214[A]:MET:HG2   | 31:a:415[A]:PL9:H102 | 1.68                     | 0.73              |
| 2:B:341:LYS:HA       | 2:B:405[A]:GLU:HG2   | 1.73                     | 0.71              |
| 24:b:624:CLA:H2      | 24:b:625:CLA:HBB2    | 1.72                     | 0.71              |
| 24:c:508:CLA:HHC     | 24:c:508:CLA:HBB1    | 1.72                     | 0.71              |
| 24:a:410:CLA:H203    | 33:d:413:LMG:H412    | 1.73                     | 0.70              |
| 31:A:419[B]:PL9:H261 | 37:E:101:LHG:H223    | 1.74                     | 0.70              |
| 24:B:615:CLA:H18     | 33:B:622:LMG:H421    | 1.73                     | 0.70              |
| 12:m:6:LEU:HD11      | 29:m:103:LMT:H11     | 1.73                     | 0.70              |
| 1:a:215[B]:HIS:ND1   | 31:a:415[B]:PL9:O1   | 2.24                     | 0.69              |
| 27:a:414:SQD:H271    | 37:d:408:LHG:H141    | 1.74                     | 0.69              |
| 41:b:899:HOH:O       | 22:v:204:CL:CL       | 2.48                     | 0.69              |
| 1:a:214[B]:MET:HG2   | 31:a:415[B]:PL9:H102 | 1.73                     | 0.68              |
| 33:c:523:LMG:H181    | 10:k:27:VAL:HG11     | 1.75                     | 0.68              |
| 15:U:51:LYS:NZ       | 41:U:301:HOH:O       | 2.27                     | 0.66              |
| 31:A:419[A]:PL9:H261 | 37:E:101:LHG:H223    | 1.77                     | 0.66              |
| 1:A:298:ASN:ND2      | 41:A:501[A]:HOH:O    | 2.29                     | 0.65              |
| 24:C:506:CLA:HMC2    | 24:C:507:CLA:H102    | 1.78                     | 0.65              |
| 37:D:409:LHG:H132    | 37:D:409:LHG:H372    | 1.79                     | 0.65              |
| 3:C:286:ALA:HB2      | 24:C:502:CLA:HMD1    | 1.78                     | 0.64              |
| 2:B:248:ALA:HA       | 24:B:604:CLA:H42     | 1.78                     | 0.64              |
| 1:a:215[A]:HIS:ND1   | 31:a:415[A]:PL9:O1   | 2.28                     | 0.64              |
| 2:B:124:ARG:O        | 7:H:12[A]:ARG:NH1    | 2.29                     | 0.64              |
| 24:C:513:CLA:H171    | 26:C:514:BCR:H373    | 1.80                     | 0.63              |
| 15:U:16:LYS:NZ       | 41:U:302:HOH:O       | 2.29                     | 0.63              |
| 24:B:617:CLA:HED2    | 24:B:617:CLA:H43     | 1.81                     | 0.63              |
| 31:a:415[B]:PL9:H28  | 37:e:102:LHG:H222    | 1.80                     | 0.63              |
| 10:k:11:LEU:HD11     | 10:k:22:VAL:HG21     | 1.81                     | 0.62              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:T:25[A]:GLU:HG3  | 28:T:101:GOL:H2     | 1.82                     | 0.62              |
| 26:t:101:BCR:H321   | 26:t:101:BCR:HC8    | 1.79                     | 0.62              |
| 24:C:513:CLA:HBB1   | 26:C:514:BCR:H24C   | 1.82                     | 0.61              |
| 24:C:505:CLA:HMD3   | 24:C:507:CLA:HAB    | 1.82                     | 0.61              |
| 26:B:619:BCR:H363   | 26:t:101:BCR:H19C   | 1.82                     | 0.60              |
| 4:D:103:ARG:NH1     | 4:D:106:GLN:OE1     | 2.34                     | 0.60              |
| 27:A:412:SQD:H251   | 37:D:409:LHG:H131   | 1.84                     | 0.60              |
| 37:D:409:LHG:H112   | 37:D:409:LHG:H382   | 1.84                     | 0.60              |
| 5:E:40:THR:HB       | 20:R:4:ARG:HG2      | 1.84                     | 0.60              |
| 24:C:513:CLA:H202   | 33:C:520:LMG:H402   | 1.82                     | 0.60              |
| 26:T:103:BCR:H321   | 26:T:103:BCR:HC8    | 1.82                     | 0.60              |
| 12:M:33:GLN:HB2     | 12:m:33:GLN:HB2     | 1.84                     | 0.59              |
| 8:I:37:LEU:O        | 41:I:201:HOH:O      | 2.16                     | 0.59              |
| 1:A:72:LEU:HD13     | 29:A:417:LMT:H11    | 1.85                     | 0.59              |
| 4:D:192:THR:HG23    | 24:D:402:CLA:HBC2   | 1.83                     | 0.59              |
| 24:C:510:CLA:H43    | 37:D:409:LHG:H383   | 1.85                     | 0.59              |
| 3:c:279:LEU:HD22    | 24:c:514:CLA:HED2   | 1.85                     | 0.59              |
| 3:C:48:LYS:HG3      | 3:C:138:GLU:HG3     | 1.84                     | 0.58              |
| 1:a:271:LEU:HD11    | 31:a:415[B]:PL9:HC8 | 1.85                     | 0.58              |
| 24:c:517:CLA:O2D    | 24:c:518:CLA:HBB2   | 2.03                     | 0.58              |
| 6:F:21:VAL:O        | 6:F:25:THR:HG23     | 2.04                     | 0.58              |
| 11:L:13:ASN:ND2     | 11:L:16:SER:H       | 2.01                     | 0.57              |
| 29:C:521:LMT:O3B    | 41:C:601:HOH:O      | 2.17                     | 0.57              |
| 4:D:157:PHE:CE2     | 4:D:171:PRO:HG2     | 2.39                     | 0.57              |
| 3:c:213[A]:LEU:HG   | 24:c:511:CLA:H202   | 1.86                     | 0.57              |
| 24:c:509:CLA:H201   | 37:d:408:LHG:H352   | 1.86                     | 0.57              |
| 2:B:171:PRO:HD3     | 7:H:66:GLY:HA2      | 1.87                     | 0.57              |
| 2:b:248:ALA:HA      | 24:b:612:CLA:H42    | 1.86                     | 0.57              |
| 28:a:420:GOL:H11    | 16:v:27:LEU:HD21    | 1.85                     | 0.57              |
| 4:D:102:THR:OG1     | 36:D:406:DGD:HG31   | 2.04                     | 0.57              |
| 2:B:472:ARG:NH2     | 41:B:703:HOH:O      | 2.30                     | 0.56              |
| 24:C:509:CLA:HBB1   | 24:C:509:CLA:HMB1   | 1.87                     | 0.56              |
| 24:C:513:CLA:HBB1   | 26:C:514:BCR:H371   | 1.86                     | 0.56              |
| 1:a:271:LEU:HD11    | 31:a:415[A]:PL9:HC8 | 1.86                     | 0.56              |
| 2:b:224:ARG:HD3     | 7:h:25:TRP:CD2      | 2.40                     | 0.56              |
| 3:c:377:LEU:HG      | 3:c:381:LYS:HE3     | 1.87                     | 0.56              |
| 26:y:101:BCR:H321   | 26:y:101:BCR:HC8    | 1.87                     | 0.56              |
| 1:a:307[B]:ILE:HG22 | 1:a:313:VAL:HA      | 1.86                     | 0.56              |
| 17:Y:28:ILE:HG23    | 26:Y:101:BCR:H10C   | 1.88                     | 0.55              |
| 2:B:50:PRO:HB2      | 28:B:630:GOL:H12    | 1.88                     | 0.55              |
| 24:b:610:CLA:H193   | 26:h:101:BCR:H353   | 1.88                     | 0.55              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 16:v:35:TYR:OH       | 41:v:301:HOH:O       | 2.15                     | 0.55              |
| 31:A:419[B]:PL9:H512 | 27:F:103:SQD:H301    | 1.88                     | 0.55              |
| 24:c:518:CLA:H171    | 26:c:528:BCR:H373    | 1.89                     | 0.55              |
| 25:A:409[A]:PHO:HBC3 | 4:D:279:LEU:HD22     | 1.89                     | 0.55              |
| 2:B:70:GLY:HA2       | 2:B:178:VAL:HG21     | 1.89                     | 0.55              |
| 3:c:320:ARG:HB2      | 28:c:503:GOL:H32     | 1.89                     | 0.55              |
| 24:b:614:CLA:HHC     | 24:b:614:CLA:HBB1    | 1.87                     | 0.55              |
| 24:b:622:CLA:H18     | 37:d:406:LHG:H202    | 1.88                     | 0.55              |
| 5:e:9:PRO:HA         | 37:e:102:LHG:HC31    | 1.89                     | 0.55              |
| 36:e:101:DGD:HAW1    | 27:f:101:SQD:H382    | 1.89                     | 0.55              |
| 24:B:602:CLA:H91     | 26:H:101:BCR:H21C    | 1.88                     | 0.54              |
| 2:B:216:HIS:HE1      | 24:B:610:CLA:C1A     | 2.20                     | 0.54              |
| 1:A:257:ARG:NH2      | 2:B:492:GLU:O        | 2.40                     | 0.54              |
| 31:a:415[A]:PL9:H28  | 37:e:102:LHG:H222    | 1.88                     | 0.54              |
| 16:V:26:TYR:O        | 41:V:301:HOH:O       | 2.19                     | 0.54              |
| 24:c:513:CLA:H201    | 33:c:523:LMG:H232    | 1.88                     | 0.54              |
| 31:a:415[A]:PL9:HC2  | 31:a:415[A]:PL9:H103 | 1.90                     | 0.54              |
| 27:A:412:SQD:H192    | 37:D:409:LHG:H201    | 1.89                     | 0.54              |
| 2:B:12:LEU:HB2       | 24:B:613:CLA:HMC2    | 1.90                     | 0.54              |
| 3:C:443:TRP:CZ2      | 24:C:508:CLA:HMD1    | 2.43                     | 0.54              |
| 24:b:624:CLA:H2      | 24:b:625:CLA:CBB     | 2.36                     | 0.53              |
| 24:c:513:CLA:H191    | 33:c:523:LMG:H232    | 1.89                     | 0.53              |
| 24:c:506:CLA:C4D     | 24:c:508:CLA:H2      | 2.38                     | 0.53              |
| 24:C:502:CLA:H61     | 24:C:512:CLA:H42     | 1.90                     | 0.53              |
| 2:B:338:GLN:HA       | 13:o:57:LYS:HE3      | 1.89                     | 0.53              |
| 36:D:406:DGD:O1B     | 36:D:406:DGD:O2D     | 2.26                     | 0.53              |
| 11:L:13:ASN:C        | 11:L:13:ASN:HD22     | 2.17                     | 0.53              |
| 33:c:501:LMG:H242    | 24:c:510:CLA:H92     | 1.91                     | 0.53              |
| 24:c:513:CLA:HBC3    | 24:c:515:CLA:H71     | 1.90                     | 0.53              |
| 29:f:102:LMT:O3'     | 29:f:102:LMT:O2B     | 2.24                     | 0.53              |
| 31:a:415[B]:PL9:HC2  | 31:a:415[B]:PL9:H103 | 1.91                     | 0.53              |
| 28:A:414:GOL:H11     | 12:M:1:FME:HG2       | 1.90                     | 0.53              |
| 37:D:409:LHG:H352    | 37:D:409:LHG:H151    | 1.91                     | 0.53              |
| 2:b:224:ARG:HD3      | 7:h:25:TRP:CE2       | 2.43                     | 0.53              |
| 1:A:50:ILE:HG12      | 29:A:417:LMT:H102    | 1.89                     | 0.53              |
| 3:C:42:LEU:HD21      | 24:C:511:CLA:H2A     | 1.91                     | 0.53              |
| 24:c:507:CLA:H61     | 24:c:517:CLA:H42     | 1.90                     | 0.52              |
| 25:A:408:PHO:HAB     | 4:D:205:LEU:HD13     | 1.91                     | 0.52              |
| 20:R:2:ASP:HB3       | 20:R:5:VAL:HG23      | 1.91                     | 0.52              |
| 2:B:30:VAL:HG12      | 24:B:606:CLA:HHD     | 1.91                     | 0.52              |
| 36:e:101:DGD:HE3     | 36:e:101:DGD:HD4     | 1.91                     | 0.52              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 13:o:179[A]:GLU:OE2  | 41:o:402:HOH:O       | 2.19                     | 0.52              |
| 1:a:183:MET:HA       | 24:a:409:CLA:HMD1    | 1.92                     | 0.52              |
| 28:c:503:GOL:H2      | 41:c:734:HOH:O       | 2.08                     | 0.52              |
| 1:A:63:ILE:HB        | 3:C:335:THR:HG21     | 1.91                     | 0.52              |
| 1:a:227:THR:HB       | 1:a:231:GLU:HG3      | 1.91                     | 0.52              |
| 33:b:629:LMG:O2      | 41:b:701:HOH:O       | 2.19                     | 0.52              |
| 1:A:183:MET:HA       | 24:A:405:CLA:HMD1    | 1.91                     | 0.52              |
| 6:F:41:GLN:OE1       | 9:J:30:GLY:HA3       | 2.10                     | 0.52              |
| 3:c:38:GLY:HA3       | 24:c:516:CLA:HMD2    | 1.90                     | 0.52              |
| 24:C:501:CLA:C4D     | 24:C:503:CLA:H2      | 2.40                     | 0.52              |
| 2:B:383:PHE:CZ       | 13:O:167:GLY:HA2     | 2.44                     | 0.52              |
| 13:O:27:ARG:NH1      | 13:O:202:ALA:O       | 2.42                     | 0.52              |
| 28:T:102:GOL:H12     | 29:m:103:LMT:H12     | 1.91                     | 0.52              |
| 24:B:607:CLA:H191    | 26:B:620:BCR:H363    | 1.92                     | 0.52              |
| 11:L:13:ASN:HD22     | 11:L:16:SER:H        | 1.58                     | 0.51              |
| 1:a:162:PRO:HB3      | 1:a:168[B]:PHE:HA    | 1.93                     | 0.51              |
| 24:b:619:CLA:OBD     | 24:b:619:CLA:H152    | 2.10                     | 0.51              |
| 19:z:47:TRP:CE2      | 33:z:101:LMG:H241    | 2.45                     | 0.51              |
| 4:D:24:ARG:HD3       | 18:X:37:VAL:HG22     | 1.92                     | 0.51              |
| 3:C:149:TYR:HB2      | 3:C:157:MET:HE1      | 1.92                     | 0.51              |
| 10:K:15:TYR:OH       | 19:Z:58:ASN:ND2      | 2.38                     | 0.51              |
| 2:b:383:PHE:CZ       | 13:o:167:GLY:HA2     | 2.46                     | 0.51              |
| 3:c:286:ALA:HB2      | 24:c:507:CLA:HMD1    | 1.92                     | 0.51              |
| 2:B:224:ARG:HD3      | 7:H:25:TRP:CD2       | 2.46                     | 0.51              |
| 16:v:95:LEU:HD11     | 16:v:112:LEU:HD11    | 1.92                     | 0.51              |
| 1:A:84:PRO:HA        | 1:A:112:TYR:CG       | 2.46                     | 0.51              |
| 25:A:409[A]:PHO:HMA2 | 31:A:419[A]:PL9:H221 | 1.93                     | 0.51              |
| 3:C:438:LEU:HD11     | 24:C:505:CLA:HBB1    | 1.91                     | 0.51              |
| 4:D:343:GLU:O        | 41:D:547[B]:HOH:O    | 2.19                     | 0.51              |
| 24:a:410:CLA:H13     | 33:d:413:LMG:H242    | 1.93                     | 0.51              |
| 15:u:58:VAL:HG12     | 15:u:79:LEU:HD22     | 1.92                     | 0.51              |
| 24:C:511:CLA:H41     | 17:Y:39:LEU:HD13     | 1.93                     | 0.51              |
| 29:M:101:LMT:H6D     | 11:l:9:PRO:HA        | 1.93                     | 0.50              |
| 28:T:102:GOL:O1      | 41:T:201:HOH:O       | 2.19                     | 0.50              |
| 2:b:498:LYS:HA       | 4:d:24:ARG:HA        | 1.94                     | 0.50              |
| 16:v:78:ASN:OD1      | 16:v:96:ARG:NH1      | 2.44                     | 0.50              |
| 24:B:616:CLA:H2      | 24:B:617:CLA:HBB2    | 1.92                     | 0.50              |
| 24:A:410:CLA:H92     | 8:I:13:THR:HG23      | 1.94                     | 0.50              |
| 24:b:613:CLA:H43     | 24:b:614:CLA:H2      | 1.92                     | 0.50              |
| 3:C:406:SER:HA       | 3:C:420:VAL:HG23     | 1.94                     | 0.50              |
| 1:a:214[A]:MET:HE2   | 1:a:255:PHE:CE1      | 2.47                     | 0.50              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 1:a:214[B]:MET:HE2   | 1:a:255:PHE:CE1    | 2.47                     | 0.50              |
| 24:c:518:CLA:HBB1    | 24:c:518:CLA:CHC   | 2.37                     | 0.50              |
| 37:d:408:LHG:H342    | 37:d:408:LHG:H151  | 1.93                     | 0.50              |
| 2:B:138:MET:HE3      | 24:B:616:CLA:CHD   | 2.41                     | 0.50              |
| 2:B:195:PRO:HD2      | 7:H:65:LEU:HD11    | 1.93                     | 0.50              |
| 24:A:410:CLA:H193    | 24:C:506:CLA:H93   | 1.93                     | 0.50              |
| 3:C:334:PRO:HA       | 13:O:153:THR:OG1   | 2.12                     | 0.50              |
| 24:b:622:CLA:HBB1    | 24:b:622:CLA:HMB1  | 1.93                     | 0.50              |
| 25:A:409[B]:PHO:HBC3 | 4:D:279:LEU:HD22   | 1.93                     | 0.49              |
| 2:B:405[B]:GLU:OE1   | 13:o:60:ARG:HD3    | 2.12                     | 0.49              |
| 2:b:216:HIS:HE1      | 24:b:618:CLA:C1A   | 2.25                     | 0.49              |
| 6:f:41:GLN:OE1       | 9:j:30:GLY:HA3     | 2.10                     | 0.49              |
| 1:a:267[B]:ASN:HB3   | 1:a:270[B]:SER:OG  | 2.12                     | 0.49              |
| 35:d:411:HTG:H1      | 7:h:25:TRP:CD1     | 2.47                     | 0.49              |
| 33:D:413:LMG:H292    | 33:D:413:LMG:H152  | 1.95                     | 0.49              |
| 2:b:224:ARG:HH11     | 29:b:630:LMT:H1'   | 1.77                     | 0.49              |
| 12:M:20:VAL:HG22     | 12:m:20:VAL:HG11   | 1.94                     | 0.49              |
| 33:A:421:LMG:C25     | 24:C:505:CLA:HBB2  | 2.42                     | 0.49              |
| 33:C:519:LMG:H161    | 33:C:519:LMG:H292  | 1.94                     | 0.49              |
| 29:a:419:LMT:O4'     | 41:a:502:HOH:O     | 2.20                     | 0.49              |
| 12:m:3:VAL:HG11      | 14:t:2:GLU:HG2     | 1.93                     | 0.49              |
| 13:O:180:GLU:CD      | 13:O:180:GLU:H     | 2.20                     | 0.49              |
| 1:a:84:PRO:HA        | 1:a:112:TYR:CG     | 2.48                     | 0.49              |
| 10:K:20:PRO:HB3      | 17:Y:21:GLN:HG3    | 1.95                     | 0.49              |
| 1:a:121[A]:LEU:HD11  | 24:c:510:CLA:H152  | 1.95                     | 0.49              |
| 8:i:36:ASP:OD1       | 8:i:36:ASP:N       | 2.40                     | 0.49              |
| 13:o:74[B]:GLU:OE1   | 41:o:401:HOH:O     | 2.18                     | 0.49              |
| 19:z:26:ALA:HB1      | 19:z:36:SER:HB3    | 1.95                     | 0.49              |
| 2:B:224:ARG:NH1      | 4:D:16:ASP:OD2     | 2.45                     | 0.49              |
| 12:M:3:VAL:HG11      | 14:T:2:GLU:HG2     | 1.93                     | 0.49              |
| 4:d:101:PHE:HB3      | 36:e:101:DGD:HG2   | 1.94                     | 0.49              |
| 29:M:101:LMT:H6'2    | 11:l:9:PRO:HB3     | 1.93                     | 0.49              |
| 33:c:524:LMG:H391    | 33:c:524:LMG:H232  | 1.95                     | 0.48              |
| 12:M:27:VAL:HG12     | 12:m:28:GLN:HB3    | 1.95                     | 0.48              |
| 24:b:620:CLA:H71     | 37:b:634:LHG:H311  | 1.96                     | 0.48              |
| 3:c:443:TRP:CZ2      | 24:c:513:CLA:HMD1  | 2.48                     | 0.48              |
| 1:a:72:LEU:HD11      | 29:a:404:LMT:H52   | 1.96                     | 0.48              |
| 28:a:402:GOL:H2      | 5:e:63[A]:ILE:HD11 | 1.96                     | 0.48              |
| 3:C:25:ASN:O         | 3:C:41:ARG:HD3     | 2.14                     | 0.48              |
| 13:o:37:THR:HG22     | 13:o:246:ALA:HB3   | 1.95                     | 0.48              |
| 2:B:243:ALA:HA       | 2:B:246:PHE:CE2    | 2.49                     | 0.48              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 25:A:409[B]:PHO:HMA2 | 31:A:419[B]:PL9:H221 | 1.96                     | 0.48              |
| 6:F:28:VAL:HB        | 6:F:29:PRO:HD3       | 1.95                     | 0.48              |
| 26:T:103:BCR:H331    | 26:T:103:BCR:HC7     | 1.63                     | 0.48              |
| 1:a:221[B]:SER:HB2   | 4:d:139:ARG:O        | 2.13                     | 0.48              |
| 4:d:14:TRP:CD1       | 35:d:411:HTG:H61     | 2.49                     | 0.48              |
| 4:D:85:MET:HE1       | 4:D:96:GLU:HG2       | 1.94                     | 0.47              |
| 24:B:611:CLA:HHC     | 24:B:611:CLA:HBB1    | 1.96                     | 0.47              |
| 8:i:17:LEU:HD22      | 8:i:21:PHE:HE2       | 1.78                     | 0.47              |
| 27:L:102:SQD:H1      | 27:L:102:SQD:H462    | 1.96                     | 0.47              |
| 2:b:98:LEU:HB2       | 35:b:601:HTG:H7'1    | 1.97                     | 0.47              |
| 3:c:223:TRP:CG       | 3:c:224:ILE:H        | 2.33                     | 0.47              |
| 4:d:139:ARG:NH2      | 41:d:505:HOH:O       | 2.47                     | 0.47              |
| 6:f:28:VAL:HB        | 6:f:29:PRO:HD3       | 1.96                     | 0.47              |
| 27:A:412:SQD:O7      | 3:C:28:GLN:NE2       | 2.46                     | 0.47              |
| 31:a:415[A]:PL9:H221 | 31:a:415[A]:PL9:H201 | 1.68                     | 0.47              |
| 24:b:619:CLA:HHC     | 24:b:619:CLA:HBB1    | 1.97                     | 0.47              |
| 13:o:53:LYS:HE3      | 13:o:65:PHE:CE1      | 2.48                     | 0.47              |
| 36:c:521:DGD:HB61    | 36:c:521:DGD:HB32    | 1.66                     | 0.47              |
| 24:a:410:CLA:HMB2    | 24:d:402:CLA:H122    | 1.96                     | 0.47              |
| 2:B:36[A]:SER:OG     | 26:B:619:BCR:H362    | 2.14                     | 0.47              |
| 17:Y:32:GLY:HA3      | 26:Y:101:BCR:C15     | 2.45                     | 0.47              |
| 10:k:10:LYS:HD2      | 10:k:10:LYS:N        | 2.30                     | 0.47              |
| 24:c:513:CLA:H122    | 24:c:513:CLA:H162    | 1.64                     | 0.47              |
| 5:e:26:THR:HB        | 38:e:103:HEM:HAB     | 1.96                     | 0.47              |
| 3:C:223:TRP:CG       | 3:C:224:ILE:H        | 2.33                     | 0.47              |
| 18:X:29:ILE:O        | 18:X:33:GLN:HG2      | 2.15                     | 0.47              |
| 2:B:162:PHE:O        | 24:B:607:CLA:HHD     | 2.15                     | 0.47              |
| 1:a:217[B]:SER:O     | 1:a:221[B]:SER:HB3   | 2.15                     | 0.47              |
| 2:B:315:ILE:HG22     | 2:B:426:PHE:HB3      | 1.96                     | 0.46              |
| 1:A:96:ILE:HG12      | 1:A:105:TRP:CE2      | 2.50                     | 0.46              |
| 26:B:618:BCR:H383    | 27:B:621:SQD:H101    | 1.96                     | 0.46              |
| 2:b:158:LEU:HB3      | 2:b:199:VAL:HG22     | 1.96                     | 0.46              |
| 2:b:160:GLY:HA3      | 2:b:180:PRO:HB3      | 1.96                     | 0.46              |
| 3:c:213[B]:LEU:HD11  | 26:c:519:BCR:H373    | 1.97                     | 0.46              |
| 26:d:404:BCR:H313    | 36:e:101:DGD:HA91    | 1.96                     | 0.46              |
| 2:b:379:ALA:HA       | 2:b:390:TYR:HB3      | 1.97                     | 0.46              |
| 24:B:614:CLA:HBB1    | 24:B:614:CLA:HMB1    | 1.97                     | 0.46              |
| 26:C:514:BCR:H20C    | 26:C:514:BCR:H361    | 1.82                     | 0.46              |
| 27:L:102:SQD:H101    | 26:b:626:BCR:H383    | 1.97                     | 0.46              |
| 26:b:626:BCR:H12C    | 33:b:629:LMG:C43     | 2.46                     | 0.46              |
| 37:d:408:LHG:H331    | 37:d:408:LHG:H361    | 1.66                     | 0.46              |

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| Atom-1               | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-------------------|--------------------------|-------------------|
| 26:t:101:BCR:H23C    | 26:t:101:BCR:H382 | 1.96                     | 0.46              |
| 3:c:334:PRO:HA       | 13:o:153:THR:OG1  | 2.15                     | 0.46              |
| 26:h:101:BCR:H331    | 26:h:101:BCR:C8   | 2.45                     | 0.46              |
| 10:k:28:ILE:HD11     | 17:y:28:ILE:HD13  | 1.98                     | 0.46              |
| 19:Z:7:LEU:HD23      | 19:Z:7:LEU:HA     | 1.85                     | 0.46              |
| 1:a:162:PRO:HB3      | 1:a:168[A]:PHE:HA | 1.97                     | 0.46              |
| 24:c:511:CLA:HMC2    | 24:c:512:CLA:H102 | 1.98                     | 0.46              |
| 2:B:76[B]:SER:HB2    | 35:B:623:HTG:HO6  | 1.81                     | 0.46              |
| 3:C:213:LEU:HD21     | 26:C:515:BCR:C20  | 2.46                     | 0.46              |
| 2:b:464:PHE:CZ       | 37:d:406:LHG:H252 | 2.50                     | 0.46              |
| 26:t:101:BCR:H331    | 26:t:101:BCR:HC7  | 1.52                     | 0.46              |
| 17:y:23:THR:O        | 17:y:27:MET:HG3   | 2.15                     | 0.46              |
| 1:A:221[B]:SER:HB2   | 4:D:139:ARG:O     | 2.15                     | 0.46              |
| 24:B:616:CLA:H112    | 24:B:616:CLA:H152 | 1.48                     | 0.46              |
| 26:y:101:BCR:H15C    | 26:y:101:BCR:H351 | 1.84                     | 0.46              |
| 24:B:607:CLA:H151    | 24:B:617:CLA:H122 | 1.98                     | 0.45              |
| 24:A:410:CLA:H72     | 24:A:410:CLA:H112 | 1.75                     | 0.45              |
| 2:B:224:ARG:HD3      | 7:H:25:TRP:CE2    | 2.51                     | 0.45              |
| 24:B:603:CLA:H111    | 24:B:603:CLA:H151 | 1.79                     | 0.45              |
| 10:K:25:LEU:HD22     | 26:Y:101:BCR:H332 | 1.98                     | 0.45              |
| 37:d:408:LHG:H122    | 37:d:408:LHG:H381 | 1.98                     | 0.45              |
| 7:h:38:PHE:HB2       | 26:h:101:BCR:C10  | 2.46                     | 0.45              |
| 27:A:416:SQD:H272    | 2:b:109:LEU:HD13  | 1.98                     | 0.45              |
| 2:B:366:PHE:CD1      | 2:B:367:PRO:HD2   | 2.50                     | 0.45              |
| 4:D:16:ASP:OD2       | 29:D:401:LMT:O6'  | 2.34                     | 0.45              |
| 10:K:11:LEU:HD11     | 10:K:22:VAL:HG21  | 1.98                     | 0.45              |
| 2:b:299:GLU:HG3      | 41:b:911:HOH:O    | 2.16                     | 0.45              |
| 6:F:27:ALA:HB1       | 38:F:102:HEM:HAC  | 1.98                     | 0.45              |
| 24:b:610:CLA:H93     | 24:b:610:CLA:H111 | 1.73                     | 0.45              |
| 24:A:405:CLA:CBD     | 24:A:406:CLA:HAC2 | 2.47                     | 0.45              |
| 26:B:620:BCR:H331    | 26:B:620:BCR:C8   | 2.45                     | 0.45              |
| 26:k:101:BCR:H371    | 26:k:101:BCR:H24C | 1.62                     | 0.45              |
| 25:A:409[A]:PHO:HMC2 | 4:D:279:LEU:HD21  | 1.98                     | 0.45              |
| 3:C:185:LEU:HB2      | 3:C:230:LEU:HD13  | 1.99                     | 0.45              |
| 3:C:279:LEU:HD22     | 24:C:509:CLA:HED2 | 1.98                     | 0.45              |
| 33:C:519:LMG:H212    | 33:C:519:LMG:H331 | 1.97                     | 0.45              |
| 24:c:513:CLA:H203    | 24:c:513:CLA:H161 | 1.78                     | 0.45              |
| 20:R:6:LEU:O         | 20:R:10:LEU:HB2   | 2.17                     | 0.45              |
| 2:b:224:ARG:NH1      | 29:b:630:LMT:H1'  | 2.32                     | 0.45              |
| 24:c:518:CLA:H202    | 33:c:524:LMG:H402 | 1.98                     | 0.45              |
| 24:A:407:CLA:HED1    | 36:C:518:DGD:HAE2 | 1.99                     | 0.45              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 27:A:412:SQD:H122    | 27:A:412:SQD:H152    | 1.66                     | 0.45              |
| 10:k:24:VAL:HG13     | 17:y:25:ILE:HD13     | 1.98                     | 0.45              |
| 2:b:224:ARG:HG3      | 7:h:24:GLY:O         | 2.17                     | 0.45              |
| 24:b:614:CLA:H62     | 24:b:614:CLA:H41     | 1.85                     | 0.45              |
| 26:b:626:BCR:H15C    | 26:b:626:BCR:H351    | 1.86                     | 0.45              |
| 24:c:514:CLA:H142    | 24:c:514:CLA:H112    | 1.78                     | 0.45              |
| 5:e:27:ILE:HB        | 5:e:28:PRO:HD3       | 1.99                     | 0.45              |
| 1:a:12:ASN:O         | 1:a:16:ARG:HG3       | 2.17                     | 0.44              |
| 24:d:403:CLA:H162    | 7:h:33:VAL:HG13      | 1.98                     | 0.44              |
| 19:z:37:LYS:HZ2      | 33:z:101:LMG:HC4     | 1.82                     | 0.44              |
| 2:B:499:VAL:HG12     | 4:D:135:LEU:HB3      | 2.00                     | 0.44              |
| 3:C:35:TRP:CD1       | 10:K:45:PHE:HB3      | 2.52                     | 0.44              |
| 26:H:101:BCR:H371    | 26:H:101:BCR:H24C    | 1.67                     | 0.44              |
| 2:b:493:TRP:CD1      | 5:e:5:THR:HG22       | 2.52                     | 0.44              |
| 26:d:404:BCR:H313    | 36:e:101:DGD:HAE1    | 1.99                     | 0.44              |
| 1:A:317:TRP:CZ3      | 4:D:180:ARG:HD2      | 2.53                     | 0.44              |
| 24:B:615:CLA:H62     | 24:B:615:CLA:H41     | 1.72                     | 0.44              |
| 24:C:513:CLA:CBB     | 26:C:514:BCR:H24C    | 2.46                     | 0.44              |
| 36:C:517:DGD:HB51    | 33:C:519:LMG:H392    | 1.99                     | 0.44              |
| 14:T:20:ALA:O        | 14:T:24:ARG:HB3      | 2.16                     | 0.44              |
| 33:Z:101:LMG:HC8     | 33:Z:101:LMG:H111    | 1.63                     | 0.44              |
| 2:b:423:LYS:HA       | 2:b:423:LYS:HD3      | 1.76                     | 0.44              |
| 1:A:192:ILE:HG13     | 1:A:293:MET:HE1      | 1.99                     | 0.44              |
| 4:D:85:MET:CE        | 4:D:96:GLU:HG2       | 2.47                     | 0.44              |
| 5:E:26:THR:HB        | 38:F:102:HEM:HAB     | 1.99                     | 0.44              |
| 1:a:259:ILE:HG22     | 1:a:260:PHE:CD1      | 2.52                     | 0.44              |
| 26:b:626:BCR:H24C    | 26:b:626:BCR:H371    | 1.79                     | 0.44              |
| 3:c:127:PHE:CE1      | 33:z:101:LMG:H152    | 2.52                     | 0.44              |
| 24:c:510:CLA:HHC     | 24:c:510:CLA:HBB1    | 1.99                     | 0.44              |
| 24:B:604:CLA:H3A     | 24:B:604:CLA:CGA     | 2.47                     | 0.44              |
| 12:M:34:LYS:HG2      | 29:M:101:LMT:O3B     | 2.17                     | 0.44              |
| 13:O:53:LYS:HE2      | 13:O:63:ALA:HB3      | 1.98                     | 0.44              |
| 26:Y:101:BCR:H321    | 26:Y:101:BCR:HC8     | 1.98                     | 0.44              |
| 1:a:96:ILE:HG12      | 1:a:105:TRP:CE2      | 2.53                     | 0.44              |
| 26:b:628:BCR:H331    | 26:b:628:BCR:C8      | 2.47                     | 0.44              |
| 26:T:103:BCR:H382    | 26:T:103:BCR:H23C    | 1.99                     | 0.44              |
| 31:A:419[A]:PL9:H421 | 31:A:419[A]:PL9:H401 | 1.79                     | 0.44              |
| 31:A:419[A]:PL9:H512 | 27:F:103:SQD:H301    | 1.98                     | 0.44              |
| 3:C:262:ARG:HG2      | 8:I:38:GLU:HG2       | 1.98                     | 0.44              |
| 8:I:2:GLU:O          | 8:I:6:ILE:HG12       | 2.17                     | 0.44              |
| 24:a:409:CLA:H192    | 24:a:409:CLA:H161    | 1.79                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:b:256:MET:HA       | 2:b:263:THR:HG21     | 1.99                     | 0.44              |
| 2:b:461:LEU:HD21     | 4:d:284:ILE:HD11     | 1.98                     | 0.44              |
| 24:b:620:CLA:H142    | 37:b:634:LHG:H361    | 2.00                     | 0.44              |
| 2:B:423:LYS:HE2      | 41:O:421:HOH:O       | 2.18                     | 0.44              |
| 26:C:515:BCR:H11C    | 26:C:515:BCR:H341    | 1.87                     | 0.44              |
| 4:D:269:PHE:CD2      | 37:D:407:LHG:HC11    | 2.53                     | 0.44              |
| 3:c:245:ILE:O        | 3:c:249:ILE:HG13     | 2.18                     | 0.44              |
| 36:e:101:DGD:HG2     | 36:e:101:DGD:HB21    | 1.84                     | 0.44              |
| 35:D:412:HTG:H1'2    | 7:H:25:TRP:CD2       | 2.53                     | 0.44              |
| 26:H:101:BCR:H331    | 26:H:101:BCR:C8      | 2.47                     | 0.44              |
| 17:Y:22:LEU:HA       | 17:Y:25:ILE:HG22     | 1.99                     | 0.44              |
| 24:a:409:CLA:CBD     | 24:d:401:CLA:HAC2    | 2.48                     | 0.44              |
| 25:a:418[A]:PHO:ND   | 25:a:418[A]:PHO:NC   | 2.66                     | 0.44              |
| 26:c:519:BCR:H24C    | 26:c:519:BCR:H371    | 1.86                     | 0.44              |
| 37:e:102:LHG:H171    | 37:e:102:LHG:H201    | 1.88                     | 0.44              |
| 26:T:103:BCR:H19C    | 26:b:627:BCR:H363    | 1.99                     | 0.43              |
| 24:c:510:CLA:HAA1    | 24:c:510:CLA:HBD     | 2.00                     | 0.43              |
| 10:k:12:PRO:HB2      | 10:k:15:TYR:HD2      | 1.83                     | 0.43              |
| 13:o:40:ILE:HD12     | 13:o:95:PHE:CD1      | 2.53                     | 0.43              |
| 27:B:621:SQD:O8      | 11:L:7:ARG:HD3       | 2.18                     | 0.43              |
| 26:C:515:BCR:H371    | 26:C:515:BCR:H24C    | 1.74                     | 0.43              |
| 2:B:314:TYR:CE2      | 2:B:316:GLY:HA3      | 2.53                     | 0.43              |
| 2:b:70:GLY:HA2       | 2:b:178:VAL:HG21     | 2.01                     | 0.43              |
| 3:c:79:LYS:HD2       | 16:v:35:TYR:CE1      | 2.53                     | 0.43              |
| 13:o:121:THR:OG1     | 13:o:123:LYS:HG3     | 2.17                     | 0.43              |
| 8:I:33:LYS:HB3       | 8:I:34:ARG:H         | 1.55                     | 0.43              |
| 2:b:62:VAL:HB        | 24:b:614:CLA:HED3    | 1.99                     | 0.43              |
| 24:c:507:CLA:H193    | 35:c:525:HTG:H4'2    | 2.01                     | 0.43              |
| 3:C:97:TRP:NE1       | 33:C:520:LMG:H131    | 2.33                     | 0.43              |
| 31:a:415[B]:PL9:H171 | 31:a:415[B]:PL9:H151 | 1.70                     | 0.43              |
| 2:b:227:LYS:NZ       | 29:b:630:LMT:O6'     | 2.51                     | 0.43              |
| 3:c:240:ILE:HD13     | 3:c:240:ILE:HA       | 1.83                     | 0.43              |
| 3:c:348:GLU:OE1      | 13:o:11:VAL:HA       | 2.18                     | 0.43              |
| 24:d:401:CLA:H162    | 24:d:401:CLA:H203    | 1.73                     | 0.43              |
| 24:C:505:CLA:HAA1    | 24:C:505:CLA:HBD     | 2.00                     | 0.43              |
| 31:a:415[A]:PL9:H171 | 31:a:415[A]:PL9:H151 | 1.75                     | 0.43              |
| 25:a:418[A]:PHO:HBC3 | 4:d:279:LEU:HD22     | 2.00                     | 0.43              |
| 2:b:231:MET:HE2      | 24:b:619:CLA:HMC2    | 2.00                     | 0.43              |
| 3:c:175:LEU:HD23     | 3:c:237:HIS:CG       | 2.54                     | 0.43              |
| 3:c:437:PHE:CE1      | 24:c:515:CLA:HMB2    | 2.54                     | 0.43              |
| 24:B:615:CLA:H92     | 24:B:615:CLA:H61     | 1.73                     | 0.43              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 24:B:616:CLA:H172  | 24:B:616:CLA:H13     | 1.85                     | 0.43              |
| 27:B:621:SQD:H462  | 27:B:621:SQD:H1      | 2.00                     | 0.43              |
| 1:a:131:TRP:CH2    | 24:c:510:CLA:HAA2    | 2.53                     | 0.43              |
| 24:b:622:CLA:H72   | 24:b:622:CLA:H111    | 1.81                     | 0.43              |
| 4:d:51:GLY:HA3     | 4:d:78:VAL:HG22      | 1.99                     | 0.43              |
| 37:d:408:LHG:H251  | 37:d:408:LHG:H281    | 1.77                     | 0.43              |
| 14:t:2:GLU:H       | 14:t:2:GLU:CD        | 2.26                     | 0.43              |
| 19:z:37:LYS:NZ     | 33:z:101:LMG:HC4     | 2.33                     | 0.43              |
| 3:C:437:PHE:CZ     | 24:C:510:CLA:HMB2    | 2.54                     | 0.43              |
| 1:a:46:ILE:HD13    | 27:a:405:SQD:H371    | 2.00                     | 0.43              |
| 1:a:215[B]:HIS:HA  | 31:a:415[B]:PL9:HC71 | 2.00                     | 0.43              |
| 24:b:612:CLA:H3A   | 24:b:612:CLA:CGA     | 2.49                     | 0.43              |
| 3:c:179:ALA:O      | 3:c:184:GLY:HA2      | 2.19                     | 0.43              |
| 2:b:36:SER:OG      | 26:b:627:BCR:H362    | 2.18                     | 0.43              |
| 2:B:223:GLN:NE2    | 2:B:227:LYS:HD3      | 2.34                     | 0.43              |
| 33:C:519:LMG:H201  | 10:K:27:VAL:HG11     | 2.00                     | 0.43              |
| 26:T:103:BCR:H11C  | 26:T:103:BCR:H341    | 1.81                     | 0.43              |
| 24:a:412:CLA:H102  | 24:a:412:CLA:H61     | 1.65                     | 0.43              |
| 2:b:30:VAL:HG12    | 24:b:614:CLA:HHD     | 2.00                     | 0.43              |
| 2:b:233:ASN:O      | 2:b:236:THR:HG22     | 2.19                     | 0.43              |
| 12:m:28:GLN:O      | 12:m:32:GLN:HG3      | 2.19                     | 0.43              |
| 24:A:406:CLA:H203  | 24:A:406:CLA:H162    | 1.63                     | 0.42              |
| 2:B:227:LYS:HE2    | 2:B:227:LYS:HB3      | 1.86                     | 0.42              |
| 13:O:42:ARG:O      | 13:O:241:ALA:HA      | 2.19                     | 0.42              |
| 2:b:487:SER:HA     | 2:b:488:PRO:HD3      | 1.79                     | 0.42              |
| 24:b:614:CLA:HAA1  | 24:b:614:CLA:HBD     | 1.99                     | 0.42              |
| 4:d:85:MET:HE1     | 4:d:96:GLU:HG2       | 2.01                     | 0.42              |
| 3:C:337:LEU:HD22   | 3:C:342:MET:HE3      | 2.01                     | 0.42              |
| 24:C:503:CLA:CBB   | 24:C:512:CLA:H41     | 2.41                     | 0.42              |
| 16:V:12:LEU:HD12   | 16:V:69:ILE:HB       | 2.01                     | 0.42              |
| 24:c:514:CLA:HBB1  | 24:c:514:CLA:HMB1    | 2.01                     | 0.42              |
| 4:d:85:MET:CE      | 4:d:96:GLU:HG2       | 2.49                     | 0.42              |
| 2:B:102:VAL:HA     | 26:B:619:BCR:C40     | 2.49                     | 0.42              |
| 24:B:614:CLA:H162  | 24:B:614:CLA:H121    | 1.75                     | 0.42              |
| 3:C:338:GLY:HA3    | 3:C:341:LEU:O        | 2.19                     | 0.42              |
| 24:D:402:CLA:HAA2  | 24:D:402:CLA:HBD     | 2.01                     | 0.42              |
| 13:O:57:LYS:NZ     | 2:b:49:ASP:OD1       | 2.48                     | 0.42              |
| 24:a:409:CLA:HAA2  | 24:a:409:CLA:HBD     | 2.01                     | 0.42              |
| 25:a:418[B]:PHO:NC | 25:a:418[B]:PHO:ND   | 2.67                     | 0.42              |
| 2:b:58:GLN:C       | 2:b:329:PRO:HB3      | 2.45                     | 0.42              |
| 3:c:217:PRO:HB2    | 36:c:520:DGD:HA21    | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:d:401:CLA:HBA1  | 24:d:401:CLA:C4A  | 2.49                     | 0.42              |
| 3:C:250:TRP:CZ3    | 3:C:254:THR:HG21  | 2.54                     | 0.42              |
| 37:D:409:LHG:H272  | 37:D:409:LHG:H242 | 1.67                     | 0.42              |
| 3:c:26:ARG:NH2     | 17:y:46:LEU:OXT   | 2.47                     | 0.42              |
| 3:c:79:LYS:HD2     | 16:v:35:TYR:HE1   | 1.84                     | 0.42              |
| 2:B:160:GLY:HA3    | 2:B:180:PRO:HB3   | 2.01                     | 0.42              |
| 2:B:422:ARG:O      | 2:B:425:ILE:HG12  | 2.20                     | 0.42              |
| 24:B:603:CLA:H41   | 7:H:46:LEU:HA     | 2.01                     | 0.42              |
| 24:B:606:CLA:HAA1  | 24:B:606:CLA:HBD  | 2.01                     | 0.42              |
| 3:C:203:THR:O      | 3:C:235:GLY:HA3   | 2.19                     | 0.42              |
| 4:D:172:SER:HB2    | 4:D:177:ALA:HB1   | 2.01                     | 0.42              |
| 3:c:95:LEU:HD21    | 24:c:506:CLA:OBD  | 2.18                     | 0.42              |
| 5:e:13:ILE:HG21    | 38:e:103:HEM:HAD2 | 2.01                     | 0.42              |
| 5:e:60:GLN:HG2     | 5:e:61:ARG:N      | 2.34                     | 0.42              |
| 24:B:607:CLA:C19   | 26:B:620:BCR:H16C | 2.50                     | 0.42              |
| 24:B:612:CLA:H192  | 24:B:612:CLA:H161 | 1.84                     | 0.42              |
| 26:B:620:BCR:H15C  | 26:B:620:BCR:H351 | 1.83                     | 0.42              |
| 19:Z:29:SER:HA     | 19:Z:30:PRO:HD3   | 1.87                     | 0.42              |
| 24:b:620:CLA:HMA3  | 24:b:621:CLA:HMC2 | 2.02                     | 0.42              |
| 26:c:528:BCR:H11C  | 26:c:528:BCR:H341 | 1.82                     | 0.42              |
| 24:A:406:CLA:C4A   | 24:A:406:CLA:HBA1 | 2.50                     | 0.42              |
| 24:B:617:CLA:H92   | 24:B:617:CLA:H61  | 1.87                     | 0.42              |
| 3:c:406:SER:HA     | 3:c:420:VAL:HG23  | 2.01                     | 0.42              |
| 4:d:49:LEU:HD13    | 26:d:404:BCR:C15  | 2.50                     | 0.42              |
| 12:m:27:VAL:HG13   | 29:m:102:LMT:H11  | 2.01                     | 0.42              |
| 1:A:214[A]:MET:HE2 | 1:A:255:PHE:CE1   | 2.55                     | 0.42              |
| 3:C:156:LYS:HE3    | 41:C:771:HOH:O    | 2.19                     | 0.42              |
| 24:C:509:CLA:H141  | 24:C:509:CLA:H161 | 1.86                     | 0.42              |
| 33:C:520:LMG:H381  | 33:C:520:LMG:H411 | 1.83                     | 0.42              |
| 27:a:414:SQD:H202  | 27:a:414:SQD:H171 | 1.90                     | 0.42              |
| 24:d:401:CLA:HMB1  | 24:d:401:CLA:HBB1 | 2.01                     | 0.42              |
| 24:d:402:CLA:HAA2  | 24:d:402:CLA:HBD  | 2.02                     | 0.42              |
| 11:l:2:GLU:HB2     | 41:l:108:HOH:O    | 2.20                     | 0.42              |
| 27:A:412:SQD:H291  | 24:C:508:CLA:H71  | 2.02                     | 0.42              |
| 26:B:618:BCR:H11C  | 26:B:618:BCR:H341 | 1.88                     | 0.42              |
| 36:C:517:DGD:HA81  | 36:C:517:DGD:HAE2 | 1.79                     | 0.42              |
| 37:D:408:LHG:H192  | 14:T:17:PHE:HZ    | 1.85                     | 0.42              |
| 16:V:126:LEU:HB3   | 16:V:129:LYS:HB2  | 2.02                     | 0.42              |
| 20:R:10:LEU:HB3    | 20:R:11:PRO:HD3   | 2.02                     | 0.42              |
| 1:a:38:ILE:HB      | 1:a:39:PRO:HD3    | 2.01                     | 0.42              |
| 4:d:136:VAL:HG12   | 4:d:138:VAL:HG13  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:d:160:TYR:HA    | 4:d:290:ALA:HB2   | 2.01                     | 0.42              |
| 19:z:29:SER:HA    | 19:z:30:PRO:HD3   | 1.85                     | 0.42              |
| 1:A:187:GLN:HB2   | 24:A:405:CLA:HAC2 | 2.02                     | 0.42              |
| 33:A:421:LMG:H242 | 33:A:421:LMG:H212 | 1.81                     | 0.42              |
| 10:K:10:LYS:N     | 41:K:202:HOH:O    | 2.53                     | 0.42              |
| 13:O:54:GLU:O     | 13:O:56:PRO:HD3   | 2.20                     | 0.42              |
| 35:V:206:HTG:H6'2 | 35:V:206:HTG:H3'2 | 1.86                     | 0.42              |
| 24:b:624:CLA:H91  | 24:b:624:CLA:H112 | 1.75                     | 0.42              |
| 3:c:225:VAL:HG13  | 3:c:289:PHE:HA    | 2.01                     | 0.42              |
| 41:d:619:HOH:O    | 28:t:102:GOL:H12  | 2.20                     | 0.42              |
| 5:e:10:PHE:HE2    | 38:e:103:HEM:HBD2 | 1.84                     | 0.42              |
| 19:z:15:LEU:O     | 19:z:19:MET:HG2   | 2.20                     | 0.42              |
| 2:B:216:HIS:CE1   | 24:B:610:CLA:NA   | 2.88                     | 0.41              |
| 24:B:617:CLA:H112 | 24:B:617:CLA:H91  | 1.80                     | 0.41              |
| 2:b:405:GLU:OE1   | 41:b:702:HOH:O    | 2.21                     | 0.41              |
| 24:b:623:CLA:H41  | 24:b:623:CLA:H62  | 1.66                     | 0.41              |
| 3:c:52:ALA:HB2    | 24:c:516:CLA:HMA2 | 2.01                     | 0.41              |
| 37:d:407:LHG:HC62 | 11:l:15:THR:HG23  | 2.02                     | 0.41              |
| 17:y:30:ILE:HA    | 17:y:30:ILE:HD12  | 1.84                     | 0.41              |
| 2:B:221:PRO:HA    | 24:B:610:CLA:HED3 | 2.02                     | 0.41              |
| 24:B:609:CLA:HAB  | 4:D:123:ILE:HG12  | 2.02                     | 0.41              |
| 26:b:628:BCR:H24C | 26:b:628:BCR:H371 | 1.82                     | 0.41              |
| 13:o:19:CYS:SG    | 13:o:46:GLN:HB2   | 2.59                     | 0.41              |
| 1:A:162:PRO:HB3   | 1:A:168[B]:PHE:HA | 2.03                     | 0.41              |
| 27:A:412:SQD:H381 | 9:J:21:ILE:HD11   | 2.02                     | 0.41              |
| 3:C:213:LEU:HD21  | 26:C:515:BCR:C19  | 2.50                     | 0.41              |
| 13:O:39:ARG:HB2   | 13:O:246:ALA:HB2  | 2.01                     | 0.41              |
| 13:o:51:LEU:HB3   | 13:o:65:PHE:HB3   | 2.01                     | 0.41              |
| 24:B:616:CLA:H51  | 26:B:620:BCR:H341 | 2.03                     | 0.41              |
| 3:C:240:ILE:HD13  | 3:C:240:ILE:HA    | 1.88                     | 0.41              |
| 24:C:508:CLA:H142 | 24:C:508:CLA:H111 | 1.84                     | 0.41              |
| 4:D:51:GLY:HA3    | 4:D:78:VAL:HG22   | 2.02                     | 0.41              |
| 24:a:412:CLA:H111 | 8:i:16:VAL:HG11   | 2.03                     | 0.41              |
| 38:e:103:HEM:CAC  | 6:f:27:ALA:HB1    | 2.51                     | 0.41              |
| 13:o:23:ASP:HB3   | 13:o:25:THR:HG23  | 2.03                     | 0.41              |
| 1:A:309:ALA:HB3   | 16:V:1:ALA:O      | 2.21                     | 0.41              |
| 33:A:421:LMG:H321 | 3:C:223:TRP:CD1   | 2.55                     | 0.41              |
| 24:B:608:CLA:C4A  | 24:B:608:CLA:HBA2 | 2.51                     | 0.41              |
| 26:C:515:BCR:H15C | 26:C:515:BCR:H351 | 1.91                     | 0.41              |
| 4:D:125:PHE:O     | 4:D:128:ARG:HB3   | 2.19                     | 0.41              |
| 4:D:191:TRP:CE3   | 4:D:289:LEU:HD11  | 2.55                     | 0.41              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 19:Z:19:MET:HE3      | 19:Z:19:MET:HB3     | 1.98                     | 0.41              |
| 19:z:9:LEU:HD13      | 19:z:54:VAL:HG11    | 2.02                     | 0.41              |
| 26:A:411:BCR:H371    | 26:A:411:BCR:H24C   | 1.75                     | 0.41              |
| 35:D:412:HTG:H1      | 7:H:25:TRP:CD1      | 2.56                     | 0.41              |
| 12:M:6:LEU:HD11      | 29:M:103:LMT:H32    | 2.01                     | 0.41              |
| 26:a:413:BCR:H24C    | 26:a:413:BCR:H371   | 1.83                     | 0.41              |
| 24:c:507:CLA:H162    | 24:c:507:CLA:H141   | 1.86                     | 0.41              |
| 13:o:42:ARG:O        | 13:o:241:ALA:HA     | 2.21                     | 0.41              |
| 1:A:300:PHE:HB3      | 1:A:302:PHE:CE1     | 2.55                     | 0.41              |
| 24:A:405:CLA:H192    | 24:A:405:CLA:H161   | 1.79                     | 0.41              |
| 26:b:627:BCR:C8      | 26:b:627:BCR:H331   | 2.50                     | 0.41              |
| 33:c:501:LMG:H182    | 33:c:501:LMG:H152   | 1.86                     | 0.41              |
| 24:c:510:CLA:HBC2    | 26:c:519:BCR:H341   | 2.03                     | 0.41              |
| 24:C:502:CLA:C6      | 24:C:512:CLA:H42    | 2.51                     | 0.41              |
| 4:D:43:LEU:HD23      | 4:D:43:LEU:HA       | 1.88                     | 0.41              |
| 5:e:10:PHE:CE2       | 38:e:103:HEM:HBD2   | 2.55                     | 0.41              |
| 24:A:410:CLA:H162    | 24:A:410:CLA:H122   | 1.72                     | 0.41              |
| 2:B:124:ARG:HD2      | 2:B:129:GLY:O       | 2.19                     | 0.41              |
| 2:B:187:PRO:HD3      | 24:B:602:CLA:HMD2   | 2.02                     | 0.41              |
| 26:B:618:BCR:H24C    | 26:B:618:BCR:H371   | 1.79                     | 0.41              |
| 3:C:154:LYS:HE2      | 3:C:261:ARG:HG2     | 2.03                     | 0.41              |
| 3:C:175:LEU:HD23     | 3:C:237:HIS:CG      | 2.55                     | 0.41              |
| 4:D:49:LEU:HD13      | 26:D:404:BCR:C15    | 2.51                     | 0.41              |
| 4:D:210:LEU:HA       | 4:D:213:ILE:HG22    | 2.02                     | 0.41              |
| 13:O:126:VAL:O       | 41:O:401:HOH:O      | 2.22                     | 0.41              |
| 24:b:613:CLA:HMD2    | 24:b:621:CLA:H203   | 2.03                     | 0.41              |
| 24:b:624:CLA:H161    | 7:h:7:LEU:HD21      | 2.02                     | 0.41              |
| 4:d:24:ARG:HD3       | 18:x:37:VAL:HG22    | 2.02                     | 0.41              |
| 35:d:411:HTG:H1      | 7:h:25:TRP:CG       | 2.56                     | 0.41              |
| 33:z:101:LMG:H142    | 33:z:101:LMG:H111   | 1.85                     | 0.41              |
| 33:A:421:LMG:H221    | 36:C:516:DGD:HAE1   | 2.02                     | 0.41              |
| 24:C:513:CLA:CBB     | 26:C:514:BCR:H371   | 2.49                     | 0.41              |
| 26:b:628:BCR:H15C    | 26:b:628:BCR:H351   | 1.91                     | 0.41              |
| 6:f:21:VAL:O         | 6:f:25:THR:HG23     | 2.21                     | 0.41              |
| 26:t:101:BCR:H11C    | 26:t:101:BCR:H341   | 1.91                     | 0.41              |
| 15:U:42:TYR:HA       | 15:U:43:PRO:HA      | 1.83                     | 0.40              |
| 2:b:298:LEU:HD12     | 2:b:298:LEU:HA      | 1.94                     | 0.40              |
| 36:e:101:DGD:O1B     | 36:e:101:DGD:O2D    | 2.39                     | 0.40              |
| 13:o:180:GLU:H       | 13:o:180:GLU:CD     | 2.30                     | 0.40              |
| 1:A:214[B]:MET:HE2   | 1:A:255:PHE:CE1     | 2.57                     | 0.40              |
| 31:D:405[B]:PL9:H471 | 31:D:405[B]:PL9:H43 | 1.89                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:L:102:SQD:H62   | 11:l:7:ARG:NH1    | 2.37                     | 0.40              |
| 12:M:28:GLN:HB3    | 12:m:27:VAL:HG12  | 2.02                     | 0.40              |
| 19:Z:36:SER:O      | 19:Z:40:ILE:HG13  | 2.20                     | 0.40              |
| 2:b:262:THR:C      | 2:b:264:PRO:HD3   | 2.46                     | 0.40              |
| 24:c:510:CLA:CMD   | 24:c:512:CLA:HAB  | 2.52                     | 0.40              |
| 2:B:172:TYR:OH     | 7:H:63:LYS:HE3    | 2.21                     | 0.40              |
| 5:E:15:THR:HB      | 9:J:7:ILE:O       | 2.21                     | 0.40              |
| 24:d:403:CLA:H2    | 18:x:14:LEU:HA    | 2.03                     | 0.40              |
| 16:v:41:HIS:HA     | 16:v:45:ILE:O     | 2.22                     | 0.40              |
| 24:B:615:CLA:HBD   | 24:B:615:CLA:HAA1 | 2.02                     | 0.40              |
| 4:D:282:SER:OG     | 24:D:402:CLA:HED3 | 2.21                     | 0.40              |
| 37:D:409:LHG:H112  | 37:D:409:LHG:C38  | 2.49                     | 0.40              |
| 2:b:63:LEU:N       | 2:b:64:PRO:HD2    | 2.36                     | 0.40              |
| 24:b:619:CLA:HHC   | 24:b:619:CLA:CBB  | 2.52                     | 0.40              |
| 4:d:103:ARG:O      | 4:d:107:LEU:HG    | 2.21                     | 0.40              |
| 19:z:52:LEU:O      | 19:z:56:VAL:HG23  | 2.21                     | 0.40              |
| 24:B:614:CLA:H192  | 24:B:614:CLA:H161 | 1.95                     | 0.40              |
| 3:C:461:ARG:NH2    | 41:C:615:HOH:O    | 2.53                     | 0.40              |
| 24:C:510:CLA:C4    | 37:D:409:LHG:H383 | 2.49                     | 0.40              |
| 1:a:272[A]:HIS:CD2 | 4:d:218:VAL:HG21  | 2.56                     | 0.40              |
| 3:c:324:LEU:HD23   | 3:c:324:LEU:HA    | 1.91                     | 0.40              |
| 26:h:101:BCR:H15C  | 26:h:101:BCR:H351 | 1.96                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 15:U:69:GLU:OE1 | 27:f:101:SQD:O3[2_554] | 2.16                     | 0.04              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 384/344 (112%) | 375 (98%) | 8 (2%)  | 1 (0%)   | 36          | 34  |
| 1   | a     | 386/344 (112%) | 377 (98%) | 8 (2%)  | 1 (0%)   | 36          | 34  |
| 2   | B     | 512/505 (101%) | 509 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 2   | b     | 513/505 (102%) | 504 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 3   | C     | 456/455 (100%) | 448 (98%) | 6 (1%)  | 2 (0%)   | 30          | 26  |
| 3   | c     | 466/455 (102%) | 454 (97%) | 10 (2%) | 2 (0%)   | 30          | 26  |
| 4   | D     | 355/342 (104%) | 346 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 4   | d     | 355/342 (104%) | 346 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 5   | E     | 81/84 (96%)    | 81 (100%) | 0       | 0        | 100         | 100 |
| 5   | e     | 81/84 (96%)    | 78 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 6   | F     | 32/44 (73%)    | 31 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 6   | f     | 30/44 (68%)    | 30 (100%) | 0       | 0        | 100         | 100 |
| 7   | H     | 64/65 (98%)    | 59 (92%)  | 5 (8%)  | 0        | 100         | 100 |
| 7   | h     | 63/65 (97%)    | 59 (94%)  | 4 (6%)  | 0        | 100         | 100 |
| 8   | I     | 36/38 (95%)    | 34 (94%)  | 2 (6%)  | 0        | 100         | 100 |
| 8   | i     | 36/38 (95%)    | 33 (92%)  | 3 (8%)  | 0        | 100         | 100 |
| 9   | J     | 36/39 (92%)    | 35 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 9   | j     | 37/39 (95%)    | 36 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 10  | K     | 35/37 (95%)    | 35 (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     | 32/36 (89%)    | 32 (100%) | 0       | 0        | 100         | 100 |
| 13  | O     | 249/244 (102%) | 244 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 13  | o     | 246/244 (101%) | 240 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 14  | T     | 29/32 (91%)    | 29 (100%) | 0       | 0        | 100         | 100 |
| 14  | t     | 29/32 (91%)    | 29 (100%) | 0       | 0        | 100         | 100 |
| 15  | U     | 95/104 (91%)   | 93 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 15  | u     | 95/104 (91%)   | 92 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 16  | V     | 136/137 (99%)  | 132 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 16  | v     | 135/137 (98%)  | 130 (96%) | 5 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 17  | Y     | 27/30 (90%)      | 27 (100%)  | 0        | 0        | 100         | 100 |
| 17  | y     | 27/30 (90%)      | 25 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 18  | X     | 37/40 (92%)      | 37 (100%)  | 0        | 0        | 100         | 100 |
| 18  | x     | 36/40 (90%)      | 36 (100%)  | 0        | 0        | 100         | 100 |
| 19  | Z     | 60/62 (97%)      | 58 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 19  | z     | 60/62 (97%)      | 58 (97%)   | 1 (2%)   | 1 (2%)   | 7           | 2   |
| 20  | R     | 28/34 (82%)      | 28 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 5419/5384 (101%) | 5300 (98%) | 112 (2%) | 7 (0%)   | 48          | 50  |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 3   | C     | 416[A] | SER  |
| 3   | C     | 416[B] | SER  |
| 3   | c     | 416[A] | SER  |
| 3   | c     | 416[B] | SER  |
| 1   | a     | 259    | ILE  |
| 19  | z     | 30     | PRO  |
| 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     | 312/279 (112%) | 312 (100%) | 0        | 100         | 100 |
| 1   | a     | 314/279 (112%) | 313 (100%) | 1 (0%)   | 86          | 91  |
| 2   | B     | 412/403 (102%) | 409 (99%)  | 3 (1%)   | 76          | 82  |
| 2   | b     | 413/403 (102%) | 407 (98%)  | 6 (2%)   | 57          | 64  |
| 3   | C     | 357/356 (100%) | 351 (98%)  | 6 (2%)   | 53          | 60  |
| 3   | c     | 367/356 (103%) | 355 (97%)  | 12 (3%)  | 33          | 34  |
| 4   | D     | 290/277 (105%) | 287 (99%)  | 3 (1%)   | 68          | 75  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | d     | 290/277 (105%) | 287 (99%)  | 3 (1%)   | 68          | 75  |
| 5   | E     | 74/73 (101%)   | 73 (99%)   | 1 (1%)   | 59          | 66  |
| 5   | e     | 74/73 (101%)   | 72 (97%)   | 2 (3%)   | 39          | 41  |
| 6   | F     | 28/38 (74%)    | 28 (100%)  | 0        | 100         | 100 |
| 6   | f     | 26/38 (68%)    | 24 (92%)   | 2 (8%)   | 12          | 7   |
| 7   | H     | 55/54 (102%)   | 54 (98%)   | 1 (2%)   | 51          | 58  |
| 7   | h     | 54/54 (100%)   | 54 (100%)  | 0        | 100         | 100 |
| 8   | I     | 34/34 (100%)   | 33 (97%)   | 1 (3%)   | 37          | 39  |
| 8   | i     | 34/34 (100%)   | 33 (97%)   | 1 (3%)   | 37          | 39  |
| 9   | J     | 26/27 (96%)    | 26 (100%)  | 0        | 100         | 100 |
| 9   | j     | 27/27 (100%)   | 26 (96%)   | 1 (4%)   | 30          | 30  |
| 10  | K     | 30/30 (100%)   | 29 (97%)   | 1 (3%)   | 33          | 34  |
| 10  | k     | 30/30 (100%)   | 28 (93%)   | 2 (7%)   | 15          | 10  |
| 11  | L     | 36/35 (103%)   | 35 (97%)   | 1 (3%)   | 38          | 40  |
| 11  | l     | 36/35 (103%)   | 35 (97%)   | 1 (3%)   | 38          | 40  |
| 12  | M     | 31/32 (97%)    | 29 (94%)   | 2 (6%)   | 15          | 11  |
| 12  | m     | 30/32 (94%)    | 29 (97%)   | 1 (3%)   | 33          | 34  |
| 13  | O     | 214/207 (103%) | 209 (98%)  | 5 (2%)   | 44          | 49  |
| 13  | o     | 211/207 (102%) | 203 (96%)  | 8 (4%)   | 29          | 29  |
| 14  | T     | 27/28 (96%)    | 25 (93%)   | 2 (7%)   | 13          | 8   |
| 14  | t     | 27/28 (96%)    | 25 (93%)   | 2 (7%)   | 13          | 8   |
| 15  | U     | 84/89 (94%)    | 82 (98%)   | 2 (2%)   | 43          | 47  |
| 15  | u     | 84/89 (94%)    | 83 (99%)   | 1 (1%)   | 63          | 70  |
| 16  | V     | 119/117 (102%) | 119 (100%) | 0        | 100         | 100 |
| 16  | v     | 118/117 (101%) | 117 (99%)  | 1 (1%)   | 73          | 79  |
| 17  | Y     | 22/23 (96%)    | 21 (96%)   | 1 (4%)   | 24          | 22  |
| 17  | y     | 22/23 (96%)    | 19 (86%)   | 3 (14%)  | 3           | 1   |
| 18  | X     | 32/33 (97%)    | 32 (100%)  | 0        | 100         | 100 |
| 18  | x     | 31/33 (94%)    | 31 (100%)  | 0        | 100         | 100 |
| 19  | Z     | 52/52 (100%)   | 49 (94%)   | 3 (6%)   | 18          | 14  |
| 19  | z     | 52/52 (100%)   | 49 (94%)   | 3 (6%)   | 18          | 14  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 20  | R     | 25/29 (86%)      | 23 (92%)   | 2 (8%)   | 11          | 7  |
| All | All   | 4500/4403 (102%) | 4416 (98%) | 84 (2%)  | 51          | 56 |

All (84) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | B     | 80     | ILE  |
| 2   | B     | 362    | PHE  |
| 2   | B     | 492    | GLU  |
| 3   | C     | 28     | GLN  |
| 3   | C     | 29     | GLU  |
| 3   | C     | 142    | GLU  |
| 3   | C     | 289    | PHE  |
| 3   | C     | 315    | MET  |
| 3   | C     | 355    | THR  |
| 4   | D     | 90     | LEU  |
| 4   | D     | 136    | VAL  |
| 4   | D     | 329    | MET  |
| 5   | E     | 71     | GLU  |
| 7   | H     | 65     | LEU  |
| 8   | I     | 38     | GLU  |
| 10  | K     | 17     | ILE  |
| 11  | L     | 13     | ASN  |
| 12  | M     | 5      | GLN  |
| 12  | M     | 9      | ILE  |
| 13  | O     | 4      | THR  |
| 13  | O     | 34     | SER  |
| 13  | O     | 69     | LYS  |
| 13  | O     | 181[A] | GLU  |
| 13  | O     | 181[B] | GLU  |
| 14  | T     | 25[A]  | GLU  |
| 14  | T     | 25[B]  | GLU  |
| 15  | U     | 59     | GLU  |
| 15  | U     | 70     | ARG  |
| 17  | Y     | 24     | MET  |
| 19  | Z     | 3      | ILE  |
| 19  | Z     | 4      | LEU  |
| 19  | Z     | 20     | VAL  |
| 20  | R     | 4      | ARG  |
| 20  | R     | 5      | VAL  |
| 1   | a     | 12     | ASN  |
| 2   | b     | 84     | THR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | b     | 315    | ILE  |
| 2   | b     | 362    | PHE  |
| 2   | b     | 467    | ILE  |
| 2   | b     | 472    | ARG  |
| 2   | b     | 479    | PHE  |
| 3   | c     | 19     | ASN  |
| 3   | c     | 21     | ILE  |
| 3   | c     | 79     | LYS  |
| 3   | c     | 142    | GLU  |
| 3   | c     | 240    | ILE  |
| 3   | c     | 255    | THR  |
| 3   | c     | 289    | PHE  |
| 3   | c     | 315    | MET  |
| 3   | c     | 416[A] | SER  |
| 3   | c     | 416[B] | SER  |
| 3   | c     | 462[A] | GLU  |
| 3   | c     | 462[B] | GLU  |
| 4   | d     | 90     | LEU  |
| 4   | d     | 293    | LEU  |
| 4   | d     | 329    | MET  |
| 5   | e     | 16     | SER  |
| 5   | e     | 71     | GLU  |
| 6   | f     | 15     | ILE  |
| 6   | f     | 44     | GLN  |
| 8   | i     | 36     | ASP  |
| 9   | j     | 1      | MET  |
| 10  | k     | 10     | LYS  |
| 10  | k     | 17     | ILE  |
| 11  | l     | 15     | THR  |
| 12  | m     | 33     | GLN  |
| 13  | o     | 4      | THR  |
| 13  | o     | 23     | ASP  |
| 13  | o     | 25     | THR  |
| 13  | o     | 37     | THR  |
| 13  | o     | 57     | LYS  |
| 13  | o     | 69     | LYS  |
| 13  | o     | 141    | ASP  |
| 13  | o     | 194    | LYS  |
| 14  | t     | 25[A]  | GLU  |
| 14  | t     | 25[B]  | GLU  |
| 15  | u     | 86     | GLU  |
| 16  | v     | 42     | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | y     | 18  | VAL  |
| 17  | y     | 24  | MET  |
| 17  | y     | 30  | ILE  |
| 19  | z     | 7   | LEU  |
| 19  | z     | 29  | SER  |
| 19  | z     | 34  | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 75  | ASN  |
| 1   | A     | 165 | GLN  |
| 2   | B     | 53  | ASN  |
| 2   | B     | 331 | ASN  |
| 3   | C     | 44  | ASN  |
| 3   | C     | 418 | ASN  |
| 4   | D     | 61  | HIS  |
| 4   | D     | 83  | ASN  |
| 4   | D     | 255 | GLN  |
| 4   | D     | 301 | GLN  |
| 4   | D     | 332 | GLN  |
| 5   | E     | 74  | GLN  |
| 11  | L     | 13  | ASN  |
| 13  | O     | 61  | GLN  |
| 13  | O     | 124 | ASN  |
| 13  | O     | 147 | ASN  |
| 19  | Z     | 58  | ASN  |
| 1   | a     | 12  | ASN  |
| 1   | a     | 165 | GLN  |
| 1   | a     | 315 | ASN  |
| 2   | b     | 53  | ASN  |
| 2   | b     | 331 | ASN  |
| 3   | c     | 28  | GLN  |
| 3   | c     | 44  | ASN  |
| 3   | c     | 201 | ASN  |
| 3   | c     | 311 | GLN  |
| 3   | c     | 373 | ASN  |
| 4   | d     | 83  | ASN  |
| 4   | d     | 301 | GLN  |
| 4   | d     | 332 | GLN  |
| 5   | e     | 74  | GLN  |
| 10  | k     | 40  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | l     | 8   | GLN  |
| 13  | o     | 124 | ASN  |
| 13  | o     | 147 | ASN  |
| 13  | o     | 155 | ASN  |
| 15  | u     | 78  | ASN  |
| 15  | u     | 81  | HIS  |
| 19  | z     | 58  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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       | 0.68 | 0           | 7,9,11      | 1.31 | 1 (14%)     |
| 8   | FME  | i     | 1   | 8    | 8,9,10       | 0.66 | 0           | 7,9,11      | 1.28 | 1 (14%)     |
| 14  | FME  | t     | 1   | 14   | 8,9,10       | 0.80 | 0           | 7,9,11      | 2.19 | 4 (57%)     |
| 14  | FME  | T     | 1   | 14   | 8,9,10       | 0.68 | 0           | 7,9,11      | 1.31 | 1 (14%)     |
| 12  | FME  | m     | 1   | 12   | 8,9,10       | 0.64 | 0           | 7,9,11      | 1.52 | 3 (42%)     |
| 8   | FME  | I     | 1   | 8    | 8,9,10       | 0.62 | 0           | 7,9,11      | 1.09 | 1 (14%)     |

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   | -       | 1/7/9/11 | -     |
| 8   | FME  | i     | 1   | 8    | -       | 0/7/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 14  | FME  | t     | 1   | 14   | -       | 1/7/9/11 | -     |
| 14  | FME  | T     | 1   | 14   | -       | 1/7/9/11 | -     |
| 12  | FME  | m     | 1   | 12   | -       | 1/7/9/11 | -     |
| 8   | FME  | I     | 1   | 8    | -       | 2/7/9/11 | -     |

There are no bond length outliers.

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 14  | t     | 1   | FME  | CA-N-CN  | -3.45 | 117.52      | 122.82   |
| 14  | t     | 1   | FME  | C-CA-N   | 2.48  | 114.20      | 109.73   |
| 14  | t     | 1   | FME  | O-C-CA   | -2.44 | 118.37      | 124.78   |
| 14  | T     | 1   | FME  | O-C-CA   | -2.44 | 118.38      | 124.78   |
| 12  | m     | 1   | FME  | CA-N-CN  | -2.29 | 119.30      | 122.82   |
| 12  | m     | 1   | FME  | O-C-CA   | -2.22 | 118.97      | 124.78   |
| 12  | m     | 1   | FME  | O1-CN-N  | -2.17 | 119.56      | 125.27   |
| 8   | I     | 1   | FME  | O-C-CA   | -2.16 | 119.13      | 124.78   |
| 8   | i     | 1   | FME  | O-C-CA   | -2.11 | 119.25      | 124.78   |
| 14  | t     | 1   | FME  | CE-SD-CG | -2.04 | 93.40       | 100.40   |
| 12  | M     | 1   | FME  | CA-N-CN  | -2.01 | 119.73      | 122.82   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 8   | I     | 1   | FME  | O1-CN-N-CA |
| 14  | T     | 1   | FME  | O1-CN-N-CA |
| 12  | m     | 1   | FME  | CB-CA-N-CN |
| 8   | I     | 1   | FME  | CB-CA-N-CN |
| 12  | M     | 1   | FME  | CB-CA-N-CN |
| 14  | t     | 1   | FME  | CB-CA-N-CN |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | M     | 1   | FME  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 267 ligands modelled in this entry, 25 are monoatomic and 18 are unknown - leaving 224 for Mogul analysis.

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

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | CLA  | c     | 518    | 3      | 69,73,73     | 2.08 | 19 (27%) | 83,113,113  | 2.85 | 30 (36%) |
| 26  | BCR  | b     | 628    | -      | 41,41,41     | 1.08 | 1 (2%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 28  | GOL  | b     | 603    | -      | 5,5,5        | 0.33 | 0        | 5,5,5       | 0.12 | 0        |
| 27  | SQD  | F     | 103    | -      | 42,43,54     | 1.16 | 3 (7%)   | 51,54,65    | 1.59 | 11 (21%) |
| 24  | CLA  | c     | 511    | 3      | 69,73,73     | 2.02 | 20 (28%) | 83,113,113  | 2.75 | 31 (37%) |
| 24  | CLA  | b     | 621    | 2      | 69,73,73     | 2.04 | 20 (28%) | 83,113,113  | 2.77 | 32 (38%) |
| 26  | BCR  | k     | 101    | -      | 41,41,41     | 1.04 | 1 (2%)   | 56,56,56    | 1.41 | 8 (14%)  |
| 26  | BCR  | B     | 618    | -      | 41,41,41     | 1.05 | 1 (2%)   | 56,56,56    | 1.31 | 6 (10%)  |
| 36  | DGD  | c     | 522    | -      | 63,63,67     | 0.90 | 2 (3%)   | 77,77,81    | 1.01 | 4 (5%)   |
| 37  | LHG  | L     | 101    | -      | 48,48,48     | 0.90 | 2 (4%)   | 51,54,54    | 1.05 | 5 (9%)   |
| 28  | GOL  | B     | 630    | -      | 5,5,5        | 0.40 | 0        | 5,5,5       | 0.25 | 0        |
| 24  | CLA  | C     | 512    | 3      | 69,73,73     | 2.02 | 19 (27%) | 83,113,113  | 2.86 | 30 (36%) |
| 24  | CLA  | c     | 515    | 3      | 69,73,73     | 2.04 | 20 (28%) | 83,113,113  | 2.74 | 31 (37%) |
| 29  | LMT  | f     | 102    | -      | 36,36,36     | 0.47 | 0        | 47,47,47    | 0.91 | 1 (2%)   |
| 31  | PL9  | D     | 405[A] | -      | 55,55,55     | 0.65 | 1 (1%)   | 68,69,69    | 1.74 | 20 (29%) |
| 26  | BCR  | C     | 514    | -      | 41,41,41     | 1.04 | 1 (2%)   | 56,56,56    | 1.50 | 9 (16%)  |
| 26  | BCR  | B     | 620    | -      | 41,41,41     | 1.06 | 1 (2%)   | 56,56,56    | 1.43 | 6 (10%)  |
| 33  | LMG  | z     | 101    | -      | 39,39,55     | 1.08 | 2 (5%)   | 47,47,63    | 1.10 | 3 (6%)   |
| 30  | OEX  | A     | 418[A] | 3,1,41 | 0,14,14      | -    | -        | -           | -    | -        |
| 25  | PHO  | a     | 418[A] | -      | 58,69,69     | 2.76 | 14 (24%) | 56,99,99    | 2.93 | 13 (23%) |
| 24  | CLA  | b     | 616    | 41     | 69,73,73     | 1.99 | 18 (26%) | 83,113,113  | 2.85 | 28 (33%) |
| 24  | CLA  | C     | 504    | 41     | 69,73,73     | 2.06 | 20 (28%) | 83,113,113  | 2.83 | 28 (33%) |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | CLA  | b     | 611    | 2    | 69,73,73     | 2.03 | 20 (28%) | 83,113,113  | 2.92 | 29 (34%) |
| 33  | LMG  | c     | 501    | -    | 51,51,55     | 0.89 | 2 (3%)   | 59,59,63    | 1.17 | 4 (6%)   |
| 37  | LHG  | b     | 634    | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.01 | 4 (7%)   |
| 24  | CLA  | B     | 612    | 2    | 69,73,73     | 2.00 | 19 (27%) | 83,113,113  | 2.84 | 30 (36%) |
| 24  | CLA  | c     | 509    | 41   | 69,73,73     | 2.03 | 20 (28%) | 83,113,113  | 2.89 | 31 (37%) |
| 28  | GOL  | B     | 631    | -    | 5,5,5        | 0.40 | 0        | 5,5,5       | 0.28 | 0        |
| 28  | GOL  | O     | 301    | -    | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.39 | 0        |
| 37  | LHG  | e     | 102    | -    | 41,41,48     | 1.02 | 2 (4%)   | 44,47,54    | 0.95 | 2 (4%)   |
| 23  | BCT  | A     | 404[A] | 21   | 2,3,3        | 0.57 | 0        | 2,3,3       | 1.28 | 0        |
| 36  | DGD  | e     | 101    | -    | 63,63,67     | 0.92 | 2 (3%)   | 77,77,81    | 1.18 | 7 (9%)   |
| 25  | PHO  | a     | 411    | -    | 58,69,69     | 2.79 | 14 (24%) | 56,99,99    | 2.75 | 17 (30%) |
| 31  | PL9  | d     | 405[B] | -    | 55,55,55     | 0.65 | 2 (3%)   | 68,69,69    | 1.55 | 13 (19%) |
| 29  | LMT  | M     | 103    | -    | 36,36,36     | 0.53 | 1 (2%)   | 47,47,47    | 0.96 | 3 (6%)   |
| 24  | CLA  | B     | 614    | 2    | 69,73,73     | 2.03 | 19 (27%) | 83,113,113  | 2.72 | 34 (40%) |
| 37  | LHG  | E     | 101    | -    | 41,41,48     | 1.03 | 2 (4%)   | 44,47,54    | 1.08 | 4 (9%)   |
| 25  | PHO  | A     | 409[B] | -    | 58,69,69     | 2.77 | 15 (25%) | 56,99,99    | 2.86 | 14 (25%) |
| 26  | BCR  | y     | 101    | -    | 41,41,41     | 1.02 | 1 (2%)   | 56,56,56    | 1.48 | 7 (12%)  |
| 24  | CLA  | B     | 604    | 2    | 69,73,73     | 2.06 | 20 (28%) | 83,113,113  | 2.83 | 31 (37%) |
| 27  | SQD  | L     | 102    | -    | 53,54,54     | 1.03 | 3 (5%)   | 62,65,65    | 1.56 | 10 (16%) |
| 35  | HTG  | D     | 412    | -    | 16,16,19     | 1.13 | 2 (12%)  | 20,21,24    | 1.50 | 1 (5%)   |
| 29  | LMT  | B     | 635    | -    | 25,25,36     | 0.52 | 0        | 30,30,47    | 0.83 | 1 (3%)   |
| 29  | LMT  | m     | 103    | -    | 36,36,36     | 0.47 | 0        | 47,47,47    | 0.99 | 3 (6%)   |
| 24  | CLA  | b     | 623    | 2    | 69,73,73     | 2.02 | 20 (28%) | 83,113,113  | 2.83 | 32 (38%) |
| 33  | LMG  | D     | 413    | 39   | 51,51,55     | 0.87 | 2 (3%)   | 59,59,63    | 1.00 | 5 (8%)   |
| 28  | GOL  | v     | 201    | -    | 5,5,5        | 0.32 | 0        | 5,5,5       | 0.24 | 0        |
| 36  | DGD  | c     | 520    | -    | 63,63,67     | 0.84 | 2 (3%)   | 77,77,81    | 1.10 | 5 (6%)   |
| 26  | BCR  | D     | 404    | -    | 41,41,41     | 1.04 | 1 (2%)   | 56,56,56    | 1.68 | 9 (16%)  |
| 35  | HTG  | B     | 624    | -    | 19,19,19     | 0.78 | 1 (5%)   | 23,24,24    | 1.64 | 3 (13%)  |
| 24  | CLA  | b     | 610    | 41   | 69,73,73     | 2.07 | 20 (28%) | 83,113,113  | 2.82 | 28 (33%) |
| 35  | HTG  | B     | 623    | -    | 19,19,19     | 1.03 | 1 (5%)   | 23,24,24    | 1.18 | 1 (4%)   |
| 24  | CLA  | c     | 507    | 3    | 69,73,73     | 2.06 | 21 (30%) | 83,113,113  | 2.71 | 27 (32%) |
| 24  | CLA  | B     | 605    | 2    | 69,73,73     | 1.98 | 20 (28%) | 83,113,113  | 2.75 | 32 (38%) |
| 40  | HEC  | V     | 205    | 16   | 50,50,50     | 1.69 | 9 (18%)  | 68,82,82    | 1.74 | 16 (23%) |
| 29  | LMT  | D     | 401    | -    | 36,36,36     | 0.43 | 0        | 47,47,47    | 1.04 | 1 (2%)   |
| 28  | GOL  | B     | 629    | -    | 5,5,5        | 0.33 | 0        | 5,5,5       | 0.36 | 0        |
| 28  | GOL  | T     | 101    | -    | 5,5,5        | 0.45 | 0        | 5,5,5       | 0.13 | 0        |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | PL9  | A     | 419[A] | -      | 55,55,55     | 0.65 | 2 (3%)   | 68,69,69    | 1.77 | 22 (32%) |
| 36  | DGD  | h     | 102    | -      | 63,63,67     | 0.89 | 3 (4%)   | 77,77,81    | 0.97 | 4 (5%)   |
| 26  | BCR  | H     | 101    | -      | 41,41,41     | 1.06 | 1 (2%)   | 56,56,56    | 1.46 | 8 (14%)  |
| 26  | BCR  | A     | 411    | -      | 41,41,41     | 0.99 | 1 (2%)   | 56,56,56    | 1.14 | 6 (10%)  |
| 29  | LMT  | A     | 417    | -      | 36,36,36     | 0.59 | 1 (2%)   | 47,47,47    | 1.25 | 4 (8%)   |
| 28  | GOL  | c     | 503    | -      | 5,5,5        | 0.39 | 0        | 5,5,5       | 0.61 | 0        |
| 29  | LMT  | M     | 101    | -      | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.90 | 0        |
| 30  | OEX  | a     | 416[A] | 3,1,41 | 0,14,14      | -    | -        | -           | -    | -        |
| 35  | HTG  | B     | 632    | -      | 19,19,19     | 1.06 | 2 (10%)  | 23,24,24    | 1.40 | 3 (13%)  |
| 26  | BCR  | T     | 103    | -      | 41,41,41     | 1.07 | 1 (2%)   | 56,56,56    | 1.54 | 12 (21%) |
| 35  | HTG  | b     | 608    | -      | 19,19,19     | 1.06 | 2 (10%)  | 23,24,24    | 1.28 | 3 (13%)  |
| 28  | GOL  | B     | 628    | -      | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.54 | 0        |
| 24  | CLA  | d     | 403    | 4      | 69,73,73     | 2.04 | 21 (30%) | 83,113,113  | 2.87 | 30 (36%) |
| 23  | BCT  | a     | 417[A] | 21     | 2,3,3        | 0.64 | 0        | 2,3,3       | 0.78 | 0        |
| 28  | GOL  | A     | 413    | -      | 5,5,5        | 0.29 | 0        | 5,5,5       | 0.40 | 0        |
| 28  | GOL  | C     | 524    | -      | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.76 | 0        |
| 29  | LMT  | a     | 419    | -      | 36,36,36     | 0.45 | 0        | 47,47,47    | 0.77 | 0        |
| 28  | GOL  | v     | 203    | -      | 5,5,5        | 0.39 | 0        | 5,5,5       | 0.23 | 0        |
| 24  | CLA  | b     | 613    | 2      | 69,73,73     | 2.01 | 19 (27%) | 83,113,113  | 2.71 | 28 (33%) |
| 24  | CLA  | c     | 512    | 41     | 69,73,73     | 1.98 | 20 (28%) | 83,113,113  | 2.83 | 28 (33%) |
| 24  | CLA  | b     | 612    | 2      | 69,73,73     | 2.05 | 20 (28%) | 83,113,113  | 2.83 | 31 (37%) |
| 24  | CLA  | B     | 615    | 2      | 69,73,73     | 2.04 | 19 (27%) | 83,113,113  | 2.84 | 29 (34%) |
| 28  | GOL  | V     | 202    | -      | 5,5,5        | 0.39 | 0        | 5,5,5       | 0.37 | 0        |
| 24  | CLA  | a     | 409    | 1      | 69,73,73     | 2.03 | 20 (28%) | 83,113,113  | 2.79 | 30 (36%) |
| 24  | CLA  | C     | 503    | 3      | 69,73,73     | 2.07 | 18 (26%) | 83,113,113  | 2.75 | 27 (32%) |
| 24  | CLA  | c     | 506    | 3      | 69,73,73     | 2.01 | 20 (28%) | 83,113,113  | 2.77 | 28 (33%) |
| 26  | BCR  | b     | 627    | -      | 41,41,41     | 1.00 | 1 (2%)   | 56,56,56    | 1.25 | 4 (7%)   |
| 24  | CLA  | a     | 410    | 41     | 69,73,73     | 2.00 | 20 (28%) | 83,113,113  | 2.90 | 32 (38%) |
| 24  | CLA  | d     | 402    | 4      | 69,73,73     | 2.01 | 19 (27%) | 83,113,113  | 2.80 | 31 (37%) |
| 28  | GOL  | T     | 102    | -      | 5,5,5        | 0.40 | 0        | 5,5,5       | 0.26 | 0        |
| 28  | GOL  | t     | 102    | -      | 5,5,5        | 0.48 | 0        | 5,5,5       | 0.11 | 0        |
| 35  | HTG  | d     | 411    | -      | 16,16,19     | 1.14 | 2 (12%)  | 20,21,24    | 1.72 | 2 (10%)  |
| 25  | PHO  | A     | 408    | -      | 58,69,69     | 2.74 | 13 (22%) | 56,99,99    | 2.73 | 12 (21%) |
| 27  | SQD  | B     | 621    | -      | 53,54,54     | 1.02 | 3 (5%)   | 62,65,65    | 1.48 | 9 (14%)  |
| 27  | SQD  | a     | 414    | -      | 53,54,54     | 0.96 | 3 (5%)   | 62,65,65    | 1.63 | 13 (20%) |
| 24  | CLA  | b     | 624    | 2      | 69,73,73     | 2.01 | 20 (28%) | 83,113,113  | 2.79 | 29 (34%) |
| 35  | HTG  | C     | 523    | -      | 19,19,19     | 1.00 | 1 (5%)   | 23,24,24    | 1.78 | 4 (17%)  |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | CLA  | A     | 410    | 1      | 69,73,73     | 2.06 | 20 (28%) | 83,113,113  | 2.78 | 34 (40%) |
| 24  | CLA  | c     | 514    | 3      | 69,73,73     | 2.09 | 20 (28%) | 83,113,113  | 2.76 | 29 (34%) |
| 26  | BCR  | t     | 101    | -      | 41,41,41     | 1.00 | 1 (2%)   | 56,56,56    | 1.62 | 15 (26%) |
| 28  | GOL  | V     | 204    | -      | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.32 | 0        |
| 26  | BCR  | a     | 413    | -      | 41,41,41     | 1.03 | 1 (2%)   | 56,56,56    | 1.14 | 6 (10%)  |
| 24  | CLA  | C     | 505    | 3      | 69,73,73     | 2.01 | 20 (28%) | 83,113,113  | 2.71 | 28 (33%) |
| 31  | PL9  | a     | 415[B] | -      | 55,55,55     | 0.62 | 2 (3%)   | 68,69,69    | 1.91 | 20 (29%) |
| 33  | LMG  | C     | 520    | -      | 51,51,55     | 0.95 | 2 (3%)   | 59,59,63    | 1.12 | 4 (6%)   |
| 24  | CLA  | B     | 613    | 2      | 69,73,73     | 1.98 | 19 (27%) | 83,113,113  | 2.93 | 31 (37%) |
| 24  | CLA  | A     | 406    | 41     | 69,73,73     | 1.97 | 21 (30%) | 83,113,113  | 2.91 | 34 (40%) |
| 29  | LMT  | F     | 101    | -      | 36,36,36     | 0.47 | 0        | 47,47,47    | 0.93 | 1 (2%)   |
| 24  | CLA  | B     | 602    | 41     | 69,73,73     | 2.07 | 20 (28%) | 83,113,113  | 2.85 | 27 (32%) |
| 37  | LHG  | d     | 408    | -      | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.02 | 2 (3%)   |
| 24  | CLA  | c     | 516    | 3      | 69,73,73     | 2.01 | 19 (27%) | 83,113,113  | 2.75 | 30 (36%) |
| 36  | DGD  | H     | 102    | -      | 63,63,67     | 0.90 | 3 (4%)   | 77,77,81    | 1.01 | 8 (10%)  |
| 33  | LMG  | C     | 519    | -      | 51,51,55     | 0.95 | 2 (3%)   | 59,59,63    | 0.99 | 4 (6%)   |
| 24  | CLA  | C     | 510    | 3      | 69,73,73     | 2.07 | 20 (28%) | 83,113,113  | 2.71 | 30 (36%) |
| 36  | DGD  | C     | 516    | -      | 63,63,67     | 0.86 | 2 (3%)   | 77,77,81    | 1.16 | 8 (10%)  |
| 36  | DGD  | D     | 406    | -      | 52,52,67     | 1.02 | 3 (5%)   | 60,60,81    | 1.18 | 5 (8%)   |
| 33  | LMG  | Z     | 101    | -      | 37,37,55     | 0.96 | 2 (5%)   | 45,45,63    | 1.39 | 6 (13%)  |
| 35  | HTG  | c     | 526    | -      | 19,19,19     | 1.02 | 2 (10%)  | 23,24,24    | 1.47 | 2 (8%)   |
| 28  | GOL  | v     | 202    | -      | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.25 | 0        |
| 24  | CLA  | C     | 506    | 3      | 69,73,73     | 2.06 | 20 (28%) | 83,113,113  | 2.66 | 30 (36%) |
| 28  | GOL  | B     | 627    | -      | 5,5,5        | 0.33 | 0        | 5,5,5       | 0.47 | 0        |
| 24  | CLA  | b     | 620    | 2      | 69,73,73     | 2.00 | 19 (27%) | 83,113,113  | 2.81 | 30 (36%) |
| 24  | CLA  | b     | 619    | 41     | 69,73,73     | 2.04 | 22 (31%) | 83,113,113  | 2.82 | 30 (36%) |
| 26  | BCR  | b     | 626    | -      | 41,41,41     | 1.02 | 1 (2%)   | 56,56,56    | 1.43 | 6 (10%)  |
| 36  | DGD  | C     | 518    | -      | 63,63,67     | 0.87 | 2 (3%)   | 77,77,81    | 0.90 | 4 (5%)   |
| 29  | LMT  | b     | 630    | -      | 25,25,36     | 0.51 | 0        | 30,30,47    | 0.67 | 0        |
| 33  | LMG  | c     | 524    | -      | 51,51,55     | 0.96 | 2 (3%)   | 59,59,63    | 1.24 | 7 (11%)  |
| 35  | HTG  | c     | 525    | -      | 19,19,19     | 1.05 | 2 (10%)  | 23,24,24    | 1.55 | 2 (8%)   |
| 24  | CLA  | C     | 513    | 3      | 69,73,73     | 2.07 | 20 (28%) | 83,113,113  | 2.79 | 30 (36%) |
| 31  | PL9  | D     | 405[B] | -      | 55,55,55     | 0.63 | 2 (3%)   | 68,69,69    | 1.65 | 20 (29%) |
| 24  | CLA  | b     | 614    | 2      | 69,73,73     | 2.01 | 19 (27%) | 83,113,113  | 2.95 | 29 (34%) |
| 28  | GOL  | b     | 605    | -      | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.30 | 0        |
| 30  | OEX  | A     | 418[B] | 3,1,41 | 0,14,14      | -    | -        | -           | -    | -        |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | PHO  | a     | 418[B] | -    | 58,69,69     | 2.76 | 14 (24%) | 56,99,99    | 2.91 | 15 (26%) |
| 31  | PL9  | d     | 405[A] | -    | 55,55,55     | 0.70 | 2 (3%)   | 68,69,69    | 1.54 | 16 (23%) |
| 24  | CLA  | C     | 507    | 41   | 69,73,73     | 2.04 | 20 (28%) | 83,113,113  | 2.71 | 30 (36%) |
| 24  | CLA  | c     | 513    | 3    | 69,73,73     | 2.07 | 20 (28%) | 83,113,113  | 2.74 | 29 (34%) |
| 37  | LHG  | D     | 408    | -    | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 0.86 | 3 (5%)   |
| 24  | CLA  | C     | 509    | 3    | 69,73,73     | 2.12 | 20 (28%) | 83,113,113  | 2.79 | 28 (33%) |
| 24  | CLA  | c     | 510    | 3    | 69,73,73     | 2.02 | 20 (28%) | 83,113,113  | 2.71 | 28 (33%) |
| 24  | CLA  | A     | 405    | 1    | 69,73,73     | 2.03 | 20 (28%) | 83,113,113  | 2.74 | 29 (34%) |
| 28  | GOL  | b     | 602    | -    | 5,5,5        | 0.43 | 0        | 5,5,5       | 0.48 | 0        |
| 25  | PHO  | A     | 409[A] | -    | 58,69,69     | 2.80 | 15 (25%) | 56,99,99    | 2.79 | 13 (23%) |
| 24  | CLA  | b     | 618    | 2    | 69,73,73     | 2.02 | 19 (27%) | 83,113,113  | 2.80 | 30 (36%) |
| 28  | GOL  | b     | 606    | -    | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.28 | 0        |
| 35  | HTG  | V     | 206    | -    | 19,19,19     | 1.02 | 2 (10%)  | 23,24,24    | 1.32 | 3 (13%)  |
| 35  | HTG  | B     | 633    | -    | 19,19,19     | 1.01 | 2 (10%)  | 23,24,24    | 1.44 | 1 (4%)   |
| 24  | CLA  | C     | 502    | 3    | 69,73,73     | 2.02 | 20 (28%) | 83,113,113  | 2.76 | 29 (34%) |
| 23  | BCT  | A     | 404[B] | 21   | 2,3,3        | 0.63 | 0        | 2,3,3       | 1.10 | 0        |
| 27  | SQD  | A     | 412    | -    | 53,54,54     | 0.97 | 3 (5%)   | 62,65,65    | 1.53 | 11 (17%) |
| 37  | LHG  | D     | 409    | -    | 48,48,48     | 0.97 | 2 (4%)   | 51,54,54    | 1.03 | 3 (5%)   |
| 33  | LMG  | c     | 523    | -    | 51,51,55     | 0.90 | 2 (3%)   | 59,59,63    | 1.12 | 4 (6%)   |
| 35  | HTG  | b     | 631    | -    | 19,19,19     | 0.81 | 1 (5%)   | 23,24,24    | 1.41 | 2 (8%)   |
| 26  | BCR  | B     | 619    | -    | 41,41,41     | 1.03 | 1 (2%)   | 56,56,56    | 1.44 | 9 (16%)  |
| 27  | SQD  | f     | 101    | -    | 42,43,54     | 1.19 | 3 (7%)   | 51,54,65    | 1.46 | 9 (17%)  |
| 29  | LMT  | C     | 521    | -    | 36,36,36     | 0.48 | 0        | 47,47,47    | 1.21 | 3 (6%)   |
| 24  | CLA  | D     | 402    | 4    | 69,73,73     | 1.99 | 20 (28%) | 83,113,113  | 2.89 | 31 (37%) |
| 24  | CLA  | B     | 617    | 2    | 69,73,73     | 2.03 | 20 (28%) | 83,113,113  | 2.80 | 29 (34%) |
| 24  | CLA  | C     | 501    | 3    | 69,73,73     | 2.04 | 19 (27%) | 83,113,113  | 2.83 | 30 (36%) |
| 38  | HEM  | F     | 102    | 6,5  | 50,50,50     | 1.56 | 6 (12%)  | 66,82,82    | 1.86 | 16 (24%) |
| 26  | BCR  | K     | 101    | -    | 41,41,41     | 1.02 | 1 (2%)   | 56,56,56    | 1.45 | 9 (16%)  |
| 28  | GOL  | V     | 203    | -    | 5,5,5        | 0.38 | 0        | 5,5,5       | 0.29 | 0        |
| 24  | CLA  | b     | 622    | 2    | 69,73,73     | 2.04 | 20 (28%) | 83,113,113  | 2.68 | 29 (34%) |
| 24  | CLA  | D     | 403    | 4    | 69,73,73     | 2.05 | 20 (28%) | 83,113,113  | 2.81 | 29 (34%) |
| 40  | HEC  | v     | 205    | 16   | 50,50,50     | 1.67 | 9 (18%)  | 68,82,82    | 1.82 | 20 (29%) |
| 24  | CLA  | c     | 517    | 3    | 69,73,73     | 2.07 | 20 (28%) | 83,113,113  | 2.93 | 32 (38%) |
| 28  | GOL  | A     | 414    | -    | 5,5,5        | 0.44 | 0        | 5,5,5       | 0.48 | 0        |
| 37  | LHG  | D     | 407    | -    | 48,48,48     | 0.84 | 2 (4%)   | 51,54,54    | 1.14 | 5 (9%)   |
| 24  | CLA  | B     | 603    | 2    | 69,73,73     | 2.06 | 20 (28%) | 83,113,113  | 2.86 | 31 (37%) |



| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | CLA  | b     | 615    | 2      | 69,73,73     | 1.99 | 19 (27%) | 83,113,113  | 2.88 | 28 (33%) |
| 28  | GOL  | o     | 301    | -      | 5,5,5        | 0.38 | 0        | 5,5,5       | 0.22 | 0        |
| 33  | LMG  | A     | 421    | -      | 51,51,55     | 0.93 | 2 (3%)   | 59,59,63    | 1.10 | 4 (6%)   |
| 28  | GOL  | C     | 525    | -      | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.48 | 0        |
| 24  | CLA  | B     | 607    | 2      | 69,73,73     | 2.01 | 20 (28%) | 83,113,113  | 2.93 | 32 (38%) |
| 33  | LMG  | B     | 622    | -      | 51,51,55     | 0.92 | 2 (3%)   | 59,59,63    | 1.07 | 5 (8%)   |
| 35  | HTG  | b     | 601    | -      | 19,19,19     | 0.97 | 1 (5%)   | 23,24,24    | 1.09 | 2 (8%)   |
| 27  | SQD  | a     | 405    | -      | 53,54,54     | 1.06 | 3 (5%)   | 62,65,65    | 1.20 | 5 (8%)   |
| 31  | PL9  | A     | 419[B] | -      | 55,55,55     | 0.62 | 1 (1%)   | 68,69,69    | 1.76 | 21 (30%) |
| 24  | CLA  | A     | 407    | 41     | 69,73,73     | 2.06 | 20 (28%) | 83,113,113  | 2.89 | 32 (38%) |
| 26  | BCR  | C     | 515    | -      | 41,41,41     | 1.00 | 1 (2%)   | 56,56,56    | 1.48 | 10 (17%) |
| 28  | GOL  | a     | 401    | -      | 5,5,5        | 0.44 | 0        | 5,5,5       | 0.48 | 0        |
| 35  | HTG  | C     | 522    | -      | 19,19,19     | 1.03 | 2 (10%)  | 23,24,24    | 1.59 | 2 (8%)   |
| 38  | HEM  | e     | 103    | 6,5    | 50,50,50     | 1.53 | 8 (16%)  | 66,82,82    | 1.76 | 15 (22%) |
| 24  | CLA  | C     | 508    | 3      | 69,73,73     | 2.09 | 20 (28%) | 83,113,113  | 2.80 | 25 (30%) |
| 24  | CLA  | B     | 610    | 2      | 69,73,73     | 2.03 | 19 (27%) | 83,113,113  | 2.76 | 29 (34%) |
| 26  | BCR  | c     | 528    | -      | 41,41,41     | 1.03 | 1 (2%)   | 56,56,56    | 1.48 | 7 (12%)  |
| 36  | DGD  | C     | 517    | -      | 63,63,67     | 0.87 | 2 (3%)   | 77,77,81    | 1.05 | 6 (7%)   |
| 29  | LMT  | m     | 102    | -      | 36,36,36     | 0.47 | 0        | 47,47,47    | 0.83 | 0        |
| 28  | GOL  | A     | 422    | 34     | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.22 | 0        |
| 37  | LHG  | d     | 406    | -      | 48,48,48     | 0.90 | 3 (6%)   | 51,54,54    | 1.04 | 4 (7%)   |
| 24  | CLA  | B     | 609    | 2      | 69,73,73     | 2.03 | 19 (27%) | 83,113,113  | 2.80 | 31 (37%) |
| 35  | HTG  | b     | 632    | -      | 19,19,19     | 1.13 | 2 (10%)  | 23,24,24    | 1.75 | 3 (13%)  |
| 30  | OEX  | a     | 416[B] | 3,1,41 | 0,14,14      | -    | -        | -           | -    | -        |
| 24  | CLA  | B     | 608    | 41     | 69,73,73     | 1.93 | 20 (28%) | 83,113,113  | 2.79 | 33 (39%) |
| 27  | SQD  | A     | 416    | -      | 53,54,54     | 1.04 | 3 (5%)   | 62,65,65    | 1.14 | 4 (6%)   |
| 24  | CLA  | b     | 617    | 2      | 69,73,73     | 2.08 | 20 (28%) | 83,113,113  | 2.69 | 30 (36%) |
| 28  | GOL  | a     | 420    | 34     | 5,5,5        | 0.33 | 0        | 5,5,5       | 0.41 | 0        |
| 35  | HTG  | b     | 607    | -      | 19,19,19     | 1.00 | 2 (10%)  | 23,24,24    | 1.22 | 1 (4%)   |
| 23  | BCT  | a     | 417[B] | 21     | 2,3,3        | 0.66 | 0        | 2,3,3       | 0.85 | 0        |
| 28  | GOL  | A     | 415    | -      | 5,5,5        | 0.41 | 0        | 5,5,5       | 0.22 | 0        |
| 28  | GOL  | V     | 201    | -      | 5,5,5        | 0.39 | 0        | 5,5,5       | 0.32 | 0        |
| 24  | CLA  | d     | 401    | 41     | 69,73,73     | 2.05 | 19 (27%) | 83,113,113  | 2.81 | 34 (40%) |
| 26  | BCR  | h     | 101    | -      | 41,41,41     | 1.05 | 1 (2%)   | 56,56,56    | 1.44 | 8 (14%)  |
| 37  | LHG  | d     | 407    | -      | 48,48,48     | 0.88 | 2 (4%)   | 51,54,54    | 0.99 | 4 (7%)   |
| 33  | LMG  | d     | 413    | 39     | 51,51,55     | 0.92 | 2 (3%)   | 59,59,63    | 0.94 | 3 (5%)   |
| 24  | CLA  | C     | 511    | 3      | 69,73,73     | 2.06 | 20 (28%) | 83,113,113  | 2.73 | 31 (37%) |



| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | BCR  | d     | 404    | -    | 41,41,41     | 1.10 | 1 (2%)   | 56,56,56    | 1.69 | 13 (23%) |
| 28  | GOL  | B     | 636    | -    | 5,5,5        | 0.40 | 0        | 5,5,5       | 0.46 | 0        |
| 28  | GOL  | B     | 626    | -    | 5,5,5        | 0.43 | 0        | 5,5,5       | 0.36 | 0        |
| 31  | PL9  | a     | 415[A] | -    | 55,55,55     | 0.63 | 2 (3%)   | 68,69,69    | 1.91 | 20 (29%) |
| 36  | DGD  | c     | 521    | -    | 63,63,67     | 0.88 | 2 (3%)   | 77,77,81    | 0.94 | 5 (6%)   |
| 26  | BCR  | Y     | 101    | -    | 41,41,41     | 1.02 | 1 (2%)   | 56,56,56    | 1.60 | 10 (17%) |
| 35  | HTG  | B     | 625    | -    | 19,19,19     | 1.06 | 2 (10%)  | 23,24,24    | 1.85 | 4 (17%)  |
| 28  | GOL  | b     | 604    | -    | 5,5,5        | 0.38 | 0        | 5,5,5       | 0.24 | 0        |
| 33  | LMG  | b     | 629    | -    | 51,51,55     | 0.90 | 2 (3%)   | 59,59,63    | 1.07 | 5 (8%)   |
| 24  | CLA  | B     | 606    | 2    | 69,73,73     | 2.04 | 19 (27%) | 83,113,113  | 2.91 | 28 (33%) |
| 24  | CLA  | c     | 508    | 3    | 69,73,73     | 2.06 | 19 (27%) | 83,113,113  | 2.85 | 27 (32%) |
| 24  | CLA  | B     | 616    | 2    | 69,73,73     | 1.99 | 18 (26%) | 83,113,113  | 2.84 | 28 (33%) |
| 28  | GOL  | a     | 402    | -    | 5,5,5        | 0.38 | 0        | 5,5,5       | 0.26 | 0        |
| 24  | CLA  | a     | 412    | 1    | 69,73,73     | 2.03 | 19 (27%) | 83,113,113  | 2.85 | 31 (37%) |
| 29  | LMT  | a     | 404    | -    | 36,36,36     | 0.46 | 0        | 47,47,47    | 1.08 | 3 (6%)   |
| 28  | GOL  | c     | 502    | -    | 5,5,5        | 0.27 | 0        | 5,5,5       | 0.47 | 0        |
| 24  | CLA  | b     | 625    | 2    | 69,73,73     | 2.01 | 19 (27%) | 83,113,113  | 2.84 | 32 (38%) |
| 26  | BCR  | c     | 519    | -    | 41,41,41     | 1.02 | 1 (2%)   | 56,56,56    | 1.44 | 7 (12%)  |
| 29  | LMT  | T     | 104    | -    | 25,25,36     | 0.50 | 0        | 30,30,47    | 0.96 | 1 (3%)   |
| 24  | CLA  | B     | 611    | 41   | 69,73,73     | 2.10 | 21 (30%) | 83,113,113  | 2.82 | 33 (39%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 24  | CLA  | c     | 518 | 3    | -       | 5/39/115/115  | -       |
| 26  | BCR  | b     | 628 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 28  | GOL  | b     | 603 | -    | -       | 0/4/4/4       | -       |
| 27  | SQD  | F     | 103 | -    | -       | 15/38/58/69   | 0/1/1/1 |
| 24  | CLA  | c     | 511 | 3    | -       | 10/39/115/115 | -       |
| 24  | CLA  | b     | 621 | 2    | -       | 3/39/115/115  | -       |
| 26  | BCR  | k     | 101 | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 26  | BCR  | B     | 618 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 36  | DGD  | c     | 522 | -    | -       | 14/51/91/95   | 0/2/2/2 |
| 37  | LHG  | L     | 101 | -    | -       | 14/53/53/53   | -       |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|--------|------|---------|---------------|---------|
| 28  | GOL  | B     | 630    | -    | -       | 4/4/4/4       | -       |
| 24  | CLA  | C     | 512    | 3    | -       | 12/39/115/115 | -       |
| 24  | CLA  | c     | 515    | 3    | -       | 9/39/115/115  | -       |
| 29  | LMT  | f     | 102    | -    | -       | 10/21/61/61   | 0/2/2/2 |
| 31  | PL9  | D     | 405[A] | -    | -       | 7/53/73/73    | 0/1/1/1 |
| 26  | BCR  | C     | 514    | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | BCR  | B     | 620    | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 33  | LMG  | z     | 101    | -    | -       | 14/34/54/70   | 0/1/1/1 |
| 25  | PHO  | a     | 418[A] | -    | -       | 0/37/103/103  | 0/5/6/6 |
| 24  | CLA  | b     | 616    | 41   | -       | 3/39/115/115  | -       |
| 24  | CLA  | C     | 504    | 41   | -       | 6/39/115/115  | -       |
| 24  | CLA  | b     | 611    | 2    | -       | 5/39/115/115  | -       |
| 33  | LMG  | c     | 501    | -    | -       | 15/46/66/70   | 0/1/1/1 |
| 37  | LHG  | b     | 634    | -    | -       | 16/53/53/53   | -       |
| 24  | CLA  | B     | 612    | 2    | -       | 4/39/115/115  | -       |
| 24  | CLA  | c     | 509    | 41   | -       | 4/39/115/115  | -       |
| 28  | GOL  | B     | 631    | -    | -       | 0/4/4/4       | -       |
| 28  | GOL  | O     | 301    | -    | -       | 2/4/4/4       | -       |
| 37  | LHG  | e     | 102    | -    | -       | 17/46/46/53   | -       |
| 36  | DGD  | e     | 101    | -    | -       | 27/51/91/95   | 0/2/2/2 |
| 25  | PHO  | a     | 411    | -    | -       | 5/37/103/103  | 0/5/6/6 |
| 31  | PL9  | d     | 405[B] | -    | -       | 8/53/73/73    | 0/1/1/1 |
| 29  | LMT  | M     | 103    | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 24  | CLA  | B     | 614    | 2    | -       | 5/39/115/115  | -       |
| 37  | LHG  | E     | 101    | -    | -       | 25/46/46/53   | -       |
| 25  | PHO  | A     | 409[B] | -    | -       | 0/37/103/103  | 0/5/6/6 |
| 26  | BCR  | y     | 101    | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 24  | CLA  | B     | 604    | 2    | -       | 4/39/115/115  | -       |
| 27  | SQD  | L     | 102    | -    | -       | 23/49/69/69   | 0/1/1/1 |
| 35  | HTG  | D     | 412    | -    | -       | 0/7/27/30     | 0/1/1/1 |
| 29  | LMT  | B     | 635    | -    | -       | 7/17/37/61    | 0/1/1/2 |
| 29  | LMT  | m     | 103    | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 24  | CLA  | b     | 623    | 2    | -       | 22/39/115/115 | -       |
| 33  | LMG  | D     | 413    | 39   | -       | 9/46/66/70    | 0/1/1/1 |
| 28  | GOL  | v     | 201    | -    | -       | 2/4/4/4       | -       |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|--------|------|---------|---------------|---------|
| 36  | DGD  | c     | 520    | -    | -       | 13/51/91/95   | 0/2/2/2 |
| 40  | HEC  | V     | 205    | 16   | 1/1/3/7 | 4/14/54/54    | -       |
| 26  | BCR  | D     | 404    | -    | -       | 8/29/63/63    | 0/2/2/2 |
| 24  | CLA  | b     | 610    | 41   | -       | 19/39/115/115 | -       |
| 35  | HTG  | B     | 623    | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 24  | CLA  | c     | 507    | 3    | -       | 9/39/115/115  | -       |
| 24  | CLA  | B     | 605    | 2    | -       | 4/39/115/115  | -       |
| 35  | HTG  | B     | 624    | -    | -       | 5/10/30/30    | 0/1/1/1 |
| 29  | LMT  | D     | 401    | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 28  | GOL  | B     | 629    | -    | -       | 2/4/4/4       | -       |
| 28  | GOL  | T     | 101    | -    | -       | 0/4/4/4       | -       |
| 31  | PL9  | A     | 419[A] | -    | -       | 14/53/73/73   | 0/1/1/1 |
| 36  | DGD  | h     | 102    | -    | -       | 12/51/91/95   | 0/2/2/2 |
| 26  | BCR  | H     | 101    | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 26  | BCR  | A     | 411    | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 29  | LMT  | A     | 417    | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 28  | GOL  | c     | 503    | -    | -       | 1/4/4/4       | -       |
| 29  | LMT  | M     | 101    | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 35  | HTG  | B     | 632    | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 26  | BCR  | T     | 103    | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 35  | HTG  | b     | 608    | -    | -       | 0/10/30/30    | 0/1/1/1 |
| 28  | GOL  | B     | 628    | -    | -       | 2/4/4/4       | -       |
| 24  | CLA  | d     | 403    | 4    | -       | 4/39/115/115  | -       |
| 29  | LMT  | a     | 419    | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 28  | GOL  | A     | 413    | -    | -       | 0/4/4/4       | -       |
| 28  | GOL  | C     | 524    | -    | -       | 2/4/4/4       | -       |
| 28  | GOL  | v     | 203    | -    | -       | 2/4/4/4       | -       |
| 24  | CLA  | b     | 613    | 2    | -       | 5/39/115/115  | -       |
| 24  | CLA  | c     | 512    | 41   | -       | 7/39/115/115  | -       |
| 24  | CLA  | b     | 612    | 2    | -       | 4/39/115/115  | -       |
| 24  | CLA  | B     | 615    | 2    | -       | 14/39/115/115 | -       |
| 28  | GOL  | V     | 202    | -    | -       | 2/4/4/4       | -       |
| 24  | CLA  | a     | 409    | 1    | -       | 4/39/115/115  | -       |
| 24  | CLA  | C     | 503    | 3    | -       | 2/39/115/115  | -       |
| 24  | CLA  | c     | 506    | 3    | -       | 4/39/115/115  | -       |
| 26  | BCR  | b     | 627    | -    | -       | 1/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|--------|------|---------|---------------|---------|
| 24  | CLA  | a     | 410    | 41   | -       | 9/39/115/115  | -       |
| 24  | CLA  | d     | 402    | 4    | -       | 4/39/115/115  | -       |
| 28  | GOL  | T     | 102    | -    | -       | 2/4/4/4       | -       |
| 28  | GOL  | t     | 102    | -    | -       | 0/4/4/4       | -       |
| 35  | HTG  | d     | 411    | -    | -       | 1/7/27/30     | 0/1/1/1 |
| 25  | PHO  | A     | 408    | -    | -       | 3/37/103/103  | 0/5/6/6 |
| 27  | SQD  | B     | 621    | -    | -       | 20/49/69/69   | 0/1/1/1 |
| 27  | SQD  | a     | 414    | -    | -       | 15/49/69/69   | 0/1/1/1 |
| 24  | CLA  | b     | 624    | 2    | -       | 3/39/115/115  | -       |
| 35  | HTG  | C     | 523    | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 24  | CLA  | A     | 410    | 1    | -       | 10/39/115/115 | -       |
| 24  | CLA  | c     | 514    | 3    | -       | 13/39/115/115 | -       |
| 26  | BCR  | t     | 101    | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 28  | GOL  | V     | 204    | -    | -       | 0/4/4/4       | -       |
| 26  | BCR  | a     | 413    | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 24  | CLA  | C     | 505    | 3    | -       | 7/39/115/115  | -       |
| 31  | PL9  | a     | 415[B] | -    | -       | 14/53/73/73   | 0/1/1/1 |
| 33  | LMG  | C     | 520    | -    | -       | 10/46/66/70   | 0/1/1/1 |
| 24  | CLA  | B     | 613    | 2    | -       | 3/39/115/115  | -       |
| 24  | CLA  | A     | 406    | 41   | -       | 4/39/115/115  | -       |
| 29  | LMT  | F     | 101    | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 24  | CLA  | B     | 602    | 41   | -       | 15/39/115/115 | -       |
| 37  | LHG  | d     | 408    | -    | -       | 10/53/53/53   | -       |
| 24  | CLA  | c     | 516    | 3    | -       | 5/39/115/115  | -       |
| 36  | DGD  | H     | 102    | -    | -       | 11/51/91/95   | 0/2/2/2 |
| 33  | LMG  | C     | 519    | -    | -       | 10/46/66/70   | 0/1/1/1 |
| 24  | CLA  | C     | 510    | 3    | -       | 9/39/115/115  | -       |
| 36  | DGD  | C     | 516    | -    | -       | 12/51/91/95   | 0/2/2/2 |
| 36  | DGD  | D     | 406    | -    | -       | 22/47/67/95   | 0/1/1/2 |
| 33  | LMG  | Z     | 101    | -    | -       | 14/31/51/70   | 0/1/1/1 |
| 35  | HTG  | c     | 526    | -    | -       | 0/10/30/30    | 0/1/1/1 |
| 28  | GOL  | v     | 202    | -    | -       | 2/4/4/4       | -       |
| 24  | CLA  | C     | 506    | 3    | -       | 7/39/115/115  | -       |
| 28  | GOL  | B     | 627    | -    | -       | 2/4/4/4       | -       |
| 24  | CLA  | b     | 620    | 2    | -       | 3/39/115/115  | -       |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|--------|------|---------|---------------|---------|
| 24  | CLA  | b     | 619    | 41   | -       | 8/39/115/115  | -       |
| 26  | BCR  | b     | 626    | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 36  | DGD  | C     | 518    | -    | -       | 10/51/91/95   | 0/2/2/2 |
| 29  | LMT  | b     | 630    | -    | -       | 4/17/37/61    | 0/1/1/2 |
| 33  | LMG  | c     | 524    | -    | -       | 4/46/66/70    | 0/1/1/1 |
| 35  | HTG  | c     | 525    | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 24  | CLA  | C     | 513    | 3    | -       | 7/39/115/115  | -       |
| 31  | PL9  | D     | 405[B] | -    | -       | 8/53/73/73    | 0/1/1/1 |
| 24  | CLA  | b     | 614    | 2    | -       | 4/39/115/115  | -       |
| 28  | GOL  | b     | 605    | -    | -       | 2/4/4/4       | -       |
| 25  | PHO  | a     | 418[B] | -    | -       | 1/37/103/103  | 0/5/6/6 |
| 31  | PL9  | d     | 405[A] | -    | -       | 5/53/73/73    | 0/1/1/1 |
| 24  | CLA  | C     | 507    | 41   | -       | 8/39/115/115  | -       |
| 24  | CLA  | c     | 513    | 3    | -       | 5/39/115/115  | -       |
| 37  | LHG  | D     | 408    | -    | -       | 8/53/53/53    | -       |
| 24  | CLA  | C     | 509    | 3    | -       | 11/39/115/115 | -       |
| 24  | CLA  | c     | 510    | 3    | -       | 3/39/115/115  | -       |
| 24  | CLA  | A     | 405    | 1    | -       | 4/39/115/115  | -       |
| 28  | GOL  | b     | 602    | -    | -       | 0/4/4/4       | -       |
| 25  | PHO  | A     | 409[A] | -    | -       | 0/37/103/103  | 0/5/6/6 |
| 24  | CLA  | b     | 618    | 2    | -       | 6/39/115/115  | -       |
| 28  | GOL  | b     | 606    | -    | -       | 2/4/4/4       | -       |
| 35  | HTG  | V     | 206    | -    | -       | 4/10/30/30    | 0/1/1/1 |
| 35  | HTG  | B     | 633    | -    | -       | 0/10/30/30    | 0/1/1/1 |
| 24  | CLA  | C     | 502    | 3    | -       | 7/39/115/115  | -       |
| 27  | SQD  | A     | 412    | -    | -       | 11/49/69/69   | 0/1/1/1 |
| 37  | LHG  | D     | 409    | -    | -       | 10/53/53/53   | -       |
| 33  | LMG  | c     | 523    | -    | -       | 13/46/66/70   | 0/1/1/1 |
| 35  | HTG  | b     | 631    | -    | -       | 2/10/30/30    | 0/1/1/1 |
| 26  | BCR  | B     | 619    | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 27  | SQD  | f     | 101    | -    | -       | 12/38/58/69   | 0/1/1/1 |
| 29  | LMT  | C     | 521    | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 24  | CLA  | D     | 402    | 4    | -       | 0/39/115/115  | -       |
| 24  | CLA  | B     | 617    | 2    | -       | 6/39/115/115  | -       |
| 24  | CLA  | C     | 501    | 3    | -       | 6/39/115/115  | -       |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|--------|------|---------|---------------|---------|
| 38  | HEM  | F     | 102    | 6,5  | -       | 8/14/54/54    | -       |
| 26  | BCR  | K     | 101    | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 28  | GOL  | V     | 203    | -    | -       | 1/4/4/4       | -       |
| 24  | CLA  | b     | 622    | 2    | -       | 3/39/115/115  | -       |
| 24  | CLA  | D     | 403    | 4    | -       | 5/39/115/115  | -       |
| 40  | HEC  | v     | 205    | 16   | 1/1/3/7 | 4/14/54/54    | -       |
| 24  | CLA  | c     | 517    | 3    | -       | 12/39/115/115 | -       |
| 28  | GOL  | A     | 414    | -    | -       | 2/4/4/4       | -       |
| 37  | LHG  | D     | 407    | -    | -       | 10/53/53/53   | -       |
| 24  | CLA  | B     | 603    | 2    | -       | 4/39/115/115  | -       |
| 24  | CLA  | b     | 615    | 2    | -       | 10/39/115/115 | -       |
| 28  | GOL  | o     | 301    | -    | -       | 4/4/4/4       | -       |
| 33  | LMG  | A     | 421    | -    | -       | 18/46/66/70   | 0/1/1/1 |
| 28  | GOL  | C     | 525    | -    | -       | 0/4/4/4       | -       |
| 24  | CLA  | B     | 607    | 2    | -       | 4/39/115/115  | -       |
| 33  | LMG  | B     | 622    | -    | -       | 6/46/66/70    | 0/1/1/1 |
| 35  | HTG  | b     | 601    | -    | -       | 3/10/30/30    | 0/1/1/1 |
| 27  | SQD  | a     | 405    | -    | -       | 15/49/69/69   | 0/1/1/1 |
| 31  | PL9  | A     | 419[B] | -    | -       | 10/53/73/73   | 0/1/1/1 |
| 24  | CLA  | A     | 407    | 41   | -       | 3/39/115/115  | -       |
| 26  | BCR  | C     | 515    | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 28  | GOL  | a     | 401    | -    | -       | 2/4/4/4       | -       |
| 35  | HTG  | C     | 522    | -    | -       | 0/10/30/30    | 0/1/1/1 |
| 38  | HEM  | e     | 103    | 6,5  | -       | 10/14/54/54   | -       |
| 24  | CLA  | C     | 508    | 3    | -       | 4/39/115/115  | -       |
| 24  | CLA  | B     | 610    | 2    | -       | 4/39/115/115  | -       |
| 26  | BCR  | c     | 528    | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 36  | DGD  | C     | 517    | -    | -       | 16/51/91/95   | 0/2/2/2 |
| 29  | LMT  | m     | 102    | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 28  | GOL  | A     | 422    | 34   | -       | 2/4/4/4       | -       |
| 37  | LHG  | d     | 406    | -    | -       | 11/53/53/53   | -       |
| 24  | CLA  | B     | 609    | 2    | -       | 1/39/115/115  | -       |
| 35  | HTG  | b     | 632    | -    | -       | 6/10/30/30    | 0/1/1/1 |
| 24  | CLA  | B     | 608    | 41   | -       | 6/39/115/115  | -       |
| 27  | SQD  | A     | 416    | -    | -       | 16/49/69/69   | 0/1/1/1 |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|--------|------|---------|---------------|---------|
| 24  | CLA  | b     | 617    | 2    | -       | 2/39/115/115  | -       |
| 28  | GOL  | a     | 420    | 34   | -       | 3/4/4/4       | -       |
| 35  | HTG  | b     | 607    | -    | -       | 1/10/30/30    | 0/1/1/1 |
| 28  | GOL  | A     | 415    | -    | -       | 2/4/4/4       | -       |
| 28  | GOL  | V     | 201    | -    | -       | 2/4/4/4       | -       |
| 24  | CLA  | d     | 401    | 41   | -       | 6/39/115/115  | -       |
| 26  | BCR  | h     | 101    | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 37  | LHG  | d     | 407    | -    | -       | 7/53/53/53    | -       |
| 33  | LMG  | d     | 413    | 39   | -       | 11/46/66/70   | 0/1/1/1 |
| 24  | CLA  | C     | 511    | 3    | -       | 3/39/115/115  | -       |
| 26  | BCR  | d     | 404    | -    | -       | 6/29/63/63    | 0/2/2/2 |
| 28  | GOL  | B     | 636    | -    | -       | 0/4/4/4       | -       |
| 28  | GOL  | B     | 626    | -    | -       | 2/4/4/4       | -       |
| 31  | PL9  | a     | 415[A] | -    | -       | 18/53/73/73   | 0/1/1/1 |
| 36  | DGD  | c     | 521    | -    | -       | 16/51/91/95   | 0/2/2/2 |
| 26  | BCR  | Y     | 101    | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 35  | HTG  | B     | 625    | -    | -       | 4/10/30/30    | 0/1/1/1 |
| 28  | GOL  | b     | 604    | -    | -       | 2/4/4/4       | -       |
| 33  | LMG  | b     | 629    | -    | -       | 11/46/66/70   | 0/1/1/1 |
| 24  | CLA  | B     | 606    | 2    | -       | 4/39/115/115  | -       |
| 24  | CLA  | c     | 508    | 3    | -       | 2/39/115/115  | -       |
| 24  | CLA  | B     | 616    | 2    | -       | 13/39/115/115 | -       |
| 28  | GOL  | a     | 402    | -    | -       | 2/4/4/4       | -       |
| 24  | CLA  | a     | 412    | 1    | -       | 11/39/115/115 | -       |
| 29  | LMT  | a     | 404    | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 28  | GOL  | c     | 502    | -    | -       | 0/4/4/4       | -       |
| 24  | CLA  | b     | 625    | 2    | -       | 8/39/115/115  | -       |
| 26  | BCR  | c     | 519    | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 29  | LMT  | T     | 104    | -    | -       | 7/17/37/61    | 0/1/1/2 |
| 24  | CLA  | B     | 611    | 41   | -       | 4/39/115/115  | -       |

All (1655) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 25  | a     | 418[A] | PHO  | C1B-C2B | 9.17 | 1.49        | 1.39     |
| 25  | A     | 408    | PHO  | C1D-C2D | 9.13 | 1.49        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 25  | A     | 408    | PHO  | C1B-C2B | 9.07 | 1.49        | 1.39     |
| 25  | a     | 411    | PHO  | C1D-C2D | 8.98 | 1.49        | 1.39     |
| 25  | A     | 409[A] | PHO  | C1D-C2D | 8.97 | 1.49        | 1.39     |
| 25  | a     | 418[B] | PHO  | C1D-C2D | 8.72 | 1.49        | 1.39     |
| 25  | a     | 411    | PHO  | C1B-C2B | 8.66 | 1.49        | 1.39     |
| 25  | a     | 418[A] | PHO  | C1D-C2D | 8.66 | 1.49        | 1.39     |
| 25  | a     | 418[B] | PHO  | C1B-C2B | 8.63 | 1.49        | 1.39     |
| 25  | A     | 409[A] | PHO  | C1B-C2B | 8.49 | 1.49        | 1.39     |
| 25  | A     | 409[B] | PHO  | C1D-C2D | 8.49 | 1.49        | 1.39     |
| 25  | A     | 409[B] | PHO  | C1B-C2B | 8.30 | 1.48        | 1.39     |
| 25  | a     | 411    | PHO  | C3B-C4B | 7.28 | 1.49        | 1.41     |
| 25  | A     | 409[A] | PHO  | C3B-C4B | 7.22 | 1.49        | 1.41     |
| 25  | A     | 409[B] | PHO  | C3B-C4B | 7.17 | 1.49        | 1.41     |
| 25  | a     | 418[A] | PHO  | C3B-C4B | 7.16 | 1.49        | 1.41     |
| 25  | a     | 418[B] | PHO  | C3B-C4B | 7.06 | 1.49        | 1.41     |
| 25  | A     | 409[A] | PHO  | C4D-CHA | 6.73 | 1.50        | 1.39     |
| 25  | A     | 409[B] | PHO  | C4D-CHA | 6.47 | 1.49        | 1.39     |
| 25  | A     | 409[B] | PHO  | C3B-C2B | 6.46 | 1.49        | 1.40     |
| 25  | A     | 408    | PHO  | C4D-CHA | 6.46 | 1.49        | 1.39     |
| 25  | a     | 418[B] | PHO  | C4D-CHA | 6.36 | 1.49        | 1.39     |
| 25  | A     | 409[A] | PHO  | C3B-C2B | 6.35 | 1.49        | 1.40     |
| 25  | a     | 411    | PHO  | C4D-CHA | 6.22 | 1.49        | 1.39     |
| 25  | a     | 418[A] | PHO  | C4D-CHA | 6.16 | 1.49        | 1.39     |
| 25  | A     | 408    | PHO  | C3B-C2B | 6.15 | 1.48        | 1.40     |
| 25  | a     | 411    | PHO  | C3B-C2B | 6.11 | 1.48        | 1.40     |
| 25  | a     | 418[B] | PHO  | C3B-C2B | 6.09 | 1.48        | 1.40     |
| 25  | a     | 418[B] | PHO  | C3C-C2C | 5.83 | 1.49        | 1.36     |
| 25  | a     | 418[A] | PHO  | C3C-C2C | 5.82 | 1.49        | 1.36     |
| 25  | A     | 409[B] | PHO  | C3C-C2C | 5.82 | 1.49        | 1.36     |
| 25  | a     | 418[A] | PHO  | C3B-C2B | 5.72 | 1.48        | 1.40     |
| 25  | A     | 409[A] | PHO  | C3D-C2D | 5.72 | 1.49        | 1.39     |
| 25  | A     | 408    | PHO  | C3C-C2C | 5.72 | 1.48        | 1.36     |
| 24  | C     | 508    | CLA  | C3C-C2C | 5.69 | 1.48        | 1.36     |
| 25  | A     | 408    | PHO  | C3B-C4B | 5.66 | 1.48        | 1.41     |
| 25  | a     | 418[A] | PHO  | C3D-C2D | 5.65 | 1.49        | 1.39     |
| 24  | b     | 610    | CLA  | C3C-C2C | 5.63 | 1.48        | 1.36     |
| 24  | D     | 403    | CLA  | C1D-ND  | 5.62 | 1.44        | 1.37     |
| 24  | C     | 509    | CLA  | C1D-ND  | 5.61 | 1.44        | 1.37     |
| 24  | B     | 614    | CLA  | C1D-ND  | 5.59 | 1.44        | 1.37     |
| 25  | a     | 411    | PHO  | C3C-C2C | 5.58 | 1.48        | 1.36     |
| 25  | a     | 418[B] | PHO  | C3D-C2D | 5.57 | 1.49        | 1.39     |
| 24  | b     | 614    | CLA  | C3C-C2C | 5.56 | 1.48        | 1.36     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 24  | b     | 622    | CLA  | C1D-ND  | 5.54 | 1.44        | 1.37     |
| 24  | B     | 617    | CLA  | C1D-ND  | 5.53 | 1.44        | 1.37     |
| 24  | B     | 611    | CLA  | C3C-C2C | 5.50 | 1.48        | 1.36     |
| 24  | b     | 619    | CLA  | C3C-C2C | 5.50 | 1.48        | 1.36     |
| 24  | c     | 514    | CLA  | C1D-ND  | 5.47 | 1.44        | 1.37     |
| 25  | a     | 411    | PHO  | C3D-C2D | 5.46 | 1.49        | 1.39     |
| 24  | B     | 606    | CLA  | O2D-CGD | 5.45 | 1.46        | 1.33     |
| 25  | A     | 409[A] | PHO  | C3C-C2C | 5.44 | 1.48        | 1.36     |
| 24  | C     | 510    | CLA  | C3C-C2C | 5.44 | 1.48        | 1.36     |
| 24  | C     | 513    | CLA  | C3C-C2C | 5.44 | 1.48        | 1.36     |
| 24  | B     | 604    | CLA  | C3C-C2C | 5.43 | 1.48        | 1.36     |
| 24  | C     | 509    | CLA  | C3C-C2C | 5.43 | 1.48        | 1.36     |
| 24  | c     | 518    | CLA  | C3C-C2C | 5.42 | 1.48        | 1.36     |
| 24  | b     | 623    | CLA  | C3C-C2C | 5.42 | 1.48        | 1.36     |
| 24  | B     | 603    | CLA  | C3C-C2C | 5.41 | 1.48        | 1.36     |
| 24  | B     | 602    | CLA  | C1D-ND  | 5.41 | 1.44        | 1.37     |
| 24  | D     | 402    | CLA  | C3C-C2C | 5.41 | 1.48        | 1.36     |
| 24  | c     | 518    | CLA  | C1D-ND  | 5.39 | 1.44        | 1.37     |
| 24  | A     | 407    | CLA  | C3C-C2C | 5.39 | 1.48        | 1.36     |
| 24  | b     | 622    | CLA  | C3C-C2C | 5.38 | 1.48        | 1.36     |
| 25  | A     | 408    | PHO  | C3D-C2D | 5.38 | 1.49        | 1.39     |
| 24  | C     | 503    | CLA  | C3C-C2C | 5.37 | 1.48        | 1.36     |
| 25  | A     | 409[B] | PHO  | C3D-C2D | 5.37 | 1.49        | 1.39     |
| 24  | D     | 403    | CLA  | C3C-C2C | 5.36 | 1.48        | 1.36     |
| 24  | b     | 611    | CLA  | C3C-C2C | 5.36 | 1.48        | 1.36     |
| 24  | C     | 512    | CLA  | C3C-C2C | 5.36 | 1.48        | 1.36     |
| 24  | c     | 513    | CLA  | C3C-C2C | 5.36 | 1.48        | 1.36     |
| 24  | B     | 605    | CLA  | C1D-ND  | 5.33 | 1.44        | 1.37     |
| 24  | b     | 617    | CLA  | C1D-ND  | 5.33 | 1.44        | 1.37     |
| 24  | c     | 515    | CLA  | C3C-C2C | 5.33 | 1.48        | 1.36     |
| 40  | V     | 205    | HEC  | FE-NB   | 5.32 | 2.11        | 1.94     |
| 24  | C     | 510    | CLA  | C1D-ND  | 5.32 | 1.44        | 1.37     |
| 24  | b     | 617    | CLA  | C3C-C2C | 5.32 | 1.48        | 1.36     |
| 24  | b     | 621    | CLA  | C3C-C2C | 5.31 | 1.48        | 1.36     |
| 24  | a     | 409    | CLA  | C1D-ND  | 5.31 | 1.44        | 1.37     |
| 24  | a     | 412    | CLA  | C3C-C2C | 5.31 | 1.48        | 1.36     |
| 24  | d     | 401    | CLA  | C3C-C2C | 5.30 | 1.48        | 1.36     |
| 24  | C     | 506    | CLA  | C1D-ND  | 5.30 | 1.44        | 1.37     |
| 24  | d     | 401    | CLA  | C1D-ND  | 5.29 | 1.44        | 1.37     |
| 24  | c     | 507    | CLA  | C3C-C2C | 5.28 | 1.48        | 1.36     |
| 24  | B     | 602    | CLA  | C3C-C2C | 5.28 | 1.48        | 1.36     |
| 24  | B     | 615    | CLA  | C3C-C2C | 5.27 | 1.47        | 1.36     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | C     | 503    | CLA  | C1D-ND  | 5.26  | 1.44        | 1.37     |
| 24  | B     | 615    | CLA  | C1D-ND  | 5.26  | 1.44        | 1.37     |
| 24  | b     | 615    | CLA  | C3C-C2C | 5.25  | 1.47        | 1.36     |
| 24  | c     | 515    | CLA  | C1D-ND  | 5.25  | 1.44        | 1.37     |
| 24  | C     | 507    | CLA  | C3C-C2C | 5.24  | 1.47        | 1.36     |
| 24  | d     | 403    | CLA  | C3C-C2C | 5.23  | 1.47        | 1.36     |
| 24  | B     | 610    | CLA  | C3C-C2C | 5.23  | 1.47        | 1.36     |
| 24  | a     | 409    | CLA  | C3C-C2C | 5.23  | 1.47        | 1.36     |
| 24  | c     | 511    | CLA  | C3C-C2C | 5.23  | 1.47        | 1.36     |
| 24  | c     | 517    | CLA  | C3C-C2C | 5.23  | 1.47        | 1.36     |
| 24  | b     | 623    | CLA  | O2D-CGD | 5.22  | 1.45        | 1.33     |
| 25  | a     | 411    | PHO  | O2D-CGD | 5.22  | 1.45        | 1.33     |
| 24  | C     | 511    | CLA  | C1D-ND  | 5.21  | 1.44        | 1.37     |
| 24  | b     | 616    | CLA  | C3C-C2C | 5.21  | 1.47        | 1.36     |
| 24  | c     | 509    | CLA  | O2D-CGD | 5.21  | 1.45        | 1.33     |
| 24  | b     | 620    | CLA  | C1D-ND  | 5.20  | 1.44        | 1.37     |
| 24  | b     | 610    | CLA  | C1D-ND  | 5.20  | 1.44        | 1.37     |
| 24  | B     | 603    | CLA  | O2D-CGD | 5.18  | 1.45        | 1.33     |
| 26  | b     | 628    | BCR  | C23-C22 | -5.18 | 1.34        | 1.45     |
| 26  | B     | 620    | BCR  | C23-C22 | -5.17 | 1.34        | 1.45     |
| 24  | A     | 410    | CLA  | C1D-ND  | 5.17  | 1.44        | 1.37     |
| 24  | C     | 502    | CLA  | C3C-C2C | 5.17  | 1.47        | 1.36     |
| 24  | b     | 618    | CLA  | C1D-ND  | 5.17  | 1.44        | 1.37     |
| 24  | B     | 612    | CLA  | C3C-C2C | 5.16  | 1.47        | 1.36     |
| 24  | c     | 508    | CLA  | C3C-C2C | 5.16  | 1.47        | 1.36     |
| 24  | c     | 512    | CLA  | C3C-C2C | 5.16  | 1.47        | 1.36     |
| 24  | c     | 513    | CLA  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 24  | b     | 620    | CLA  | C3C-C2C | 5.15  | 1.47        | 1.36     |
| 24  | C     | 505    | CLA  | C3C-C2C | 5.15  | 1.47        | 1.36     |
| 40  | v     | 205    | HEC  | FE-NB   | 5.15  | 2.10        | 1.94     |
| 24  | B     | 612    | CLA  | C1D-ND  | 5.14  | 1.44        | 1.37     |
| 24  | b     | 622    | CLA  | O2D-CGD | 5.13  | 1.45        | 1.33     |
| 24  | b     | 613    | CLA  | C3C-C2C | 5.13  | 1.47        | 1.36     |
| 24  | B     | 607    | CLA  | C3C-C2C | 5.13  | 1.47        | 1.36     |
| 24  | c     | 514    | CLA  | C3C-C2C | 5.12  | 1.47        | 1.36     |
| 24  | B     | 608    | CLA  | C3C-C2C | 5.12  | 1.47        | 1.36     |
| 38  | F     | 102    | HEM  | FE-NB   | 5.11  | 2.10        | 1.94     |
| 25  | A     | 409[B] | PHO  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 24  | C     | 502    | CLA  | C1D-ND  | 5.11  | 1.44        | 1.37     |
| 24  | b     | 623    | CLA  | C1D-ND  | 5.11  | 1.44        | 1.37     |
| 24  | B     | 609    | CLA  | C3C-C2C | 5.11  | 1.47        | 1.36     |
| 24  | b     | 618    | CLA  | C3C-C2C | 5.11  | 1.47        | 1.36     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | C     | 511    | CLA  | C3C-C2C | 5.11  | 1.47        | 1.36     |
| 24  | B     | 607    | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 24  | A     | 406    | CLA  | C3C-C2C | 5.10  | 1.47        | 1.36     |
| 24  | C     | 501    | CLA  | C1D-ND  | 5.10  | 1.44        | 1.37     |
| 24  | d     | 401    | CLA  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 38  | e     | 103    | HEM  | FE-NB   | 5.10  | 2.10        | 1.94     |
| 24  | C     | 504    | CLA  | C1D-ND  | 5.10  | 1.44        | 1.37     |
| 24  | B     | 614    | CLA  | C3C-C2C | 5.10  | 1.47        | 1.36     |
| 24  | c     | 509    | CLA  | C3C-C2C | 5.09  | 1.47        | 1.36     |
| 26  | k     | 101    | BCR  | C23-C22 | -5.09 | 1.35        | 1.45     |
| 24  | c     | 506    | CLA  | C3C-C2C | 5.09  | 1.47        | 1.36     |
| 24  | c     | 516    | CLA  | C3C-C2C | 5.09  | 1.47        | 1.36     |
| 24  | c     | 508    | CLA  | CHC-C1C | 5.08  | 1.48        | 1.38     |
| 24  | c     | 517    | CLA  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 24  | C     | 504    | CLA  | C3C-C2C | 5.08  | 1.47        | 1.36     |
| 24  | c     | 511    | CLA  | C1D-ND  | 5.08  | 1.44        | 1.37     |
| 24  | C     | 506    | CLA  | C3C-C2C | 5.08  | 1.47        | 1.36     |
| 24  | c     | 507    | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 24  | b     | 621    | CLA  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 24  | b     | 625    | CLA  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 24  | B     | 606    | CLA  | C3C-C2C | 5.05  | 1.47        | 1.36     |
| 24  | d     | 403    | CLA  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 24  | b     | 624    | CLA  | C3C-C2C | 5.05  | 1.47        | 1.36     |
| 24  | B     | 611    | CLA  | C1D-ND  | 5.05  | 1.44        | 1.37     |
| 24  | C     | 508    | CLA  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 24  | b     | 611    | CLA  | C1D-ND  | 5.04  | 1.44        | 1.37     |
| 24  | b     | 613    | CLA  | C1D-ND  | 5.04  | 1.44        | 1.37     |
| 24  | c     | 514    | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 24  | b     | 618    | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 24  | b     | 612    | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 24  | c     | 518    | CLA  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 24  | A     | 410    | CLA  | C3C-C2C | 5.03  | 1.47        | 1.36     |
| 25  | A     | 409[A] | PHO  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 24  | C     | 513    | CLA  | C1D-ND  | 5.02  | 1.44        | 1.37     |
| 26  | T     | 103    | BCR  | C23-C22 | -5.02 | 1.35        | 1.45     |
| 24  | B     | 616    | CLA  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 24  | C     | 513    | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 24  | b     | 624    | CLA  | C1D-ND  | 5.01  | 1.43        | 1.37     |
| 24  | C     | 503    | CLA  | CHC-C1C | 5.01  | 1.48        | 1.38     |
| 24  | C     | 509    | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 24  | B     | 614    | CLA  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 24  | c     | 513    | CLA  | C1D-ND  | 5.00  | 1.43        | 1.37     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | c     | 508    | CLA  | C1D-ND  | 5.00  | 1.43        | 1.37     |
| 24  | b     | 612    | CLA  | C3C-C2C | 5.00  | 1.47        | 1.36     |
| 24  | c     | 510    | CLA  | C3C-C2C | 4.99  | 1.47        | 1.36     |
| 24  | c     | 509    | CLA  | C1D-ND  | 4.99  | 1.43        | 1.37     |
| 25  | a     | 418[B] | PHO  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 24  | B     | 603    | CLA  | CHC-C1C | 4.98  | 1.48        | 1.38     |
| 24  | B     | 602    | CLA  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 24  | b     | 619    | CLA  | C1D-ND  | 4.98  | 1.43        | 1.37     |
| 24  | B     | 617    | CLA  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 24  | b     | 616    | CLA  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 24  | c     | 511    | CLA  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 24  | c     | 506    | CLA  | C1D-ND  | 4.97  | 1.43        | 1.37     |
| 24  | b     | 610    | CLA  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 24  | b     | 614    | CLA  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 24  | C     | 507    | CLA  | C1D-ND  | 4.97  | 1.43        | 1.37     |
| 24  | c     | 517    | CLA  | C1D-ND  | 4.97  | 1.43        | 1.37     |
| 24  | C     | 508    | CLA  | C1D-ND  | 4.96  | 1.43        | 1.37     |
| 24  | b     | 620    | CLA  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 24  | C     | 510    | CLA  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 24  | d     | 402    | CLA  | C3C-C2C | 4.95  | 1.47        | 1.36     |
| 24  | B     | 606    | CLA  | C1D-ND  | 4.95  | 1.43        | 1.37     |
| 24  | C     | 506    | CLA  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 24  | B     | 604    | CLA  | CHC-C1C | 4.95  | 1.48        | 1.38     |
| 24  | A     | 407    | CLA  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 25  | a     | 411    | PHO  | OBD-CAD | 4.94  | 1.29        | 1.22     |
| 24  | d     | 403    | CLA  | C1D-ND  | 4.94  | 1.43        | 1.37     |
| 24  | b     | 615    | CLA  | C1D-ND  | 4.93  | 1.43        | 1.37     |
| 24  | b     | 614    | CLA  | C1D-ND  | 4.93  | 1.43        | 1.37     |
| 24  | B     | 605    | CLA  | C3C-C2C | 4.92  | 1.47        | 1.36     |
| 24  | C     | 501    | CLA  | C3C-C2C | 4.92  | 1.47        | 1.36     |
| 24  | A     | 407    | CLA  | C1D-ND  | 4.92  | 1.43        | 1.37     |
| 24  | c     | 516    | CLA  | C1D-ND  | 4.91  | 1.43        | 1.37     |
| 26  | C     | 514    | BCR  | C23-C22 | -4.91 | 1.35        | 1.45     |
| 24  | C     | 512    | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 24  | A     | 406    | CLA  | C1D-ND  | 4.90  | 1.43        | 1.37     |
| 24  | c     | 517    | CLA  | CHC-C1C | 4.90  | 1.48        | 1.38     |
| 24  | B     | 612    | CLA  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 24  | C     | 501    | CLA  | CHC-C1C | 4.88  | 1.48        | 1.38     |
| 26  | d     | 404    | BCR  | C23-C22 | -4.88 | 1.35        | 1.45     |
| 24  | b     | 612    | CLA  | C1D-ND  | 4.88  | 1.43        | 1.37     |
| 24  | A     | 410    | CLA  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 24  | b     | 619    | CLA  | O2D-CGD | 4.87  | 1.45        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | B     | 606    | CLA  | CHC-C1C | 4.86  | 1.48        | 1.38     |
| 24  | a     | 412    | CLA  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 24  | A     | 405    | CLA  | C3C-C2C | 4.86  | 1.47        | 1.36     |
| 24  | c     | 507    | CLA  | C1D-ND  | 4.86  | 1.43        | 1.37     |
| 24  | b     | 624    | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 25  | A     | 408    | PHO  | OBD-CAD | 4.85  | 1.29        | 1.22     |
| 24  | b     | 621    | CLA  | C1D-ND  | 4.84  | 1.43        | 1.37     |
| 24  | C     | 505    | CLA  | CHC-C1C | 4.84  | 1.48        | 1.38     |
| 24  | D     | 403    | CLA  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 24  | A     | 407    | CLA  | CHC-C1C | 4.83  | 1.48        | 1.38     |
| 26  | h     | 101    | BCR  | C23-C22 | -4.83 | 1.35        | 1.45     |
| 24  | c     | 515    | CLA  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 24  | A     | 405    | CLA  | C1D-ND  | 4.82  | 1.43        | 1.37     |
| 24  | B     | 617    | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 24  | C     | 511    | CLA  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 24  | a     | 410    | CLA  | C3C-C2C | 4.82  | 1.47        | 1.36     |
| 24  | C     | 504    | CLA  | CHC-C1C | 4.82  | 1.48        | 1.38     |
| 24  | d     | 402    | CLA  | CHC-C1C | 4.81  | 1.48        | 1.38     |
| 24  | C     | 508    | CLA  | CHC-C1C | 4.81  | 1.48        | 1.38     |
| 24  | C     | 513    | CLA  | CHC-C1C | 4.81  | 1.48        | 1.38     |
| 24  | b     | 615    | CLA  | O2D-CGD | 4.81  | 1.44        | 1.33     |
| 24  | A     | 405    | CLA  | CHC-C1C | 4.81  | 1.48        | 1.38     |
| 24  | a     | 409    | CLA  | O2D-CGD | 4.81  | 1.44        | 1.33     |
| 26  | K     | 101    | BCR  | C23-C22 | -4.80 | 1.35        | 1.45     |
| 24  | A     | 405    | CLA  | O2D-CGD | 4.79  | 1.44        | 1.33     |
| 24  | B     | 602    | CLA  | O2A-CGA | 4.79  | 1.47        | 1.33     |
| 24  | B     | 609    | CLA  | C1D-ND  | 4.79  | 1.43        | 1.37     |
| 24  | C     | 501    | CLA  | O2D-CGD | 4.79  | 1.44        | 1.33     |
| 24  | d     | 403    | CLA  | CHC-C1C | 4.78  | 1.48        | 1.38     |
| 24  | B     | 613    | CLA  | O2D-CGD | 4.78  | 1.44        | 1.33     |
| 24  | a     | 410    | CLA  | CHC-C1C | 4.78  | 1.48        | 1.38     |
| 26  | H     | 101    | BCR  | C23-C22 | -4.77 | 1.35        | 1.45     |
| 24  | B     | 616    | CLA  | C1D-ND  | 4.77  | 1.43        | 1.37     |
| 26  | C     | 515    | BCR  | C23-C22 | -4.77 | 1.35        | 1.45     |
| 25  | a     | 418[A] | PHO  | O2D-CGD | 4.77  | 1.44        | 1.33     |
| 26  | y     | 101    | BCR  | C23-C22 | -4.76 | 1.35        | 1.45     |
| 24  | B     | 616    | CLA  | C3C-C2C | 4.76  | 1.46        | 1.36     |
| 24  | C     | 502    | CLA  | CHC-C1C | 4.76  | 1.48        | 1.38     |
| 24  | b     | 617    | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 24  | B     | 610    | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 24  | c     | 510    | CLA  | CHC-C1C | 4.74  | 1.48        | 1.38     |
| 24  | c     | 506    | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | B     | 613 | CLA  | C3C-C2C | 4.73  | 1.46        | 1.36     |
| 24  | C     | 507 | CLA  | CHC-C1C | 4.73  | 1.48        | 1.38     |
| 24  | C     | 509 | CLA  | CHC-C1C | 4.72  | 1.48        | 1.38     |
| 24  | B     | 604 | CLA  | C1D-ND  | 4.71  | 1.43        | 1.37     |
| 24  | B     | 609 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 24  | c     | 508 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 24  | B     | 616 | CLA  | CHC-C1C | 4.71  | 1.48        | 1.38     |
| 24  | b     | 614 | CLA  | CHC-C1C | 4.71  | 1.48        | 1.38     |
| 24  | C     | 512 | CLA  | C1D-ND  | 4.70  | 1.43        | 1.37     |
| 24  | b     | 611 | CLA  | CHC-C1C | 4.70  | 1.48        | 1.38     |
| 24  | c     | 510 | CLA  | O2D-CGD | 4.69  | 1.44        | 1.33     |
| 24  | b     | 625 | CLA  | C3C-C2C | 4.68  | 1.46        | 1.36     |
| 24  | B     | 610 | CLA  | C1D-ND  | 4.67  | 1.43        | 1.37     |
| 24  | B     | 607 | CLA  | C1D-ND  | 4.67  | 1.43        | 1.37     |
| 24  | B     | 615 | CLA  | CHC-C1C | 4.67  | 1.48        | 1.38     |
| 24  | C     | 512 | CLA  | CHC-C1C | 4.67  | 1.48        | 1.38     |
| 24  | a     | 412 | CLA  | C1D-ND  | 4.67  | 1.43        | 1.37     |
| 24  | B     | 611 | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 24  | b     | 611 | CLA  | O2D-CGD | 4.66  | 1.44        | 1.33     |
| 27  | a     | 405 | SQD  | O48-C23 | 4.66  | 1.47        | 1.33     |
| 24  | C     | 507 | CLA  | O2D-CGD | 4.66  | 1.44        | 1.33     |
| 24  | B     | 610 | CLA  | CHC-C1C | 4.65  | 1.48        | 1.38     |
| 24  | b     | 623 | CLA  | CHC-C1C | 4.65  | 1.48        | 1.38     |
| 24  | B     | 603 | CLA  | C1D-ND  | 4.65  | 1.43        | 1.37     |
| 26  | c     | 528 | BCR  | C23-C22 | -4.65 | 1.36        | 1.45     |
| 24  | c     | 507 | CLA  | CHC-C1C | 4.65  | 1.48        | 1.38     |
| 26  | Y     | 101 | BCR  | C23-C22 | -4.64 | 1.36        | 1.45     |
| 24  | B     | 602 | CLA  | CHC-C1C | 4.64  | 1.48        | 1.38     |
| 24  | c     | 513 | CLA  | O2A-CGA | 4.64  | 1.46        | 1.33     |
| 24  | b     | 617 | CLA  | CHD-C1D | 4.64  | 1.47        | 1.38     |
| 24  | D     | 402 | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 24  | c     | 509 | CLA  | CHC-C1C | 4.63  | 1.47        | 1.38     |
| 24  | B     | 608 | CLA  | O2D-CGD | 4.63  | 1.44        | 1.33     |
| 24  | c     | 518 | CLA  | CHC-C1C | 4.63  | 1.47        | 1.38     |
| 24  | B     | 605 | CLA  | CHC-C1C | 4.63  | 1.47        | 1.38     |
| 25  | A     | 408 | PHO  | O2D-CGD | 4.63  | 1.44        | 1.33     |
| 24  | b     | 612 | CLA  | CHC-C1C | 4.62  | 1.47        | 1.38     |
| 26  | t     | 101 | BCR  | C23-C22 | -4.62 | 1.36        | 1.45     |
| 24  | c     | 512 | CLA  | C1D-ND  | 4.62  | 1.43        | 1.37     |
| 24  | C     | 504 | CLA  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 24  | c     | 516 | CLA  | CHC-C1C | 4.62  | 1.47        | 1.38     |
| 24  | a     | 410 | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | c     | 512 | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 24  | b     | 616 | CLA  | CHC-C1C | 4.61  | 1.47        | 1.38     |
| 24  | C     | 505 | CLA  | O2D-CGD | 4.60  | 1.44        | 1.33     |
| 27  | A     | 416 | SQD  | O48-C23 | 4.60  | 1.46        | 1.33     |
| 24  | b     | 617 | CLA  | CHC-C1C | 4.60  | 1.47        | 1.38     |
| 24  | B     | 617 | CLA  | CHC-C1C | 4.60  | 1.47        | 1.38     |
| 24  | b     | 618 | CLA  | CHC-C1C | 4.60  | 1.47        | 1.38     |
| 24  | C     | 502 | CLA  | O2D-CGD | 4.59  | 1.44        | 1.33     |
| 24  | C     | 506 | CLA  | CHD-C1D | 4.59  | 1.47        | 1.38     |
| 24  | B     | 615 | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |
| 24  | B     | 605 | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |
| 27  | f     | 101 | SQD  | O47-C7  | 4.56  | 1.47        | 1.34     |
| 24  | b     | 610 | CLA  | CHC-C1C | 4.56  | 1.47        | 1.38     |
| 24  | B     | 608 | CLA  | C1D-ND  | 4.56  | 1.43        | 1.37     |
| 24  | c     | 516 | CLA  | O2D-CGD | 4.56  | 1.44        | 1.33     |
| 24  | b     | 613 | CLA  | O2D-CGD | 4.56  | 1.44        | 1.33     |
| 24  | c     | 510 | CLA  | C1D-ND  | 4.55  | 1.43        | 1.37     |
| 24  | B     | 610 | CLA  | O2A-CGA | 4.54  | 1.46        | 1.33     |
| 36  | D     | 406 | DGD  | O1G-C1A | 4.54  | 1.46        | 1.33     |
| 24  | C     | 510 | CLA  | CHC-C1C | 4.54  | 1.47        | 1.38     |
| 24  | A     | 410 | CLA  | CHC-C1C | 4.53  | 1.47        | 1.38     |
| 24  | D     | 402 | CLA  | C1D-ND  | 4.53  | 1.43        | 1.37     |
| 26  | D     | 404 | BCR  | C23-C22 | -4.53 | 1.36        | 1.45     |
| 24  | C     | 506 | CLA  | CHC-C1C | 4.53  | 1.47        | 1.38     |
| 26  | a     | 413 | BCR  | C23-C22 | -4.53 | 1.36        | 1.45     |
| 24  | b     | 625 | CLA  | C1D-ND  | 4.52  | 1.43        | 1.37     |
| 24  | c     | 517 | CLA  | CHD-C1D | 4.52  | 1.47        | 1.38     |
| 24  | B     | 607 | CLA  | CHC-C1C | 4.52  | 1.47        | 1.38     |
| 24  | c     | 514 | CLA  | CHC-C1C | 4.51  | 1.47        | 1.38     |
| 26  | b     | 626 | BCR  | C23-C22 | -4.50 | 1.36        | 1.45     |
| 24  | a     | 409 | CLA  | CHD-C1D | 4.50  | 1.47        | 1.38     |
| 24  | d     | 402 | CLA  | O2D-CGD | 4.50  | 1.44        | 1.33     |
| 24  | C     | 503 | CLA  | O2D-CGD | 4.49  | 1.44        | 1.33     |
| 27  | F     | 103 | SQD  | O47-C7  | 4.48  | 1.46        | 1.34     |
| 24  | D     | 403 | CLA  | CHC-C1C | 4.48  | 1.47        | 1.38     |
| 24  | C     | 509 | CLA  | O2A-CGA | 4.47  | 1.46        | 1.33     |
| 24  | B     | 604 | CLA  | O2D-CGD | 4.47  | 1.44        | 1.33     |
| 24  | c     | 512 | CLA  | CHC-C1C | 4.47  | 1.47        | 1.38     |
| 26  | B     | 618 | BCR  | C23-C22 | -4.47 | 1.36        | 1.45     |
| 33  | C     | 519 | LMG  | O8-C28  | 4.46  | 1.46        | 1.33     |
| 24  | b     | 613 | CLA  | CHC-C1C | 4.46  | 1.47        | 1.38     |
| 24  | b     | 610 | CLA  | CHD-C1D | 4.45  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | d     | 401 | CLA  | CHD-C1D | 4.45  | 1.47        | 1.38     |
| 33  | z     | 101 | LMG  | O8-C28  | 4.45  | 1.46        | 1.33     |
| 26  | c     | 519 | BCR  | C23-C22 | -4.45 | 1.36        | 1.45     |
| 24  | b     | 623 | CLA  | CHD-C1D | 4.43  | 1.47        | 1.38     |
| 24  | c     | 511 | CLA  | CHC-C1C | 4.43  | 1.47        | 1.38     |
| 24  | B     | 609 | CLA  | CHD-C1D | 4.41  | 1.47        | 1.38     |
| 24  | c     | 514 | CLA  | CHD-C1D | 4.41  | 1.47        | 1.38     |
| 24  | b     | 615 | CLA  | CHC-C1C | 4.41  | 1.47        | 1.38     |
| 24  | d     | 402 | CLA  | O2A-CGA | 4.41  | 1.46        | 1.33     |
| 24  | c     | 515 | CLA  | CHD-C1D | 4.41  | 1.46        | 1.38     |
| 24  | C     | 512 | CLA  | O2A-CGA | 4.41  | 1.46        | 1.33     |
| 24  | C     | 507 | CLA  | CHD-C1D | 4.41  | 1.46        | 1.38     |
| 24  | C     | 508 | CLA  | O2A-CGA | 4.41  | 1.46        | 1.33     |
| 24  | B     | 612 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 36  | D     | 406 | DGD  | O2G-C1B | 4.40  | 1.46        | 1.34     |
| 24  | C     | 506 | CLA  | O2A-CGA | 4.40  | 1.46        | 1.33     |
| 24  | b     | 622 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 24  | C     | 503 | CLA  | O2A-CGA | 4.40  | 1.46        | 1.33     |
| 24  | A     | 407 | CLA  | CHD-C1D | 4.39  | 1.46        | 1.38     |
| 24  | C     | 508 | CLA  | CHD-C1D | 4.39  | 1.46        | 1.38     |
| 26  | A     | 411 | BCR  | C23-C22 | -4.38 | 1.36        | 1.45     |
| 24  | b     | 610 | CLA  | O2A-CGA | 4.38  | 1.46        | 1.33     |
| 24  | b     | 624 | CLA  | O2A-CGA | 4.38  | 1.46        | 1.33     |
| 24  | d     | 402 | CLA  | C1D-ND  | 4.38  | 1.43        | 1.37     |
| 24  | c     | 515 | CLA  | CHC-C1C | 4.37  | 1.47        | 1.38     |
| 24  | C     | 505 | CLA  | C1D-ND  | 4.37  | 1.43        | 1.37     |
| 24  | b     | 621 | CLA  | CHC-C1C | 4.37  | 1.47        | 1.38     |
| 24  | a     | 412 | CLA  | CHC-C1C | 4.37  | 1.47        | 1.38     |
| 24  | c     | 516 | CLA  | O2A-CGA | 4.37  | 1.46        | 1.33     |
| 37  | E     | 101 | LHG  | O8-C23  | 4.37  | 1.46        | 1.33     |
| 36  | e     | 101 | DGD  | O2G-C1B | 4.37  | 1.46        | 1.34     |
| 24  | c     | 514 | CLA  | O2A-CGA | 4.37  | 1.46        | 1.33     |
| 24  | B     | 608 | CLA  | CHC-C1C | 4.35  | 1.47        | 1.38     |
| 24  | D     | 403 | CLA  | CHD-C1D | 4.35  | 1.46        | 1.38     |
| 26  | b     | 627 | BCR  | C23-C22 | -4.35 | 1.36        | 1.45     |
| 24  | a     | 410 | CLA  | O2A-CGA | 4.34  | 1.46        | 1.33     |
| 24  | B     | 602 | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 24  | B     | 610 | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 24  | B     | 613 | CLA  | CHC-C1C | 4.34  | 1.47        | 1.38     |
| 33  | A     | 421 | LMG  | O7-C10  | 4.33  | 1.46        | 1.34     |
| 24  | b     | 624 | CLA  | CHC-C1C | 4.33  | 1.47        | 1.38     |
| 27  | a     | 405 | SQD  | O47-C7  | 4.33  | 1.46        | 1.34     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | A     | 410    | CLA  | CHD-C1D | 4.33  | 1.46        | 1.38     |
| 33  | C     | 520    | LMG  | O7-C10  | 4.32  | 1.46        | 1.34     |
| 24  | C     | 513    | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 24  | B     | 603    | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 24  | C     | 510    | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 24  | B     | 611    | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 24  | b     | 616    | CLA  | C1D-ND  | 4.32  | 1.43        | 1.37     |
| 24  | c     | 510    | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 24  | B     | 613    | CLA  | C1B-NB  | -4.31 | 1.32        | 1.37     |
| 27  | B     | 621    | SQD  | O47-C7  | 4.31  | 1.46        | 1.34     |
| 37  | D     | 409    | LHG  | O7-C7   | 4.31  | 1.46        | 1.34     |
| 38  | e     | 103    | HEM  | FE-NC   | 4.31  | 2.09        | 1.95     |
| 24  | b     | 625    | CLA  | CHC-C1C | 4.31  | 1.47        | 1.38     |
| 36  | e     | 101    | DGD  | O1G-C1A | 4.30  | 1.45        | 1.33     |
| 24  | C     | 511    | CLA  | CHC-C1C | 4.30  | 1.47        | 1.38     |
| 24  | C     | 507    | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 24  | B     | 617    | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 24  | c     | 511    | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 24  | c     | 513    | CLA  | CHC-C1C | 4.29  | 1.47        | 1.38     |
| 24  | B     | 614    | CLA  | CHC-C1C | 4.29  | 1.47        | 1.38     |
| 24  | B     | 611    | CLA  | CHC-C1C | 4.29  | 1.47        | 1.38     |
| 24  | C     | 511    | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 24  | b     | 620    | CLA  | CHC-C1C | 4.28  | 1.47        | 1.38     |
| 24  | b     | 619    | CLA  | CHC-C1C | 4.28  | 1.47        | 1.38     |
| 24  | C     | 509    | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 33  | c     | 524    | LMG  | O7-C10  | 4.27  | 1.46        | 1.34     |
| 24  | c     | 516    | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 24  | C     | 510    | CLA  | CHB-C1B | 4.27  | 1.49        | 1.39     |
| 24  | c     | 518    | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 24  | b     | 612    | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 24  | a     | 410    | CLA  | C1D-ND  | 4.27  | 1.43        | 1.37     |
| 24  | b     | 618    | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 37  | e     | 102    | LHG  | O8-C23  | 4.26  | 1.45        | 1.33     |
| 36  | H     | 102    | DGD  | O1G-C1A | 4.26  | 1.45        | 1.33     |
| 37  | b     | 634    | LHG  | O8-C23  | 4.26  | 1.45        | 1.33     |
| 24  | d     | 401    | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 24  | C     | 501    | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 24  | b     | 613    | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 24  | c     | 514    | CLA  | CHB-C1B | 4.25  | 1.48        | 1.39     |
| 24  | B     | 609    | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 25  | a     | 418[B] | PHO  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 24  | c     | 506    | CLA  | CHC-C1C | 4.23  | 1.47        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 24  | c     | 512    | CLA  | O2A-CGA | 4.23 | 1.45        | 1.33     |
| 24  | A     | 406    | CLA  | O2D-CGD | 4.23 | 1.43        | 1.33     |
| 27  | f     | 101    | SQD  | O48-C23 | 4.23 | 1.45        | 1.33     |
| 24  | C     | 511    | CLA  | CHD-C1D | 4.23 | 1.46        | 1.38     |
| 24  | c     | 513    | CLA  | C3D-C2D | 4.22 | 1.50        | 1.39     |
| 24  | C     | 503    | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 24  | c     | 518    | CLA  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 24  | C     | 501    | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 25  | A     | 409[B] | PHO  | OBD-CAD | 4.22 | 1.28        | 1.22     |
| 27  | L     | 102    | SQD  | O47-C7  | 4.22 | 1.46        | 1.34     |
| 33  | B     | 622    | LMG  | O8-C28  | 4.22 | 1.45        | 1.33     |
| 33  | A     | 421    | LMG  | O8-C28  | 4.22 | 1.45        | 1.33     |
| 24  | c     | 513    | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 24  | c     | 506    | CLA  | CHD-C1D | 4.21 | 1.46        | 1.38     |
| 33  | C     | 520    | LMG  | O8-C28  | 4.21 | 1.45        | 1.33     |
| 25  | A     | 409[A] | PHO  | OBD-CAD | 4.20 | 1.28        | 1.22     |
| 24  | B     | 616    | CLA  | O2A-CGA | 4.20 | 1.45        | 1.33     |
| 33  | c     | 524    | LMG  | O8-C28  | 4.20 | 1.45        | 1.33     |
| 24  | c     | 517    | CLA  | O2A-CGA | 4.20 | 1.45        | 1.33     |
| 24  | d     | 402    | CLA  | CHD-C1D | 4.20 | 1.46        | 1.38     |
| 24  | C     | 513    | CLA  | O2A-CGA | 4.19 | 1.45        | 1.33     |
| 24  | B     | 606    | CLA  | O2A-CGA | 4.19 | 1.45        | 1.33     |
| 24  | B     | 610    | CLA  | C3D-C2D | 4.18 | 1.50        | 1.39     |
| 24  | C     | 509    | CLA  | C3D-C2D | 4.18 | 1.50        | 1.39     |
| 37  | d     | 408    | LHG  | O8-C23  | 4.18 | 1.45        | 1.33     |
| 36  | c     | 522    | DGD  | O1G-C1A | 4.18 | 1.45        | 1.33     |
| 24  | B     | 607    | CLA  | CHD-C1D | 4.17 | 1.46        | 1.38     |
| 24  | b     | 618    | CLA  | O2A-CGA | 4.17 | 1.45        | 1.33     |
| 24  | B     | 611    | CLA  | OBD-CAD | 4.17 | 1.29        | 1.22     |
| 24  | a     | 412    | CLA  | CHD-C4C | 4.17 | 1.48        | 1.39     |
| 24  | B     | 617    | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 37  | e     | 102    | LHG  | O7-C7   | 4.16 | 1.46        | 1.34     |
| 24  | C     | 506    | CLA  | CHD-C4C | 4.16 | 1.48        | 1.39     |
| 33  | b     | 629    | LMG  | O8-C28  | 4.16 | 1.45        | 1.33     |
| 24  | B     | 615    | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 24  | a     | 409    | CLA  | CHC-C1C | 4.15 | 1.47        | 1.38     |
| 24  | b     | 617    | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 24  | c     | 507    | CLA  | CHD-C1D | 4.15 | 1.46        | 1.38     |
| 24  | B     | 616    | CLA  | CHC-C4B | 4.15 | 1.48        | 1.39     |
| 24  | b     | 624    | CLA  | CHD-C1D | 4.15 | 1.46        | 1.38     |
| 33  | d     | 413    | LMG  | O7-C10  | 4.15 | 1.46        | 1.34     |
| 24  | b     | 625    | CLA  | CHD-C1D | 4.15 | 1.46        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 36  | C     | 518    | DGD  | O1G-C1A | 4.15 | 1.45        | 1.33     |
| 33  | c     | 501    | LMG  | O8-C28  | 4.14 | 1.45        | 1.33     |
| 24  | A     | 407    | CLA  | CHC-C4B | 4.14 | 1.48        | 1.39     |
| 24  | C     | 502    | CLA  | CHD-C1D | 4.14 | 1.46        | 1.38     |
| 24  | c     | 508    | CLA  | CHD-C1D | 4.14 | 1.46        | 1.38     |
| 37  | d     | 408    | LHG  | O7-C7   | 4.13 | 1.46        | 1.34     |
| 24  | C     | 503    | CLA  | CHD-C4C | 4.13 | 1.48        | 1.39     |
| 27  | L     | 102    | SQD  | O48-C23 | 4.13 | 1.45        | 1.33     |
| 25  | a     | 418[B] | PHO  | OBD-CAD | 4.13 | 1.28        | 1.22     |
| 33  | c     | 523    | LMG  | O8-C28  | 4.13 | 1.45        | 1.33     |
| 24  | b     | 611    | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 25  | a     | 418[A] | PHO  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 27  | a     | 414    | SQD  | O48-C23 | 4.13 | 1.45        | 1.33     |
| 24  | B     | 607    | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 24  | b     | 623    | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 36  | C     | 517    | DGD  | O1G-C1A | 4.12 | 1.45        | 1.33     |
| 33  | Z     | 101    | LMG  | O7-C10  | 4.12 | 1.45        | 1.34     |
| 24  | b     | 621    | CLA  | CHD-C1D | 4.12 | 1.46        | 1.38     |
| 37  | E     | 101    | LHG  | O7-C7   | 4.12 | 1.45        | 1.34     |
| 25  | A     | 409[B] | PHO  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 24  | A     | 410    | CLA  | O2A-CGA | 4.11 | 1.45        | 1.33     |
| 24  | B     | 612    | CLA  | CHB-C1B | 4.11 | 1.48        | 1.39     |
| 24  | c     | 508    | CLA  | O2A-CGA | 4.11 | 1.45        | 1.33     |
| 24  | C     | 505    | CLA  | CHD-C1D | 4.11 | 1.46        | 1.38     |
| 24  | B     | 609    | CLA  | CHC-C1C | 4.11 | 1.46        | 1.38     |
| 24  | B     | 604    | CLA  | CHD-C1D | 4.11 | 1.46        | 1.38     |
| 24  | b     | 617    | CLA  | CHB-C1B | 4.11 | 1.48        | 1.39     |
| 24  | B     | 613    | CLA  | C1D-ND  | 4.11 | 1.42        | 1.37     |
| 24  | C     | 505    | CLA  | CHC-C4B | 4.11 | 1.48        | 1.39     |
| 24  | d     | 401    | CLA  | CHC-C1C | 4.10 | 1.46        | 1.38     |
| 24  | b     | 625    | CLA  | C3D-C2D | 4.10 | 1.50        | 1.39     |
| 24  | A     | 406    | CLA  | O2A-CGA | 4.10 | 1.45        | 1.33     |
| 24  | a     | 410    | CLA  | CHD-C1D | 4.10 | 1.46        | 1.38     |
| 24  | b     | 625    | CLA  | O2A-CGA | 4.10 | 1.45        | 1.33     |
| 24  | D     | 402    | CLA  | CHC-C1C | 4.10 | 1.46        | 1.38     |
| 36  | c     | 521    | DGD  | O1G-C1A | 4.10 | 1.45        | 1.33     |
| 24  | C     | 511    | CLA  | C3D-C2D | 4.10 | 1.50        | 1.39     |
| 24  | c     | 518    | CLA  | CHD-C4C | 4.10 | 1.48        | 1.39     |
| 24  | b     | 623    | CLA  | C3D-C2D | 4.10 | 1.50        | 1.39     |
| 36  | h     | 102    | DGD  | O1G-C1A | 4.10 | 1.45        | 1.33     |
| 24  | b     | 620    | CLA  | CHD-C1D | 4.09 | 1.46        | 1.38     |
| 24  | C     | 512    | CLA  | CHD-C1D | 4.09 | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | C     | 510 | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 24  | C     | 501 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 24  | B     | 605 | CLA  | CHD-C1D | 4.09  | 1.46        | 1.38     |
| 24  | B     | 615 | CLA  | CHB-C1B | 4.09  | 1.48        | 1.39     |
| 24  | c     | 509 | CLA  | CHD-C1D | 4.09  | 1.46        | 1.38     |
| 24  | C     | 503 | CLA  | CHC-C4B | 4.09  | 1.48        | 1.39     |
| 33  | z     | 101 | LMG  | O7-C10  | 4.09  | 1.45        | 1.34     |
| 37  | D     | 408 | LHG  | O7-C7   | 4.09  | 1.45        | 1.34     |
| 24  | b     | 617 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 24  | A     | 407 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 24  | c     | 515 | CLA  | CHB-C1B | 4.08  | 1.48        | 1.39     |
| 24  | b     | 612 | CLA  | CHD-C1D | 4.08  | 1.46        | 1.38     |
| 24  | B     | 612 | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 24  | C     | 510 | CLA  | CHD-C4C | 4.07  | 1.48        | 1.39     |
| 24  | D     | 402 | CLA  | C1B-NB  | -4.07 | 1.32        | 1.37     |
| 38  | F     | 102 | HEM  | FE-NC   | 4.07  | 2.08        | 1.95     |
| 24  | C     | 511 | CLA  | CHB-C1B | 4.07  | 1.48        | 1.39     |
| 27  | F     | 103 | SQD  | O48-C23 | 4.07  | 1.45        | 1.33     |
| 24  | c     | 506 | CLA  | O2A-CGA | 4.07  | 1.45        | 1.33     |
| 24  | d     | 402 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 24  | c     | 507 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 24  | d     | 403 | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 24  | d     | 403 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 27  | A     | 416 | SQD  | O47-C7  | 4.05  | 1.45        | 1.34     |
| 24  | C     | 506 | CLA  | C3D-C2D | 4.05  | 1.50        | 1.39     |
| 24  | A     | 407 | CLA  | OBD-CAD | 4.05  | 1.29        | 1.22     |
| 26  | B     | 619 | BCR  | C23-C22 | -4.05 | 1.37        | 1.45     |
| 24  | B     | 606 | CLA  | CHC-C4B | 4.05  | 1.48        | 1.39     |
| 24  | a     | 410 | CLA  | OBD-CAD | 4.05  | 1.29        | 1.22     |
| 24  | c     | 516 | CLA  | C3D-C2D | 4.05  | 1.50        | 1.39     |
| 24  | B     | 614 | CLA  | CHB-C1B | 4.05  | 1.48        | 1.39     |
| 24  | A     | 407 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 37  | D     | 409 | LHG  | O8-C23  | 4.04  | 1.45        | 1.33     |
| 24  | b     | 616 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 25  | A     | 408 | PHO  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 24  | C     | 511 | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 24  | B     | 612 | CLA  | C3D-C2D | 4.04  | 1.50        | 1.39     |
| 24  | C     | 504 | CLA  | C3D-C2D | 4.04  | 1.50        | 1.39     |
| 27  | B     | 621 | SQD  | O48-C23 | 4.04  | 1.45        | 1.33     |
| 24  | c     | 514 | CLA  | OBD-CAD | 4.04  | 1.29        | 1.22     |
| 24  | b     | 612 | CLA  | OBD-CAD | 4.04  | 1.29        | 1.22     |
| 24  | b     | 619 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | c     | 522 | DGD  | O2G-C1B | 4.04  | 1.45        | 1.34     |
| 24  | b     | 610 | CLA  | C3D-C2D | 4.04  | 1.50        | 1.39     |
| 24  | c     | 507 | CLA  | C3D-C2D | 4.03  | 1.50        | 1.39     |
| 24  | a     | 409 | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 24  | c     | 508 | CLA  | OBD-CAD | 4.03  | 1.29        | 1.22     |
| 24  | C     | 505 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 36  | c     | 520 | DGD  | O1G-C1A | 4.03  | 1.45        | 1.33     |
| 24  | b     | 625 | CLA  | CHB-C1B | 4.03  | 1.48        | 1.39     |
| 24  | B     | 604 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 24  | c     | 508 | CLA  | CHC-C4B | 4.03  | 1.48        | 1.39     |
| 24  | B     | 613 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 37  | L     | 101 | LHG  | O8-C23  | 4.03  | 1.45        | 1.33     |
| 24  | d     | 401 | CLA  | CHD-C4C | 4.02  | 1.48        | 1.39     |
| 24  | B     | 613 | CLA  | CHB-C1B | 4.02  | 1.48        | 1.39     |
| 24  | b     | 614 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 24  | b     | 622 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 24  | C     | 504 | CLA  | CHB-C1B | 4.02  | 1.48        | 1.39     |
| 24  | C     | 504 | CLA  | O2A-CGA | 4.01  | 1.45        | 1.33     |
| 24  | C     | 504 | CLA  | CHD-C1D | 4.01  | 1.46        | 1.38     |
| 33  | d     | 413 | LMG  | O8-C28  | 4.01  | 1.45        | 1.33     |
| 24  | b     | 611 | CLA  | CHD-C1D | 4.01  | 1.46        | 1.38     |
| 24  | a     | 412 | CLA  | O2A-CGA | 4.01  | 1.45        | 1.33     |
| 24  | b     | 614 | CLA  | CHB-C1B | 4.01  | 1.48        | 1.39     |
| 24  | C     | 509 | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 37  | D     | 408 | LHG  | O8-C23  | 4.01  | 1.45        | 1.33     |
| 40  | v     | 205 | HEC  | CBC-CAC | -4.00 | 1.33        | 1.51     |
| 24  | c     | 507 | CLA  | O2A-CGA | 4.00  | 1.45        | 1.33     |
| 24  | b     | 624 | CLA  | C3D-C2D | 4.00  | 1.50        | 1.39     |
| 24  | B     | 602 | CLA  | CHD-C4C | 3.99  | 1.48        | 1.39     |
| 24  | b     | 619 | CLA  | CHD-C1D | 3.99  | 1.46        | 1.38     |
| 24  | a     | 412 | CLA  | CHD-C1D | 3.99  | 1.46        | 1.38     |
| 24  | A     | 406 | CLA  | C3D-C2D | 3.99  | 1.50        | 1.39     |
| 24  | b     | 612 | CLA  | CHB-C1B | 3.98  | 1.48        | 1.39     |
| 24  | b     | 615 | CLA  | CHB-C1B | 3.98  | 1.48        | 1.39     |
| 24  | C     | 508 | CLA  | CHD-C4C | 3.98  | 1.48        | 1.39     |
| 24  | B     | 614 | CLA  | O2A-CGA | 3.98  | 1.45        | 1.33     |
| 24  | d     | 401 | CLA  | C3D-C2D | 3.98  | 1.50        | 1.39     |
| 24  | b     | 613 | CLA  | CHB-C1B | 3.98  | 1.48        | 1.39     |
| 27  | A     | 412 | SQD  | O47-C7  | 3.98  | 1.45        | 1.34     |
| 24  | b     | 615 | CLA  | CHD-C1D | 3.97  | 1.46        | 1.38     |
| 35  | b     | 632 | HTG  | C1'-S1  | -3.97 | 1.76        | 1.81     |
| 24  | C     | 512 | CLA  | C3D-C2D | 3.97  | 1.50        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | b     | 620    | CLA  | O2A-CGA | 3.97  | 1.44        | 1.33     |
| 24  | C     | 513    | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 24  | B     | 611    | CLA  | C3D-C2D | 3.97  | 1.50        | 1.39     |
| 24  | C     | 504    | CLA  | OBD-CAD | 3.97  | 1.29        | 1.22     |
| 24  | D     | 403    | CLA  | C3D-C2D | 3.96  | 1.49        | 1.39     |
| 24  | c     | 517    | CLA  | C3D-C2D | 3.96  | 1.49        | 1.39     |
| 36  | H     | 102    | DGD  | O2G-C1B | 3.96  | 1.45        | 1.34     |
| 33  | c     | 523    | LMG  | O7-C10  | 3.96  | 1.45        | 1.34     |
| 24  | A     | 405    | CLA  | O2A-CGA | 3.96  | 1.44        | 1.33     |
| 24  | A     | 405    | CLA  | OBD-CAD | 3.96  | 1.29        | 1.22     |
| 24  | D     | 402    | CLA  | O2A-CGA | 3.96  | 1.44        | 1.33     |
| 24  | b     | 621    | CLA  | O2A-CGA | 3.95  | 1.44        | 1.33     |
| 24  | D     | 403    | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 25  | A     | 409[A] | PHO  | O2A-CGA | 3.95  | 1.44        | 1.33     |
| 24  | c     | 510    | CLA  | CHB-C1B | 3.95  | 1.48        | 1.39     |
| 24  | b     | 621    | CLA  | C3D-C2D | 3.95  | 1.49        | 1.39     |
| 33  | D     | 413    | LMG  | O8-C28  | 3.95  | 1.44        | 1.33     |
| 24  | B     | 614    | CLA  | OBD-CAD | 3.94  | 1.29        | 1.22     |
| 33  | B     | 622    | LMG  | O7-C10  | 3.94  | 1.45        | 1.34     |
| 24  | c     | 513    | CLA  | OBD-CAD | 3.94  | 1.29        | 1.22     |
| 24  | a     | 412    | CLA  | C3D-C2D | 3.94  | 1.49        | 1.39     |
| 24  | c     | 511    | CLA  | O2A-CGA | 3.94  | 1.44        | 1.33     |
| 24  | c     | 517    | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 24  | C     | 504    | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 24  | C     | 503    | CLA  | C3D-C2D | 3.93  | 1.49        | 1.39     |
| 33  | C     | 519    | LMG  | O7-C10  | 3.93  | 1.45        | 1.34     |
| 24  | c     | 515    | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 24  | C     | 513    | CLA  | CHC-C4B | 3.93  | 1.48        | 1.39     |
| 24  | c     | 511    | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 35  | B     | 623    | HTG  | C1'-S1  | -3.93 | 1.76        | 1.81     |
| 24  | c     | 508    | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 24  | B     | 611    | CLA  | O2A-CGA | 3.92  | 1.44        | 1.33     |
| 24  | B     | 602    | CLA  | CHC-C4B | 3.92  | 1.48        | 1.39     |
| 36  | C     | 516    | DGD  | O1G-C1A | 3.92  | 1.44        | 1.33     |
| 24  | b     | 618    | CLA  | OBD-CAD | 3.92  | 1.29        | 1.22     |
| 24  | b     | 615    | CLA  | O2A-CGA | 3.92  | 1.44        | 1.33     |
| 24  | b     | 623    | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 24  | d     | 403    | CLA  | CHC-C4B | 3.92  | 1.48        | 1.39     |
| 24  | B     | 605    | CLA  | O2A-CGA | 3.92  | 1.44        | 1.33     |
| 24  | b     | 610    | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 24  | a     | 410    | CLA  | CHB-C1B | 3.92  | 1.48        | 1.39     |
| 24  | c     | 509    | CLA  | CHB-C1B | 3.91  | 1.48        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 24  | B     | 617    | CLA  | CHB-C1B | 3.91 | 1.48        | 1.39     |
| 24  | c     | 517    | CLA  | OBD-CAD | 3.91 | 1.29        | 1.22     |
| 24  | B     | 603    | CLA  | CHD-C4C | 3.91 | 1.48        | 1.39     |
| 24  | B     | 605    | CLA  | CHB-C1B | 3.91 | 1.48        | 1.39     |
| 24  | B     | 604    | CLA  | CHB-C1B | 3.90 | 1.48        | 1.39     |
| 24  | b     | 615    | CLA  | CHD-C4C | 3.90 | 1.48        | 1.39     |
| 24  | c     | 514    | CLA  | C3D-C2D | 3.90 | 1.49        | 1.39     |
| 24  | b     | 616    | CLA  | CHC-C4B | 3.90 | 1.48        | 1.39     |
| 24  | c     | 506    | CLA  | CHD-C4C | 3.90 | 1.48        | 1.39     |
| 25  | a     | 418[A] | PHO  | OBD-CAD | 3.90 | 1.27        | 1.22     |
| 24  | B     | 609    | CLA  | CHD-C4C | 3.90 | 1.48        | 1.39     |
| 24  | B     | 606    | CLA  | OBD-CAD | 3.89 | 1.29        | 1.22     |
| 24  | c     | 514    | CLA  | CHD-C4C | 3.89 | 1.48        | 1.39     |
| 24  | B     | 610    | CLA  | OBD-CAD | 3.89 | 1.29        | 1.22     |
| 24  | B     | 611    | CLA  | CHD-C4C | 3.89 | 1.48        | 1.39     |
| 24  | c     | 515    | CLA  | OBD-CAD | 3.89 | 1.29        | 1.22     |
| 24  | B     | 606    | CLA  | CHD-C4C | 3.89 | 1.48        | 1.39     |
| 24  | A     | 405    | CLA  | CHD-C4C | 3.89 | 1.48        | 1.39     |
| 24  | B     | 608    | CLA  | CHD-C1D | 3.89 | 1.45        | 1.38     |
| 24  | c     | 512    | CLA  | C3D-C2D | 3.89 | 1.49        | 1.39     |
| 24  | c     | 509    | CLA  | O2A-CGA | 3.89 | 1.44        | 1.33     |
| 24  | b     | 622    | CLA  | CHB-C1B | 3.89 | 1.48        | 1.39     |
| 24  | A     | 410    | CLA  | CHC-C4B | 3.88 | 1.48        | 1.39     |
| 24  | b     | 619    | CLA  | CHB-C1B | 3.88 | 1.48        | 1.39     |
| 24  | c     | 509    | CLA  | CHD-C4C | 3.88 | 1.48        | 1.39     |
| 24  | B     | 603    | CLA  | OBD-CAD | 3.88 | 1.29        | 1.22     |
| 40  | v     | 205    | HEC  | FE-NC   | 3.88 | 2.08        | 1.95     |
| 24  | B     | 602    | CLA  | C3D-C2D | 3.88 | 1.49        | 1.39     |
| 24  | c     | 512    | CLA  | CHD-C1D | 3.88 | 1.45        | 1.38     |
| 24  | C     | 508    | CLA  | C3D-C2D | 3.88 | 1.49        | 1.39     |
| 24  | a     | 410    | CLA  | CHD-C4C | 3.88 | 1.48        | 1.39     |
| 24  | C     | 502    | CLA  | O2A-CGA | 3.87 | 1.44        | 1.33     |
| 24  | B     | 604    | CLA  | CHC-C4B | 3.87 | 1.48        | 1.39     |
| 24  | D     | 403    | CLA  | O2A-CGA | 3.87 | 1.44        | 1.33     |
| 24  | C     | 501    | CLA  | OBD-CAD | 3.87 | 1.29        | 1.22     |
| 27  | A     | 412    | SQD  | O48-C23 | 3.87 | 1.44        | 1.33     |
| 24  | A     | 410    | CLA  | CHB-C1B | 3.87 | 1.48        | 1.39     |
| 24  | A     | 410    | CLA  | OBD-CAD | 3.87 | 1.29        | 1.22     |
| 24  | A     | 405    | CLA  | CHD-C1D | 3.87 | 1.45        | 1.38     |
| 24  | b     | 617    | CLA  | C3D-C2D | 3.87 | 1.49        | 1.39     |
| 24  | B     | 603    | CLA  | O2A-CGA | 3.87 | 1.44        | 1.33     |
| 36  | h     | 102    | DGD  | O2G-C1B | 3.87 | 1.45        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 614 | CLA  | O2A-CGA | 3.86  | 1.44        | 1.33     |
| 24  | A     | 406 | CLA  | C1B-NB  | -3.86 | 1.33        | 1.37     |
| 24  | c     | 509 | CLA  | C3D-C2D | 3.86  | 1.49        | 1.39     |
| 24  | c     | 517 | CLA  | CHC-C4B | 3.86  | 1.48        | 1.39     |
| 33  | b     | 629 | LMG  | O7-C10  | 3.86  | 1.45        | 1.34     |
| 24  | D     | 402 | CLA  | C3D-C2D | 3.86  | 1.49        | 1.39     |
| 24  | D     | 402 | CLA  | CHD-C1D | 3.85  | 1.45        | 1.38     |
| 24  | B     | 608 | CLA  | O2A-CGA | 3.85  | 1.44        | 1.33     |
| 24  | b     | 617 | CLA  | CHC-C4B | 3.85  | 1.48        | 1.39     |
| 24  | A     | 410 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 24  | c     | 513 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 37  | d     | 407 | LHG  | O7-C7   | 3.85  | 1.45        | 1.34     |
| 24  | B     | 616 | CLA  | CHD-C1D | 3.85  | 1.45        | 1.38     |
| 24  | B     | 609 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 24  | a     | 412 | CLA  | C4B-NB  | -3.84 | 1.33        | 1.37     |
| 24  | d     | 401 | CLA  | CHB-C1B | 3.84  | 1.48        | 1.39     |
| 24  | C     | 507 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 24  | B     | 614 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 24  | a     | 412 | CLA  | OBD-CAD | 3.84  | 1.29        | 1.22     |
| 24  | B     | 603 | CLA  | CHC-C4B | 3.84  | 1.48        | 1.39     |
| 24  | A     | 406 | CLA  | CHC-C1C | 3.84  | 1.46        | 1.38     |
| 35  | B     | 632 | HTG  | C1'-S1  | -3.84 | 1.76        | 1.81     |
| 24  | A     | 407 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 24  | b     | 613 | CLA  | O2A-CGA | 3.83  | 1.44        | 1.33     |
| 40  | V     | 205 | HEC  | CBC-CAC | -3.83 | 1.34        | 1.51     |
| 24  | B     | 607 | CLA  | C1B-NB  | -3.83 | 1.33        | 1.37     |
| 24  | B     | 606 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 33  | c     | 501 | LMG  | O7-C10  | 3.83  | 1.45        | 1.34     |
| 37  | D     | 407 | LHG  | O8-C23  | 3.82  | 1.44        | 1.33     |
| 24  | b     | 619 | CLA  | CHC-C4B | 3.82  | 1.48        | 1.39     |
| 24  | b     | 610 | CLA  | CHC-C4B | 3.82  | 1.48        | 1.39     |
| 24  | c     | 506 | CLA  | CHB-C1B | 3.82  | 1.48        | 1.39     |
| 24  | C     | 502 | CLA  | CHB-C1B | 3.82  | 1.48        | 1.39     |
| 36  | C     | 518 | DGD  | O2G-C1B | 3.82  | 1.45        | 1.34     |
| 24  | C     | 507 | CLA  | CHD-C4C | 3.82  | 1.47        | 1.39     |
| 24  | C     | 507 | CLA  | CHC-C4B | 3.81  | 1.48        | 1.39     |
| 36  | C     | 516 | DGD  | O2G-C1B | 3.81  | 1.45        | 1.34     |
| 40  | v     | 205 | HEC  | CBB-CAB | -3.81 | 1.34        | 1.51     |
| 24  | B     | 606 | CLA  | CHD-C1D | 3.81  | 1.45        | 1.38     |
| 37  | b     | 634 | LHG  | O7-C7   | 3.81  | 1.45        | 1.34     |
| 24  | B     | 606 | CLA  | CHB-C1B | 3.81  | 1.47        | 1.39     |
| 24  | c     | 509 | CLA  | CHC-C4B | 3.80  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 622 | CLA  | O2A-CGA | 3.80  | 1.44        | 1.33     |
| 24  | b     | 618 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 24  | c     | 518 | CLA  | CHC-C4B | 3.80  | 1.47        | 1.39     |
| 24  | B     | 604 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 24  | b     | 614 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 24  | d     | 402 | CLA  | C1B-NB  | -3.80 | 1.33        | 1.37     |
| 24  | B     | 604 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 27  | a     | 414 | SQD  | O47-C7  | 3.80  | 1.45        | 1.34     |
| 24  | d     | 403 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 24  | b     | 624 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 24  | b     | 622 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 24  | b     | 614 | CLA  | CHC-C4B | 3.79  | 1.47        | 1.39     |
| 24  | b     | 618 | CLA  | CHB-C1B | 3.79  | 1.47        | 1.39     |
| 24  | C     | 502 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 24  | c     | 518 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 24  | b     | 613 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 24  | C     | 505 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 24  | C     | 502 | CLA  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 24  | b     | 617 | CLA  | OBD-CAD | 3.78  | 1.29        | 1.22     |
| 24  | A     | 406 | CLA  | CHD-C1D | 3.78  | 1.45        | 1.38     |
| 24  | c     | 511 | CLA  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 24  | b     | 621 | CLA  | CHB-C1B | 3.78  | 1.47        | 1.39     |
| 24  | d     | 403 | CLA  | CHB-C1B | 3.78  | 1.47        | 1.39     |
| 24  | C     | 501 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 24  | B     | 603 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 36  | c     | 521 | DGD  | O2G-C1B | 3.77  | 1.44        | 1.34     |
| 24  | B     | 614 | CLA  | CHC-C4B | 3.77  | 1.47        | 1.39     |
| 24  | B     | 612 | CLA  | O2A-CGA | 3.77  | 1.44        | 1.33     |
| 36  | C     | 517 | DGD  | O2G-C1B | 3.77  | 1.44        | 1.34     |
| 24  | D     | 402 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 24  | D     | 403 | CLA  | CHB-C1B | 3.76  | 1.47        | 1.39     |
| 24  | c     | 515 | CLA  | O2A-CGA | 3.76  | 1.44        | 1.33     |
| 24  | B     | 602 | CLA  | CHB-C1B | 3.76  | 1.47        | 1.39     |
| 24  | B     | 607 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 24  | b     | 620 | CLA  | CHB-C1B | 3.76  | 1.47        | 1.39     |
| 24  | B     | 612 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 24  | C     | 512 | CLA  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 24  | b     | 615 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 40  | V     | 205 | HEC  | FE-NC   | 3.75  | 2.07        | 1.95     |
| 24  | B     | 609 | CLA  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 24  | b     | 611 | CLA  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 24  | a     | 412 | CLA  | CHB-C1B | 3.75  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 37  | d     | 406 | LHG  | O8-C23  | 3.75  | 1.44        | 1.33     |
| 24  | c     | 510 | CLA  | CHC-C4B | 3.75  | 1.47        | 1.39     |
| 24  | C     | 509 | CLA  | CHB-C1B | 3.75  | 1.47        | 1.39     |
| 24  | C     | 505 | CLA  | CHB-C1B | 3.75  | 1.47        | 1.39     |
| 24  | C     | 501 | CLA  | CHC-C4B | 3.75  | 1.47        | 1.39     |
| 24  | B     | 610 | CLA  | CHB-C1B | 3.75  | 1.47        | 1.39     |
| 24  | c     | 510 | CLA  | O2A-CGA | 3.75  | 1.44        | 1.33     |
| 24  | b     | 616 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 24  | c     | 511 | CLA  | CHB-C1B | 3.74  | 1.47        | 1.39     |
| 24  | B     | 607 | CLA  | CHC-C4B | 3.74  | 1.47        | 1.39     |
| 24  | b     | 620 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 24  | B     | 613 | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 24  | C     | 513 | CLA  | C3D-C2D | 3.74  | 1.49        | 1.39     |
| 24  | C     | 512 | CLA  | CHC-C4B | 3.74  | 1.47        | 1.39     |
| 24  | C     | 512 | CLA  | CHB-C1B | 3.73  | 1.47        | 1.39     |
| 24  | c     | 506 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 40  | V     | 205 | HEC  | CBB-CAB | -3.73 | 1.34        | 1.51     |
| 24  | b     | 619 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 24  | C     | 506 | CLA  | CHB-C1B | 3.73  | 1.47        | 1.39     |
| 24  | b     | 612 | CLA  | CHC-C4B | 3.73  | 1.47        | 1.39     |
| 24  | c     | 513 | CLA  | CHB-C1B | 3.73  | 1.47        | 1.39     |
| 24  | d     | 402 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 38  | F     | 102 | HEM  | C4D-ND  | -3.72 | 1.33        | 1.40     |
| 24  | B     | 613 | CLA  | CHC-C4B | 3.72  | 1.47        | 1.39     |
| 24  | C     | 504 | CLA  | CHC-C4B | 3.72  | 1.47        | 1.39     |
| 24  | B     | 614 | CLA  | CHD-C1D | 3.72  | 1.45        | 1.38     |
| 24  | B     | 611 | CLA  | CHB-C1B | 3.72  | 1.47        | 1.39     |
| 24  | B     | 613 | CLA  | CHD-C1D | 3.72  | 1.45        | 1.38     |
| 24  | B     | 617 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 24  | B     | 615 | CLA  | CHC-C4B | 3.72  | 1.47        | 1.39     |
| 24  | d     | 401 | CLA  | C4B-NB  | -3.71 | 1.33        | 1.37     |
| 24  | b     | 619 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 24  | B     | 611 | CLA  | CHC-C4B | 3.71  | 1.47        | 1.39     |
| 24  | b     | 611 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 24  | C     | 512 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 24  | b     | 618 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 24  | B     | 609 | CLA  | CHB-C1B | 3.71  | 1.47        | 1.39     |
| 24  | b     | 621 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 24  | a     | 409 | CLA  | CHC-C4B | 3.71  | 1.47        | 1.39     |
| 24  | A     | 406 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 37  | L     | 101 | LHG  | O7-C7   | 3.70  | 1.44        | 1.34     |
| 24  | C     | 508 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35  | V     | 206 | HTG  | C1'-S1  | -3.70 | 1.76        | 1.81     |
| 24  | D     | 402 | CLA  | CHB-C1B | 3.70  | 1.47        | 1.39     |
| 24  | B     | 617 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 24  | b     | 616 | CLA  | O2A-CGA | 3.70  | 1.44        | 1.33     |
| 24  | b     | 621 | CLA  | CHC-C4B | 3.70  | 1.47        | 1.39     |
| 24  | d     | 402 | CLA  | CHB-C1B | 3.69  | 1.47        | 1.39     |
| 24  | C     | 510 | CLA  | CHC-C4B | 3.69  | 1.47        | 1.39     |
| 24  | d     | 402 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 36  | c     | 520 | DGD  | O2G-C1B | 3.69  | 1.44        | 1.34     |
| 24  | B     | 604 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 24  | C     | 507 | CLA  | CHB-C1B | 3.69  | 1.47        | 1.39     |
| 24  | C     | 501 | CLA  | CHB-C1B | 3.69  | 1.47        | 1.39     |
| 24  | b     | 620 | CLA  | CHC-C4B | 3.69  | 1.47        | 1.39     |
| 24  | b     | 625 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 24  | c     | 507 | CLA  | CHB-C1B | 3.69  | 1.47        | 1.39     |
| 24  | d     | 403 | CLA  | C1B-NB  | -3.68 | 1.33        | 1.37     |
| 35  | d     | 411 | HTG  | C1'-S1  | -3.68 | 1.76        | 1.81     |
| 24  | C     | 511 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 24  | b     | 623 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 24  | b     | 614 | CLA  | C3D-C2D | 3.68  | 1.49        | 1.39     |
| 24  | B     | 610 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 24  | C     | 509 | CLA  | CHC-C4B | 3.67  | 1.47        | 1.39     |
| 24  | B     | 608 | CLA  | CHC-C4B | 3.67  | 1.47        | 1.39     |
| 24  | c     | 512 | CLA  | CHB-C1B | 3.67  | 1.47        | 1.39     |
| 24  | B     | 612 | CLA  | CHC-C4B | 3.67  | 1.47        | 1.39     |
| 24  | B     | 613 | CLA  | C3D-C2D | 3.67  | 1.49        | 1.39     |
| 33  | D     | 413 | LMG  | O7-C10  | 3.67  | 1.44        | 1.34     |
| 35  | B     | 625 | HTG  | C1'-S1  | -3.67 | 1.76        | 1.81     |
| 24  | c     | 512 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 35  | D     | 412 | HTG  | C1'-S1  | -3.66 | 1.76        | 1.81     |
| 24  | B     | 608 | CLA  | CHD-C4C | 3.65  | 1.47        | 1.39     |
| 24  | c     | 511 | CLA  | C1B-NB  | -3.65 | 1.33        | 1.37     |
| 24  | b     | 624 | CLA  | CHB-C1B | 3.65  | 1.47        | 1.39     |
| 37  | d     | 407 | LHG  | O8-C23  | 3.65  | 1.44        | 1.33     |
| 24  | c     | 516 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 24  | c     | 515 | CLA  | C3D-C2D | 3.65  | 1.49        | 1.39     |
| 35  | b     | 608 | HTG  | C1'-S1  | -3.64 | 1.76        | 1.81     |
| 24  | B     | 615 | CLA  | C3D-C2D | 3.64  | 1.49        | 1.39     |
| 24  | C     | 504 | CLA  | C1B-NB  | -3.64 | 1.33        | 1.37     |
| 24  | C     | 502 | CLA  | CHC-C4B | 3.64  | 1.47        | 1.39     |
| 24  | B     | 605 | CLA  | CHC-C4B | 3.64  | 1.47        | 1.39     |
| 24  | c     | 510 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | A     | 410 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 24  | B     | 616 | CLA  | CHB-C1B | 3.63  | 1.47        | 1.39     |
| 24  | B     | 615 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 24  | b     | 611 | CLA  | C3D-C2D | 3.63  | 1.49        | 1.39     |
| 24  | C     | 510 | CLA  | C3D-C2D | 3.63  | 1.49        | 1.39     |
| 24  | c     | 518 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 24  | a     | 412 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 24  | D     | 402 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 37  | d     | 406 | LHG  | O7-C7   | 3.62  | 1.44        | 1.34     |
| 24  | b     | 620 | CLA  | C3D-C2D | 3.62  | 1.49        | 1.39     |
| 24  | B     | 616 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 24  | d     | 403 | CLA  | C3D-C2D | 3.62  | 1.49        | 1.39     |
| 24  | B     | 615 | CLA  | CHD-C1D | 3.62  | 1.45        | 1.38     |
| 35  | c     | 525 | HTG  | C1'-S1  | -3.61 | 1.76        | 1.81     |
| 24  | b     | 622 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 24  | B     | 617 | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 24  | B     | 605 | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 24  | c     | 516 | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 24  | b     | 620 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 24  | C     | 506 | CLA  | C1B-NB  | -3.60 | 1.33        | 1.37     |
| 24  | a     | 410 | CLA  | C3D-C2D | 3.59  | 1.48        | 1.39     |
| 24  | C     | 503 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 24  | B     | 616 | CLA  | C3D-C2D | 3.59  | 1.48        | 1.39     |
| 24  | b     | 616 | CLA  | C3D-C2D | 3.58  | 1.48        | 1.39     |
| 24  | B     | 608 | CLA  | CHB-C1B | 3.58  | 1.47        | 1.39     |
| 24  | c     | 507 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 24  | B     | 614 | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 24  | b     | 616 | CLA  | C1B-NB  | -3.58 | 1.33        | 1.37     |
| 24  | B     | 610 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 24  | b     | 613 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 24  | B     | 608 | CLA  | C3D-C2D | 3.57  | 1.48        | 1.39     |
| 24  | B     | 611 | CLA  | C1B-NB  | -3.57 | 1.33        | 1.37     |
| 24  | c     | 510 | CLA  | C3D-C2D | 3.57  | 1.48        | 1.39     |
| 24  | A     | 405 | CLA  | CHC-C4B | 3.56  | 1.47        | 1.39     |
| 24  | a     | 409 | CLA  | O2A-CGA | 3.56  | 1.43        | 1.33     |
| 24  | A     | 405 | CLA  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 24  | C     | 509 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 24  | c     | 516 | CLA  | CHD-C4C | 3.56  | 1.47        | 1.39     |
| 24  | b     | 619 | CLA  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 24  | b     | 612 | CLA  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 24  | b     | 618 | CLA  | CHC-C4B | 3.56  | 1.47        | 1.39     |
| 24  | a     | 409 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35  | c     | 526 | HTG  | C1'-S1  | -3.55 | 1.76        | 1.81     |
| 24  | b     | 621 | CLA  | CHD-C4C | 3.55  | 1.47        | 1.39     |
| 24  | b     | 624 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 24  | C     | 503 | CLA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 24  | c     | 507 | CLA  | CHC-C4B | 3.54  | 1.47        | 1.39     |
| 24  | A     | 405 | CLA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 24  | B     | 607 | CLA  | CHB-C1B | 3.53  | 1.47        | 1.39     |
| 24  | C     | 505 | CLA  | C1B-NB  | -3.53 | 1.33        | 1.37     |
| 35  | B     | 633 | HTG  | C1'-S1  | -3.53 | 1.76        | 1.81     |
| 24  | B     | 603 | CLA  | CHB-C1B | 3.53  | 1.47        | 1.39     |
| 24  | b     | 611 | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 24  | D     | 403 | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 24  | B     | 615 | CLA  | C1B-NB  | -3.52 | 1.33        | 1.37     |
| 24  | d     | 403 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 35  | C     | 522 | HTG  | C1'-S1  | -3.52 | 1.76        | 1.81     |
| 24  | B     | 616 | CLA  | CHD-C4C | 3.52  | 1.47        | 1.39     |
| 24  | B     | 615 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 24  | c     | 516 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 24  | c     | 508 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 24  | c     | 508 | CLA  | C3D-C2D | 3.51  | 1.48        | 1.39     |
| 24  | B     | 609 | CLA  | C4B-NB  | -3.51 | 1.33        | 1.37     |
| 24  | b     | 612 | CLA  | CHD-C4C | 3.50  | 1.47        | 1.39     |
| 24  | b     | 613 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 24  | b     | 624 | CLA  | CHC-C4B | 3.49  | 1.47        | 1.39     |
| 24  | d     | 401 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 24  | C     | 507 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 24  | B     | 611 | CLA  | C4B-NB  | -3.48 | 1.33        | 1.37     |
| 24  | d     | 401 | CLA  | CHC-C4B | 3.48  | 1.47        | 1.39     |
| 24  | b     | 616 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 24  | c     | 518 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 24  | C     | 513 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 24  | b     | 622 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 35  | C     | 523 | HTG  | C1'-S1  | -3.48 | 1.77        | 1.81     |
| 24  | a     | 409 | CLA  | C3D-C2D | 3.48  | 1.48        | 1.39     |
| 24  | C     | 513 | CLA  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 40  | V     | 205 | HEC  | C1D-ND  | -3.47 | 1.34        | 1.40     |
| 24  | d     | 402 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 24  | B     | 607 | CLA  | C3D-C2D | 3.47  | 1.48        | 1.39     |
| 24  | c     | 514 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 24  | B     | 603 | CLA  | C1B-NB  | -3.47 | 1.33        | 1.37     |
| 24  | c     | 509 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 24  | C     | 510 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | c     | 515 | CLA  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 24  | b     | 623 | CLA  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 35  | b     | 601 | HTG  | C1'-S1  | -3.46 | 1.77        | 1.81     |
| 24  | D     | 403 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 24  | b     | 625 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 24  | b     | 625 | CLA  | C4B-NB  | -3.45 | 1.33        | 1.37     |
| 24  | b     | 611 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 24  | B     | 604 | CLA  | C1B-NB  | -3.45 | 1.33        | 1.37     |
| 24  | c     | 512 | CLA  | CHC-C4B | 3.45  | 1.47        | 1.39     |
| 35  | b     | 607 | HTG  | C1'-S1  | -3.45 | 1.77        | 1.81     |
| 24  | A     | 406 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 24  | B     | 602 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 24  | B     | 617 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 24  | A     | 406 | CLA  | C4B-NB  | -3.43 | 1.33        | 1.37     |
| 24  | B     | 612 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 24  | b     | 623 | CLA  | CHB-C1B | 3.43  | 1.47        | 1.39     |
| 24  | C     | 509 | CLA  | C1B-NB  | -3.43 | 1.33        | 1.37     |
| 24  | c     | 506 | CLA  | C1B-NB  | -3.43 | 1.33        | 1.37     |
| 24  | b     | 625 | CLA  | CHC-C4B | 3.41  | 1.47        | 1.39     |
| 24  | b     | 618 | CLA  | C1B-NB  | -3.40 | 1.33        | 1.37     |
| 38  | F     | 102 | HEM  | C1B-NB  | -3.39 | 1.34        | 1.40     |
| 24  | c     | 511 | CLA  | CHC-C4B | 3.39  | 1.47        | 1.39     |
| 38  | e     | 103 | HEM  | C4D-ND  | -3.38 | 1.34        | 1.40     |
| 24  | B     | 613 | CLA  | C1C-C2C | 3.37  | 1.51        | 1.44     |
| 24  | a     | 409 | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 24  | C     | 508 | CLA  | CHC-C4B | 3.37  | 1.47        | 1.39     |
| 24  | C     | 506 | CLA  | CHC-C4B | 3.37  | 1.47        | 1.39     |
| 24  | b     | 610 | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 24  | A     | 406 | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 24  | B     | 605 | CLA  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 24  | c     | 512 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 24  | c     | 516 | CLA  | C4B-NB  | -3.36 | 1.33        | 1.37     |
| 24  | b     | 610 | CLA  | C3B-C4B | 3.36  | 1.50        | 1.42     |
| 24  | B     | 610 | CLA  | C1B-NB  | -3.35 | 1.33        | 1.37     |
| 24  | C     | 502 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 24  | c     | 510 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 24  | c     | 506 | CLA  | CHC-C4B | 3.35  | 1.46        | 1.39     |
| 24  | c     | 511 | CLA  | OBD-CAD | 3.34  | 1.28        | 1.22     |
| 24  | C     | 505 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 24  | b     | 610 | CLA  | OBD-CAD | 3.34  | 1.28        | 1.22     |
| 24  | b     | 615 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 24  | a     | 410 | CLA  | CHC-C4B | 3.33  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | C     | 508 | CLA  | CHB-C1B | 3.32  | 1.46        | 1.39     |
| 24  | b     | 610 | CLA  | C1B-NB  | -3.31 | 1.33        | 1.37     |
| 24  | c     | 514 | CLA  | C1B-NB  | -3.31 | 1.33        | 1.37     |
| 24  | A     | 407 | CLA  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 24  | c     | 506 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 24  | B     | 609 | CLA  | CHC-C4B | 3.30  | 1.46        | 1.39     |
| 24  | C     | 501 | CLA  | C1B-NB  | -3.30 | 1.33        | 1.37     |
| 24  | C     | 506 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 40  | v     | 205 | HEC  | C1D-ND  | -3.30 | 1.34        | 1.40     |
| 24  | c     | 517 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 24  | c     | 513 | CLA  | CHC-C4B | 3.29  | 1.46        | 1.39     |
| 24  | C     | 511 | CLA  | C1B-C2B | 3.28  | 1.51        | 1.43     |
| 24  | b     | 611 | CLA  | C1B-NB  | -3.27 | 1.33        | 1.37     |
| 24  | A     | 407 | CLA  | C3B-C4B | 3.26  | 1.50        | 1.42     |
| 24  | b     | 613 | CLA  | CHD-C4C | 3.26  | 1.46        | 1.39     |
| 24  | B     | 607 | CLA  | C4B-NB  | -3.25 | 1.33        | 1.37     |
| 37  | D     | 407 | LHG  | O7-C7   | 3.25  | 1.43        | 1.34     |
| 24  | b     | 615 | CLA  | CHC-C4B | 3.25  | 1.46        | 1.39     |
| 24  | b     | 619 | CLA  | C4B-NB  | -3.25 | 1.33        | 1.37     |
| 24  | b     | 619 | CLA  | C1B-NB  | -3.24 | 1.33        | 1.37     |
| 24  | B     | 615 | CLA  | C4B-NB  | -3.24 | 1.33        | 1.37     |
| 24  | b     | 611 | CLA  | C4B-NB  | -3.23 | 1.33        | 1.37     |
| 38  | e     | 103 | HEM  | C1B-NB  | -3.23 | 1.34        | 1.40     |
| 24  | C     | 513 | CLA  | C3B-C4B | 3.22  | 1.50        | 1.42     |
| 24  | b     | 615 | CLA  | C1B-NB  | -3.22 | 1.33        | 1.37     |
| 24  | C     | 513 | CLA  | C1B-NB  | -3.21 | 1.33        | 1.37     |
| 24  | A     | 405 | CLA  | C4B-NB  | -3.21 | 1.33        | 1.37     |
| 24  | c     | 507 | CLA  | C4B-NB  | -3.20 | 1.33        | 1.37     |
| 24  | c     | 510 | CLA  | C1B-NB  | -3.20 | 1.33        | 1.37     |
| 25  | a     | 411 | PHO  | O2A-CGA | 3.19  | 1.42        | 1.33     |
| 24  | c     | 509 | CLA  | C1B-NB  | -3.19 | 1.33        | 1.37     |
| 24  | b     | 616 | CLA  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 24  | c     | 517 | CLA  | C1B-NB  | -3.17 | 1.33        | 1.37     |
| 24  | b     | 614 | CLA  | OBD-CAD | 3.17  | 1.27        | 1.22     |
| 24  | c     | 518 | CLA  | C3B-C4B | 3.17  | 1.50        | 1.42     |
| 24  | C     | 502 | CLA  | C1B-NB  | -3.17 | 1.33        | 1.37     |
| 24  | c     | 508 | CLA  | C3B-C4B | 3.17  | 1.50        | 1.42     |
| 24  | C     | 511 | CLA  | CHC-C4B | 3.16  | 1.46        | 1.39     |
| 24  | b     | 613 | CLA  | OBD-CAD | 3.16  | 1.27        | 1.22     |
| 24  | C     | 508 | CLA  | C4C-C3C | 3.16  | 1.50        | 1.45     |
| 24  | B     | 607 | CLA  | OBD-CAD | 3.16  | 1.27        | 1.22     |
| 24  | b     | 625 | CLA  | C1B-NB  | -3.16 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | b     | 616 | CLA  | C1B-C2B | 3.16  | 1.50        | 1.43     |
| 24  | A     | 410 | CLA  | C4B-NB  | -3.16 | 1.33        | 1.37     |
| 24  | C     | 508 | CLA  | C1B-NB  | -3.16 | 1.33        | 1.37     |
| 24  | B     | 613 | CLA  | CHD-C4C | 3.16  | 1.46        | 1.39     |
| 24  | C     | 503 | CLA  | C3B-C4B | 3.15  | 1.50        | 1.42     |
| 24  | c     | 517 | CLA  | C4B-NB  | -3.15 | 1.33        | 1.37     |
| 24  | c     | 508 | CLA  | C1C-C2C | 3.15  | 1.50        | 1.44     |
| 24  | C     | 505 | CLA  | OBD-CAD | 3.14  | 1.27        | 1.22     |
| 24  | c     | 506 | CLA  | C4B-NB  | -3.14 | 1.33        | 1.37     |
| 24  | c     | 513 | CLA  | C1B-NB  | -3.14 | 1.33        | 1.37     |
| 24  | b     | 621 | CLA  | C1B-NB  | -3.14 | 1.33        | 1.37     |
| 24  | c     | 509 | CLA  | C4B-NB  | -3.13 | 1.33        | 1.37     |
| 24  | b     | 616 | CLA  | C3B-C4B | 3.13  | 1.50        | 1.42     |
| 24  | C     | 507 | CLA  | C1B-NB  | -3.12 | 1.33        | 1.37     |
| 24  | C     | 510 | CLA  | C1B-NB  | -3.12 | 1.33        | 1.37     |
| 24  | b     | 621 | CLA  | C4B-NB  | -3.12 | 1.33        | 1.37     |
| 24  | D     | 403 | CLA  | C4B-NB  | -3.11 | 1.34        | 1.37     |
| 24  | a     | 410 | CLA  | C1B-NB  | -3.11 | 1.34        | 1.37     |
| 40  | V     | 205 | HEC  | C4B-NB  | -3.11 | 1.34        | 1.40     |
| 24  | c     | 515 | CLA  | C1B-NB  | -3.11 | 1.34        | 1.37     |
| 24  | C     | 508 | CLA  | C3B-C4B | 3.11  | 1.50        | 1.42     |
| 24  | b     | 624 | CLA  | C1B-NB  | -3.10 | 1.34        | 1.37     |
| 24  | c     | 514 | CLA  | C4B-NB  | -3.10 | 1.34        | 1.37     |
| 24  | B     | 602 | CLA  | C3B-C4B | 3.10  | 1.50        | 1.42     |
| 24  | b     | 622 | CLA  | C4B-NB  | -3.10 | 1.34        | 1.37     |
| 24  | C     | 511 | CLA  | C4B-NB  | -3.10 | 1.34        | 1.37     |
| 24  | b     | 622 | CLA  | CHC-C4B | 3.10  | 1.46        | 1.39     |
| 24  | b     | 620 | CLA  | C1B-NB  | -3.09 | 1.34        | 1.37     |
| 24  | c     | 510 | CLA  | C3B-C4B | 3.08  | 1.50        | 1.42     |
| 24  | A     | 405 | CLA  | C4C-C3C | 3.08  | 1.50        | 1.45     |
| 24  | A     | 406 | CLA  | OBD-CAD | 3.08  | 1.27        | 1.22     |
| 24  | c     | 514 | CLA  | C1B-C2B | 3.07  | 1.50        | 1.43     |
| 24  | b     | 625 | CLA  | C1B-C2B | 3.07  | 1.50        | 1.43     |
| 24  | a     | 409 | CLA  | C1B-NB  | -3.07 | 1.34        | 1.37     |
| 24  | A     | 405 | CLA  | C1B-NB  | -3.06 | 1.34        | 1.37     |
| 24  | B     | 606 | CLA  | C1C-C2C | 3.06  | 1.50        | 1.44     |
| 24  | c     | 512 | CLA  | C4B-NB  | -3.05 | 1.34        | 1.37     |
| 24  | b     | 614 | CLA  | C3B-C4B | 3.05  | 1.49        | 1.42     |
| 24  | b     | 623 | CLA  | C1B-NB  | -3.05 | 1.34        | 1.37     |
| 24  | c     | 516 | CLA  | C1B-NB  | -3.04 | 1.34        | 1.37     |
| 24  | a     | 410 | CLA  | C3B-C4B | 3.03  | 1.49        | 1.42     |
| 24  | a     | 409 | CLA  | C4B-NB  | -3.03 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | B     | 613 | CLA  | C4B-NB  | -3.03 | 1.34        | 1.37     |
| 24  | b     | 613 | CLA  | C1B-C2B | 3.03  | 1.50        | 1.43     |
| 24  | c     | 517 | CLA  | C3B-C4B | 3.03  | 1.49        | 1.42     |
| 24  | b     | 612 | CLA  | C4B-NB  | -3.02 | 1.34        | 1.37     |
| 24  | c     | 515 | CLA  | C4B-NB  | -3.02 | 1.34        | 1.37     |
| 24  | C     | 505 | CLA  | C4B-NB  | -3.01 | 1.34        | 1.37     |
| 24  | B     | 605 | CLA  | C1B-C2B | 3.01  | 1.50        | 1.43     |
| 24  | B     | 612 | CLA  | C1B-NB  | -3.00 | 1.34        | 1.37     |
| 24  | c     | 512 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 24  | B     | 617 | CLA  | C4B-NB  | -3.00 | 1.34        | 1.37     |
| 24  | A     | 410 | CLA  | C1B-NB  | -3.00 | 1.34        | 1.37     |
| 24  | b     | 622 | CLA  | C1B-C2B | 2.99  | 1.50        | 1.43     |
| 24  | B     | 608 | CLA  | C1B-NB  | -2.99 | 1.34        | 1.37     |
| 27  | f     | 101 | SQD  | C6-S    | -2.98 | 1.66        | 1.77     |
| 24  | B     | 616 | CLA  | C1B-NB  | -2.98 | 1.34        | 1.37     |
| 24  | b     | 611 | CLA  | C3B-C4B | 2.98  | 1.49        | 1.42     |
| 24  | B     | 605 | CLA  | C1B-NB  | -2.97 | 1.34        | 1.37     |
| 27  | A     | 416 | SQD  | C6-S    | -2.97 | 1.66        | 1.77     |
| 35  | b     | 631 | HTG  | C1'-S1  | -2.97 | 1.77        | 1.81     |
| 24  | C     | 512 | CLA  | C1B-NB  | -2.96 | 1.34        | 1.37     |
| 24  | A     | 407 | CLA  | C1B-NB  | -2.96 | 1.34        | 1.37     |
| 24  | C     | 502 | CLA  | C1B-C2B | 2.96  | 1.50        | 1.43     |
| 24  | C     | 507 | CLA  | C3B-C4B | 2.96  | 1.49        | 1.42     |
| 24  | B     | 610 | CLA  | C1B-C2B | 2.96  | 1.50        | 1.43     |
| 24  | c     | 518 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 24  | c     | 510 | CLA  | C1B-C2B | 2.95  | 1.50        | 1.43     |
| 24  | C     | 505 | CLA  | C1B-C2B | 2.94  | 1.50        | 1.43     |
| 24  | B     | 611 | CLA  | C3B-C4B | 2.94  | 1.49        | 1.42     |
| 24  | C     | 511 | CLA  | C4C-C3C | 2.94  | 1.50        | 1.45     |
| 24  | c     | 518 | CLA  | C1B-NB  | -2.93 | 1.34        | 1.37     |
| 24  | b     | 612 | CLA  | C1B-NB  | -2.93 | 1.34        | 1.37     |
| 24  | a     | 409 | CLA  | C4C-C3C | 2.93  | 1.50        | 1.45     |
| 24  | C     | 506 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 24  | b     | 613 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 24  | C     | 501 | CLA  | C3B-C4B | 2.93  | 1.49        | 1.42     |
| 24  | c     | 515 | CLA  | C1B-C2B | 2.92  | 1.50        | 1.43     |
| 24  | B     | 602 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 24  | B     | 610 | CLA  | C3B-C4B | 2.92  | 1.49        | 1.42     |
| 24  | b     | 615 | CLA  | C1B-C2B | 2.92  | 1.50        | 1.43     |
| 24  | c     | 508 | CLA  | C1B-NB  | -2.92 | 1.34        | 1.37     |
| 24  | C     | 510 | CLA  | C1B-C2B | 2.92  | 1.50        | 1.43     |
| 24  | c     | 512 | CLA  | C1B-C2B | 2.91  | 1.50        | 1.43     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | C     | 504    | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 24  | C     | 509    | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 24  | d     | 401    | CLA  | C1B-NB  | -2.91 | 1.34        | 1.37     |
| 24  | B     | 612    | CLA  | C1B-C2B | 2.90  | 1.50        | 1.43     |
| 24  | b     | 617    | CLA  | C3B-C4B | 2.90  | 1.49        | 1.42     |
| 35  | B     | 624    | HTG  | C1'-S1  | -2.90 | 1.77        | 1.81     |
| 24  | b     | 612    | CLA  | C3B-C4B | 2.89  | 1.49        | 1.42     |
| 24  | b     | 610    | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 24  | b     | 622    | CLA  | C1B-NB  | -2.89 | 1.34        | 1.37     |
| 24  | B     | 616    | CLA  | C1B-C2B | 2.89  | 1.50        | 1.43     |
| 24  | a     | 412    | CLA  | C3B-C4B | 2.89  | 1.49        | 1.42     |
| 24  | B     | 604    | CLA  | C1C-C2C | 2.89  | 1.50        | 1.44     |
| 24  | C     | 507    | CLA  | C1C-C2C | 2.87  | 1.50        | 1.44     |
| 24  | C     | 509    | CLA  | C1B-C2B | 2.87  | 1.50        | 1.43     |
| 24  | b     | 615    | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 24  | c     | 513    | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 24  | b     | 624    | CLA  | C3B-C4B | 2.85  | 1.49        | 1.42     |
| 24  | b     | 613    | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 24  | C     | 512    | CLA  | C1B-C2B | 2.85  | 1.50        | 1.43     |
| 24  | b     | 614    | CLA  | C1B-NB  | -2.85 | 1.34        | 1.37     |
| 24  | b     | 612    | CLA  | C1B-C2B | 2.85  | 1.50        | 1.43     |
| 24  | B     | 609    | CLA  | C1B-NB  | -2.84 | 1.34        | 1.37     |
| 24  | b     | 612    | CLA  | C1C-C2C | 2.84  | 1.50        | 1.44     |
| 24  | b     | 621    | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 24  | B     | 606    | CLA  | C3B-C4B | 2.84  | 1.49        | 1.42     |
| 24  | c     | 506    | CLA  | C1B-C2B | 2.84  | 1.49        | 1.43     |
| 40  | v     | 205    | HEC  | C4B-NB  | -2.84 | 1.35        | 1.40     |
| 24  | B     | 616    | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 24  | B     | 608    | CLA  | C1B-C2B | 2.83  | 1.49        | 1.43     |
| 24  | C     | 503    | CLA  | C1B-NB  | -2.83 | 1.34        | 1.37     |
| 24  | B     | 617    | CLA  | C1B-NB  | -2.83 | 1.34        | 1.37     |
| 24  | C     | 505    | CLA  | C3B-C4B | 2.83  | 1.49        | 1.42     |
| 24  | c     | 513    | CLA  | C1B-C2B | 2.83  | 1.49        | 1.43     |
| 24  | B     | 614    | CLA  | C1C-C2C | 2.83  | 1.50        | 1.44     |
| 24  | c     | 507    | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 24  | c     | 518    | CLA  | C1C-C2C | 2.82  | 1.50        | 1.44     |
| 24  | c     | 511    | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 24  | C     | 509    | CLA  | C3B-C4B | 2.82  | 1.49        | 1.42     |
| 24  | b     | 619    | CLA  | C3B-C4B | 2.82  | 1.49        | 1.42     |
| 24  | c     | 512    | CLA  | C1B-NB  | -2.82 | 1.34        | 1.37     |
| 25  | A     | 409[A] | PHO  | CHA-CBD | -2.81 | 1.48        | 1.51     |
| 24  | C     | 502    | CLA  | C3B-C4B | 2.81  | 1.49        | 1.42     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | B     | 604    | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 24  | C     | 512    | CLA  | C3B-C4B | 2.81  | 1.49        | 1.42     |
| 24  | B     | 607    | CLA  | C1C-C2C | 2.80  | 1.50        | 1.44     |
| 24  | B     | 609    | CLA  | C3B-C4B | 2.80  | 1.49        | 1.42     |
| 24  | b     | 622    | CLA  | C4C-C3C | 2.80  | 1.49        | 1.45     |
| 24  | b     | 624    | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 24  | c     | 507    | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 24  | b     | 617    | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 24  | A     | 405    | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 24  | c     | 507    | CLA  | C3B-C4B | 2.80  | 1.49        | 1.42     |
| 27  | a     | 405    | SQD  | C6-S    | -2.79 | 1.67        | 1.77     |
| 24  | B     | 608    | CLA  | OBD-CAD | 2.79  | 1.27        | 1.22     |
| 24  | c     | 514    | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 24  | B     | 609    | CLA  | C1B-C2B | 2.79  | 1.49        | 1.43     |
| 24  | D     | 402    | CLA  | OBD-CAD | 2.79  | 1.27        | 1.22     |
| 24  | B     | 614    | CLA  | C4C-C3C | 2.79  | 1.49        | 1.45     |
| 24  | A     | 406    | CLA  | C1B-C2B | 2.79  | 1.49        | 1.43     |
| 24  | D     | 402    | CLA  | C1C-C2C | 2.78  | 1.50        | 1.44     |
| 24  | b     | 625    | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 24  | b     | 621    | CLA  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 24  | B     | 614    | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 24  | C     | 510    | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 24  | C     | 503    | CLA  | C1C-C2C | 2.78  | 1.49        | 1.44     |
| 24  | C     | 510    | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 24  | B     | 605    | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 24  | B     | 616    | CLA  | C3B-C4B | 2.77  | 1.49        | 1.42     |
| 24  | C     | 511    | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 24  | A     | 406    | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 24  | D     | 403    | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 24  | D     | 402    | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 24  | C     | 504    | CLA  | C1C-C2C | 2.76  | 1.49        | 1.44     |
| 24  | C     | 502    | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 27  | F     | 103    | SQD  | C6-S    | -2.75 | 1.67        | 1.77     |
| 24  | c     | 516    | CLA  | C3B-C4B | 2.75  | 1.49        | 1.42     |
| 25  | a     | 418[A] | PHO  | C3A-C2A | -2.74 | 1.52        | 1.54     |
| 24  | c     | 506    | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 24  | c     | 509    | CLA  | C1C-C2C | 2.74  | 1.49        | 1.44     |
| 24  | C     | 507    | CLA  | C4D-CHA | 2.73  | 1.48        | 1.38     |
| 38  | F     | 102    | HEM  | C1C-C2C | -2.73 | 1.39        | 1.45     |
| 24  | B     | 613    | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 24  | b     | 620    | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 24  | B     | 604    | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | B     | 605 | CLA  | OBD-CAD | 2.72  | 1.27        | 1.22     |
| 24  | D     | 403 | CLA  | C3B-C4B | 2.72  | 1.49        | 1.42     |
| 24  | B     | 614 | CLA  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 24  | C     | 504 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 24  | d     | 403 | CLA  | C1C-C2C | 2.71  | 1.49        | 1.44     |
| 24  | A     | 410 | CLA  | C1C-C2C | 2.71  | 1.49        | 1.44     |
| 24  | B     | 612 | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 24  | B     | 617 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 24  | b     | 620 | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 24  | C     | 505 | CLA  | C1C-C2C | 2.70  | 1.49        | 1.44     |
| 24  | b     | 614 | CLA  | C1C-C2C | 2.70  | 1.49        | 1.44     |
| 24  | c     | 516 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 24  | C     | 513 | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 24  | b     | 623 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 24  | b     | 620 | CLA  | C3B-C4B | 2.69  | 1.49        | 1.42     |
| 24  | c     | 517 | CLA  | C1C-C2C | 2.68  | 1.49        | 1.44     |
| 24  | b     | 617 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 24  | A     | 410 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 24  | B     | 603 | CLA  | C3B-C4B | 2.68  | 1.49        | 1.42     |
| 24  | C     | 509 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 24  | b     | 617 | CLA  | C1C-C2C | 2.68  | 1.49        | 1.44     |
| 24  | c     | 511 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 29  | A     | 417 | LMT  | O1'-C1' | 2.68  | 1.44        | 1.40     |
| 24  | A     | 410 | CLA  | C3B-C4B | 2.67  | 1.49        | 1.42     |
| 24  | c     | 512 | CLA  | C1C-C2C | 2.67  | 1.49        | 1.44     |
| 24  | d     | 403 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 24  | a     | 410 | CLA  | C1C-C2C | 2.67  | 1.49        | 1.44     |
| 24  | b     | 621 | CLA  | C3B-C4B | 2.67  | 1.49        | 1.42     |
| 24  | B     | 607 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 24  | D     | 402 | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 24  | d     | 403 | CLA  | C3B-C4B | 2.66  | 1.49        | 1.42     |
| 24  | B     | 615 | CLA  | C1C-C2C | 2.66  | 1.49        | 1.44     |
| 24  | C     | 511 | CLA  | C1B-NB  | -2.66 | 1.34        | 1.37     |
| 24  | C     | 509 | CLA  | C1C-C2C | 2.66  | 1.49        | 1.44     |
| 24  | d     | 401 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 27  | B     | 621 | SQD  | C6-S    | -2.66 | 1.67        | 1.77     |
| 24  | B     | 607 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 24  | a     | 412 | CLA  | C1B-NB  | -2.65 | 1.34        | 1.37     |
| 24  | C     | 502 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 24  | b     | 624 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 24  | c     | 506 | CLA  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 24  | b     | 615 | CLA  | C1C-C2C | 2.65  | 1.49        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | C     | 504 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 24  | a     | 412 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 24  | C     | 506 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 24  | C     | 501 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 24  | b     | 620 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 24  | D     | 403 | CLA  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 24  | b     | 615 | CLA  | C3B-C4B | 2.64  | 1.48        | 1.42     |
| 24  | B     | 611 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 24  | c     | 513 | CLA  | C3B-C4B | 2.63  | 1.48        | 1.42     |
| 24  | c     | 508 | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 24  | b     | 617 | CLA  | C1B-NB  | -2.62 | 1.34        | 1.37     |
| 27  | A     | 412 | SQD  | C6-S    | -2.62 | 1.67        | 1.77     |
| 24  | B     | 612 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 24  | B     | 614 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 24  | C     | 504 | CLA  | C3B-C4B | 2.62  | 1.48        | 1.42     |
| 24  | C     | 502 | CLA  | C1C-C2C | 2.61  | 1.49        | 1.44     |
| 24  | B     | 606 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 24  | B     | 617 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 24  | C     | 513 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 24  | b     | 622 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 24  | b     | 620 | CLA  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 24  | C     | 508 | CLA  | C1C-C2C | 2.61  | 1.49        | 1.44     |
| 24  | a     | 412 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 27  | a     | 414 | SQD  | C6-S    | -2.60 | 1.67        | 1.77     |
| 24  | c     | 507 | CLA  | C1B-NB  | -2.60 | 1.34        | 1.37     |
| 24  | C     | 508 | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 27  | L     | 102 | SQD  | C6-S    | -2.60 | 1.67        | 1.77     |
| 24  | c     | 518 | CLA  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 24  | C     | 501 | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 24  | b     | 619 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 24  | B     | 610 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 33  | Z     | 101 | LMG  | O8-C28  | 2.60  | 1.46        | 1.33     |
| 24  | C     | 509 | CLA  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 24  | C     | 513 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 24  | B     | 611 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 24  | A     | 410 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 24  | C     | 512 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 24  | B     | 603 | CLA  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 24  | A     | 407 | CLA  | C1C-C2C | 2.59  | 1.49        | 1.44     |
| 24  | B     | 616 | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 40  | V     | 205 | HEC  | C4B-C3B | 2.58  | 1.49        | 1.45     |
| 24  | C     | 510 | CLA  | C3B-C4B | 2.58  | 1.48        | 1.42     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | b     | 610    | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 31  | a     | 415[B] | PL9  | C6-C5   | 2.58  | 1.48        | 1.35     |
| 24  | A     | 405    | CLA  | C3B-C4B | 2.58  | 1.48        | 1.42     |
| 24  | b     | 617    | CLA  | C4B-NB  | -2.58 | 1.34        | 1.37     |
| 24  | c     | 510    | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 25  | A     | 409[B] | PHO  | CHA-CBD | -2.58 | 1.48        | 1.51     |
| 31  | a     | 415[A] | PL9  | C6-C5   | 2.58  | 1.48        | 1.35     |
| 24  | c     | 515    | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 24  | B     | 615    | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 24  | b     | 615    | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 24  | b     | 622    | CLA  | C1C-C2C | 2.57  | 1.49        | 1.44     |
| 24  | b     | 613    | CLA  | C3B-C4B | 2.57  | 1.48        | 1.42     |
| 24  | b     | 616    | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 24  | C     | 512    | CLA  | C1C-C2C | 2.57  | 1.49        | 1.44     |
| 24  | B     | 608    | CLA  | C3B-C4B | 2.57  | 1.48        | 1.42     |
| 24  | c     | 510    | CLA  | C1C-C2C | 2.57  | 1.49        | 1.44     |
| 24  | B     | 607    | CLA  | C3B-C4B | 2.56  | 1.48        | 1.42     |
| 24  | B     | 608    | CLA  | C4D-CHA | 2.56  | 1.47        | 1.38     |
| 31  | D     | 405[B] | PL9  | C6-C5   | 2.56  | 1.48        | 1.35     |
| 24  | d     | 402    | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 24  | C     | 508    | CLA  | C4D-CHA | 2.56  | 1.47        | 1.38     |
| 24  | a     | 410    | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 25  | a     | 418[A] | PHO  | C4B-NB  | -2.55 | 1.33        | 1.38     |
| 31  | A     | 419[B] | PL9  | C6-C5   | 2.55  | 1.48        | 1.35     |
| 24  | c     | 513    | CLA  | C4D-CHA | 2.55  | 1.47        | 1.38     |
| 24  | c     | 509    | CLA  | C4D-CHA | 2.55  | 1.47        | 1.38     |
| 24  | B     | 612    | CLA  | C1C-C2C | 2.55  | 1.49        | 1.44     |
| 24  | B     | 603    | CLA  | C4D-CHA | 2.55  | 1.47        | 1.38     |
| 24  | D     | 403    | CLA  | C1B-NB  | -2.55 | 1.34        | 1.37     |
| 24  | b     | 611    | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 24  | B     | 609    | CLA  | C4C-C3C | 2.54  | 1.49        | 1.45     |
| 24  | A     | 405    | CLA  | C4D-CHA | 2.54  | 1.47        | 1.38     |
| 31  | A     | 419[A] | PL9  | C6-C5   | 2.54  | 1.48        | 1.35     |
| 24  | B     | 602    | CLA  | C4D-CHA | 2.54  | 1.47        | 1.38     |
| 24  | B     | 617    | CLA  | C4C-C3C | 2.54  | 1.49        | 1.45     |
| 24  | d     | 403    | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 24  | C     | 507    | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 31  | d     | 405[A] | PL9  | C6-C5   | 2.53  | 1.48        | 1.35     |
| 31  | d     | 405[B] | PL9  | C6-C5   | 2.53  | 1.48        | 1.35     |
| 24  | C     | 505    | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 24  | c     | 508    | CLA  | C3D-C4D | -2.53 | 1.38        | 1.44     |
| 24  | b     | 618    | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | B     | 602 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 24  | c     | 510 | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 24  | B     | 605 | CLA  | C3B-C4B | 2.53  | 1.48        | 1.42     |
| 24  | B     | 609 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 24  | B     | 615 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 25  | a     | 411 | PHO  | CHA-CBD | -2.52 | 1.48        | 1.51     |
| 24  | b     | 614 | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 24  | a     | 409 | CLA  | C1C-C2C | 2.51  | 1.49        | 1.44     |
| 24  | C     | 506 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 24  | A     | 405 | CLA  | C1C-C2C | 2.51  | 1.49        | 1.44     |
| 24  | B     | 604 | CLA  | C4D-CHA | 2.51  | 1.47        | 1.38     |
| 24  | C     | 510 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 24  | B     | 606 | CLA  | C1B-NB  | -2.50 | 1.34        | 1.37     |
| 24  | B     | 615 | CLA  | C3B-C4B | 2.50  | 1.48        | 1.42     |
| 24  | a     | 409 | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 24  | c     | 509 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 24  | d     | 402 | CLA  | C4B-NB  | -2.50 | 1.34        | 1.37     |
| 24  | B     | 613 | CLA  | C4D-CHA | 2.49  | 1.47        | 1.38     |
| 24  | B     | 608 | CLA  | C4B-NB  | -2.49 | 1.34        | 1.37     |
| 24  | b     | 611 | CLA  | C4D-CHA | 2.49  | 1.47        | 1.38     |
| 24  | b     | 621 | CLA  | C3B-C2B | 2.49  | 1.49        | 1.41     |
| 24  | B     | 605 | CLA  | C3B-C2B | 2.49  | 1.49        | 1.41     |
| 24  | B     | 603 | CLA  | C4B-NB  | -2.49 | 1.34        | 1.37     |
| 24  | D     | 402 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 24  | c     | 518 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 24  | C     | 510 | CLA  | C1C-C2C | 2.48  | 1.49        | 1.44     |
| 24  | B     | 614 | CLA  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 24  | c     | 516 | CLA  | C4D-CHA | 2.48  | 1.47        | 1.38     |
| 24  | c     | 517 | CLA  | C4D-CHA | 2.48  | 1.47        | 1.38     |
| 24  | b     | 622 | CLA  | C3B-C4B | 2.48  | 1.48        | 1.42     |
| 24  | c     | 511 | CLA  | C3B-C4B | 2.48  | 1.48        | 1.42     |
| 24  | a     | 410 | CLA  | C4B-NB  | -2.48 | 1.34        | 1.37     |
| 24  | C     | 501 | CLA  | C1C-C2C | 2.48  | 1.49        | 1.44     |
| 24  | C     | 512 | CLA  | C4B-NB  | -2.47 | 1.34        | 1.37     |
| 24  | B     | 617 | CLA  | C3B-C4B | 2.47  | 1.48        | 1.42     |
| 24  | C     | 511 | CLA  | C3B-C4B | 2.47  | 1.48        | 1.42     |
| 24  | B     | 603 | CLA  | C1C-C2C | 2.46  | 1.49        | 1.44     |
| 24  | B     | 604 | CLA  | C3B-C4B | 2.46  | 1.48        | 1.42     |
| 24  | B     | 616 | CLA  | C4D-CHA | 2.46  | 1.47        | 1.38     |
| 24  | b     | 621 | CLA  | C1C-C2C | 2.46  | 1.49        | 1.44     |
| 24  | c     | 515 | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 24  | b     | 612 | CLA  | C4D-CHA | 2.46  | 1.47        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | A     | 410    | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 24  | b     | 618    | CLA  | C4B-NB  | -2.46 | 1.34        | 1.37     |
| 24  | C     | 505    | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 24  | d     | 403    | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 24  | c     | 511    | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 24  | C     | 507    | CLA  | C4B-NB  | -2.45 | 1.34        | 1.37     |
| 24  | b     | 614    | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 24  | d     | 402    | CLA  | C3B-C4B | 2.45  | 1.48        | 1.42     |
| 24  | d     | 403    | CLA  | C4D-CHA | 2.44  | 1.47        | 1.38     |
| 24  | c     | 507    | CLA  | C1C-C2C | 2.44  | 1.49        | 1.44     |
| 24  | c     | 518    | CLA  | C4D-CHA | 2.44  | 1.47        | 1.38     |
| 24  | b     | 625    | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 24  | a     | 409    | CLA  | C3B-C4B | 2.44  | 1.48        | 1.42     |
| 24  | B     | 603    | CLA  | C1B-C2B | 2.44  | 1.49        | 1.43     |
| 24  | D     | 403    | CLA  | C4D-CHA | 2.44  | 1.47        | 1.38     |
| 24  | b     | 623    | CLA  | C3B-C4B | 2.44  | 1.48        | 1.42     |
| 24  | C     | 508    | CLA  | C1B-C2B | 2.44  | 1.49        | 1.43     |
| 24  | d     | 401    | CLA  | C4D-CHA | 2.43  | 1.47        | 1.38     |
| 24  | C     | 501    | CLA  | C4D-CHA | 2.43  | 1.47        | 1.38     |
| 38  | e     | 103    | HEM  | C3C-C4C | -2.43 | 1.41        | 1.46     |
| 35  | b     | 607    | HTG  | C1-S1   | -2.43 | 1.77        | 1.80     |
| 24  | B     | 609    | CLA  | C1C-C2C | 2.43  | 1.49        | 1.44     |
| 24  | B     | 617    | CLA  | C3D-C4D | -2.43 | 1.38        | 1.44     |
| 31  | D     | 405[A] | PL9  | C6-C5   | 2.42  | 1.47        | 1.35     |
| 24  | c     | 511    | CLA  | C4D-CHA | 2.42  | 1.47        | 1.38     |
| 24  | D     | 403    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 24  | c     | 515    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 24  | B     | 603    | CLA  | C3D-C4D | -2.42 | 1.38        | 1.44     |
| 25  | a     | 418[B] | PHO  | C4B-NB  | -2.42 | 1.34        | 1.38     |
| 24  | b     | 618    | CLA  | C3B-C4B | 2.42  | 1.48        | 1.42     |
| 24  | C     | 513    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 24  | b     | 622    | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 24  | b     | 611    | CLA  | C1C-C2C | 2.41  | 1.49        | 1.44     |
| 24  | d     | 402    | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 24  | A     | 407    | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 24  | C     | 511    | CLA  | C1C-C2C | 2.41  | 1.49        | 1.44     |
| 24  | c     | 508    | CLA  | C4D-CHA | 2.41  | 1.47        | 1.38     |
| 24  | c     | 515    | CLA  | C3B-C4B | 2.41  | 1.48        | 1.42     |
| 24  | b     | 616    | CLA  | C1C-C2C | 2.41  | 1.49        | 1.44     |
| 24  | b     | 618    | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 24  | D     | 402    | CLA  | C4D-CHA | 2.41  | 1.47        | 1.38     |
| 24  | d     | 402    | CLA  | C4D-CHA | 2.41  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | B     | 611 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 35  | c     | 525 | HTG  | C1-S1   | -2.40 | 1.77        | 1.80     |
| 24  | b     | 625 | CLA  | C3B-C4B | 2.40  | 1.48        | 1.42     |
| 24  | b     | 621 | CLA  | C1C-NC  | -2.40 | 1.34        | 1.37     |
| 24  | B     | 605 | CLA  | C1C-C2C | 2.40  | 1.49        | 1.44     |
| 24  | A     | 407 | CLA  | C4D-CHA | 2.40  | 1.46        | 1.38     |
| 24  | C     | 503 | CLA  | C4D-CHA | 2.40  | 1.46        | 1.38     |
| 24  | b     | 619 | CLA  | C4D-CHA | 2.40  | 1.46        | 1.38     |
| 40  | V     | 205 | HEC  | C1B-NB  | -2.40 | 1.33        | 1.38     |
| 24  | B     | 608 | CLA  | C1C-C2C | 2.39  | 1.49        | 1.44     |
| 24  | C     | 504 | CLA  | C3B-C2B | 2.39  | 1.49        | 1.41     |
| 24  | C     | 506 | CLA  | C3B-C4B | 2.39  | 1.48        | 1.42     |
| 24  | C     | 506 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 24  | A     | 406 | CLA  | C3B-C4B | 2.39  | 1.48        | 1.42     |
| 24  | b     | 613 | CLA  | C1C-C2C | 2.39  | 1.49        | 1.44     |
| 24  | B     | 606 | CLA  | C4D-CHA | 2.39  | 1.46        | 1.38     |
| 24  | c     | 514 | CLA  | C1C-C2C | 2.38  | 1.49        | 1.44     |
| 24  | b     | 614 | CLA  | C4D-CHA | 2.38  | 1.46        | 1.38     |
| 24  | D     | 402 | CLA  | C3B-C4B | 2.38  | 1.48        | 1.42     |
| 24  | a     | 409 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 24  | B     | 602 | CLA  | C1B-NB  | -2.38 | 1.34        | 1.37     |
| 24  | C     | 509 | CLA  | C3B-C2B | 2.38  | 1.49        | 1.41     |
| 24  | C     | 504 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 24  | C     | 506 | CLA  | C3D-C4D | -2.38 | 1.38        | 1.44     |
| 35  | D     | 412 | HTG  | C1-S1   | -2.38 | 1.77        | 1.80     |
| 24  | c     | 513 | CLA  | C3B-C2B | 2.38  | 1.49        | 1.41     |
| 35  | b     | 632 | HTG  | C1-S1   | -2.37 | 1.77        | 1.80     |
| 24  | B     | 607 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 24  | b     | 616 | CLA  | C4B-NB  | -2.37 | 1.34        | 1.37     |
| 24  | A     | 406 | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 24  | B     | 615 | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 24  | c     | 507 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 35  | d     | 411 | HTG  | C1-S1   | -2.36 | 1.77        | 1.80     |
| 40  | V     | 205 | HEC  | C4D-ND  | -2.36 | 1.33        | 1.38     |
| 24  | B     | 602 | CLA  | C1C-C2C | 2.36  | 1.49        | 1.44     |
| 24  | B     | 617 | CLA  | C3B-C2B | 2.36  | 1.49        | 1.41     |
| 24  | B     | 608 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 24  | B     | 611 | CLA  | C1C-NC  | -2.35 | 1.34        | 1.37     |
| 24  | C     | 503 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 24  | b     | 610 | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 24  | B     | 606 | CLA  | C4B-NB  | -2.35 | 1.34        | 1.37     |
| 24  | C     | 513 | CLA  | C3D-C4D | -2.35 | 1.38        | 1.44     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | c     | 510    | CLA  | C3D-C4D | -2.35 | 1.38        | 1.44     |
| 25  | A     | 409[B] | PHO  | C3A-C2A | -2.35 | 1.52        | 1.54     |
| 24  | c     | 508    | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 24  | b     | 618    | CLA  | C1C-C2C | 2.34  | 1.49        | 1.44     |
| 24  | B     | 613    | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 35  | b     | 608    | HTG  | C1-S1   | -2.34 | 1.77        | 1.80     |
| 35  | C     | 522    | HTG  | C1-S1   | -2.34 | 1.77        | 1.80     |
| 36  | D     | 406    | DGD  | O3G-C1D | 2.34  | 1.44        | 1.40     |
| 24  | D     | 403    | CLA  | C3D-C4D | -2.34 | 1.38        | 1.44     |
| 25  | a     | 418[B] | PHO  | C3A-C2A | -2.34 | 1.52        | 1.54     |
| 24  | B     | 614    | CLA  | C3B-C4B | 2.33  | 1.48        | 1.42     |
| 24  | c     | 511    | CLA  | C3B-C2B | 2.33  | 1.49        | 1.41     |
| 24  | c     | 514    | CLA  | C3B-C4B | 2.33  | 1.48        | 1.42     |
| 24  | B     | 614    | CLA  | C3B-C2B | 2.33  | 1.49        | 1.41     |
| 24  | a     | 410    | CLA  | C4D-CHA | 2.33  | 1.46        | 1.38     |
| 24  | c     | 506    | CLA  | C3B-C4B | 2.33  | 1.48        | 1.42     |
| 24  | C     | 513    | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 24  | b     | 616    | CLA  | C3D-C4D | -2.32 | 1.38        | 1.44     |
| 24  | b     | 617    | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 24  | b     | 610    | CLA  | C1B-C2B | 2.32  | 1.48        | 1.43     |
| 24  | b     | 611    | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 25  | A     | 409[A] | PHO  | C1B-NB  | -2.31 | 1.34        | 1.38     |
| 24  | c     | 515    | CLA  | C3B-C2B | 2.31  | 1.49        | 1.41     |
| 24  | A     | 407    | CLA  | C4B-NB  | -2.31 | 1.34        | 1.37     |
| 24  | b     | 619    | CLA  | C3B-C2B | 2.31  | 1.49        | 1.41     |
| 24  | c     | 509    | CLA  | C3B-C4B | 2.31  | 1.48        | 1.42     |
| 24  | C     | 502    | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 24  | B     | 615    | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 24  | c     | 510    | CLA  | C4B-NB  | -2.31 | 1.34        | 1.37     |
| 24  | c     | 509    | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 24  | B     | 610    | CLA  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 24  | d     | 402    | CLA  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 25  | a     | 411    | PHO  | C4B-NB  | -2.30 | 1.34        | 1.38     |
| 24  | c     | 512    | CLA  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 24  | a     | 412    | CLA  | C1C-C2C | 2.30  | 1.49        | 1.44     |
| 24  | A     | 405    | CLA  | C3B-C2B | 2.30  | 1.49        | 1.41     |
| 38  | F     | 102    | HEM  | C1D-ND  | -2.30 | 1.34        | 1.38     |
| 24  | C     | 508    | CLA  | C3B-C2B | 2.30  | 1.49        | 1.41     |
| 40  | v     | 205    | HEC  | C4B-C3B | 2.29  | 1.49        | 1.45     |
| 24  | c     | 508    | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 24  | c     | 515    | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 24  | b     | 623    | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | B     | 604    | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |
| 24  | b     | 614    | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 24  | B     | 609    | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 24  | C     | 504    | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 24  | b     | 624    | CLA  | C1C-C2C | 2.28  | 1.49        | 1.44     |
| 24  | C     | 505    | CLA  | C4C-C3C | 2.27  | 1.49        | 1.45     |
| 24  | C     | 510    | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 24  | a     | 409    | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 24  | D     | 402    | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 24  | b     | 617    | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 24  | b     | 622    | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 24  | c     | 513    | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 35  | c     | 526    | HTG  | C1-S1   | -2.27 | 1.77        | 1.80     |
| 24  | c     | 514    | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 36  | h     | 102    | DGD  | O5D-C1E | 2.27  | 1.44        | 1.40     |
| 24  | b     | 613    | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 24  | b     | 617    | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 24  | C     | 501    | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 24  | C     | 503    | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 24  | c     | 518    | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 24  | b     | 624    | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 24  | b     | 618    | CLA  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 24  | D     | 402    | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 25  | A     | 409[B] | PHO  | C1B-NB  | -2.25 | 1.34        | 1.38     |
| 24  | C     | 507    | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 24  | B     | 606    | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 24  | b     | 619    | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 24  | c     | 517    | CLA  | C1B-C2B | 2.25  | 1.48        | 1.43     |
| 24  | b     | 615    | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 25  | A     | 409[A] | PHO  | C3A-C2A | -2.25 | 1.52        | 1.54     |
| 24  | b     | 620    | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 24  | b     | 624    | CLA  | C4B-NB  | -2.24 | 1.35        | 1.37     |
| 24  | B     | 607    | CLA  | C3D-C4D | -2.24 | 1.39        | 1.44     |
| 24  | d     | 401    | CLA  | C1C-NC  | -2.24 | 1.34        | 1.37     |
| 24  | B     | 612    | CLA  | C3B-C4B | 2.24  | 1.48        | 1.42     |
| 24  | b     | 619    | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 24  | c     | 512    | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 24  | A     | 410    | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 24  | c     | 517    | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 24  | b     | 623    | CLA  | C1C-C2C | 2.23  | 1.48        | 1.44     |
| 35  | B     | 632    | HTG  | C1-S1   | -2.23 | 1.77        | 1.80     |
| 24  | B     | 611    | CLA  | C1C-C2C | 2.23  | 1.48        | 1.44     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | c     | 514    | CLA  | C3B-C2B | 2.23  | 1.48        | 1.41     |
| 25  | A     | 409[B] | PHO  | C4B-NB  | -2.23 | 1.34        | 1.38     |
| 24  | b     | 625    | CLA  | C3B-C2B | 2.23  | 1.48        | 1.41     |
| 24  | b     | 612    | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 35  | V     | 206    | HTG  | C1-S1   | -2.23 | 1.77        | 1.80     |
| 24  | a     | 410    | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 24  | c     | 516    | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 24  | A     | 406    | CLA  | C1C-C2C | 2.22  | 1.48        | 1.44     |
| 24  | d     | 403    | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 24  | c     | 509    | CLA  | C3B-C2B | 2.22  | 1.48        | 1.41     |
| 24  | C     | 509    | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 24  | A     | 406    | CLA  | C3B-C2B | 2.22  | 1.48        | 1.41     |
| 24  | d     | 401    | CLA  | C3B-C2B | 2.22  | 1.48        | 1.41     |
| 24  | B     | 611    | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 24  | d     | 401    | CLA  | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 24  | c     | 506    | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 24  | B     | 613    | CLA  | C3B-C4B | 2.21  | 1.48        | 1.42     |
| 24  | C     | 508    | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 24  | a     | 412    | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 24  | C     | 510    | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 24  | B     | 610    | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 38  | e     | 103    | HEM  | C1C-C2C | -2.21 | 1.41        | 1.45     |
| 24  | b     | 612    | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 24  | C     | 507    | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 24  | B     | 604    | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 24  | B     | 605    | CLA  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 24  | b     | 620    | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 24  | b     | 619    | CLA  | C1C-C2C | 2.20  | 1.48        | 1.44     |
| 24  | c     | 513    | CLA  | C1C-C2C | 2.20  | 1.48        | 1.44     |
| 24  | C     | 506    | CLA  | C1C-C2C | 2.20  | 1.48        | 1.44     |
| 25  | A     | 409[A] | PHO  | C4B-NB  | -2.20 | 1.34        | 1.38     |
| 24  | a     | 409    | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 24  | b     | 610    | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 24  | C     | 503    | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 24  | c     | 506    | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 24  | c     | 516    | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 24  | c     | 512    | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 24  | c     | 517    | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 24  | a     | 410    | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 24  | A     | 407    | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 25  | a     | 418[A] | PHO  | CHA-CBD | -2.18 | 1.49        | 1.51     |
| 24  | B     | 607    | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | c     | 514    | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 24  | B     | 603    | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 24  | b     | 624    | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 24  | A     | 407    | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 24  | c     | 506    | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 24  | b     | 610    | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 24  | b     | 613    | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 24  | B     | 616    | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 24  | b     | 623    | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 24  | c     | 516    | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 24  | B     | 608    | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 24  | c     | 511    | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 24  | D     | 403    | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 24  | B     | 617    | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 24  | c     | 511    | CLA  | C4C-C3C | 2.16  | 1.48        | 1.45     |
| 24  | b     | 619    | CLA  | C1C-NC  | -2.16 | 1.34        | 1.37     |
| 24  | b     | 612    | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 24  | B     | 602    | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 24  | A     | 410    | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 24  | b     | 625    | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 24  | C     | 502    | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 24  | C     | 507    | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 24  | b     | 621    | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 24  | c     | 517    | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 25  | A     | 408    | PHO  | C4B-NB  | -2.14 | 1.34        | 1.38     |
| 24  | B     | 604    | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 37  | d     | 406    | LHG  | O7-C5   | -2.14 | 1.41        | 1.46     |
| 35  | B     | 633    | HTG  | C1-S1   | -2.14 | 1.77        | 1.80     |
| 35  | B     | 625    | HTG  | C1-S1   | -2.14 | 1.77        | 1.80     |
| 24  | C     | 501    | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 24  | c     | 507    | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 24  | b     | 623    | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 25  | a     | 418[B] | PHO  | CHA-CBD | -2.13 | 1.49        | 1.51     |
| 24  | B     | 612    | CLA  | C4C-C3C | 2.13  | 1.48        | 1.45     |
| 40  | v     | 205    | HEC  | C4A-C3A | -2.12 | 1.41        | 1.45     |
| 25  | a     | 418[B] | PHO  | C1B-NB  | -2.12 | 1.34        | 1.38     |
| 24  | c     | 513    | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 24  | C     | 511    | CLA  | C3B-C2B | 2.12  | 1.48        | 1.41     |
| 24  | A     | 407    | CLA  | C3B-C2B | 2.12  | 1.48        | 1.41     |
| 24  | b     | 623    | CLA  | C4D-CHA | 2.12  | 1.45        | 1.38     |
| 24  | b     | 611    | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 25  | A     | 408    | PHO  | C1B-NB  | -2.11 | 1.34        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | b     | 615    | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 25  | A     | 409[A] | PHO  | C1D-ND  | -2.11 | 1.34        | 1.38     |
| 24  | B     | 610    | CLA  | C4B-NB  | -2.11 | 1.35        | 1.37     |
| 24  | B     | 605    | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 24  | B     | 602    | CLA  | C1D-C2D | 2.11  | 1.49        | 1.45     |
| 24  | a     | 412    | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 24  | b     | 623    | CLA  | C4B-NB  | -2.11 | 1.35        | 1.37     |
| 24  | B     | 610    | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 24  | c     | 507    | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 24  | b     | 614    | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 25  | a     | 411    | PHO  | C3A-C2A | -2.10 | 1.52        | 1.54     |
| 24  | B     | 605    | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 31  | d     | 405[A] | PL9  | C2-C3   | 2.10  | 1.40        | 1.34     |
| 24  | c     | 507    | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 24  | c     | 510    | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 31  | a     | 415[A] | PL9  | C2-C3   | 2.09  | 1.40        | 1.34     |
| 24  | d     | 403    | CLA  | C3B-C2B | 2.09  | 1.48        | 1.41     |
| 24  | B     | 613    | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 24  | C     | 512    | CLA  | C3B-C2B | 2.08  | 1.48        | 1.41     |
| 24  | C     | 513    | CLA  | C3B-C2B | 2.08  | 1.48        | 1.41     |
| 24  | b     | 618    | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 24  | b     | 610    | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 24  | B     | 612    | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 25  | A     | 409[B] | PHO  | C3D-C4D | -2.07 | 1.38        | 1.41     |
| 29  | M     | 103    | LMT  | O1'-C1' | 2.07  | 1.43        | 1.40     |
| 24  | b     | 611    | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 40  | v     | 205    | HEC  | C1D-C2D | 2.06  | 1.48        | 1.44     |
| 31  | D     | 405[B] | PL9  | C2-C3   | 2.06  | 1.40        | 1.34     |
| 24  | C     | 505    | CLA  | C3B-C2B | 2.06  | 1.48        | 1.41     |
| 24  | C     | 512    | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 31  | A     | 419[A] | PL9  | C2-C3   | 2.05  | 1.40        | 1.34     |
| 24  | d     | 401    | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 25  | A     | 408    | PHO  | C3A-C2A | -2.05 | 1.52        | 1.54     |
| 24  | c     | 509    | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 38  | e     | 103    | HEM  | C3B-C4B | 2.05  | 1.49        | 1.44     |
| 24  | C     | 511    | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 31  | d     | 405[B] | PL9  | C2-C3   | 2.05  | 1.40        | 1.34     |
| 24  | d     | 402    | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 25  | a     | 411    | PHO  | CBD-CGD | -2.04 | 1.49        | 1.52     |
| 24  | B     | 602    | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 36  | H     | 102    | DGD  | O5D-C1E | 2.04  | 1.43        | 1.40     |
| 25  | a     | 418[A] | PHO  | C1B-NB  | -2.04 | 1.34        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 38  | e     | 103    | HEM  | C1D-ND  | -2.03 | 1.34        | 1.38     |
| 24  | B     | 608    | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 31  | a     | 415[B] | PL9  | C2-C3   | 2.03  | 1.40        | 1.34     |
| 24  | c     | 512    | CLA  | C3B-C4B | 2.03  | 1.47        | 1.42     |
| 24  | a     | 410    | CLA  | C3B-C2B | 2.02  | 1.48        | 1.41     |
| 24  | b     | 619    | CLA  | C1D-C2D | 2.02  | 1.49        | 1.45     |
| 24  | A     | 405    | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 24  | d     | 403    | CLA  | C1D-C2D | 2.01  | 1.49        | 1.45     |
| 24  | A     | 406    | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 24  | C     | 506    | CLA  | C3B-C2B | 2.01  | 1.48        | 1.41     |
| 24  | B     | 606    | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 24  | C     | 502    | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 24  | b     | 624    | CLA  | C3B-C2B | 2.01  | 1.48        | 1.41     |
| 24  | B     | 611    | CLA  | C1D-C2D | 2.00  | 1.49        | 1.45     |
| 24  | A     | 406    | CLA  | C1C-NC  | -2.00 | 1.34        | 1.37     |

All (2859) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|--------|-------------|----------|
| 25  | A     | 409[B] | PHO  | C2D-C1D-ND | 11.62  | 117.55      | 109.53   |
| 25  | A     | 409[A] | PHO  | C2D-C1D-ND | 11.51  | 117.47      | 109.53   |
| 25  | A     | 408    | PHO  | C2D-C1D-ND | 11.39  | 117.39      | 109.53   |
| 25  | a     | 418[A] | PHO  | C2D-C1D-ND | 11.24  | 117.29      | 109.53   |
| 25  | a     | 418[B] | PHO  | C2D-C1D-ND | 11.17  | 117.24      | 109.53   |
| 24  | B     | 613    | CLA  | C1D-ND-C4D | -10.71 | 98.72       | 106.33   |
| 25  | a     | 411    | PHO  | C2D-C1D-ND | 10.60  | 116.84      | 109.53   |
| 24  | a     | 410    | CLA  | C1D-ND-C4D | -10.56 | 98.84       | 106.33   |
| 24  | b     | 614    | CLA  | C1D-ND-C4D | -10.36 | 98.98       | 106.33   |
| 24  | A     | 407    | CLA  | C1D-ND-C4D | -10.21 | 99.08       | 106.33   |
| 24  | B     | 606    | CLA  | C1D-ND-C4D | -10.07 | 99.18       | 106.33   |
| 24  | B     | 613    | CLA  | C2D-C1D-ND | 10.00  | 117.47      | 110.10   |
| 24  | c     | 508    | CLA  | C1D-ND-C4D | -9.95  | 99.27       | 106.33   |
| 24  | B     | 616    | CLA  | C1D-ND-C4D | -9.83  | 99.35       | 106.33   |
| 24  | C     | 503    | CLA  | C1D-ND-C4D | -9.75  | 99.41       | 106.33   |
| 24  | C     | 501    | CLA  | C1D-ND-C4D | -9.73  | 99.42       | 106.33   |
| 24  | c     | 516    | CLA  | C1D-ND-C4D | -9.69  | 99.45       | 106.33   |
| 24  | b     | 618    | CLA  | C1D-ND-C4D | -9.66  | 99.47       | 106.33   |
| 24  | C     | 502    | CLA  | C1D-ND-C4D | -9.64  | 99.49       | 106.33   |
| 24  | d     | 403    | CLA  | C1D-ND-C4D | -9.61  | 99.51       | 106.33   |
| 24  | b     | 620    | CLA  | C1D-ND-C4D | -9.59  | 99.52       | 106.33   |
| 24  | B     | 602    | CLA  | C1D-ND-C4D | -9.56  | 99.55       | 106.33   |
| 24  | D     | 402    | CLA  | C1D-ND-C4D | -9.47  | 99.61       | 106.33   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 24  | c     | 518 | CLA  | C1D-ND-C4D | -9.46 | 99.61       | 106.33   |
| 24  | c     | 509 | CLA  | C1D-ND-C4D | -9.45 | 99.62       | 106.33   |
| 24  | B     | 612 | CLA  | C1D-ND-C4D | -9.41 | 99.65       | 106.33   |
| 24  | a     | 412 | CLA  | C1D-ND-C4D | -9.39 | 99.66       | 106.33   |
| 24  | b     | 619 | CLA  | C1D-ND-C4D | -9.31 | 99.72       | 106.33   |
| 24  | b     | 615 | CLA  | C1D-ND-C4D | -9.30 | 99.72       | 106.33   |
| 24  | B     | 615 | CLA  | C1D-ND-C4D | -9.29 | 99.73       | 106.33   |
| 24  | C     | 513 | CLA  | C1D-ND-C4D | -9.26 | 99.76       | 106.33   |
| 24  | d     | 402 | CLA  | C1D-ND-C4D | -9.24 | 99.77       | 106.33   |
| 24  | C     | 512 | CLA  | C1D-ND-C4D | -9.23 | 99.78       | 106.33   |
| 24  | b     | 624 | CLA  | C1D-ND-C4D | -9.19 | 99.81       | 106.33   |
| 24  | b     | 612 | CLA  | C1D-ND-C4D | -9.18 | 99.81       | 106.33   |
| 24  | c     | 517 | CLA  | C1D-ND-C4D | -9.16 | 99.83       | 106.33   |
| 24  | b     | 611 | CLA  | C1D-ND-C4D | -9.16 | 99.83       | 106.33   |
| 24  | B     | 608 | CLA  | C1D-ND-C4D | -9.14 | 99.84       | 106.33   |
| 24  | C     | 511 | CLA  | C1D-ND-C4D | -9.09 | 99.88       | 106.33   |
| 24  | b     | 621 | CLA  | C1D-ND-C4D | -9.09 | 99.88       | 106.33   |
| 24  | A     | 410 | CLA  | C1D-ND-C4D | -9.08 | 99.88       | 106.33   |
| 24  | b     | 623 | CLA  | C1D-ND-C4D | -9.07 | 99.89       | 106.33   |
| 24  | B     | 607 | CLA  | C1D-ND-C4D | -9.05 | 99.91       | 106.33   |
| 24  | B     | 603 | CLA  | C1D-ND-C4D | -9.03 | 99.92       | 106.33   |
| 24  | B     | 611 | CLA  | C1D-ND-C4D | -9.00 | 99.94       | 106.33   |
| 24  | A     | 406 | CLA  | C1D-ND-C4D | -8.95 | 99.97       | 106.33   |
| 24  | C     | 504 | CLA  | C1D-ND-C4D | -8.95 | 99.98       | 106.33   |
| 24  | C     | 510 | CLA  | C1D-ND-C4D | -8.94 | 99.98       | 106.33   |
| 24  | a     | 410 | CLA  | C2D-C1D-ND | 8.93  | 116.68      | 110.10   |
| 24  | b     | 625 | CLA  | C1D-ND-C4D | -8.92 | 100.00      | 106.33   |
| 24  | B     | 609 | CLA  | C1D-ND-C4D | -8.89 | 100.02      | 106.33   |
| 24  | B     | 617 | CLA  | C1D-ND-C4D | -8.87 | 100.03      | 106.33   |
| 24  | B     | 614 | CLA  | C1D-ND-C4D | -8.87 | 100.03      | 106.33   |
| 24  | b     | 616 | CLA  | C1D-ND-C4D | -8.84 | 100.05      | 106.33   |
| 24  | c     | 514 | CLA  | C1D-ND-C4D | -8.84 | 100.05      | 106.33   |
| 24  | c     | 512 | CLA  | C1D-ND-C4D | -8.83 | 100.06      | 106.33   |
| 24  | D     | 402 | CLA  | C2D-C1D-ND | 8.82  | 116.60      | 110.10   |
| 24  | B     | 604 | CLA  | C1D-ND-C4D | -8.81 | 100.08      | 106.33   |
| 24  | C     | 508 | CLA  | C1D-ND-C4D | -8.81 | 100.08      | 106.33   |
| 24  | c     | 517 | CLA  | C2B-C1B-NB | 8.77  | 116.11      | 110.23   |
| 24  | B     | 610 | CLA  | C1D-ND-C4D | -8.76 | 100.11      | 106.33   |
| 24  | a     | 409 | CLA  | C1D-ND-C4D | -8.74 | 100.13      | 106.33   |
| 24  | B     | 606 | CLA  | C2D-C1D-ND | 8.74  | 116.54      | 110.10   |
| 24  | B     | 612 | CLA  | C2D-C1D-ND | 8.73  | 116.54      | 110.10   |
| 24  | d     | 401 | CLA  | C1D-ND-C4D | -8.72 | 100.14      | 106.33   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 24  | C     | 507 | CLA  | C1D-ND-C4D | -8.72 | 100.14      | 106.33   |
| 24  | c     | 511 | CLA  | C1D-ND-C4D | -8.71 | 100.15      | 106.33   |
| 24  | c     | 506 | CLA  | C1D-ND-C4D | -8.70 | 100.15      | 106.33   |
| 24  | C     | 509 | CLA  | C1D-ND-C4D | -8.69 | 100.16      | 106.33   |
| 24  | C     | 512 | CLA  | C2D-C1D-ND | 8.68  | 116.50      | 110.10   |
| 24  | C     | 502 | CLA  | C2D-C1D-ND | 8.68  | 116.50      | 110.10   |
| 24  | B     | 614 | CLA  | C2D-C1D-ND | 8.68  | 116.50      | 110.10   |
| 24  | b     | 610 | CLA  | C1D-ND-C4D | -8.66 | 100.18      | 106.33   |
| 24  | b     | 614 | CLA  | C2D-C1D-ND | 8.66  | 116.48      | 110.10   |
| 24  | c     | 507 | CLA  | C1D-ND-C4D | -8.63 | 100.20      | 106.33   |
| 24  | D     | 403 | CLA  | C1D-ND-C4D | -8.62 | 100.21      | 106.33   |
| 24  | b     | 621 | CLA  | C2D-C1D-ND | 8.61  | 116.45      | 110.10   |
| 24  | c     | 512 | CLA  | C2D-C1D-ND | 8.61  | 116.45      | 110.10   |
| 24  | B     | 605 | CLA  | C1D-ND-C4D | -8.58 | 100.24      | 106.33   |
| 24  | B     | 608 | CLA  | C2D-C1D-ND | 8.56  | 116.41      | 110.10   |
| 24  | b     | 617 | CLA  | C1D-ND-C4D | -8.52 | 100.28      | 106.33   |
| 24  | c     | 515 | CLA  | C1D-ND-C4D | -8.52 | 100.28      | 106.33   |
| 24  | c     | 513 | CLA  | C1D-ND-C4D | -8.51 | 100.29      | 106.33   |
| 24  | c     | 509 | CLA  | C2D-C1D-ND | 8.49  | 116.36      | 110.10   |
| 24  | C     | 504 | CLA  | C2D-C1D-ND | 8.45  | 116.33      | 110.10   |
| 24  | c     | 508 | CLA  | C2D-C1D-ND | 8.42  | 116.31      | 110.10   |
| 24  | C     | 508 | CLA  | C2B-C1B-NB | 8.41  | 115.87      | 110.23   |
| 24  | A     | 406 | CLA  | C2D-C1D-ND | 8.39  | 116.29      | 110.10   |
| 24  | C     | 505 | CLA  | C1D-ND-C4D | -8.39 | 100.37      | 106.33   |
| 24  | B     | 607 | CLA  | C2D-C1D-ND | 8.38  | 116.28      | 110.10   |
| 24  | a     | 412 | CLA  | C2D-C1D-ND | 8.35  | 116.26      | 110.10   |
| 24  | c     | 516 | CLA  | C2D-C1D-ND | 8.35  | 116.25      | 110.10   |
| 24  | B     | 616 | CLA  | C2D-C1D-ND | 8.33  | 116.24      | 110.10   |
| 24  | d     | 403 | CLA  | C2D-C1D-ND | 8.32  | 116.24      | 110.10   |
| 24  | b     | 615 | CLA  | C2D-C1D-ND | 8.26  | 116.19      | 110.10   |
| 24  | A     | 407 | CLA  | C2D-C1D-ND | 8.25  | 116.19      | 110.10   |
| 24  | c     | 510 | CLA  | C1D-ND-C4D | -8.24 | 100.48      | 106.33   |
| 24  | b     | 616 | CLA  | C2D-C1D-ND | 8.23  | 116.17      | 110.10   |
| 24  | b     | 620 | CLA  | C2D-C1D-ND | 8.21  | 116.16      | 110.10   |
| 24  | C     | 501 | CLA  | C2D-C1D-ND | 8.21  | 116.15      | 110.10   |
| 24  | b     | 610 | CLA  | C2B-C1B-NB | 8.19  | 115.72      | 110.23   |
| 24  | b     | 625 | CLA  | C2D-C1D-ND | 8.14  | 116.11      | 110.10   |
| 24  | b     | 623 | CLA  | C2D-C1D-ND | 8.14  | 116.10      | 110.10   |
| 24  | b     | 611 | CLA  | C2B-C1B-NB | 8.10  | 115.66      | 110.23   |
| 24  | B     | 602 | CLA  | C2D-C1D-ND | 8.06  | 116.05      | 110.10   |
| 24  | A     | 405 | CLA  | C1D-ND-C4D | -8.05 | 100.61      | 106.33   |
| 24  | c     | 517 | CLA  | C2D-C1D-ND | 8.02  | 116.02      | 110.10   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 511    | CLA  | C2D-C1D-ND  | 8.01  | 116.01      | 110.10   |
| 24  | C     | 503    | CLA  | C2D-C1D-ND  | 8.00  | 116.00      | 110.10   |
| 24  | b     | 622    | CLA  | C1D-ND-C4D  | -7.99 | 100.66      | 106.33   |
| 24  | B     | 610    | CLA  | C2D-C1D-ND  | 7.99  | 115.99      | 110.10   |
| 24  | b     | 618    | CLA  | C2D-C1D-ND  | 7.99  | 115.99      | 110.10   |
| 24  | c     | 506    | CLA  | C2D-C1D-ND  | 7.99  | 115.99      | 110.10   |
| 24  | B     | 615    | CLA  | C2D-C1D-ND  | 7.97  | 115.98      | 110.10   |
| 24  | A     | 410    | CLA  | C2D-C1D-ND  | 7.94  | 115.96      | 110.10   |
| 24  | C     | 506    | CLA  | C1D-ND-C4D  | -7.93 | 100.70      | 106.33   |
| 24  | b     | 624    | CLA  | C2D-C1D-ND  | 7.93  | 115.94      | 110.10   |
| 24  | C     | 507    | CLA  | C2D-C1D-ND  | 7.90  | 115.93      | 110.10   |
| 24  | B     | 605    | CLA  | C2D-C1D-ND  | 7.89  | 115.92      | 110.10   |
| 24  | B     | 611    | CLA  | C2B-C1B-NB  | 7.87  | 115.51      | 110.23   |
| 24  | d     | 401    | CLA  | C2D-C1D-ND  | 7.86  | 115.90      | 110.10   |
| 24  | B     | 617    | CLA  | C2D-C1D-ND  | 7.84  | 115.88      | 110.10   |
| 24  | C     | 513    | CLA  | C2B-C1B-NB  | 7.83  | 115.48      | 110.23   |
| 24  | b     | 611    | CLA  | C2D-C1D-ND  | 7.81  | 115.86      | 110.10   |
| 24  | C     | 508    | CLA  | C2D-C1D-ND  | 7.81  | 115.86      | 110.10   |
| 24  | A     | 406    | CLA  | C2B-C1B-NB  | 7.76  | 115.44      | 110.23   |
| 24  | c     | 514    | CLA  | C2D-C1D-ND  | 7.76  | 115.82      | 110.10   |
| 24  | c     | 518    | CLA  | C2B-C1B-NB  | 7.72  | 115.41      | 110.23   |
| 24  | B     | 609    | CLA  | C2D-C1D-ND  | 7.71  | 115.78      | 110.10   |
| 25  | a     | 418[A] | PHO  | O2D-CGD-CBD | 7.71  | 120.76      | 111.00   |
| 25  | a     | 418[B] | PHO  | O2D-CGD-CBD | 7.69  | 120.74      | 111.00   |
| 24  | b     | 619    | CLA  | C2D-C1D-ND  | 7.68  | 115.77      | 110.10   |
| 24  | C     | 513    | CLA  | C2D-C1D-ND  | 7.65  | 115.74      | 110.10   |
| 24  | B     | 607    | CLA  | C2B-C1B-NB  | 7.65  | 115.36      | 110.23   |
| 24  | B     | 611    | CLA  | C2D-C1D-ND  | 7.62  | 115.72      | 110.10   |
| 24  | c     | 518    | CLA  | C2D-C1D-ND  | 7.62  | 115.72      | 110.10   |
| 24  | A     | 405    | CLA  | C2B-C1B-NB  | 7.61  | 115.34      | 110.23   |
| 24  | b     | 612    | CLA  | C2D-C1D-ND  | 7.59  | 115.70      | 110.10   |
| 24  | c     | 507    | CLA  | C2D-C1D-ND  | 7.59  | 115.69      | 110.10   |
| 24  | b     | 613    | CLA  | C2D-C1D-ND  | 7.58  | 115.69      | 110.10   |
| 24  | A     | 407    | CLA  | C2B-C1B-NB  | 7.58  | 115.31      | 110.23   |
| 24  | c     | 516    | CLA  | C2B-C1B-NB  | 7.57  | 115.31      | 110.23   |
| 25  | a     | 411    | PHO  | O2D-CGD-CBD | 7.56  | 120.58      | 111.00   |
| 24  | C     | 509    | CLA  | C2D-C1D-ND  | 7.56  | 115.67      | 110.10   |
| 24  | c     | 513    | CLA  | C2D-C1D-ND  | 7.55  | 115.67      | 110.10   |
| 24  | c     | 511    | CLA  | C2D-C1D-ND  | 7.53  | 115.65      | 110.10   |
| 24  | B     | 604    | CLA  | C2D-C1D-ND  | 7.51  | 115.64      | 110.10   |
| 24  | B     | 609    | CLA  | C2B-C1B-NB  | 7.50  | 115.26      | 110.23   |
| 24  | D     | 403    | CLA  | C2B-C1B-NB  | 7.50  | 115.26      | 110.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 622    | CLA  | C2D-C1D-ND  | 7.49  | 115.62      | 110.10   |
| 24  | B     | 603    | CLA  | C2D-C1D-ND  | 7.48  | 115.61      | 110.10   |
| 24  | C     | 510    | CLA  | C2D-C1D-ND  | 7.47  | 115.61      | 110.10   |
| 24  | D     | 403    | CLA  | C2D-C1D-ND  | 7.44  | 115.59      | 110.10   |
| 24  | b     | 610    | CLA  | C2D-C1D-ND  | 7.43  | 115.58      | 110.10   |
| 25  | a     | 418[B] | PHO  | C2B-C1B-NB  | 7.40  | 114.64      | 109.53   |
| 24  | C     | 509    | CLA  | C2B-C1B-NB  | 7.40  | 115.19      | 110.23   |
| 24  | b     | 617    | CLA  | C2D-C1D-ND  | 7.39  | 115.55      | 110.10   |
| 24  | B     | 605    | CLA  | CMD-C2D-C1D | 7.39  | 137.74      | 124.71   |
| 24  | B     | 603    | CLA  | C2B-C1B-NB  | 7.34  | 115.16      | 110.23   |
| 24  | c     | 513    | CLA  | C2B-C1B-NB  | 7.34  | 115.15      | 110.23   |
| 24  | a     | 409    | CLA  | C2B-C1B-NB  | 7.34  | 115.15      | 110.23   |
| 24  | C     | 503    | CLA  | C2B-C1B-NB  | 7.34  | 115.15      | 110.23   |
| 24  | c     | 507    | CLA  | C2B-C1B-NB  | 7.34  | 115.15      | 110.23   |
| 24  | A     | 410    | CLA  | C2B-C1B-NB  | 7.30  | 115.13      | 110.23   |
| 24  | C     | 512    | CLA  | C2B-C1B-NB  | 7.28  | 115.11      | 110.23   |
| 24  | d     | 402    | CLA  | C2D-C1D-ND  | 7.28  | 115.47      | 110.10   |
| 24  | B     | 602    | CLA  | C2B-C1B-NB  | 7.25  | 115.09      | 110.23   |
| 24  | c     | 508    | CLA  | C2B-C1B-NB  | 7.20  | 115.06      | 110.23   |
| 24  | b     | 615    | CLA  | C2B-C1B-NB  | 7.18  | 115.05      | 110.23   |
| 24  | B     | 606    | CLA  | CHD-C4C-C3C | -7.17 | 114.30      | 124.84   |
| 24  | d     | 403    | CLA  | C2B-C1B-NB  | 7.15  | 115.03      | 110.23   |
| 24  | b     | 613    | CLA  | C1D-ND-C4D  | -7.14 | 101.26      | 106.33   |
| 24  | a     | 409    | CLA  | C2D-C1D-ND  | 7.09  | 115.33      | 110.10   |
| 25  | a     | 411    | PHO  | C2B-C1B-NB  | 7.08  | 114.42      | 109.53   |
| 24  | C     | 505    | CLA  | C2B-C1B-NB  | 7.05  | 114.96      | 110.23   |
| 24  | C     | 506    | CLA  | C2D-C1D-ND  | 7.05  | 115.30      | 110.10   |
| 24  | b     | 619    | CLA  | C2B-C1B-NB  | 7.04  | 114.95      | 110.23   |
| 24  | c     | 517    | CLA  | C4A-NA-C1A  | -7.02 | 103.55      | 106.71   |
| 24  | c     | 506    | CLA  | C2B-C1B-NB  | 7.02  | 114.94      | 110.23   |
| 25  | a     | 418[A] | PHO  | C2B-C1B-NB  | 7.00  | 114.36      | 109.53   |
| 24  | b     | 617    | CLA  | C2B-C1B-NB  | 7.00  | 114.92      | 110.23   |
| 24  | C     | 507    | CLA  | C2B-C1B-NB  | 6.98  | 114.91      | 110.23   |
| 24  | d     | 403    | CLA  | CMD-C2D-C1D | 6.97  | 137.00      | 124.71   |
| 25  | a     | 418[A] | PHO  | C4D-ND-C1D  | -6.97 | 101.74      | 108.83   |
| 24  | B     | 616    | CLA  | C2B-C1B-NB  | 6.95  | 114.89      | 110.23   |
| 24  | C     | 510    | CLA  | CMD-C2D-C1D | 6.95  | 136.96      | 124.71   |
| 24  | a     | 412    | CLA  | C2B-C1B-NB  | 6.94  | 114.88      | 110.23   |
| 24  | b     | 623    | CLA  | C2B-C1B-NB  | 6.92  | 114.87      | 110.23   |
| 24  | b     | 616    | CLA  | CMD-C2D-C1D | 6.92  | 136.90      | 124.71   |
| 25  | A     | 408    | PHO  | C4D-ND-C1D  | -6.91 | 101.80      | 108.83   |
| 24  | B     | 615    | CLA  | C2B-C1B-NB  | 6.90  | 114.86      | 110.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25  | A     | 409[B] | PHO  | C4D-ND-C1D  | -6.89 | 101.82      | 108.83   |
| 24  | b     | 614    | CLA  | CHD-C4C-C3C | -6.89 | 114.71      | 124.84   |
| 25  | A     | 409[B] | PHO  | C2B-C1B-NB  | 6.89  | 114.28      | 109.53   |
| 24  | a     | 410    | CLA  | C2B-C1B-NB  | 6.88  | 114.84      | 110.23   |
| 24  | c     | 515    | CLA  | C2D-C1D-ND  | 6.83  | 115.14      | 110.10   |
| 25  | a     | 418[B] | PHO  | C4D-ND-C1D  | -6.83 | 101.89      | 108.83   |
| 24  | B     | 603    | CLA  | C4A-NA-C1A  | -6.82 | 103.64      | 106.71   |
| 24  | a     | 409    | CLA  | CMD-C2D-C1D | 6.82  | 136.74      | 124.71   |
| 25  | A     | 409[A] | PHO  | C2B-C1B-NB  | 6.82  | 114.23      | 109.53   |
| 24  | b     | 614    | CLA  | C4A-NA-C1A  | -6.79 | 103.66      | 106.71   |
| 24  | c     | 508    | CLA  | CMD-C2D-C1D | 6.77  | 136.64      | 124.71   |
| 24  | c     | 512    | CLA  | O2D-CGD-CBD | 6.76  | 123.28      | 111.27   |
| 24  | A     | 405    | CLA  | C2D-C1D-ND  | 6.75  | 115.08      | 110.10   |
| 24  | b     | 611    | CLA  | CMD-C2D-C1D | 6.74  | 136.60      | 124.71   |
| 24  | C     | 505    | CLA  | C2D-C1D-ND  | 6.74  | 115.07      | 110.10   |
| 24  | c     | 518    | CLA  | CMD-C2D-C1D | 6.72  | 136.56      | 124.71   |
| 24  | B     | 613    | CLA  | CHD-C4C-C3C | -6.72 | 114.96      | 124.84   |
| 24  | b     | 621    | CLA  | C2B-C1B-NB  | 6.72  | 114.73      | 110.23   |
| 24  | b     | 624    | CLA  | C2B-C1B-NB  | 6.71  | 114.73      | 110.23   |
| 24  | d     | 402    | CLA  | C4A-NA-C1A  | -6.71 | 103.69      | 106.71   |
| 24  | b     | 622    | CLA  | C2B-C1B-NB  | 6.68  | 114.71      | 110.23   |
| 24  | b     | 614    | CLA  | CHD-C1D-ND  | -6.67 | 118.32      | 124.45   |
| 25  | A     | 408    | PHO  | C1C-C2C-C3C | -6.66 | 103.07      | 108.61   |
| 24  | d     | 402    | CLA  | CMD-C2D-C1D | 6.66  | 136.45      | 124.71   |
| 24  | b     | 616    | CLA  | C2B-C1B-NB  | 6.66  | 114.69      | 110.23   |
| 24  | b     | 620    | CLA  | C2B-C1B-NB  | 6.65  | 114.69      | 110.23   |
| 24  | c     | 509    | CLA  | CMD-C2D-C1D | 6.65  | 136.43      | 124.71   |
| 24  | D     | 402    | CLA  | C2B-C1B-NB  | 6.64  | 114.69      | 110.23   |
| 24  | b     | 619    | CLA  | CMD-C2D-C1D | 6.64  | 136.42      | 124.71   |
| 24  | b     | 610    | CLA  | O2D-CGD-CBD | 6.63  | 123.06      | 111.27   |
| 24  | C     | 504    | CLA  | C2B-C1B-NB  | 6.58  | 114.64      | 110.23   |
| 24  | b     | 614    | CLA  | C2B-C1B-NB  | 6.58  | 114.64      | 110.23   |
| 24  | A     | 407    | CLA  | CHD-C1D-ND  | -6.58 | 118.41      | 124.45   |
| 24  | B     | 612    | CLA  | CHD-C4C-C3C | -6.58 | 115.17      | 124.84   |
| 24  | C     | 501    | CLA  | CMD-C2D-C1D | 6.57  | 136.30      | 124.71   |
| 24  | C     | 513    | CLA  | CMD-C2D-C1D | 6.57  | 136.29      | 124.71   |
| 24  | b     | 612    | CLA  | CMD-C2D-C1D | 6.57  | 136.29      | 124.71   |
| 24  | B     | 606    | CLA  | C2B-C1B-NB  | 6.56  | 114.63      | 110.23   |
| 24  | c     | 514    | CLA  | C2B-C1B-NB  | 6.55  | 114.62      | 110.23   |
| 24  | B     | 610    | CLA  | C2B-C1B-NB  | 6.55  | 114.62      | 110.23   |
| 24  | b     | 613    | CLA  | CMD-C2D-C1D | 6.54  | 136.24      | 124.71   |
| 24  | C     | 504    | CLA  | CMD-C2D-C1D | 6.54  | 136.24      | 124.71   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | B     | 602    | CLA  | CMD-C2D-C1D | 6.53  | 136.23      | 124.71   |
| 24  | B     | 614    | CLA  | CMD-C2D-C1D | 6.52  | 136.21      | 124.71   |
| 24  | b     | 616    | CLA  | CHD-C1D-ND  | -6.50 | 118.48      | 124.45   |
| 24  | c     | 511    | CLA  | C2B-C1B-NB  | 6.50  | 114.59      | 110.23   |
| 24  | c     | 510    | CLA  | C4A-NA-C1A  | -6.49 | 103.79      | 106.71   |
| 24  | c     | 515    | CLA  | CMD-C2D-C1D | 6.49  | 136.15      | 124.71   |
| 25  | A     | 409[B] | PHO  | O2D-CGD-CBD | 6.49  | 119.22      | 111.00   |
| 24  | C     | 511    | CLA  | C2B-C1B-NB  | 6.47  | 114.57      | 110.23   |
| 24  | c     | 510    | CLA  | C2B-C1B-NB  | 6.47  | 114.57      | 110.23   |
| 24  | B     | 603    | CLA  | CMD-C2D-C1D | 6.47  | 136.12      | 124.71   |
| 24  | D     | 403    | CLA  | CMD-C2D-C1D | 6.47  | 136.12      | 124.71   |
| 35  | d     | 411    | HTG  | C1'-S1-C1   | 6.46  | 112.18      | 100.09   |
| 24  | b     | 625    | CLA  | C2B-C1B-NB  | 6.45  | 114.56      | 110.23   |
| 24  | b     | 620    | CLA  | CMD-C2D-C1D | 6.45  | 136.08      | 124.71   |
| 24  | c     | 508    | CLA  | CHD-C4C-C3C | -6.44 | 115.38      | 124.84   |
| 24  | c     | 515    | CLA  | C2B-C1B-NB  | 6.44  | 114.55      | 110.23   |
| 24  | b     | 614    | CLA  | CMD-C2D-C1D | 6.43  | 136.04      | 124.71   |
| 24  | B     | 616    | CLA  | CHD-C4C-C3C | -6.43 | 115.39      | 124.84   |
| 25  | A     | 409[A] | PHO  | O2D-CGD-CBD | 6.42  | 119.14      | 111.00   |
| 24  | c     | 512    | CLA  | CHD-C4C-C3C | -6.42 | 115.41      | 124.84   |
| 24  | c     | 511    | CLA  | CMD-C2D-C1D | 6.41  | 136.01      | 124.71   |
| 24  | B     | 608    | CLA  | C2B-C1B-NB  | 6.39  | 114.52      | 110.23   |
| 24  | B     | 607    | CLA  | CMD-C2D-C1D | 6.39  | 135.98      | 124.71   |
| 35  | C     | 522    | HTG  | C1'-S1-C1   | 6.39  | 112.04      | 100.09   |
| 24  | b     | 611    | CLA  | CHD-C1D-ND  | -6.39 | 118.58      | 124.45   |
| 24  | B     | 617    | CLA  | CMD-C2D-C1D | 6.38  | 135.96      | 124.71   |
| 24  | B     | 608    | CLA  | CMD-C2D-C1D | 6.37  | 135.94      | 124.71   |
| 25  | A     | 409[A] | PHO  | C4D-ND-C1D  | -6.37 | 102.35      | 108.83   |
| 24  | d     | 402    | CLA  | CHD-C1D-ND  | -6.37 | 118.60      | 124.45   |
| 24  | b     | 613    | CLA  | C2C-C1C-NC  | 6.37  | 115.94      | 109.97   |
| 24  | B     | 604    | CLA  | CHD-C4C-C3C | -6.35 | 115.50      | 124.84   |
| 24  | b     | 611    | CLA  | C4A-NA-C1A  | -6.35 | 103.85      | 106.71   |
| 24  | C     | 513    | CLA  | CHD-C1D-ND  | -6.35 | 118.62      | 124.45   |
| 24  | c     | 508    | CLA  | C4A-NA-C1A  | -6.34 | 103.85      | 106.71   |
| 24  | C     | 512    | CLA  | CHD-C4C-C3C | -6.34 | 115.52      | 124.84   |
| 24  | B     | 616    | CLA  | CMD-C2D-C1D | 6.33  | 135.88      | 124.71   |
| 24  | B     | 604    | CLA  | O2D-CGD-CBD | 6.32  | 122.50      | 111.27   |
| 24  | C     | 503    | CLA  | CHD-C4C-C3C | -6.32 | 115.55      | 124.84   |
| 24  | C     | 505    | CLA  | C4A-NA-C1A  | -6.32 | 103.86      | 106.71   |
| 24  | d     | 403    | CLA  | CHD-C1D-ND  | -6.32 | 118.65      | 124.45   |
| 24  | B     | 613    | CLA  | C2B-C1B-NB  | 6.32  | 114.47      | 110.23   |
| 25  | A     | 408    | PHO  | O2D-CGD-CBD | 6.31  | 118.99      | 111.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | b     | 623 | CLA  | O2D-CGD-CBD | 6.31  | 122.48      | 111.27   |
| 24  | c     | 510 | CLA  | C2D-C1D-ND  | 6.31  | 114.75      | 110.10   |
| 24  | C     | 501 | CLA  | C2B-C1B-NB  | 6.31  | 114.46      | 110.23   |
| 24  | B     | 617 | CLA  | O2D-CGD-CBD | 6.30  | 122.46      | 111.27   |
| 24  | C     | 505 | CLA  | CHD-C4C-C3C | -6.29 | 115.59      | 124.84   |
| 24  | C     | 504 | CLA  | CHD-C1D-ND  | -6.28 | 118.69      | 124.45   |
| 24  | C     | 502 | CLA  | C2B-C1B-NB  | 6.27  | 114.44      | 110.23   |
| 24  | c     | 509 | CLA  | CHD-C1D-ND  | -6.26 | 118.70      | 124.45   |
| 24  | b     | 612 | CLA  | C2B-C1B-NB  | 6.25  | 114.42      | 110.23   |
| 24  | C     | 507 | CLA  | CMD-C2D-C1D | 6.25  | 135.72      | 124.71   |
| 24  | D     | 402 | CLA  | C4A-NA-C1A  | -6.24 | 103.90      | 106.71   |
| 24  | b     | 615 | CLA  | CHD-C4C-C3C | -6.24 | 115.66      | 124.84   |
| 24  | C     | 501 | CLA  | CHD-C1D-ND  | -6.24 | 118.72      | 124.45   |
| 24  | b     | 621 | CLA  | CHD-C4C-C3C | -6.23 | 115.68      | 124.84   |
| 24  | b     | 622 | CLA  | CMD-C2D-C1D | 6.23  | 135.69      | 124.71   |
| 24  | b     | 612 | CLA  | CHD-C4C-C3C | -6.22 | 115.70      | 124.84   |
| 24  | D     | 402 | CLA  | CHD-C1D-ND  | -6.22 | 118.74      | 124.45   |
| 25  | a     | 411 | PHO  | C4D-ND-C1D  | -6.22 | 102.50      | 108.83   |
| 24  | B     | 616 | CLA  | CHD-C1D-ND  | -6.22 | 118.74      | 124.45   |
| 24  | d     | 401 | CLA  | C2B-C1B-NB  | 6.21  | 114.40      | 110.23   |
| 24  | b     | 616 | CLA  | CHD-C4C-C3C | -6.21 | 115.71      | 124.84   |
| 24  | a     | 410 | CLA  | CHD-C1D-ND  | -6.20 | 118.75      | 124.45   |
| 25  | a     | 411 | PHO  | C1C-C2C-C3C | -6.20 | 103.45      | 108.61   |
| 24  | d     | 402 | CLA  | C2B-C1B-NB  | 6.20  | 114.39      | 110.23   |
| 24  | C     | 508 | CLA  | CMD-C2D-C1D | 6.20  | 135.63      | 124.71   |
| 24  | a     | 409 | CLA  | C2C-C1C-NC  | 6.20  | 115.78      | 109.97   |
| 24  | B     | 617 | CLA  | C2B-C1B-NB  | 6.19  | 114.38      | 110.23   |
| 24  | C     | 511 | CLA  | C2C-C1C-NC  | 6.19  | 115.77      | 109.97   |
| 24  | a     | 409 | CLA  | CHD-C1D-ND  | -6.18 | 118.77      | 124.45   |
| 24  | b     | 615 | CLA  | C4A-NA-C1A  | -6.17 | 103.93      | 106.71   |
| 24  | d     | 401 | CLA  | C2C-C1C-NC  | 6.17  | 115.75      | 109.97   |
| 24  | C     | 501 | CLA  | O2D-CGD-CBD | 6.17  | 122.23      | 111.27   |
| 24  | B     | 604 | CLA  | C2B-C1B-NB  | 6.17  | 114.36      | 110.23   |
| 24  | d     | 403 | CLA  | CHD-C4C-C3C | -6.16 | 115.78      | 124.84   |
| 24  | B     | 606 | CLA  | CMD-C2D-C1D | 6.16  | 135.57      | 124.71   |
| 24  | b     | 618 | CLA  | CHD-C4C-C3C | -6.16 | 115.79      | 124.84   |
| 24  | C     | 506 | CLA  | CMD-C2D-C1D | 6.16  | 135.56      | 124.71   |
| 24  | B     | 605 | CLA  | C2C-C1C-NC  | 6.14  | 115.72      | 109.97   |
| 24  | b     | 618 | CLA  | CMD-C2D-C1D | 6.14  | 135.53      | 124.71   |
| 24  | c     | 510 | CLA  | CHD-C4C-C3C | -6.14 | 115.82      | 124.84   |
| 24  | B     | 609 | CLA  | CMD-C2D-C1D | 6.13  | 135.52      | 124.71   |
| 24  | C     | 507 | CLA  | CHD-C4C-C3C | -6.12 | 115.84      | 124.84   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | B     | 608    | CLA  | CHD-C1D-ND  | -6.12 | 118.83      | 124.45   |
| 24  | b     | 613    | CLA  | C2B-C1B-NB  | 6.12  | 114.33      | 110.23   |
| 24  | C     | 503    | CLA  | CHD-C1D-ND  | -6.12 | 118.83      | 124.45   |
| 24  | c     | 518    | CLA  | CHD-C1D-ND  | -6.12 | 118.83      | 124.45   |
| 24  | b     | 624    | CLA  | CHD-C4C-C3C | -6.11 | 115.86      | 124.84   |
| 24  | a     | 410    | CLA  | CHD-C4C-C3C | -6.11 | 115.86      | 124.84   |
| 24  | C     | 509    | CLA  | CMD-C2D-C1D | 6.10  | 135.47      | 124.71   |
| 24  | C     | 505    | CLA  | CMD-C2D-C1D | 6.10  | 135.47      | 124.71   |
| 24  | b     | 610    | CLA  | CHD-C4C-C3C | -6.10 | 115.88      | 124.84   |
| 24  | b     | 624    | CLA  | C4A-NA-C1A  | -6.09 | 103.97      | 106.71   |
| 24  | B     | 609    | CLA  | C2C-C1C-NC  | 6.08  | 115.67      | 109.97   |
| 24  | B     | 602    | CLA  | CHD-C1D-ND  | -6.08 | 118.87      | 124.45   |
| 24  | b     | 610    | CLA  | CMD-C2D-C1D | 6.08  | 135.42      | 124.71   |
| 24  | c     | 509    | CLA  | CHD-C4C-C3C | -6.07 | 115.92      | 124.84   |
| 24  | C     | 503    | CLA  | CMD-C2D-C1D | 6.07  | 135.41      | 124.71   |
| 24  | B     | 612    | CLA  | C2B-C1B-NB  | 6.07  | 114.30      | 110.23   |
| 24  | c     | 517    | CLA  | O2D-CGD-CBD | 6.06  | 122.04      | 111.27   |
| 24  | B     | 603    | CLA  | CHD-C1D-ND  | -6.06 | 118.89      | 124.45   |
| 24  | b     | 625    | CLA  | CHD-C4C-C3C | -6.06 | 115.94      | 124.84   |
| 24  | b     | 624    | CLA  | CMD-C2D-C1D | 6.05  | 135.37      | 124.71   |
| 24  | c     | 512    | CLA  | C2C-C1C-NC  | 6.04  | 115.63      | 109.97   |
| 24  | c     | 506    | CLA  | CMD-C2D-C1D | 6.04  | 135.35      | 124.71   |
| 25  | A     | 409[A] | PHO  | C1C-C2C-C3C | -6.02 | 103.60      | 108.61   |
| 24  | b     | 613    | CLA  | O2D-CGD-CBD | 6.02  | 121.96      | 111.27   |
| 24  | B     | 602    | CLA  | CHD-C4C-C3C | -6.02 | 116.00      | 124.84   |
| 24  | B     | 607    | CLA  | CHD-C4C-C3C | -6.02 | 116.00      | 124.84   |
| 24  | B     | 617    | CLA  | CHD-C4C-C3C | -6.00 | 116.02      | 124.84   |
| 24  | D     | 402    | CLA  | CHD-C4C-C3C | -6.00 | 116.02      | 124.84   |
| 24  | c     | 506    | CLA  | C2C-C1C-NC  | 5.99  | 115.59      | 109.97   |
| 24  | A     | 407    | CLA  | CHD-C4C-C3C | -5.99 | 116.03      | 124.84   |
| 24  | b     | 622    | CLA  | C2C-C1C-NC  | 5.99  | 115.58      | 109.97   |
| 24  | b     | 625    | CLA  | O2D-CGD-CBD | 5.99  | 121.91      | 111.27   |
| 25  | A     | 409[B] | PHO  | C1C-C2C-C3C | -5.98 | 103.63      | 108.61   |
| 24  | c     | 510    | CLA  | C2C-C1C-NC  | 5.98  | 115.58      | 109.97   |
| 24  | c     | 511    | CLA  | CHD-C1D-ND  | -5.98 | 118.96      | 124.45   |
| 24  | b     | 617    | CLA  | CMD-C2D-C1D | 5.97  | 135.24      | 124.71   |
| 24  | D     | 402    | CLA  | C2C-C1C-NC  | 5.97  | 115.56      | 109.97   |
| 24  | d     | 401    | CLA  | CHD-C4C-C3C | -5.97 | 116.07      | 124.84   |
| 24  | B     | 615    | CLA  | CMD-C2D-C1D | 5.96  | 135.22      | 124.71   |
| 24  | C     | 510    | CLA  | CHD-C4C-C3C | -5.96 | 116.08      | 124.84   |
| 24  | B     | 610    | CLA  | C4A-NA-C1A  | -5.96 | 104.03      | 106.71   |
| 24  | c     | 514    | CLA  | CHD-C4C-C3C | -5.96 | 116.08      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 607 | CLA  | CHD-C1D-ND  | -5.96 | 118.98      | 124.45   |
| 24  | C     | 506 | CLA  | C2B-C1B-NB  | 5.95  | 114.22      | 110.23   |
| 24  | A     | 405 | CLA  | CMD-C2D-C1D | 5.95  | 135.20      | 124.71   |
| 24  | A     | 406 | CLA  | CHD-C4C-C3C | -5.95 | 116.09      | 124.84   |
| 24  | A     | 410 | CLA  | CMD-C2D-C1D | 5.95  | 135.19      | 124.71   |
| 24  | A     | 407 | CLA  | CMD-C2D-C1D | 5.94  | 135.19      | 124.71   |
| 24  | C     | 502 | CLA  | CHD-C4C-C3C | -5.93 | 116.12      | 124.84   |
| 24  | B     | 614 | CLA  | CHD-C4C-C3C | -5.93 | 116.12      | 124.84   |
| 24  | c     | 518 | CLA  | C4A-NA-C1A  | -5.93 | 104.04      | 106.71   |
| 24  | B     | 611 | CLA  | CMD-C2D-C1D | 5.93  | 135.16      | 124.71   |
| 24  | c     | 507 | CLA  | CHD-C4C-C3C | -5.92 | 116.13      | 124.84   |
| 24  | c     | 514 | CLA  | CMD-C2D-C1D | 5.92  | 135.15      | 124.71   |
| 24  | B     | 610 | CLA  | CHD-C4C-C3C | -5.92 | 116.14      | 124.84   |
| 24  | B     | 616 | CLA  | C4A-NA-C1A  | -5.91 | 104.05      | 106.71   |
| 35  | c     | 525 | HTG  | C1'-S1-C1   | 5.91  | 111.14      | 100.09   |
| 24  | B     | 610 | CLA  | CMD-C2D-C1D | 5.90  | 135.12      | 124.71   |
| 24  | B     | 615 | CLA  | CHD-C4C-C3C | -5.90 | 116.17      | 124.84   |
| 24  | c     | 515 | CLA  | C2C-C1C-NC  | 5.90  | 115.50      | 109.97   |
| 24  | b     | 625 | CLA  | CMD-C2D-C1D | 5.90  | 135.11      | 124.71   |
| 24  | b     | 618 | CLA  | C2B-C1B-NB  | 5.90  | 114.19      | 110.23   |
| 24  | B     | 604 | CLA  | CMD-C2D-C1D | 5.89  | 135.10      | 124.71   |
| 24  | B     | 611 | CLA  | CHD-C1D-ND  | -5.88 | 119.05      | 124.45   |
| 24  | c     | 509 | CLA  | C2B-C1B-NB  | 5.88  | 114.17      | 110.23   |
| 24  | b     | 618 | CLA  | C4A-NA-C1A  | -5.88 | 104.06      | 106.71   |
| 24  | A     | 406 | CLA  | C2C-C1C-NC  | 5.88  | 115.48      | 109.97   |
| 24  | a     | 410 | CLA  | CMD-C2D-C1D | 5.87  | 135.06      | 124.71   |
| 24  | B     | 612 | CLA  | C2C-C1C-NC  | 5.87  | 115.47      | 109.97   |
| 24  | b     | 615 | CLA  | CMD-C2D-C1D | 5.86  | 135.03      | 124.71   |
| 24  | d     | 401 | CLA  | CMD-C2D-C1D | 5.86  | 135.03      | 124.71   |
| 24  | b     | 611 | CLA  | CHD-C4C-C3C | -5.85 | 116.25      | 124.84   |
| 24  | C     | 508 | CLA  | CHD-C1D-ND  | -5.84 | 119.08      | 124.45   |
| 24  | C     | 506 | CLA  | C2C-C1C-NC  | 5.84  | 115.44      | 109.97   |
| 24  | c     | 516 | CLA  | CHD-C1D-ND  | -5.83 | 119.09      | 124.45   |
| 24  | A     | 410 | CLA  | CHD-C4C-C3C | -5.83 | 116.26      | 124.84   |
| 24  | B     | 614 | CLA  | C2B-C1B-NB  | 5.83  | 114.14      | 110.23   |
| 24  | B     | 615 | CLA  | O2D-CGD-CBD | 5.83  | 121.62      | 111.27   |
| 24  | B     | 602 | CLA  | O2D-CGD-CBD | 5.83  | 121.62      | 111.27   |
| 24  | d     | 402 | CLA  | C2C-C1C-NC  | 5.83  | 115.43      | 109.97   |
| 24  | b     | 617 | CLA  | CHD-C4C-C3C | -5.82 | 116.28      | 124.84   |
| 24  | c     | 517 | CLA  | CHD-C4C-C3C | -5.82 | 116.28      | 124.84   |
| 24  | c     | 506 | CLA  | CHD-C1D-ND  | -5.82 | 119.11      | 124.45   |
| 24  | b     | 620 | CLA  | C2C-C1C-NC  | 5.81  | 115.42      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 617 | CLA  | C4A-NA-C1A  | -5.81 | 104.09      | 106.71   |
| 24  | b     | 615 | CLA  | CHD-C1D-ND  | -5.80 | 119.12      | 124.45   |
| 24  | B     | 609 | CLA  | CHD-C1D-ND  | -5.80 | 119.12      | 124.45   |
| 24  | C     | 512 | CLA  | O2D-CGD-CBD | 5.80  | 121.57      | 111.27   |
| 24  | c     | 510 | CLA  | O2D-CGD-CBD | 5.80  | 121.57      | 111.27   |
| 35  | B     | 633 | HTG  | C1'-S1-C1   | 5.79  | 110.93      | 100.09   |
| 24  | A     | 405 | CLA  | C2C-C1C-NC  | 5.79  | 115.40      | 109.97   |
| 24  | B     | 605 | CLA  | CHD-C4C-C3C | -5.79 | 116.33      | 124.84   |
| 24  | b     | 616 | CLA  | C2C-C1C-NC  | 5.79  | 115.40      | 109.97   |
| 24  | b     | 623 | CLA  | CHD-C1D-ND  | -5.79 | 119.14      | 124.45   |
| 24  | b     | 619 | CLA  | CHD-C4C-C3C | -5.79 | 116.33      | 124.84   |
| 24  | A     | 406 | CLA  | CMD-C2D-C1D | 5.78  | 134.91      | 124.71   |
| 24  | A     | 405 | CLA  | C4A-NA-C1A  | -5.78 | 104.11      | 106.71   |
| 24  | b     | 624 | CLA  | CHD-C1D-ND  | -5.78 | 119.14      | 124.45   |
| 24  | C     | 502 | CLA  | CHD-C1D-ND  | -5.77 | 119.15      | 124.45   |
| 24  | a     | 412 | CLA  | CHD-C4C-C3C | -5.76 | 116.37      | 124.84   |
| 24  | c     | 511 | CLA  | C2C-C1C-NC  | 5.75  | 115.36      | 109.97   |
| 24  | b     | 610 | CLA  | C4A-NA-C1A  | -5.75 | 104.12      | 106.71   |
| 24  | B     | 603 | CLA  | CHD-C4C-C3C | -5.74 | 116.40      | 124.84   |
| 24  | A     | 407 | CLA  | C4A-NA-C1A  | -5.74 | 104.12      | 106.71   |
| 24  | c     | 510 | CLA  | CMD-C2D-C1D | 5.74  | 134.83      | 124.71   |
| 24  | a     | 412 | CLA  | C2C-C1C-NC  | 5.74  | 115.35      | 109.97   |
| 24  | D     | 403 | CLA  | C2C-C1C-NC  | 5.73  | 115.34      | 109.97   |
| 24  | c     | 516 | CLA  | CHD-C4C-C3C | -5.73 | 116.42      | 124.84   |
| 24  | c     | 518 | CLA  | CHD-C4C-C3C | -5.73 | 116.42      | 124.84   |
| 24  | B     | 615 | CLA  | CHD-C1D-ND  | -5.72 | 119.20      | 124.45   |
| 24  | A     | 406 | CLA  | CHD-C1D-ND  | -5.72 | 119.20      | 124.45   |
| 24  | b     | 620 | CLA  | CHD-C4C-C3C | -5.71 | 116.45      | 124.84   |
| 24  | b     | 617 | CLA  | C4A-NA-C1A  | -5.70 | 104.14      | 106.71   |
| 24  | D     | 403 | CLA  | C4A-NA-C1A  | -5.69 | 104.15      | 106.71   |
| 24  | D     | 403 | CLA  | CHD-C1D-ND  | -5.69 | 119.23      | 124.45   |
| 35  | D     | 412 | HTG  | C1'-S1-C1   | 5.68  | 110.72      | 100.09   |
| 24  | b     | 610 | CLA  | CHD-C1D-ND  | -5.68 | 119.23      | 124.45   |
| 24  | c     | 509 | CLA  | C2C-C1C-NC  | 5.68  | 115.29      | 109.97   |
| 24  | C     | 511 | CLA  | CHD-C4C-C3C | -5.68 | 116.49      | 124.84   |
| 24  | C     | 502 | CLA  | CMD-C2D-C1D | 5.68  | 134.72      | 124.71   |
| 24  | B     | 608 | CLA  | CHD-C4C-C3C | -5.67 | 116.51      | 124.84   |
| 24  | b     | 612 | CLA  | CHD-C1D-ND  | -5.66 | 119.25      | 124.45   |
| 24  | c     | 512 | CLA  | CMD-C2D-C1D | 5.66  | 134.68      | 124.71   |
| 24  | B     | 607 | CLA  | C4A-NA-C1A  | -5.65 | 104.16      | 106.71   |
| 25  | A     | 408 | PHO  | C2B-C1B-NB  | 5.65  | 113.43      | 109.53   |
| 24  | B     | 610 | CLA  | CHD-C1D-ND  | -5.65 | 119.26      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | c     | 513 | CLA  | CHD-C4C-C3C | -5.65 | 116.54      | 124.84   |
| 24  | c     | 508 | CLA  | CHD-C1D-ND  | -5.64 | 119.27      | 124.45   |
| 24  | b     | 618 | CLA  | CHD-C1D-ND  | -5.64 | 119.27      | 124.45   |
| 24  | C     | 509 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.84   |
| 24  | C     | 503 | CLA  | C4A-NA-C1A  | -5.63 | 104.17      | 106.71   |
| 24  | c     | 513 | CLA  | C2C-C1C-NC  | 5.63  | 115.24      | 109.97   |
| 24  | c     | 511 | CLA  | CHD-C4C-C3C | -5.62 | 116.57      | 124.84   |
| 24  | B     | 607 | CLA  | C2C-C1C-NC  | 5.62  | 115.24      | 109.97   |
| 24  | c     | 507 | CLA  | C4A-NA-C1A  | -5.62 | 104.18      | 106.71   |
| 24  | C     | 507 | CLA  | CHD-C1D-ND  | -5.61 | 119.30      | 124.45   |
| 24  | B     | 614 | CLA  | C2C-C1C-NC  | 5.61  | 115.23      | 109.97   |
| 24  | d     | 403 | CLA  | C4A-NA-C1A  | -5.61 | 104.18      | 106.71   |
| 24  | c     | 515 | CLA  | CHD-C4C-C3C | -5.61 | 116.60      | 124.84   |
| 24  | C     | 510 | CLA  | C2B-C1B-NB  | 5.61  | 113.99      | 110.23   |
| 24  | b     | 619 | CLA  | CHD-C1D-ND  | -5.60 | 119.31      | 124.45   |
| 24  | C     | 509 | CLA  | CHD-C1D-ND  | -5.59 | 119.31      | 124.45   |
| 24  | b     | 612 | CLA  | O2D-CGD-CBD | 5.58  | 121.19      | 111.27   |
| 24  | B     | 613 | CLA  | CHD-C1D-ND  | -5.58 | 119.32      | 124.45   |
| 24  | b     | 623 | CLA  | CHD-C4C-C3C | -5.58 | 116.64      | 124.84   |
| 24  | b     | 623 | CLA  | CMD-C2D-C1D | 5.58  | 134.54      | 124.71   |
| 35  | B     | 625 | HTG  | C1'-S1-C1   | 5.57  | 110.51      | 100.09   |
| 24  | C     | 504 | CLA  | CHD-C4C-C3C | -5.57 | 116.66      | 124.84   |
| 24  | D     | 402 | CLA  | CMD-C2D-C1D | 5.56  | 134.52      | 124.71   |
| 24  | C     | 508 | CLA  | C2C-C1C-NC  | 5.55  | 115.17      | 109.97   |
| 24  | b     | 624 | CLA  | C2C-C1C-NC  | 5.54  | 115.17      | 109.97   |
| 24  | b     | 613 | CLA  | CHD-C4C-C3C | -5.54 | 116.70      | 124.84   |
| 24  | C     | 506 | CLA  | CHD-C1D-ND  | -5.54 | 119.36      | 124.45   |
| 24  | c     | 514 | CLA  | C2C-C1C-NC  | 5.54  | 115.16      | 109.97   |
| 24  | b     | 615 | CLA  | C2C-C1C-NC  | 5.54  | 115.16      | 109.97   |
| 24  | B     | 610 | CLA  | C2C-C1C-NC  | 5.53  | 115.16      | 109.97   |
| 24  | b     | 620 | CLA  | CHD-C1D-ND  | -5.53 | 119.37      | 124.45   |
| 24  | C     | 510 | CLA  | CHD-C1D-ND  | -5.53 | 119.37      | 124.45   |
| 24  | b     | 623 | CLA  | C2C-C1C-NC  | 5.52  | 115.15      | 109.97   |
| 24  | B     | 606 | CLA  | CHD-C1D-ND  | -5.50 | 119.40      | 124.45   |
| 24  | C     | 513 | CLA  | CHD-C4C-C3C | -5.49 | 116.77      | 124.84   |
| 24  | b     | 625 | CLA  | CHD-C1D-ND  | -5.49 | 119.41      | 124.45   |
| 24  | B     | 617 | CLA  | C2C-C1C-NC  | 5.49  | 115.12      | 109.97   |
| 24  | C     | 508 | CLA  | O2D-CGD-CBD | 5.48  | 121.01      | 111.27   |
| 24  | C     | 512 | CLA  | CHD-C1D-ND  | -5.48 | 119.42      | 124.45   |
| 24  | B     | 611 | CLA  | CHD-C4C-C3C | -5.48 | 116.79      | 124.84   |
| 24  | a     | 410 | CLA  | C4A-NA-C1A  | -5.48 | 104.24      | 106.71   |
| 24  | B     | 611 | CLA  | C2C-C1C-NC  | 5.48  | 115.10      | 109.97   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 619    | CLA  | C4A-NA-C1A  | -5.47 | 104.25      | 106.71   |
| 24  | c     | 512    | CLA  | C2B-C1B-NB  | 5.47  | 113.90      | 110.23   |
| 24  | b     | 622    | CLA  | CHD-C4C-C3C | -5.47 | 116.80      | 124.84   |
| 24  | B     | 609    | CLA  | CHD-C4C-C3C | -5.46 | 116.81      | 124.84   |
| 24  | C     | 511    | CLA  | CMD-C2D-C1D | 5.45  | 134.31      | 124.71   |
| 24  | B     | 607    | CLA  | O2D-CGD-CBD | 5.44  | 120.94      | 111.27   |
| 24  | c     | 515    | CLA  | CHD-C1D-ND  | -5.44 | 119.45      | 124.45   |
| 24  | C     | 504    | CLA  | C2C-C1C-NC  | 5.44  | 115.06      | 109.97   |
| 24  | B     | 614    | CLA  | CHD-C1D-ND  | -5.43 | 119.46      | 124.45   |
| 24  | b     | 625    | CLA  | C4A-NA-C1A  | -5.43 | 104.27      | 106.71   |
| 26  | Y     | 101    | BCR  | C33-C5-C6   | -5.43 | 118.44      | 124.53   |
| 24  | c     | 512    | CLA  | CHD-C1D-ND  | -5.42 | 119.47      | 124.45   |
| 24  | c     | 517    | CLA  | CHD-C1D-ND  | -5.42 | 119.47      | 124.45   |
| 24  | B     | 604    | CLA  | C2C-C1C-NC  | 5.41  | 115.04      | 109.97   |
| 24  | C     | 509    | CLA  | C2C-C1C-NC  | 5.41  | 115.04      | 109.97   |
| 24  | B     | 604    | CLA  | C4A-NA-C1A  | -5.41 | 104.28      | 106.71   |
| 24  | c     | 517    | CLA  | CMD-C2D-C1D | 5.41  | 134.24      | 124.71   |
| 24  | C     | 501    | CLA  | CHD-C4C-C3C | -5.40 | 116.90      | 124.84   |
| 25  | a     | 418[A] | PHO  | C1C-C2C-C3C | -5.40 | 104.12      | 108.61   |
| 38  | F     | 102    | HEM  | CHC-C4B-NB  | 5.39  | 130.28      | 124.42   |
| 24  | A     | 410    | CLA  | C2C-C1C-NC  | 5.38  | 115.02      | 109.97   |
| 27  | f     | 101    | SQD  | O47-C7-C8   | 5.38  | 123.10      | 111.50   |
| 24  | C     | 505    | CLA  | C2C-C1C-NC  | 5.38  | 115.01      | 109.97   |
| 24  | B     | 612    | CLA  | CMD-C2D-C1D | 5.38  | 134.19      | 124.71   |
| 24  | b     | 612    | CLA  | C4A-NA-C1A  | -5.37 | 104.29      | 106.71   |
| 35  | B     | 624    | HTG  | C1'-S1-C1   | 5.37  | 110.13      | 100.09   |
| 25  | a     | 418[B] | PHO  | C1C-C2C-C3C | -5.37 | 104.15      | 108.61   |
| 24  | b     | 618    | CLA  | C2C-C1C-NC  | 5.36  | 115.00      | 109.97   |
| 24  | c     | 506    | CLA  | O2D-CGD-CBD | 5.36  | 120.80      | 111.27   |
| 24  | D     | 403    | CLA  | CHD-C4C-C3C | -5.36 | 116.96      | 124.84   |
| 24  | B     | 605    | CLA  | CHD-C1D-ND  | -5.36 | 119.53      | 124.45   |
| 24  | b     | 619    | CLA  | C2C-C1C-NC  | 5.34  | 114.97      | 109.97   |
| 24  | B     | 613    | CLA  | C3C-C4C-NC  | 5.34  | 116.56      | 110.57   |
| 24  | b     | 612    | CLA  | C2C-C1C-NC  | 5.34  | 114.97      | 109.97   |
| 24  | b     | 617    | CLA  | C2C-C1C-NC  | 5.34  | 114.97      | 109.97   |
| 24  | B     | 605    | CLA  | C2B-C1B-NB  | 5.33  | 113.81      | 110.23   |
| 24  | C     | 511    | CLA  | CHD-C1D-ND  | -5.33 | 119.56      | 124.45   |
| 24  | C     | 507    | CLA  | O2D-CGD-CBD | 5.32  | 120.72      | 111.27   |
| 24  | a     | 412    | CLA  | CHD-C1D-ND  | -5.32 | 119.56      | 124.45   |
| 24  | c     | 506    | CLA  | CHD-C4C-C3C | -5.32 | 117.02      | 124.84   |
| 35  | c     | 526    | HTG  | C1'-S1-C1   | 5.31  | 110.02      | 100.09   |
| 35  | b     | 632    | HTG  | C1'-S1-C1   | 5.31  | 110.02      | 100.09   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 506    | CLA  | CHD-C4C-C3C | -5.31 | 117.04      | 124.84   |
| 24  | C     | 510    | CLA  | C2C-C1C-NC  | 5.30  | 114.94      | 109.97   |
| 24  | B     | 613    | CLA  | O2D-CGD-CBD | 5.30  | 120.69      | 111.27   |
| 24  | C     | 508    | CLA  | CHD-C4C-C3C | -5.30 | 117.05      | 124.84   |
| 25  | A     | 408    | PHO  | C3D-C4D-ND  | 5.30  | 114.94      | 107.72   |
| 26  | D     | 404    | BCR  | C7-C8-C9    | -5.30 | 118.23      | 126.23   |
| 24  | c     | 509    | CLA  | O2D-CGD-CBD | 5.29  | 120.67      | 111.27   |
| 35  | b     | 631    | HTG  | C1'-S1-C1   | 5.27  | 109.95      | 100.09   |
| 24  | C     | 501    | CLA  | C2C-C1C-NC  | 5.27  | 114.91      | 109.97   |
| 24  | c     | 507    | CLA  | C2C-C1C-NC  | 5.27  | 114.91      | 109.97   |
| 24  | c     | 517    | CLA  | C3B-C2B-C1B | -5.26 | 100.81      | 107.16   |
| 24  | B     | 603    | CLA  | O2D-CGD-CBD | 5.26  | 120.62      | 111.27   |
| 24  | d     | 401    | CLA  | CHD-C1D-ND  | -5.26 | 119.62      | 124.45   |
| 24  | a     | 412    | CLA  | CMD-C2D-C1D | 5.26  | 133.98      | 124.71   |
| 27  | L     | 102    | SQD  | O6-C1-C2    | 5.25  | 116.50      | 108.30   |
| 24  | C     | 512    | CLA  | CMD-C2D-C1D | 5.25  | 133.97      | 124.71   |
| 24  | B     | 612    | CLA  | CHD-C1D-ND  | -5.25 | 119.63      | 124.45   |
| 24  | a     | 412    | CLA  | O2D-CGD-CBD | 5.24  | 120.58      | 111.27   |
| 24  | B     | 606    | CLA  | C4A-NA-C1A  | -5.24 | 104.35      | 106.71   |
| 24  | b     | 621    | CLA  | C2C-C1C-NC  | 5.24  | 114.88      | 109.97   |
| 24  | A     | 406    | CLA  | O2D-CGD-CBD | 5.23  | 120.56      | 111.27   |
| 24  | b     | 615    | CLA  | O2D-CGD-CBD | 5.23  | 120.56      | 111.27   |
| 24  | c     | 518    | CLA  | C2C-C1C-NC  | 5.23  | 114.87      | 109.97   |
| 24  | B     | 608    | CLA  | C2C-C1C-NC  | 5.22  | 114.86      | 109.97   |
| 24  | c     | 513    | CLA  | C4A-NA-C1A  | -5.22 | 104.36      | 106.71   |
| 24  | c     | 513    | CLA  | O2D-CGD-CBD | 5.20  | 120.51      | 111.27   |
| 24  | c     | 507    | CLA  | CHD-C1D-ND  | -5.19 | 119.68      | 124.45   |
| 24  | c     | 516    | CLA  | CMD-C2D-C1D | 5.17  | 133.83      | 124.71   |
| 24  | A     | 407    | CLA  | O2D-CGD-CBD | 5.17  | 120.46      | 111.27   |
| 24  | b     | 613    | CLA  | C4A-NA-C1A  | -5.16 | 104.39      | 106.71   |
| 24  | C     | 512    | CLA  | C4A-NA-C1A  | -5.16 | 104.39      | 106.71   |
| 24  | B     | 603    | CLA  | C2C-C1C-NC  | 5.15  | 114.79      | 109.97   |
| 27  | F     | 103    | SQD  | O47-C7-C8   | 5.13  | 122.56      | 111.50   |
| 24  | a     | 409    | CLA  | CHD-C4C-C3C | -5.13 | 117.30      | 124.84   |
| 24  | B     | 613    | CLA  | C3D-C2D-C1D | -5.12 | 98.84       | 105.83   |
| 27  | a     | 414    | SQD  | O6-C1-C2    | 5.11  | 116.28      | 108.30   |
| 24  | C     | 509    | CLA  | C1-C2-C3    | -5.10 | 117.22      | 126.04   |
| 25  | a     | 418[B] | PHO  | C3D-C4D-ND  | 5.10  | 114.67      | 107.72   |
| 24  | b     | 611    | CLA  | O2D-CGD-CBD | 5.10  | 120.33      | 111.27   |
| 25  | a     | 418[A] | PHO  | C1-C2-C3    | -5.10 | 117.22      | 126.04   |
| 24  | a     | 409    | CLA  | C4A-NA-C1A  | -5.09 | 104.42      | 106.71   |
| 35  | C     | 523    | HTG  | C1'-S1-C1   | 5.09  | 109.62      | 100.09   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | B     | 604    | CLA  | CHD-C1D-ND  | -5.09 | 119.78      | 124.45   |
| 24  | b     | 616    | CLA  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 24  | c     | 510    | CLA  | C3C-C4C-NC  | 5.09  | 116.28      | 110.57   |
| 24  | b     | 617    | CLA  | CHD-C1D-ND  | -5.08 | 119.78      | 124.45   |
| 24  | B     | 608    | CLA  | C3D-C2D-C1D | -5.07 | 98.91       | 105.83   |
| 24  | B     | 613    | CLA  | CMD-C2D-C1D | 5.07  | 133.65      | 124.71   |
| 24  | B     | 615    | CLA  | C2C-C1C-NC  | 5.07  | 114.72      | 109.97   |
| 24  | b     | 621    | CLA  | C3C-C4C-NC  | 5.06  | 116.25      | 110.57   |
| 24  | B     | 614    | CLA  | C3D-C2D-C1D | -5.06 | 98.92       | 105.83   |
| 24  | B     | 602    | CLA  | C4A-NA-C1A  | -5.06 | 104.43      | 106.71   |
| 24  | b     | 614    | CLA  | C2C-C1C-NC  | 5.06  | 114.71      | 109.97   |
| 24  | c     | 516    | CLA  | C3B-C2B-C1B | -5.05 | 101.06      | 107.16   |
| 24  | A     | 406    | CLA  | C3D-C2D-C1D | -5.05 | 98.94       | 105.83   |
| 24  | C     | 510    | CLA  | O2D-CGD-CBD | 5.04  | 120.22      | 111.27   |
| 24  | b     | 611    | CLA  | C3B-C2B-C1B | -5.04 | 101.08      | 107.16   |
| 24  | B     | 611    | CLA  | C4A-NA-C1A  | -5.04 | 104.44      | 106.71   |
| 24  | C     | 513    | CLA  | C2C-C1C-NC  | 5.04  | 114.69      | 109.97   |
| 24  | A     | 410    | CLA  | CHD-C1D-ND  | -5.04 | 119.83      | 124.45   |
| 24  | C     | 504    | CLA  | C3D-C2D-C1D | -5.03 | 98.96       | 105.83   |
| 24  | C     | 502    | CLA  | C2C-C1C-NC  | 5.03  | 114.68      | 109.97   |
| 25  | A     | 409[A] | PHO  | C1-C2-C3    | -5.03 | 117.34      | 126.04   |
| 24  | B     | 602    | CLA  | C2C-C1C-NC  | 5.03  | 114.68      | 109.97   |
| 24  | C     | 513    | CLA  | C4A-NA-C1A  | -5.02 | 104.45      | 106.71   |
| 24  | C     | 503    | CLA  | C2C-C1C-NC  | 5.02  | 114.68      | 109.97   |
| 24  | b     | 619    | CLA  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 24  | C     | 512    | CLA  | C2C-C1C-NC  | 5.02  | 114.68      | 109.97   |
| 25  | a     | 418[A] | PHO  | C3D-C4D-ND  | 5.02  | 114.56      | 107.72   |
| 24  | c     | 513    | CLA  | CMD-C2D-C1D | 5.01  | 133.55      | 124.71   |
| 24  | c     | 516    | CLA  | C2C-C1C-NC  | 5.01  | 114.67      | 109.97   |
| 35  | B     | 625    | HTG  | O5-C1-C2    | 5.01  | 116.61      | 110.31   |
| 24  | C     | 505    | CLA  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 24  | a     | 410    | CLA  | C2C-C1C-NC  | 5.00  | 114.66      | 109.97   |
| 24  | B     | 611    | CLA  | C3B-C2B-C1B | -5.00 | 101.13      | 107.16   |
| 24  | C     | 504    | CLA  | O2D-CGD-CBD | 4.98  | 120.12      | 111.27   |
| 24  | c     | 507    | CLA  | C3B-C2B-C1B | -4.98 | 101.15      | 107.16   |
| 24  | D     | 403    | CLA  | O2D-CGD-CBD | 4.97  | 120.11      | 111.27   |
| 24  | C     | 505    | CLA  | C3C-C4C-NC  | 4.97  | 116.15      | 110.57   |
| 24  | C     | 505    | CLA  | C3B-C2B-C1B | -4.97 | 101.16      | 107.16   |
| 25  | A     | 409[B] | PHO  | C1-C2-C3    | -4.97 | 117.45      | 126.04   |
| 24  | c     | 512    | CLA  | C3D-C2D-C1D | -4.97 | 99.05       | 105.83   |
| 24  | b     | 616    | CLA  | O2D-CGD-CBD | 4.97  | 120.09      | 111.27   |
| 24  | A     | 407    | CLA  | C3D-C4D-ND  | 4.96  | 118.26      | 110.24   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | A     | 405    | CLA  | C3B-C2B-C1B | -4.96 | 101.17      | 107.16   |
| 24  | D     | 403    | CLA  | C3B-C2B-C1B | -4.96 | 101.18      | 107.16   |
| 27  | B     | 621    | SQD  | O47-C7-C8   | 4.96  | 122.18      | 111.50   |
| 24  | b     | 622    | CLA  | C3D-C2D-C1D | -4.95 | 99.07       | 105.83   |
| 24  | B     | 607    | CLA  | C3D-C2D-C1D | -4.95 | 99.07       | 105.83   |
| 24  | B     | 605    | CLA  | C3D-C2D-C1D | -4.95 | 99.07       | 105.83   |
| 24  | B     | 607    | CLA  | C3B-C2B-C1B | -4.95 | 101.19      | 107.16   |
| 27  | B     | 621    | SQD  | O6-C1-C2    | 4.95  | 116.03      | 108.30   |
| 24  | b     | 611    | CLA  | C2C-C1C-NC  | 4.94  | 114.60      | 109.97   |
| 24  | b     | 613    | CLA  | C3D-C2D-C1D | -4.92 | 99.12       | 105.83   |
| 24  | c     | 508    | CLA  | C3D-C2D-C1D | -4.91 | 99.14       | 105.83   |
| 25  | A     | 409[B] | PHO  | C3D-C4D-ND  | 4.91  | 114.41      | 107.72   |
| 35  | C     | 523    | HTG  | C1-O5-C5    | 4.90  | 121.62      | 112.58   |
| 24  | c     | 509    | CLA  | C3D-C2D-C1D | -4.90 | 99.14       | 105.83   |
| 24  | A     | 410    | CLA  | C3B-C2B-C1B | -4.90 | 101.25      | 107.16   |
| 24  | B     | 616    | CLA  | C2C-C1C-NC  | 4.90  | 114.56      | 109.97   |
| 24  | B     | 609    | CLA  | C3B-C2B-C1B | -4.90 | 101.25      | 107.16   |
| 24  | a     | 409    | CLA  | C3B-C2B-C1B | -4.90 | 101.25      | 107.16   |
| 24  | a     | 410    | CLA  | C3D-C4D-ND  | 4.90  | 118.16      | 110.24   |
| 24  | d     | 403    | CLA  | C3D-C2D-C1D | -4.89 | 99.16       | 105.83   |
| 24  | c     | 507    | CLA  | CMD-C2D-C1D | 4.89  | 133.33      | 124.71   |
| 24  | d     | 403    | CLA  | C2C-C1C-NC  | 4.89  | 114.55      | 109.97   |
| 24  | D     | 402    | CLA  | C3C-C4C-NC  | 4.89  | 116.05      | 110.57   |
| 24  | d     | 401    | CLA  | C4A-NA-C1A  | -4.88 | 104.51      | 106.71   |
| 24  | c     | 517    | CLA  | C2C-C1C-NC  | 4.88  | 114.55      | 109.97   |
| 24  | c     | 512    | CLA  | C3B-C2B-C1B | -4.88 | 101.28      | 107.16   |
| 24  | b     | 610    | CLA  | C2C-C1C-NC  | 4.87  | 114.54      | 109.97   |
| 24  | b     | 623    | CLA  | C4A-NA-C1A  | -4.87 | 104.52      | 106.71   |
| 24  | c     | 514    | CLA  | O2D-CGD-CBD | 4.87  | 119.91      | 111.27   |
| 24  | B     | 605    | CLA  | C4A-NA-C1A  | -4.86 | 104.52      | 106.71   |
| 24  | c     | 518    | CLA  | C3B-C2B-C1B | -4.85 | 101.31      | 107.16   |
| 36  | C     | 516    | DGD  | O2G-C1B-C2B | 4.85  | 121.94      | 111.50   |
| 38  | F     | 102    | HEM  | CAD-CBD-CGD | 4.84  | 124.03      | 113.60   |
| 24  | A     | 406    | CLA  | C3B-C2B-C1B | -4.83 | 101.33      | 107.16   |
| 24  | B     | 609    | CLA  | O2D-CGD-CBD | 4.83  | 119.84      | 111.27   |
| 25  | a     | 411    | PHO  | C3D-C4D-ND  | 4.82  | 114.30      | 107.72   |
| 24  | c     | 514    | CLA  | CHD-C1D-ND  | -4.82 | 120.03      | 124.45   |
| 24  | A     | 405    | CLA  | CHD-C1D-ND  | -4.81 | 120.03      | 124.45   |
| 24  | B     | 615    | CLA  | C4A-NA-C1A  | -4.81 | 104.54      | 106.71   |
| 24  | B     | 608    | CLA  | O2D-CGD-CBD | 4.81  | 119.82      | 111.27   |
| 24  | C     | 513    | CLA  | C3B-C2B-C1B | -4.81 | 101.36      | 107.16   |
| 24  | c     | 506    | CLA  | C3B-C2B-C1B | -4.81 | 101.36      | 107.16   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 509    | CLA  | C3B-C2B-C1B | -4.81 | 101.36      | 107.16   |
| 27  | A     | 412    | SQD  | O47-C7-C8   | 4.80  | 121.86      | 111.50   |
| 24  | d     | 401    | CLA  | C3D-C2D-C1D | -4.80 | 99.28       | 105.83   |
| 24  | d     | 402    | CLA  | C3D-C4D-ND  | 4.80  | 118.00      | 110.24   |
| 24  | c     | 506    | CLA  | C3D-C2D-C1D | -4.79 | 99.30       | 105.83   |
| 24  | A     | 405    | CLA  | CAC-C3C-C4C | 4.78  | 131.02      | 124.81   |
| 24  | B     | 612    | CLA  | C3D-C2D-C1D | -4.78 | 99.31       | 105.83   |
| 25  | a     | 418[B] | PHO  | C1-C2-C3    | -4.78 | 117.78      | 126.04   |
| 24  | B     | 606    | CLA  | O2D-CGD-CBD | 4.78  | 119.76      | 111.27   |
| 24  | B     | 605    | CLA  | O2D-CGD-CBD | 4.78  | 119.76      | 111.27   |
| 24  | D     | 402    | CLA  | C3D-C2D-C1D | -4.78 | 99.31       | 105.83   |
| 24  | B     | 616    | CLA  | C3B-C2B-C1B | -4.77 | 101.40      | 107.16   |
| 24  | a     | 412    | CLA  | C3B-C2B-C1B | -4.77 | 101.41      | 107.16   |
| 25  | A     | 409[A] | PHO  | C3D-C4D-ND  | 4.77  | 114.22      | 107.72   |
| 24  | c     | 512    | CLA  | C3C-C4C-NC  | 4.76  | 115.91      | 110.57   |
| 24  | C     | 502    | CLA  | C3D-C2D-C1D | -4.75 | 99.34       | 105.83   |
| 24  | b     | 625    | CLA  | C2C-C1C-NC  | 4.75  | 114.42      | 109.97   |
| 24  | B     | 606    | CLA  | C3C-C4C-NC  | 4.75  | 115.90      | 110.57   |
| 24  | c     | 516    | CLA  | C3D-C4D-ND  | 4.75  | 117.92      | 110.24   |
| 26  | b     | 626    | BCR  | C33-C5-C6   | -4.74 | 119.20      | 124.53   |
| 24  | C     | 506    | CLA  | C4A-NA-C1A  | -4.74 | 104.58      | 106.71   |
| 24  | B     | 606    | CLA  | C2C-C1C-NC  | 4.73  | 114.41      | 109.97   |
| 24  | B     | 610    | CLA  | C3D-C2D-C1D | -4.73 | 99.37       | 105.83   |
| 24  | C     | 509    | CLA  | C4A-NA-C1A  | -4.73 | 104.58      | 106.71   |
| 24  | C     | 507    | CLA  | C3B-C2B-C1B | -4.73 | 101.46      | 107.16   |
| 24  | c     | 511    | CLA  | C3D-C2D-C1D | -4.72 | 99.38       | 105.83   |
| 24  | d     | 402    | CLA  | CHD-C4C-C3C | -4.72 | 117.90      | 124.84   |
| 24  | b     | 620    | CLA  | C4A-NA-C1A  | -4.72 | 104.58      | 106.71   |
| 24  | b     | 614    | CLA  | C3D-C4D-ND  | 4.72  | 117.87      | 110.24   |
| 24  | a     | 410    | CLA  | O2D-CGD-CBD | 4.72  | 119.65      | 111.27   |
| 24  | b     | 613    | CLA  | C3C-C4C-NC  | 4.72  | 115.86      | 110.57   |
| 24  | C     | 512    | CLA  | C3D-C2D-C1D | -4.71 | 99.40       | 105.83   |
| 24  | b     | 619    | CLA  | C3B-C2B-C1B | -4.71 | 101.47      | 107.16   |
| 29  | A     | 417    | LMT  | C1'-O5'-C5' | 4.71  | 122.94      | 113.69   |
| 24  | c     | 509    | CLA  | C4A-NA-C1A  | -4.70 | 104.59      | 106.71   |
| 24  | c     | 513    | CLA  | CHD-C1D-ND  | -4.70 | 120.13      | 124.45   |
| 24  | d     | 403    | CLA  | O2D-CGD-CBD | 4.70  | 119.63      | 111.27   |
| 24  | C     | 512    | CLA  | C3B-C2B-C1B | -4.70 | 101.48      | 107.16   |
| 24  | D     | 403    | CLA  | C3D-C2D-C1D | -4.70 | 99.42       | 105.83   |
| 24  | b     | 614    | CLA  | C3D-C2D-C1D | -4.69 | 99.43       | 105.83   |
| 24  | b     | 621    | CLA  | O2D-CGD-CBD | 4.69  | 119.60      | 111.27   |
| 24  | c     | 513    | CLA  | C3B-C2B-C1B | -4.69 | 101.50      | 107.16   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | b     | 615 | CLA  | C3D-C2D-C1D | -4.69 | 99.43       | 105.83   |
| 24  | C     | 508 | CLA  | C3B-C2B-C1B | -4.68 | 101.51      | 107.16   |
| 24  | B     | 617 | CLA  | C3D-C2D-C1D | -4.68 | 99.44       | 105.83   |
| 24  | c     | 508 | CLA  | C3C-C4C-NC  | 4.68  | 115.82      | 110.57   |
| 24  | b     | 615 | CLA  | C3C-C4C-NC  | 4.68  | 115.82      | 110.57   |
| 24  | B     | 614 | CLA  | C3C-C4C-NC  | 4.67  | 115.81      | 110.57   |
| 26  | t     | 101 | BCR  | C33-C5-C6   | -4.67 | 119.28      | 124.53   |
| 24  | C     | 508 | CLA  | C3D-C2D-C1D | -4.67 | 99.46       | 105.83   |
| 24  | b     | 613 | CLA  | CHD-C1D-ND  | -4.67 | 120.16      | 124.45   |
| 27  | L     | 102 | SQD  | O47-C7-C8   | 4.67  | 121.56      | 111.50   |
| 24  | b     | 625 | CLA  | C3B-C2B-C1B | -4.67 | 101.53      | 107.16   |
| 24  | b     | 617 | CLA  | C3B-C2B-C1B | -4.66 | 101.53      | 107.16   |
| 24  | c     | 506 | CLA  | C4A-NA-C1A  | -4.66 | 104.61      | 106.71   |
| 24  | B     | 615 | CLA  | C3D-C2D-C1D | -4.65 | 99.49       | 105.83   |
| 24  | B     | 612 | CLA  | O2D-CGD-CBD | 4.65  | 119.53      | 111.27   |
| 24  | b     | 614 | CLA  | O2D-CGD-CBD | 4.64  | 119.52      | 111.27   |
| 24  | C     | 507 | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 24  | b     | 625 | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 24  | C     | 508 | CLA  | C4A-NA-C1A  | -4.64 | 104.62      | 106.71   |
| 24  | B     | 602 | CLA  | C3B-C2B-C1B | -4.64 | 101.57      | 107.16   |
| 24  | c     | 515 | CLA  | O2D-CGD-CBD | 4.63  | 119.50      | 111.27   |
| 24  | B     | 605 | CLA  | C3C-C4C-NC  | 4.63  | 115.76      | 110.57   |
| 24  | B     | 617 | CLA  | CHD-C1D-ND  | -4.63 | 120.20      | 124.45   |
| 24  | C     | 506 | CLA  | C3D-C2D-C1D | -4.63 | 99.52       | 105.83   |
| 24  | b     | 622 | CLA  | C3B-C2B-C1B | -4.63 | 101.58      | 107.16   |
| 24  | A     | 410 | CLA  | C3D-C2D-C1D | -4.62 | 99.52       | 105.83   |
| 24  | B     | 606 | CLA  | C3D-C2D-C1D | -4.62 | 99.52       | 105.83   |
| 24  | B     | 602 | CLA  | C3D-C2D-C1D | -4.62 | 99.52       | 105.83   |
| 24  | C     | 511 | CLA  | C3B-C4B-NB  | 4.62  | 114.80      | 110.52   |
| 24  | C     | 505 | CLA  | CHD-C1D-ND  | -4.61 | 120.22      | 124.45   |
| 24  | b     | 615 | CLA  | C3B-C2B-C1B | -4.61 | 101.60      | 107.16   |
| 24  | A     | 406 | CLA  | C1C-C2C-C3C | -4.61 | 102.11      | 106.96   |
| 24  | B     | 613 | CLA  | C3D-C4D-ND  | 4.60  | 117.69      | 110.24   |
| 24  | C     | 507 | CLA  | C4A-NA-C1A  | -4.60 | 104.64      | 106.71   |
| 24  | C     | 503 | CLA  | C3D-C4D-ND  | 4.60  | 117.68      | 110.24   |
| 24  | b     | 611 | CLA  | C3D-C2D-C1D | -4.60 | 99.56       | 105.83   |
| 33  | c     | 524 | LMG  | O7-C10-C11  | 4.60  | 121.41      | 111.50   |
| 24  | A     | 406 | CLA  | C3B-C4B-NB  | 4.60  | 114.78      | 110.52   |
| 24  | b     | 612 | CLA  | C3C-C4C-NC  | 4.59  | 115.72      | 110.57   |
| 24  | B     | 615 | CLA  | C3B-C2B-C1B | -4.59 | 101.62      | 107.16   |
| 24  | c     | 509 | CLA  | C3C-C4C-NC  | 4.59  | 115.72      | 110.57   |
| 24  | c     | 514 | CLA  | C3B-C2B-C1B | -4.58 | 101.63      | 107.16   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 606 | CLA  | C3D-C4D-ND  | 4.58  | 117.65      | 110.24   |
| 33  | A     | 421 | LMG  | O7-C10-C11  | 4.58  | 121.38      | 111.50   |
| 24  | b     | 621 | CLA  | C4A-NA-C1A  | -4.58 | 104.65      | 106.71   |
| 24  | B     | 603 | CLA  | C3B-C2B-C1B | -4.58 | 101.63      | 107.16   |
| 24  | C     | 501 | CLA  | C3D-C2D-C1D | -4.58 | 99.58       | 105.83   |
| 24  | b     | 618 | CLA  | C3D-C2D-C1D | -4.58 | 99.58       | 105.83   |
| 24  | C     | 507 | CLA  | C2C-C1C-NC  | 4.58  | 114.26      | 109.97   |
| 24  | A     | 405 | CLA  | CHD-C4C-C3C | -4.58 | 118.11      | 124.84   |
| 24  | a     | 410 | CLA  | C3D-C2D-C1D | -4.58 | 99.59       | 105.83   |
| 24  | A     | 410 | CLA  | C3C-C4C-NC  | 4.57  | 115.70      | 110.57   |
| 24  | c     | 518 | CLA  | C3D-C4D-ND  | 4.57  | 117.64      | 110.24   |
| 24  | B     | 612 | CLA  | C4A-NA-C1A  | -4.57 | 104.65      | 106.71   |
| 24  | b     | 619 | CLA  | C3D-C2D-C1D | -4.57 | 99.60       | 105.83   |
| 24  | B     | 613 | CLA  | C2C-C1C-NC  | 4.57  | 114.25      | 109.97   |
| 24  | d     | 401 | CLA  | C3B-C2B-C1B | -4.57 | 101.65      | 107.16   |
| 24  | B     | 604 | CLA  | C3C-C4C-NC  | 4.57  | 115.69      | 110.57   |
| 24  | d     | 403 | CLA  | C3B-C2B-C1B | -4.57 | 101.65      | 107.16   |
| 24  | b     | 623 | CLA  | C3D-C2D-C1D | -4.57 | 99.60       | 105.83   |
| 24  | b     | 621 | CLA  | C3B-C2B-C1B | -4.56 | 101.66      | 107.16   |
| 26  | B     | 620 | BCR  | C15-C14-C13 | -4.56 | 120.80      | 127.31   |
| 24  | b     | 620 | CLA  | C3D-C2D-C1D | -4.56 | 99.61       | 105.83   |
| 24  | A     | 407 | CLA  | C3B-C2B-C1B | -4.56 | 101.66      | 107.16   |
| 24  | d     | 401 | CLA  | C3B-C4B-NB  | 4.55  | 114.74      | 110.52   |
| 24  | B     | 604 | CLA  | O2D-CGD-O1D | -4.55 | 114.95      | 123.84   |
| 24  | c     | 511 | CLA  | C4A-NA-C1A  | -4.55 | 104.66      | 106.71   |
| 24  | C     | 501 | CLA  | C3D-C4D-ND  | 4.54  | 117.58      | 110.24   |
| 40  | V     | 205 | HEC  | C4B-NB-C1B  | 4.54  | 109.76      | 105.07   |
| 24  | B     | 612 | CLA  | C3C-C4C-NC  | 4.54  | 115.66      | 110.57   |
| 24  | c     | 508 | CLA  | C3B-C2B-C1B | -4.54 | 101.69      | 107.16   |
| 24  | a     | 412 | CLA  | C4A-NA-C1A  | -4.53 | 104.67      | 106.71   |
| 24  | B     | 615 | CLA  | C3C-C4C-NC  | 4.53  | 115.65      | 110.57   |
| 24  | B     | 606 | CLA  | C3B-C2B-C1B | -4.52 | 101.70      | 107.16   |
| 24  | C     | 511 | CLA  | C3B-C2B-C1B | -4.52 | 101.70      | 107.16   |
| 24  | b     | 610 | CLA  | C3B-C2B-C1B | -4.51 | 101.72      | 107.16   |
| 24  | B     | 613 | CLA  | C3B-C2B-C1B | -4.50 | 101.73      | 107.16   |
| 24  | a     | 412 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 24  | c     | 508 | CLA  | C3D-C4D-ND  | 4.50  | 117.51      | 110.24   |
| 24  | C     | 506 | CLA  | O2D-CGD-CBD | 4.50  | 119.26      | 111.27   |
| 36  | e     | 101 | DGD  | O2G-C1B-C2B | 4.50  | 121.19      | 111.50   |
| 24  | A     | 407 | CLA  | C2C-C1C-NC  | 4.49  | 114.18      | 109.97   |
| 24  | c     | 514 | CLA  | C3D-C2D-C1D | -4.49 | 99.71       | 105.83   |
| 24  | C     | 503 | CLA  | C3C-C4C-NC  | 4.49  | 115.60      | 110.57   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 602 | CLA  | C3D-C4D-ND  | 4.48  | 117.49      | 110.24   |
| 24  | c     | 513 | CLA  | C3C-C4C-NC  | 4.48  | 115.60      | 110.57   |
| 24  | C     | 502 | CLA  | C1-C2-C3    | -4.48 | 118.29      | 126.04   |
| 24  | b     | 616 | CLA  | C3C-C4C-NC  | 4.48  | 115.60      | 110.57   |
| 33  | C     | 520 | LMG  | O7-C10-C11  | 4.48  | 121.16      | 111.50   |
| 24  | C     | 504 | CLA  | C4A-NA-C1A  | -4.48 | 104.69      | 106.71   |
| 24  | C     | 509 | CLA  | O2D-CGD-CBD | 4.48  | 119.22      | 111.27   |
| 24  | B     | 616 | CLA  | C3D-C2D-C1D | -4.47 | 99.72       | 105.83   |
| 24  | C     | 513 | CLA  | C3D-C2D-C1D | -4.47 | 99.72       | 105.83   |
| 24  | B     | 604 | CLA  | C3B-C2B-C1B | -4.47 | 101.76      | 107.16   |
| 24  | A     | 406 | CLA  | CBC-CAC-C3C | -4.47 | 100.11      | 112.43   |
| 24  | C     | 512 | CLA  | C3C-C4C-NC  | 4.47  | 115.58      | 110.57   |
| 24  | B     | 616 | CLA  | C3D-C4D-ND  | 4.47  | 117.46      | 110.24   |
| 24  | b     | 617 | CLA  | C3D-C2D-C1D | -4.46 | 99.74       | 105.83   |
| 24  | b     | 618 | CLA  | C3D-C4D-ND  | 4.46  | 117.46      | 110.24   |
| 24  | b     | 616 | CLA  | C1C-C2C-C3C | -4.46 | 102.27      | 106.96   |
| 24  | b     | 622 | CLA  | C3C-C4C-NC  | 4.46  | 115.57      | 110.57   |
| 24  | b     | 618 | CLA  | O2D-CGD-CBD | 4.46  | 119.19      | 111.27   |
| 24  | b     | 619 | CLA  | C3D-C4D-ND  | 4.46  | 117.44      | 110.24   |
| 24  | d     | 402 | CLA  | O2D-CGD-CBD | 4.45  | 119.18      | 111.27   |
| 24  | B     | 617 | CLA  | C3B-C2B-C1B | -4.45 | 101.79      | 107.16   |
| 35  | B     | 632 | HTG  | C1'-S1-C1   | 4.45  | 108.41      | 100.09   |
| 24  | B     | 611 | CLA  | C3D-C2D-C1D | -4.45 | 99.76       | 105.83   |
| 24  | b     | 623 | CLA  | C3B-C2B-C1B | -4.45 | 101.80      | 107.16   |
| 24  | c     | 514 | CLA  | C4A-NA-C1A  | -4.44 | 104.71      | 106.71   |
| 24  | b     | 621 | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 24  | b     | 618 | CLA  | CMB-C2B-C1B | 4.44  | 132.13      | 125.37   |
| 24  | B     | 609 | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 24  | c     | 513 | CLA  | C3D-C2D-C1D | -4.43 | 99.78       | 105.83   |
| 24  | C     | 510 | CLA  | C3D-C2D-C1D | -4.43 | 99.78       | 105.83   |
| 24  | a     | 412 | CLA  | C1C-C2C-C3C | -4.43 | 102.30      | 106.96   |
| 40  | v     | 205 | HEC  | C4C-NC-C1C  | 4.43  | 109.68      | 105.35   |
| 24  | B     | 616 | CLA  | C3C-C4C-NC  | 4.43  | 115.53      | 110.57   |
| 24  | B     | 610 | CLA  | CMB-C2B-C1B | 4.42  | 132.10      | 125.37   |
| 25  | a     | 411 | PHO  | O1D-CGD-CBD | -4.42 | 117.38      | 124.74   |
| 24  | c     | 515 | CLA  | C3B-C2B-C1B | -4.42 | 101.83      | 107.16   |
| 24  | b     | 614 | CLA  | C3C-C4C-NC  | 4.42  | 115.52      | 110.57   |
| 24  | a     | 412 | CLA  | C3D-C4D-ND  | 4.41  | 117.38      | 110.24   |
| 24  | b     | 610 | CLA  | C3D-C2D-C1D | -4.41 | 99.81       | 105.83   |
| 24  | b     | 620 | CLA  | C3B-C2B-C1B | -4.41 | 101.84      | 107.16   |
| 24  | c     | 518 | CLA  | C3D-C2D-C1D | -4.41 | 99.81       | 105.83   |
| 24  | d     | 403 | CLA  | C3D-C4D-ND  | 4.41  | 117.37      | 110.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | C     | 509 | CLA  | C3D-C2D-C1D | -4.41 | 99.82       | 105.83   |
| 24  | c     | 517 | CLA  | C3D-C2D-C1D | -4.40 | 99.82       | 105.83   |
| 24  | C     | 511 | CLA  | C3D-C2D-C1D | -4.40 | 99.82       | 105.83   |
| 35  | b     | 632 | HTG  | O5-C1-C2    | 4.40  | 115.85      | 110.31   |
| 24  | C     | 513 | CLA  | C3D-C4D-ND  | 4.40  | 117.35      | 110.24   |
| 24  | C     | 502 | CLA  | C4A-NA-C1A  | -4.39 | 104.73      | 106.71   |
| 24  | A     | 410 | CLA  | O2D-CGD-CBD | 4.39  | 119.07      | 111.27   |
| 40  | v     | 205 | HEC  | C4B-NB-C1B  | 4.39  | 109.61      | 105.07   |
| 24  | c     | 508 | CLA  | C2C-C1C-NC  | 4.39  | 114.08      | 109.97   |
| 24  | B     | 611 | CLA  | C3D-C4D-ND  | 4.38  | 117.33      | 110.24   |
| 24  | B     | 616 | CLA  | CMB-C2B-C1B | 4.38  | 132.04      | 125.37   |
| 24  | c     | 510 | CLA  | CHD-C1D-ND  | -4.38 | 120.43      | 124.45   |
| 24  | b     | 618 | CLA  | C3C-C4C-NC  | 4.38  | 115.48      | 110.57   |
| 38  | e     | 103 | HEM  | CHC-C4B-NB  | 4.37  | 129.17      | 124.42   |
| 24  | C     | 503 | CLA  | C3D-C2D-C1D | -4.37 | 99.87       | 105.83   |
| 24  | B     | 617 | CLA  | C1D-CHD-C4C | -4.37 | 116.64      | 126.06   |
| 24  | D     | 402 | CLA  | C3D-C4D-ND  | 4.37  | 117.30      | 110.24   |
| 24  | B     | 603 | CLA  | C3D-C4D-ND  | 4.36  | 117.30      | 110.24   |
| 24  | c     | 509 | CLA  | C3B-C2B-C1B | -4.36 | 101.90      | 107.16   |
| 24  | c     | 511 | CLA  | O2D-CGD-CBD | 4.35  | 119.00      | 111.27   |
| 24  | C     | 510 | CLA  | C4A-NA-C1A  | -4.35 | 104.75      | 106.71   |
| 24  | c     | 515 | CLA  | C4A-NA-C1A  | -4.35 | 104.75      | 106.71   |
| 24  | B     | 610 | CLA  | C3D-C4D-ND  | 4.35  | 117.28      | 110.24   |
| 24  | c     | 507 | CLA  | C3C-C4C-NC  | 4.35  | 115.45      | 110.57   |
| 24  | c     | 517 | CLA  | C3D-C4D-ND  | 4.35  | 117.27      | 110.24   |
| 24  | a     | 409 | CLA  | C3D-C2D-C1D | -4.35 | 99.90       | 105.83   |
| 24  | c     | 510 | CLA  | C3B-C2B-C1B | -4.35 | 101.92      | 107.16   |
| 24  | B     | 607 | CLA  | C3C-C4C-NC  | 4.34  | 115.43      | 110.57   |
| 24  | C     | 502 | CLA  | O2D-CGD-CBD | 4.33  | 118.97      | 111.27   |
| 24  | c     | 516 | CLA  | C3D-C2D-C1D | -4.33 | 99.92       | 105.83   |
| 24  | C     | 503 | CLA  | C3B-C2B-C1B | -4.33 | 101.94      | 107.16   |
| 26  | B     | 618 | BCR  | C33-C5-C6   | -4.33 | 119.67      | 124.53   |
| 24  | b     | 625 | CLA  | C3D-C4D-ND  | 4.33  | 117.24      | 110.24   |
| 24  | A     | 407 | CLA  | C3D-C2D-C1D | -4.33 | 99.93       | 105.83   |
| 24  | b     | 624 | CLA  | C3D-C2D-C1D | -4.32 | 99.93       | 105.83   |
| 24  | c     | 513 | CLA  | C3D-C4D-ND  | 4.32  | 117.23      | 110.24   |
| 24  | B     | 611 | CLA  | O2D-CGD-CBD | 4.32  | 118.94      | 111.27   |
| 24  | b     | 623 | CLA  | C3D-C4D-ND  | 4.32  | 117.22      | 110.24   |
| 24  | C     | 502 | CLA  | C3B-C2B-C1B | -4.32 | 101.95      | 107.16   |
| 35  | b     | 607 | HTG  | C1'-S1-C1   | 4.31  | 108.15      | 100.09   |
| 24  | B     | 608 | CLA  | C3B-C2B-C1B | -4.31 | 101.96      | 107.16   |
| 24  | b     | 611 | CLA  | C3D-C4D-ND  | 4.31  | 117.20      | 110.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | c     | 501 | LMG  | O7-C10-C11  | 4.31  | 120.78      | 111.50   |
| 24  | a     | 410 | CLA  | C3B-C2B-C1B | -4.31 | 101.96      | 107.16   |
| 24  | a     | 410 | CLA  | C3C-C4C-NC  | 4.30  | 115.40      | 110.57   |
| 24  | B     | 612 | CLA  | CMC-C2C-C1C | 4.30  | 131.58      | 125.04   |
| 24  | d     | 401 | CLA  | C1D-CHD-C4C | -4.30 | 116.79      | 126.06   |
| 24  | d     | 401 | CLA  | C1C-C2C-C3C | -4.29 | 102.44      | 106.96   |
| 24  | b     | 610 | CLA  | C3D-C4D-ND  | 4.29  | 117.18      | 110.24   |
| 24  | b     | 620 | CLA  | C3D-C4D-ND  | 4.29  | 117.18      | 110.24   |
| 24  | B     | 612 | CLA  | C3B-C2B-C1B | -4.29 | 101.98      | 107.16   |
| 24  | C     | 513 | CLA  | O2D-CGD-CBD | 4.29  | 118.89      | 111.27   |
| 24  | B     | 603 | CLA  | C3D-C2D-C1D | -4.29 | 99.98       | 105.83   |
| 24  | c     | 514 | CLA  | C3B-C4B-NB  | 4.29  | 114.49      | 110.52   |
| 38  | e     | 103 | HEM  | C1B-NB-C4B  | 4.29  | 109.50      | 105.07   |
| 24  | b     | 624 | CLA  | C3D-C4D-ND  | 4.28  | 117.17      | 110.24   |
| 24  | b     | 620 | CLA  | O2D-CGD-CBD | 4.28  | 118.88      | 111.27   |
| 24  | b     | 624 | CLA  | C3C-C4C-NC  | 4.28  | 115.37      | 110.57   |
| 24  | c     | 514 | CLA  | C1D-CHD-C4C | -4.28 | 116.83      | 126.06   |
| 24  | b     | 616 | CLA  | C3B-C2B-C1B | -4.27 | 102.00      | 107.16   |
| 24  | c     | 508 | CLA  | O2D-CGD-CBD | 4.27  | 118.86      | 111.27   |
| 24  | C     | 511 | CLA  | C3D-C4D-ND  | 4.27  | 117.14      | 110.24   |
| 24  | D     | 402 | CLA  | C3B-C2B-C1B | -4.27 | 102.01      | 107.16   |
| 24  | B     | 604 | CLA  | C3D-C4D-ND  | 4.26  | 117.14      | 110.24   |
| 24  | C     | 504 | CLA  | C3B-C2B-C1B | -4.26 | 102.02      | 107.16   |
| 24  | b     | 612 | CLA  | C3B-C2B-C1B | -4.26 | 102.02      | 107.16   |
| 24  | C     | 502 | CLA  | C3D-C4D-ND  | 4.26  | 117.13      | 110.24   |
| 24  | b     | 625 | CLA  | C1D-CHD-C4C | -4.26 | 116.87      | 126.06   |
| 24  | B     | 615 | CLA  | O2D-CGD-O1D | -4.25 | 115.52      | 123.84   |
| 36  | c     | 522 | DGD  | O2G-C1B-C2B | 4.25  | 120.67      | 111.50   |
| 24  | b     | 621 | CLA  | CHD-C1D-ND  | -4.25 | 120.55      | 124.45   |
| 36  | e     | 101 | DGD  | O6E-C5E-C4E | 4.25  | 117.41      | 109.69   |
| 24  | b     | 613 | CLA  | C1C-C2C-C3C | -4.25 | 102.49      | 106.96   |
| 26  | d     | 404 | BCR  | C24-C23-C22 | -4.24 | 119.82      | 126.23   |
| 27  | A     | 412 | SQD  | O6-C1-C2    | 4.24  | 114.92      | 108.30   |
| 27  | a     | 414 | SQD  | O47-C7-C8   | 4.24  | 120.64      | 111.50   |
| 24  | B     | 612 | CLA  | C3D-C4D-ND  | 4.24  | 117.09      | 110.24   |
| 24  | c     | 509 | CLA  | C3D-C4D-ND  | 4.24  | 117.09      | 110.24   |
| 24  | d     | 401 | CLA  | C3D-C4D-ND  | 4.23  | 117.09      | 110.24   |
| 24  | B     | 609 | CLA  | C3D-C4D-ND  | 4.23  | 117.09      | 110.24   |
| 24  | A     | 410 | CLA  | C3D-C4D-ND  | 4.23  | 117.08      | 110.24   |
| 24  | c     | 516 | CLA  | C4A-NA-C1A  | -4.23 | 104.80      | 106.71   |
| 24  | b     | 612 | CLA  | C3D-C4D-ND  | 4.23  | 117.08      | 110.24   |
| 24  | B     | 606 | CLA  | C1D-CHD-C4C | -4.23 | 116.94      | 126.06   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | B     | 609    | CLA  | C1C-C2C-C3C | -4.23 | 102.51      | 106.96   |
| 24  | B     | 614    | CLA  | C3B-C2B-C1B | -4.22 | 102.06      | 107.16   |
| 24  | b     | 617    | CLA  | C3C-C4C-NC  | 4.22  | 115.30      | 110.57   |
| 24  | B     | 608    | CLA  | C3C-C4C-NC  | 4.22  | 115.30      | 110.57   |
| 24  | C     | 507    | CLA  | C3C-C4C-NC  | 4.22  | 115.30      | 110.57   |
| 38  | e     | 103    | HEM  | CHD-C1D-ND  | 4.21  | 128.99      | 124.42   |
| 25  | a     | 418[A] | PHO  | O2D-CGD-O1D | -4.21 | 115.62      | 123.84   |
| 24  | c     | 515    | CLA  | C3B-C4B-NB  | 4.20  | 114.42      | 110.52   |
| 24  | c     | 508    | CLA  | C1D-CHD-C4C | -4.20 | 116.99      | 126.06   |
| 24  | b     | 612    | CLA  | C3D-C2D-C1D | -4.20 | 100.10      | 105.83   |
| 24  | A     | 406    | CLA  | C3D-C4D-ND  | 4.20  | 117.04      | 110.24   |
| 24  | c     | 511    | CLA  | C1C-C2C-C3C | -4.20 | 102.54      | 106.96   |
| 24  | b     | 613    | CLA  | C3B-C4B-NB  | 4.20  | 114.41      | 110.52   |
| 24  | a     | 409    | CLA  | C1C-C2C-C3C | -4.20 | 102.54      | 106.96   |
| 24  | c     | 507    | CLA  | C3D-C4D-ND  | 4.19  | 117.02      | 110.24   |
| 24  | C     | 511    | CLA  | O2D-CGD-CBD | 4.19  | 118.72      | 111.27   |
| 24  | B     | 617    | CLA  | C3C-C4C-NC  | 4.19  | 115.27      | 110.57   |
| 24  | c     | 507    | CLA  | C3D-C2D-C1D | -4.19 | 100.11      | 105.83   |
| 24  | c     | 507    | CLA  | O2D-CGD-CBD | 4.19  | 118.71      | 111.27   |
| 38  | F     | 102    | HEM  | C1B-NB-C4B  | 4.19  | 109.40      | 105.07   |
| 24  | C     | 512    | CLA  | C3D-C4D-ND  | 4.19  | 117.01      | 110.24   |
| 24  | b     | 612    | CLA  | CAA-C2A-C3A | -4.18 | 101.33      | 112.78   |
| 38  | e     | 103    | HEM  | CHD-C4C-NC  | 4.18  | 128.96      | 124.44   |
| 24  | C     | 508    | CLA  | C3D-C4D-ND  | 4.17  | 116.99      | 110.24   |
| 24  | b     | 625    | CLA  | C3B-C4B-NB  | 4.17  | 114.39      | 110.52   |
| 24  | c     | 512    | CLA  | C1C-C2C-C3C | -4.17 | 102.57      | 106.96   |
| 27  | a     | 414    | SQD  | O9-S-C6     | 4.17  | 111.90      | 106.94   |
| 24  | b     | 615    | CLA  | C3D-C4D-ND  | 4.17  | 116.98      | 110.24   |
| 24  | B     | 606    | CLA  | CMB-C2B-C1B | 4.17  | 131.72      | 125.37   |
| 24  | B     | 606    | CLA  | CMC-C2C-C1C | 4.17  | 131.38      | 125.04   |
| 24  | c     | 510    | CLA  | C3D-C4D-ND  | 4.17  | 116.98      | 110.24   |
| 24  | C     | 501    | CLA  | C4A-NA-C1A  | -4.16 | 104.84      | 106.71   |
| 26  | C     | 514    | BCR  | C7-C8-C9    | -4.16 | 119.95      | 126.23   |
| 24  | C     | 510    | CLA  | C3C-C4C-NC  | 4.15  | 115.23      | 110.57   |
| 24  | b     | 625    | CLA  | CAC-C3C-C4C | 4.15  | 130.19      | 124.81   |
| 24  | C     | 510    | CLA  | C3D-C4D-ND  | 4.15  | 116.95      | 110.24   |
| 24  | D     | 402    | CLA  | O2D-CGD-CBD | 4.15  | 118.64      | 111.27   |
| 26  | y     | 101    | BCR  | C33-C5-C6   | -4.15 | 119.87      | 124.53   |
| 24  | C     | 502    | CLA  | C3C-C4C-NC  | 4.14  | 115.22      | 110.57   |
| 26  | c     | 519    | BCR  | C7-C8-C9    | -4.14 | 119.97      | 126.23   |
| 24  | C     | 509    | CLA  | C3C-C4C-NC  | 4.14  | 115.22      | 110.57   |
| 24  | b     | 612    | CLA  | C1D-CHD-C4C | -4.14 | 117.13      | 126.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | b     | 622 | CLA  | C4A-NA-C1A  | -4.14 | 104.84      | 106.71   |
| 24  | B     | 612 | CLA  | C1D-CHD-C4C | -4.14 | 117.13      | 126.06   |
| 24  | c     | 511 | CLA  | C3B-C4B-NB  | 4.14  | 114.35      | 110.52   |
| 24  | b     | 625 | CLA  | C3C-C4C-NC  | 4.13  | 115.21      | 110.57   |
| 24  | c     | 514 | CLA  | C3C-C4C-NC  | 4.13  | 115.20      | 110.57   |
| 24  | c     | 515 | CLA  | C3D-C4D-ND  | 4.13  | 116.92      | 110.24   |
| 26  | d     | 404 | BCR  | C38-C26-C25 | -4.13 | 119.89      | 124.53   |
| 24  | b     | 624 | CLA  | C3B-C2B-C1B | -4.13 | 102.18      | 107.16   |
| 24  | c     | 511 | CLA  | C3D-C4D-ND  | 4.13  | 116.91      | 110.24   |
| 24  | B     | 607 | CLA  | C1C-C2C-C3C | -4.12 | 102.62      | 106.96   |
| 24  | b     | 619 | CLA  | C3C-C4C-NC  | 4.12  | 115.19      | 110.57   |
| 24  | d     | 401 | CLA  | O2D-CGD-CBD | 4.12  | 118.59      | 111.27   |
| 24  | b     | 621 | CLA  | CMD-C2D-C1D | 4.12  | 131.97      | 124.71   |
| 24  | c     | 511 | CLA  | C3B-C2B-C1B | -4.12 | 102.19      | 107.16   |
| 36  | D     | 406 | DGD  | O2G-C1B-C2B | 4.12  | 120.37      | 111.50   |
| 24  | c     | 515 | CLA  | C1-C2-C3    | -4.11 | 118.93      | 126.04   |
| 24  | c     | 509 | CLA  | C1C-C2C-C3C | -4.11 | 102.64      | 106.96   |
| 24  | d     | 402 | CLA  | C3D-C2D-C1D | -4.11 | 100.23      | 105.83   |
| 24  | a     | 409 | CLA  | C3D-C4D-ND  | 4.10  | 116.87      | 110.24   |
| 24  | c     | 512 | CLA  | C4A-NA-C1A  | -4.09 | 104.86      | 106.71   |
| 24  | B     | 604 | CLA  | C3D-C2D-C1D | -4.09 | 100.24      | 105.83   |
| 24  | B     | 610 | CLA  | C3C-C4C-NC  | 4.09  | 115.16      | 110.57   |
| 38  | e     | 103 | HEM  | C4C-NC-C1C  | 4.09  | 109.36      | 105.35   |
| 24  | b     | 613 | CLA  | C3B-C2B-C1B | -4.09 | 102.22      | 107.16   |
| 24  | A     | 405 | CLA  | C1D-CHD-C4C | -4.09 | 117.23      | 126.06   |
| 24  | b     | 622 | CLA  | C3B-C4B-NB  | 4.09  | 114.31      | 110.52   |
| 24  | B     | 609 | CLA  | C4A-NA-C1A  | -4.08 | 104.87      | 106.71   |
| 24  | b     | 610 | CLA  | C1D-CHD-C4C | -4.08 | 117.25      | 126.06   |
| 24  | b     | 622 | CLA  | CHD-C1D-ND  | -4.08 | 120.71      | 124.45   |
| 24  | D     | 403 | CLA  | C3D-C4D-ND  | 4.07  | 116.83      | 110.24   |
| 24  | C     | 503 | CLA  | C1D-CHD-C4C | -4.07 | 117.27      | 126.06   |
| 24  | B     | 615 | CLA  | C3D-C4D-ND  | 4.07  | 116.82      | 110.24   |
| 24  | b     | 623 | CLA  | C3C-C4C-NC  | 4.07  | 115.14      | 110.57   |
| 24  | b     | 616 | CLA  | C3D-C4D-ND  | 4.06  | 116.81      | 110.24   |
| 24  | b     | 615 | CLA  | C3B-C4B-NB  | 4.06  | 114.28      | 110.52   |
| 24  | c     | 509 | CLA  | C1D-CHD-C4C | -4.06 | 117.30      | 126.06   |
| 24  | c     | 506 | CLA  | C3C-C4C-NC  | 4.06  | 115.12      | 110.57   |
| 24  | C     | 511 | CLA  | C1D-CHD-C4C | -4.06 | 117.31      | 126.06   |
| 24  | B     | 604 | CLA  | C1D-CHD-C4C | -4.06 | 117.31      | 126.06   |
| 24  | B     | 611 | CLA  | CAA-C2A-C3A | -4.06 | 101.67      | 112.78   |
| 24  | D     | 403 | CLA  | C3C-C4C-NC  | 4.06  | 115.12      | 110.57   |
| 24  | B     | 603 | CLA  | C3C-C4C-NC  | 4.05  | 115.11      | 110.57   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | c     | 512 | CLA  | O2D-CGD-O1D | -4.05 | 115.92      | 123.84   |
| 26  | b     | 626 | BCR  | C7-C8-C9    | -4.05 | 120.12      | 126.23   |
| 24  | c     | 515 | CLA  | C3D-C2D-C1D | -4.04 | 100.31      | 105.83   |
| 24  | c     | 510 | CLA  | C1D-CHD-C4C | -4.04 | 117.33      | 126.06   |
| 24  | c     | 518 | CLA  | C1D-CHD-C4C | -4.04 | 117.33      | 126.06   |
| 24  | C     | 509 | CLA  | C3D-C4D-ND  | 4.04  | 116.78      | 110.24   |
| 33  | Z     | 101 | LMG  | O7-C10-C11  | 4.04  | 120.21      | 111.50   |
| 24  | b     | 621 | CLA  | C1D-CHD-C4C | -4.04 | 117.34      | 126.06   |
| 24  | c     | 518 | CLA  | O2D-CGD-CBD | 4.04  | 118.45      | 111.27   |
| 24  | C     | 505 | CLA  | CMB-C2B-C1B | 4.04  | 131.52      | 125.37   |
| 24  | C     | 504 | CLA  | C1C-C2C-C3C | -4.04 | 102.71      | 106.96   |
| 24  | D     | 402 | CLA  | C1C-C2C-C3C | -4.04 | 102.71      | 106.96   |
| 26  | k     | 101 | BCR  | C24-C23-C22 | -4.04 | 120.14      | 126.23   |
| 24  | c     | 514 | CLA  | C3D-C4D-ND  | 4.04  | 116.77      | 110.24   |
| 24  | c     | 506 | CLA  | O2D-CGD-O1D | -4.03 | 115.96      | 123.84   |
| 24  | B     | 614 | CLA  | C4A-NA-C1A  | -4.03 | 104.89      | 106.71   |
| 24  | c     | 515 | CLA  | C3C-C4C-NC  | 4.03  | 115.08      | 110.57   |
| 24  | b     | 615 | CLA  | C1D-CHD-C4C | -4.02 | 117.38      | 126.06   |
| 24  | C     | 511 | CLA  | C3C-C4C-NC  | 4.02  | 115.08      | 110.57   |
| 24  | B     | 608 | CLA  | C3D-C4D-ND  | 4.02  | 116.74      | 110.24   |
| 26  | H     | 101 | BCR  | C38-C26-C25 | -4.02 | 120.01      | 124.53   |
| 29  | C     | 521 | LMT  | O1B-C4'-C3' | 4.02  | 117.97      | 107.28   |
| 24  | C     | 504 | CLA  | C3C-C4C-NC  | 4.02  | 115.08      | 110.57   |
| 24  | b     | 617 | CLA  | C3D-C4D-ND  | 4.02  | 116.74      | 110.24   |
| 24  | b     | 610 | CLA  | C3C-C4C-NC  | 4.01  | 115.07      | 110.57   |
| 29  | A     | 417 | LMT  | O5'-C5'-C4' | 4.01  | 118.22      | 109.75   |
| 24  | c     | 512 | CLA  | C1D-CHD-C4C | -4.01 | 117.40      | 126.06   |
| 24  | A     | 405 | CLA  | C3D-C4D-ND  | 4.01  | 116.73      | 110.24   |
| 24  | B     | 602 | CLA  | C1D-CHD-C4C | -4.01 | 117.41      | 126.06   |
| 24  | C     | 504 | CLA  | C3D-C4D-ND  | 4.01  | 116.72      | 110.24   |
| 26  | D     | 404 | BCR  | C33-C5-C6   | -4.00 | 120.03      | 124.53   |
| 24  | c     | 513 | CLA  | C3B-C4B-NB  | 4.00  | 114.23      | 110.52   |
| 24  | b     | 614 | CLA  | C3B-C2B-C1B | -4.00 | 102.33      | 107.16   |
| 24  | b     | 621 | CLA  | C3D-C4D-ND  | 4.00  | 116.71      | 110.24   |
| 24  | B     | 607 | CLA  | C1D-CHD-C4C | -4.00 | 117.43      | 126.06   |
| 24  | b     | 624 | CLA  | C1D-CHD-C4C | -4.00 | 117.44      | 126.06   |
| 24  | A     | 405 | CLA  | C3B-C4B-NB  | 3.99  | 114.22      | 110.52   |
| 24  | B     | 615 | CLA  | CAC-C3C-C4C | 3.99  | 129.98      | 124.81   |
| 24  | C     | 505 | CLA  | C1D-CHD-C4C | -3.98 | 117.47      | 126.06   |
| 24  | c     | 507 | CLA  | C1D-CHD-C4C | -3.98 | 117.47      | 126.06   |
| 24  | C     | 507 | CLA  | C3D-C4D-ND  | 3.98  | 116.67      | 110.24   |
| 24  | B     | 611 | CLA  | C3C-C4C-NC  | 3.98  | 115.03      | 110.57   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 510    | CLA  | C3B-C2B-C1B | -3.98 | 102.36      | 107.16   |
| 24  | A     | 405    | CLA  | C3C-C4C-NC  | 3.98  | 115.03      | 110.57   |
| 24  | d     | 402    | CLA  | C1C-C2C-C3C | -3.97 | 102.78      | 106.96   |
| 27  | a     | 405    | SQD  | O47-C7-C8   | 3.97  | 120.06      | 111.50   |
| 24  | B     | 609    | CLA  | C3C-C4C-NC  | 3.97  | 115.03      | 110.57   |
| 24  | b     | 610    | CLA  | O2D-CGD-O1D | -3.97 | 116.07      | 123.84   |
| 24  | b     | 614    | CLA  | C1C-C2C-C3C | -3.97 | 102.78      | 106.96   |
| 24  | b     | 615    | CLA  | C1C-C2C-C3C | -3.97 | 102.78      | 106.96   |
| 27  | a     | 414    | SQD  | O8-S-C6     | 3.97  | 112.06      | 105.74   |
| 24  | C     | 508    | CLA  | C3C-C4C-NC  | 3.97  | 115.02      | 110.57   |
| 26  | y     | 101    | BCR  | C15-C14-C13 | -3.96 | 121.65      | 127.31   |
| 24  | a     | 412    | CLA  | C3C-C4C-NC  | 3.96  | 115.01      | 110.57   |
| 24  | d     | 401    | CLA  | C3C-C4C-NC  | 3.96  | 115.01      | 110.57   |
| 24  | b     | 614    | CLA  | C1D-CHD-C4C | -3.95 | 117.53      | 126.06   |
| 24  | C     | 505    | CLA  | C3D-C4D-ND  | 3.95  | 116.63      | 110.24   |
| 27  | L     | 102    | SQD  | C3-C4-C5    | 3.95  | 117.29      | 110.24   |
| 24  | c     | 514    | CLA  | C1-C2-C3    | -3.95 | 119.21      | 126.04   |
| 24  | B     | 604    | CLA  | CAA-C2A-C3A | -3.95 | 101.96      | 112.78   |
| 38  | F     | 102    | HEM  | CHD-C4C-NC  | 3.95  | 128.71      | 124.44   |
| 24  | d     | 401    | CLA  | CBC-CAC-C3C | -3.95 | 101.55      | 112.43   |
| 37  | D     | 409    | LHG  | O7-C7-C8    | 3.94  | 120.00      | 111.50   |
| 24  | b     | 611    | CLA  | C3C-C4C-NC  | 3.94  | 114.99      | 110.57   |
| 24  | b     | 623    | CLA  | O2D-CGD-O1D | -3.94 | 116.13      | 123.84   |
| 24  | b     | 623    | CLA  | C1C-C2C-C3C | -3.94 | 102.82      | 106.96   |
| 31  | a     | 415[A] | PL9  | C22-C23-C24 | -3.94 | 118.19      | 127.66   |
| 29  | D     | 401    | LMT  | O1B-C4'-C3' | 3.93  | 117.74      | 107.28   |
| 27  | B     | 621    | SQD  | O7-S-C6     | 3.93  | 111.61      | 106.94   |
| 24  | C     | 510    | CLA  | C1-C2-C3    | -3.93 | 119.25      | 126.04   |
| 24  | B     | 612    | CLA  | C1C-C2C-C3C | -3.92 | 102.83      | 106.96   |
| 24  | c     | 515    | CLA  | C1C-C2C-C3C | -3.92 | 102.83      | 106.96   |
| 24  | D     | 402    | CLA  | C3B-C4B-NB  | 3.92  | 114.16      | 110.52   |
| 26  | H     | 101    | BCR  | C16-C17-C18 | -3.92 | 121.71      | 127.31   |
| 24  | b     | 623    | CLA  | C1-C2-C3    | -3.92 | 119.27      | 126.04   |
| 33  | b     | 629    | LMG  | O7-C10-C11  | 3.92  | 119.95      | 111.50   |
| 31  | a     | 415[A] | PL9  | C15-C14-C16 | 3.92  | 121.86      | 115.27   |
| 24  | C     | 501    | CLA  | C1C-C2C-C3C | -3.92 | 102.84      | 106.96   |
| 24  | C     | 501    | CLA  | C3B-C2B-C1B | -3.91 | 102.44      | 107.16   |
| 24  | c     | 506    | CLA  | C3D-C4D-ND  | 3.91  | 116.57      | 110.24   |
| 24  | d     | 402    | CLA  | C3B-C4B-NB  | 3.91  | 114.14      | 110.52   |
| 24  | A     | 405    | CLA  | C3D-C2D-C1D | -3.91 | 100.50      | 105.83   |
| 24  | b     | 618    | CLA  | C3B-C2B-C1B | -3.90 | 102.45      | 107.16   |
| 24  | B     | 602    | CLA  | C3C-C4C-NC  | 3.90  | 114.95      | 110.57   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | c     | 515    | CLA  | C4-C3-C5    | 3.90  | 121.83      | 115.27   |
| 24  | C     | 506    | CLA  | C3D-C4D-ND  | 3.90  | 116.54      | 110.24   |
| 24  | B     | 604    | CLA  | C1C-C2C-C3C | -3.89 | 102.86      | 106.96   |
| 26  | D     | 404    | BCR  | C24-C23-C22 | -3.89 | 120.36      | 126.23   |
| 24  | B     | 617    | CLA  | C3D-C4D-ND  | 3.89  | 116.53      | 110.24   |
| 24  | B     | 612    | CLA  | C3B-C4B-NB  | 3.88  | 114.11      | 110.52   |
| 24  | B     | 607    | CLA  | C3D-C4D-ND  | 3.88  | 116.51      | 110.24   |
| 31  | a     | 415[A] | PL9  | C32-C33-C34 | -3.87 | 118.33      | 127.66   |
| 24  | a     | 409    | CLA  | C1D-CHD-C4C | -3.87 | 117.70      | 126.06   |
| 24  | B     | 605    | CLA  | C1C-C2C-C3C | -3.87 | 102.89      | 106.96   |
| 24  | B     | 610    | CLA  | C3B-C2B-C1B | -3.87 | 102.49      | 107.16   |
| 37  | D     | 407    | LHG  | O7-C7-C8    | 3.87  | 119.85      | 111.50   |
| 40  | v     | 205    | HEC  | CHA-C4D-ND  | 3.87  | 128.62      | 124.42   |
| 24  | B     | 605    | CLA  | C3B-C4B-NB  | 3.87  | 114.10      | 110.52   |
| 24  | C     | 506    | CLA  | C1C-C2C-C3C | -3.86 | 102.90      | 106.96   |
| 24  | d     | 403    | CLA  | C3C-C4C-NC  | 3.86  | 114.90      | 110.57   |
| 24  | c     | 512    | CLA  | C3D-C4D-ND  | 3.86  | 116.48      | 110.24   |
| 24  | B     | 616    | CLA  | C1D-CHD-C4C | -3.86 | 117.74      | 126.06   |
| 24  | b     | 621    | CLA  | C4C-C3C-C2C | -3.86 | 101.28      | 106.90   |
| 24  | b     | 620    | CLA  | C1D-CHD-C4C | -3.85 | 117.75      | 126.06   |
| 24  | c     | 518    | CLA  | C3C-C4C-NC  | 3.85  | 114.89      | 110.57   |
| 24  | c     | 517    | CLA  | C3C-C4C-NC  | 3.85  | 114.89      | 110.57   |
| 31  | a     | 415[B] | PL9  | C22-C23-C24 | -3.85 | 118.39      | 127.66   |
| 24  | C     | 506    | CLA  | C3B-C2B-C1B | -3.85 | 102.51      | 107.16   |
| 36  | c     | 520    | DGD  | O2G-C1B-C2B | 3.85  | 119.80      | 111.50   |
| 27  | A     | 416    | SQD  | O47-C7-C8   | 3.85  | 119.80      | 111.50   |
| 36  | D     | 406    | DGD  | C1D-C2D-C3D | 3.85  | 118.00      | 110.00   |
| 33  | C     | 519    | LMG  | O7-C10-C11  | 3.84  | 119.78      | 111.50   |
| 24  | b     | 620    | CLA  | C1C-C2C-C3C | -3.84 | 102.92      | 106.96   |
| 24  | b     | 624    | CLA  | O2D-CGD-CBD | 3.84  | 118.08      | 111.27   |
| 31  | a     | 415[A] | PL9  | C7-C3-C4    | 3.83  | 119.99      | 116.88   |
| 24  | b     | 620    | CLA  | C3C-C4C-NC  | 3.83  | 114.86      | 110.57   |
| 24  | C     | 504    | CLA  | C3B-C4B-NB  | 3.82  | 114.06      | 110.52   |
| 24  | c     | 506    | CLA  | C3B-C4B-NB  | 3.82  | 114.06      | 110.52   |
| 31  | a     | 415[B] | PL9  | C32-C33-C34 | -3.82 | 118.45      | 127.66   |
| 36  | c     | 521    | DGD  | O2G-C1B-C2B | 3.82  | 119.74      | 111.50   |
| 24  | b     | 618    | CLA  | C1D-CHD-C4C | -3.82 | 117.82      | 126.06   |
| 24  | C     | 506    | CLA  | C3C-C4C-NC  | 3.82  | 114.85      | 110.57   |
| 24  | c     | 506    | CLA  | CAC-C3C-C4C | 3.82  | 129.76      | 124.81   |
| 24  | b     | 611    | CLA  | CAA-C2A-C3A | -3.82 | 102.33      | 112.78   |
| 24  | c     | 511    | CLA  | C3C-C4C-NC  | 3.81  | 114.85      | 110.57   |
| 24  | B     | 610    | CLA  | C1D-CHD-C4C | -3.81 | 117.83      | 126.06   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 512    | CLA  | C1D-CHD-C4C | -3.81 | 117.84      | 126.06   |
| 24  | B     | 604    | CLA  | CMC-C2C-C1C | 3.81  | 130.84      | 125.04   |
| 35  | B     | 623    | HTG  | C1'-S1-C1   | 3.81  | 107.21      | 100.09   |
| 24  | c     | 506    | CLA  | C1C-C2C-C3C | -3.81 | 102.95      | 106.96   |
| 24  | b     | 624    | CLA  | CMB-C2B-C1B | 3.81  | 131.16      | 125.37   |
| 24  | B     | 610    | CLA  | O2D-CGD-CBD | 3.80  | 118.03      | 111.27   |
| 24  | C     | 504    | CLA  | CBC-CAC-C3C | -3.80 | 101.96      | 112.43   |
| 24  | b     | 616    | CLA  | C4A-NA-C1A  | -3.80 | 105.00      | 106.71   |
| 24  | a     | 409    | CLA  | C3C-C4C-NC  | 3.80  | 114.83      | 110.57   |
| 24  | b     | 622    | CLA  | C1C-C2C-C3C | -3.80 | 102.97      | 106.96   |
| 24  | C     | 507    | CLA  | C1D-CHD-C4C | -3.80 | 117.87      | 126.06   |
| 36  | C     | 517    | DGD  | O2G-C1B-C2B | 3.79  | 119.67      | 111.50   |
| 24  | C     | 513    | CLA  | C3C-C4C-NC  | 3.79  | 114.82      | 110.57   |
| 24  | c     | 517    | CLA  | C1D-CHD-C4C | -3.79 | 117.88      | 126.06   |
| 24  | C     | 512    | CLA  | C1-C2-C3    | -3.79 | 119.49      | 126.04   |
| 27  | A     | 412    | SQD  | C45-O47-C7  | -3.79 | 108.47      | 117.79   |
| 36  | e     | 101    | DGD  | C3E-C4E-C5E | 3.78  | 116.98      | 110.24   |
| 24  | b     | 620    | CLA  | C1-C2-C3    | -3.78 | 119.51      | 126.04   |
| 24  | c     | 516    | CLA  | C3C-C4C-NC  | 3.78  | 114.81      | 110.57   |
| 24  | A     | 405    | CLA  | CAA-C2A-C3A | -3.77 | 102.45      | 112.78   |
| 24  | A     | 407    | CLA  | C3C-C4C-NC  | 3.77  | 114.80      | 110.57   |
| 24  | c     | 511    | CLA  | C1D-CHD-C4C | -3.77 | 117.93      | 126.06   |
| 24  | B     | 602    | CLA  | O2D-CGD-O1D | -3.77 | 116.47      | 123.84   |
| 26  | h     | 101    | BCR  | C16-C17-C18 | -3.77 | 121.93      | 127.31   |
| 24  | A     | 406    | CLA  | C1D-CHD-C4C | -3.77 | 117.93      | 126.06   |
| 24  | B     | 612    | CLA  | CAC-C3C-C4C | 3.77  | 129.70      | 124.81   |
| 24  | D     | 403    | CLA  | C1C-C2C-C3C | -3.76 | 103.00      | 106.96   |
| 24  | c     | 517    | CLA  | C1C-C2C-C3C | -3.76 | 103.01      | 106.96   |
| 24  | a     | 412    | CLA  | CMB-C2B-C1B | 3.75  | 131.09      | 125.37   |
| 24  | c     | 516    | CLA  | C1D-CHD-C4C | -3.75 | 117.97      | 126.06   |
| 24  | c     | 512    | CLA  | CMB-C2B-C1B | 3.75  | 131.08      | 125.37   |
| 24  | a     | 409    | CLA  | C1-C2-C3    | -3.75 | 119.56      | 126.04   |
| 24  | C     | 510    | CLA  | C1D-CHD-C4C | -3.75 | 117.97      | 126.06   |
| 24  | d     | 402    | CLA  | C3B-C2B-C1B | -3.75 | 102.64      | 107.16   |
| 24  | D     | 402    | CLA  | C1-C2-C3    | -3.75 | 119.56      | 126.04   |
| 37  | E     | 101    | LHG  | O7-C7-C8    | 3.75  | 119.57      | 111.50   |
| 31  | a     | 415[B] | PL9  | C7-C3-C4    | 3.75  | 119.92      | 116.88   |
| 24  | c     | 513    | CLA  | C1D-CHD-C4C | -3.74 | 117.98      | 126.06   |
| 24  | a     | 412    | CLA  | C1-C2-C3    | -3.74 | 119.57      | 126.04   |
| 40  | v     | 205    | HEC  | CHC-C4B-NB  | 3.74  | 128.99      | 124.37   |
| 24  | A     | 410    | CLA  | CAC-C3C-C4C | 3.74  | 129.66      | 124.81   |
| 24  | C     | 513    | CLA  | C1D-CHD-C4C | -3.73 | 118.00      | 126.06   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | A     | 410    | CLA  | C1D-CHD-C4C | -3.73 | 118.01      | 126.06   |
| 24  | C     | 511    | CLA  | C1C-C2C-C3C | -3.73 | 103.04      | 106.96   |
| 24  | B     | 605    | CLA  | C3B-C2B-C1B | -3.73 | 102.66      | 107.16   |
| 26  | t     | 101    | BCR  | C15-C16-C17 | -3.72 | 115.84      | 123.47   |
| 24  | b     | 621    | CLA  | C3B-C4B-NB  | 3.72  | 113.97      | 110.52   |
| 24  | c     | 518    | CLA  | C1C-C2C-C3C | -3.72 | 103.04      | 106.96   |
| 24  | B     | 603    | CLA  | C1D-CHD-C4C | -3.72 | 118.02      | 126.06   |
| 31  | A     | 419[B] | PL9  | C7-C3-C4    | 3.72  | 119.90      | 116.88   |
| 33  | c     | 524    | LMG  | O6-C5-C4    | 3.71  | 116.44      | 109.69   |
| 27  | a     | 405    | SQD  | O8-S-C6     | 3.71  | 111.66      | 105.74   |
| 24  | a     | 412    | CLA  | C1D-CHD-C4C | -3.71 | 118.05      | 126.06   |
| 24  | d     | 403    | CLA  | C1C-C2C-C3C | -3.71 | 103.06      | 106.96   |
| 24  | b     | 617    | CLA  | C1D-CHD-C4C | -3.71 | 118.05      | 126.06   |
| 24  | d     | 402    | CLA  | C3C-C4C-NC  | 3.70  | 114.72      | 110.57   |
| 24  | b     | 611    | CLA  | C1D-CHD-C4C | -3.70 | 118.07      | 126.06   |
| 24  | C     | 509    | CLA  | C1C-C2C-C3C | -3.70 | 103.07      | 106.96   |
| 24  | C     | 510    | CLA  | C3B-C4B-NB  | 3.70  | 113.94      | 110.52   |
| 27  | A     | 416    | SQD  | O48-C23-C24 | 3.70  | 123.51      | 111.91   |
| 24  | C     | 504    | CLA  | O2D-CGD-O1D | -3.69 | 116.62      | 123.84   |
| 24  | b     | 617    | CLA  | C1C-C2C-C3C | -3.69 | 103.08      | 106.96   |
| 24  | a     | 412    | CLA  | O2D-CGD-O1D | -3.69 | 116.62      | 123.84   |
| 24  | D     | 403    | CLA  | C1D-CHD-C4C | -3.69 | 118.10      | 126.06   |
| 26  | T     | 103    | BCR  | C33-C5-C6   | -3.69 | 120.39      | 124.53   |
| 24  | C     | 505    | CLA  | C3D-C2D-C1D | -3.68 | 100.81      | 105.83   |
| 24  | A     | 405    | CLA  | O2D-CGD-CBD | 3.68  | 117.80      | 111.27   |
| 24  | B     | 608    | CLA  | C4A-NA-C1A  | -3.68 | 105.05      | 106.71   |
| 24  | b     | 612    | CLA  | C1C-C2C-C3C | -3.68 | 103.09      | 106.96   |
| 29  | a     | 404    | LMT  | C1'-O5'-C5' | 3.68  | 120.90      | 113.69   |
| 24  | B     | 607    | CLA  | CMC-C2C-C1C | 3.68  | 130.64      | 125.04   |
| 24  | C     | 506    | CLA  | CAC-C3C-C4C | 3.67  | 129.58      | 124.81   |
| 24  | b     | 619    | CLA  | C1-C2-C3    | -3.67 | 119.70      | 126.04   |
| 24  | b     | 619    | CLA  | C1D-CHD-C4C | -3.67 | 118.15      | 126.06   |
| 24  | C     | 501    | CLA  | CMB-C2B-C1B | 3.66  | 130.95      | 125.37   |
| 24  | B     | 613    | CLA  | C4A-NA-C1A  | -3.66 | 105.06      | 106.71   |
| 27  | a     | 405    | SQD  | O48-C23-C24 | 3.66  | 123.40      | 111.91   |
| 24  | C     | 504    | CLA  | C1D-CHD-C4C | -3.66 | 118.16      | 126.06   |
| 31  | d     | 405[A] | PL9  | C42-C43-C44 | -3.66 | 118.84      | 127.66   |
| 24  | A     | 406    | CLA  | C3C-C4C-NC  | 3.66  | 114.67      | 110.57   |
| 24  | b     | 617    | CLA  | O2D-CGD-CBD | 3.66  | 117.77      | 111.27   |
| 24  | B     | 605    | CLA  | C1D-CHD-C4C | -3.66 | 118.17      | 126.06   |
| 24  | c     | 513    | CLA  | C1C-C2C-C3C | -3.66 | 103.11      | 106.96   |
| 24  | c     | 509    | CLA  | C4-C3-C5    | 3.65  | 121.42      | 115.27   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | B     | 609    | CLA  | C3B-C4B-NB  | 3.65  | 113.90      | 110.52   |
| 24  | c     | 510    | CLA  | O2D-CGD-O1D | -3.65 | 116.70      | 123.84   |
| 24  | C     | 508    | CLA  | C1C-C2C-C3C | -3.65 | 103.12      | 106.96   |
| 40  | V     | 205    | HEC  | C4C-NC-C1C  | 3.64  | 108.92      | 105.35   |
| 24  | b     | 612    | CLA  | CMC-C2C-C1C | 3.64  | 130.59      | 125.04   |
| 24  | C     | 501    | CLA  | C3C-C4C-NC  | 3.64  | 114.65      | 110.57   |
| 24  | d     | 402    | CLA  | C1-C2-C3    | -3.64 | 119.75      | 126.04   |
| 24  | C     | 511    | CLA  | CAC-C3C-C4C | 3.63  | 129.53      | 124.81   |
| 31  | a     | 415[B] | PL9  | C15-C14-C16 | 3.63  | 121.39      | 115.27   |
| 31  | a     | 415[B] | PL9  | C7-C8-C9    | -3.63 | 120.75      | 126.79   |
| 24  | d     | 403    | CLA  | C1D-CHD-C4C | -3.63 | 118.23      | 126.06   |
| 24  | a     | 410    | CLA  | C1D-CHD-C4C | -3.62 | 118.24      | 126.06   |
| 24  | D     | 403    | CLA  | CAC-C3C-C4C | 3.61  | 129.50      | 124.81   |
| 24  | c     | 514    | CLA  | C1C-C2C-C3C | -3.61 | 103.16      | 106.96   |
| 37  | L     | 101    | LHG  | O7-C7-C8    | 3.61  | 119.29      | 111.50   |
| 24  | B     | 611    | CLA  | C1C-C2C-C3C | -3.61 | 103.16      | 106.96   |
| 24  | B     | 614    | CLA  | C3D-C4D-ND  | 3.61  | 116.08      | 110.24   |
| 24  | C     | 513    | CLA  | C1C-C2C-C3C | -3.61 | 103.16      | 106.96   |
| 24  | B     | 616    | CLA  | C1C-C2C-C3C | -3.61 | 103.16      | 106.96   |
| 27  | a     | 414    | SQD  | C1-C2-C3    | -3.61 | 102.48      | 110.00   |
| 26  | C     | 514    | BCR  | C33-C5-C6   | -3.61 | 120.48      | 124.53   |
| 24  | a     | 410    | CLA  | CMC-C2C-C1C | 3.60  | 130.53      | 125.04   |
| 24  | B     | 610    | CLA  | C1C-C2C-C3C | -3.60 | 103.17      | 106.96   |
| 24  | b     | 613    | CLA  | C1D-CHD-C4C | -3.60 | 118.28      | 126.06   |
| 24  | b     | 618    | CLA  | C1C-C2C-C3C | -3.60 | 103.17      | 106.96   |
| 24  | B     | 608    | CLA  | C1D-CHD-C4C | -3.60 | 118.30      | 126.06   |
| 24  | C     | 506    | CLA  | C1D-CHD-C4C | -3.60 | 118.30      | 126.06   |
| 33  | z     | 101    | LMG  | O7-C10-C11  | 3.59  | 119.24      | 111.50   |
| 24  | b     | 622    | CLA  | C3D-C4D-ND  | 3.59  | 116.05      | 110.24   |
| 24  | B     | 602    | CLA  | C1C-C2C-C3C | -3.59 | 103.18      | 106.96   |
| 24  | C     | 501    | CLA  | C1D-CHD-C4C | -3.59 | 118.32      | 126.06   |
| 24  | B     | 610    | CLA  | C3B-C4B-NB  | 3.59  | 113.84      | 110.52   |
| 24  | C     | 501    | CLA  | O2D-CGD-O1D | -3.58 | 116.83      | 123.84   |
| 33  | c     | 524    | LMG  | C3-C4-C5    | 3.58  | 116.63      | 110.24   |
| 24  | C     | 502    | CLA  | C1C-C2C-C3C | -3.58 | 103.19      | 106.96   |
| 24  | B     | 616    | CLA  | CMC-C2C-C1C | 3.58  | 130.48      | 125.04   |
| 40  | v     | 205    | HEC  | CHB-C1B-NB  | 3.57  | 128.30      | 124.42   |
| 24  | B     | 603    | CLA  | C1C-C2C-C3C | -3.57 | 103.21      | 106.96   |
| 24  | b     | 623    | CLA  | C1D-CHD-C4C | -3.57 | 118.37      | 126.06   |
| 38  | F     | 102    | HEM  | C4C-NC-C1C  | 3.56  | 108.84      | 105.35   |
| 24  | b     | 622    | CLA  | C1D-CHD-C4C | -3.56 | 118.37      | 126.06   |
| 24  | c     | 515    | CLA  | C1D-CHD-C4C | -3.56 | 118.37      | 126.06   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 509    | CLA  | C1D-CHD-C4C | -3.56 | 118.38      | 126.06   |
| 29  | a     | 404    | LMT  | O5'-C5'-C4' | 3.56  | 117.25      | 109.75   |
| 24  | B     | 615    | CLA  | C1C-C2C-C3C | -3.55 | 103.22      | 106.96   |
| 24  | B     | 606    | CLA  | CHD-C4C-NC  | 3.55  | 129.80      | 124.20   |
| 24  | B     | 603    | CLA  | O2D-CGD-O1D | -3.54 | 116.91      | 123.84   |
| 24  | C     | 512    | CLA  | CMB-C2B-C1B | 3.54  | 130.76      | 125.37   |
| 24  | c     | 511    | CLA  | CBC-CAC-C3C | -3.54 | 102.67      | 112.43   |
| 31  | D     | 405[A] | PL9  | C40-C39-C41 | 3.54  | 121.23      | 115.27   |
| 24  | C     | 503    | CLA  | O2D-CGD-CBD | 3.54  | 117.56      | 111.27   |
| 24  | C     | 502    | CLA  | C1D-CHD-C4C | -3.54 | 118.43      | 126.06   |
| 24  | c     | 516    | CLA  | O2D-CGD-CBD | 3.54  | 117.55      | 111.27   |
| 33  | c     | 523    | LMG  | O7-C10-C11  | 3.54  | 119.12      | 111.50   |
| 26  | c     | 519    | BCR  | C33-C5-C6   | -3.53 | 120.56      | 124.53   |
| 24  | B     | 608    | CLA  | C1C-C2C-C3C | -3.53 | 103.24      | 106.96   |
| 24  | C     | 506    | CLA  | C3B-C4B-NB  | 3.53  | 113.79      | 110.52   |
| 35  | b     | 608    | HTG  | C1'-S1-C1   | 3.53  | 106.69      | 100.09   |
| 26  | D     | 404    | BCR  | C38-C26-C25 | -3.53 | 120.57      | 124.53   |
| 24  | b     | 614    | CLA  | CHD-C4C-NC  | 3.53  | 129.76      | 124.20   |
| 24  | c     | 510    | CLA  | C1C-C2C-C3C | -3.52 | 103.25      | 106.96   |
| 31  | D     | 405[A] | PL9  | C42-C43-C44 | -3.52 | 119.18      | 127.66   |
| 24  | B     | 614    | CLA  | C3B-C4B-NB  | 3.52  | 113.78      | 110.52   |
| 24  | B     | 606    | CLA  | C4-C3-C5    | 3.52  | 121.19      | 115.27   |
| 24  | A     | 405    | CLA  | O2A-CGA-CBA | 3.52  | 122.94      | 111.91   |
| 29  | C     | 521    | LMT  | C1'-O5'-C5' | 3.52  | 120.59      | 113.69   |
| 24  | b     | 621    | CLA  | O2A-CGA-CBA | 3.51  | 122.94      | 111.91   |
| 24  | C     | 509    | CLA  | C3B-C4B-NB  | 3.51  | 113.77      | 110.52   |
| 25  | A     | 409[B] | PHO  | C1A-C2A-C3A | -3.51 | 99.50       | 102.84   |
| 25  | a     | 418[A] | PHO  | C4-C3-C5    | 3.51  | 121.17      | 115.27   |
| 24  | D     | 403    | CLA  | O2D-CGD-O1D | -3.50 | 116.99      | 123.84   |
| 24  | A     | 405    | CLA  | C1C-C2C-C3C | -3.50 | 103.28      | 106.96   |
| 24  | D     | 403    | CLA  | C3B-C4B-NB  | 3.50  | 113.76      | 110.52   |
| 24  | a     | 410    | CLA  | C1C-C2C-C3C | -3.50 | 103.28      | 106.96   |
| 24  | A     | 407    | CLA  | C1C-C2C-C3C | -3.50 | 103.28      | 106.96   |
| 26  | b     | 626    | BCR  | C15-C14-C13 | -3.50 | 122.32      | 127.31   |
| 24  | b     | 611    | CLA  | C1C-C2C-C3C | -3.49 | 103.28      | 106.96   |
| 24  | B     | 607    | CLA  | O2D-CGD-O1D | -3.49 | 117.01      | 123.84   |
| 24  | c     | 510    | CLA  | C4C-C3C-C2C | -3.49 | 101.81      | 106.90   |
| 24  | C     | 508    | CLA  | C3B-C4B-NB  | 3.49  | 113.75      | 110.52   |
| 25  | a     | 418[A] | PHO  | C1A-C2A-C3A | -3.49 | 99.52       | 102.84   |
| 27  | A     | 412    | SQD  | O8-S-C6     | 3.49  | 111.30      | 105.74   |
| 25  | a     | 418[A] | PHO  | C4D-CHA-CBD | 3.49  | 110.09      | 108.52   |
| 24  | B     | 614    | CLA  | C1C-C2C-C3C | -3.49 | 103.29      | 106.96   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | B     | 605    | CLA  | C3D-C4D-ND  | 3.49  | 115.88      | 110.24   |
| 24  | A     | 407    | CLA  | C4-C3-C5    | 3.48  | 121.13      | 115.27   |
| 24  | b     | 625    | CLA  | C4C-C3C-C2C | -3.48 | 101.83      | 106.90   |
| 24  | B     | 607    | CLA  | C3B-C4B-NB  | 3.48  | 113.74      | 110.52   |
| 25  | a     | 418[B] | PHO  | C1A-C2A-C3A | -3.48 | 99.53       | 102.84   |
| 24  | c     | 508    | CLA  | C4C-C3C-C2C | -3.48 | 101.83      | 106.90   |
| 26  | k     | 101    | BCR  | C7-C8-C9    | -3.47 | 120.98      | 126.23   |
| 31  | a     | 415[A] | PL9  | C7-C8-C9    | -3.47 | 121.01      | 126.79   |
| 24  | b     | 611    | CLA  | O2D-CGD-O1D | -3.47 | 117.06      | 123.84   |
| 27  | F     | 103    | SQD  | O6-C1-C2    | 3.47  | 113.72      | 108.30   |
| 24  | A     | 406    | CLA  | C4A-NA-C1A  | -3.47 | 105.15      | 106.71   |
| 24  | b     | 612    | CLA  | C3B-C4B-NB  | 3.46  | 113.73      | 110.52   |
| 26  | T     | 103    | BCR  | C11-C10-C9  | -3.46 | 122.37      | 127.31   |
| 24  | c     | 510    | CLA  | C3D-C2D-C1D | -3.46 | 101.11      | 105.83   |
| 26  | d     | 404    | BCR  | C7-C8-C9    | -3.46 | 121.01      | 126.23   |
| 33  | c     | 523    | LMG  | O8-C28-C29  | 3.46  | 122.76      | 111.91   |
| 37  | d     | 407    | LHG  | O7-C7-C8    | 3.46  | 118.95      | 111.50   |
| 24  | B     | 613    | CLA  | C3B-C4B-NB  | 3.45  | 113.72      | 110.52   |
| 24  | c     | 516    | CLA  | C1C-C2C-C3C | -3.45 | 103.33      | 106.96   |
| 24  | d     | 403    | CLA  | CMC-C2C-C1C | 3.45  | 130.30      | 125.04   |
| 24  | B     | 609    | CLA  | C1D-CHD-C4C | -3.45 | 118.61      | 126.06   |
| 25  | a     | 418[B] | PHO  | O2D-CGD-O1D | -3.45 | 117.09      | 123.84   |
| 24  | A     | 410    | CLA  | C4A-NA-C1A  | -3.45 | 105.16      | 106.71   |
| 24  | b     | 614    | CLA  | C4-C3-C5    | 3.45  | 121.07      | 115.27   |
| 24  | c     | 508    | CLA  | CMB-C2B-C1B | 3.45  | 130.62      | 125.37   |
| 26  | H     | 101    | BCR  | C24-C23-C22 | -3.44 | 121.03      | 126.23   |
| 24  | C     | 512    | CLA  | C1C-C2C-C3C | -3.44 | 103.34      | 106.96   |
| 24  | B     | 608    | CLA  | C3B-C4B-NB  | 3.44  | 113.71      | 110.52   |
| 24  | A     | 407    | CLA  | C1D-CHD-C4C | -3.44 | 118.64      | 126.06   |
| 36  | h     | 102    | DGD  | O2G-C1B-C2B | 3.44  | 118.91      | 111.50   |
| 24  | C     | 501    | CLA  | CMC-C2C-C1C | 3.44  | 130.28      | 125.04   |
| 24  | C     | 505    | CLA  | C4C-C3C-C2C | -3.44 | 101.89      | 106.90   |
| 24  | B     | 613    | CLA  | CMC-C2C-C1C | 3.43  | 130.27      | 125.04   |
| 40  | V     | 205    | HEC  | CHC-C4B-NB  | 3.43  | 128.61      | 124.37   |
| 26  | B     | 619    | BCR  | C28-C27-C26 | -3.43 | 107.96      | 114.08   |
| 24  | b     | 614    | CLA  | O2D-CGD-O1D | -3.43 | 117.14      | 123.84   |
| 24  | C     | 508    | CLA  | C1D-CHD-C4C | -3.42 | 118.67      | 126.06   |
| 24  | b     | 622    | CLA  | C1-C2-C3    | -3.42 | 120.13      | 126.04   |
| 24  | B     | 603    | CLA  | CAA-C2A-C3A | -3.42 | 103.41      | 112.78   |
| 26  | b     | 627    | BCR  | C29-C30-C25 | 3.42  | 115.75      | 110.48   |
| 24  | B     | 617    | CLA  | C3B-C4B-NB  | 3.42  | 113.69      | 110.52   |
| 27  | A     | 412    | SQD  | O9-S-C6     | 3.42  | 111.00      | 106.94   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 38  | F     | 102    | HEM  | C4A-NA-C1A  | 3.42  | 108.69      | 105.35   |
| 31  | A     | 419[A] | PL9  | C7-C3-C4    | 3.41  | 119.65      | 116.88   |
| 31  | A     | 419[A] | PL9  | C37-C38-C39 | -3.41 | 119.44      | 127.66   |
| 27  | f     | 101    | SQD  | C1-O5-C5    | 3.41  | 120.37      | 113.69   |
| 24  | c     | 506    | CLA  | C1D-CHD-C4C | -3.41 | 118.71      | 126.06   |
| 31  | A     | 419[B] | PL9  | C32-C33-C34 | -3.41 | 119.46      | 127.66   |
| 35  | B     | 624    | HTG  | C1-O5-C5    | 3.40  | 118.86      | 112.58   |
| 24  | b     | 624    | CLA  | C3B-C4B-NB  | 3.40  | 113.67      | 110.52   |
| 26  | c     | 528    | BCR  | C15-C14-C13 | -3.40 | 122.46      | 127.31   |
| 40  | V     | 205    | HEC  | CHB-C1B-NB  | 3.40  | 128.11      | 124.42   |
| 26  | C     | 515    | BCR  | C33-C5-C6   | -3.39 | 120.72      | 124.53   |
| 24  | B     | 613    | CLA  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 24  | B     | 615    | CLA  | C1D-CHD-C4C | -3.39 | 118.75      | 126.06   |
| 24  | b     | 623    | CLA  | C3B-C4B-NB  | 3.39  | 113.66      | 110.52   |
| 24  | B     | 613    | CLA  | C4C-C3C-C2C | -3.39 | 101.96      | 106.90   |
| 24  | b     | 610    | CLA  | C1C-C2C-C3C | -3.39 | 103.40      | 106.96   |
| 26  | C     | 515    | BCR  | C7-C8-C9    | -3.38 | 121.12      | 126.23   |
| 24  | B     | 614    | CLA  | C4C-C3C-C2C | -3.38 | 101.97      | 106.90   |
| 40  | v     | 205    | HEC  | CHA-C1A-NA  | 3.38  | 128.10      | 124.44   |
| 31  | A     | 419[A] | PL9  | C20-C19-C21 | 3.38  | 120.96      | 115.27   |
| 29  | T     | 104    | LMT  | C1'-O5'-C5' | 3.38  | 120.33      | 113.69   |
| 24  | C     | 510    | CLA  | C1C-C2C-C3C | -3.38 | 103.41      | 106.96   |
| 40  | V     | 205    | HEC  | CHA-C4D-ND  | 3.38  | 128.09      | 124.42   |
| 24  | C     | 507    | CLA  | CMC-C2C-C1C | 3.37  | 130.18      | 125.04   |
| 24  | b     | 615    | CLA  | C4-C3-C5    | 3.37  | 120.94      | 115.27   |
| 24  | b     | 614    | CLA  | C2A-C1A-CHA | -3.37 | 117.97      | 123.86   |
| 24  | a     | 409    | CLA  | CAA-C2A-C3A | -3.37 | 103.56      | 112.78   |
| 24  | c     | 518    | CLA  | CMC-C2C-C1C | 3.37  | 130.16      | 125.04   |
| 24  | b     | 616    | CLA  | CMB-C2B-C1B | 3.36  | 130.49      | 125.37   |
| 24  | c     | 510    | CLA  | CMB-C2B-C1B | 3.36  | 130.48      | 125.37   |
| 24  | c     | 507    | CLA  | C4C-C3C-C2C | -3.36 | 102.01      | 106.90   |
| 24  | b     | 624    | CLA  | C1C-C2C-C3C | -3.36 | 103.43      | 106.96   |
| 24  | c     | 508    | CLA  | CMC-C2C-C1C | 3.35  | 130.15      | 125.04   |
| 24  | A     | 410    | CLA  | C1C-C2C-C3C | -3.35 | 103.43      | 106.96   |
| 24  | B     | 604    | CLA  | O2A-CGA-O1A | -3.35 | 115.13      | 123.59   |
| 24  | C     | 511    | CLA  | C4A-NA-C1A  | -3.35 | 105.20      | 106.71   |
| 26  | A     | 411    | BCR  | C33-C5-C6   | -3.34 | 120.77      | 124.53   |
| 31  | D     | 405[A] | PL9  | C7-C8-C9    | -3.34 | 121.23      | 126.79   |
| 24  | B     | 605    | CLA  | C1-C2-C3    | -3.34 | 120.26      | 126.04   |
| 26  | C     | 514    | BCR  | C15-C14-C13 | -3.34 | 122.55      | 127.31   |
| 31  | d     | 405[B] | PL9  | C42-C43-C44 | -3.33 | 119.63      | 127.66   |
| 27  | a     | 414    | SQD  | C44-O6-C1   | -3.33 | 107.23      | 113.74   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 619    | CLA  | C1C-C2C-C3C | -3.33 | 103.45      | 106.96   |
| 24  | B     | 611    | CLA  | C1D-CHD-C4C | -3.32 | 118.89      | 126.06   |
| 25  | A     | 409[B] | PHO  | CMB-C2B-C3B | 3.32  | 130.89      | 124.68   |
| 24  | B     | 615    | CLA  | C3B-C4B-NB  | 3.32  | 113.60      | 110.52   |
| 24  | c     | 507    | CLA  | C1C-C2C-C3C | -3.31 | 103.47      | 106.96   |
| 24  | b     | 619    | CLA  | C4C-C3C-C2C | -3.31 | 102.07      | 106.90   |
| 24  | B     | 615    | CLA  | O2A-CGA-O1A | -3.31 | 115.24      | 123.59   |
| 24  | C     | 501    | CLA  | C1-C2-C3    | -3.31 | 120.32      | 126.04   |
| 31  | a     | 415[B] | PL9  | C17-C18-C19 | -3.31 | 119.69      | 127.66   |
| 24  | c     | 508    | CLA  | CAC-C3C-C4C | 3.31  | 129.10      | 124.81   |
| 24  | B     | 613    | CLA  | C1D-CHD-C4C | -3.31 | 118.93      | 126.06   |
| 24  | b     | 620    | CLA  | C3B-C4B-NB  | 3.30  | 113.58      | 110.52   |
| 24  | D     | 403    | CLA  | CMB-C2B-C1B | 3.30  | 130.40      | 125.37   |
| 24  | C     | 502    | CLA  | C3B-C4B-NB  | 3.30  | 113.58      | 110.52   |
| 27  | F     | 103    | SQD  | O7-S-C6     | 3.30  | 110.86      | 106.94   |
| 24  | A     | 410    | CLA  | C4C-C3C-C2C | -3.30 | 102.09      | 106.90   |
| 24  | d     | 402    | CLA  | O2D-CGD-O1D | -3.30 | 117.39      | 123.84   |
| 24  | C     | 503    | CLA  | C1C-C2C-C3C | -3.30 | 103.49      | 106.96   |
| 24  | C     | 501    | CLA  | CBC-CAC-C3C | -3.29 | 103.36      | 112.43   |
| 35  | V     | 206    | HTG  | C1'-S1-C1   | 3.29  | 106.25      | 100.09   |
| 31  | A     | 419[A] | PL9  | C32-C33-C34 | -3.29 | 119.75      | 127.66   |
| 24  | c     | 507    | CLA  | CMB-C2B-C1B | 3.28  | 130.37      | 125.37   |
| 24  | c     | 509    | CLA  | CMC-C2C-C1C | 3.28  | 130.03      | 125.04   |
| 31  | a     | 415[A] | PL9  | C17-C18-C19 | -3.28 | 119.76      | 127.66   |
| 24  | B     | 617    | CLA  | CAC-C3C-C4C | 3.28  | 129.06      | 124.81   |
| 24  | A     | 407    | CLA  | CBC-CAC-C3C | -3.27 | 103.41      | 112.43   |
| 24  | b     | 621    | CLA  | O2A-CGA-O1A | -3.27 | 115.34      | 123.59   |
| 24  | b     | 616    | CLA  | C1D-CHD-C4C | -3.27 | 119.00      | 126.06   |
| 24  | B     | 602    | CLA  | O2A-CGA-CBA | 3.27  | 122.17      | 111.91   |
| 24  | B     | 617    | CLA  | C4C-C3C-C2C | -3.26 | 102.14      | 106.90   |
| 24  | A     | 407    | CLA  | CMB-C2B-C1B | 3.26  | 130.34      | 125.37   |
| 31  | D     | 405[A] | PL9  | C10-C9-C11  | 3.26  | 120.76      | 115.27   |
| 25  | A     | 409[A] | PHO  | C4-C3-C5    | 3.26  | 120.76      | 115.27   |
| 24  | b     | 624    | CLA  | CAC-C3C-C4C | 3.26  | 129.04      | 124.81   |
| 24  | B     | 606    | CLA  | C1C-C2C-C3C | -3.26 | 103.53      | 106.96   |
| 24  | c     | 509    | CLA  | C1-C2-C3    | -3.26 | 120.41      | 126.04   |
| 24  | d     | 401    | CLA  | CAA-C2A-C3A | -3.25 | 103.86      | 112.78   |
| 24  | c     | 513    | CLA  | CAC-C3C-C4C | 3.25  | 129.03      | 124.81   |
| 24  | c     | 513    | CLA  | C4C-C3C-C2C | -3.25 | 102.16      | 106.90   |
| 24  | c     | 514    | CLA  | CAC-C3C-C4C | 3.25  | 129.02      | 124.81   |
| 24  | c     | 507    | CLA  | C3B-C4B-NB  | 3.25  | 113.53      | 110.52   |
| 24  | c     | 516    | CLA  | C3B-C4B-NB  | 3.24  | 113.53      | 110.52   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | d     | 403    | CLA  | CHD-C4C-NC  | 3.24  | 129.31      | 124.20   |
| 24  | B     | 611    | CLA  | C4C-C3C-C2C | -3.24 | 102.17      | 106.90   |
| 24  | C     | 509    | CLA  | CAC-C3C-C4C | 3.24  | 129.01      | 124.81   |
| 24  | b     | 615    | CLA  | CMC-C2C-C1C | 3.24  | 129.97      | 125.04   |
| 25  | A     | 409[B] | PHO  | C4-C3-C5    | 3.24  | 120.72      | 115.27   |
| 24  | C     | 507    | CLA  | C1C-C2C-C3C | -3.24 | 103.56      | 106.96   |
| 24  | C     | 505    | CLA  | C1C-C2C-C3C | -3.23 | 103.56      | 106.96   |
| 24  | B     | 605    | CLA  | CAC-C3C-C4C | 3.23  | 129.00      | 124.81   |
| 24  | d     | 402    | CLA  | CAC-C3C-C4C | 3.22  | 128.99      | 124.81   |
| 33  | c     | 501    | LMG  | C8-O7-C10   | -3.22 | 109.86      | 117.79   |
| 24  | B     | 610    | CLA  | CHC-C1C-C2C | -3.22 | 117.78      | 126.73   |
| 24  | B     | 607    | CLA  | CBC-CAC-C3C | -3.22 | 103.55      | 112.43   |
| 25  | A     | 408    | PHO  | C1A-C2A-C3A | -3.22 | 99.77       | 102.84   |
| 24  | b     | 619    | CLA  | CAC-C3C-C4C | 3.22  | 128.99      | 124.81   |
| 37  | d     | 408    | LHG  | O7-C7-C8    | 3.22  | 118.44      | 111.50   |
| 24  | A     | 410    | CLA  | C4-C3-C5    | 3.22  | 120.69      | 115.27   |
| 24  | B     | 617    | CLA  | O2D-CGD-O1D | -3.22 | 117.55      | 123.84   |
| 33  | D     | 413    | LMG  | O7-C10-C11  | 3.21  | 118.42      | 111.50   |
| 24  | C     | 512    | CLA  | O2D-CGD-O1D | -3.21 | 117.56      | 123.84   |
| 31  | a     | 415[A] | PL9  | C20-C19-C21 | 3.21  | 120.67      | 115.27   |
| 24  | C     | 506    | CLA  | CHC-C1C-C2C | -3.21 | 117.82      | 126.73   |
| 26  | B     | 619    | BCR  | C29-C30-C25 | 3.21  | 115.42      | 110.48   |
| 24  | A     | 410    | CLA  | C3B-C4B-NB  | 3.20  | 113.49      | 110.52   |
| 31  | D     | 405[B] | PL9  | C42-C43-C44 | -3.20 | 119.94      | 127.66   |
| 24  | b     | 622    | CLA  | C4C-C3C-C2C | -3.20 | 102.23      | 106.90   |
| 24  | C     | 503    | CLA  | CMB-C2B-C1B | 3.20  | 130.25      | 125.37   |
| 25  | a     | 418[B] | PHO  | C4-C3-C5    | 3.20  | 120.66      | 115.27   |
| 24  | B     | 608    | CLA  | CAA-C2A-C3A | -3.20 | 104.01      | 112.78   |
| 24  | c     | 510    | CLA  | CAC-C3C-C4C | 3.20  | 128.96      | 124.81   |
| 26  | c     | 528    | BCR  | C11-C10-C9  | -3.20 | 122.74      | 127.31   |
| 33  | B     | 622    | LMG  | O8-C28-C29  | 3.20  | 121.95      | 111.91   |
| 31  | A     | 419[B] | PL9  | C20-C19-C21 | 3.20  | 120.66      | 115.27   |
| 31  | a     | 415[A] | PL9  | C42-C43-C44 | -3.20 | 119.95      | 127.66   |
| 25  | a     | 418[B] | PHO  | CMB-C2B-C3B | 3.20  | 130.66      | 124.68   |
| 24  | A     | 406    | CLA  | CHC-C1C-C2C | -3.20 | 117.85      | 126.73   |
| 31  | a     | 415[A] | PL9  | C10-C9-C11  | 3.20  | 120.65      | 115.27   |
| 31  | D     | 405[B] | PL9  | C7-C8-C9    | -3.20 | 121.47      | 126.79   |
| 24  | B     | 606    | CLA  | C2A-C1A-CHA | -3.19 | 118.27      | 123.86   |
| 24  | D     | 402    | CLA  | C4C-C3C-C2C | -3.19 | 102.24      | 106.90   |
| 24  | B     | 614    | CLA  | C1-C2-C3    | -3.19 | 120.52      | 126.04   |
| 24  | B     | 606    | CLA  | C4C-C3C-C2C | -3.19 | 102.25      | 106.90   |
| 24  | c     | 513    | CLA  | C1-C2-C3    | -3.19 | 120.52      | 126.04   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 511    | CLA  | CHC-C1C-C2C | -3.19 | 117.87      | 126.73   |
| 24  | b     | 625    | CLA  | O2A-CGA-CBA | 3.19  | 121.92      | 111.91   |
| 24  | b     | 624    | CLA  | C4C-C3C-C2C | -3.19 | 102.25      | 106.90   |
| 31  | a     | 415[B] | PL9  | C37-C38-C39 | -3.19 | 119.98      | 127.66   |
| 24  | A     | 406    | CLA  | CHD-C4C-NC  | 3.19  | 129.23      | 124.20   |
| 24  | B     | 607    | CLA  | CAC-C3C-C4C | 3.19  | 128.94      | 124.81   |
| 24  | B     | 613    | CLA  | C1C-C2C-C3C | -3.18 | 103.61      | 106.96   |
| 24  | C     | 510    | CLA  | C4-C3-C5    | 3.18  | 120.62      | 115.27   |
| 24  | c     | 514    | CLA  | CHB-C1B-NB  | -3.18 | 120.89      | 124.26   |
| 31  | a     | 415[B] | PL9  | C10-C9-C11  | 3.18  | 120.62      | 115.27   |
| 26  | B     | 618    | BCR  | C7-C8-C9    | -3.18 | 121.43      | 126.23   |
| 40  | V     | 205    | HEC  | C1D-ND-C4D  | 3.18  | 108.36      | 105.07   |
| 24  | b     | 613    | CLA  | CAC-C3C-C4C | 3.18  | 128.93      | 124.81   |
| 35  | b     | 601    | HTG  | C1'-S1-C1   | 3.18  | 106.03      | 100.09   |
| 37  | b     | 634    | LHG  | O7-C7-C8    | 3.17  | 118.34      | 111.50   |
| 24  | b     | 620    | CLA  | CMB-C2B-C1B | 3.17  | 130.20      | 125.37   |
| 24  | C     | 512    | CLA  | C3B-C4B-NB  | 3.17  | 113.46      | 110.52   |
| 24  | b     | 622    | CLA  | CAC-C3C-C4C | 3.17  | 128.92      | 124.81   |
| 31  | a     | 415[B] | PL9  | C27-C28-C29 | -3.17 | 120.03      | 127.66   |
| 31  | d     | 405[B] | PL9  | C37-C38-C39 | -3.17 | 120.04      | 127.66   |
| 24  | C     | 506    | CLA  | CBC-CAC-C3C | -3.16 | 103.71      | 112.43   |
| 24  | c     | 518    | CLA  | CMB-C2B-C1B | 3.16  | 130.19      | 125.37   |
| 24  | d     | 402    | CLA  | C1D-CHD-C4C | -3.16 | 119.24      | 126.06   |
| 35  | C     | 523    | HTG  | O5-C5-C4    | 3.16  | 115.43      | 109.69   |
| 24  | b     | 616    | CLA  | C3B-C4B-NB  | 3.16  | 113.44      | 110.52   |
| 31  | a     | 415[B] | PL9  | C20-C19-C21 | 3.16  | 120.58      | 115.27   |
| 31  | A     | 419[B] | PL9  | C37-C38-C39 | -3.15 | 120.06      | 127.66   |
| 24  | A     | 407    | CLA  | CHD-C4C-NC  | 3.15  | 129.17      | 124.20   |
| 24  | B     | 614    | CLA  | C1D-CHD-C4C | -3.15 | 119.26      | 126.06   |
| 24  | C     | 505    | CLA  | O2D-CGD-O1D | -3.15 | 117.69      | 123.84   |
| 26  | K     | 101    | BCR  | C24-C23-C22 | -3.15 | 121.48      | 126.23   |
| 40  | V     | 205    | HEC  | CBC-CAC-C3C | 3.15  | 121.10      | 112.43   |
| 24  | D     | 402    | CLA  | C1D-CHD-C4C | -3.15 | 119.27      | 126.06   |
| 24  | C     | 510    | CLA  | C4C-C3C-C2C | -3.15 | 102.31      | 106.90   |
| 24  | B     | 612    | CLA  | CHD-C4C-NC  | 3.14  | 129.16      | 124.20   |
| 24  | B     | 615    | CLA  | CMC-C2C-C1C | 3.14  | 129.83      | 125.04   |
| 24  | c     | 511    | CLA  | C1-C2-C3    | -3.14 | 120.61      | 126.04   |
| 31  | D     | 405[B] | PL9  | C37-C38-C39 | -3.14 | 120.10      | 127.66   |
| 24  | C     | 502    | CLA  | O2D-CGD-O1D | -3.14 | 117.70      | 123.84   |
| 24  | c     | 512    | CLA  | CMC-C2C-C1C | 3.14  | 129.82      | 125.04   |
| 40  | v     | 205    | HEC  | CBC-CAC-C3C | 3.14  | 121.08      | 112.43   |
| 24  | b     | 622    | CLA  | CHC-C1C-C2C | -3.14 | 118.01      | 126.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31  | A     | 419[B] | PL9  | C7-C8-C9    | -3.14 | 121.57      | 126.79   |
| 24  | a     | 412    | CLA  | C3B-C4B-NB  | 3.14  | 113.42      | 110.52   |
| 24  | C     | 504    | CLA  | CAC-C3C-C4C | 3.13  | 128.88      | 124.81   |
| 24  | b     | 610    | CLA  | C3B-C4B-NB  | 3.13  | 113.42      | 110.52   |
| 24  | b     | 610    | CLA  | C4C-C3C-C2C | -3.13 | 102.33      | 106.90   |
| 24  | a     | 409    | CLA  | CHC-C1C-C2C | -3.13 | 118.04      | 126.73   |
| 24  | C     | 512    | CLA  | C4C-C3C-C2C | -3.13 | 102.34      | 106.90   |
| 24  | B     | 615    | CLA  | C4C-C3C-C2C | -3.13 | 102.34      | 106.90   |
| 24  | C     | 508    | CLA  | C4C-C3C-C2C | -3.12 | 102.34      | 106.90   |
| 24  | b     | 621    | CLA  | CAC-C3C-C4C | 3.12  | 128.86      | 124.81   |
| 31  | d     | 405[A] | PL9  | C40-C39-C41 | 3.12  | 120.52      | 115.27   |
| 24  | B     | 604    | CLA  | O2A-CGA-CBA | 3.12  | 121.70      | 111.91   |
| 24  | B     | 608    | CLA  | CAC-C3C-C4C | 3.12  | 128.86      | 124.81   |
| 31  | D     | 405[B] | PL9  | C10-C9-C11  | 3.12  | 120.52      | 115.27   |
| 40  | v     | 205    | HEC  | C1D-ND-C4D  | 3.12  | 108.29      | 105.07   |
| 24  | B     | 615    | CLA  | O2A-CGA-CBA | 3.12  | 121.69      | 111.91   |
| 24  | C     | 503    | CLA  | C4C-C3C-C2C | -3.12 | 102.35      | 106.90   |
| 24  | d     | 402    | CLA  | C2A-C1A-CHA | -3.11 | 118.41      | 123.86   |
| 33  | Z     | 101    | LMG  | O6-C5-C4    | 3.11  | 115.35      | 109.69   |
| 24  | c     | 517    | CLA  | CMC-C2C-C1C | 3.11  | 129.78      | 125.04   |
| 26  | T     | 103    | BCR  | C15-C16-C17 | -3.11 | 117.10      | 123.47   |
| 38  | F     | 102    | HEM  | CBD-CAD-C3D | -3.11 | 103.99      | 112.63   |
| 24  | b     | 613    | CLA  | CHC-C1C-C2C | -3.11 | 118.10      | 126.73   |
| 24  | B     | 611    | CLA  | CAC-C3C-C4C | 3.11  | 128.84      | 124.81   |
| 24  | C     | 508    | CLA  | CHC-C1C-C2C | -3.10 | 118.11      | 126.73   |
| 24  | b     | 616    | CLA  | CMC-C2C-C1C | 3.10  | 129.76      | 125.04   |
| 31  | A     | 419[A] | PL9  | C53-C6-C1   | 3.10  | 121.33      | 114.99   |
| 24  | C     | 506    | CLA  | C4-C3-C5    | 3.10  | 120.49      | 115.27   |
| 24  | B     | 611    | CLA  | O2A-CGA-CBA | 3.10  | 121.64      | 111.91   |
| 36  | C     | 518    | DGD  | O2G-C1B-C2B | 3.10  | 118.18      | 111.50   |
| 24  | B     | 614    | CLA  | O2D-CGD-CBD | 3.10  | 116.78      | 111.27   |
| 24  | a     | 409    | CLA  | C3B-C4B-NB  | 3.10  | 113.39      | 110.52   |
| 25  | A     | 409[A] | PHO  | CMB-C2B-C3B | 3.10  | 130.47      | 124.68   |
| 33  | C     | 519    | LMG  | O8-C28-C29  | 3.10  | 121.63      | 111.91   |
| 26  | d     | 404    | BCR  | C33-C5-C6   | -3.10 | 121.05      | 124.53   |
| 24  | C     | 504    | CLA  | C4-C3-C5    | 3.10  | 120.48      | 115.27   |
| 24  | c     | 511    | CLA  | CHC-C1C-C2C | -3.10 | 118.13      | 126.73   |
| 24  | B     | 608    | CLA  | C1-C2-C3    | -3.10 | 120.69      | 126.04   |
| 24  | C     | 501    | CLA  | C3B-C4B-NB  | 3.09  | 113.38      | 110.52   |
| 24  | B     | 616    | CLA  | CHD-C4C-NC  | 3.09  | 129.07      | 124.20   |
| 24  | b     | 620    | CLA  | CHC-C1C-C2C | -3.09 | 118.15      | 126.73   |
| 36  | H     | 102    | DGD  | O1G-C1A-C2A | 3.09  | 121.60      | 111.91   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | B     | 617    | CLA  | CBC-CAC-C3C | -3.09 | 103.92      | 112.43   |
| 24  | b     | 619    | CLA  | C3B-C4B-NB  | 3.09  | 113.38      | 110.52   |
| 26  | c     | 528    | BCR  | C33-C5-C6   | -3.08 | 121.06      | 124.53   |
| 24  | c     | 516    | CLA  | CAC-C3C-C4C | 3.08  | 128.81      | 124.81   |
| 31  | D     | 405[A] | PL9  | C36-C37-C38 | -3.08 | 101.75      | 111.88   |
| 26  | D     | 404    | BCR  | C28-C27-C26 | -3.08 | 108.58      | 114.08   |
| 26  | C     | 514    | BCR  | C16-C17-C18 | -3.08 | 122.91      | 127.31   |
| 24  | b     | 613    | CLA  | CMC-C2C-C1C | 3.08  | 129.73      | 125.04   |
| 24  | c     | 517    | CLA  | C4-C3-C5    | 3.08  | 120.45      | 115.27   |
| 31  | a     | 415[A] | PL9  | C27-C28-C29 | -3.08 | 120.25      | 127.66   |
| 37  | D     | 407    | LHG  | O8-C23-C24  | 3.08  | 121.56      | 111.91   |
| 24  | b     | 610    | CLA  | CHD-C4C-NC  | 3.08  | 129.05      | 124.20   |
| 24  | B     | 609    | CLA  | C1-C2-C3    | -3.08 | 120.72      | 126.04   |
| 27  | F     | 103    | SQD  | O5-C5-C4    | 3.08  | 115.28      | 109.69   |
| 37  | D     | 407    | LHG  | O8-C23-O10  | -3.08 | 115.83      | 123.59   |
| 31  | a     | 415[B] | PL9  | C7-C3-C2    | -3.08 | 119.26      | 123.30   |
| 24  | b     | 611    | CLA  | C4C-C3C-C2C | -3.07 | 102.42      | 106.90   |
| 24  | B     | 602    | CLA  | CHD-C4C-NC  | 3.07  | 129.05      | 124.20   |
| 31  | a     | 415[B] | PL9  | C42-C43-C44 | -3.07 | 120.26      | 127.66   |
| 31  | A     | 419[B] | PL9  | C7-C3-C2    | -3.07 | 119.26      | 123.30   |
| 24  | B     | 617    | CLA  | C1C-C2C-C3C | -3.07 | 103.73      | 106.96   |
| 36  | H     | 102    | DGD  | O2G-C1B-C2B | 3.07  | 118.12      | 111.50   |
| 24  | B     | 616    | CLA  | O2D-CGD-CBD | 3.07  | 116.72      | 111.27   |
| 24  | b     | 615    | CLA  | O2A-CGA-O1A | -3.06 | 115.86      | 123.59   |
| 37  | b     | 634    | LHG  | O8-C23-C24  | 3.06  | 121.52      | 111.91   |
| 24  | B     | 617    | CLA  | CHC-C1C-C2C | -3.06 | 118.22      | 126.73   |
| 26  | K     | 101    | BCR  | C15-C14-C13 | -3.06 | 122.94      | 127.31   |
| 31  | d     | 405[B] | PL9  | C27-C28-C29 | -3.06 | 120.29      | 127.66   |
| 25  | A     | 408    | PHO  | CBC-CAC-C3C | -3.06 | 108.40      | 112.88   |
| 26  | D     | 404    | BCR  | C29-C30-C25 | 3.06  | 115.19      | 110.48   |
| 24  | c     | 506    | CLA  | CHC-C1C-C2C | -3.06 | 118.24      | 126.73   |
| 24  | c     | 515    | CLA  | CHC-C1C-C2C | -3.05 | 118.25      | 126.73   |
| 24  | C     | 507    | CLA  | CMB-C2B-C1B | 3.05  | 130.02      | 125.37   |
| 24  | a     | 409    | CLA  | CAA-C2A-C1A | -3.05 | 101.97      | 111.97   |
| 24  | B     | 608    | CLA  | CMC-C2C-C1C | 3.05  | 129.68      | 125.04   |
| 24  | c     | 513    | CLA  | CHC-C1C-C2C | -3.05 | 118.26      | 126.73   |
| 24  | C     | 513    | CLA  | C1-C2-C3    | -3.05 | 120.77      | 126.04   |
| 31  | A     | 419[A] | PL9  | C45-C44-C46 | 3.05  | 120.39      | 115.27   |
| 26  | b     | 627    | BCR  | C38-C26-C25 | -3.04 | 121.11      | 124.53   |
| 24  | d     | 401    | CLA  | C2A-C1A-CHA | -3.04 | 118.54      | 123.86   |
| 24  | C     | 511    | CLA  | C4C-C3C-C2C | -3.04 | 102.47      | 106.90   |
| 24  | b     | 617    | CLA  | CMC-C2C-C1C | 3.04  | 129.67      | 125.04   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31  | A     | 419[A] | PL9  | C22-C23-C24 | -3.04 | 120.34      | 127.66   |
| 24  | b     | 625    | CLA  | CHC-C1C-C2C | -3.04 | 118.29      | 126.73   |
| 24  | B     | 613    | CLA  | C4-C3-C5    | 3.04  | 120.38      | 115.27   |
| 24  | A     | 405    | CLA  | CHC-C1C-C2C | -3.04 | 118.29      | 126.73   |
| 24  | C     | 502    | CLA  | CMB-C2B-C1B | 3.04  | 130.00      | 125.37   |
| 24  | c     | 509    | CLA  | C3B-C4B-NB  | 3.04  | 113.33      | 110.52   |
| 24  | C     | 504    | CLA  | CMC-C2C-C1C | 3.03  | 129.66      | 125.04   |
| 24  | b     | 611    | CLA  | CMB-C2B-C1B | 3.03  | 129.99      | 125.37   |
| 38  | e     | 103    | HEM  | CHB-C1B-NB  | 3.03  | 128.12      | 124.37   |
| 24  | c     | 511    | CLA  | CAA-C2A-C3A | -3.03 | 104.47      | 112.78   |
| 24  | A     | 406    | CLA  | O2D-CGD-O1D | -3.03 | 117.91      | 123.84   |
| 26  | h     | 101    | BCR  | C38-C26-C25 | -3.03 | 121.12      | 124.53   |
| 24  | C     | 505    | CLA  | CAC-C3C-C4C | 3.03  | 128.74      | 124.81   |
| 24  | A     | 405    | CLA  | C4C-C3C-C2C | -3.03 | 102.48      | 106.90   |
| 24  | d     | 401    | CLA  | CHC-C1C-C2C | -3.03 | 118.32      | 126.73   |
| 24  | b     | 620    | CLA  | CAC-C3C-C4C | 3.03  | 128.74      | 124.81   |
| 24  | A     | 407    | CLA  | C2A-C1A-CHA | -3.02 | 118.57      | 123.86   |
| 24  | a     | 410    | CLA  | O2A-CGA-O1A | -3.02 | 115.96      | 123.59   |
| 24  | c     | 508    | CLA  | C1-C2-C3    | -3.02 | 120.81      | 126.04   |
| 31  | D     | 405[A] | PL9  | C15-C14-C16 | 3.02  | 120.36      | 115.27   |
| 24  | B     | 609    | CLA  | CHC-C1C-C2C | -3.02 | 118.34      | 126.73   |
| 24  | b     | 615    | CLA  | O2D-CGD-O1D | -3.02 | 117.94      | 123.84   |
| 24  | b     | 617    | CLA  | C3B-C4B-NB  | 3.02  | 113.31      | 110.52   |
| 24  | a     | 410    | CLA  | C4C-C3C-C2C | -3.02 | 102.50      | 106.90   |
| 37  | D     | 408    | LHG  | O7-C7-C8    | 3.01  | 118.00      | 111.50   |
| 24  | B     | 611    | CLA  | C3B-C4B-NB  | 3.01  | 113.31      | 110.52   |
| 24  | b     | 624    | CLA  | CHC-C1C-C2C | -3.01 | 118.37      | 126.73   |
| 24  | C     | 509    | CLA  | O2D-CGD-O1D | -3.01 | 117.95      | 123.84   |
| 24  | c     | 518    | CLA  | CAC-C3C-C4C | 3.01  | 128.71      | 124.81   |
| 24  | c     | 512    | CLA  | C4C-C3C-C2C | -3.01 | 102.51      | 106.90   |
| 24  | a     | 412    | CLA  | C4-C3-C5    | 3.01  | 120.33      | 115.27   |
| 37  | D     | 409    | LHG  | O8-C23-C24  | 3.00  | 121.34      | 111.91   |
| 33  | B     | 622    | LMG  | O7-C10-C11  | 3.00  | 117.98      | 111.50   |
| 24  | D     | 403    | CLA  | C4C-C3C-C2C | -3.00 | 102.52      | 106.90   |
| 37  | E     | 101    | LHG  | O8-C23-C24  | 3.00  | 121.33      | 111.91   |
| 24  | b     | 610    | CLA  | C4-C3-C5    | 3.00  | 120.32      | 115.27   |
| 24  | c     | 506    | CLA  | C4C-C3C-C2C | -3.00 | 102.52      | 106.90   |
| 26  | b     | 628    | BCR  | C38-C26-C25 | -3.00 | 121.16      | 124.53   |
| 24  | b     | 616    | CLA  | CHC-C1C-C2C | -3.00 | 118.40      | 126.73   |
| 24  | B     | 608    | CLA  | C4C-C3C-C2C | -3.00 | 102.53      | 106.90   |
| 24  | D     | 402    | CLA  | O2D-CGD-O1D | -3.00 | 117.98      | 123.84   |
| 24  | b     | 616    | CLA  | CAA-C2A-C3A | -3.00 | 104.58      | 112.78   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | d     | 402    | CLA  | CMB-C2B-C1B | 2.99  | 129.93      | 125.37   |
| 27  | f     | 101    | SQD  | O5-C5-C4    | 2.99  | 115.13      | 109.69   |
| 24  | B     | 613    | CLA  | C2A-C1A-CHA | -2.99 | 118.63      | 123.86   |
| 24  | b     | 622    | CLA  | CMB-C2B-C1B | 2.99  | 129.93      | 125.37   |
| 31  | a     | 415[A] | PL9  | C35-C34-C36 | 2.99  | 120.30      | 115.27   |
| 24  | B     | 611    | CLA  | CHC-C1C-C2C | -2.99 | 118.42      | 126.73   |
| 24  | d     | 401    | CLA  | CHD-C4C-NC  | 2.99  | 128.91      | 124.20   |
| 24  | B     | 602    | CLA  | CMB-C2B-C1B | 2.99  | 129.92      | 125.37   |
| 26  | C     | 515    | BCR  | C24-C23-C22 | -2.99 | 121.72      | 126.23   |
| 27  | L     | 102    | SQD  | O8-S-C6     | 2.99  | 110.50      | 105.74   |
| 24  | B     | 610    | CLA  | CAC-C3C-C4C | 2.99  | 128.68      | 124.81   |
| 24  | c     | 507    | CLA  | CHC-C1C-C2C | -2.99 | 118.44      | 126.73   |
| 24  | b     | 618    | CLA  | C4C-C3C-C2C | -2.99 | 102.55      | 106.90   |
| 26  | B     | 620    | BCR  | C38-C26-C25 | -2.98 | 121.18      | 124.53   |
| 24  | b     | 621    | CLA  | C1C-C2C-C3C | -2.98 | 103.82      | 106.96   |
| 24  | b     | 612    | CLA  | C4C-C3C-C2C | -2.98 | 102.55      | 106.90   |
| 24  | C     | 506    | CLA  | C1-C2-C3    | -2.98 | 120.88      | 126.04   |
| 24  | B     | 603    | CLA  | C4C-C3C-C2C | -2.98 | 102.55      | 106.90   |
| 31  | d     | 405[A] | PL9  | C10-C9-C11  | 2.98  | 120.29      | 115.27   |
| 24  | C     | 509    | CLA  | C1-O2A-CGA  | 2.98  | 124.27      | 116.44   |
| 24  | B     | 613    | CLA  | CAC-C3C-C4C | 2.98  | 128.68      | 124.81   |
| 24  | b     | 611    | CLA  | C3B-C4B-NB  | 2.98  | 113.28      | 110.52   |
| 25  | a     | 411    | PHO  | C1A-C2A-C3A | -2.98 | 100.00      | 102.84   |
| 24  | B     | 605    | CLA  | CHC-C1C-C2C | -2.98 | 118.45      | 126.73   |
| 24  | c     | 514    | CLA  | CHC-C1C-C2C | -2.98 | 118.45      | 126.73   |
| 24  | B     | 613    | CLA  | CHB-C1B-NB  | -2.98 | 121.10      | 124.26   |
| 24  | C     | 512    | CLA  | CHD-C4C-NC  | 2.98  | 128.90      | 124.20   |
| 24  | C     | 509    | CLA  | C4C-C3C-C2C | -2.98 | 102.56      | 106.90   |
| 24  | C     | 508    | CLA  | CAC-C3C-C4C | 2.97  | 128.67      | 124.81   |
| 24  | D     | 403    | CLA  | C4-C3-C5    | 2.97  | 120.26      | 115.27   |
| 24  | b     | 624    | CLA  | C4-C3-C5    | 2.97  | 120.26      | 115.27   |
| 26  | d     | 404    | BCR  | C15-C14-C13 | -2.96 | 123.08      | 127.31   |
| 24  | b     | 622    | CLA  | CED-O2D-CGD | 2.96  | 122.64      | 115.94   |
| 24  | B     | 605    | CLA  | C4C-C3C-C2C | -2.96 | 102.58      | 106.90   |
| 24  | B     | 603    | CLA  | CHC-C1C-C2C | -2.96 | 118.51      | 126.73   |
| 31  | A     | 419[B] | PL9  | C22-C23-C24 | -2.96 | 120.53      | 127.66   |
| 24  | b     | 613    | CLA  | CMB-C2B-C1B | 2.96  | 129.87      | 125.37   |
| 24  | C     | 501    | CLA  | CAC-C3C-C4C | 2.96  | 128.65      | 124.81   |
| 24  | C     | 507    | CLA  | C4C-C3C-C2C | -2.96 | 102.59      | 106.90   |
| 24  | a     | 410    | CLA  | C2A-C1A-CHA | -2.96 | 118.69      | 123.86   |
| 24  | b     | 613    | CLA  | C3D-C4D-ND  | 2.96  | 115.02      | 110.24   |
| 24  | B     | 613    | CLA  | C1-C2-C3    | -2.95 | 120.93      | 126.04   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | A     | 405    | CLA  | O2A-CGA-O1A | -2.95 | 116.14      | 123.59   |
| 24  | a     | 412    | CLA  | CAA-C2A-C3A | -2.95 | 104.69      | 112.78   |
| 24  | b     | 614    | CLA  | O2A-CGA-O1A | -2.95 | 116.14      | 123.59   |
| 24  | c     | 515    | CLA  | CBC-CAC-C3C | -2.95 | 104.29      | 112.43   |
| 35  | b     | 608    | HTG  | O5-C1-C2    | 2.95  | 114.03      | 110.31   |
| 24  | A     | 410    | CLA  | C1-C2-C3    | -2.95 | 120.94      | 126.04   |
| 24  | b     | 625    | CLA  | CHD-C4C-NC  | 2.95  | 128.85      | 124.20   |
| 24  | D     | 402    | CLA  | CMC-C2C-C1C | 2.95  | 129.53      | 125.04   |
| 37  | e     | 102    | LHG  | O7-C7-C8    | 2.95  | 117.86      | 111.50   |
| 24  | b     | 621    | CLA  | C4-C3-C5    | 2.95  | 120.23      | 115.27   |
| 24  | C     | 507    | CLA  | CHD-C4C-NC  | 2.95  | 128.85      | 124.20   |
| 24  | b     | 616    | CLA  | C4-C3-C5    | 2.95  | 120.23      | 115.27   |
| 24  | c     | 517    | CLA  | C1-C2-C3    | -2.95 | 120.94      | 126.04   |
| 26  | K     | 101    | BCR  | C7-C8-C9    | -2.95 | 121.78      | 126.23   |
| 24  | C     | 504    | CLA  | CHC-C1C-C2C | -2.95 | 118.55      | 126.73   |
| 24  | C     | 503    | CLA  | CHD-C4C-NC  | 2.95  | 128.84      | 124.20   |
| 31  | a     | 415[A] | PL9  | C53-C6-C1   | 2.95  | 121.01      | 114.99   |
| 24  | c     | 514    | CLA  | C4C-C3C-C2C | -2.94 | 102.61      | 106.90   |
| 24  | a     | 409    | CLA  | O2A-CGA-CBA | 2.94  | 121.14      | 111.91   |
| 27  | F     | 103    | SQD  | O48-C23-C24 | 2.94  | 121.13      | 111.91   |
| 31  | A     | 419[A] | PL9  | C7-C8-C9    | -2.94 | 121.90      | 126.79   |
| 24  | d     | 402    | CLA  | CHC-C1C-C2C | -2.94 | 118.57      | 126.73   |
| 38  | F     | 102    | HEM  | CHD-C1D-ND  | 2.94  | 127.61      | 124.42   |
| 24  | B     | 604    | CLA  | C4C-C3C-C2C | -2.94 | 102.62      | 106.90   |
| 24  | B     | 605    | CLA  | CMC-C2C-C1C | 2.93  | 129.51      | 125.04   |
| 31  | A     | 419[A] | PL9  | C8-C7-C3    | 2.93  | 120.27      | 111.98   |
| 24  | c     | 517    | CLA  | CHD-C4C-NC  | 2.93  | 128.83      | 124.20   |
| 24  | B     | 610    | CLA  | C4C-C3C-C2C | -2.93 | 102.62      | 106.90   |
| 24  | C     | 509    | CLA  | CMC-C2C-C1C | 2.93  | 129.50      | 125.04   |
| 24  | C     | 508    | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 24  | C     | 511    | CLA  | C4-C3-C5    | 2.93  | 120.20      | 115.27   |
| 24  | A     | 406    | CLA  | C4-C3-C5    | 2.93  | 120.19      | 115.27   |
| 31  | d     | 405[B] | PL9  | C40-C39-C41 | 2.92  | 120.19      | 115.27   |
| 24  | a     | 410    | CLA  | CMB-C2B-C1B | 2.92  | 129.82      | 125.37   |
| 35  | b     | 608    | HTG  | C1-O5-C5    | 2.92  | 117.97      | 112.58   |
| 24  | a     | 412    | CLA  | CBC-CAC-C3C | -2.92 | 104.38      | 112.43   |
| 24  | B     | 604    | CLA  | CHD-C4C-NC  | 2.92  | 128.81      | 124.20   |
| 26  | c     | 528    | BCR  | C16-C17-C18 | -2.92 | 123.14      | 127.31   |
| 24  | c     | 518    | CLA  | C1-C2-C3    | -2.92 | 120.99      | 126.04   |
| 31  | a     | 415[A] | PL9  | C40-C39-C41 | 2.92  | 120.18      | 115.27   |
| 24  | c     | 513    | CLA  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |
| 26  | y     | 101    | BCR  | C16-C17-C18 | -2.92 | 123.15      | 127.31   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | c     | 508    | CLA  | CHD-C4C-NC  | 2.92  | 128.80      | 124.20   |
| 24  | d     | 403    | CLA  | C2A-C1A-CHA | -2.92 | 118.76      | 123.86   |
| 31  | d     | 405[A] | PL9  | C37-C38-C39 | -2.92 | 120.64      | 127.66   |
| 24  | A     | 410    | CLA  | CMB-C2B-C1B | 2.92  | 129.81      | 125.37   |
| 31  | A     | 419[B] | PL9  | C27-C28-C29 | -2.91 | 120.64      | 127.66   |
| 24  | C     | 511    | CLA  | O2D-CGD-O1D | -2.91 | 118.14      | 123.84   |
| 26  | h     | 101    | BCR  | C11-C10-C9  | -2.91 | 123.15      | 127.31   |
| 24  | b     | 623    | CLA  | CHC-C1C-C2C | -2.91 | 118.64      | 126.73   |
| 24  | d     | 403    | CLA  | C3B-C4B-NB  | 2.91  | 113.22      | 110.52   |
| 24  | a     | 410    | CLA  | O2D-CGD-O1D | -2.91 | 118.15      | 123.84   |
| 36  | c     | 520    | DGD  | C2G-O2G-C1B | -2.91 | 110.62      | 117.79   |
| 24  | b     | 625    | CLA  | O2D-CGD-O1D | -2.91 | 118.15      | 123.84   |
| 26  | B     | 619    | BCR  | C33-C5-C6   | -2.91 | 121.26      | 124.53   |
| 26  | Y     | 101    | BCR  | C37-C22-C23 | 2.90  | 122.65      | 118.08   |
| 26  | B     | 619    | BCR  | C37-C22-C21 | -2.90 | 118.86      | 122.92   |
| 24  | B     | 615    | CLA  | C4-C3-C5    | 2.90  | 120.16      | 115.27   |
| 24  | C     | 502    | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.90   |
| 24  | c     | 516    | CLA  | C1-C2-C3    | -2.90 | 121.02      | 126.04   |
| 24  | b     | 622    | CLA  | C4-C3-C5    | 2.90  | 120.15      | 115.27   |
| 24  | D     | 403    | CLA  | CHC-C1C-C2C | -2.90 | 118.67      | 126.73   |
| 25  | a     | 411    | PHO  | C1-O2A-CGA  | 2.90  | 124.05      | 116.44   |
| 24  | c     | 516    | CLA  | CHD-C4C-NC  | 2.90  | 128.77      | 124.20   |
| 24  | B     | 616    | CLA  | CBC-CAC-C3C | -2.90 | 104.44      | 112.43   |
| 24  | b     | 620    | CLA  | CBC-CAC-C3C | -2.90 | 104.44      | 112.43   |
| 24  | c     | 506    | CLA  | CMC-C2C-C1C | 2.90  | 129.45      | 125.04   |
| 24  | B     | 604    | CLA  | C3B-C4B-NB  | 2.90  | 113.20      | 110.52   |
| 26  | C     | 515    | BCR  | C11-C10-C9  | -2.90 | 123.18      | 127.31   |
| 24  | b     | 614    | CLA  | C4C-C3C-C2C | -2.90 | 102.68      | 106.90   |
| 36  | C     | 517    | DGD  | C2G-O2G-C1B | -2.89 | 110.67      | 117.79   |
| 24  | b     | 624    | CLA  | CHD-C4C-NC  | 2.89  | 128.76      | 124.20   |
| 36  | D     | 406    | DGD  | O1G-C1A-C2A | 2.89  | 120.99      | 111.91   |
| 24  | B     | 617    | CLA  | CMB-C2B-C1B | 2.89  | 129.77      | 125.37   |
| 24  | b     | 611    | CLA  | CHD-C4C-NC  | 2.89  | 128.76      | 124.20   |
| 24  | A     | 407    | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 31  | A     | 419[B] | PL9  | C42-C43-C44 | -2.89 | 120.70      | 127.66   |
| 36  | C     | 517    | DGD  | O1G-C1A-C2A | 2.89  | 120.97      | 111.91   |
| 24  | B     | 603    | CLA  | C3B-C4B-NB  | 2.89  | 113.19      | 110.52   |
| 24  | b     | 612    | CLA  | O2D-CGD-O1D | -2.88 | 118.20      | 123.84   |
| 24  | C     | 501    | CLA  | C1-O2A-CGA  | 2.88  | 124.00      | 116.44   |
| 24  | B     | 614    | CLA  | CAC-C3C-C4C | 2.88  | 128.54      | 124.81   |
| 24  | c     | 507    | CLA  | C1-C2-C3    | -2.88 | 121.07      | 126.04   |
| 24  | c     | 510    | CLA  | CHC-C1C-C2C | -2.88 | 118.74      | 126.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | A     | 410    | CLA  | CAA-C2A-C3A | -2.87 | 104.91      | 112.78   |
| 31  | a     | 415[A] | PL9  | C37-C38-C39 | -2.87 | 120.74      | 127.66   |
| 24  | b     | 618    | CLA  | CHD-C4C-NC  | 2.87  | 128.73      | 124.20   |
| 24  | b     | 615    | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.90   |
| 24  | a     | 410    | CLA  | CHD-C4C-NC  | 2.87  | 128.73      | 124.20   |
| 24  | c     | 514    | CLA  | CMB-C2B-C1B | 2.87  | 129.74      | 125.37   |
| 37  | d     | 406    | LHG  | O8-C23-O10  | -2.87 | 116.35      | 123.59   |
| 26  | d     | 404    | BCR  | C29-C30-C25 | 2.87  | 114.90      | 110.48   |
| 24  | b     | 623    | CLA  | CMC-C2C-C1C | 2.87  | 129.41      | 125.04   |
| 37  | D     | 409    | LHG  | O8-C23-O10  | -2.87 | 116.36      | 123.59   |
| 24  | b     | 621    | CLA  | C1-C2-C3    | -2.87 | 121.08      | 126.04   |
| 36  | h     | 102    | DGD  | O1G-C1A-C2A | 2.87  | 120.90      | 111.91   |
| 24  | b     | 610    | CLA  | CHC-C1C-C2C | -2.87 | 118.77      | 126.73   |
| 24  | C     | 513    | CLA  | C4C-C3C-C2C | -2.86 | 102.72      | 106.90   |
| 24  | B     | 617    | CLA  | CHD-C4C-NC  | 2.86  | 128.71      | 124.20   |
| 31  | a     | 415[B] | PL9  | C35-C34-C36 | 2.86  | 120.08      | 115.27   |
| 24  | c     | 514    | CLA  | CHD-C4C-NC  | 2.86  | 128.71      | 124.20   |
| 24  | B     | 616    | CLA  | C3B-C4B-NB  | 2.86  | 113.17      | 110.52   |
| 24  | c     | 516    | CLA  | CMC-C2C-C1C | 2.86  | 129.39      | 125.04   |
| 37  | d     | 406    | LHG  | O8-C23-C24  | 2.86  | 120.88      | 111.91   |
| 26  | c     | 519    | BCR  | C38-C26-C25 | -2.86 | 121.32      | 124.53   |
| 24  | b     | 612    | CLA  | CAC-C3C-C4C | 2.86  | 128.52      | 124.81   |
| 24  | B     | 609    | CLA  | CMB-C2B-C1B | 2.86  | 129.72      | 125.37   |
| 24  | b     | 622    | CLA  | CHB-C1B-NB  | -2.86 | 121.23      | 124.26   |
| 24  | C     | 506    | CLA  | CAA-C2A-C3A | -2.86 | 104.95      | 112.78   |
| 24  | d     | 403    | CLA  | C4-C3-C5    | 2.86  | 120.08      | 115.27   |
| 31  | D     | 405[A] | PL9  | C53-C6-C1   | 2.86  | 120.83      | 114.99   |
| 24  | b     | 613    | CLA  | C4C-C3C-C2C | -2.86 | 102.74      | 106.90   |
| 24  | B     | 607    | CLA  | CHC-C1C-C2C | -2.85 | 118.80      | 126.73   |
| 40  | V     | 205    | HEC  | CHA-C1A-NA  | 2.85  | 127.53      | 124.44   |
| 24  | C     | 510    | CLA  | CHD-C4C-NC  | 2.85  | 128.70      | 124.20   |
| 24  | A     | 406    | CLA  | CAA-C2A-C3A | -2.85 | 104.97      | 112.78   |
| 31  | A     | 419[A] | PL9  | C12-C13-C14 | -2.85 | 120.80      | 127.66   |
| 24  | B     | 602    | CLA  | C4C-C3C-C2C | -2.85 | 102.74      | 106.90   |
| 24  | b     | 622    | CLA  | O2D-CGD-CBD | 2.85  | 116.33      | 111.27   |
| 24  | b     | 625    | CLA  | C1-C2-C3    | -2.85 | 121.11      | 126.04   |
| 24  | b     | 616    | CLA  | CHD-C4C-NC  | 2.85  | 128.69      | 124.20   |
| 24  | c     | 518    | CLA  | C4C-C3C-C2C | -2.85 | 102.75      | 106.90   |
| 31  | a     | 415[B] | PL9  | C53-C6-C1   | 2.85  | 120.81      | 114.99   |
| 24  | B     | 607    | CLA  | C1-C2-C3    | -2.85 | 121.12      | 126.04   |
| 24  | c     | 518    | CLA  | CHD-C4C-NC  | 2.85  | 128.69      | 124.20   |
| 24  | B     | 610    | CLA  | CHD-C4C-NC  | 2.84  | 128.69      | 124.20   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 620    | CLA  | CHD-C4C-NC  | 2.84  | 128.69      | 124.20   |
| 24  | b     | 611    | CLA  | CHC-C1C-C2C | -2.84 | 118.83      | 126.73   |
| 31  | A     | 419[B] | PL9  | C53-C6-C1   | 2.84  | 120.80      | 114.99   |
| 31  | a     | 415[B] | PL9  | C25-C24-C26 | 2.84  | 120.05      | 115.27   |
| 24  | B     | 611    | CLA  | CMB-C2B-C1B | 2.84  | 129.69      | 125.37   |
| 24  | B     | 612    | CLA  | CHC-C1C-C2C | -2.84 | 118.84      | 126.73   |
| 27  | L     | 102    | SQD  | C44-O6-C1   | -2.84 | 108.19      | 113.74   |
| 26  | Y     | 101    | BCR  | C10-C11-C12 | -2.84 | 114.36      | 123.22   |
| 24  | c     | 507    | CLA  | CAC-C3C-C4C | 2.84  | 128.49      | 124.81   |
| 31  | D     | 405[B] | PL9  | C40-C39-C41 | 2.84  | 120.04      | 115.27   |
| 24  | B     | 612    | CLA  | CMB-C2B-C1B | 2.84  | 129.69      | 125.37   |
| 38  | e     | 103    | HEM  | C4D-ND-C1D  | 2.84  | 108.00      | 105.07   |
| 24  | c     | 511    | CLA  | C4-C3-C5    | 2.83  | 120.04      | 115.27   |
| 24  | C     | 503    | CLA  | O2A-CGA-CBA | 2.83  | 120.80      | 111.91   |
| 24  | C     | 502    | CLA  | O2A-CGA-O1A | -2.83 | 116.44      | 123.59   |
| 24  | b     | 623    | CLA  | C2A-C1A-CHA | -2.83 | 118.91      | 123.86   |
| 24  | c     | 512    | CLA  | CHD-C4C-NC  | 2.83  | 128.66      | 124.20   |
| 31  | A     | 419[A] | PL9  | C27-C28-C29 | -2.83 | 120.84      | 127.66   |
| 24  | B     | 602    | CLA  | C3B-C4B-NB  | 2.83  | 113.14      | 110.52   |
| 24  | C     | 502    | CLA  | CHD-C4C-NC  | 2.83  | 128.66      | 124.20   |
| 24  | a     | 410    | CLA  | CAC-C3C-C4C | 2.83  | 128.48      | 124.81   |
| 26  | k     | 101    | BCR  | C20-C21-C22 | -2.83 | 123.28      | 127.31   |
| 24  | a     | 409    | CLA  | O2A-CGA-O1A | -2.83 | 116.46      | 123.59   |
| 24  | b     | 617    | CLA  | C4C-C3C-C2C | -2.83 | 102.78      | 106.90   |
| 24  | a     | 410    | CLA  | CAA-C2A-C3A | -2.83 | 105.04      | 112.78   |
| 24  | c     | 515    | CLA  | C4C-C3C-C2C | -2.82 | 102.78      | 106.90   |
| 24  | B     | 603    | CLA  | CAC-C3C-C4C | 2.82  | 128.47      | 124.81   |
| 24  | C     | 512    | CLA  | CHC-C1C-C2C | -2.82 | 118.90      | 126.73   |
| 24  | d     | 402    | CLA  | O2A-CGA-CBA | 2.82  | 120.76      | 111.91   |
| 36  | c     | 522    | DGD  | O1G-C1A-C2A | 2.82  | 120.76      | 111.91   |
| 24  | b     | 612    | CLA  | O2A-CGA-CBA | 2.82  | 120.74      | 111.91   |
| 31  | a     | 415[A] | PL9  | C25-C24-C26 | 2.81  | 120.00      | 115.27   |
| 24  | c     | 509    | CLA  | C4C-C3C-C2C | -2.81 | 102.80      | 106.90   |
| 35  | V     | 206    | HTG  | C1-C2-C3    | -2.81 | 105.04      | 110.59   |
| 24  | b     | 623    | CLA  | C4C-C3C-C2C | -2.81 | 102.80      | 106.90   |
| 33  | d     | 413    | LMG  | O7-C10-C11  | 2.81  | 117.56      | 111.50   |
| 24  | B     | 616    | CLA  | C4C-C3C-C2C | -2.81 | 102.80      | 106.90   |
| 24  | D     | 402    | CLA  | CHC-C1C-C2C | -2.81 | 118.93      | 126.73   |
| 24  | B     | 604    | CLA  | CMB-C2B-C1B | 2.81  | 129.64      | 125.37   |
| 24  | c     | 511    | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 24  | a     | 412    | CLA  | CHC-C1C-C2C | -2.81 | 118.94      | 126.73   |
| 27  | L     | 102    | SQD  | O7-S-C6     | 2.81  | 110.27      | 106.94   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | B     | 609    | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 24  | B     | 615    | CLA  | CHC-C1C-C2C | -2.80 | 118.94      | 126.73   |
| 38  | e     | 103    | HEM  | C4A-NA-C1A  | 2.80  | 108.09      | 105.35   |
| 24  | C     | 510    | CLA  | CHC-C1C-C2C | -2.80 | 118.95      | 126.73   |
| 24  | a     | 412    | CLA  | CHD-C4C-NC  | 2.80  | 128.61      | 124.20   |
| 24  | c     | 515    | CLA  | O2A-CGA-CBA | 2.79  | 120.67      | 111.91   |
| 24  | b     | 611    | CLA  | C4-C3-C5    | 2.79  | 119.97      | 115.27   |
| 24  | d     | 402    | CLA  | C4-C3-C5    | 2.79  | 119.97      | 115.27   |
| 24  | a     | 409    | CLA  | O2D-CGD-CBD | 2.79  | 116.23      | 111.27   |
| 31  | D     | 405[B] | PL9  | C22-C23-C24 | -2.79 | 120.94      | 127.66   |
| 24  | D     | 402    | CLA  | O2A-CGA-CBA | 2.79  | 120.67      | 111.91   |
| 24  | b     | 618    | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 24  | C     | 505    | CLA  | CMC-C2C-C1C | 2.79  | 129.29      | 125.04   |
| 24  | c     | 516    | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.90   |
| 24  | b     | 620    | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.90   |
| 24  | b     | 618    | CLA  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 24  | C     | 506    | CLA  | C4C-C3C-C2C | -2.78 | 102.84      | 106.90   |
| 24  | B     | 607    | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 24  | b     | 618    | CLA  | CHC-C1C-C2C | -2.78 | 119.00      | 126.73   |
| 31  | D     | 405[B] | PL9  | C27-C28-C29 | -2.78 | 120.96      | 127.66   |
| 24  | b     | 617    | CLA  | CBC-CAC-C3C | -2.78 | 104.77      | 112.43   |
| 26  | Y     | 101    | BCR  | C15-C14-C13 | -2.78 | 123.35      | 127.31   |
| 24  | C     | 513    | CLA  | CMB-C2B-C1B | 2.78  | 129.60      | 125.37   |
| 24  | c     | 511    | CLA  | CHD-C4C-NC  | 2.78  | 128.58      | 124.20   |
| 24  | A     | 407    | CLA  | C4C-C3C-C2C | -2.78 | 102.85      | 106.90   |
| 24  | c     | 517    | CLA  | O2A-CGA-CBA | 2.78  | 120.62      | 111.91   |
| 24  | B     | 609    | CLA  | O2A-CGA-CBA | 2.77  | 120.61      | 111.91   |
| 24  | c     | 518    | CLA  | C2A-C1A-CHA | -2.77 | 119.01      | 123.86   |
| 24  | B     | 608    | CLA  | CBC-CAC-C3C | -2.77 | 104.78      | 112.43   |
| 24  | b     | 612    | CLA  | CHD-C4C-NC  | 2.77  | 128.57      | 124.20   |
| 24  | d     | 401    | CLA  | CMA-C3A-C2A | -2.77 | 102.64      | 113.83   |
| 26  | c     | 519    | BCR  | C15-C14-C13 | -2.77 | 123.35      | 127.31   |
| 24  | c     | 510    | CLA  | C1-C2-C3    | -2.77 | 121.25      | 126.04   |
| 24  | B     | 603    | CLA  | C1-C2-C3    | -2.77 | 121.25      | 126.04   |
| 26  | K     | 101    | BCR  | C3-C4-C5    | -2.77 | 109.13      | 114.08   |
| 24  | B     | 607    | CLA  | CHD-C4C-NC  | 2.77  | 128.57      | 124.20   |
| 24  | b     | 619    | CLA  | CHC-C1C-C2C | -2.77 | 119.05      | 126.73   |
| 24  | c     | 512    | CLA  | C4-C3-C5    | 2.76  | 119.92      | 115.27   |
| 24  | b     | 615    | CLA  | CHC-C1C-C2C | -2.76 | 119.05      | 126.73   |
| 24  | B     | 609    | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.90   |
| 24  | b     | 625    | CLA  | CMB-C2B-C1B | 2.76  | 129.57      | 125.37   |
| 31  | d     | 405[B] | PL9  | C53-C6-C1   | 2.76  | 120.64      | 114.99   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 617    | CLA  | O2D-CGD-O1D | -2.76 | 118.44      | 123.84   |
| 31  | D     | 405[B] | PL9  | C25-C24-C26 | 2.76  | 119.91      | 115.27   |
| 24  | d     | 403    | CLA  | CAC-C3C-C4C | 2.76  | 128.39      | 124.81   |
| 26  | t     | 101    | BCR  | C11-C10-C9  | -2.76 | 123.37      | 127.31   |
| 24  | B     | 608    | CLA  | CHC-C1C-C2C | -2.76 | 119.07      | 126.73   |
| 24  | b     | 617    | CLA  | CHC-C1C-C2C | -2.76 | 119.07      | 126.73   |
| 24  | C     | 507    | CLA  | O2A-CGA-CBA | 2.76  | 120.57      | 111.91   |
| 24  | D     | 402    | CLA  | C2A-C1A-CHA | -2.76 | 119.03      | 123.86   |
| 38  | e     | 103    | HEM  | CAD-CBD-CGD | 2.76  | 119.53      | 113.60   |
| 24  | C     | 509    | CLA  | CHC-C1C-C2C | -2.76 | 119.08      | 126.73   |
| 24  | B     | 613    | CLA  | CBC-CAC-C3C | -2.76 | 104.83      | 112.43   |
| 24  | b     | 613    | CLA  | O2D-CGD-O1D | -2.75 | 118.45      | 123.84   |
| 24  | B     | 604    | CLA  | C2A-C1A-CHA | -2.75 | 119.05      | 123.86   |
| 31  | D     | 405[A] | PL9  | C7-C3-C4    | 2.75  | 119.11      | 116.88   |
| 24  | C     | 507    | CLA  | CAC-C3C-C4C | 2.75  | 128.38      | 124.81   |
| 31  | d     | 405[B] | PL9  | C15-C14-C16 | 2.75  | 119.90      | 115.27   |
| 24  | a     | 410    | CLA  | O2A-CGA-CBA | 2.75  | 120.55      | 111.91   |
| 24  | a     | 412    | CLA  | CMA-C3A-C2A | -2.75 | 102.72      | 113.83   |
| 40  | V     | 205    | HEC  | CHD-C1D-ND  | 2.75  | 127.77      | 124.37   |
| 24  | c     | 516    | CLA  | O2A-CGA-CBA | 2.75  | 120.54      | 111.91   |
| 31  | d     | 405[A] | PL9  | C27-C28-C29 | -2.75 | 121.04      | 127.66   |
| 24  | C     | 508    | CLA  | C1-C2-C3    | -2.75 | 121.29      | 126.04   |
| 24  | A     | 410    | CLA  | CMA-C3A-C4A | -2.75 | 104.39      | 111.77   |
| 24  | b     | 619    | CLA  | O2A-CGA-CBA | 2.75  | 120.53      | 111.91   |
| 31  | a     | 415[B] | PL9  | C40-C39-C41 | 2.75  | 119.89      | 115.27   |
| 24  | b     | 616    | CLA  | CBC-CAC-C3C | -2.75 | 104.86      | 112.43   |
| 24  | c     | 507    | CLA  | O2A-CGA-CBA | 2.74  | 120.52      | 111.91   |
| 24  | A     | 410    | CLA  | CHC-C1C-C2C | -2.74 | 119.11      | 126.73   |
| 27  | F     | 103    | SQD  | O9-S-C6     | 2.74  | 110.20      | 106.94   |
| 24  | a     | 412    | CLA  | C2A-C1A-CHA | -2.74 | 119.06      | 123.86   |
| 24  | c     | 516    | CLA  | CHC-C1C-C2C | -2.74 | 119.11      | 126.73   |
| 24  | C     | 513    | CLA  | O2A-CGA-CBA | 2.74  | 120.51      | 111.91   |
| 24  | B     | 602    | CLA  | CHC-C1C-C2C | -2.74 | 119.12      | 126.73   |
| 24  | c     | 509    | CLA  | CHC-C1C-C2C | -2.74 | 119.12      | 126.73   |
| 24  | B     | 606    | CLA  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 24  | B     | 612    | CLA  | C4C-C3C-C2C | -2.74 | 102.91      | 106.90   |
| 26  | B     | 619    | BCR  | C2-C1-C6    | 2.74  | 114.69      | 110.48   |
| 24  | C     | 513    | CLA  | CHC-C1C-C2C | -2.74 | 119.13      | 126.73   |
| 24  | c     | 518    | CLA  | O2A-CGA-CBA | 2.74  | 120.50      | 111.91   |
| 24  | c     | 514    | CLA  | O2A-CGA-CBA | 2.74  | 120.49      | 111.91   |
| 33  | z     | 101    | LMG  | O8-C28-C29  | 2.73  | 120.49      | 111.91   |
| 38  | F     | 102    | HEM  | CHB-C1B-NB  | 2.73  | 127.75      | 124.37   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 35  | B     | 625    | HTG  | C1-O5-C5    | 2.73  | 117.62      | 112.58   |
| 24  | b     | 615    | CLA  | CHD-C4C-NC  | 2.73  | 128.51      | 124.20   |
| 24  | c     | 516    | CLA  | C4-C3-C5    | 2.73  | 119.86      | 115.27   |
| 36  | C     | 516    | DGD  | C3G-C2G-C1G | -2.73 | 105.34      | 111.79   |
| 27  | B     | 621    | SQD  | C3-C4-C5    | 2.72  | 115.10      | 110.24   |
| 24  | C     | 509    | CLA  | O2A-CGA-CBA | 2.72  | 120.46      | 111.91   |
| 25  | a     | 411    | PHO  | CMA-C3A-C4A | -2.72 | 108.41      | 114.38   |
| 24  | b     | 612    | CLA  | CMA-C3A-C2A | -2.72 | 102.84      | 113.83   |
| 26  | b     | 628    | BCR  | C2-C1-C6    | 2.72  | 114.67      | 110.48   |
| 24  | c     | 518    | CLA  | CAA-C2A-C3A | -2.72 | 105.32      | 112.78   |
| 31  | d     | 405[A] | PL9  | C20-C19-C21 | 2.72  | 119.85      | 115.27   |
| 24  | B     | 615    | CLA  | C2A-C1A-CHA | -2.72 | 119.10      | 123.86   |
| 25  | A     | 409[A] | PHO  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 24  | A     | 410    | CLA  | CHB-C4A-NA  | 2.72  | 128.27      | 124.51   |
| 24  | B     | 603    | CLA  | CHD-C4C-NC  | 2.72  | 128.49      | 124.20   |
| 24  | c     | 517    | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 24  | b     | 616    | CLA  | C4C-C3C-C2C | -2.72 | 102.94      | 106.90   |
| 24  | c     | 509    | CLA  | CMB-C2B-C1B | 2.72  | 129.51      | 125.37   |
| 25  | A     | 409[A] | PHO  | C4A-C3A-C2A | -2.71 | 100.26      | 102.84   |
| 33  | b     | 629    | LMG  | O8-C28-C29  | 2.71  | 120.42      | 111.91   |
| 24  | D     | 403    | CLA  | C2A-C1A-CHA | -2.71 | 119.11      | 123.86   |
| 31  | A     | 419[B] | PL9  | C45-C44-C46 | 2.71  | 119.83      | 115.27   |
| 24  | B     | 606    | CLA  | O2A-CGA-O1A | -2.71 | 116.75      | 123.59   |
| 24  | b     | 623    | CLA  | CBC-CAC-C3C | -2.71 | 104.96      | 112.43   |
| 24  | c     | 512    | CLA  | CHC-C1C-C2C | -2.71 | 119.20      | 126.73   |
| 35  | b     | 632    | HTG  | C1-O5-C5    | 2.71  | 117.58      | 112.58   |
| 24  | D     | 402    | CLA  | CAA-C2A-C3A | -2.71 | 105.36      | 112.78   |
| 24  | B     | 606    | CLA  | O2A-CGA-CBA | 2.71  | 120.40      | 111.91   |
| 24  | B     | 613    | CLA  | CHD-C4C-NC  | 2.71  | 128.47      | 124.20   |
| 24  | b     | 619    | CLA  | CHD-C4C-NC  | 2.71  | 128.47      | 124.20   |
| 26  | b     | 628    | BCR  | C24-C23-C22 | -2.71 | 122.15      | 126.23   |
| 31  | A     | 419[B] | PL9  | C15-C14-C16 | 2.71  | 119.82      | 115.27   |
| 25  | a     | 418[B] | PHO  | C4D-CHA-CBD | 2.71  | 109.74      | 108.52   |
| 40  | v     | 205    | HEC  | C3C-C4C-NC  | -2.70 | 107.12      | 110.15   |
| 24  | C     | 502    | CLA  | CHC-C1C-C2C | -2.70 | 119.22      | 126.73   |
| 31  | d     | 405[B] | PL9  | C20-C19-C21 | 2.70  | 119.82      | 115.27   |
| 27  | a     | 414    | SQD  | C45-O47-C7  | -2.70 | 111.14      | 117.79   |
| 26  | B     | 620    | BCR  | C10-C11-C12 | -2.70 | 114.78      | 123.22   |
| 29  | f     | 102    | LMT  | C1B-O5B-C5B | 2.70  | 118.99      | 113.69   |
| 31  | a     | 415[B] | PL9  | C30-C29-C31 | 2.70  | 119.81      | 115.27   |
| 27  | L     | 102    | SQD  | O48-C23-C24 | 2.70  | 120.37      | 111.91   |
| 24  | C     | 503    | CLA  | CMC-C2C-C1C | 2.70  | 129.15      | 125.04   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 511    | CLA  | CMB-C2B-C1B | 2.70  | 129.48      | 125.37   |
| 24  | C     | 501    | CLA  | CHD-C4C-NC  | 2.70  | 128.45      | 124.20   |
| 31  | A     | 419[B] | PL9  | C25-C24-C26 | 2.70  | 119.81      | 115.27   |
| 24  | C     | 506    | CLA  | O2D-CGD-O1D | -2.69 | 118.57      | 123.84   |
| 24  | c     | 510    | CLA  | C4-C3-C5    | 2.69  | 119.80      | 115.27   |
| 24  | B     | 614    | CLA  | CMB-C2B-C1B | 2.69  | 129.47      | 125.37   |
| 25  | a     | 418[A] | PHO  | CMB-C2B-C3B | 2.69  | 129.72      | 124.68   |
| 24  | a     | 409    | CLA  | C2A-C1A-CHA | -2.69 | 119.15      | 123.86   |
| 24  | b     | 611    | CLA  | CAC-C3C-C4C | 2.69  | 128.30      | 124.81   |
| 24  | d     | 403    | CLA  | CAA-C2A-C3A | -2.69 | 105.42      | 112.78   |
| 24  | d     | 402    | CLA  | C4C-C3C-C2C | -2.69 | 102.98      | 106.90   |
| 25  | A     | 409[A] | PHO  | C1A-C2A-C3A | -2.69 | 100.28      | 102.84   |
| 24  | b     | 618    | CLA  | O2A-CGA-O1A | -2.68 | 116.82      | 123.59   |
| 24  | d     | 401    | CLA  | C4C-C3C-C2C | -2.68 | 102.99      | 106.90   |
| 24  | d     | 401    | CLA  | CMB-C2B-C1B | 2.68  | 129.45      | 125.37   |
| 24  | a     | 409    | CLA  | C4C-C3C-C2C | -2.68 | 102.99      | 106.90   |
| 26  | h     | 101    | BCR  | C7-C8-C9    | -2.68 | 122.19      | 126.23   |
| 27  | A     | 412    | SQD  | O48-C23-C24 | 2.68  | 120.32      | 111.91   |
| 24  | d     | 403    | CLA  | C4C-C3C-C2C | -2.68 | 102.99      | 106.90   |
| 24  | B     | 602    | CLA  | C2A-C1A-CHA | -2.68 | 119.17      | 123.86   |
| 24  | a     | 412    | CLA  | C4C-C3C-C2C | -2.68 | 102.99      | 106.90   |
| 24  | B     | 609    | CLA  | CBC-CAC-C3C | -2.68 | 105.05      | 112.43   |
| 24  | b     | 621    | CLA  | CHC-C1C-C2C | -2.68 | 119.30      | 126.73   |
| 24  | C     | 511    | CLA  | CHD-C4C-NC  | 2.68  | 128.42      | 124.20   |
| 26  | C     | 514    | BCR  | C20-C21-C22 | -2.68 | 123.49      | 127.31   |
| 24  | c     | 514    | CLA  | CMC-C2C-C1C | 2.67  | 129.11      | 125.04   |
| 24  | c     | 507    | CLA  | CHD-C4C-NC  | 2.67  | 128.42      | 124.20   |
| 35  | c     | 526    | HTG  | C1-O5-C5    | 2.67  | 117.51      | 112.58   |
| 24  | b     | 617    | CLA  | CHD-C4C-NC  | 2.67  | 128.41      | 124.20   |
| 25  | a     | 418[B] | PHO  | CMA-C3A-C4A | -2.67 | 108.53      | 114.38   |
| 24  | B     | 607    | CLA  | O2A-CGA-CBA | 2.67  | 120.29      | 111.91   |
| 24  | A     | 407    | CLA  | CMC-C2C-C1C | 2.67  | 129.10      | 125.04   |
| 31  | d     | 405[B] | PL9  | C10-C9-C11  | 2.67  | 119.76      | 115.27   |
| 36  | C     | 516    | DGD  | O1G-C1A-O1A | -2.67 | 116.86      | 123.59   |
| 24  | C     | 513    | CLA  | CHD-C4C-NC  | 2.67  | 128.41      | 124.20   |
| 24  | b     | 615    | CLA  | O2A-CGA-CBA | 2.67  | 120.28      | 111.91   |
| 24  | c     | 508    | CLA  | C1C-C2C-C3C | -2.67 | 104.15      | 106.96   |
| 36  | h     | 102    | DGD  | O1G-C1A-O1A | -2.67 | 116.86      | 123.59   |
| 24  | A     | 405    | CLA  | CAA-C2A-C1A | -2.66 | 103.25      | 111.97   |
| 24  | C     | 505    | CLA  | CHC-C1C-C2C | -2.66 | 119.33      | 126.73   |
| 24  | C     | 504    | CLA  | C2A-C1A-CHA | -2.66 | 119.20      | 123.86   |
| 26  | Y     | 101    | BCR  | C16-C17-C18 | -2.66 | 123.51      | 127.31   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 33  | c     | 501    | LMG  | O8-C28-C29  | 2.66  | 120.26      | 111.91   |
| 24  | C     | 506    | CLA  | CMC-C2C-C1C | 2.66  | 129.09      | 125.04   |
| 26  | t     | 101    | BCR  | C1-C6-C7    | 2.66  | 123.31      | 115.78   |
| 24  | c     | 517    | CLA  | C4C-C3C-C2C | -2.66 | 103.02      | 106.90   |
| 24  | B     | 611    | CLA  | CMA-C3A-C4A | -2.66 | 104.63      | 111.77   |
| 31  | A     | 419[A] | PL9  | C25-C24-C26 | 2.66  | 119.74      | 115.27   |
| 24  | B     | 606    | CLA  | CAC-C3C-C4C | 2.66  | 128.26      | 124.81   |
| 24  | b     | 611    | CLA  | O2A-CGA-CBA | 2.66  | 120.25      | 111.91   |
| 31  | D     | 405[A] | PL9  | C25-C24-C26 | 2.66  | 119.74      | 115.27   |
| 25  | A     | 409[B] | PHO  | O2D-CGD-O1D | -2.66 | 118.65      | 123.84   |
| 24  | B     | 614    | CLA  | CHC-C1C-C2C | -2.66 | 119.36      | 126.73   |
| 24  | c     | 512    | CLA  | C3B-C4B-NB  | 2.65  | 112.98      | 110.52   |
| 37  | e     | 102    | LHG  | O8-C23-C24  | 2.65  | 120.24      | 111.91   |
| 27  | F     | 103    | SQD  | C44-O6-C1   | -2.65 | 108.56      | 113.74   |
| 24  | c     | 509    | CLA  | CBC-CAC-C3C | -2.65 | 105.12      | 112.43   |
| 24  | B     | 609    | CLA  | CMA-C3A-C4A | -2.65 | 104.65      | 111.77   |
| 35  | V     | 206    | HTG  | O5-C1-C2    | -2.65 | 106.98      | 110.31   |
| 24  | b     | 616    | CLA  | O2D-CGD-O1D | -2.65 | 118.66      | 123.84   |
| 27  | F     | 103    | SQD  | C3-C4-C5    | 2.65  | 114.96      | 110.24   |
| 40  | V     | 205    | HEC  | CAB-C3B-C4B | 2.65  | 128.25      | 124.81   |
| 26  | c     | 519    | BCR  | C3-C4-C5    | -2.65 | 109.35      | 114.08   |
| 24  | c     | 517    | CLA  | CMB-C2B-C1B | 2.65  | 129.40      | 125.37   |
| 24  | C     | 501    | CLA  | CHC-C1C-C2C | -2.65 | 119.38      | 126.73   |
| 24  | C     | 504    | CLA  | C1-O2A-CGA  | 2.64  | 123.38      | 116.44   |
| 38  | e     | 103    | HEM  | CHA-C4D-ND  | 2.64  | 127.63      | 124.37   |
| 24  | c     | 509    | CLA  | CHD-C4C-NC  | 2.64  | 128.36      | 124.20   |
| 31  | A     | 419[A] | PL9  | C30-C29-C31 | 2.64  | 119.71      | 115.27   |
| 24  | b     | 614    | CLA  | C3B-C4B-NB  | 2.64  | 112.96      | 110.52   |
| 24  | b     | 618    | CLA  | CMC-C2C-C1C | 2.64  | 129.06      | 125.04   |
| 24  | B     | 607    | CLA  | O2A-CGA-O1A | -2.64 | 116.94      | 123.59   |
| 26  | B     | 620    | BCR  | C2-C1-C6    | 2.64  | 114.54      | 110.48   |
| 24  | B     | 616    | CLA  | CAC-C3C-C4C | 2.63  | 128.23      | 124.81   |
| 24  | d     | 403    | CLA  | CHC-C1C-C2C | -2.63 | 119.42      | 126.73   |
| 33  | Z     | 101    | LMG  | C1-O6-C5    | 2.63  | 118.85      | 113.69   |
| 27  | A     | 412    | SQD  | O48-C23-O10 | -2.63 | 116.95      | 123.59   |
| 36  | C     | 518    | DGD  | O1G-C1A-C2A | 2.63  | 120.16      | 111.91   |
| 24  | A     | 406    | CLA  | CHB-C1B-NB  | -2.63 | 121.47      | 124.26   |
| 26  | t     | 101    | BCR  | C15-C14-C13 | 2.63  | 131.06      | 127.31   |
| 24  | b     | 613    | CLA  | O2A-CGA-CBA | 2.63  | 120.16      | 111.91   |
| 24  | b     | 614    | CLA  | CHC-C1C-C2C | -2.63 | 119.43      | 126.73   |
| 31  | d     | 405[A] | PL9  | C53-C6-C1   | 2.63  | 120.36      | 114.99   |
| 27  | A     | 416    | SQD  | O48-C23-O10 | -2.63 | 116.96      | 123.59   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 501    | CLA  | C4-C3-C5    | 2.63  | 119.69      | 115.27   |
| 24  | c     | 511    | CLA  | C4C-C3C-C2C | -2.63 | 103.07      | 106.90   |
| 24  | C     | 505    | CLA  | C3B-C4B-NB  | 2.63  | 112.95      | 110.52   |
| 24  | a     | 410    | CLA  | C3B-C4B-NB  | 2.63  | 112.95      | 110.52   |
| 24  | c     | 517    | CLA  | CBC-CAC-C3C | -2.63 | 105.19      | 112.43   |
| 36  | H     | 102    | DGD  | O1G-C1A-O1A | -2.63 | 116.97      | 123.59   |
| 27  | B     | 621    | SQD  | O48-C23-C24 | 2.63  | 120.15      | 111.91   |
| 24  | a     | 412    | CLA  | CMC-C2C-C1C | 2.63  | 129.04      | 125.04   |
| 24  | C     | 507    | CLA  | CHC-C1C-C2C | -2.62 | 119.44      | 126.73   |
| 24  | b     | 619    | CLA  | C4-C3-C5    | 2.62  | 119.68      | 115.27   |
| 24  | c     | 517    | CLA  | C3B-C4B-NB  | 2.62  | 112.95      | 110.52   |
| 26  | B     | 619    | BCR  | C31-C1-C6   | -2.62 | 106.05      | 110.30   |
| 24  | B     | 609    | CLA  | CAC-C3C-C4C | 2.62  | 128.21      | 124.81   |
| 24  | b     | 613    | CLA  | C1-C2-C3    | -2.62 | 121.52      | 126.04   |
| 24  | B     | 605    | CLA  | O2A-CGA-O1A | -2.62 | 116.99      | 123.59   |
| 24  | A     | 410    | CLA  | CMC-C2C-C1C | 2.62  | 129.02      | 125.04   |
| 24  | B     | 609    | CLA  | CHB-C4A-NA  | 2.61  | 128.13      | 124.51   |
| 26  | T     | 103    | BCR  | C35-C13-C12 | 2.61  | 122.20      | 118.08   |
| 36  | e     | 101    | DGD  | C1E-O6E-C5E | 2.61  | 118.82      | 113.69   |
| 24  | b     | 618    | CLA  | C3B-C4B-NB  | 2.61  | 112.94      | 110.52   |
| 31  | D     | 405[A] | PL9  | C37-C38-C39 | -2.61 | 121.37      | 127.66   |
| 24  | B     | 617    | CLA  | C2A-C1A-CHA | -2.61 | 119.29      | 123.86   |
| 24  | c     | 512    | CLA  | C1-C2-C3    | -2.61 | 121.52      | 126.04   |
| 26  | b     | 627    | BCR  | C37-C22-C21 | -2.61 | 119.26      | 122.92   |
| 24  | c     | 510    | CLA  | C3B-C4B-NB  | 2.61  | 112.94      | 110.52   |
| 24  | B     | 607    | CLA  | C4C-C3C-C2C | -2.61 | 103.09      | 106.90   |
| 24  | c     | 515    | CLA  | CHD-C4C-NC  | 2.61  | 128.32      | 124.20   |
| 24  | C     | 508    | CLA  | C4-C3-C5    | 2.61  | 119.66      | 115.27   |
| 24  | c     | 509    | CLA  | C2A-C1A-CHA | -2.61 | 119.29      | 123.86   |
| 31  | D     | 405[A] | PL9  | C22-C23-C24 | -2.61 | 121.37      | 127.66   |
| 31  | A     | 419[B] | PL9  | C30-C29-C31 | 2.61  | 119.66      | 115.27   |
| 24  | B     | 614    | CLA  | CMC-C2C-C1C | 2.61  | 129.01      | 125.04   |
| 33  | c     | 501    | LMG  | C7-O1-C1    | -2.61 | 108.64      | 113.74   |
| 24  | b     | 623    | CLA  | O2A-CGA-CBA | 2.61  | 120.09      | 111.91   |
| 24  | D     | 403    | CLA  | CAA-C2A-C3A | -2.61 | 105.64      | 112.78   |
| 31  | d     | 405[B] | PL9  | C12-C13-C14 | -2.61 | 121.38      | 127.66   |
| 26  | t     | 101    | BCR  | C20-C21-C22 | -2.60 | 123.59      | 127.31   |
| 24  | c     | 518    | CLA  | CHC-C1C-C2C | -2.60 | 119.50      | 126.73   |
| 26  | y     | 101    | BCR  | C10-C11-C12 | -2.60 | 115.09      | 123.22   |
| 24  | C     | 513    | CLA  | C4-C3-C5    | 2.60  | 119.65      | 115.27   |
| 24  | b     | 620    | CLA  | O2A-CGA-O1A | -2.60 | 117.03      | 123.59   |
| 26  | T     | 103    | BCR  | C34-C9-C10  | -2.60 | 119.28      | 122.92   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31  | A     | 419[A] | PL9  | C15-C14-C16 | 2.60  | 119.65      | 115.27   |
| 38  | e     | 103    | HEM  | CHA-C1A-NA  | 2.60  | 128.63      | 123.85   |
| 24  | c     | 518    | CLA  | C4-C3-C5    | 2.60  | 119.64      | 115.27   |
| 26  | t     | 101    | BCR  | C3-C4-C5    | -2.60 | 109.44      | 114.08   |
| 31  | a     | 415[A] | PL9  | C30-C29-C31 | 2.60  | 119.64      | 115.27   |
| 24  | b     | 615    | CLA  | CAC-C3C-C4C | 2.60  | 128.18      | 124.81   |
| 24  | D     | 402    | CLA  | C4-C3-C5    | 2.60  | 119.64      | 115.27   |
| 24  | B     | 606    | CLA  | C1-C2-C3    | -2.60 | 121.55      | 126.04   |
| 26  | h     | 101    | BCR  | C16-C15-C14 | -2.60 | 118.16      | 123.47   |
| 26  | d     | 404    | BCR  | C28-C27-C26 | -2.59 | 109.44      | 114.08   |
| 24  | B     | 612    | CLA  | O2D-CGD-O1D | -2.59 | 118.77      | 123.84   |
| 37  | d     | 408    | LHG  | O8-C23-C24  | 2.59  | 120.05      | 111.91   |
| 24  | a     | 410    | CLA  | C4-C3-C5    | 2.59  | 119.63      | 115.27   |
| 37  | D     | 407    | LHG  | C5-O7-C7    | -2.59 | 111.41      | 117.79   |
| 24  | b     | 617    | CLA  | O2A-CGA-CBA | 2.59  | 120.04      | 111.91   |
| 24  | a     | 409    | CLA  | CAC-C3C-C4C | 2.59  | 128.17      | 124.81   |
| 24  | C     | 511    | CLA  | CBC-CAC-C3C | -2.59 | 105.29      | 112.43   |
| 24  | b     | 625    | CLA  | C4-C3-C5    | 2.59  | 119.63      | 115.27   |
| 24  | C     | 502    | CLA  | CMC-C2C-C1C | 2.59  | 128.98      | 125.04   |
| 36  | C     | 516    | DGD  | O3G-C3G-C2G | -2.59 | 104.65      | 110.90   |
| 31  | A     | 419[B] | PL9  | C12-C13-C14 | -2.59 | 121.43      | 127.66   |
| 24  | B     | 610    | CLA  | CBC-CAC-C3C | -2.59 | 105.30      | 112.43   |
| 24  | A     | 407    | CLA  | CAA-C2A-C3A | -2.59 | 105.70      | 112.78   |
| 24  | b     | 618    | CLA  | O2A-CGA-CBA | 2.58  | 120.01      | 111.91   |
| 24  | c     | 506    | CLA  | CBC-CAC-C3C | -2.58 | 105.31      | 112.43   |
| 24  | c     | 517    | CLA  | CHC-C1C-C2C | -2.58 | 119.56      | 126.73   |
| 24  | C     | 511    | CLA  | O2A-CGA-CBA | 2.58  | 120.01      | 111.91   |
| 24  | C     | 513    | CLA  | O2D-CGD-O1D | -2.58 | 118.80      | 123.84   |
| 24  | B     | 609    | CLA  | CMC-C2C-C1C | 2.58  | 128.97      | 125.04   |
| 24  | B     | 608    | CLA  | C2A-C1A-CHA | -2.58 | 119.35      | 123.86   |
| 24  | C     | 504    | CLA  | CHD-C4C-NC  | 2.58  | 128.26      | 124.20   |
| 24  | c     | 508    | CLA  | C2A-C1A-CHA | -2.58 | 119.35      | 123.86   |
| 24  | C     | 503    | CLA  | CHC-C1C-C2C | -2.58 | 119.57      | 126.73   |
| 33  | c     | 523    | LMG  | C8-O7-C10   | -2.58 | 111.45      | 117.79   |
| 24  | B     | 614    | CLA  | C4-C3-C5    | 2.57  | 119.60      | 115.27   |
| 24  | C     | 505    | CLA  | CHD-C4C-NC  | 2.57  | 128.26      | 124.20   |
| 35  | C     | 523    | HTG  | O5-C1-C2    | 2.57  | 113.55      | 110.31   |
| 24  | c     | 509    | CLA  | O2A-CGA-O1A | -2.57 | 117.10      | 123.59   |
| 24  | b     | 623    | CLA  | CAC-C3C-C4C | 2.57  | 128.15      | 124.81   |
| 36  | c     | 520    | DGD  | O2G-C1B-O1B | -2.57 | 117.49      | 123.70   |
| 36  | C     | 517    | DGD  | O1G-C1A-O1A | -2.57 | 117.11      | 123.59   |
| 26  | H     | 101    | BCR  | C10-C11-C12 | -2.57 | 115.20      | 123.22   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 27  | A     | 416    | SQD  | O8-S-C6     | 2.57  | 109.83      | 105.74   |
| 27  | L     | 102    | SQD  | O47-C7-O49  | -2.57 | 117.50      | 123.70   |
| 27  | f     | 101    | SQD  | O7-S-C6     | 2.57  | 109.99      | 106.94   |
| 24  | c     | 513    | CLA  | C4-C3-C5    | 2.57  | 119.59      | 115.27   |
| 24  | C     | 510    | CLA  | CAC-C3C-C4C | 2.57  | 128.14      | 124.81   |
| 33  | C     | 520    | LMG  | O8-C28-C29  | 2.56  | 119.95      | 111.91   |
| 27  | f     | 101    | SQD  | O47-C7-O49  | -2.56 | 117.51      | 123.70   |
| 26  | h     | 101    | BCR  | C10-C11-C12 | -2.56 | 115.22      | 123.22   |
| 24  | b     | 614    | CLA  | O2A-CGA-CBA | 2.56  | 119.94      | 111.91   |
| 24  | C     | 504    | CLA  | C4C-C3C-C2C | -2.56 | 103.17      | 106.90   |
| 24  | B     | 614    | CLA  | CHB-C1B-NB  | -2.56 | 121.55      | 124.26   |
| 24  | b     | 618    | CLA  | C2A-C1A-CHA | -2.56 | 119.38      | 123.86   |
| 31  | D     | 405[B] | PL9  | C53-C6-C1   | 2.56  | 120.22      | 114.99   |
| 24  | b     | 619    | CLA  | CMB-C2B-C1B | 2.56  | 129.27      | 125.37   |
| 24  | d     | 403    | CLA  | O2D-CGD-O1D | -2.56 | 118.84      | 123.84   |
| 24  | c     | 509    | CLA  | O2D-CGD-O1D | -2.56 | 118.84      | 123.84   |
| 33  | D     | 413    | LMG  | C7-O1-C1    | -2.56 | 108.74      | 113.74   |
| 27  | a     | 414    | SQD  | O48-C23-C24 | 2.56  | 119.93      | 111.91   |
| 24  | b     | 617    | CLA  | CAC-C3C-C4C | 2.56  | 128.13      | 124.81   |
| 24  | C     | 509    | CLA  | CHD-C4C-NC  | 2.56  | 128.23      | 124.20   |
| 36  | e     | 101    | DGD  | O1G-C1A-C2A | 2.55  | 119.92      | 111.91   |
| 31  | a     | 415[A] | PL9  | C51-C49-C50 | 2.55  | 120.25      | 114.60   |
| 26  | B     | 618    | BCR  | C15-C14-C13 | -2.55 | 123.67      | 127.31   |
| 24  | b     | 623    | CLA  | CHD-C4C-NC  | 2.55  | 128.23      | 124.20   |
| 24  | B     | 608    | CLA  | C4-C3-C5    | 2.55  | 119.57      | 115.27   |
| 24  | b     | 624    | CLA  | CBC-CAC-C3C | -2.55 | 105.39      | 112.43   |
| 24  | b     | 612    | CLA  | O2A-CGA-O1A | -2.55 | 117.15      | 123.59   |
| 24  | b     | 614    | CLA  | CMB-C2B-C1B | 2.55  | 129.26      | 125.37   |
| 24  | b     | 612    | CLA  | CHC-C1C-C2C | -2.55 | 119.64      | 126.73   |
| 31  | D     | 405[A] | PL9  | C27-C28-C29 | -2.55 | 121.52      | 127.66   |
| 24  | C     | 513    | CLA  | C3B-C4B-NB  | 2.55  | 112.88      | 110.52   |
| 31  | a     | 415[B] | PL9  | C51-C49-C50 | 2.55  | 120.23      | 114.60   |
| 24  | b     | 623    | CLA  | CMB-C2B-C1B | 2.55  | 129.25      | 125.37   |
| 24  | C     | 502    | CLA  | C4-C3-C5    | 2.55  | 119.56      | 115.27   |
| 37  | L     | 101    | LHG  | O8-C23-C24  | 2.55  | 119.90      | 111.91   |
| 24  | b     | 620    | CLA  | O2A-CGA-CBA | 2.54  | 119.89      | 111.91   |
| 24  | c     | 510    | CLA  | CMC-C2C-C1C | 2.54  | 128.91      | 125.04   |
| 24  | B     | 608    | CLA  | CMB-C2B-C1B | 2.54  | 129.24      | 125.37   |
| 24  | C     | 509    | CLA  | C4-C3-C5    | 2.54  | 119.55      | 115.27   |
| 24  | b     | 619    | CLA  | CAA-C2A-C3A | -2.54 | 105.82      | 112.78   |
| 26  | y     | 101    | BCR  | C24-C23-C22 | -2.54 | 122.39      | 126.23   |
| 24  | c     | 509    | CLA  | CAC-C3C-C4C | 2.54  | 128.11      | 124.81   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 612    | CLA  | C2A-C1A-CHA | -2.54 | 119.42      | 123.86   |
| 24  | b     | 619    | CLA  | O2D-CGD-O1D | -2.54 | 118.87      | 123.84   |
| 24  | c     | 506    | CLA  | CMB-C2B-C1B | 2.54  | 129.24      | 125.37   |
| 24  | B     | 605    | CLA  | CMB-C2B-C1B | 2.54  | 129.23      | 125.37   |
| 31  | A     | 419[B] | PL9  | C17-C18-C19 | -2.54 | 121.56      | 127.66   |
| 24  | b     | 625    | CLA  | C1C-C2C-C3C | -2.53 | 104.29      | 106.96   |
| 24  | B     | 617    | CLA  | C1-O2A-CGA  | 2.53  | 123.09      | 116.44   |
| 24  | A     | 407    | CLA  | CHC-C1C-C2C | -2.53 | 119.69      | 126.73   |
| 24  | C     | 513    | CLA  | CAC-C3C-C4C | 2.53  | 128.09      | 124.81   |
| 31  | D     | 405[B] | PL9  | C20-C19-C21 | 2.53  | 119.53      | 115.27   |
| 27  | f     | 101    | SQD  | O48-C23-C24 | 2.53  | 119.85      | 111.91   |
| 24  | B     | 608    | CLA  | CHD-C4C-NC  | 2.53  | 128.19      | 124.20   |
| 24  | B     | 611    | CLA  | C4-C3-C5    | 2.53  | 119.53      | 115.27   |
| 26  | K     | 101    | BCR  | C20-C21-C22 | -2.53 | 123.70      | 127.31   |
| 24  | C     | 501    | CLA  | C4C-C3C-C2C | -2.52 | 103.22      | 106.90   |
| 24  | C     | 502    | CLA  | CAC-C3C-C4C | 2.52  | 128.08      | 124.81   |
| 24  | C     | 511    | CLA  | CMC-C2C-C1C | 2.52  | 128.88      | 125.04   |
| 36  | C     | 516    | DGD  | C2G-O2G-C1B | -2.52 | 111.58      | 117.79   |
| 24  | c     | 517    | CLA  | CBA-CAA-C2A | -2.52 | 106.42      | 113.86   |
| 24  | b     | 614    | CLA  | CAC-C3C-C2C | 2.52  | 131.84      | 127.53   |
| 24  | B     | 611    | CLA  | CBC-CAC-C3C | -2.52 | 105.48      | 112.43   |
| 24  | B     | 611    | CLA  | CHD-C4C-NC  | 2.52  | 128.17      | 124.20   |
| 24  | C     | 512    | CLA  | CMC-C2C-C1C | 2.52  | 128.88      | 125.04   |
| 25  | A     | 408    | PHO  | C4-C3-C5    | 2.52  | 119.50      | 115.27   |
| 25  | A     | 409[B] | PHO  | C4D-CHA-CBD | 2.52  | 109.66      | 108.52   |
| 26  | H     | 101    | BCR  | C7-C8-C9    | -2.51 | 122.44      | 126.23   |
| 25  | A     | 408    | PHO  | CMA-C3A-C4A | -2.51 | 108.87      | 114.38   |
| 24  | B     | 603    | CLA  | C2A-C1A-CHA | -2.51 | 119.46      | 123.86   |
| 24  | B     | 609    | CLA  | CHD-C4C-NC  | 2.51  | 128.16      | 124.20   |
| 24  | B     | 615    | CLA  | CHD-C4C-NC  | 2.51  | 128.16      | 124.20   |
| 24  | b     | 620    | CLA  | O2D-CGD-O1D | -2.51 | 118.94      | 123.84   |
| 24  | C     | 505    | CLA  | CHB-C1B-NB  | -2.51 | 121.60      | 124.26   |
| 35  | B     | 624    | HTG  | C1-C2-C3    | 2.51  | 115.54      | 110.59   |
| 24  | A     | 406    | CLA  | O2A-CGA-O1A | -2.50 | 117.27      | 123.59   |
| 24  | b     | 620    | CLA  | CMC-C2C-C1C | 2.50  | 128.85      | 125.04   |
| 33  | c     | 524    | LMG  | O8-C28-C29  | 2.50  | 119.77      | 111.91   |
| 38  | F     | 102    | HEM  | CHA-C1A-NA  | 2.50  | 128.45      | 123.85   |
| 26  | h     | 101    | BCR  | C20-C21-C22 | -2.50 | 123.74      | 127.31   |
| 24  | c     | 512    | CLA  | O2A-CGA-CBA | 2.50  | 119.76      | 111.91   |
| 24  | C     | 502    | CLA  | CBC-CAC-C3C | -2.50 | 105.53      | 112.43   |
| 24  | C     | 509    | CLA  | CHB-C1B-NB  | -2.50 | 121.61      | 124.26   |
| 26  | k     | 101    | BCR  | C11-C10-C9  | -2.50 | 123.74      | 127.31   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 27  | A     | 412    | SQD  | C1-C2-C3    | -2.50 | 104.79      | 110.00   |
| 24  | c     | 507    | CLA  | O2D-CGD-O1D | -2.50 | 118.95      | 123.84   |
| 24  | c     | 514    | CLA  | C4-C3-C5    | 2.50  | 119.47      | 115.27   |
| 31  | a     | 415[A] | PL9  | C7-C3-C2    | -2.50 | 120.01      | 123.30   |
| 26  | t     | 101    | BCR  | C7-C6-C5    | -2.50 | 115.41      | 121.46   |
| 24  | C     | 507    | CLA  | O2A-CGA-O1A | -2.50 | 117.29      | 123.59   |
| 24  | c     | 515    | CLA  | CMB-C2B-C1B | 2.50  | 129.17      | 125.37   |
| 26  | K     | 101    | BCR  | C2-C1-C6    | 2.50  | 114.32      | 110.48   |
| 24  | C     | 513    | CLA  | CMC-C2C-C1C | 2.50  | 128.84      | 125.04   |
| 31  | A     | 419[A] | PL9  | C42-C43-C44 | -2.50 | 121.65      | 127.66   |
| 29  | m     | 103    | LMT  | O5'-C5'-C4' | 2.49  | 115.01      | 109.75   |
| 24  | A     | 405    | CLA  | CMA-C3A-C4A | -2.49 | 105.07      | 111.77   |
| 24  | B     | 617    | CLA  | O2A-CGA-CBA | 2.49  | 119.73      | 111.91   |
| 24  | c     | 513    | CLA  | CAA-C2A-C3A | -2.49 | 105.95      | 112.78   |
| 24  | C     | 511    | CLA  | CHB-C1B-NB  | -2.49 | 121.62      | 124.26   |
| 24  | a     | 410    | CLA  | CHC-C1C-C2C | -2.49 | 119.81      | 126.73   |
| 24  | b     | 624    | CLA  | CMC-C2C-C1C | 2.49  | 128.83      | 125.04   |
| 24  | d     | 401    | CLA  | CHB-C1B-NB  | -2.49 | 121.62      | 124.26   |
| 24  | A     | 405    | CLA  | C2A-C1A-CHA | -2.49 | 119.51      | 123.86   |
| 24  | d     | 402    | CLA  | CMC-C2C-C1C | 2.49  | 128.83      | 125.04   |
| 38  | e     | 103    | HEM  | CHD-C1D-C2D | -2.49 | 121.09      | 124.98   |
| 26  | C     | 515    | BCR  | C21-C20-C19 | -2.48 | 115.48      | 123.22   |
| 26  | T     | 103    | BCR  | C21-C20-C19 | -2.48 | 115.48      | 123.22   |
| 24  | b     | 625    | CLA  | CHB-C1B-NB  | -2.48 | 121.63      | 124.26   |
| 24  | C     | 506    | CLA  | CHD-C4C-NC  | 2.48  | 128.11      | 124.20   |
| 24  | C     | 511    | CLA  | C1-C2-C3    | -2.48 | 121.76      | 126.04   |
| 24  | B     | 603    | CLA  | CMB-C2B-C1B | 2.48  | 129.14      | 125.37   |
| 31  | D     | 405[A] | PL9  | C42-C41-C39 | -2.48 | 104.83      | 112.98   |
| 24  | B     | 609    | CLA  | CAA-C2A-C3A | -2.47 | 106.01      | 112.78   |
| 24  | B     | 610    | CLA  | O2D-CGD-O1D | -2.47 | 119.01      | 123.84   |
| 24  | b     | 615    | CLA  | CAA-C2A-C3A | -2.47 | 106.01      | 112.78   |
| 26  | K     | 101    | BCR  | C33-C5-C6   | -2.47 | 121.76      | 124.53   |
| 24  | c     | 513    | CLA  | O2A-CGA-CBA | 2.47  | 119.65      | 111.91   |
| 31  | A     | 419[A] | PL9  | C10-C9-C11  | 2.47  | 119.42      | 115.27   |
| 24  | c     | 515    | CLA  | O2A-CGA-O1A | -2.47 | 117.36      | 123.59   |
| 24  | c     | 517    | CLA  | O1D-CGD-CBD | -2.47 | 119.44      | 124.48   |
| 24  | B     | 614    | CLA  | O2A-CGA-CBA | 2.46  | 119.64      | 111.91   |
| 24  | c     | 507    | CLA  | O2A-CGA-O1A | -2.46 | 117.37      | 123.59   |
| 24  | C     | 512    | CLA  | CBC-CAC-C3C | -2.46 | 105.64      | 112.43   |
| 26  | a     | 413    | BCR  | C33-C5-C6   | -2.46 | 121.76      | 124.53   |
| 37  | d     | 406    | LHG  | O7-C7-C8    | 2.46  | 116.81      | 111.50   |
| 24  | c     | 514    | CLA  | O2D-CGD-O1D | -2.46 | 119.03      | 123.84   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | B     | 604    | CLA  | CHC-C1C-C2C | -2.46 | 119.89      | 126.73   |
| 24  | A     | 410    | CLA  | CED-O2D-CGD | 2.46  | 121.50      | 115.94   |
| 24  | B     | 614    | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 24  | B     | 616    | CLA  | CHC-C1C-C2C | -2.46 | 119.91      | 126.73   |
| 24  | B     | 613    | CLA  | O2A-CGA-CBA | 2.46  | 119.61      | 111.91   |
| 26  | T     | 103    | BCR  | C2-C1-C6    | 2.45  | 114.26      | 110.48   |
| 24  | b     | 622    | CLA  | O2A-CGA-CBA | 2.45  | 119.61      | 111.91   |
| 26  | T     | 103    | BCR  | C29-C28-C27 | -2.45 | 105.89      | 111.38   |
| 29  | M     | 103    | LMT  | O1B-C1B-C2B | 2.45  | 114.45      | 108.10   |
| 26  | b     | 627    | BCR  | C28-C27-C26 | -2.45 | 109.70      | 114.08   |
| 24  | b     | 617    | CLA  | OBD-CAD-C3D | -2.45 | 122.63      | 128.52   |
| 24  | B     | 614    | CLA  | CHD-C4C-NC  | 2.45  | 128.06      | 124.20   |
| 26  | d     | 404    | BCR  | C3-C4-C5    | -2.45 | 109.71      | 114.08   |
| 24  | b     | 625    | CLA  | O2A-CGA-O1A | -2.44 | 117.42      | 123.59   |
| 24  | C     | 513    | CLA  | CAA-C2A-C3A | -2.44 | 106.09      | 112.78   |
| 24  | b     | 613    | CLA  | O1D-CGD-CBD | -2.44 | 119.48      | 124.48   |
| 24  | C     | 502    | CLA  | C2A-C1A-CHA | -2.44 | 119.59      | 123.86   |
| 24  | A     | 405    | CLA  | O2D-CGD-O1D | -2.44 | 119.07      | 123.84   |
| 24  | C     | 510    | CLA  | C2A-C1A-CHA | -2.44 | 119.59      | 123.86   |
| 24  | b     | 616    | CLA  | C2A-C1A-CHA | -2.44 | 119.59      | 123.86   |
| 26  | y     | 101    | BCR  | C21-C20-C19 | -2.44 | 115.61      | 123.22   |
| 24  | c     | 511    | CLA  | O2A-CGA-O1A | -2.44 | 117.44      | 123.59   |
| 24  | b     | 621    | CLA  | CHD-C4C-NC  | 2.44  | 128.04      | 124.20   |
| 24  | a     | 410    | CLA  | CBC-CAC-C3C | -2.44 | 105.72      | 112.43   |
| 31  | D     | 405[A] | PL9  | C51-C49-C50 | 2.44  | 119.98      | 114.60   |
| 24  | b     | 611    | CLA  | C1-C2-C3    | -2.44 | 121.83      | 126.04   |
| 31  | D     | 405[A] | PL9  | C12-C13-C14 | -2.44 | 121.80      | 127.66   |
| 24  | C     | 507    | CLA  | O2D-CGD-O1D | -2.44 | 119.08      | 123.84   |
| 26  | H     | 101    | BCR  | C29-C30-C25 | 2.43  | 114.23      | 110.48   |
| 24  | b     | 621    | CLA  | CED-O2D-CGD | 2.43  | 121.44      | 115.94   |
| 24  | b     | 622    | CLA  | CMA-C3A-C4A | -2.43 | 105.23      | 111.77   |
| 24  | d     | 402    | CLA  | CAA-C2A-C3A | -2.43 | 106.11      | 112.78   |
| 24  | A     | 410    | CLA  | CHD-C4C-NC  | 2.43  | 128.03      | 124.20   |
| 24  | b     | 617    | CLA  | C2A-C1A-CHA | -2.43 | 119.61      | 123.86   |
| 24  | c     | 508    | CLA  | O2A-CGA-CBA | 2.43  | 119.53      | 111.91   |
| 33  | C     | 520    | LMG  | C8-O7-C10   | -2.43 | 111.81      | 117.79   |
| 24  | B     | 604    | CLA  | CAC-C3C-C4C | 2.43  | 127.96      | 124.81   |
| 26  | t     | 101    | BCR  | C21-C20-C19 | -2.43 | 115.64      | 123.22   |
| 31  | A     | 419[B] | PL9  | C10-C9-C11  | 2.43  | 119.35      | 115.27   |
| 24  | B     | 602    | CLA  | CBC-CAC-C3C | -2.43 | 105.74      | 112.43   |
| 24  | A     | 407    | CLA  | O2A-CGA-O1A | -2.42 | 117.47      | 123.59   |
| 24  | a     | 412    | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26  | d     | 404    | BCR  | C2-C1-C6    | 2.42  | 114.21      | 110.48   |
| 24  | C     | 513    | CLA  | CBC-CAC-C3C | -2.42 | 105.76      | 112.43   |
| 24  | b     | 618    | CLA  | CAC-C3C-C4C | 2.42  | 127.95      | 124.81   |
| 24  | b     | 621    | CLA  | O2D-CGD-O1D | -2.42 | 119.11      | 123.84   |
| 24  | D     | 403    | CLA  | CMC-C2C-C1C | 2.42  | 128.72      | 125.04   |
| 40  | v     | 205    | HEC  | CHD-C1D-ND  | 2.41  | 127.35      | 124.37   |
| 24  | A     | 406    | CLA  | C4C-C3C-C2C | -2.41 | 103.38      | 106.90   |
| 24  | b     | 617    | CLA  | CMB-C2B-C1B | 2.41  | 129.04      | 125.37   |
| 24  | C     | 512    | CLA  | CAC-C3C-C4C | 2.41  | 127.94      | 124.81   |
| 31  | D     | 405[B] | PL9  | C12-C13-C14 | -2.41 | 121.85      | 127.66   |
| 40  | V     | 205    | HEC  | O2D-CGD-CBD | 2.41  | 121.78      | 114.03   |
| 24  | D     | 403    | CLA  | O2A-CGA-O1A | -2.41 | 117.52      | 123.59   |
| 24  | c     | 515    | CLA  | CAC-C3C-C4C | 2.41  | 127.93      | 124.81   |
| 33  | c     | 524    | LMG  | C8-O7-C10   | -2.41 | 111.87      | 117.79   |
| 27  | a     | 414    | SQD  | O47-C7-O49  | -2.40 | 117.90      | 123.70   |
| 24  | b     | 623    | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 24  | C     | 503    | CLA  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 31  | D     | 405[B] | PL9  | C15-C14-C16 | 2.40  | 119.31      | 115.27   |
| 26  | C     | 514    | BCR  | C37-C22-C23 | 2.40  | 121.85      | 118.08   |
| 24  | B     | 603    | CLA  | C1-O2A-CGA  | 2.40  | 122.73      | 116.44   |
| 24  | b     | 623    | CLA  | CAA-C2A-C3A | -2.39 | 106.23      | 112.78   |
| 37  | D     | 407    | LHG  | O7-C7-O9    | -2.39 | 117.93      | 123.70   |
| 37  | L     | 101    | LHG  | C5-O7-C7    | -2.39 | 111.91      | 117.79   |
| 24  | B     | 605    | CLA  | C4-C3-C5    | 2.39  | 119.29      | 115.27   |
| 26  | C     | 515    | BCR  | C15-C16-C17 | -2.39 | 118.58      | 123.47   |
| 24  | C     | 505    | CLA  | C1-O2A-CGA  | 2.39  | 122.71      | 116.44   |
| 24  | C     | 502    | CLA  | O2A-CGA-CBA | 2.39  | 119.40      | 111.91   |
| 24  | C     | 508    | CLA  | O2A-CGA-CBA | 2.38  | 119.39      | 111.91   |
| 24  | c     | 516    | CLA  | CED-O2D-CGD | 2.38  | 121.33      | 115.94   |
| 24  | d     | 403    | CLA  | O2A-CGA-CBA | 2.38  | 119.39      | 111.91   |
| 27  | a     | 405    | SQD  | O48-C23-O10 | -2.38 | 117.57      | 123.59   |
| 26  | Y     | 101    | BCR  | C34-C9-C8   | 2.38  | 121.83      | 118.08   |
| 24  | c     | 506    | CLA  | O2A-CGA-CBA | 2.38  | 119.38      | 111.91   |
| 24  | c     | 517    | CLA  | CAC-C3C-C4C | 2.38  | 127.90      | 124.81   |
| 24  | B     | 605    | CLA  | O2A-CGA-CBA | 2.38  | 119.38      | 111.91   |
| 25  | A     | 408    | PHO  | O2D-CGD-O1D | -2.38 | 119.19      | 123.84   |
| 24  | b     | 624    | CLA  | C11-C10-C8  | -2.38 | 108.23      | 115.92   |
| 36  | D     | 406    | DGD  | C4D-C3D-C2D | 2.38  | 114.97      | 110.82   |
| 24  | A     | 410    | CLA  | O2A-CGA-CBA | 2.38  | 119.37      | 111.91   |
| 33  | Z     | 101    | LMG  | C1-C2-C3    | 2.38  | 114.94      | 110.00   |
| 27  | L     | 102    | SQD  | C1-C2-C3    | -2.38 | 105.05      | 110.00   |
| 24  | b     | 617    | CLA  | C1-C2-C3    | -2.37 | 121.94      | 126.04   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31  | D     | 405[B] | PL9  | C45-C44-C46 | 2.37  | 119.26      | 115.27   |
| 24  | d     | 401    | CLA  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 24  | B     | 612    | CLA  | C1-C2-C3    | -2.37 | 121.94      | 126.04   |
| 31  | D     | 405[B] | PL9  | C17-C18-C19 | -2.37 | 121.95      | 127.66   |
| 33  | c     | 523    | LMG  | O8-C28-O10  | -2.37 | 117.61      | 123.59   |
| 27  | A     | 412    | SQD  | O47-C7-O49  | -2.37 | 117.97      | 123.70   |
| 36  | H     | 102    | DGD  | C3G-O3G-C1D | -2.37 | 109.11      | 113.74   |
| 33  | Z     | 101    | LMG  | C9-O8-C28   | 2.37  | 123.05      | 117.10   |
| 24  | c     | 513    | CLA  | C2A-C1A-CHA | -2.37 | 119.72      | 123.86   |
| 24  | b     | 610    | CLA  | C2A-C1A-CHA | -2.37 | 119.72      | 123.86   |
| 24  | b     | 612    | CLA  | CBC-CAC-C3C | -2.37 | 105.91      | 112.43   |
| 24  | c     | 518    | CLA  | C3B-C4B-NB  | 2.37  | 112.71      | 110.52   |
| 36  | c     | 521    | DGD  | O1G-C1A-C2A | 2.37  | 119.33      | 111.91   |
| 38  | F     | 102    | HEM  | C4D-ND-C1D  | 2.37  | 107.52      | 105.07   |
| 26  | k     | 101    | BCR  | C10-C11-C12 | -2.36 | 115.84      | 123.22   |
| 24  | c     | 511    | CLA  | O2A-CGA-CBA | 2.36  | 119.33      | 111.91   |
| 24  | b     | 615    | CLA  | CBC-CAC-C3C | -2.36 | 105.91      | 112.43   |
| 24  | b     | 616    | CLA  | O2A-CGA-O1A | -2.36 | 117.63      | 123.59   |
| 24  | C     | 508    | CLA  | CHD-C4C-NC  | 2.36  | 127.93      | 124.20   |
| 24  | D     | 402    | CLA  | CHD-C4C-NC  | 2.36  | 127.93      | 124.20   |
| 24  | C     | 503    | CLA  | C2A-C1A-CHA | -2.36 | 119.73      | 123.86   |
| 26  | t     | 101    | BCR  | C16-C15-C14 | 2.36  | 128.31      | 123.47   |
| 24  | c     | 506    | CLA  | OBD-CAD-C3D | -2.36 | 122.84      | 128.52   |
| 36  | e     | 101    | DGD  | O5D-C1E-C2E | 2.36  | 111.99      | 108.30   |
| 24  | b     | 621    | CLA  | CHB-C1B-NB  | -2.36 | 121.76      | 124.26   |
| 24  | C     | 510    | CLA  | O2A-CGA-CBA | 2.36  | 119.31      | 111.91   |
| 24  | B     | 611    | CLA  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 40  | v     | 205    | HEC  | CBB-CAB-C3B | 2.36  | 118.93      | 112.43   |
| 24  | D     | 403    | CLA  | CHD-C4C-NC  | 2.36  | 127.92      | 124.20   |
| 26  | C     | 515    | BCR  | C15-C14-C13 | -2.35 | 123.95      | 127.31   |
| 24  | C     | 512    | CLA  | C1-O2A-CGA  | 2.35  | 122.62      | 116.44   |
| 24  | B     | 607    | CLA  | C1-O2A-CGA  | 2.35  | 122.62      | 116.44   |
| 24  | c     | 516    | CLA  | O2D-CGD-O1D | -2.35 | 119.24      | 123.84   |
| 24  | c     | 516    | CLA  | C1-O2A-CGA  | 2.35  | 122.61      | 116.44   |
| 24  | d     | 403    | CLA  | CMB-C2B-C1B | 2.35  | 128.95      | 125.37   |
| 24  | b     | 623    | CLA  | O2A-CGA-O1A | -2.35 | 117.66      | 123.59   |
| 24  | B     | 605    | CLA  | CHD-C4C-NC  | 2.35  | 127.91      | 124.20   |
| 24  | B     | 615    | CLA  | CMB-C2B-C1B | 2.35  | 128.95      | 125.37   |
| 31  | d     | 405[A] | PL9  | C12-C13-C14 | -2.35 | 122.00      | 127.66   |
| 24  | A     | 406    | CLA  | CMA-C3A-C4A | -2.35 | 105.46      | 111.77   |
| 26  | B     | 620    | BCR  | C32-C1-C6   | -2.35 | 106.49      | 110.30   |
| 24  | c     | 510    | CLA  | CHD-C4C-NC  | 2.35  | 127.90      | 124.20   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | a     | 409    | CLA  | CMC-C2C-C1C | 2.35  | 128.61      | 125.04   |
| 24  | B     | 614    | CLA  | OBD-CAD-C3D | -2.34 | 122.88      | 128.52   |
| 24  | d     | 402    | CLA  | CMA-C3A-C2A | -2.34 | 104.37      | 113.83   |
| 24  | c     | 509    | CLA  | O2A-CGA-CBA | 2.34  | 119.27      | 111.91   |
| 31  | D     | 405[A] | PL9  | C40-C39-C38 | -2.34 | 117.67      | 123.68   |
| 31  | D     | 405[A] | PL9  | C32-C33-C34 | -2.34 | 122.02      | 127.66   |
| 27  | a     | 414    | SQD  | O48-C23-O10 | -2.34 | 117.68      | 123.59   |
| 24  | b     | 625    | CLA  | C2A-C1A-CHA | -2.34 | 119.76      | 123.86   |
| 24  | B     | 604    | CLA  | C4-C3-C5    | 2.34  | 119.21      | 115.27   |
| 29  | M     | 103    | LMT  | O5'-C5'-C4' | 2.34  | 114.69      | 109.75   |
| 24  | c     | 511    | CLA  | CMC-C2C-C1C | 2.34  | 128.60      | 125.04   |
| 24  | b     | 615    | CLA  | C2A-C1A-CHA | -2.34 | 119.77      | 123.86   |
| 24  | C     | 503    | CLA  | C4-C3-C5    | 2.34  | 119.21      | 115.27   |
| 36  | C     | 517    | DGD  | O2G-C1B-O1B | -2.34 | 118.05      | 123.70   |
| 24  | C     | 506    | CLA  | CMB-C2B-C1B | 2.34  | 128.93      | 125.37   |
| 24  | D     | 402    | CLA  | CAC-C3C-C4C | 2.34  | 127.84      | 124.81   |
| 24  | C     | 512    | CLA  | O2A-CGA-CBA | 2.34  | 119.24      | 111.91   |
| 31  | a     | 415[B] | PL9  | C45-C44-C46 | 2.34  | 119.20      | 115.27   |
| 33  | B     | 622    | LMG  | O6-C5-C4    | 2.33  | 113.93      | 109.69   |
| 24  | c     | 513    | CLA  | CMB-C2B-C1B | 2.33  | 128.92      | 125.37   |
| 24  | B     | 611    | CLA  | CAA-CBA-CGA | -2.33 | 106.43      | 113.25   |
| 33  | D     | 413    | LMG  | O8-C28-O10  | -2.33 | 117.70      | 123.59   |
| 24  | B     | 616    | CLA  | O2D-CGD-O1D | -2.33 | 119.28      | 123.84   |
| 24  | C     | 509    | CLA  | C2A-C1A-CHA | -2.33 | 119.78      | 123.86   |
| 24  | a     | 412    | CLA  | O2A-CGA-CBA | 2.33  | 119.22      | 111.91   |
| 31  | A     | 419[B] | PL9  | C40-C39-C41 | 2.33  | 119.19      | 115.27   |
| 31  | D     | 405[B] | PL9  | C35-C34-C36 | 2.33  | 119.19      | 115.27   |
| 24  | b     | 612    | CLA  | C4-C3-C5    | 2.33  | 119.19      | 115.27   |
| 24  | B     | 607    | CLA  | CAA-C2A-C3A | -2.33 | 106.41      | 112.78   |
| 24  | c     | 506    | CLA  | O2A-CGA-O1A | -2.33 | 117.72      | 123.59   |
| 24  | A     | 407    | CLA  | C1-C2-C3    | -2.33 | 122.02      | 126.04   |
| 24  | c     | 515    | CLA  | C2A-C1A-CHA | -2.33 | 119.79      | 123.86   |
| 24  | B     | 614    | CLA  | O2D-CGD-O1D | -2.33 | 119.29      | 123.84   |
| 24  | C     | 510    | CLA  | CMC-C2C-C1C | 2.32  | 128.58      | 125.04   |
| 24  | A     | 410    | CLA  | C2A-C1A-CHA | -2.32 | 119.80      | 123.86   |
| 40  | V     | 205    | HEC  | CBB-CAB-C3B | 2.32  | 118.83      | 112.43   |
| 24  | c     | 516    | CLA  | CBC-CAC-C3C | -2.32 | 106.03      | 112.43   |
| 24  | c     | 513    | CLA  | CHB-C1B-NB  | -2.32 | 121.80      | 124.26   |
| 24  | D     | 402    | CLA  | CED-O2D-CGD | 2.32  | 121.19      | 115.94   |
| 31  | d     | 405[A] | PL9  | C25-C24-C26 | 2.32  | 119.17      | 115.27   |
| 24  | c     | 513    | CLA  | CHD-C4C-NC  | 2.32  | 127.86      | 124.20   |
| 24  | b     | 619    | CLA  | CMC-C2C-C1C | 2.32  | 128.57      | 125.04   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | a     | 409    | CLA  | CHD-C4C-NC  | 2.32  | 127.86      | 124.20   |
| 37  | D     | 408    | LHG  | O8-C23-O10  | -2.32 | 117.75      | 123.59   |
| 31  | d     | 405[A] | PL9  | C15-C14-C16 | 2.32  | 119.17      | 115.27   |
| 27  | F     | 103    | SQD  | O47-C7-O49  | -2.32 | 118.11      | 123.70   |
| 24  | c     | 506    | CLA  | CHD-C4C-NC  | 2.32  | 127.85      | 124.20   |
| 29  | C     | 521    | LMT  | O5'-C5'-C4' | 2.32  | 114.63      | 109.75   |
| 24  | B     | 612    | CLA  | O2A-CGA-CBA | 2.31  | 119.17      | 111.91   |
| 25  | a     | 411    | PHO  | CBA-CAA-C2A | -2.31 | 107.05      | 113.81   |
| 24  | B     | 603    | CLA  | C4-C3-C5    | 2.31  | 119.16      | 115.27   |
| 24  | c     | 508    | CLA  | C4-C3-C5    | 2.31  | 119.16      | 115.27   |
| 24  | b     | 616    | CLA  | CED-O2D-CGD | 2.31  | 121.16      | 115.94   |
| 31  | d     | 405[B] | PL9  | C45-C44-C46 | 2.31  | 119.16      | 115.27   |
| 33  | d     | 413    | LMG  | O6-C5-C4    | 2.31  | 113.89      | 109.69   |
| 24  | B     | 603    | CLA  | CMC-C2C-C1C | 2.31  | 128.56      | 125.04   |
| 24  | B     | 613    | CLA  | CMB-C2B-C1B | 2.31  | 128.88      | 125.37   |
| 29  | B     | 635    | LMT  | C1'-O5'-C5' | 2.31  | 118.22      | 113.69   |
| 27  | A     | 412    | SQD  | C1-O5-C5    | -2.30 | 109.17      | 113.69   |
| 26  | b     | 628    | BCR  | C15-C14-C13 | -2.30 | 124.02      | 127.31   |
| 24  | B     | 612    | CLA  | CBC-CAC-C3C | -2.30 | 106.09      | 112.43   |
| 24  | B     | 612    | CLA  | C2A-C1A-CHA | -2.30 | 119.83      | 123.86   |
| 24  | C     | 501    | CLA  | C2A-C1A-CHA | -2.30 | 119.84      | 123.86   |
| 24  | b     | 621    | CLA  | CAA-C2A-C3A | -2.30 | 106.48      | 112.78   |
| 26  | K     | 101    | BCR  | C16-C17-C18 | -2.30 | 124.03      | 127.31   |
| 24  | c     | 510    | CLA  | CBC-CAC-C3C | -2.30 | 106.09      | 112.43   |
| 40  | v     | 205    | HEC  | C3B-C4B-NB  | -2.30 | 107.61      | 110.17   |
| 24  | d     | 401    | CLA  | C4-C3-C5    | 2.30  | 119.14      | 115.27   |
| 27  | A     | 412    | SQD  | C44-O6-C1   | -2.30 | 109.25      | 113.74   |
| 33  | A     | 421    | LMG  | C8-O7-C10   | -2.30 | 112.14      | 117.79   |
| 27  | a     | 414    | SQD  | C1-O5-C5    | -2.30 | 109.18      | 113.69   |
| 24  | d     | 401    | CLA  | C1-C2-C3    | -2.30 | 122.07      | 126.04   |
| 26  | t     | 101    | BCR  | C29-C28-C27 | -2.29 | 106.25      | 111.38   |
| 27  | F     | 103    | SQD  | C1-C2-C3    | -2.29 | 105.22      | 110.00   |
| 24  | B     | 603    | CLA  | CMA-C3A-C4A | -2.29 | 105.61      | 111.77   |
| 24  | b     | 611    | CLA  | CMC-C2C-C1C | 2.29  | 128.53      | 125.04   |
| 31  | D     | 405[B] | PL9  | C32-C33-C34 | -2.29 | 122.14      | 127.66   |
| 24  | A     | 410    | CLA  | O2D-CGD-O1D | -2.29 | 119.36      | 123.84   |
| 31  | A     | 419[A] | PL9  | C17-C18-C19 | -2.29 | 122.14      | 127.66   |
| 26  | k     | 101    | BCR  | C39-C30-C25 | -2.29 | 106.58      | 110.30   |
| 24  | A     | 406    | CLA  | CED-O2D-CGD | 2.29  | 121.12      | 115.94   |
| 24  | C     | 503    | CLA  | CAC-C3C-C4C | 2.29  | 127.78      | 124.81   |
| 37  | d     | 407    | LHG  | O8-C23-C24  | 2.29  | 119.09      | 111.91   |
| 24  | c     | 515    | CLA  | CMC-C2C-C1C | 2.29  | 128.52      | 125.04   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | A     | 410    | CLA  | O2A-CGA-O1A | -2.29 | 117.82      | 123.59   |
| 25  | a     | 418[A] | PHO  | C4A-C3A-C2A | -2.29 | 100.66      | 102.84   |
| 35  | B     | 632    | HTG  | C6-C5-C4    | -2.29 | 107.65      | 113.00   |
| 26  | C     | 515    | BCR  | C28-C27-C26 | -2.29 | 110.00      | 114.08   |
| 24  | B     | 610    | CLA  | C1-O2A-CGA  | 2.28  | 122.44      | 116.44   |
| 26  | D     | 404    | BCR  | C10-C11-C12 | -2.28 | 116.09      | 123.22   |
| 24  | B     | 606    | CLA  | CHC-C1C-C2C | -2.28 | 120.39      | 126.73   |
| 26  | B     | 618    | BCR  | C34-C9-C10  | -2.28 | 119.72      | 122.92   |
| 27  | B     | 621    | SQD  | O47-C7-O49  | -2.28 | 118.19      | 123.70   |
| 24  | b     | 625    | CLA  | CBC-CAC-C3C | -2.28 | 106.15      | 112.43   |
| 26  | T     | 103    | BCR  | C16-C17-C18 | -2.28 | 124.06      | 127.31   |
| 36  | C     | 516    | DGD  | O1G-C1A-C2A | 2.28  | 119.06      | 111.91   |
| 35  | B     | 625    | HTG  | C1-C2-C3    | 2.28  | 115.09      | 110.59   |
| 24  | D     | 402    | CLA  | O2A-CGA-O1A | -2.28 | 117.84      | 123.59   |
| 40  | v     | 205    | HEC  | C2A-C1A-NA  | -2.28 | 108.11      | 110.32   |
| 24  | b     | 620    | CLA  | CMA-C3A-C4A | -2.27 | 105.66      | 111.77   |
| 24  | b     | 624    | CLA  | O2A-CGA-O1A | -2.27 | 117.85      | 123.59   |
| 24  | c     | 511    | CLA  | C2A-C1A-CHA | -2.27 | 119.88      | 123.86   |
| 24  | b     | 622    | CLA  | O2A-CGA-O1A | -2.27 | 117.86      | 123.59   |
| 24  | c     | 516    | CLA  | CMB-C2B-C1B | 2.27  | 128.83      | 125.37   |
| 24  | B     | 616    | CLA  | C2A-C1A-CHA | -2.27 | 119.89      | 123.86   |
| 36  | c     | 521    | DGD  | C3B-C2B-C1B | -2.27 | 105.36      | 113.62   |
| 24  | A     | 406    | CLA  | CAC-C3C-C4C | 2.27  | 127.76      | 124.81   |
| 24  | C     | 510    | CLA  | CMB-C2B-C1B | 2.27  | 128.83      | 125.37   |
| 37  | D     | 408    | LHG  | O8-C23-C24  | 2.27  | 119.03      | 111.91   |
| 24  | c     | 515    | CLA  | CHB-C1B-NB  | -2.27 | 121.86      | 124.26   |
| 33  | A     | 421    | LMG  | O8-C28-C29  | 2.27  | 119.02      | 111.91   |
| 24  | B     | 612    | CLA  | O2A-CGA-O1A | -2.27 | 117.87      | 123.59   |
| 24  | d     | 401    | CLA  | CAC-C3C-C4C | 2.26  | 127.75      | 124.81   |
| 24  | C     | 513    | CLA  | C2A-C1A-CHA | -2.26 | 119.90      | 123.86   |
| 24  | C     | 504    | CLA  | CAA-C2A-C3A | -2.26 | 106.59      | 112.78   |
| 26  | B     | 620    | BCR  | C28-C27-C26 | -2.26 | 110.04      | 114.08   |
| 26  | c     | 528    | BCR  | C29-C30-C25 | 2.26  | 113.96      | 110.48   |
| 25  | A     | 409[B] | PHO  | O2A-CGA-CBA | 2.26  | 119.00      | 111.91   |
| 24  | b     | 611    | CLA  | C1-O2A-CGA  | 2.26  | 122.37      | 116.44   |
| 24  | B     | 614    | CLA  | CMA-C3A-C2A | -2.26 | 104.73      | 113.83   |
| 24  | c     | 511    | CLA  | CGD-CBD-CAD | -2.26 | 103.43      | 110.73   |
| 24  | b     | 618    | CLA  | C1-O2A-CGA  | 2.26  | 122.36      | 116.44   |
| 24  | b     | 624    | CLA  | C1-C2-C3    | -2.25 | 122.14      | 126.04   |
| 37  | d     | 407    | LHG  | C6-C5-C4    | -2.25 | 106.46      | 111.79   |
| 31  | D     | 405[B] | PL9  | C51-C49-C50 | 2.25  | 119.58      | 114.60   |
| 35  | B     | 632    | HTG  | C3-C4-C5    | 2.25  | 114.26      | 110.24   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 618    | CLA  | CMA-C3A-C4A | -2.25 | 105.72      | 111.77   |
| 36  | C     | 518    | DGD  | O3G-C3G-C2G | -2.25 | 105.47      | 110.90   |
| 36  | C     | 518    | DGD  | C3G-C2G-C1G | -2.25 | 106.47      | 111.79   |
| 24  | b     | 613    | CLA  | CHA-C1A-NA  | -2.25 | 121.25      | 126.40   |
| 26  | B     | 618    | BCR  | C11-C10-C9  | -2.25 | 124.10      | 127.31   |
| 25  | a     | 411    | PHO  | CAA-CBA-CGA | -2.25 | 106.68      | 113.25   |
| 24  | c     | 518    | CLA  | O2D-CGD-O1D | -2.25 | 119.44      | 123.84   |
| 24  | b     | 612    | CLA  | C7-C6-C5    | -2.25 | 107.25      | 113.36   |
| 40  | v     | 205    | HEC  | CAB-C3B-C4B | 2.25  | 127.73      | 124.81   |
| 26  | k     | 101    | BCR  | C2-C1-C6    | 2.25  | 113.94      | 110.48   |
| 26  | c     | 528    | BCR  | C34-C9-C10  | -2.24 | 119.78      | 122.92   |
| 40  | v     | 205    | HEC  | CHD-C4C-NC  | 2.24  | 127.98      | 123.85   |
| 24  | C     | 503    | CLA  | C3B-C4B-NB  | 2.24  | 112.60      | 110.52   |
| 33  | b     | 629    | LMG  | O7-C10-O9   | -2.24 | 118.28      | 123.70   |
| 24  | C     | 508    | CLA  | C2A-C1A-CHA | -2.24 | 119.94      | 123.86   |
| 24  | c     | 507    | CLA  | O2A-C1-C2   | 2.24  | 114.53      | 108.64   |
| 26  | T     | 103    | BCR  | C1-C6-C7    | 2.24  | 122.12      | 115.78   |
| 31  | A     | 419[B] | PL9  | C8-C7-C3    | 2.24  | 118.31      | 111.98   |
| 24  | B     | 602    | CLA  | CHB-C4A-NA  | 2.24  | 127.61      | 124.51   |
| 24  | A     | 407    | CLA  | C3B-C4B-NB  | 2.24  | 112.59      | 110.52   |
| 24  | B     | 605    | CLA  | C11-C10-C8  | -2.24 | 108.69      | 115.92   |
| 24  | B     | 616    | CLA  | C1-C2-C3    | -2.24 | 122.18      | 126.04   |
| 24  | B     | 611    | CLA  | O2D-CGD-O1D | -2.23 | 119.47      | 123.84   |
| 24  | b     | 610    | CLA  | CAC-C3C-C4C | 2.23  | 127.71      | 124.81   |
| 24  | C     | 511    | CLA  | O2A-CGA-O1A | -2.23 | 117.96      | 123.59   |
| 24  | B     | 617    | CLA  | C4-C3-C5    | 2.23  | 119.02      | 115.27   |
| 36  | c     | 522    | DGD  | C2G-O2G-C1B | -2.23 | 112.30      | 117.79   |
| 24  | C     | 512    | CLA  | C4-C3-C5    | 2.23  | 119.02      | 115.27   |
| 24  | a     | 409    | CLA  | C4-C3-C5    | 2.23  | 119.02      | 115.27   |
| 24  | C     | 513    | CLA  | O2A-CGA-O1A | -2.23 | 117.97      | 123.59   |
| 29  | m     | 103    | LMT  | C1'-O5'-C5' | 2.23  | 118.06      | 113.69   |
| 24  | c     | 517    | CLA  | CHB-C1B-C2B | -2.23 | 120.94      | 127.24   |
| 24  | B     | 610    | CLA  | O2A-CGA-CBA | 2.23  | 118.90      | 111.91   |
| 24  | C     | 507    | CLA  | CBC-CAC-C3C | -2.23 | 106.30      | 112.43   |
| 24  | c     | 510    | CLA  | C2A-C1A-CHA | -2.22 | 119.97      | 123.86   |
| 31  | A     | 419[A] | PL9  | C7-C3-C2    | -2.22 | 120.38      | 123.30   |
| 24  | d     | 401    | CLA  | O2A-CGA-O1A | -2.22 | 117.99      | 123.59   |
| 36  | c     | 521    | DGD  | C2G-O2G-C1B | -2.22 | 112.33      | 117.79   |
| 40  | v     | 205    | HEC  | CMD-C2D-C1D | 2.22  | 128.42      | 125.04   |
| 24  | d     | 402    | CLA  | CBC-CAC-C3C | -2.22 | 106.32      | 112.43   |
| 37  | L     | 101    | LHG  | O7-C7-O9    | -2.22 | 118.34      | 123.70   |
| 24  | b     | 625    | CLA  | O1D-CGD-CBD | -2.22 | 119.95      | 124.48   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26  | a     | 413    | BCR  | C7-C8-C9    | -2.22 | 122.88      | 126.23   |
| 33  | Z     | 101    | LMG  | C8-O7-C10   | -2.22 | 112.33      | 117.79   |
| 24  | b     | 622    | CLA  | C2A-C1A-CHA | -2.22 | 119.98      | 123.86   |
| 24  | D     | 402    | CLA  | CMA-C3A-C4A | -2.21 | 105.82      | 111.77   |
| 36  | C     | 516    | DGD  | O2G-C1B-O1B | -2.21 | 118.35      | 123.70   |
| 24  | C     | 507    | CLA  | C4-C3-C5    | 2.21  | 118.99      | 115.27   |
| 24  | c     | 511    | CLA  | CAC-C3C-C4C | 2.21  | 127.68      | 124.81   |
| 25  | a     | 411    | PHO  | CMB-C2B-C3B | 2.21  | 128.81      | 124.68   |
| 24  | B     | 610    | CLA  | C7-C6-C5    | -2.21 | 107.35      | 113.36   |
| 24  | c     | 509    | CLA  | C11-C10-C8  | -2.21 | 108.77      | 115.92   |
| 25  | a     | 418[B] | PHO  | O2A-CGA-CBA | 2.21  | 118.84      | 111.91   |
| 24  | C     | 505    | CLA  | C4-C3-C5    | 2.21  | 118.99      | 115.27   |
| 24  | B     | 604    | CLA  | CMA-C3A-C2A | -2.21 | 104.91      | 113.83   |
| 24  | B     | 614    | CLA  | O2A-CGA-O1A | -2.21 | 118.02      | 123.59   |
| 29  | A     | 417    | LMT  | C4B-C3B-C2B | -2.21 | 106.97      | 110.82   |
| 24  | b     | 619    | CLA  | C2A-C1A-CHA | -2.21 | 120.00      | 123.86   |
| 31  | d     | 405[B] | PL9  | C22-C23-C24 | -2.21 | 122.35      | 127.66   |
| 38  | e     | 103    | HEM  | C2A-C1A-NA  | -2.21 | 107.68      | 110.15   |
| 31  | A     | 419[B] | PL9  | C35-C34-C36 | 2.21  | 118.98      | 115.27   |
| 24  | B     | 602    | CLA  | CMC-C2C-C1C | 2.21  | 128.40      | 125.04   |
| 24  | b     | 621    | CLA  | C2A-C1A-CHA | -2.21 | 120.00      | 123.86   |
| 26  | T     | 103    | BCR  | C12-C13-C14 | -2.20 | 115.56      | 118.94   |
| 26  | B     | 619    | BCR  | C30-C25-C26 | -2.20 | 119.51      | 122.61   |
| 24  | b     | 624    | CLA  | O2A-CGA-CBA | 2.20  | 118.82      | 111.91   |
| 24  | c     | 514    | CLA  | O2A-CGA-O1A | -2.20 | 118.03      | 123.59   |
| 24  | A     | 406    | CLA  | C2A-C1A-CHA | -2.20 | 120.01      | 123.86   |
| 24  | c     | 508    | CLA  | CHC-C1C-C2C | -2.20 | 120.62      | 126.73   |
| 24  | A     | 406    | CLA  | CAA-CBA-CGA | 2.20  | 119.68      | 113.25   |
| 36  | H     | 102    | DGD  | C2G-O2G-C1B | -2.20 | 112.38      | 117.79   |
| 24  | B     | 617    | CLA  | O1D-CGD-CBD | -2.20 | 119.98      | 124.48   |
| 24  | d     | 403    | CLA  | CBC-CAC-C3C | -2.20 | 106.37      | 112.43   |
| 26  | B     | 619    | BCR  | C37-C22-C23 | 2.20  | 121.54      | 118.08   |
| 26  | d     | 404    | BCR  | C38-C26-C27 | 2.20  | 117.84      | 113.62   |
| 24  | B     | 608    | CLA  | O2A-CGA-O1A | -2.20 | 118.05      | 123.59   |
| 24  | b     | 614    | CLA  | CMC-C2C-C1C | 2.20  | 128.38      | 125.04   |
| 24  | c     | 510    | CLA  | CED-O2D-CGD | 2.19  | 120.90      | 115.94   |
| 26  | h     | 101    | BCR  | C37-C22-C21 | -2.19 | 119.85      | 122.92   |
| 33  | D     | 413    | LMG  | O8-C28-C29  | 2.19  | 118.79      | 111.91   |
| 24  | a     | 410    | CLA  | C1-C2-C3    | -2.19 | 122.25      | 126.04   |
| 24  | d     | 403    | CLA  | C1-C2-C3    | -2.19 | 122.25      | 126.04   |
| 36  | D     | 406    | DGD  | O6D-C5D-C6D | 2.19  | 111.09      | 106.67   |
| 37  | d     | 407    | LHG  | O8-C23-O10  | -2.19 | 118.06      | 123.59   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 610    | CLA  | O2A-CGA-CBA | 2.19  | 118.78      | 111.91   |
| 35  | d     | 411    | HTG  | C1-O5-C5    | 2.19  | 116.61      | 112.58   |
| 26  | d     | 404    | BCR  | C10-C11-C12 | -2.19 | 116.39      | 123.22   |
| 24  | A     | 405    | CLA  | CMA-C3A-C2A | -2.19 | 105.01      | 113.83   |
| 24  | B     | 610    | CLA  | CMC-C2C-C1C | 2.18  | 128.36      | 125.04   |
| 26  | C     | 515    | BCR  | C38-C26-C25 | -2.18 | 122.08      | 124.53   |
| 24  | C     | 506    | CLA  | CED-O2D-CGD | 2.18  | 120.87      | 115.94   |
| 40  | v     | 205    | HEC  | C4A-NA-C1A  | 2.18  | 107.48      | 105.35   |
| 24  | a     | 409    | CLA  | CHB-C1B-C2B | -2.18 | 121.08      | 127.24   |
| 24  | B     | 614    | CLA  | C2A-C1A-CHA | -2.18 | 120.05      | 123.86   |
| 24  | b     | 617    | CLA  | O2A-CGA-O1A | -2.18 | 118.09      | 123.59   |
| 26  | t     | 101    | BCR  | C37-C22-C23 | 2.18  | 121.51      | 118.08   |
| 24  | d     | 401    | CLA  | O2A-CGA-CBA | 2.18  | 118.75      | 111.91   |
| 24  | c     | 513    | CLA  | O2A-CGA-O1A | -2.18 | 118.09      | 123.59   |
| 24  | d     | 401    | CLA  | CMC-C2C-C1C | 2.18  | 128.36      | 125.04   |
| 27  | B     | 621    | SQD  | C44-O6-C1   | -2.18 | 109.48      | 113.74   |
| 24  | B     | 612    | CLA  | CHB-C1B-NB  | -2.18 | 121.95      | 124.26   |
| 26  | Y     | 101    | BCR  | C21-C20-C19 | -2.18 | 116.43      | 123.22   |
| 24  | c     | 515    | CLA  | C4-C3-C2    | -2.17 | 118.10      | 123.68   |
| 24  | B     | 610    | CLA  | C2A-C1A-CHA | -2.17 | 120.06      | 123.86   |
| 24  | B     | 616    | CLA  | O2A-CGA-O1A | -2.17 | 118.11      | 123.59   |
| 25  | a     | 418[B] | PHO  | C4A-C3A-C2A | -2.17 | 100.77      | 102.84   |
| 26  | y     | 101    | BCR  | C38-C26-C25 | -2.17 | 122.09      | 124.53   |
| 24  | C     | 512    | CLA  | CHB-C1B-NB  | -2.17 | 121.96      | 124.26   |
| 24  | b     | 613    | CLA  | O2A-CGA-O1A | -2.17 | 118.11      | 123.59   |
| 24  | b     | 622    | CLA  | CHD-C4C-NC  | 2.17  | 127.62      | 124.20   |
| 36  | h     | 102    | DGD  | C2G-O2G-C1B | -2.17 | 112.45      | 117.79   |
| 40  | V     | 205    | HEC  | C3B-C4B-NB  | -2.17 | 107.75      | 110.17   |
| 24  | A     | 405    | CLA  | CMC-C2C-C1C | 2.17  | 128.34      | 125.04   |
| 40  | V     | 205    | HEC  | CHD-C4C-NC  | 2.17  | 127.84      | 123.85   |
| 37  | L     | 101    | LHG  | O8-C23-O10  | -2.17 | 118.12      | 123.59   |
| 24  | C     | 510    | CLA  | O2D-CGD-O1D | -2.17 | 119.60      | 123.84   |
| 33  | A     | 421    | LMG  | C7-O1-C1    | -2.17 | 109.51      | 113.74   |
| 38  | F     | 102    | HEM  | O2A-CGA-CBA | 2.17  | 120.99      | 114.03   |
| 24  | D     | 403    | CLA  | CHB-C4A-NA  | 2.16  | 127.50      | 124.51   |
| 24  | A     | 410    | CLA  | CBC-CAC-C3C | -2.16 | 106.47      | 112.43   |
| 25  | a     | 411    | PHO  | O2A-CGA-CBA | 2.16  | 118.69      | 111.91   |
| 24  | b     | 624    | CLA  | CHA-C1A-NA  | -2.16 | 121.44      | 126.40   |
| 31  | d     | 405[B] | PL9  | C25-C24-C26 | 2.16  | 118.91      | 115.27   |
| 26  | t     | 101    | BCR  | C12-C13-C14 | -2.16 | 115.62      | 118.94   |
| 24  | B     | 609    | CLA  | O2A-CGA-O1A | -2.16 | 118.14      | 123.59   |
| 24  | B     | 616    | CLA  | O2A-CGA-CBA | 2.16  | 118.69      | 111.91   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | c     | 506    | CLA  | C4-C3-C5    | 2.16  | 118.91      | 115.27   |
| 24  | b     | 620    | CLA  | CHB-C4A-NA  | 2.16  | 127.50      | 124.51   |
| 24  | d     | 403    | CLA  | O2A-CGA-O1A | -2.16 | 118.15      | 123.59   |
| 24  | B     | 607    | CLA  | OBD-CAD-C3D | -2.16 | 123.33      | 128.52   |
| 29  | a     | 404    | LMT  | C1B-O1B-C4' | -2.16 | 112.63      | 117.96   |
| 25  | A     | 409[B] | PHO  | C4A-C3A-C2A | -2.16 | 100.79      | 102.84   |
| 40  | v     | 205    | HEC  | O2D-CGD-CBD | 2.16  | 120.95      | 114.03   |
| 24  | b     | 619    | CLA  | CMA-C3A-C2A | -2.15 | 105.14      | 113.83   |
| 24  | B     | 604    | CLA  | CBC-CAC-C3C | -2.15 | 106.50      | 112.43   |
| 24  | c     | 508    | CLA  | C1-O2A-CGA  | 2.15  | 122.09      | 116.44   |
| 24  | b     | 617    | CLA  | CMA-C3A-C2A | -2.15 | 105.15      | 113.83   |
| 24  | C     | 507    | CLA  | C1-C2-C3    | -2.15 | 122.33      | 126.04   |
| 25  | A     | 408    | PHO  | C1-C2-C3    | -2.15 | 122.33      | 126.04   |
| 26  | Y     | 101    | BCR  | C15-C16-C17 | -2.15 | 119.07      | 123.47   |
| 24  | D     | 402    | CLA  | CHB-C1B-NB  | -2.15 | 121.98      | 124.26   |
| 31  | d     | 405[A] | PL9  | C40-C39-C38 | -2.15 | 118.17      | 123.68   |
| 24  | A     | 406    | CLA  | CMB-C2B-C1B | 2.15  | 128.64      | 125.37   |
| 40  | V     | 205    | HEC  | CAA-C2A-C3A | -2.15 | 123.88      | 127.88   |
| 31  | a     | 415[A] | PL9  | C8-C7-C3    | 2.15  | 118.05      | 111.98   |
| 24  | B     | 611    | CLA  | CHB-C1B-NB  | -2.15 | 121.99      | 124.26   |
| 38  | F     | 102    | HEM  | C4B-C3B-C2B | -2.14 | 105.41      | 107.11   |
| 24  | c     | 518    | CLA  | O2A-CGA-O1A | -2.14 | 118.18      | 123.59   |
| 24  | b     | 621    | CLA  | CMC-C2C-C1C | 2.14  | 128.31      | 125.04   |
| 24  | A     | 407    | CLA  | CMA-C3A-C2A | -2.14 | 105.18      | 113.83   |
| 26  | D     | 404    | BCR  | C3-C4-C5    | -2.14 | 110.25      | 114.08   |
| 31  | D     | 405[A] | PL9  | C35-C34-C36 | 2.14  | 118.87      | 115.27   |
| 35  | b     | 631    | HTG  | C1-C2-C3    | 2.14  | 114.81      | 110.59   |
| 24  | B     | 613    | CLA  | CMA-C3A-C2A | -2.14 | 105.20      | 113.83   |
| 24  | B     | 613    | CLA  | CHC-C1C-C2C | -2.14 | 120.79      | 126.73   |
| 24  | d     | 402    | CLA  | O2A-CGA-O1A | -2.14 | 118.20      | 123.59   |
| 26  | H     | 101    | BCR  | C15-C14-C13 | -2.14 | 124.26      | 127.31   |
| 33  | z     | 101    | LMG  | C8-O7-C10   | -2.14 | 112.53      | 117.79   |
| 24  | B     | 606    | CLA  | C3B-C4B-NB  | 2.14  | 112.50      | 110.52   |
| 24  | A     | 407    | CLA  | CAA-CBA-CGA | 2.14  | 119.49      | 113.25   |
| 27  | a     | 414    | SQD  | O9-S-O7     | -2.13 | 106.56      | 113.95   |
| 37  | E     | 101    | LHG  | C5-O7-C7    | -2.13 | 112.53      | 117.79   |
| 37  | b     | 634    | LHG  | O8-C23-O10  | -2.13 | 118.20      | 123.59   |
| 24  | b     | 618    | CLA  | CBC-CAC-C3C | -2.13 | 106.55      | 112.43   |
| 36  | C     | 516    | DGD  | O6D-C5D-C6D | 2.13  | 110.97      | 106.67   |
| 24  | C     | 504    | CLA  | OBD-CAD-C3D | -2.13 | 123.39      | 128.52   |
| 35  | b     | 601    | HTG  | C1-O5-C5    | 2.13  | 116.52      | 112.58   |
| 31  | a     | 415[A] | PL9  | C45-C44-C46 | 2.13  | 118.86      | 115.27   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 27  | f     | 101    | SQD  | O48-C23-O10 | -2.13 | 118.21      | 123.59   |
| 26  | H     | 101    | BCR  | C39-C30-C25 | -2.13 | 106.84      | 110.30   |
| 24  | b     | 621    | CLA  | CHB-C4A-NA  | 2.13  | 127.46      | 124.51   |
| 24  | d     | 401    | CLA  | CED-O2D-CGD | 2.13  | 120.76      | 115.94   |
| 24  | B     | 608    | CLA  | C1-O2A-CGA  | 2.13  | 122.03      | 116.44   |
| 24  | a     | 409    | CLA  | O2D-CGD-O1D | -2.13 | 119.67      | 123.84   |
| 26  | b     | 628    | BCR  | C16-C17-C18 | -2.13 | 124.27      | 127.31   |
| 40  | v     | 205    | HEC  | O2A-CGA-CBA | 2.13  | 120.87      | 114.03   |
| 24  | C     | 511    | CLA  | C1-O2A-CGA  | 2.13  | 122.03      | 116.44   |
| 26  | c     | 519    | BCR  | C21-C20-C19 | -2.13 | 116.58      | 123.22   |
| 24  | C     | 505    | CLA  | C2A-C1A-CHA | -2.13 | 120.14      | 123.86   |
| 25  | A     | 409[A] | PHO  | O2A-CGA-CBA | 2.13  | 118.58      | 111.91   |
| 36  | C     | 517    | DGD  | C3G-O3G-C1D | -2.13 | 109.59      | 113.74   |
| 24  | b     | 619    | CLA  | O2A-CGA-O1A | -2.12 | 118.23      | 123.59   |
| 31  | A     | 419[B] | PL9  | C51-C49-C50 | 2.12  | 119.29      | 114.60   |
| 24  | B     | 614    | CLA  | CMA-C3A-C4A | -2.12 | 106.07      | 111.77   |
| 31  | D     | 405[A] | PL9  | C20-C19-C21 | 2.12  | 118.84      | 115.27   |
| 24  | B     | 604    | CLA  | CBA-CAA-C2A | 2.12  | 120.12      | 113.86   |
| 24  | B     | 615    | CLA  | OBD-CAD-C3D | -2.12 | 123.42      | 128.52   |
| 26  | C     | 514    | BCR  | C38-C26-C25 | -2.12 | 122.15      | 124.53   |
| 31  | d     | 405[A] | PL9  | C36-C37-C38 | -2.12 | 104.92      | 111.88   |
| 24  | b     | 623    | CLA  | C4-C3-C5    | 2.12  | 118.83      | 115.27   |
| 36  | e     | 101    | DGD  | O2G-C1B-O1B | -2.12 | 118.59      | 123.70   |
| 24  | c     | 512    | CLA  | O2A-CGA-O1A | -2.12 | 118.25      | 123.59   |
| 38  | e     | 103    | HEM  | C4C-CHD-C1D | -2.12 | 121.49      | 126.06   |
| 24  | b     | 610    | CLA  | CAA-C2A-C3A | -2.12 | 106.98      | 112.78   |
| 29  | m     | 103    | LMT  | C1B-O1B-C4' | -2.12 | 112.73      | 117.96   |
| 26  | d     | 404    | BCR  | C39-C30-C25 | -2.12 | 106.87      | 110.30   |
| 27  | B     | 621    | SQD  | O9-S-C6     | 2.11  | 109.45      | 106.94   |
| 24  | B     | 615    | CLA  | CAA-C2A-C3A | -2.11 | 106.99      | 112.78   |
| 24  | A     | 406    | CLA  | CMA-C3A-C2A | -2.11 | 105.30      | 113.83   |
| 26  | C     | 514    | BCR  | C23-C24-C25 | -2.11 | 121.27      | 127.20   |
| 36  | c     | 521    | DGD  | O1G-C1A-O1A | -2.11 | 118.26      | 123.59   |
| 36  | c     | 520    | DGD  | O1G-C1A-C2A | 2.11  | 118.53      | 111.91   |
| 24  | c     | 507    | CLA  | C2A-C1A-CHA | -2.11 | 120.17      | 123.86   |
| 24  | C     | 505    | CLA  | CHA-C1A-NA  | -2.11 | 121.57      | 126.40   |
| 24  | A     | 406    | CLA  | CMC-C2C-C1C | 2.11  | 128.25      | 125.04   |
| 24  | B     | 611    | CLA  | CGD-CBD-CAD | -2.11 | 103.91      | 110.73   |
| 24  | C     | 510    | CLA  | O1D-CGD-CBD | -2.11 | 120.17      | 124.48   |
| 26  | A     | 411    | BCR  | C3-C4-C5    | -2.11 | 110.32      | 114.08   |
| 33  | B     | 622    | LMG  | O8-C28-O10  | -2.11 | 118.28      | 123.59   |
| 26  | T     | 103    | BCR  | C28-C27-C26 | -2.10 | 110.32      | 114.08   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 38  | F     | 102    | HEM  | C2A-C1A-NA  | -2.10 | 107.80      | 110.15   |
| 24  | a     | 410    | CLA  | CAA-CBA-CGA | 2.10  | 119.40      | 113.25   |
| 31  | a     | 415[B] | PL9  | C12-C13-C14 | -2.10 | 122.59      | 127.66   |
| 24  | B     | 610    | CLA  | CED-O2D-CGD | 2.10  | 120.69      | 115.94   |
| 24  | B     | 611    | CLA  | C1-C2-C3    | -2.10 | 122.41      | 126.04   |
| 24  | A     | 405    | CLA  | CHB-C4A-NA  | 2.10  | 127.42      | 124.51   |
| 27  | a     | 405    | SQD  | C3-C4-C5    | 2.10  | 113.99      | 110.24   |
| 31  | A     | 419[A] | PL9  | C47-C46-C44 | -2.10 | 106.06      | 112.98   |
| 26  | a     | 413    | BCR  | C38-C26-C25 | -2.10 | 122.17      | 124.53   |
| 33  | C     | 519    | LMG  | O7-C10-O9   | -2.10 | 118.63      | 123.70   |
| 33  | b     | 629    | LMG  | O8-C28-O10  | -2.10 | 118.30      | 123.59   |
| 27  | B     | 621    | SQD  | O8-S-C6     | 2.10  | 109.08      | 105.74   |
| 24  | B     | 612    | CLA  | CED-O2D-CGD | 2.10  | 120.68      | 115.94   |
| 24  | C     | 507    | CLA  | O1D-CGD-CBD | -2.10 | 120.20      | 124.48   |
| 31  | D     | 405[A] | PL9  | C47-C48-C49 | -2.10 | 120.59      | 127.75   |
| 24  | b     | 610    | CLA  | CHB-C1B-C2B | -2.09 | 121.33      | 127.24   |
| 24  | b     | 610    | CLA  | C1-O2A-CGA  | 2.09  | 121.93      | 116.44   |
| 40  | V     | 205    | HEC  | CAD-CBD-CGD | 2.09  | 118.10      | 113.60   |
| 29  | M     | 103    | LMT  | O5B-C5B-C4B | 2.09  | 113.49      | 109.69   |
| 26  | a     | 413    | BCR  | C8-C7-C6    | -2.09 | 121.33      | 127.20   |
| 36  | c     | 520    | DGD  | O6D-C5D-C6D | 2.09  | 110.88      | 106.67   |
| 31  | A     | 419[A] | PL9  | C51-C49-C50 | 2.09  | 119.21      | 114.60   |
| 24  | b     | 620    | CLA  | C2A-C1A-CHA | -2.09 | 120.21      | 123.86   |
| 24  | c     | 517    | CLA  | C1-O2A-CGA  | 2.09  | 121.92      | 116.44   |
| 31  | A     | 419[A] | PL9  | C40-C39-C41 | 2.09  | 118.78      | 115.27   |
| 36  | c     | 522    | DGD  | O1G-C1A-O1A | -2.08 | 118.34      | 123.59   |
| 24  | A     | 406    | CLA  | O2A-CGA-CBA | 2.08  | 118.44      | 111.91   |
| 24  | B     | 607    | CLA  | C2A-C1A-CHA | -2.08 | 120.22      | 123.86   |
| 33  | d     | 413    | LMG  | C1-O6-C5    | 2.08  | 117.77      | 113.69   |
| 24  | B     | 611    | CLA  | O2A-CGA-O1A | -2.08 | 118.35      | 123.59   |
| 26  | Y     | 101    | BCR  | C40-C30-C25 | -2.08 | 106.93      | 110.30   |
| 26  | B     | 619    | BCR  | C8-C7-C6    | -2.08 | 121.37      | 127.20   |
| 36  | H     | 102    | DGD  | C3B-C2B-C1B | -2.07 | 106.08      | 113.62   |
| 24  | d     | 401    | CLA  | C1-O2A-CGA  | 2.07  | 121.88      | 116.44   |
| 26  | A     | 411    | BCR  | C8-C7-C6    | -2.07 | 121.38      | 127.20   |
| 24  | c     | 517    | CLA  | CMA-C3A-C4A | -2.07 | 106.21      | 111.77   |
| 26  | b     | 626    | BCR  | C29-C30-C25 | 2.07  | 113.67      | 110.48   |
| 38  | e     | 103    | HEM  | CBD-CAD-C3D | -2.07 | 106.88      | 112.63   |
| 35  | c     | 525    | HTG  | C6-C5-C4    | -2.07 | 108.16      | 113.00   |
| 24  | C     | 511    | CLA  | C2A-C1A-CHA | -2.07 | 120.24      | 123.86   |
| 26  | Y     | 101    | BCR  | C28-C27-C26 | -2.07 | 110.39      | 114.08   |
| 31  | d     | 405[A] | PL9  | C22-C23-C24 | -2.06 | 122.69      | 127.66   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | D     | 403    | CLA  | O2A-CGA-CBA | 2.06  | 118.38      | 111.91   |
| 24  | B     | 602    | CLA  | CAC-C3C-C4C | 2.06  | 127.49      | 124.81   |
| 24  | C     | 503    | CLA  | O2A-CGA-O1A | -2.06 | 118.39      | 123.59   |
| 27  | L     | 102    | SQD  | O5-C5-C4    | 2.06  | 113.44      | 109.69   |
| 29  | A     | 417    | LMT  | C6'-C5'-C4' | -2.06 | 107.33      | 113.33   |
| 26  | b     | 628    | BCR  | C21-C20-C19 | -2.06 | 116.79      | 123.22   |
| 27  | f     | 101    | SQD  | O9-S-C6     | 2.06  | 109.39      | 106.94   |
| 25  | a     | 411    | PHO  | CAC-C3C-C4C | 2.06  | 129.49      | 124.27   |
| 26  | c     | 519    | BCR  | C16-C17-C18 | -2.06 | 124.37      | 127.31   |
| 26  | t     | 101    | BCR  | C2-C1-C6    | 2.06  | 113.65      | 110.48   |
| 31  | d     | 405[B] | PL9  | C35-C34-C36 | 2.06  | 118.73      | 115.27   |
| 24  | b     | 623    | CLA  | C4-C3-C2    | -2.06 | 118.40      | 123.68   |
| 24  | A     | 407    | CLA  | O2A-CGA-CBA | 2.06  | 118.36      | 111.91   |
| 24  | b     | 611    | CLA  | C2A-C1A-CHA | -2.06 | 120.26      | 123.86   |
| 27  | f     | 101    | SQD  | C4-C3-C2    | -2.06 | 107.23      | 110.82   |
| 33  | c     | 524    | LMG  | O7-C10-O9   | -2.06 | 118.73      | 123.70   |
| 24  | b     | 613    | CLA  | CHD-C4C-NC  | 2.06  | 127.44      | 124.20   |
| 24  | c     | 509    | CLA  | C6-C7-C8    | -2.06 | 109.28      | 115.92   |
| 26  | b     | 626    | BCR  | C16-C17-C18 | -2.05 | 124.38      | 127.31   |
| 24  | c     | 514    | CLA  | CBC-CAC-C3C | -2.05 | 106.77      | 112.43   |
| 24  | B     | 608    | CLA  | O2D-CGD-O1D | -2.05 | 119.82      | 123.84   |
| 27  | F     | 103    | SQD  | O48-C23-O10 | -2.05 | 118.41      | 123.59   |
| 26  | A     | 411    | BCR  | C24-C23-C22 | -2.05 | 123.14      | 126.23   |
| 24  | B     | 603    | CLA  | O2A-CGA-CBA | 2.05  | 118.34      | 111.91   |
| 31  | d     | 405[A] | PL9  | C35-C34-C36 | 2.05  | 118.72      | 115.27   |
| 24  | c     | 512    | CLA  | OBD-CAD-C3D | -2.05 | 123.59      | 128.52   |
| 26  | A     | 411    | BCR  | C38-C26-C25 | -2.05 | 122.23      | 124.53   |
| 35  | C     | 522    | HTG  | C1-O5-C5    | 2.05  | 116.36      | 112.58   |
| 26  | a     | 413    | BCR  | C3-C4-C5    | -2.05 | 110.42      | 114.08   |
| 24  | B     | 607    | CLA  | CMB-C2B-C1B | 2.05  | 128.49      | 125.37   |
| 25  | a     | 411    | PHO  | C4A-C3A-C2A | -2.05 | 100.89      | 102.84   |
| 26  | K     | 101    | BCR  | C36-C18-C19 | 2.05  | 121.30      | 118.08   |
| 24  | B     | 609    | CLA  | C2A-C1A-CHA | -2.05 | 120.28      | 123.86   |
| 24  | a     | 410    | CLA  | CMA-C3A-C2A | -2.05 | 105.57      | 113.83   |
| 26  | b     | 626    | BCR  | C10-C11-C12 | -2.05 | 116.83      | 123.22   |
| 24  | B     | 605    | CLA  | O2D-CGD-O1D | -2.04 | 119.84      | 123.84   |
| 33  | D     | 413    | LMG  | O7-C10-O9   | -2.04 | 118.76      | 123.70   |
| 24  | B     | 605    | CLA  | OBD-CAD-C3D | -2.04 | 123.60      | 128.52   |
| 33  | b     | 629    | LMG  | C9-C8-C7    | -2.04 | 106.96      | 111.79   |
| 36  | H     | 102    | DGD  | O6E-C5E-C6E | 2.04  | 111.51      | 106.44   |
| 24  | b     | 610    | CLA  | CMB-C2B-C1B | 2.04  | 128.48      | 125.37   |
| 31  | D     | 405[B] | PL9  | C7-C3-C4    | 2.04  | 118.53      | 116.88   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 614    | CLA  | CHB-C1B-C2B | -2.04 | 121.47      | 127.24   |
| 33  | B     | 622    | LMG  | C9-C8-C7    | -2.04 | 106.96      | 111.79   |
| 24  | c     | 516    | CLA  | C2A-C1A-CHA | -2.04 | 120.29      | 123.86   |
| 26  | d     | 404    | BCR  | C21-C20-C19 | -2.04 | 116.86      | 123.22   |
| 24  | C     | 507    | CLA  | CHB-C1B-C2B | -2.04 | 121.48      | 127.24   |
| 38  | F     | 102    | HEM  | CHA-C4D-ND  | 2.04  | 126.89      | 124.37   |
| 24  | B     | 614    | CLA  | CAA-C2A-C3A | -2.04 | 107.20      | 112.78   |
| 37  | E     | 101    | LHG  | O8-C23-O10  | -2.04 | 118.45      | 123.59   |
| 24  | C     | 506    | CLA  | O2A-CGA-CBA | 2.04  | 118.30      | 111.91   |
| 37  | d     | 406    | LHG  | O7-C7-O9    | -2.03 | 118.79      | 123.70   |
| 24  | b     | 625    | CLA  | CHC-C1C-NC  | 2.03  | 127.29      | 124.20   |
| 40  | v     | 205    | HEC  | C1A-CHA-C4D | -2.03 | 121.67      | 126.06   |
| 24  | A     | 410    | CLA  | CHB-C1B-NB  | -2.03 | 122.10      | 124.26   |
| 24  | B     | 608    | CLA  | CED-O2D-CGD | 2.03  | 120.53      | 115.94   |
| 24  | b     | 621    | CLA  | CMB-C2B-C1B | 2.03  | 128.46      | 125.37   |
| 24  | c     | 511    | CLA  | CHB-C4A-NA  | 2.03  | 127.32      | 124.51   |
| 25  | a     | 411    | PHO  | CMC-C2C-C1C | 2.03  | 128.56      | 124.73   |
| 33  | c     | 524    | LMG  | O8-C28-O10  | -2.03 | 118.48      | 123.59   |
| 24  | c     | 508    | CLA  | CHB-C1B-C2B | -2.03 | 121.52      | 127.24   |
| 24  | B     | 605    | CLA  | O1D-CGD-CBD | -2.02 | 120.34      | 124.48   |
| 24  | C     | 501    | CLA  | CHB-C1B-NB  | -2.02 | 122.11      | 124.26   |
| 24  | A     | 407    | CLA  | CAC-C3C-C4C | 2.02  | 127.44      | 124.81   |
| 24  | b     | 614    | CLA  | OBD-CAD-C3D | -2.02 | 123.65      | 128.52   |
| 24  | b     | 625    | CLA  | CAA-C2A-C3A | -2.02 | 107.24      | 112.78   |
| 24  | C     | 512    | CLA  | CHB-C4A-NA  | 2.02  | 127.31      | 124.51   |
| 31  | d     | 405[A] | PL9  | O1-C4-C3    | -2.02 | 118.49      | 120.72   |
| 24  | B     | 613    | CLA  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |
| 27  | a     | 414    | SQD  | O6-C44-C45  | -2.02 | 106.03      | 110.90   |
| 33  | C     | 519    | LMG  | O8-C28-O10  | -2.02 | 118.50      | 123.59   |
| 24  | B     | 608    | CLA  | O1D-CGD-CBD | -2.02 | 120.36      | 124.48   |
| 24  | B     | 605    | CLA  | CHA-C1A-NA  | -2.02 | 121.78      | 126.40   |
| 26  | a     | 413    | BCR  | C15-C14-C13 | -2.02 | 124.43      | 127.31   |
| 26  | k     | 101    | BCR  | C38-C26-C25 | -2.02 | 122.26      | 124.53   |
| 31  | D     | 405[B] | PL9  | C30-C29-C31 | 2.02  | 118.66      | 115.27   |
| 26  | D     | 404    | BCR  | C38-C26-C27 | 2.02  | 117.49      | 113.62   |
| 24  | d     | 402    | CLA  | CHD-C4C-NC  | 2.01  | 127.38      | 124.20   |
| 24  | C     | 501    | CLA  | C6-C7-C8    | -2.01 | 109.41      | 115.92   |
| 24  | C     | 507    | CLA  | CED-O2D-CGD | 2.01  | 120.49      | 115.94   |
| 24  | C     | 510    | CLA  | C4-C3-C2    | -2.01 | 118.51      | 123.68   |
| 37  | b     | 634    | LHG  | O4-P-O5     | 2.01  | 122.19      | 112.24   |
| 24  | c     | 515    | CLA  | C6-C7-C8    | -2.01 | 109.42      | 115.92   |
| 26  | A     | 411    | BCR  | C7-C8-C9    | -2.01 | 123.19      | 126.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | c     | 512    | CLA  | CHB-C4A-NA  | 2.01  | 127.29      | 124.51   |
| 24  | C     | 506    | CLA  | C2A-C1A-CHA | -2.01 | 120.34      | 123.86   |
| 24  | a     | 412    | CLA  | OBD-CAD-C3D | -2.01 | 123.69      | 128.52   |
| 26  | t     | 101    | BCR  | C37-C22-C21 | -2.01 | 120.11      | 122.92   |
| 24  | B     | 608    | CLA  | CHB-C4A-NA  | 2.01  | 127.29      | 124.51   |
| 29  | F     | 101    | LMT  | C1B-O5B-C5B | 2.01  | 117.63      | 113.69   |
| 31  | D     | 405[B] | PL9  | C7-C3-C2    | -2.01 | 120.66      | 123.30   |
| 26  | C     | 514    | BCR  | C11-C10-C9  | -2.01 | 124.45      | 127.31   |
| 26  | B     | 618    | BCR  | C29-C30-C25 | 2.01  | 113.57      | 110.48   |
| 24  | B     | 603    | CLA  | CHB-C1B-C2B | -2.01 | 121.57      | 127.24   |
| 26  | c     | 528    | BCR  | C28-C27-C26 | -2.00 | 110.50      | 114.08   |
| 38  | F     | 102    | HEM  | CBA-CAA-C2A | -2.00 | 107.06      | 112.63   |
| 24  | c     | 518    | CLA  | CHB-C1B-C2B | -2.00 | 121.58      | 127.24   |
| 26  | C     | 515    | BCR  | C40-C30-C25 | -2.00 | 107.05      | 110.30   |
| 33  | C     | 520    | LMG  | C3-C4-C5    | 2.00  | 113.81      | 110.24   |
| 24  | C     | 510    | CLA  | O2A-CGA-O1A | -2.00 | 118.54      | 123.59   |
| 24  | B     | 605    | CLA  | CHB-C1B-NB  | -2.00 | 122.14      | 124.26   |
| 24  | B     | 617    | CLA  | CHB-C1B-NB  | -2.00 | 122.14      | 124.26   |
| 31  | d     | 405[A] | PL9  | C45-C44-C46 | 2.00  | 118.64      | 115.27   |
| 36  | H     | 102    | DGD  | C3E-C4E-C5E | -2.00 | 106.67      | 110.24   |
| 24  | b     | 612    | CLA  | CMB-C2B-C1B | 2.00  | 128.42      | 125.37   |
| 31  | A     | 419[A] | PL9  | C16-C17-C18 | -2.00 | 105.31      | 111.88   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 40  | V     | 205 | HEC  | NA   |
| 40  | v     | 205 | HEC  | NA   |

All (1331) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | A     | 406 | CLA  | CHA-CBD-CGD-O1D |
| 24  | A     | 406 | CLA  | CHA-CBD-CGD-O2D |
| 24  | B     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 24  | B     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 24  | B     | 602 | CLA  | CAD-CBD-CGD-O1D |
| 24  | B     | 603 | CLA  | C14-C13-C15-C16 |
| 24  | B     | 606 | CLA  | C2-C3-C5-C6     |
| 24  | B     | 606 | CLA  | C4-C3-C5-C6     |
| 24  | B     | 607 | CLA  | CHA-CBD-CGD-O1D |
| 24  | B     | 607 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | B     | 615 | CLA  | CHA-CBD-CGD-O1D |
| 24  | B     | 615 | CLA  | CHA-CBD-CGD-O2D |
| 24  | B     | 615 | CLA  | CAD-CBD-CGD-O1D |
| 24  | B     | 615 | CLA  | CAD-CBD-CGD-O2D |
| 24  | B     | 615 | CLA  | C2-C3-C5-C6     |
| 24  | B     | 615 | CLA  | C4-C3-C5-C6     |
| 24  | C     | 507 | CLA  | C2B-C3B-CAB-CBB |
| 24  | C     | 507 | CLA  | C4B-C3B-CAB-CBB |
| 24  | C     | 508 | CLA  | CHA-CBD-CGD-O1D |
| 24  | C     | 509 | CLA  | C2-C1-O2A-CGA   |
| 24  | b     | 614 | CLA  | C2-C3-C5-C6     |
| 24  | b     | 614 | CLA  | C4-C3-C5-C6     |
| 24  | b     | 615 | CLA  | CHA-CBD-CGD-O1D |
| 24  | b     | 615 | CLA  | CHA-CBD-CGD-O2D |
| 24  | b     | 623 | CLA  | CHA-CBD-CGD-O1D |
| 24  | b     | 623 | CLA  | CHA-CBD-CGD-O2D |
| 24  | b     | 623 | CLA  | CAD-CBD-CGD-O1D |
| 24  | b     | 623 | CLA  | C2-C3-C5-C6     |
| 24  | b     | 623 | CLA  | C4-C3-C5-C6     |
| 24  | c     | 513 | CLA  | CHA-CBD-CGD-O1D |
| 24  | c     | 513 | CLA  | CHA-CBD-CGD-O2D |
| 24  | c     | 517 | CLA  | C2B-C3B-CAB-CBB |
| 24  | c     | 517 | CLA  | C4B-C3B-CAB-CBB |
| 26  | D     | 404 | BCR  | C21-C22-C23-C24 |
| 26  | D     | 404 | BCR  | C37-C22-C23-C24 |
| 26  | Y     | 101 | BCR  | C1-C6-C7-C8     |
| 26  | Y     | 101 | BCR  | C5-C6-C7-C8     |
| 26  | b     | 626 | BCR  | C1-C6-C7-C8     |
| 26  | d     | 404 | BCR  | C21-C22-C23-C24 |
| 26  | d     | 404 | BCR  | C37-C22-C23-C24 |
| 26  | y     | 101 | BCR  | C1-C6-C7-C8     |
| 26  | y     | 101 | BCR  | C5-C6-C7-C8     |
| 27  | A     | 416 | SQD  | O6-C44-C45-O47  |
| 27  | B     | 621 | SQD  | O49-C7-O47-C45  |
| 27  | B     | 621 | SQD  | C5-C6-S-O7      |
| 27  | B     | 621 | SQD  | C5-C6-S-O9      |
| 27  | F     | 103 | SQD  | O49-C7-O47-C45  |
| 27  | F     | 103 | SQD  | C5-C6-S-O7      |
| 27  | L     | 102 | SQD  | O5-C1-O6-C44    |
| 27  | L     | 102 | SQD  | O49-C7-O47-C45  |
| 27  | a     | 405 | SQD  | O6-C44-C45-O47  |
| 27  | a     | 405 | SQD  | O5-C5-C6-S      |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 27  | f     | 101    | SQD  | O49-C7-O47-C45  |
| 27  | f     | 101    | SQD  | C8-C7-O47-C45   |
| 27  | f     | 101    | SQD  | C5-C6-S-O7      |
| 27  | f     | 101    | SQD  | C5-C6-S-O8      |
| 27  | f     | 101    | SQD  | C5-C6-S-O9      |
| 28  | A     | 414    | GOL  | C1-C2-C3-O3     |
| 28  | A     | 415    | GOL  | C1-C2-C3-O3     |
| 28  | A     | 422    | GOL  | O1-C1-C2-C3     |
| 28  | B     | 627    | GOL  | O1-C1-C2-C3     |
| 28  | B     | 628    | GOL  | O1-C1-C2-C3     |
| 28  | B     | 630    | GOL  | O1-C1-C2-C3     |
| 28  | B     | 630    | GOL  | C1-C2-C3-O3     |
| 28  | C     | 524    | GOL  | O1-C1-C2-C3     |
| 28  | T     | 102    | GOL  | O1-C1-C2-O2     |
| 28  | T     | 102    | GOL  | O1-C1-C2-C3     |
| 28  | V     | 201    | GOL  | C1-C2-C3-O3     |
| 28  | a     | 402    | GOL  | O1-C1-C2-C3     |
| 28  | a     | 420    | GOL  | O1-C1-C2-C3     |
| 28  | b     | 604    | GOL  | O1-C1-C2-C3     |
| 29  | A     | 417    | LMT  | C2'-C1'-O1'-C1  |
| 29  | A     | 417    | LMT  | O5'-C1'-O1'-C1  |
| 29  | B     | 635    | LMT  | C2'-C1'-O1'-C1  |
| 29  | B     | 635    | LMT  | O5'-C1'-O1'-C1  |
| 29  | C     | 521    | LMT  | C2'-C1'-O1'-C1  |
| 29  | C     | 521    | LMT  | O5'-C1'-O1'-C1  |
| 29  | F     | 101    | LMT  | C2'-C1'-O1'-C1  |
| 29  | F     | 101    | LMT  | O5'-C1'-O1'-C1  |
| 29  | M     | 103    | LMT  | O5'-C1'-O1'-C1  |
| 29  | T     | 104    | LMT  | C2'-C1'-O1'-C1  |
| 29  | T     | 104    | LMT  | O5'-C1'-O1'-C1  |
| 29  | a     | 404    | LMT  | C2'-C1'-O1'-C1  |
| 29  | a     | 404    | LMT  | O5'-C1'-O1'-C1  |
| 29  | a     | 419    | LMT  | C2'-C1'-O1'-C1  |
| 29  | a     | 419    | LMT  | O5'-C1'-O1'-C1  |
| 29  | b     | 630    | LMT  | C2'-C1'-O1'-C1  |
| 29  | b     | 630    | LMT  | O5'-C1'-O1'-C1  |
| 29  | f     | 102    | LMT  | C2'-C1'-O1'-C1  |
| 29  | f     | 102    | LMT  | O5'-C1'-O1'-C1  |
| 31  | a     | 415[B] | PL9  | C12-C11-C9-C10  |
| 31  | a     | 415[B] | PL9  | C18-C19-C21-C22 |
| 31  | a     | 415[B] | PL9  | C20-C19-C21-C22 |
| 33  | C     | 520    | LMG  | C11-C10-O7-C8   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | Z     | 101 | LMG  | O6-C1-O1-C7     |
| 33  | Z     | 101 | LMG  | O9-C10-O7-C8    |
| 33  | Z     | 101 | LMG  | C11-C10-O7-C8   |
| 33  | z     | 101 | LMG  | O6-C1-O1-C7     |
| 33  | z     | 101 | LMG  | O9-C10-O7-C8    |
| 35  | B     | 624 | HTG  | C2'-C1'-S1-C1   |
| 35  | B     | 625 | HTG  | O5-C1-S1-C1'    |
| 35  | b     | 632 | HTG  | O5-C1-S1-C1'    |
| 35  | b     | 632 | HTG  | C2'-C1'-S1-C1   |
| 35  | c     | 525 | HTG  | C2'-C1'-S1-C1   |
| 36  | D     | 406 | DGD  | C2B-C1B-O2G-C2G |
| 36  | D     | 406 | DGD  | C2D-C1D-O3G-C3G |
| 36  | D     | 406 | DGD  | O6D-C1D-O3G-C3G |
| 36  | e     | 101 | DGD  | C2B-C1B-O2G-C2G |
| 36  | e     | 101 | DGD  | O1B-C1B-O2G-C2G |
| 36  | e     | 101 | DGD  | O6E-C1E-O5D-C6D |
| 37  | D     | 408 | LHG  | C4-O6-P-O4      |
| 37  | E     | 101 | LHG  | C3-O3-P-O4      |
| 37  | E     | 101 | LHG  | C3-O3-P-O5      |
| 37  | E     | 101 | LHG  | C3-O3-P-O6      |
| 37  | E     | 101 | LHG  | C4-O6-P-O5      |
| 37  | L     | 101 | LHG  | C4-O6-P-O4      |
| 37  | L     | 101 | LHG  | C4-O6-P-O5      |
| 37  | b     | 634 | LHG  | C4-O6-P-O4      |
| 37  | d     | 407 | LHG  | C3-O3-P-O4      |
| 37  | e     | 102 | LHG  | C3-O3-P-O5      |
| 37  | e     | 102 | LHG  | C3-O3-P-O6      |
| 38  | F     | 102 | HEM  | C2B-C3B-CAB-CBB |
| 38  | F     | 102 | HEM  | C2C-C3C-CAC-CBC |
| 37  | e     | 102 | LHG  | O10-C23-O8-C6   |
| 29  | C     | 521 | LMT  | C3'-C4'-O1B-C1B |
| 29  | D     | 401 | LMT  | C3'-C4'-O1B-C1B |
| 37  | E     | 101 | LHG  | O10-C23-O8-C6   |
| 24  | c     | 516 | CLA  | CBD-CGD-O2D-CED |
| 33  | C     | 520 | LMG  | O9-C10-O7-C8    |
| 36  | D     | 406 | DGD  | O1B-C1B-O2G-C2G |
| 24  | A     | 410 | CLA  | C3-C5-C6-C7     |
| 24  | B     | 617 | CLA  | C3-C5-C6-C7     |
| 24  | b     | 623 | CLA  | C3-C5-C6-C7     |
| 37  | E     | 101 | LHG  | C24-C23-O8-C6   |
| 37  | e     | 102 | LHG  | C24-C23-O8-C6   |
| 27  | B     | 621 | SQD  | C8-C7-O47-C45   |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 27  | F     | 103    | SQD  | C8-C7-O47-C45   |
| 27  | L     | 102    | SQD  | C8-C7-O47-C45   |
| 33  | z     | 101    | LMG  | C11-C10-O7-C8   |
| 31  | a     | 415[A] | PL9  | C12-C11-C9-C10  |
| 31  | a     | 415[A] | PL9  | C20-C19-C21-C22 |
| 36  | C     | 516    | DGD  | C2A-C3A-C4A-C5A |
| 24  | B     | 615    | CLA  | C3-C5-C6-C7     |
| 24  | c     | 511    | CLA  | C3-C5-C6-C7     |
| 35  | b     | 632    | HTG  | S1-C1'-C2'-C3'  |
| 33  | z     | 101    | LMG  | O6-C5-C6-O5     |
| 37  | E     | 101    | LHG  | O2-C2-C3-O3     |
| 37  | d     | 407    | LHG  | O2-C2-C3-O3     |
| 29  | M     | 103    | LMT  | O5'-C5'-C6'-O6' |
| 33  | A     | 421    | LMG  | C11-C10-O7-C8   |
| 29  | f     | 102    | LMT  | C4'-C5'-C6'-O6' |
| 29  | M     | 103    | LMT  | O5B-C5B-C6B-O6B |
| 29  | f     | 102    | LMT  | O5'-C5'-C6'-O6' |
| 24  | B     | 602    | CLA  | C3-C5-C6-C7     |
| 35  | V     | 206    | HTG  | S1-C1'-C2'-C3'  |
| 33  | C     | 520    | LMG  | O6-C5-C6-O5     |
| 38  | e     | 103    | HEM  | C3D-CAD-CBD-CGD |
| 29  | M     | 101    | LMT  | O5B-C5B-C6B-O6B |
| 31  | A     | 419[A] | PL9  | C25-C24-C26-C27 |
| 31  | A     | 419[B] | PL9  | C25-C24-C26-C27 |
| 31  | a     | 415[A] | PL9  | C15-C14-C16-C17 |
| 31  | a     | 415[A] | PL9  | C25-C24-C26-C27 |
| 31  | a     | 415[B] | PL9  | C15-C14-C16-C17 |
| 31  | a     | 415[B] | PL9  | C25-C24-C26-C27 |
| 31  | A     | 419[A] | PL9  | C23-C24-C26-C27 |
| 31  | A     | 419[B] | PL9  | C23-C24-C26-C27 |
| 31  | a     | 415[A] | PL9  | C13-C14-C16-C17 |
| 31  | a     | 415[A] | PL9  | C23-C24-C26-C27 |
| 31  | a     | 415[B] | PL9  | C13-C14-C16-C17 |
| 31  | a     | 415[B] | PL9  | C23-C24-C26-C27 |
| 24  | B     | 607    | CLA  | C2A-CAA-CBA-CGA |
| 24  | b     | 615    | CLA  | C2A-CAA-CBA-CGA |
| 33  | z     | 101    | LMG  | C4-C5-C6-O5     |
| 27  | B     | 621    | SQD  | O5-C1-O6-C44    |
| 31  | D     | 405[A] | PL9  | C39-C41-C42-C43 |
| 31  | d     | 405[A] | PL9  | C39-C41-C42-C43 |
| 31  | d     | 405[B] | PL9  | C39-C41-C42-C43 |
| 24  | C     | 509    | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 29  | M     | 103    | LMT  | C4'-C5'-C6'-O6' |
| 29  | m     | 103    | LMT  | O5'-C5'-C6'-O6' |
| 33  | A     | 421    | LMG  | O9-C10-O7-C8    |
| 24  | C     | 509    | CLA  | O1A-CGA-O2A-C1  |
| 24  | C     | 509    | CLA  | CBA-CGA-O2A-C1  |
| 24  | B     | 615    | CLA  | C5-C6-C7-C8     |
| 29  | D     | 401    | LMT  | O5B-C5B-C6B-O6B |
| 33  | c     | 501    | LMG  | C17-C18-C19-C20 |
| 24  | B     | 602    | CLA  | C10-C11-C12-C13 |
| 24  | B     | 615    | CLA  | C8-C10-C11-C12  |
| 33  | Z     | 101    | LMG  | C10-C11-C12-C13 |
| 33  | Z     | 101    | LMG  | C2-C1-O1-C7     |
| 36  | e     | 101    | DGD  | C2E-C1E-O5D-C6D |
| 31  | a     | 415[A] | PL9  | C12-C11-C9-C8   |
| 24  | B     | 602    | CLA  | C11-C10-C8-C9   |
| 24  | B     | 617    | CLA  | C6-C7-C8-C9     |
| 24  | C     | 501    | CLA  | C11-C12-C13-C14 |
| 24  | b     | 619    | CLA  | C11-C12-C13-C14 |
| 24  | c     | 511    | CLA  | C6-C7-C8-C9     |
| 24  | c     | 514    | CLA  | C11-C10-C8-C9   |
| 33  | B     | 622    | LMG  | C15-C16-C17-C18 |
| 24  | B     | 616    | CLA  | C8-C10-C11-C12  |
| 26  | D     | 404    | BCR  | C7-C8-C9-C34    |
| 27  | B     | 621    | SQD  | C7-C8-C9-C10    |
| 24  | b     | 624    | CLA  | C10-C11-C12-C13 |
| 24  | C     | 501    | CLA  | C15-C16-C17-C18 |
| 35  | B     | 625    | HTG  | O5-C5-C6-O6     |
| 33  | C     | 520    | LMG  | C28-C29-C30-C31 |
| 35  | b     | 601    | HTG  | C1'-C2'-C3'-C4' |
| 35  | c     | 525    | HTG  | C1'-C2'-C3'-C4' |
| 24  | A     | 410    | CLA  | C13-C15-C16-C17 |
| 24  | B     | 615    | CLA  | C10-C11-C12-C13 |
| 24  | C     | 508    | CLA  | C10-C11-C12-C13 |
| 24  | c     | 513    | CLA  | C15-C16-C17-C18 |
| 28  | B     | 627    | GOL  | O1-C1-C2-O2     |
| 28  | V     | 202    | GOL  | O1-C1-C2-O2     |
| 28  | a     | 402    | GOL  | O1-C1-C2-O2     |
| 28  | a     | 420    | GOL  | O1-C1-C2-O2     |
| 28  | b     | 605    | GOL  | O1-C1-C2-O2     |
| 28  | v     | 203    | GOL  | O1-C1-C2-O2     |
| 27  | A     | 416    | SQD  | C23-C24-C25-C26 |
| 33  | c     | 523    | LMG  | C10-C11-C12-C13 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | c     | 522    | DGD  | C1A-C2A-C3A-C4A |
| 29  | A     | 417    | LMT  | O5B-C5B-C6B-O6B |
| 24  | b     | 610    | CLA  | C2-C1-O2A-CGA   |
| 29  | M     | 101    | LMT  | C4B-C5B-C6B-O6B |
| 33  | c     | 501    | LMG  | C10-C11-C12-C13 |
| 24  | c     | 516    | CLA  | O1D-CGD-O2D-CED |
| 24  | C     | 506    | CLA  | C6-C7-C8-C10    |
| 24  | b     | 615    | CLA  | C12-C13-C15-C16 |
| 24  | c     | 514    | CLA  | C12-C13-C15-C16 |
| 24  | C     | 508    | CLA  | C5-C6-C7-C8     |
| 24  | b     | 623    | CLA  | C5-C6-C7-C8     |
| 29  | T     | 104    | LMT  | O1'-C1-C2-C3    |
| 36  | e     | 101    | DGD  | O6D-C1D-O3G-C3G |
| 24  | a     | 412    | CLA  | C8-C10-C11-C12  |
| 31  | a     | 415[A] | PL9  | C9-C11-C12-C13  |
| 31  | a     | 415[B] | PL9  | C9-C11-C12-C13  |
| 27  | A     | 416    | SQD  | C26-C27-C28-C29 |
| 37  | e     | 102    | LHG  | C11-C12-C13-C14 |
| 24  | C     | 506    | CLA  | C13-C15-C16-C17 |
| 24  | c     | 514    | CLA  | C13-C15-C16-C17 |
| 24  | C     | 504    | CLA  | C15-C16-C17-C18 |
| 24  | C     | 506    | CLA  | C5-C6-C7-C8     |
| 24  | b     | 623    | CLA  | C13-C15-C16-C17 |
| 29  | M     | 103    | LMT  | C4B-C5B-C6B-O6B |
| 33  | C     | 520    | LMG  | C4-C5-C6-O5     |
| 27  | F     | 103    | SQD  | C26-C27-C28-C29 |
| 24  | B     | 617    | CLA  | C10-C11-C12-C13 |
| 24  | b     | 610    | CLA  | C8-C10-C11-C12  |
| 24  | b     | 615    | CLA  | C13-C15-C16-C17 |
| 37  | L     | 101    | LHG  | C4-O6-P-O3      |
| 37  | b     | 634    | LHG  | C4-O6-P-O3      |
| 37  | d     | 407    | LHG  | C3-O3-P-O6      |
| 37  | D     | 407    | LHG  | C23-C24-C25-C26 |
| 35  | b     | 632    | HTG  | C1'-C2'-C3'-C4' |
| 35  | c     | 525    | HTG  | S1-C1'-C2'-C3'  |
| 35  | b     | 632    | HTG  | O5-C5-C6-O6     |
| 37  | E     | 101    | LHG  | C1-C2-C3-O3     |
| 24  | c     | 515    | CLA  | C4-C3-C5-C6     |
| 31  | a     | 415[A] | PL9  | C30-C29-C31-C32 |
| 24  | c     | 514    | CLA  | C15-C16-C17-C18 |
| 37  | D     | 408    | LHG  | C32-C33-C34-C35 |
| 35  | C     | 523    | HTG  | O5-C5-C6-O6     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | D     | 403    | CLA  | C3-C5-C6-C7     |
| 24  | c     | 509    | CLA  | C15-C16-C17-C18 |
| 27  | A     | 416    | SQD  | C30-C31-C32-C33 |
| 29  | M     | 103    | LMT  | C2-C3-C4-C5     |
| 33  | A     | 421    | LMG  | C14-C15-C16-C17 |
| 33  | c     | 523    | LMG  | C11-C10-O7-C8   |
| 29  | m     | 102    | LMT  | O5'-C5'-C6'-O6' |
| 27  | A     | 412    | SQD  | C9-C10-C11-C12  |
| 29  | T     | 104    | LMT  | C11-C10-C9-C8   |
| 35  | B     | 624    | HTG  | C2'-C3'-C4'-C5' |
| 36  | D     | 406    | DGD  | C6A-C7A-C8A-C9A |
| 36  | H     | 102    | DGD  | CBB-CCB-CDB-CEB |
| 37  | e     | 102    | LHG  | C24-C25-C26-C27 |
| 24  | a     | 412    | CLA  | C16-C17-C18-C19 |
| 24  | b     | 623    | CLA  | C16-C17-C18-C19 |
| 33  | c     | 501    | LMG  | C21-C22-C23-C24 |
| 33  | d     | 413    | LMG  | C17-C18-C19-C20 |
| 36  | C     | 516    | DGD  | C4B-C5B-C6B-C7B |
| 36  | C     | 517    | DGD  | C9A-CAA-CBA-CCA |
| 36  | C     | 518    | DGD  | CAA-CBA-CCA-CDA |
| 36  | c     | 521    | DGD  | C9A-CAA-CBA-CCA |
| 33  | c     | 523    | LMG  | O9-C10-O7-C8    |
| 24  | a     | 412    | CLA  | C10-C11-C12-C13 |
| 24  | c     | 518    | CLA  | C10-C11-C12-C13 |
| 29  | B     | 635    | LMT  | C3-C4-C5-C6     |
| 33  | B     | 622    | LMG  | C29-C30-C31-C32 |
| 27  | B     | 621    | SQD  | C30-C31-C32-C33 |
| 27  | L     | 102    | SQD  | C27-C28-C29-C30 |
| 29  | T     | 104    | LMT  | C4-C5-C6-C7     |
| 27  | A     | 416    | SQD  | C2-C1-O6-C44    |
| 29  | D     | 401    | LMT  | C2'-C1'-O1'-C1  |
| 29  | m     | 102    | LMT  | C2'-C1'-O1'-C1  |
| 36  | C     | 517    | DGD  | C2E-C1E-O5D-C6D |
| 36  | c     | 521    | DGD  | C2E-C1E-O5D-C6D |
| 36  | e     | 101    | DGD  | C2D-C1D-O3G-C3G |
| 33  | c     | 523    | LMG  | C34-C35-C36-C37 |
| 36  | e     | 101    | DGD  | CCA-CDA-CEA-CFA |
| 33  | d     | 413    | LMG  | O6-C5-C6-O5     |
| 31  | d     | 405[A] | PL9  | C45-C44-C46-C47 |
| 27  | L     | 102    | SQD  | C12-C13-C14-C15 |
| 36  | c     | 522    | DGD  | C6A-C7A-C8A-C9A |
| 31  | d     | 405[B] | PL9  | C13-C14-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | C     | 505 | CLA  | C11-C12-C13-C14 |
| 24  | a     | 410 | CLA  | C11-C12-C13-C14 |
| 24  | b     | 610 | CLA  | C11-C10-C8-C9   |
| 24  | b     | 612 | CLA  | C6-C7-C8-C9     |
| 36  | c     | 520 | DGD  | O6D-C5D-C6D-O5D |
| 36  | c     | 521 | DGD  | C4A-C5A-C6A-C7A |
| 36  | e     | 101 | DGD  | C8B-C9B-CAB-CBB |
| 37  | D     | 409 | LHG  | C29-C30-C31-C32 |
| 33  | z     | 101 | LMG  | C12-C13-C14-C15 |
| 36  | h     | 102 | DGD  | CAA-CBA-CCA-CDA |
| 37  | D     | 407 | LHG  | C34-C35-C36-C37 |
| 37  | d     | 406 | LHG  | C32-C33-C34-C35 |
| 28  | B     | 626 | GOL  | C1-C2-C3-O3     |
| 28  | B     | 629 | GOL  | O1-C1-C2-C3     |
| 28  | V     | 202 | GOL  | O1-C1-C2-C3     |
| 28  | b     | 605 | GOL  | O1-C1-C2-C3     |
| 28  | o     | 301 | GOL  | O1-C1-C2-C3     |
| 28  | o     | 301 | GOL  | C1-C2-C3-O3     |
| 28  | v     | 201 | GOL  | O1-C1-C2-C3     |
| 28  | v     | 202 | GOL  | O1-C1-C2-C3     |
| 28  | v     | 203 | GOL  | O1-C1-C2-C3     |
| 37  | D     | 407 | LHG  | O1-C1-C2-C3     |
| 36  | C     | 516 | DGD  | C3B-C4B-C5B-C6B |
| 36  | c     | 520 | DGD  | C5A-C6A-C7A-C8A |
| 29  | a     | 404 | LMT  | C4B-C5B-C6B-O6B |
| 37  | e     | 102 | LHG  | C23-C24-C25-C26 |
| 27  | a     | 414 | SQD  | C11-C12-C13-C14 |
| 33  | A     | 421 | LMG  | C11-C12-C13-C14 |
| 33  | b     | 629 | LMG  | C38-C39-C40-C41 |
| 36  | C     | 516 | DGD  | C5B-C6B-C7B-C8B |
| 36  | c     | 522 | DGD  | C7A-C8A-C9A-CAA |
| 36  | c     | 522 | DGD  | C6B-C7B-C8B-C9B |
| 37  | L     | 101 | LHG  | C14-C15-C16-C17 |
| 24  | C     | 502 | CLA  | C4B-C3B-CAB-CBB |
| 24  | C     | 512 | CLA  | C4B-C3B-CAB-CBB |
| 24  | b     | 616 | CLA  | C4B-C3B-CAB-CBB |
| 24  | b     | 618 | CLA  | C4B-C3B-CAB-CBB |
| 24  | c     | 507 | CLA  | C4B-C3B-CAB-CBB |
| 24  | d     | 402 | CLA  | C4B-C3B-CAB-CBB |
| 24  | b     | 620 | CLA  | C16-C17-C18-C19 |
| 35  | B     | 632 | HTG  | C4-C5-C6-O6     |
| 29  | m     | 102 | LMT  | O5'-C1'-O1'-C1  |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | B     | 614    | CLA  | C13-C15-C16-C17 |
| 33  | C     | 519    | LMG  | C11-C12-C13-C14 |
| 36  | c     | 522    | DGD  | C7B-C8B-C9B-CAB |
| 29  | A     | 417    | LMT  | C6-C7-C8-C9     |
| 36  | c     | 520    | DGD  | C9A-CAA-CBA-CCA |
| 37  | D     | 407    | LHG  | C24-C25-C26-C27 |
| 37  | E     | 101    | LHG  | C24-C25-C26-C27 |
| 36  | c     | 520    | DGD  | C8B-C9B-CAB-CBB |
| 36  | c     | 522    | DGD  | CBA-CCA-CDA-CEA |
| 37  | d     | 408    | LHG  | C29-C30-C31-C32 |
| 24  | c     | 514    | CLA  | C3-C5-C6-C7     |
| 27  | L     | 102    | SQD  | C24-C23-O48-C46 |
| 29  | M     | 103    | LMT  | C2-C1-O1'-C1'   |
| 33  | b     | 629    | LMG  | C32-C33-C34-C35 |
| 33  | d     | 413    | LMG  | C36-C37-C38-C39 |
| 37  | D     | 409    | LHG  | C24-C25-C26-C27 |
| 33  | z     | 101    | LMG  | C15-C16-C17-C18 |
| 35  | b     | 631    | HTG  | C2'-C3'-C4'-C5' |
| 29  | C     | 521    | LMT  | O5B-C5B-C6B-O6B |
| 27  | B     | 621    | SQD  | C31-C32-C33-C34 |
| 33  | c     | 501    | LMG  | C14-C15-C16-C17 |
| 36  | D     | 406    | DGD  | C2A-C3A-C4A-C5A |
| 29  | T     | 104    | LMT  | C1-C2-C3-C4     |
| 25  | A     | 408    | PHO  | C4-C3-C5-C6     |
| 31  | D     | 405[A] | PL9  | C15-C14-C16-C17 |
| 24  | C     | 510    | CLA  | C2-C3-C5-C6     |
| 24  | c     | 515    | CLA  | C2-C3-C5-C6     |
| 25  | A     | 408    | PHO  | C2-C3-C5-C6     |
| 31  | a     | 415[A] | PL9  | C18-C19-C21-C22 |
| 31  | d     | 405[B] | PL9  | C43-C44-C46-C47 |
| 27  | a     | 405    | SQD  | C25-C26-C27-C28 |
| 28  | A     | 414    | GOL  | O2-C2-C3-O3     |
| 28  | B     | 628    | GOL  | O1-C1-C2-O2     |
| 28  | B     | 630    | GOL  | O1-C1-C2-O2     |
| 28  | B     | 630    | GOL  | O2-C2-C3-O3     |
| 28  | v     | 201    | GOL  | O1-C1-C2-O2     |
| 27  | a     | 414    | SQD  | C29-C30-C31-C32 |
| 29  | a     | 404    | LMT  | C2-C3-C4-C5     |
| 33  | A     | 421    | LMG  | C30-C31-C32-C33 |
| 24  | a     | 412    | CLA  | C16-C17-C18-C20 |
| 24  | b     | 624    | CLA  | C16-C17-C18-C19 |
| 33  | Z     | 101    | LMG  | C19-C20-C21-C22 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | C     | 502    | CLA  | C2B-C3B-CAB-CBB |
| 24  | C     | 512    | CLA  | C2B-C3B-CAB-CBB |
| 24  | b     | 616    | CLA  | C2B-C3B-CAB-CBB |
| 24  | b     | 618    | CLA  | C2B-C3B-CAB-CBB |
| 24  | c     | 507    | CLA  | C2B-C3B-CAB-CBB |
| 24  | d     | 402    | CLA  | C2B-C3B-CAB-CBB |
| 24  | c     | 511    | CLA  | C15-C16-C17-C18 |
| 29  | T     | 104    | LMT  | C7-C8-C9-C10    |
| 33  | D     | 413    | LMG  | C19-C20-C21-C22 |
| 36  | h     | 102    | DGD  | C4E-C5E-C6E-O5E |
| 33  | B     | 622    | LMG  | C31-C32-C33-C34 |
| 24  | B     | 617    | CLA  | C2-C1-O2A-CGA   |
| 24  | c     | 514    | CLA  | C2-C1-O2A-CGA   |
| 36  | H     | 102    | DGD  | C7A-C8A-C9A-CAA |
| 36  | c     | 520    | DGD  | CAB-CBB-CCB-CDB |
| 27  | a     | 405    | SQD  | C31-C32-C33-C34 |
| 26  | B     | 618    | BCR  | C1-C6-C7-C8     |
| 26  | B     | 618    | BCR  | C5-C6-C7-C8     |
| 26  | b     | 626    | BCR  | C5-C6-C7-C8     |
| 26  | d     | 404    | BCR  | C23-C24-C25-C26 |
| 26  | d     | 404    | BCR  | C23-C24-C25-C30 |
| 33  | d     | 413    | LMG  | C19-C20-C21-C22 |
| 35  | B     | 632    | HTG  | C2'-C3'-C4'-C5' |
| 37  | b     | 634    | LHG  | C27-C28-C29-C30 |
| 38  | e     | 103    | HEM  | C2A-CAA-CBA-CGA |
| 27  | a     | 414    | SQD  | C9-C10-C11-C12  |
| 36  | e     | 101    | DGD  | C2A-C3A-C4A-C5A |
| 29  | C     | 521    | LMT  | O5'-C5'-C6'-O6' |
| 24  | B     | 602    | CLA  | C8-C10-C11-C12  |
| 27  | A     | 412    | SQD  | C13-C14-C15-C16 |
| 36  | e     | 101    | DGD  | C5A-C6A-C7A-C8A |
| 31  | D     | 405[B] | PL9  | C15-C14-C16-C17 |
| 31  | d     | 405[B] | PL9  | C45-C44-C46-C47 |
| 24  | B     | 603    | CLA  | C12-C13-C15-C16 |
| 24  | B     | 616    | CLA  | C11-C12-C13-C15 |
| 24  | C     | 505    | CLA  | C11-C12-C13-C15 |
| 24  | a     | 410    | CLA  | C11-C12-C13-C15 |
| 24  | b     | 612    | CLA  | C6-C7-C8-C10    |
| 24  | b     | 625    | CLA  | C11-C12-C13-C15 |
| 31  | D     | 405[A] | PL9  | C13-C14-C16-C17 |
| 31  | D     | 405[B] | PL9  | C28-C29-C31-C32 |
| 31  | d     | 405[A] | PL9  | C43-C44-C46-C47 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 35  | C     | 523    | HTG  | S1-C1'-C2'-C3'  |
| 24  | C     | 511    | CLA  | O1A-CGA-O2A-C1  |
| 27  | L     | 102    | SQD  | O10-C23-O48-C46 |
| 27  | L     | 102    | SQD  | C31-C32-C33-C34 |
| 24  | B     | 616    | CLA  | C5-C6-C7-C8     |
| 24  | c     | 515    | CLA  | C8-C10-C11-C12  |
| 26  | t     | 101    | BCR  | C13-C14-C15-C16 |
| 24  | b     | 623    | CLA  | C16-C17-C18-C20 |
| 36  | e     | 101    | DGD  | O6D-C5D-C6D-O5D |
| 24  | C     | 511    | CLA  | CBA-CGA-O2A-C1  |
| 36  | e     | 101    | DGD  | C2A-C1A-O1G-C1G |
| 27  | A     | 412    | SQD  | C14-C15-C16-C17 |
| 33  | B     | 622    | LMG  | C36-C37-C38-C39 |
| 35  | b     | 631    | HTG  | C3'-C4'-C5'-C6' |
| 37  | d     | 406    | LHG  | C29-C30-C31-C32 |
| 36  | C     | 517    | DGD  | C4B-C5B-C6B-C7B |
| 38  | e     | 103    | HEM  | C2C-C3C-CAC-CBC |
| 27  | B     | 621    | SQD  | C24-C23-O48-C46 |
| 36  | c     | 520    | DGD  | C4D-C5D-C6D-O5D |
| 27  | A     | 416    | SQD  | O5-C1-O6-C44    |
| 29  | D     | 401    | LMT  | O5'-C1'-O1'-C1  |
| 36  | C     | 517    | DGD  | O6E-C1E-O5D-C6D |
| 36  | c     | 521    | DGD  | O6E-C1E-O5D-C6D |
| 24  | a     | 412    | CLA  | C15-C16-C17-C18 |
| 27  | L     | 102    | SQD  | C29-C30-C31-C32 |
| 29  | B     | 635    | LMT  | C2-C3-C4-C5     |
| 29  | B     | 635    | LMT  | C7-C8-C9-C10    |
| 29  | a     | 419    | LMT  | C6-C7-C8-C9     |
| 29  | f     | 102    | LMT  | C5-C6-C7-C8     |
| 33  | b     | 629    | LMG  | C33-C34-C35-C36 |
| 33  | c     | 501    | LMG  | C29-C30-C31-C32 |
| 38  | F     | 102    | HEM  | C4B-C3B-CAB-CBB |
| 38  | F     | 102    | HEM  | C4C-C3C-CAC-CBC |
| 36  | C     | 517    | DGD  | C8A-C9A-CAA-CBA |
| 27  | F     | 103    | SQD  | C2-C1-O6-C44    |
| 24  | b     | 620    | CLA  | C16-C17-C18-C20 |
| 33  | d     | 413    | LMG  | C35-C36-C37-C38 |
| 36  | D     | 406    | DGD  | C8B-C9B-CAB-CBB |
| 24  | b     | 613    | CLA  | C13-C15-C16-C17 |
| 24  | c     | 517    | CLA  | C15-C16-C17-C18 |
| 24  | C     | 510    | CLA  | C4-C3-C5-C6     |
| 31  | D     | 405[A] | PL9  | C45-C44-C46-C47 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 31  | D     | 405[B] | PL9  | C45-C44-C46-C47 |
| 31  | d     | 405[B] | PL9  | C15-C14-C16-C17 |
| 31  | a     | 415[B] | PL9  | C12-C11-C9-C8   |
| 31  | A     | 419[A] | PL9  | C4-C3-C7-C8     |
| 31  | A     | 419[B] | PL9  | C4-C3-C7-C8     |
| 31  | a     | 415[A] | PL9  | C4-C3-C7-C8     |
| 31  | a     | 415[B] | PL9  | C4-C3-C7-C8     |
| 33  | c     | 501    | LMG  | C33-C34-C35-C36 |
| 24  | C     | 506    | CLA  | C6-C7-C8-C9     |
| 24  | a     | 410    | CLA  | C14-C13-C15-C16 |
| 24  | b     | 610    | CLA  | C6-C7-C8-C9     |
| 24  | b     | 623    | CLA  | C11-C12-C13-C14 |
| 24  | b     | 625    | CLA  | C11-C12-C13-C14 |
| 24  | c     | 514    | CLA  | C14-C13-C15-C16 |
| 36  | c     | 520    | DGD  | O6E-C5E-C6E-O5E |
| 27  | L     | 102    | SQD  | C30-C31-C32-C33 |
| 24  | c     | 517    | CLA  | CBA-CGA-O2A-C1  |
| 37  | d     | 408    | LHG  | C31-C32-C33-C34 |
| 24  | C     | 506    | CLA  | C1A-C2A-CAA-CBA |
| 24  | b     | 624    | CLA  | C16-C17-C18-C20 |
| 27  | a     | 414    | SQD  | C15-C16-C17-C18 |
| 36  | h     | 102    | DGD  | C6A-C7A-C8A-C9A |
| 37  | D     | 407    | LHG  | C25-C26-C27-C28 |
| 37  | b     | 634    | LHG  | C33-C34-C35-C36 |
| 37  | D     | 408    | LHG  | C4-O6-P-O3      |
| 33  | A     | 421    | LMG  | C10-C11-C12-C13 |
| 24  | b     | 623    | CLA  | CBD-CGD-O2D-CED |
| 24  | C     | 512    | CLA  | CBA-CGA-O2A-C1  |
| 29  | B     | 635    | LMT  | C11-C10-C9-C8   |
| 36  | c     | 520    | DGD  | C7B-C8B-C9B-CAB |
| 36  | h     | 102    | DGD  | C5B-C6B-C7B-C8B |
| 27  | L     | 102    | SQD  | C32-C33-C34-C35 |
| 27  | A     | 416    | SQD  | C11-C12-C13-C14 |
| 27  | L     | 102    | SQD  | C24-C25-C26-C27 |
| 36  | D     | 406    | DGD  | C1B-C2B-C3B-C4B |
| 35  | b     | 601    | HTG  | C2'-C3'-C4'-C5' |
| 36  | C     | 516    | DGD  | O6E-C5E-C6E-O5E |
| 27  | B     | 621    | SQD  | C35-C36-C37-C38 |
| 27  | F     | 103    | SQD  | C31-C32-C33-C34 |
| 33  | Z     | 101    | LMG  | O6-C5-C6-O5     |
| 27  | A     | 412    | SQD  | C18-C19-C20-C21 |
| 27  | A     | 416    | SQD  | O6-C44-C45-C46  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | B     | 621 | SQD  | C44-C45-C46-O48 |
| 27  | F     | 103 | SQD  | C44-C45-C46-O48 |
| 27  | a     | 405 | SQD  | O6-C44-C45-C46  |
| 33  | A     | 421 | LMG  | C7-C8-C9-O8     |
| 33  | c     | 501 | LMG  | C7-C8-C9-O8     |
| 36  | D     | 406 | DGD  | O1G-C1G-C2G-C3G |
| 36  | e     | 101 | DGD  | O1G-C1G-C2G-C3G |
| 37  | E     | 101 | LHG  | C4-C5-C6-O8     |
| 37  | d     | 406 | LHG  | C25-C26-C27-C28 |
| 33  | C     | 520 | LMG  | C8-C7-O1-C1     |
| 36  | c     | 521 | DGD  | C2G-C3G-O3G-C1D |
| 36  | c     | 521 | DGD  | C5D-C6D-O5D-C1E |
| 27  | a     | 405 | SQD  | C28-C29-C30-C31 |
| 29  | a     | 404 | LMT  | C3-C4-C5-C6     |
| 29  | a     | 404 | LMT  | O5B-C5B-C6B-O6B |
| 37  | E     | 101 | LHG  | C10-C11-C12-C13 |
| 24  | C     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 24  | c     | 517 | CLA  | O1A-CGA-O2A-C1  |
| 36  | e     | 101 | DGD  | O1A-C1A-O1G-C1G |
| 33  | b     | 629 | LMG  | C40-C41-C42-C43 |
| 24  | b     | 619 | CLA  | C16-C17-C18-C20 |
| 36  | H     | 102 | DGD  | CDA-CEA-CFA-CGA |
| 37  | E     | 101 | LHG  | C19-C20-C21-C22 |
| 28  | A     | 415 | GOL  | O2-C2-C3-O3     |
| 28  | A     | 422 | GOL  | O1-C1-C2-O2     |
| 28  | C     | 524 | GOL  | O1-C1-C2-O2     |
| 28  | V     | 201 | GOL  | O2-C2-C3-O3     |
| 29  | b     | 630 | LMT  | C3'-C4'-O1B-C1B |
| 29  | a     | 404 | LMT  | C7-C8-C9-C10    |
| 27  | L     | 102 | SQD  | C28-C29-C30-C31 |
| 36  | H     | 102 | DGD  | CDB-CEB-CFB-CGB |
| 37  | L     | 101 | LHG  | C13-C14-C15-C16 |
| 24  | B     | 602 | CLA  | CBA-CGA-O2A-C1  |
| 27  | L     | 102 | SQD  | C35-C36-C37-C38 |
| 33  | C     | 519 | LMG  | C14-C15-C16-C17 |
| 24  | B     | 604 | CLA  | C5-C6-C7-C8     |
| 24  | c     | 512 | CLA  | C5-C6-C7-C8     |
| 29  | C     | 521 | LMT  | C9-C10-C11-C12  |
| 33  | d     | 413 | LMG  | C38-C39-C40-C41 |
| 36  | C     | 517 | DGD  | CAB-CBB-CCB-CDB |
| 37  | D     | 409 | LHG  | C12-C13-C14-C15 |
| 33  | D     | 413 | LMG  | O6-C5-C6-O5     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | b     | 612    | CLA  | C5-C6-C7-C8     |
| 24  | C     | 513    | CLA  | C2-C1-O2A-CGA   |
| 36  | C     | 516    | DGD  | O6D-C5D-C6D-O5D |
| 27  | B     | 621    | SQD  | C11-C10-C9-C8   |
| 36  | D     | 406    | DGD  | C7A-C8A-C9A-CAA |
| 29  | A     | 417    | LMT  | O1'-C1-C2-C3    |
| 36  | c     | 521    | DGD  | C2B-C3B-C4B-C5B |
| 27  | F     | 103    | SQD  | C30-C31-C32-C33 |
| 27  | B     | 621    | SQD  | O10-C23-O48-C46 |
| 33  | A     | 421    | LMG  | C13-C14-C15-C16 |
| 33  | A     | 421    | LMG  | C36-C37-C38-C39 |
| 24  | a     | 410    | CLA  | C10-C11-C12-C13 |
| 24  | b     | 623    | CLA  | C10-C11-C12-C13 |
| 27  | f     | 101    | SQD  | O6-C44-C45-O47  |
| 33  | Z     | 101    | LMG  | O1-C7-C8-O7     |
| 33  | C     | 520    | LMG  | C11-C12-C13-C14 |
| 33  | c     | 501    | LMG  | C35-C36-C37-C38 |
| 24  | c     | 509    | CLA  | C4-C3-C5-C6     |
| 24  | B     | 602    | CLA  | C11-C10-C8-C7   |
| 24  | B     | 615    | CLA  | C12-C13-C15-C16 |
| 24  | C     | 512    | CLA  | C11-C10-C8-C7   |
| 24  | b     | 610    | CLA  | C6-C7-C8-C10    |
| 24  | b     | 623    | CLA  | C11-C12-C13-C15 |
| 24  | c     | 511    | CLA  | C6-C7-C8-C10    |
| 31  | D     | 405[B] | PL9  | C13-C14-C16-C17 |
| 24  | B     | 602    | CLA  | O1A-CGA-O2A-C1  |
| 24  | B     | 615    | CLA  | C14-C13-C15-C16 |
| 24  | B     | 616    | CLA  | C14-C13-C15-C16 |
| 24  | C     | 512    | CLA  | C11-C10-C8-C9   |
| 24  | D     | 403    | CLA  | C11-C10-C8-C9   |
| 24  | b     | 615    | CLA  | C14-C13-C15-C16 |
| 24  | c     | 511    | CLA  | C11-C10-C8-C9   |
| 24  | c     | 514    | CLA  | C6-C7-C8-C9     |
| 37  | D     | 409    | LHG  | C28-C29-C30-C31 |
| 24  | b     | 610    | CLA  | CBA-CGA-O2A-C1  |
| 26  | d     | 404    | BCR  | C7-C8-C9-C34    |
| 24  | b     | 619    | CLA  | C16-C17-C18-C19 |
| 37  | D     | 408    | LHG  | C26-C27-C28-C29 |
| 26  | D     | 404    | BCR  | C7-C8-C9-C10    |
| 24  | C     | 512    | CLA  | C3-C5-C6-C7     |
| 37  | d     | 407    | LHG  | C1-C2-C3-O3     |
| 33  | C     | 519    | LMG  | C31-C32-C33-C34 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | z     | 101    | LMG  | C13-C14-C15-C16 |
| 24  | a     | 412    | CLA  | CBA-CGA-O2A-C1  |
| 24  | c     | 516    | CLA  | CBA-CGA-O2A-C1  |
| 29  | m     | 102    | LMT  | C1-C2-C3-C4     |
| 27  | a     | 405    | SQD  | C23-C24-C25-C26 |
| 33  | b     | 629    | LMG  | C39-C40-C41-C42 |
| 35  | B     | 625    | HTG  | C3'-C4'-C5'-C6' |
| 33  | d     | 413    | LMG  | C13-C14-C15-C16 |
| 24  | A     | 410    | CLA  | C4B-C3B-CAB-CBB |
| 24  | B     | 608    | CLA  | C4B-C3B-CAB-CBB |
| 24  | b     | 611    | CLA  | C4B-C3B-CAB-CBB |
| 24  | c     | 506    | CLA  | C4B-C3B-CAB-CBB |
| 24  | c     | 512    | CLA  | C4B-C3B-CAB-CBB |
| 24  | d     | 403    | CLA  | C4B-C3B-CAB-CBB |
| 24  | B     | 611    | CLA  | C16-C17-C18-C20 |
| 37  | e     | 102    | LHG  | O6-C4-C5-C6     |
| 31  | a     | 415[A] | PL9  | C39-C41-C42-C43 |
| 33  | C     | 519    | LMG  | C30-C31-C32-C33 |
| 36  | c     | 522    | DGD  | C2A-C1A-O1G-C1G |
| 33  | d     | 413    | LMG  | C29-C30-C31-C32 |
| 31  | a     | 415[A] | PL9  | C28-C29-C31-C32 |
| 24  | B     | 612    | CLA  | C15-C16-C17-C18 |
| 36  | C     | 517    | DGD  | C5A-C6A-C7A-C8A |
| 36  | h     | 102    | DGD  | O2G-C1B-C2B-C3B |
| 27  | F     | 103    | SQD  | C34-C35-C36-C37 |
| 24  | b     | 613    | CLA  | CBD-CGD-O2D-CED |
| 24  | C     | 513    | CLA  | C3A-C2A-CAA-CBA |
| 29  | B     | 635    | LMT  | C4-C5-C6-C7     |
| 36  | e     | 101    | DGD  | CAA-CBA-CCA-CDA |
| 27  | A     | 416    | SQD  | C24-C25-C26-C27 |
| 36  | h     | 102    | DGD  | O6E-C5E-C6E-O5E |
| 27  | A     | 416    | SQD  | C24-C23-O48-C46 |
| 37  | D     | 409    | LHG  | C24-C23-O8-C6   |
| 29  | D     | 401    | LMT  | O5B-C1B-O1B-C4' |
| 24  | c     | 514    | CLA  | C10-C11-C12-C13 |
| 27  | L     | 102    | SQD  | C44-C45-C46-O48 |
| 27  | a     | 414    | SQD  | O6-C44-C45-C46  |
| 33  | Z     | 101    | LMG  | C7-C8-C9-O8     |
| 33  | c     | 523    | LMG  | O1-C7-C8-C9     |
| 33  | c     | 523    | LMG  | C7-C8-C9-O8     |
| 37  | e     | 102    | LHG  | C4-C5-C6-O8     |
| 33  | d     | 413    | LMG  | C14-C15-C16-C17 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | e     | 101    | DGD  | C4D-C5D-C6D-O5D |
| 29  | F     | 101    | LMT  | O1'-C1-C2-C3    |
| 36  | c     | 521    | DGD  | C3B-C4B-C5B-C6B |
| 36  | e     | 101    | DGD  | C4A-C5A-C6A-C7A |
| 31  | a     | 415[A] | PL9  | C45-C44-C46-C47 |
| 33  | b     | 629    | LMG  | C37-C38-C39-C40 |
| 36  | C     | 517    | DGD  | C4A-C5A-C6A-C7A |
| 28  | b     | 604    | GOL  | O1-C1-C2-O2     |
| 28  | c     | 503    | GOL  | O1-C1-C2-O2     |
| 28  | o     | 301    | GOL  | O1-C1-C2-O2     |
| 27  | a     | 414    | SQD  | C34-C35-C36-C37 |
| 33  | c     | 501    | LMG  | C12-C13-C14-C15 |
| 37  | e     | 102    | LHG  | O6-C4-C5-O7     |
| 33  | C     | 519    | LMG  | C29-C28-O8-C9   |
| 36  | C     | 518    | DGD  | C2A-C1A-O1G-C1G |
| 29  | a     | 404    | LMT  | C6-C7-C8-C9     |
| 37  | d     | 407    | LHG  | C34-C35-C36-C37 |
| 24  | a     | 412    | CLA  | O1A-CGA-O2A-C1  |
| 24  | c     | 516    | CLA  | O1A-CGA-O2A-C1  |
| 37  | d     | 406    | LHG  | C11-C10-C9-C8   |
| 27  | A     | 412    | SQD  | C15-C16-C17-C18 |
| 27  | L     | 102    | SQD  | C11-C12-C13-C14 |
| 27  | f     | 101    | SQD  | C24-C25-C26-C27 |
| 35  | b     | 607    | HTG  | C4'-C5'-C6'-C7' |
| 27  | a     | 414    | SQD  | O6-C44-C45-O47  |
| 33  | Z     | 101    | LMG  | O7-C8-C9-O8     |
| 36  | D     | 406    | DGD  | O2G-C2G-C3G-O3G |
| 25  | a     | 411    | PHO  | C2C-C3C-CAC-CBC |
| 24  | B     | 611    | CLA  | C16-C17-C18-C19 |
| 31  | D     | 405[B] | PL9  | C9-C11-C12-C13  |
| 31  | D     | 405[B] | PL9  | C39-C41-C42-C43 |
| 33  | c     | 523    | LMG  | C40-C41-C42-C43 |
| 35  | b     | 601    | HTG  | C3'-C4'-C5'-C6' |
| 24  | c     | 516    | CLA  | C2-C1-O2A-CGA   |
| 24  | B     | 604    | CLA  | C6-C7-C8-C9     |
| 24  | b     | 623    | CLA  | C11-C10-C8-C9   |
| 24  | c     | 514    | CLA  | C11-C12-C13-C14 |
| 24  | A     | 410    | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 419[A] | PL9  | C2-C3-C7-C8     |
| 27  | F     | 103    | SQD  | C32-C33-C34-C35 |
| 36  | c     | 520    | DGD  | CBA-CCA-CDA-CEA |
| 24  | A     | 405    | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | B     | 614    | CLA  | C15-C16-C17-C18 |
| 24  | b     | 610    | CLA  | O1A-CGA-O2A-C1  |
| 36  | c     | 521    | DGD  | C6A-C7A-C8A-C9A |
| 36  | e     | 101    | DGD  | C2B-C3B-C4B-C5B |
| 26  | C     | 514    | BCR  | C1-C6-C7-C8     |
| 26  | C     | 514    | BCR  | C5-C6-C7-C8     |
| 26  | C     | 515    | BCR  | C1-C6-C7-C8     |
| 26  | C     | 515    | BCR  | C5-C6-C7-C8     |
| 26  | D     | 404    | BCR  | C1-C6-C7-C8     |
| 26  | D     | 404    | BCR  | C5-C6-C7-C8     |
| 26  | D     | 404    | BCR  | C23-C24-C25-C26 |
| 26  | D     | 404    | BCR  | C23-C24-C25-C30 |
| 36  | C     | 518    | DGD  | CDA-CEA-CFA-CGA |
| 36  | H     | 102    | DGD  | O2G-C1B-C2B-C3B |
| 33  | C     | 519    | LMG  | C29-C30-C31-C32 |
| 26  | d     | 404    | BCR  | C7-C8-C9-C10    |
| 36  | C     | 516    | DGD  | C4D-C5D-C6D-O5D |
| 33  | b     | 629    | LMG  | C30-C31-C32-C33 |
| 24  | b     | 625    | CLA  | C10-C11-C12-C13 |
| 36  | h     | 102    | DGD  | CDB-CEB-CFB-CGB |
| 24  | C     | 509    | CLA  | C16-C17-C18-C19 |
| 24  | C     | 513    | CLA  | C3-C5-C6-C7     |
| 27  | F     | 103    | SQD  | C7-C8-C9-C10    |
| 35  | B     | 625    | HTG  | C4-C5-C6-O6     |
| 36  | C     | 518    | DGD  | C8A-C9A-CAA-CBA |
| 33  | A     | 421    | LMG  | C12-C13-C14-C15 |
| 24  | b     | 610    | CLA  | CAA-CBA-CGA-O2A |
| 37  | D     | 408    | LHG  | O2-C2-C3-O3     |
| 36  | c     | 522    | DGD  | C5B-C6B-C7B-C8B |
| 24  | B     | 612    | CLA  | C12-C13-C15-C16 |
| 24  | B     | 616    | CLA  | C12-C13-C15-C16 |
| 24  | B     | 617    | CLA  | C6-C7-C8-C10    |
| 24  | a     | 410    | CLA  | C12-C13-C15-C16 |
| 24  | c     | 509    | CLA  | C2-C3-C5-C6     |
| 24  | c     | 511    | CLA  | C11-C10-C8-C7   |
| 24  | c     | 514    | CLA  | C6-C7-C8-C10    |
| 24  | c     | 517    | CLA  | C11-C10-C8-C7   |
| 31  | a     | 415[A] | PL9  | C43-C44-C46-C47 |
| 24  | C     | 503    | CLA  | C8-C10-C11-C12  |
| 24  | c     | 508    | CLA  | C8-C10-C11-C12  |
| 26  | T     | 103    | BCR  | C13-C14-C15-C16 |
| 27  | a     | 414    | SQD  | C27-C28-C29-C30 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | b     | 610    | CLA  | C10-C11-C12-C13 |
| 37  | E     | 101    | LHG  | C8-C7-O7-C5     |
| 29  | f     | 102    | LMT  | C4-C5-C6-C7     |
| 33  | c     | 524    | LMG  | C10-C11-C12-C13 |
| 24  | d     | 403    | CLA  | C15-C16-C17-C18 |
| 24  | C     | 510    | CLA  | CBA-CGA-O2A-C1  |
| 33  | d     | 413    | LMG  | C16-C17-C18-C19 |
| 35  | d     | 411    | HTG  | C4-C5-C6-O6     |
| 27  | a     | 405    | SQD  | C19-C20-C21-C22 |
| 27  | f     | 101    | SQD  | C31-C32-C33-C34 |
| 29  | C     | 521    | LMT  | O1'-C1-C2-C3    |
| 37  | D     | 409    | LHG  | C25-C26-C27-C28 |
| 24  | C     | 509    | CLA  | CBD-CGD-O2D-CED |
| 33  | A     | 421    | LMG  | C32-C33-C34-C35 |
| 24  | B     | 602    | CLA  | CAD-CBD-CGD-O2D |
| 24  | B     | 617    | CLA  | CAD-CBD-CGD-O2D |
| 24  | C     | 505    | CLA  | CAD-CBD-CGD-O2D |
| 24  | C     | 510    | CLA  | CAD-CBD-CGD-O2D |
| 24  | C     | 512    | CLA  | CAD-CBD-CGD-O2D |
| 24  | D     | 403    | CLA  | CAD-CBD-CGD-O2D |
| 24  | b     | 613    | CLA  | CAD-CBD-CGD-O2D |
| 24  | b     | 623    | CLA  | CAD-CBD-CGD-O2D |
| 24  | b     | 625    | CLA  | CAD-CBD-CGD-O2D |
| 24  | c     | 508    | CLA  | CAD-CBD-CGD-O2D |
| 24  | c     | 518    | CLA  | CAD-CBD-CGD-O2D |
| 38  | e     | 103    | HEM  | C2B-C3B-CAB-CBB |
| 29  | m     | 103    | LMT  | C1-C2-C3-C4     |
| 37  | e     | 102    | LHG  | C14-C15-C16-C17 |
| 24  | b     | 625    | CLA  | C4-C3-C5-C6     |
| 31  | A     | 419[A] | PL9  | C15-C14-C16-C17 |
| 27  | F     | 103    | SQD  | O5-C1-O6-C44    |
| 24  | D     | 403    | CLA  | C8-C10-C11-C12  |
| 24  | b     | 623    | CLA  | C15-C16-C17-C18 |
| 24  | B     | 610    | CLA  | C2-C3-C5-C6     |
| 24  | b     | 625    | CLA  | C2-C3-C5-C6     |
| 31  | D     | 405[A] | PL9  | C9-C11-C12-C13  |
| 36  | C     | 516    | DGD  | C1B-C2B-C3B-C4B |
| 37  | L     | 101    | LHG  | C7-C8-C9-C10    |
| 33  | A     | 421    | LMG  | O1-C7-C8-C9     |
| 33  | z     | 101    | LMG  | O1-C7-C8-C9     |
| 37  | D     | 409    | LHG  | C2-C3-O3-P      |
| 37  | d     | 408    | LHG  | C2-C3-O3-P      |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 37  | D     | 409    | LHG  | O10-C23-O8-C6   |
| 24  | b     | 614    | CLA  | C8-C10-C11-C12  |
| 33  | C     | 520    | LMG  | C16-C17-C18-C19 |
| 24  | C     | 502    | CLA  | CHA-CBD-CGD-O1D |
| 24  | C     | 502    | CLA  | CHA-CBD-CGD-O2D |
| 24  | C     | 507    | CLA  | CHA-CBD-CGD-O1D |
| 24  | C     | 507    | CLA  | CHA-CBD-CGD-O2D |
| 24  | C     | 508    | CLA  | CHA-CBD-CGD-O2D |
| 24  | b     | 610    | CLA  | CHA-CBD-CGD-O1D |
| 24  | b     | 610    | CLA  | CHA-CBD-CGD-O2D |
| 24  | c     | 507    | CLA  | CHA-CBD-CGD-O1D |
| 24  | c     | 512    | CLA  | CHA-CBD-CGD-O1D |
| 24  | c     | 512    | CLA  | CHA-CBD-CGD-O2D |
| 24  | A     | 410    | CLA  | O1A-CGA-O2A-C1  |
| 24  | C     | 510    | CLA  | O1A-CGA-O2A-C1  |
| 33  | C     | 519    | LMG  | O10-C28-O8-C9   |
| 36  | c     | 522    | DGD  | O1A-C1A-O1G-C1G |
| 36  | h     | 102    | DGD  | C9B-CAB-CBB-CCB |
| 37  | E     | 101    | LHG  | C15-C16-C17-C18 |
| 27  | L     | 102    | SQD  | O47-C45-C46-O48 |
| 33  | c     | 501    | LMG  | O7-C8-C9-O8     |
| 33  | c     | 523    | LMG  | O1-C7-C8-O7     |
| 33  | c     | 523    | LMG  | O7-C8-C9-O8     |
| 36  | D     | 406    | DGD  | O1G-C1G-C2G-O2G |
| 37  | E     | 101    | LHG  | O7-C5-C6-O8     |
| 37  | e     | 102    | LHG  | O7-C5-C6-O8     |
| 27  | A     | 416    | SQD  | O10-C23-O48-C46 |
| 28  | a     | 401    | GOL  | O2-C2-C3-O3     |
| 28  | v     | 202    | GOL  | O1-C1-C2-O2     |
| 37  | D     | 407    | LHG  | O1-C1-C2-O2     |
| 27  | a     | 414    | SQD  | C35-C36-C37-C38 |
| 36  | c     | 520    | DGD  | C3A-C4A-C5A-C6A |
| 37  | d     | 406    | LHG  | C33-C34-C35-C36 |
| 31  | A     | 419[B] | PL9  | C15-C14-C16-C17 |
| 33  | B     | 622    | LMG  | C16-C17-C18-C19 |
| 36  | C     | 518    | DGD  | O1A-C1A-O1G-C1G |
| 31  | A     | 419[A] | PL9  | C13-C14-C16-C17 |
| 31  | d     | 405[B] | PL9  | C28-C29-C31-C32 |
| 37  | E     | 101    | LHG  | O9-C7-O7-C5     |
| 24  | B     | 612    | CLA  | C14-C13-C15-C16 |
| 24  | c     | 517    | CLA  | C11-C10-C8-C9   |
| 33  | c     | 523    | LMG  | C39-C40-C41-C42 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | c     | 522    | DGD  | C2A-C3A-C4A-C5A |
| 27  | B     | 621    | SQD  | C5-C6-S-O8      |
| 27  | F     | 103    | SQD  | C5-C6-S-O8      |
| 33  | c     | 524    | LMG  | O6-C5-C6-O5     |
| 35  | B     | 632    | HTG  | O5-C5-C6-O6     |
| 27  | a     | 414    | SQD  | C19-C20-C21-C22 |
| 36  | H     | 102    | DGD  | C3B-C4B-C5B-C6B |
| 28  | O     | 301    | GOL  | O1-C1-C2-C3     |
| 29  | C     | 521    | LMT  | C1-C2-C3-C4     |
| 24  | c     | 513    | CLA  | C1A-C2A-CAA-CBA |
| 37  | E     | 101    | LHG  | C23-C24-C25-C26 |
| 24  | c     | 507    | CLA  | C16-C17-C18-C19 |
| 37  | D     | 408    | LHG  | C3-O3-P-O6      |
| 37  | E     | 101    | LHG  | C4-O6-P-O3      |
| 27  | B     | 621    | SQD  | C17-C18-C19-C20 |
| 29  | m     | 103    | LMT  | C11-C10-C9-C8   |
| 24  | c     | 512    | CLA  | C4-C3-C5-C6     |
| 24  | b     | 617    | CLA  | C13-C15-C16-C17 |
| 31  | D     | 405[A] | PL9  | C43-C44-C46-C47 |
| 27  | a     | 405    | SQD  | C29-C30-C31-C32 |
| 36  | e     | 101    | DGD  | C6A-C7A-C8A-C9A |
| 37  | E     | 101    | LHG  | C25-C26-C27-C28 |
| 37  | d     | 406    | LHG  | C30-C31-C32-C33 |
| 24  | B     | 616    | CLA  | C4B-C3B-CAB-CBB |
| 24  | C     | 505    | CLA  | C4B-C3B-CAB-CBB |
| 37  | D     | 408    | LHG  | C4-O6-P-O5      |
| 37  | b     | 634    | LHG  | C4-O6-P-O5      |
| 24  | B     | 616    | CLA  | C16-C17-C18-C20 |
| 33  | D     | 413    | LMG  | C13-C14-C15-C16 |
| 36  | C     | 517    | DGD  | CBB-CCB-CDB-CEB |
| 31  | a     | 415[A] | PL9  | C14-C16-C17-C18 |
| 33  | c     | 523    | LMG  | C36-C37-C38-C39 |
| 36  | C     | 518    | DGD  | C9A-CAA-CBA-CCA |
| 24  | B     | 606    | CLA  | CAD-CBD-CGD-O1D |
| 24  | B     | 610    | CLA  | CAD-CBD-CGD-O1D |
| 24  | C     | 502    | CLA  | CAD-CBD-CGD-O1D |
| 24  | b     | 610    | CLA  | CAD-CBD-CGD-O1D |
| 24  | b     | 614    | CLA  | CAD-CBD-CGD-O1D |
| 24  | c     | 507    | CLA  | CAD-CBD-CGD-O1D |
| 24  | c     | 511    | CLA  | CAD-CBD-CGD-O1D |
| 27  | A     | 416    | SQD  | O5-C5-C6-S      |
| 29  | D     | 401    | LMT  | C2B-C1B-O1B-C4' |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | c     | 515    | CLA  | CBA-CGA-O2A-C1  |
| 37  | b     | 634    | LHG  | C10-C11-C12-C13 |
| 24  | A     | 407    | CLA  | C11-C10-C8-C7   |
| 24  | a     | 410    | CLA  | C11-C10-C8-C7   |
| 24  | d     | 402    | CLA  | C11-C12-C13-C15 |
| 35  | V     | 206    | HTG  | C2-C1-S1-C1'    |
| 37  | E     | 101    | LHG  | C7-C8-C9-C10    |
| 29  | m     | 102    | LMT  | C5-C6-C7-C8     |
| 33  | c     | 501    | LMG  | C31-C32-C33-C34 |
| 24  | a     | 409    | CLA  | C2C-C3C-CAC-CBC |
| 27  | B     | 621    | SQD  | C12-C13-C14-C15 |
| 35  | V     | 206    | HTG  | C2'-C3'-C4'-C5' |
| 27  | L     | 102    | SQD  | C11-C10-C9-C8   |
| 27  | a     | 414    | SQD  | C30-C31-C32-C33 |
| 29  | D     | 401    | LMT  | C4B-C5B-C6B-O6B |
| 37  | d     | 408    | LHG  | C30-C31-C32-C33 |
| 24  | C     | 509    | CLA  | C10-C11-C12-C13 |
| 27  | a     | 405    | SQD  | C27-C28-C29-C30 |
| 27  | f     | 101    | SQD  | O6-C44-C45-C46  |
| 33  | Z     | 101    | LMG  | O1-C7-C8-C9     |
| 36  | e     | 101    | DGD  | C7B-C8B-C9B-CAB |
| 27  | F     | 103    | SQD  | O47-C45-C46-O48 |
| 33  | A     | 421    | LMG  | O1-C7-C8-O7     |
| 33  | z     | 101    | LMG  | O1-C7-C8-O7     |
| 36  | e     | 101    | DGD  | O1G-C1G-C2G-O2G |
| 29  | m     | 103    | LMT  | C2-C3-C4-C5     |
| 29  | f     | 102    | LMT  | C2B-C1B-O1B-C4' |
| 27  | A     | 412    | SQD  | C16-C17-C18-C19 |
| 36  | H     | 102    | DGD  | CCA-CDA-CEA-CFA |
| 36  | D     | 406    | DGD  | C3B-C4B-C5B-C6B |
| 27  | a     | 405    | SQD  | C24-C25-C26-C27 |
| 25  | a     | 411    | PHO  | C2-C3-C5-C6     |
| 33  | C     | 520    | LMG  | C15-C16-C17-C18 |
| 24  | B     | 613    | CLA  | C8-C10-C11-C12  |
| 24  | b     | 621    | CLA  | C8-C10-C11-C12  |
| 24  | a     | 410    | CLA  | C6-C7-C8-C9     |
| 37  | D     | 407    | LHG  | C17-C18-C19-C20 |
| 24  | B     | 616    | CLA  | C16-C17-C18-C19 |
| 31  | a     | 415[B] | PL9  | C14-C16-C17-C18 |
| 37  | b     | 634    | LHG  | C17-C18-C19-C20 |
| 24  | c     | 515    | CLA  | O1A-CGA-O2A-C1  |
| 28  | O     | 301    | GOL  | O1-C1-C2-O2     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | a     | 405 | SQD  | C35-C36-C37-C38 |
| 24  | d     | 401 | CLA  | C2C-C3C-CAC-CBC |
| 33  | A     | 421 | LMG  | C17-C18-C19-C20 |
| 24  | A     | 410 | CLA  | C2B-C3B-CAB-CBB |
| 24  | B     | 608 | CLA  | C2B-C3B-CAB-CBB |
| 24  | C     | 505 | CLA  | C2B-C3B-CAB-CBB |
| 24  | b     | 611 | CLA  | C2B-C3B-CAB-CBB |
| 24  | c     | 506 | CLA  | C2B-C3B-CAB-CBB |
| 24  | c     | 512 | CLA  | C2B-C3B-CAB-CBB |
| 24  | d     | 403 | CLA  | C2B-C3B-CAB-CBB |
| 36  | c     | 521 | DGD  | C1A-C2A-C3A-C4A |
| 37  | d     | 407 | LHG  | O10-C23-O8-C6   |
| 29  | m     | 103 | LMT  | C4'-C5'-C6'-O6' |
| 27  | A     | 412 | SQD  | C7-C8-C9-C10    |
| 24  | A     | 405 | CLA  | C16-C17-C18-C19 |
| 37  | d     | 408 | LHG  | C33-C34-C35-C36 |
| 36  | c     | 522 | DGD  | C4A-C5A-C6A-C7A |
| 24  | C     | 502 | CLA  | C3-C5-C6-C7     |
| 27  | B     | 621 | SQD  | C46-C45-O47-C7  |
| 27  | L     | 102 | SQD  | C46-C45-O47-C7  |
| 24  | b     | 619 | CLA  | C2A-CAA-CBA-CGA |
| 24  | B     | 602 | CLA  | C2-C1-O2A-CGA   |
| 24  | C     | 511 | CLA  | C2-C1-O2A-CGA   |
| 24  | b     | 623 | CLA  | C2-C1-O2A-CGA   |
| 27  | L     | 102 | SQD  | C33-C34-C35-C36 |
| 36  | C     | 518 | DGD  | C2A-C3A-C4A-C5A |
| 36  | D     | 406 | DGD  | C4B-C5B-C6B-C7B |
| 36  | e     | 101 | DGD  | C9B-CAB-CBB-CCB |
| 24  | C     | 509 | CLA  | C8-C10-C11-C12  |
| 25  | a     | 411 | PHO  | C4-C3-C5-C6     |
| 26  | c     | 519 | BCR  | C1-C6-C7-C8     |
| 26  | c     | 519 | BCR  | C5-C6-C7-C8     |
| 24  | b     | 618 | CLA  | C2-C3-C5-C6     |
| 24  | C     | 509 | CLA  | C13-C15-C16-C17 |
| 40  | v     | 205 | HEC  | C2B-C3B-CAB-CBB |
| 24  | a     | 409 | CLA  | C4C-C3C-CAC-CBC |
| 24  | b     | 610 | CLA  | C16-C17-C18-C20 |
| 29  | m     | 103 | LMT  | O5'-C1'-O1'-C1  |
| 36  | c     | 520 | DGD  | O6E-C1E-O5D-C6D |
| 33  | c     | 501 | LMG  | C22-C23-C24-C25 |
| 27  | B     | 621 | SQD  | O47-C45-C46-O48 |
| 33  | A     | 421 | LMG  | C18-C19-C20-C21 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 37  | e     | 102    | LHG  | C13-C14-C15-C16 |
| 37  | e     | 102    | LHG  | C4-O6-P-O3      |
| 37  | b     | 634    | LHG  | C12-C13-C14-C15 |
| 24  | A     | 405    | CLA  | C15-C16-C17-C18 |
| 36  | D     | 406    | DGD  | C2B-C3B-C4B-C5B |
| 24  | B     | 607    | CLA  | C10-C11-C12-C13 |
| 36  | D     | 406    | DGD  | C1G-C2G-C3G-O3G |
| 31  | a     | 415[B] | PL9  | C45-C44-C46-C47 |
| 33  | b     | 629    | LMG  | C20-C21-C22-C23 |
| 24  | B     | 604    | CLA  | C6-C7-C8-C10    |
| 24  | D     | 403    | CLA  | C11-C10-C8-C7   |
| 24  | b     | 610    | CLA  | C11-C10-C8-C7   |
| 24  | b     | 619    | CLA  | C12-C13-C15-C16 |
| 24  | c     | 514    | CLA  | C11-C10-C8-C7   |
| 33  | D     | 413    | LMG  | C34-C35-C36-C37 |
| 24  | A     | 407    | CLA  | C11-C10-C8-C9   |
| 24  | B     | 616    | CLA  | C11-C12-C13-C14 |
| 24  | a     | 410    | CLA  | C11-C10-C8-C9   |
| 24  | b     | 619    | CLA  | C14-C13-C15-C16 |
| 36  | C     | 517    | DGD  | C1A-C2A-C3A-C4A |
| 40  | V     | 205    | HEC  | C2B-C3B-CAB-CBB |
| 37  | d     | 407    | LHG  | C24-C23-O8-C6   |
| 37  | D     | 407    | LHG  | C33-C34-C35-C36 |
| 29  | M     | 101    | LMT  | C3-C4-C5-C6     |
| 36  | c     | 522    | DGD  | O6D-C5D-C6D-O5D |
| 29  | a     | 419    | LMT  | C7-C8-C9-C10    |
| 24  | B     | 610    | CLA  | C4-C3-C5-C6     |
| 24  | a     | 412    | CLA  | C4-C3-C5-C6     |
| 27  | L     | 102    | SQD  | C7-C8-C9-C10    |
| 28  | B     | 626    | GOL  | O2-C2-C3-O3     |
| 28  | B     | 629    | GOL  | O1-C1-C2-O2     |
| 28  | a     | 420    | GOL  | O2-C2-C3-O3     |
| 28  | o     | 301    | GOL  | O2-C2-C3-O3     |
| 24  | c     | 507    | CLA  | C16-C17-C18-C20 |
| 35  | B     | 623    | HTG  | C4-C5-C6-O6     |
| 35  | B     | 624    | HTG  | C1'-C2'-C3'-C4' |
| 24  | B     | 605    | CLA  | CBD-CGD-O2D-CED |
| 24  | B     | 602    | CLA  | C4B-C3B-CAB-CBB |
| 24  | a     | 412    | CLA  | C4B-C3B-CAB-CBB |
| 29  | m     | 102    | LMT  | C4'-C5'-C6'-O6' |
| 26  | h     | 101    | BCR  | C9-C10-C11-C12  |
| 31  | A     | 419[A] | PL9  | C19-C21-C22-C23 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | b     | 615    | CLA  | C8-C10-C11-C12  |
| 33  | c     | 501    | LMG  | C30-C31-C32-C33 |
| 38  | e     | 103    | HEM  | C4C-C3C-CAC-CBC |
| 24  | B     | 616    | CLA  | C4-C3-C5-C6     |
| 24  | b     | 618    | CLA  | C4-C3-C5-C6     |
| 31  | d     | 405[A] | PL9  | C30-C29-C31-C32 |
| 24  | B     | 616    | CLA  | C13-C15-C16-C17 |
| 31  | A     | 419[B] | PL9  | C13-C14-C16-C17 |
| 31  | d     | 405[A] | PL9  | C28-C29-C31-C32 |
| 24  | C     | 513    | CLA  | O1A-CGA-O2A-C1  |
| 27  | a     | 414    | SQD  | C17-C18-C19-C20 |
| 37  | b     | 634    | LHG  | C34-C35-C36-C37 |
| 24  | b     | 622    | CLA  | C2-C1-O2A-CGA   |
| 24  | c     | 517    | CLA  | C2-C1-O2A-CGA   |
| 29  | M     | 103    | LMT  | C2'-C1'-O1'-C1  |
| 36  | c     | 520    | DGD  | C2E-C1E-O5D-C6D |
| 24  | A     | 406    | CLA  | C2C-C3C-CAC-CBC |
| 36  | C     | 518    | DGD  | C6B-C7B-C8B-C9B |
| 38  | F     | 102    | HEM  | CAD-CBD-CGD-O1D |
| 36  | D     | 406    | DGD  | C1A-C2A-C3A-C4A |
| 36  | e     | 101    | DGD  | CAB-CBB-CCB-CDB |
| 24  | b     | 618    | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 419[A] | PL9  | C45-C44-C46-C47 |
| 31  | d     | 405[B] | PL9  | C30-C29-C31-C32 |
| 37  | D     | 407    | LHG  | C11-C10-C9-C8   |
| 31  | a     | 415[B] | PL9  | C43-C44-C46-C47 |
| 33  | D     | 413    | LMG  | C20-C21-C22-C23 |
| 36  | c     | 520    | DGD  | C2A-C3A-C4A-C5A |
| 24  | B     | 608    | CLA  | C6-C7-C8-C9     |
| 24  | B     | 615    | CLA  | C6-C7-C8-C9     |
| 36  | C     | 517    | DGD  | C3A-C4A-C5A-C6A |
| 24  | C     | 504    | CLA  | C13-C15-C16-C17 |
| 27  | a     | 414    | SQD  | C12-C13-C14-C15 |
| 37  | E     | 101    | LHG  | C14-C15-C16-C17 |
| 24  | c     | 511    | CLA  | C10-C11-C12-C13 |
| 36  | h     | 102    | DGD  | O1G-C1G-C2G-C3G |
| 33  | d     | 413    | LMG  | C18-C19-C20-C21 |
| 36  | H     | 102    | DGD  | C5B-C6B-C7B-C8B |
| 33  | C     | 519    | LMG  | C16-C17-C18-C19 |
| 24  | b     | 621    | CLA  | C1A-C2A-CAA-CBA |
| 24  | c     | 511    | CLA  | C1A-C2A-CAA-CBA |
| 24  | C     | 504    | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | C     | 507    | CLA  | C11-C10-C8-C7   |
| 24  | b     | 623    | CLA  | C12-C13-C15-C16 |
| 24  | c     | 515    | CLA  | C12-C13-C15-C16 |
| 38  | F     | 102    | HEM  | CAD-CBD-CGD-O2D |
| 28  | b     | 606    | GOL  | O1-C1-C2-O2     |
| 24  | b     | 615    | CLA  | C10-C11-C12-C13 |
| 36  | c     | 521    | DGD  | C2A-C3A-C4A-C5A |
| 27  | A     | 412    | SQD  | O49-C7-O47-C45  |
| 24  | C     | 513    | CLA  | CBA-CGA-O2A-C1  |
| 37  | L     | 101    | LHG  | O6-C4-C5-C6     |
| 37  | b     | 634    | LHG  | O6-C4-C5-C6     |
| 27  | A     | 416    | SQD  | C17-C18-C19-C20 |
| 40  | V     | 205    | HEC  | CAD-CBD-CGD-O2D |
| 24  | c     | 518    | CLA  | C4-C3-C5-C6     |
| 29  | D     | 401    | LMT  | C5-C6-C7-C8     |
| 33  | C     | 519    | LMG  | C12-C13-C14-C15 |
| 36  | c     | 521    | DGD  | C3A-C4A-C5A-C6A |
| 36  | H     | 102    | DGD  | C4E-C5E-C6E-O5E |
| 24  | a     | 412    | CLA  | C2-C3-C5-C6     |
| 24  | B     | 602    | CLA  | C2B-C3B-CAB-CBB |
| 24  | B     | 616    | CLA  | C2B-C3B-CAB-CBB |
| 24  | a     | 412    | CLA  | C2B-C3B-CAB-CBB |
| 33  | c     | 523    | LMG  | C20-C21-C22-C23 |
| 24  | C     | 501    | CLA  | C13-C15-C16-C17 |
| 24  | b     | 610    | CLA  | C13-C15-C16-C17 |
| 33  | D     | 413    | LMG  | C16-C17-C18-C19 |
| 33  | c     | 523    | LMG  | C17-C18-C19-C20 |
| 37  | d     | 408    | LHG  | C28-C29-C30-C31 |
| 24  | B     | 609    | CLA  | C13-C15-C16-C17 |
| 24  | b     | 610    | CLA  | C16-C17-C18-C19 |
| 29  | b     | 630    | LMT  | C6-C7-C8-C9     |
| 36  | c     | 521    | DGD  | C7A-C8A-C9A-CAA |
| 37  | d     | 408    | LHG  | C9-C10-C11-C12  |
| 31  | A     | 419[B] | PL9  | C19-C21-C22-C23 |
| 31  | a     | 415[B] | PL9  | C39-C41-C42-C43 |
| 35  | B     | 623    | HTG  | C3'-C4'-C5'-C6' |
| 37  | D     | 408    | LHG  | C13-C14-C15-C16 |
| 24  | A     | 406    | CLA  | C15-C16-C17-C18 |
| 24  | b     | 623    | CLA  | O1D-CGD-O2D-CED |
| 37  | D     | 409    | LHG  | C9-C10-C11-C12  |
| 24  | c     | 518    | CLA  | C2-C1-O2A-CGA   |
| 24  | B     | 616    | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 31  | A     | 419[A] | PL9  | C43-C44-C46-C47 |
| 31  | A     | 419[B] | PL9  | C43-C44-C46-C47 |
| 29  | f     | 102    | LMT  | C9-C10-C11-C12  |
| 24  | B     | 602    | CLA  | CAA-CBA-CGA-O2A |
| 37  | L     | 101    | LHG  | C26-C27-C28-C29 |
| 36  | D     | 406    | DGD  | CBA-CCA-CDA-CEA |
| 24  | B     | 611    | CLA  | C2A-CAA-CBA-CGA |
| 24  | b     | 611    | CLA  | C16-C17-C18-C19 |
| 26  | H     | 101    | BCR  | C23-C24-C25-C30 |
| 26  | b     | 627    | BCR  | C23-C24-C25-C30 |
| 27  | A     | 416    | SQD  | C25-C26-C27-C28 |
| 28  | a     | 401    | GOL  | C1-C2-C3-O3     |
| 28  | b     | 606    | GOL  | O1-C1-C2-C3     |
| 27  | A     | 412    | SQD  | C12-C13-C14-C15 |
| 24  | B     | 605    | CLA  | C4-C3-C5-C6     |
| 33  | B     | 622    | LMG  | O8-C28-C29-C30  |
| 33  | Z     | 101    | LMG  | C8-C7-O1-C1     |
| 36  | C     | 517    | DGD  | C2G-C3G-O3G-C1D |
| 36  | C     | 517    | DGD  | C5D-C6D-O5D-C1E |
| 36  | D     | 406    | DGD  | C2G-C3G-O3G-C1D |
| 36  | h     | 102    | DGD  | CDA-CEA-CFA-CGA |
| 24  | b     | 620    | CLA  | C8-C10-C11-C12  |
| 40  | V     | 205    | HEC  | CAD-CBD-CGD-O1D |
| 36  | C     | 516    | DGD  | O2G-C1B-C2B-C3B |
| 29  | M     | 101    | LMT  | O5'-C1'-O1'-C1  |
| 29  | D     | 401    | LMT  | O1'-C1-C2-C3    |
| 24  | b     | 610    | CLA  | C4-C3-C5-C6     |
| 24  | d     | 403    | CLA  | C4-C3-C5-C6     |
| 31  | A     | 419[A] | PL9  | C20-C19-C21-C22 |
| 31  | A     | 419[A] | PL9  | C40-C39-C41-C42 |
| 31  | A     | 419[B] | PL9  | C30-C29-C31-C32 |
| 27  | A     | 412    | SQD  | C8-C7-O47-C45   |
| 31  | A     | 419[A] | PL9  | C9-C11-C12-C13  |
| 27  | A     | 416    | SQD  | C12-C13-C14-C15 |
| 24  | a     | 410    | CLA  | C6-C7-C8-C10    |
| 24  | b     | 625    | CLA  | C12-C13-C15-C16 |
| 24  | c     | 507    | CLA  | C11-C12-C13-C15 |
| 40  | v     | 205    | HEC  | CAD-CBD-CGD-O2D |
| 36  | C     | 516    | DGD  | CAA-CBA-CCA-CDA |
| 37  | b     | 634    | LHG  | C13-C14-C15-C16 |
| 37  | L     | 101    | LHG  | C33-C34-C35-C36 |
| 37  | d     | 406    | LHG  | C34-C35-C36-C37 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | A     | 421    | LMG  | O7-C8-C9-O8     |
| 33  | c     | 524    | LMG  | O7-C8-C9-O8     |
| 24  | d     | 401    | CLA  | C15-C16-C17-C18 |
| 35  | V     | 206    | HTG  | O5-C1-S1-C1'    |
| 37  | e     | 102    | LHG  | O8-C23-C24-C25  |
| 29  | a     | 404    | LMT  | C1-C2-C3-C4     |
| 31  | A     | 419[A] | PL9  | C30-C29-C31-C32 |
| 31  | D     | 405[B] | PL9  | C35-C34-C36-C37 |
| 38  | e     | 103    | HEM  | CAD-CBD-CGD-O1D |
| 24  | c     | 512    | CLA  | C2-C3-C5-C6     |
| 37  | b     | 634    | LHG  | C7-C8-C9-C10    |
| 37  | d     | 406    | LHG  | C26-C27-C28-C29 |
| 33  | z     | 101    | LMG  | O7-C10-C11-C12  |
| 29  | m     | 102    | LMT  | C9-C10-C11-C12  |
| 33  | C     | 519    | LMG  | C21-C22-C23-C24 |
| 24  | C     | 505    | CLA  | C11-C10-C8-C9   |
| 24  | C     | 507    | CLA  | C11-C10-C8-C9   |
| 24  | b     | 625    | CLA  | C14-C13-C15-C16 |
| 24  | c     | 513    | CLA  | C6-C7-C8-C9     |
| 24  | c     | 515    | CLA  | C11-C12-C13-C14 |
| 24  | d     | 402    | CLA  | C11-C12-C13-C14 |
| 36  | e     | 101    | DGD  | C3A-C4A-C5A-C6A |
| 33  | A     | 421    | LMG  | C37-C38-C39-C40 |
| 24  | B     | 608    | CLA  | C3A-C2A-CAA-CBA |
| 24  | B     | 610    | CLA  | C3A-C2A-CAA-CBA |
| 24  | C     | 510    | CLA  | CAA-CBA-CGA-O2A |
| 24  | C     | 512    | CLA  | CAA-CBA-CGA-O2A |
| 27  | f     | 101    | SQD  | O47-C7-C8-C9    |
| 37  | d     | 406    | LHG  | O8-C23-C24-C25  |
| 27  | A     | 416    | SQD  | C29-C30-C31-C32 |
| 27  | B     | 621    | SQD  | C19-C20-C21-C22 |
| 33  | z     | 101    | LMG  | C11-C12-C13-C14 |
| 24  | B     | 604    | CLA  | CAD-CBD-CGD-O2D |
| 24  | B     | 605    | CLA  | CAD-CBD-CGD-O2D |
| 24  | B     | 611    | CLA  | CAD-CBD-CGD-O2D |
| 24  | C     | 501    | CLA  | CAD-CBD-CGD-O2D |
| 24  | C     | 503    | CLA  | CAD-CBD-CGD-O2D |
| 24  | b     | 612    | CLA  | CAD-CBD-CGD-O2D |
| 24  | b     | 619    | CLA  | CAD-CBD-CGD-O2D |
| 24  | b     | 621    | CLA  | CAD-CBD-CGD-O2D |
| 24  | c     | 517    | CLA  | CAD-CBD-CGD-O2D |
| 25  | A     | 408    | PHO  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 25  | a     | 411    | PHO  | CAD-CBD-CGD-O2D |
| 24  | B     | 615    | CLA  | C16-C17-C18-C19 |
| 40  | V     | 205    | HEC  | C4B-C3B-CAB-CBB |
| 33  | D     | 413    | LMG  | C30-C31-C32-C33 |
| 29  | f     | 102    | LMT  | C1-C2-C3-C4     |
| 33  | c     | 524    | LMG  | C32-C33-C34-C35 |
| 33  | Z     | 101    | LMG  | O7-C10-C11-C12  |
| 27  | a     | 405    | SQD  | C24-C23-O48-C46 |
| 31  | A     | 419[B] | PL9  | C20-C19-C21-C22 |
| 31  | A     | 419[B] | PL9  | C45-C44-C46-C47 |
| 31  | D     | 405[A] | PL9  | C35-C34-C36-C37 |
| 24  | b     | 613    | CLA  | C3-C5-C6-C7     |
| 38  | e     | 103    | HEM  | CAA-CBA-CGA-O1A |
| 40  | v     | 205    | HEC  | CAD-CBD-CGD-O1D |
| 24  | c     | 518    | CLA  | C2-C3-C5-C6     |
| 24  | c     | 517    | CLA  | CAA-CBA-CGA-O2A |
| 33  | c     | 501    | LMG  | C18-C19-C20-C21 |
| 37  | L     | 101    | LHG  | C30-C31-C32-C33 |
| 26  | K     | 101    | BCR  | C7-C8-C9-C10    |
| 26  | Y     | 101    | BCR  | C21-C22-C23-C24 |
| 27  | a     | 405    | SQD  | O10-C23-O48-C46 |
| 35  | B     | 624    | HTG  | C3'-C4'-C5'-C6' |
| 24  | B     | 614    | CLA  | O2A-C1-C2-C3    |
| 24  | b     | 613    | CLA  | O2A-C1-C2-C3    |
| 25  | a     | 411    | PHO  | O2A-C1-C2-C3    |
| 37  | d     | 408    | LHG  | C11-C12-C13-C14 |
| 38  | e     | 103    | HEM  | C4B-C3B-CAB-CBB |
| 38  | F     | 102    | HEM  | CAA-CBA-CGA-O1A |
| 24  | B     | 603    | CLA  | CHA-CBD-CGD-O1D |
| 24  | B     | 603    | CLA  | CHA-CBD-CGD-O2D |
| 24  | B     | 606    | CLA  | CHA-CBD-CGD-O1D |
| 24  | B     | 608    | CLA  | CHA-CBD-CGD-O1D |
| 24  | C     | 512    | CLA  | CHA-CBD-CGD-O1D |
| 24  | c     | 507    | CLA  | CHA-CBD-CGD-O2D |
| 24  | d     | 401    | CLA  | CHA-CBD-CGD-O1D |
| 24  | d     | 401    | CLA  | CHA-CBD-CGD-O2D |
| 38  | F     | 102    | HEM  | CAA-CBA-CGA-O2A |
| 36  | C     | 517    | DGD  | C6B-C7B-C8B-C9B |
| 37  | e     | 102    | LHG  | C28-C29-C30-C31 |
| 24  | B     | 612    | CLA  | C2-C3-C5-C6     |
| 24  | b     | 610    | CLA  | C3-C5-C6-C7     |
| 24  | C     | 509    | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | c     | 515    | CLA  | CAA-CBA-CGA-O2A |
| 36  | c     | 522    | DGD  | O1G-C1A-C2A-C3A |
| 36  | e     | 101    | DGD  | O2G-C1B-C2B-C3B |
| 37  | L     | 101    | LHG  | O7-C7-C8-C9     |
| 27  | A     | 412    | SQD  | O6-C44-C45-O47  |
| 27  | a     | 414    | SQD  | C7-C8-C9-C10    |
| 37  | L     | 101    | LHG  | C18-C19-C20-C21 |
| 29  | F     | 101    | LMT  | C1-C2-C3-C4     |
| 40  | v     | 205    | HEC  | C4B-C3B-CAB-CBB |
| 24  | C     | 513    | CLA  | C5-C6-C7-C8     |
| 36  | D     | 406    | DGD  | O1G-C1A-C2A-C3A |
| 37  | E     | 101    | LHG  | O8-C23-C24-C25  |
| 28  | V     | 203    | GOL  | O2-C2-C3-O3     |
| 24  | d     | 401    | CLA  | C4C-C3C-CAC-CBC |
| 24  | c     | 517    | CLA  | C3-C5-C6-C7     |
| 35  | B     | 624    | HTG  | C4'-C5'-C6'-C7' |
| 29  | f     | 102    | LMT  | O5B-C1B-O1B-C4' |
| 24  | A     | 407    | CLA  | C12-C13-C15-C16 |
| 31  | A     | 419[A] | PL9  | C28-C29-C31-C32 |
| 37  | D     | 409    | LHG  | C33-C34-C35-C36 |
| 35  | b     | 632    | HTG  | C4-C5-C6-O6     |
| 24  | B     | 613    | CLA  | CAA-CBA-CGA-O2A |
| 24  | B     | 614    | CLA  | CAA-CBA-CGA-O2A |
| 38  | e     | 103    | HEM  | CAD-CBD-CGD-O2D |
| 33  | c     | 501    | LMG  | C13-C14-C15-C16 |
| 24  | b     | 615    | CLA  | C11-C10-C8-C9   |
| 24  | c     | 507    | CLA  | C11-C12-C13-C14 |
| 24  | c     | 510    | CLA  | C11-C12-C13-C14 |
| 36  | h     | 102    | DGD  | O1B-C1B-C2B-C3B |
| 26  | k     | 101    | BCR  | C9-C10-C11-C12  |
| 24  | C     | 504    | CLA  | C2B-C3B-CAB-CBB |
| 24  | c     | 514    | CLA  | C2B-C3B-CAB-CBB |
| 29  | M     | 103    | LMT  | C2B-C1B-O1B-C4' |
| 33  | b     | 629    | LMG  | C29-C28-O8-C9   |
| 35  | B     | 623    | HTG  | C4'-C5'-C6'-C7' |
| 38  | e     | 103    | HEM  | CAA-CBA-CGA-O2A |
| 24  | a     | 409    | CLA  | C2A-CAA-CBA-CGA |
| 27  | a     | 405    | SQD  | C12-C13-C14-C15 |
| 37  | d     | 408    | LHG  | C25-C26-C27-C28 |
| 37  | b     | 634    | LHG  | C14-C15-C16-C17 |
| 33  | z     | 101    | LMG  | C16-C17-C18-C19 |
| 26  | K     | 101    | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | z     | 101    | LMG  | O9-C10-C11-C12  |
| 37  | d     | 406    | LHG  | O10-C23-C24-C25 |
| 24  | b     | 615    | CLA  | C15-C16-C17-C18 |
| 29  | m     | 103    | LMT  | C5-C6-C7-C8     |
| 36  | C     | 518    | DGD  | C8B-C9B-CAB-CBB |
| 24  | C     | 506    | CLA  | C4-C3-C5-C6     |
| 37  | b     | 634    | LHG  | O1-C1-C2-C3     |
| 37  | D     | 407    | LHG  | C26-C27-C28-C29 |
| 24  | C     | 513    | CLA  | C1A-C2A-CAA-CBA |
| 25  | a     | 418[B] | PHO  | C2C-C3C-CAC-CBC |
| 27  | B     | 621    | SQD  | C14-C15-C16-C17 |
| 37  | L     | 101    | LHG  | C16-C17-C18-C19 |
| 24  | C     | 509    | CLA  | O1D-CGD-O2D-CED |
| 24  | B     | 614    | CLA  | C2-C1-O2A-CGA   |
| 24  | C     | 510    | CLA  | C2-C1-O2A-CGA   |
| 24  | b     | 617    | CLA  | C2-C1-O2A-CGA   |
| 37  | e     | 102    | LHG  | O10-C23-C24-C25 |
| 37  | b     | 634    | LHG  | O7-C7-C8-C9     |
| 24  | b     | 611    | CLA  | C2A-CAA-CBA-CGA |
| 24  | b     | 623    | CLA  | C2A-CAA-CBA-CGA |
| 24  | c     | 506    | CLA  | C2A-CAA-CBA-CGA |
| 24  | c     | 510    | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 415[A] | PL9  | C2-C3-C7-C8     |
| 24  | C     | 512    | CLA  | CAA-CBA-CGA-O1A |
| 27  | f     | 101    | SQD  | O49-C7-C8-C9    |
| 24  | B     | 605    | CLA  | C13-C15-C16-C17 |
| 24  | a     | 409    | CLA  | C15-C16-C17-C18 |
| 29  | C     | 521    | LMT  | C3-C4-C5-C6     |
| 36  | C     | 518    | DGD  | CBB-CCB-CDB-CEB |
| 36  | H     | 102    | DGD  | C8A-C9A-CAA-CBA |
| 24  | C     | 510    | CLA  | CAA-CBA-CGA-O1A |
| 36  | c     | 522    | DGD  | O1A-C1A-C2A-C3A |
| 29  | m     | 103    | LMT  | C2'-C1'-O1'-C1  |
| 24  | C     | 502    | CLA  | C13-C15-C16-C17 |
| 31  | a     | 415[A] | PL9  | C3-C7-C8-C9     |
| 24  | b     | 611    | CLA  | C16-C17-C18-C20 |
| 24  | b     | 622    | CLA  | CAA-CBA-CGA-O2A |
| 33  | C     | 520    | LMG  | C13-C14-C15-C16 |
| 36  | D     | 406    | DGD  | C5B-C6B-C7B-C8B |
| 24  | c     | 517    | CLA  | CAA-CBA-CGA-O1A |
| 36  | D     | 406    | DGD  | O1A-C1A-C2A-C3A |
| 36  | e     | 101    | DGD  | O1B-C1B-C2B-C3B |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | A     | 421    | LMG  | O6-C5-C6-O5     |
| 24  | A     | 405    | CLA  | C2A-CAA-CBA-CGA |
| 24  | C     | 507    | CLA  | C2A-CAA-CBA-CGA |
| 27  | F     | 103    | SQD  | C33-C34-C35-C36 |
| 24  | C     | 510    | CLA  | C8-C10-C11-C12  |
| 29  | F     | 101    | LMT  | C2-C3-C4-C5     |
| 36  | h     | 102    | DGD  | CBB-CCB-CDB-CEB |
| 27  | L     | 102    | SQD  | C23-C24-C25-C26 |
| 24  | b     | 610    | CLA  | CAA-CBA-CGA-O1A |
| 33  | Z     | 101    | LMG  | O9-C10-C11-C12  |
| 24  | B     | 608    | CLA  | CAD-CBD-CGD-O1D |
| 24  | C     | 504    | CLA  | CAD-CBD-CGD-O1D |
| 24  | C     | 506    | CLA  | CAD-CBD-CGD-O1D |
| 24  | b     | 616    | CLA  | CAD-CBD-CGD-O1D |
| 24  | b     | 618    | CLA  | CAD-CBD-CGD-O1D |
| 24  | c     | 509    | CLA  | CAD-CBD-CGD-O1D |
| 27  | L     | 102    | SQD  | O5-C5-C6-S      |
| 37  | d     | 406    | LHG  | C7-C8-C9-C10    |
| 27  | f     | 101    | SQD  | C30-C31-C32-C33 |
| 36  | c     | 521    | DGD  | CCB-CDB-CEB-CFB |
| 24  | C     | 504    | CLA  | C14-C13-C15-C16 |
| 24  | C     | 512    | CLA  | C6-C7-C8-C9     |
| 36  | C     | 516    | DGD  | C6A-C7A-C8A-C9A |
| 36  | H     | 102    | DGD  | O1B-C1B-C2B-C3B |
| 37  | L     | 101    | LHG  | O9-C7-C8-C9     |
| 33  | b     | 629    | LMG  | O8-C28-C29-C30  |
| 36  | c     | 521    | DGD  | O2G-C1B-C2B-C3B |
| 24  | d     | 401    | CLA  | C13-C15-C16-C17 |
| 24  | C     | 507    | CLA  | C5-C6-C7-C8     |
| 27  | a     | 414    | SQD  | C10-C11-C12-C13 |
| 33  | D     | 413    | LMG  | C12-C13-C14-C15 |
| 24  | C     | 505    | CLA  | CAA-CBA-CGA-O2A |
| 24  | c     | 506    | CLA  | CAA-CBA-CGA-O2A |
| 33  | D     | 413    | LMG  | O7-C10-C11-C12  |
| 37  | d     | 408    | LHG  | O8-C23-C24-C25  |
| 24  | c     | 511    | CLA  | C13-C15-C16-C17 |
| 37  | E     | 101    | LHG  | O10-C23-C24-C25 |
| 31  | D     | 405[B] | PL9  | C30-C29-C31-C32 |
| 24  | A     | 410    | CLA  | C6-C7-C8-C10    |
| 24  | A     | 410    | CLA  | C12-C13-C15-C16 |
| 24  | C     | 501    | CLA  | C11-C12-C13-C15 |
| 24  | b     | 619    | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 31  | d     | 405[B] | PL9  | C18-C19-C21-C22 |
| 36  | C     | 517    | DGD  | CAA-CBA-CCA-CDA |
| 37  | E     | 101    | LHG  | O7-C7-C8-C9     |
| 36  | e     | 101    | DGD  | C6B-C7B-C8B-C9B |
| 24  | B     | 613    | CLA  | CAA-CBA-CGA-O1A |
| 24  | c     | 515    | CLA  | CAA-CBA-CGA-O1A |
| 37  | E     | 101    | LHG  | O9-C7-C8-C9     |
| 29  | m     | 102    | LMT  | O1'-C1-C2-C3    |
| 36  | C     | 517    | DGD  | O2G-C1B-C2B-C3B |
| 36  | C     | 516    | DGD  | O6E-C1E-O5D-C6D |
| 24  | A     | 410    | CLA  | C8-C10-C11-C12  |
| 24  | A     | 410    | CLA  | C15-C16-C17-C18 |
| 33  | b     | 629    | LMG  | O10-C28-O8-C9   |
| 37  | b     | 634    | LHG  | C11-C12-C13-C14 |
| 24  | C     | 501    | CLA  | CAA-CBA-CGA-O2A |
| 24  | c     | 510    | CLA  | CAA-CBA-CGA-O2A |
| 24  | b     | 622    | CLA  | CAA-CBA-CGA-O1A |
| 24  | b     | 623    | CLA  | C8-C10-C11-C12  |
| 36  | c     | 521    | DGD  | O1B-C1B-C2B-C3B |

There are no ring outliers.

159 monomers are involved in 345 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 24  | c     | 518    | CLA  | 5       | 0            |
| 26  | b     | 628    | BCR  | 3       | 0            |
| 27  | F     | 103    | SQD  | 2       | 0            |
| 24  | c     | 511    | CLA  | 2       | 0            |
| 24  | b     | 621    | CLA  | 2       | 0            |
| 26  | k     | 101    | BCR  | 1       | 0            |
| 26  | B     | 618    | BCR  | 3       | 0            |
| 28  | B     | 630    | GOL  | 1       | 0            |
| 24  | C     | 512    | CLA  | 4       | 0            |
| 24  | c     | 515    | CLA  | 2       | 0            |
| 29  | f     | 102    | LMT  | 1       | 0            |
| 26  | C     | 514    | BCR  | 6       | 0            |
| 26  | B     | 620    | BCR  | 5       | 0            |
| 33  | z     | 101    | LMG  | 5       | 0            |
| 25  | a     | 418[A] | PHO  | 2       | 0            |
| 33  | c     | 501    | LMG  | 2       | 0            |
| 37  | b     | 634    | LHG  | 3       | 0            |
| 24  | B     | 612    | CLA  | 1       | 0            |

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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 24  | c     | 509    | CLA  | 1       | 0            |
| 37  | e     | 102    | LHG  | 4       | 0            |
| 36  | e     | 101    | DGD  | 7       | 0            |
| 29  | M     | 103    | LMT  | 1       | 0            |
| 24  | B     | 614    | CLA  | 3       | 0            |
| 37  | E     | 101    | LHG  | 2       | 0            |
| 25  | A     | 409[B] | PHO  | 2       | 0            |
| 26  | y     | 101    | BCR  | 2       | 0            |
| 24  | B     | 604    | CLA  | 2       | 0            |
| 27  | L     | 102    | SQD  | 3       | 0            |
| 35  | D     | 412    | HTG  | 2       | 0            |
| 29  | m     | 103    | LMT  | 2       | 0            |
| 24  | b     | 623    | CLA  | 1       | 0            |
| 33  | D     | 413    | LMG  | 1       | 0            |
| 28  | v     | 201    | GOL  | 1       | 0            |
| 36  | c     | 520    | DGD  | 1       | 0            |
| 26  | D     | 404    | BCR  | 1       | 0            |
| 24  | b     | 610    | CLA  | 2       | 0            |
| 35  | B     | 623    | HTG  | 1       | 0            |
| 24  | c     | 507    | CLA  | 4       | 0            |
| 29  | D     | 401    | LMT  | 1       | 0            |
| 28  | T     | 101    | GOL  | 1       | 0            |
| 31  | A     | 419[A] | PL9  | 5       | 0            |
| 26  | H     | 101    | BCR  | 3       | 0            |
| 26  | A     | 411    | BCR  | 1       | 0            |
| 29  | A     | 417    | LMT  | 2       | 0            |
| 28  | c     | 503    | GOL  | 2       | 0            |
| 29  | M     | 101    | LMT  | 3       | 0            |
| 26  | T     | 103    | BCR  | 5       | 0            |
| 24  | d     | 403    | CLA  | 2       | 0            |
| 29  | a     | 419    | LMT  | 1       | 0            |
| 24  | b     | 613    | CLA  | 2       | 0            |
| 24  | c     | 512    | CLA  | 3       | 0            |
| 24  | b     | 612    | CLA  | 2       | 0            |
| 24  | B     | 615    | CLA  | 4       | 0            |
| 24  | a     | 409    | CLA  | 4       | 0            |
| 24  | C     | 503    | CLA  | 3       | 0            |
| 24  | c     | 506    | CLA  | 3       | 0            |
| 26  | b     | 627    | BCR  | 3       | 0            |
| 24  | a     | 410    | CLA  | 3       | 0            |
| 24  | d     | 402    | CLA  | 3       | 0            |
| 28  | T     | 102    | GOL  | 2       | 0            |

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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 28  | t     | 102    | GOL  | 1       | 0            |
| 35  | d     | 411    | HTG  | 3       | 0            |
| 25  | A     | 408    | PHO  | 1       | 0            |
| 27  | B     | 621    | SQD  | 3       | 0            |
| 27  | a     | 414    | SQD  | 2       | 0            |
| 24  | b     | 624    | CLA  | 5       | 0            |
| 24  | A     | 410    | CLA  | 4       | 0            |
| 24  | c     | 514    | CLA  | 3       | 0            |
| 26  | t     | 101    | BCR  | 5       | 0            |
| 26  | a     | 413    | BCR  | 1       | 0            |
| 24  | C     | 505    | CLA  | 5       | 0            |
| 31  | a     | 415[B] | PL9  | 7       | 0            |
| 33  | C     | 520    | LMG  | 3       | 0            |
| 24  | B     | 613    | CLA  | 1       | 0            |
| 24  | A     | 406    | CLA  | 3       | 0            |
| 24  | B     | 602    | CLA  | 2       | 0            |
| 37  | d     | 408    | LHG  | 6       | 0            |
| 24  | c     | 516    | CLA  | 2       | 0            |
| 33  | C     | 519    | LMG  | 4       | 0            |
| 24  | C     | 510    | CLA  | 3       | 0            |
| 36  | C     | 516    | DGD  | 1       | 0            |
| 36  | D     | 406    | DGD  | 2       | 0            |
| 33  | Z     | 101    | LMG  | 1       | 0            |
| 24  | C     | 506    | CLA  | 2       | 0            |
| 24  | b     | 620    | CLA  | 3       | 0            |
| 24  | b     | 619    | CLA  | 4       | 0            |
| 26  | b     | 626    | BCR  | 4       | 0            |
| 36  | C     | 518    | DGD  | 1       | 0            |
| 29  | b     | 630    | LMT  | 3       | 0            |
| 33  | c     | 524    | LMG  | 2       | 0            |
| 35  | c     | 525    | HTG  | 1       | 0            |
| 24  | C     | 513    | CLA  | 6       | 0            |
| 31  | D     | 405[B] | PL9  | 1       | 0            |
| 24  | b     | 614    | CLA  | 6       | 0            |
| 25  | a     | 418[B] | PHO  | 1       | 0            |
| 24  | C     | 507    | CLA  | 3       | 0            |
| 24  | c     | 513    | CLA  | 6       | 0            |
| 37  | D     | 408    | LHG  | 1       | 0            |
| 24  | C     | 509    | CLA  | 3       | 0            |
| 24  | c     | 510    | CLA  | 7       | 0            |
| 24  | A     | 405    | CLA  | 4       | 0            |
| 25  | A     | 409[A] | PHO  | 3       | 0            |

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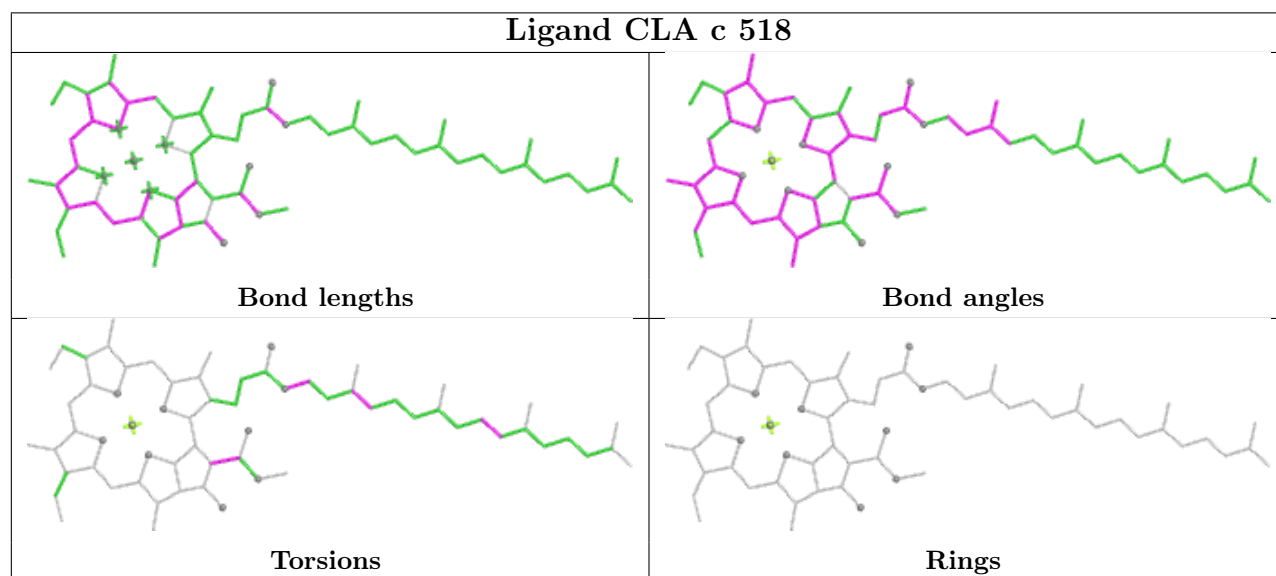
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 24  | b     | 618    | CLA  | 1       | 0            |
| 35  | V     | 206    | HTG  | 1       | 0            |
| 24  | C     | 502    | CLA  | 3       | 0            |
| 27  | A     | 412    | SQD  | 6       | 0            |
| 37  | D     | 409    | LHG  | 9       | 0            |
| 33  | c     | 523    | LMG  | 3       | 0            |
| 26  | B     | 619    | BCR  | 3       | 0            |
| 27  | f     | 101    | SQD  | 1       | 1            |
| 29  | C     | 521    | LMT  | 1       | 0            |
| 24  | D     | 402    | CLA  | 3       | 0            |
| 24  | B     | 617    | CLA  | 6       | 0            |
| 24  | C     | 501    | CLA  | 1       | 0            |
| 38  | F     | 102    | HEM  | 2       | 0            |
| 24  | b     | 622    | CLA  | 3       | 0            |
| 24  | D     | 403    | CLA  | 1       | 0            |
| 24  | c     | 517    | CLA  | 2       | 0            |
| 28  | A     | 414    | GOL  | 1       | 0            |
| 37  | D     | 407    | LHG  | 1       | 0            |
| 24  | B     | 603    | CLA  | 2       | 0            |
| 33  | A     | 421    | LMG  | 4       | 0            |
| 24  | B     | 607    | CLA  | 4       | 0            |
| 33  | B     | 622    | LMG  | 1       | 0            |
| 35  | b     | 601    | HTG  | 1       | 0            |
| 27  | a     | 405    | SQD  | 1       | 0            |
| 31  | A     | 419[B] | PL9  | 4       | 0            |
| 24  | A     | 407    | CLA  | 1       | 0            |
| 26  | C     | 515    | BCR  | 5       | 0            |
| 38  | e     | 103    | HEM  | 5       | 0            |
| 24  | C     | 508    | CLA  | 3       | 0            |
| 24  | B     | 610    | CLA  | 3       | 0            |
| 26  | c     | 528    | BCR  | 2       | 0            |
| 36  | C     | 517    | DGD  | 2       | 0            |
| 29  | m     | 102    | LMT  | 1       | 0            |
| 37  | d     | 406    | LHG  | 2       | 0            |
| 24  | B     | 609    | CLA  | 1       | 0            |
| 24  | B     | 608    | CLA  | 1       | 0            |
| 27  | A     | 416    | SQD  | 1       | 0            |
| 28  | a     | 420    | GOL  | 1       | 0            |
| 24  | d     | 401    | CLA  | 4       | 0            |
| 26  | h     | 101    | BCR  | 4       | 0            |
| 37  | d     | 407    | LHG  | 1       | 0            |
| 33  | d     | 413    | LMG  | 2       | 0            |

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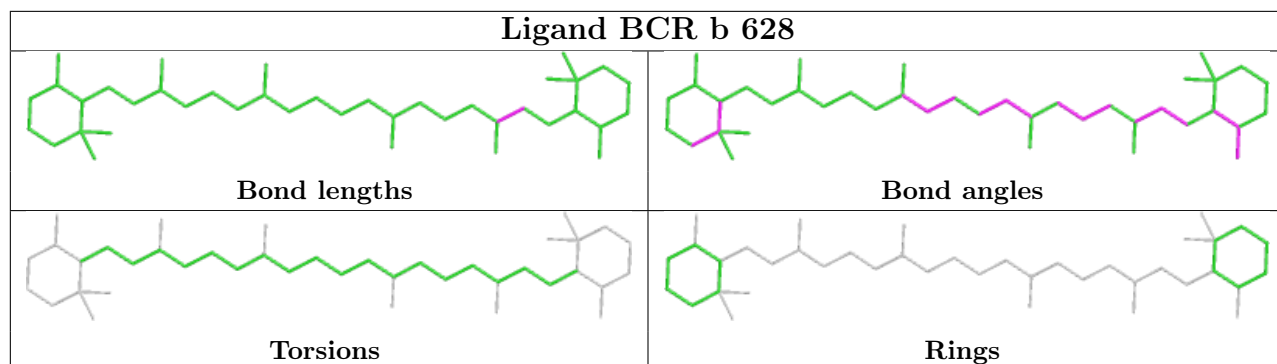
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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 24  | C     | 511    | CLA  | 2       | 0            |
| 26  | d     | 404    | BCR  | 3       | 0            |
| 31  | a     | 415[A] | PL9  | 7       | 0            |
| 36  | c     | 521    | DGD  | 1       | 0            |
| 26  | Y     | 101    | BCR  | 4       | 0            |
| 33  | b     | 629    | LMG  | 3       | 0            |
| 24  | B     | 606    | CLA  | 2       | 0            |
| 24  | c     | 508    | CLA  | 2       | 0            |
| 24  | B     | 616    | CLA  | 6       | 0            |
| 28  | a     | 402    | GOL  | 1       | 0            |
| 24  | a     | 412    | CLA  | 2       | 0            |
| 29  | a     | 404    | LMT  | 1       | 0            |
| 24  | b     | 625    | CLA  | 2       | 0            |
| 26  | c     | 519    | BCR  | 3       | 0            |
| 24  | B     | 611    | CLA  | 1       | 0            |

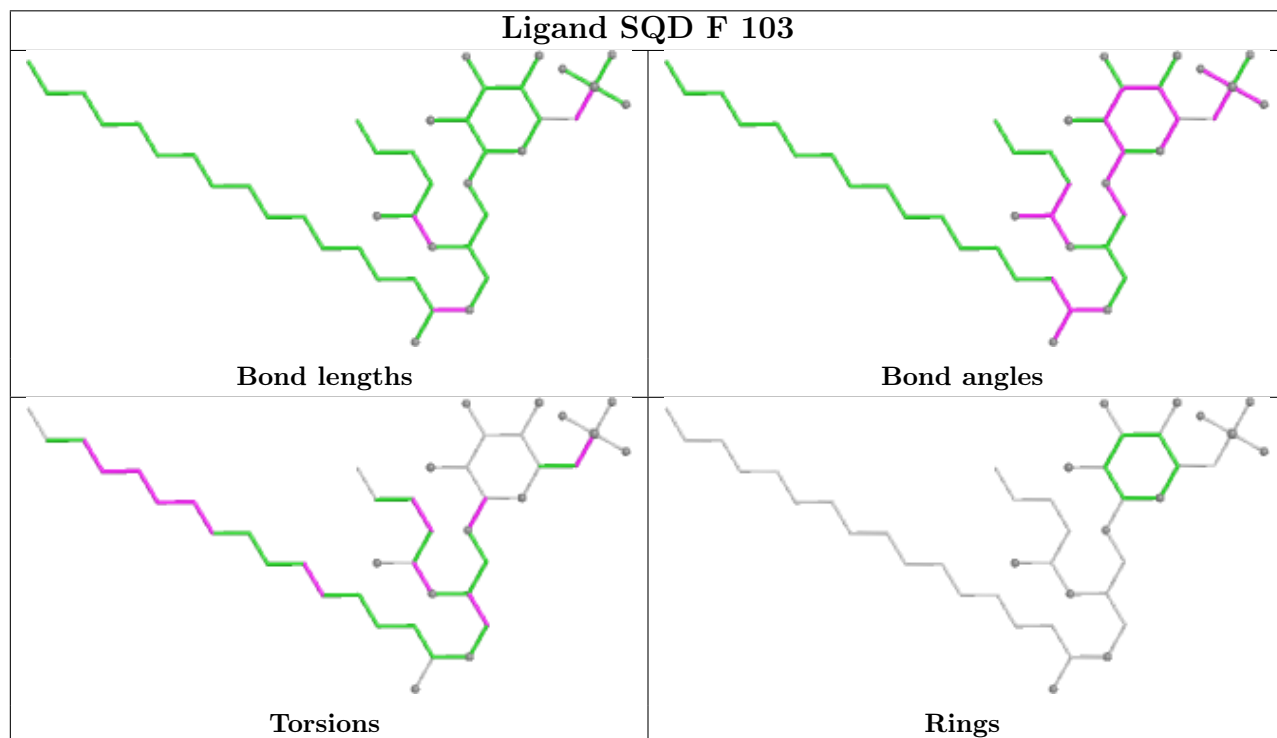
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



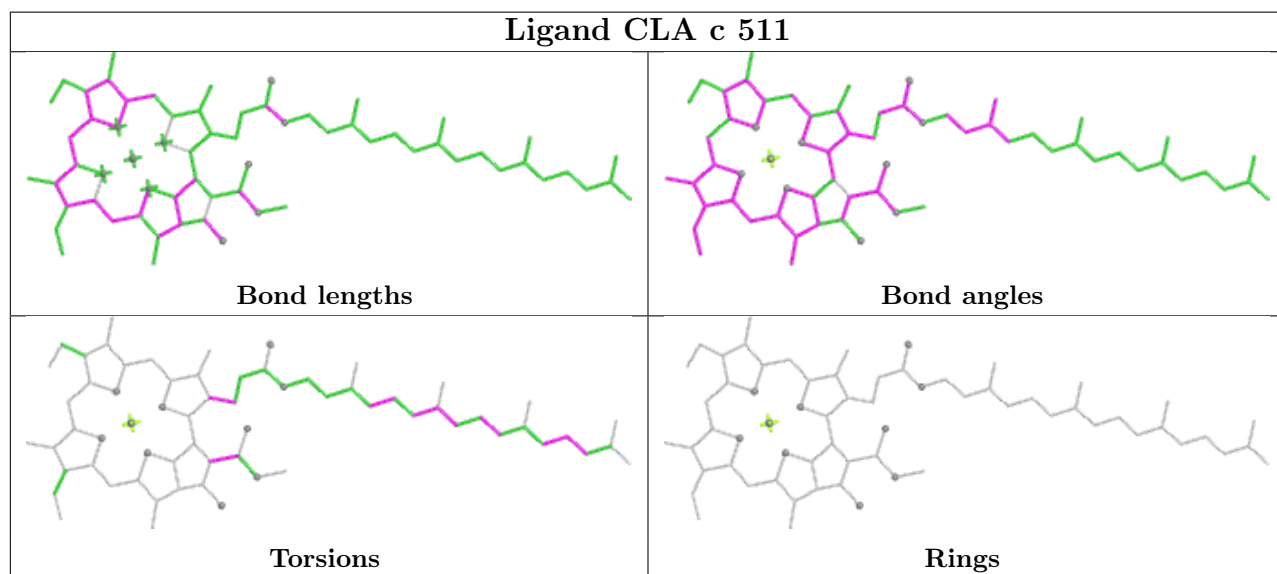
## Ligand BCR b 628



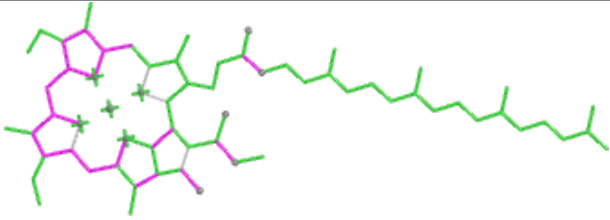
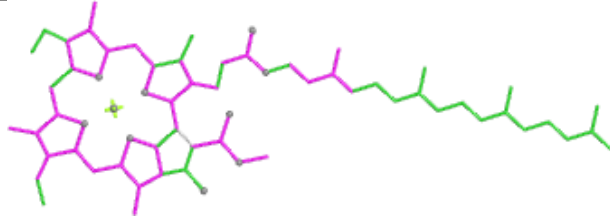
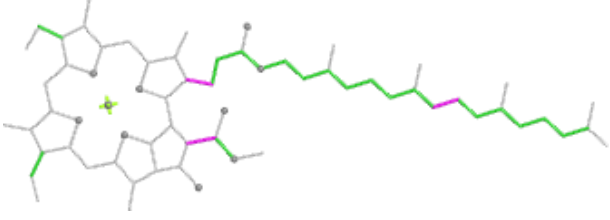
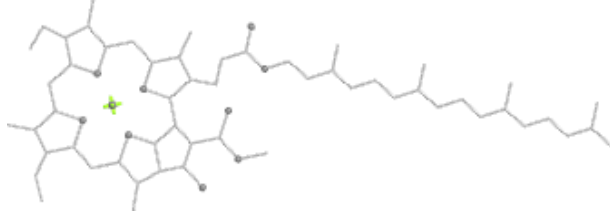
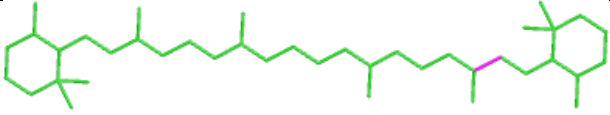
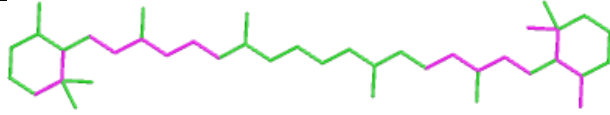
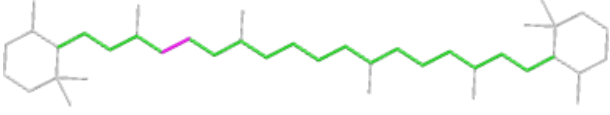
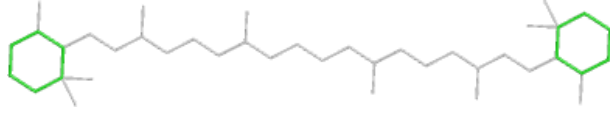
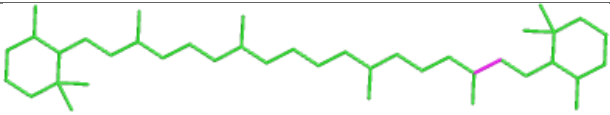
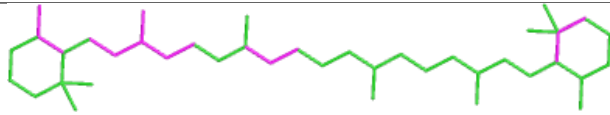
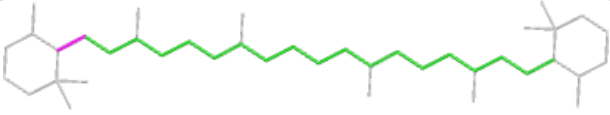
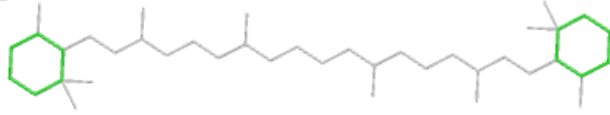
## Ligand SQD F 103

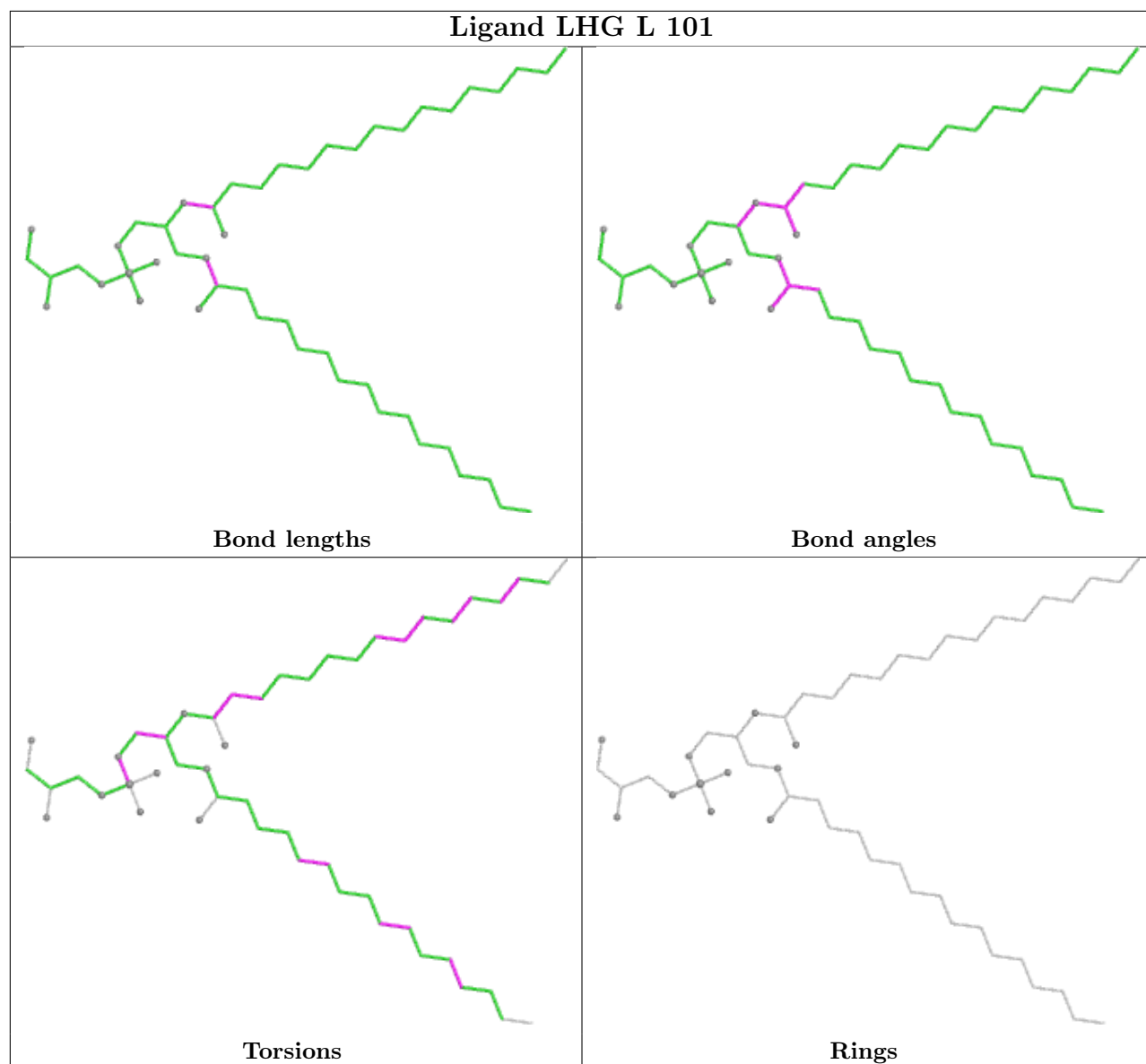
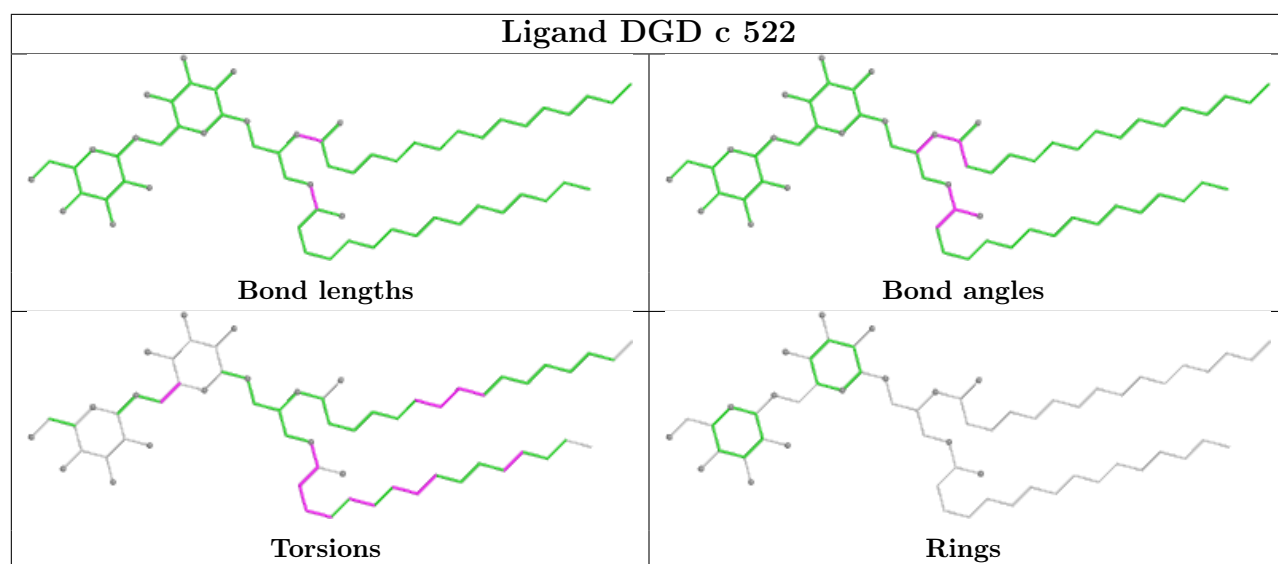


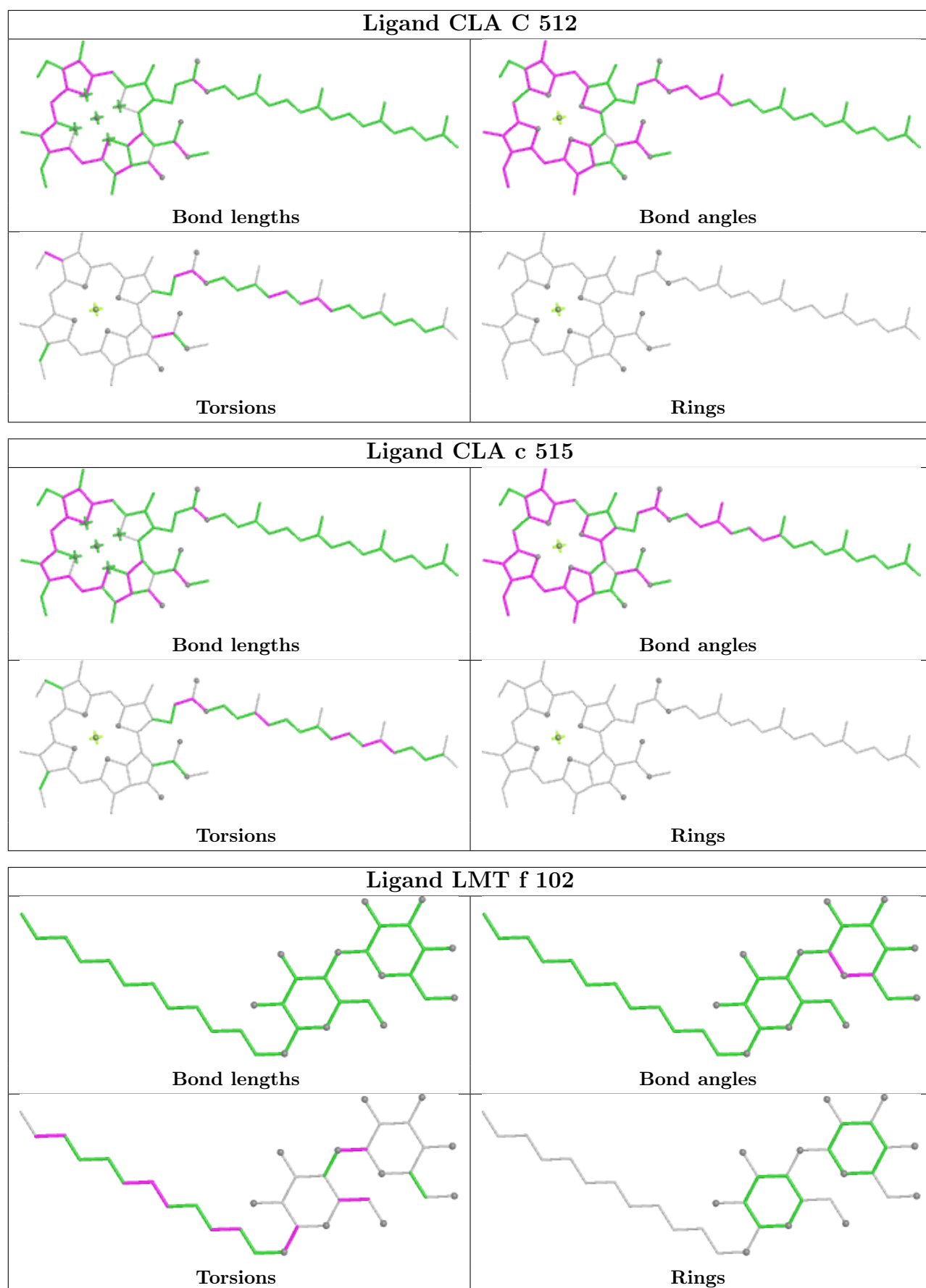
## Ligand CLA c 511

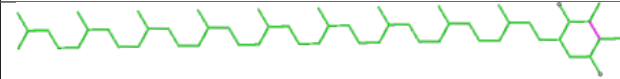
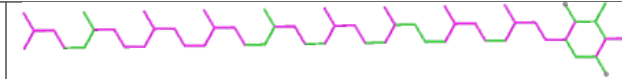
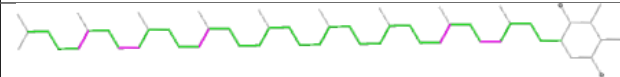
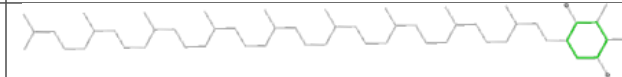
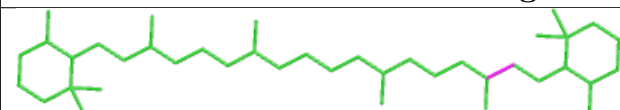
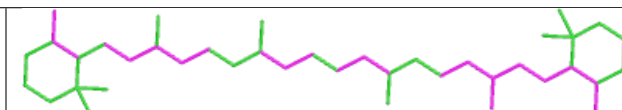
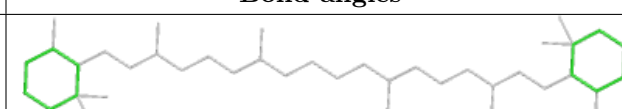
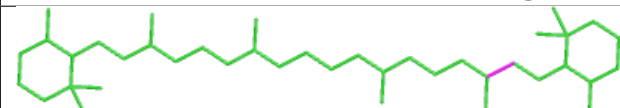
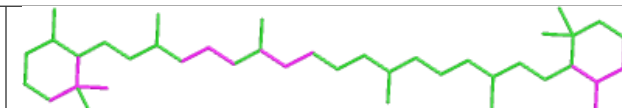
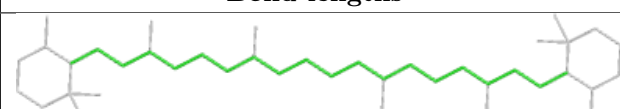
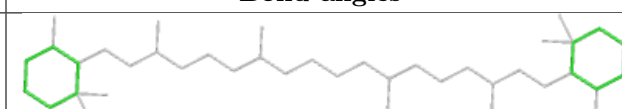
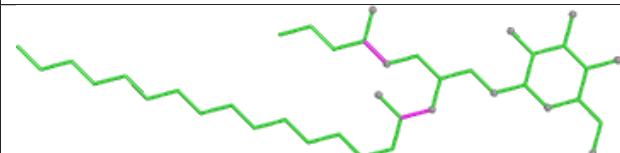
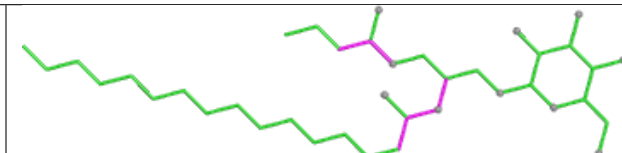
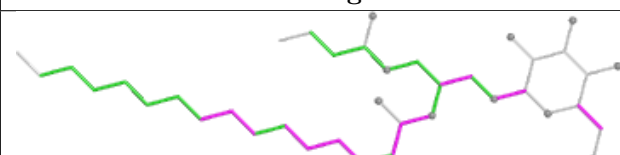
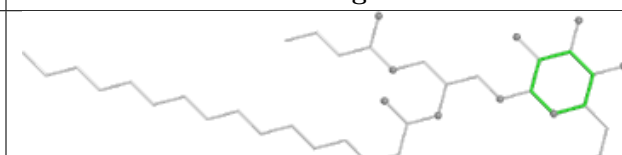


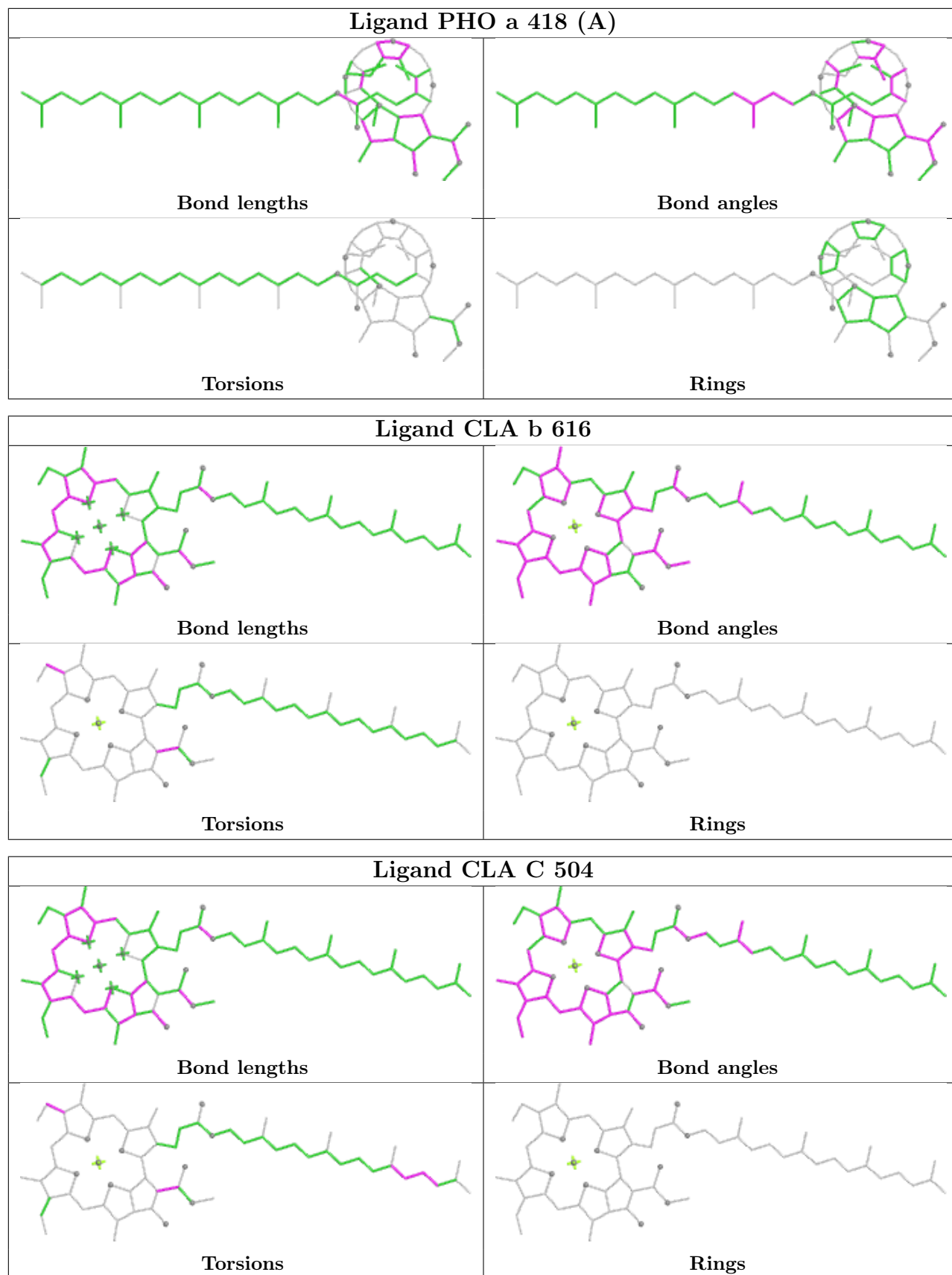


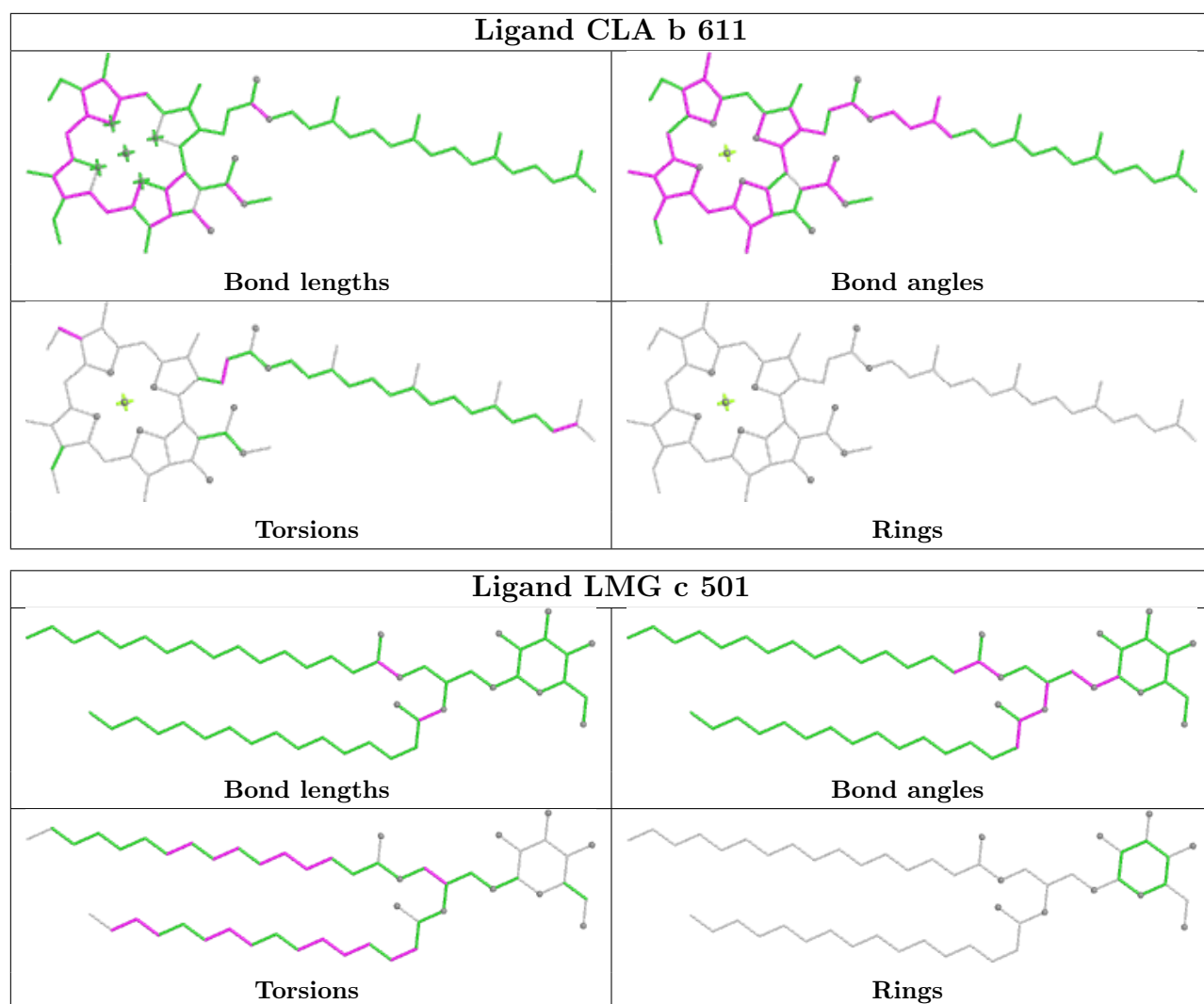
| Ligand CLA b 621                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <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 BCR B 618                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

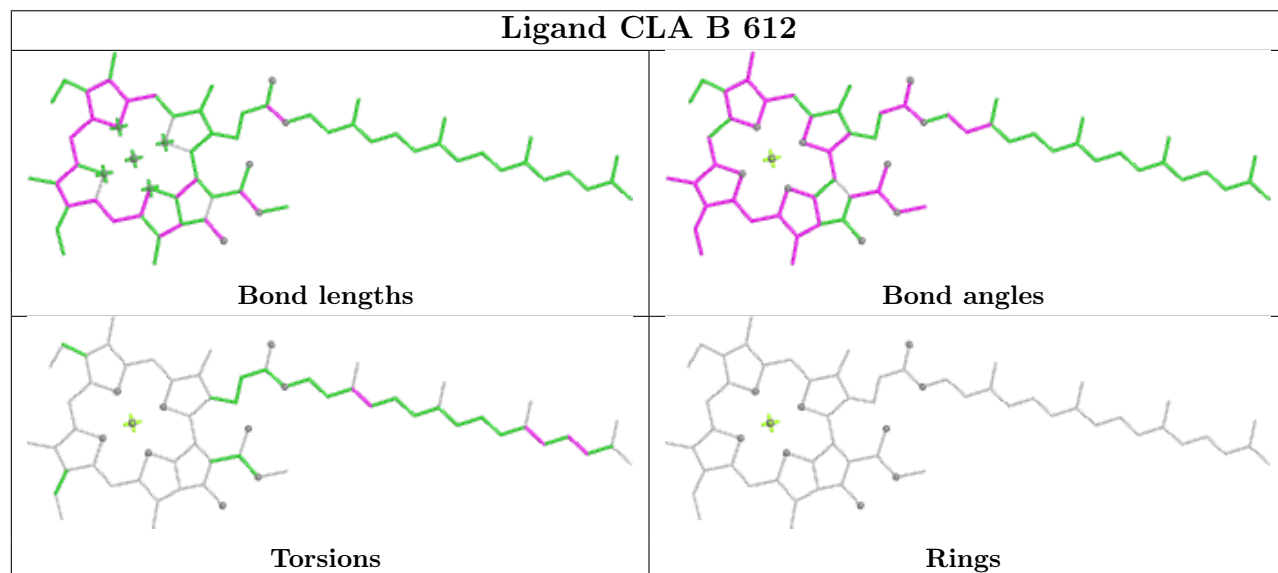
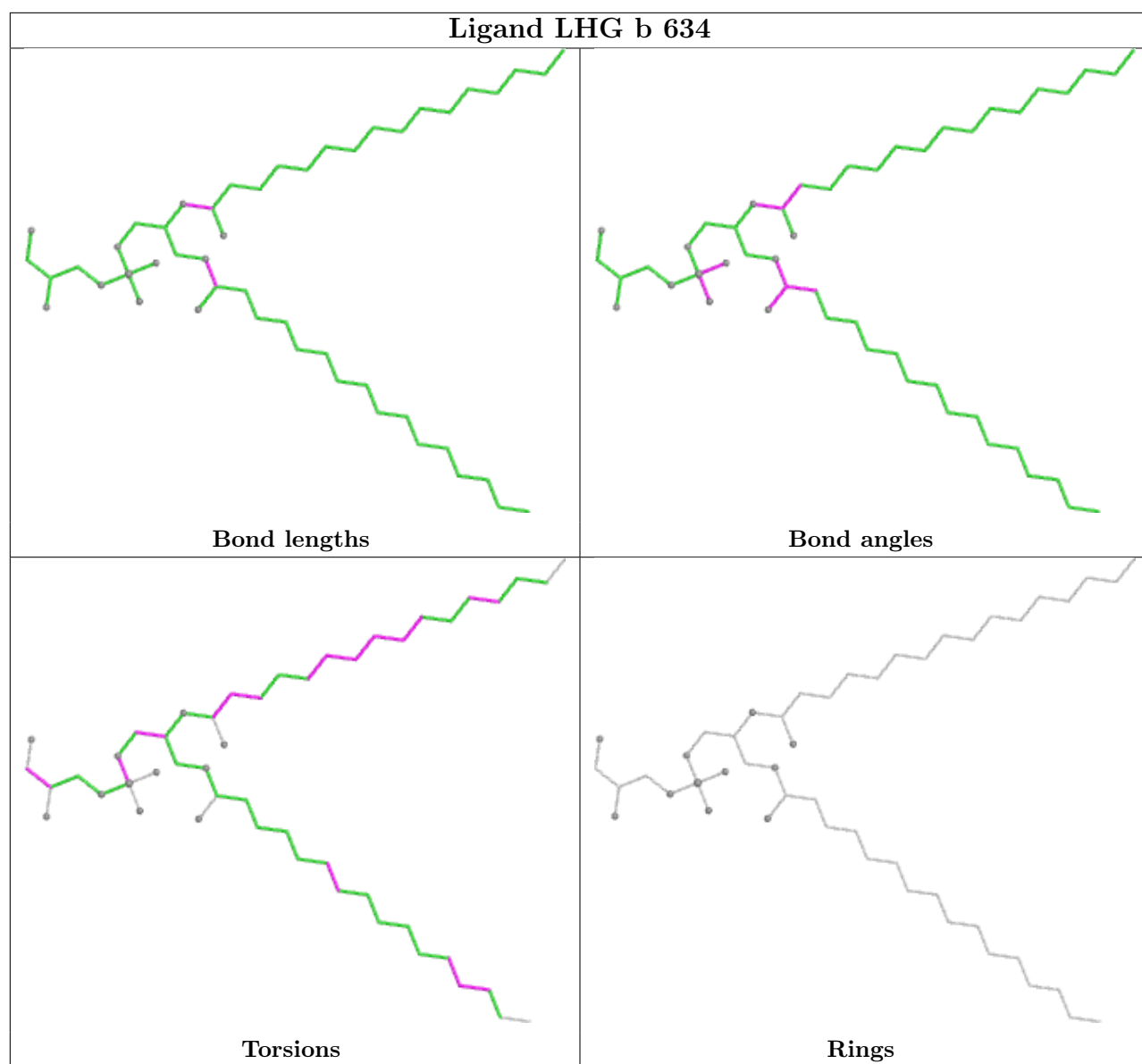




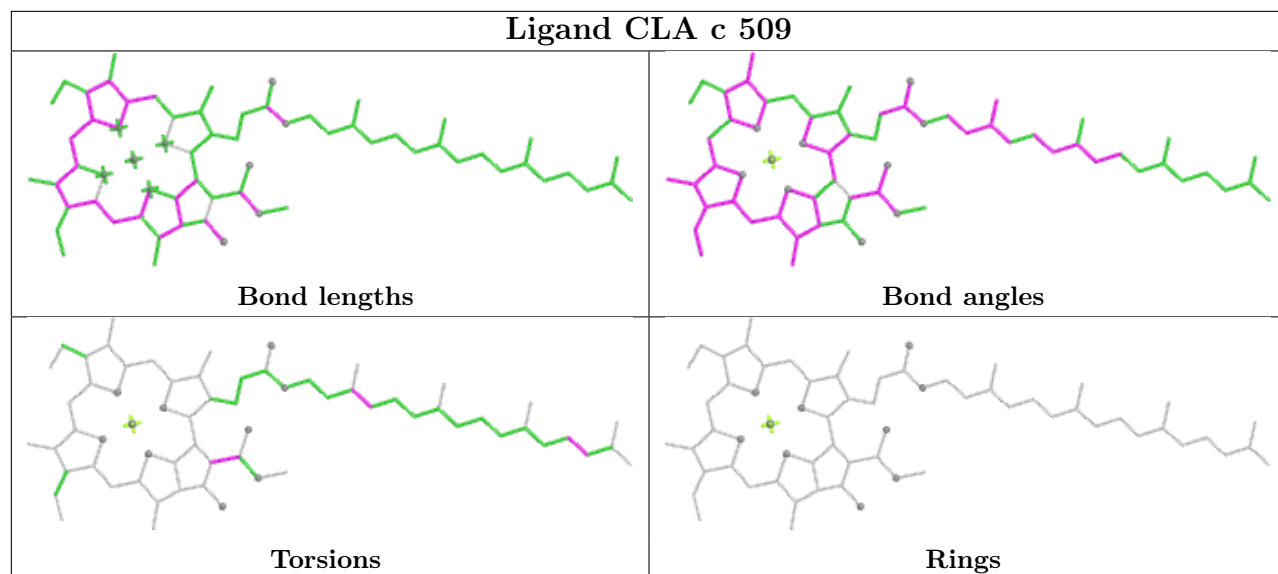
| Ligand PL9 D 405 (A)                                                                                    |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR C 514                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR B 620                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand LMG z 101                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |



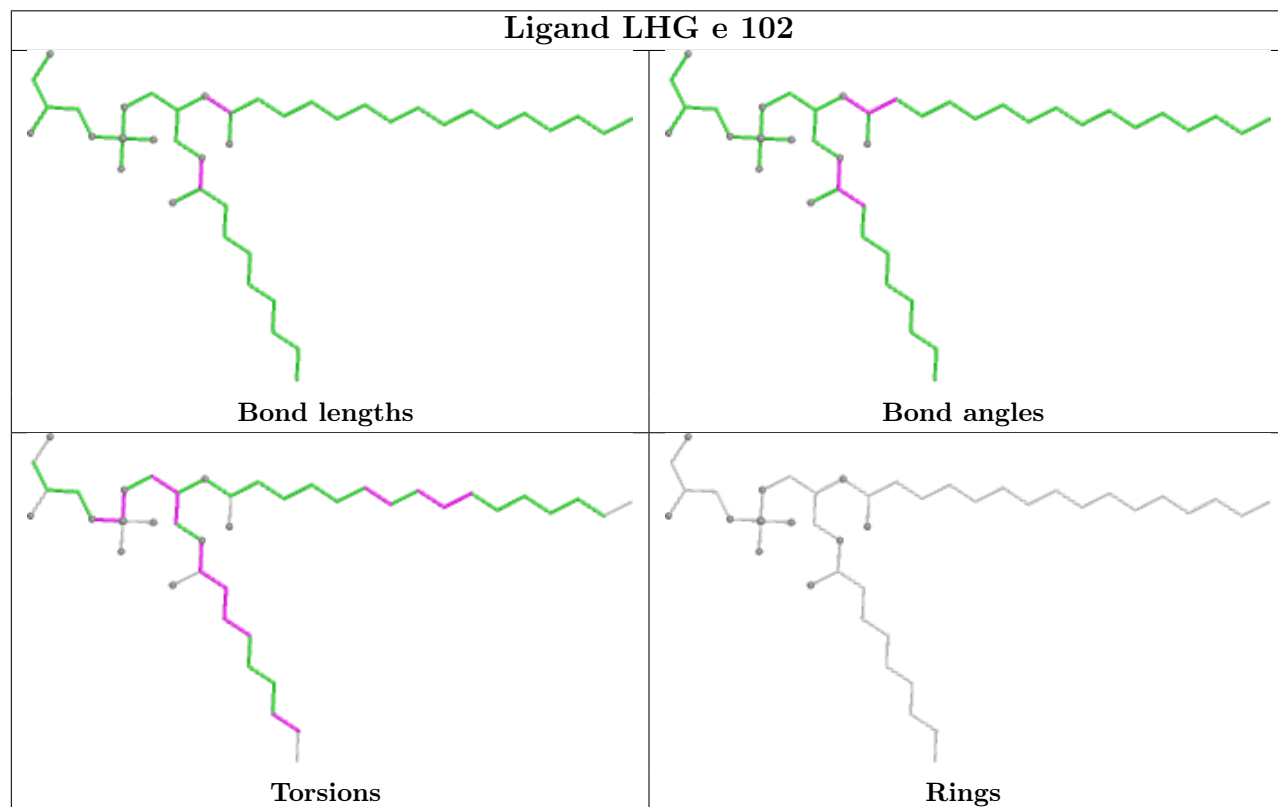




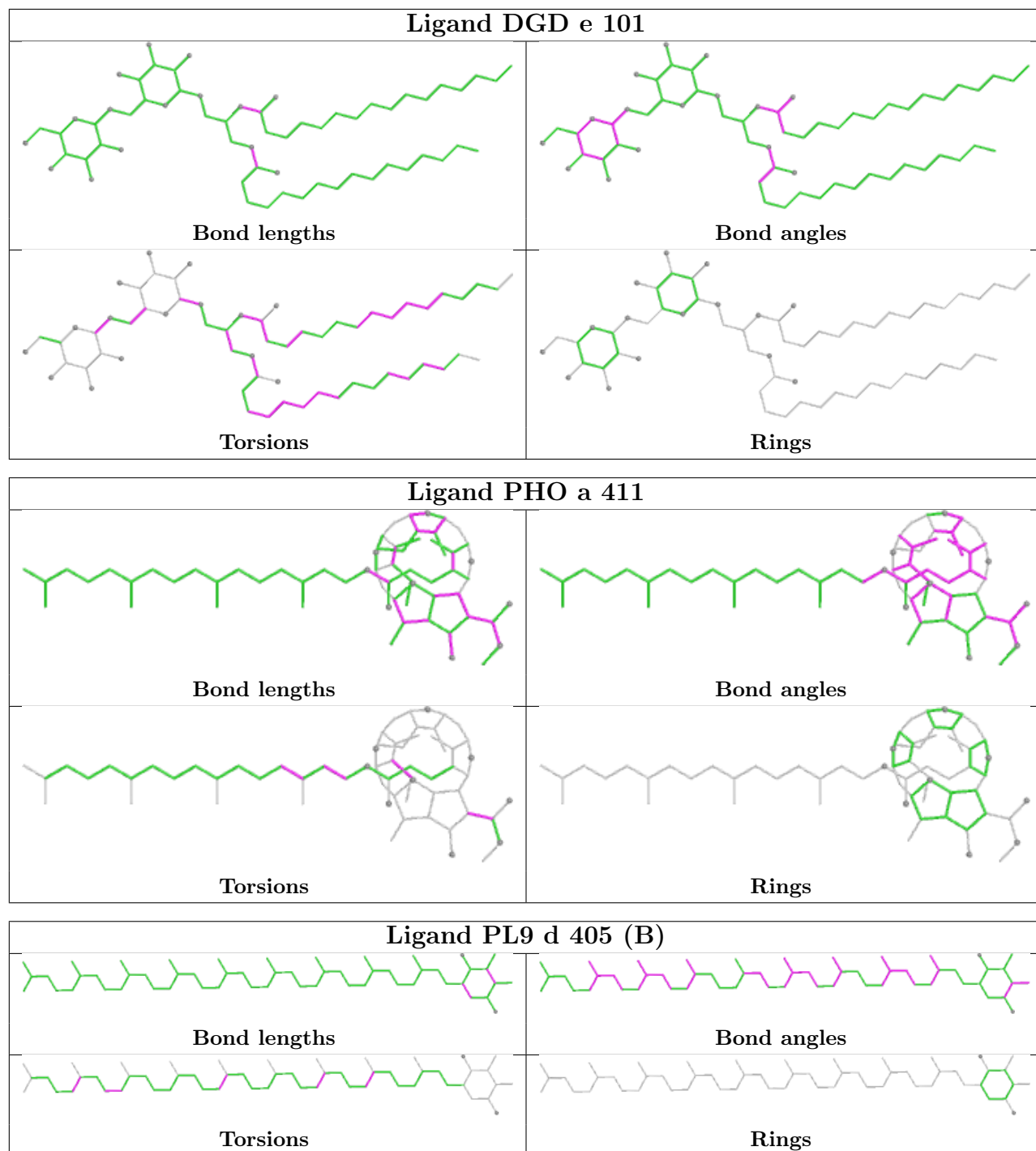
## Ligand CLA c 509

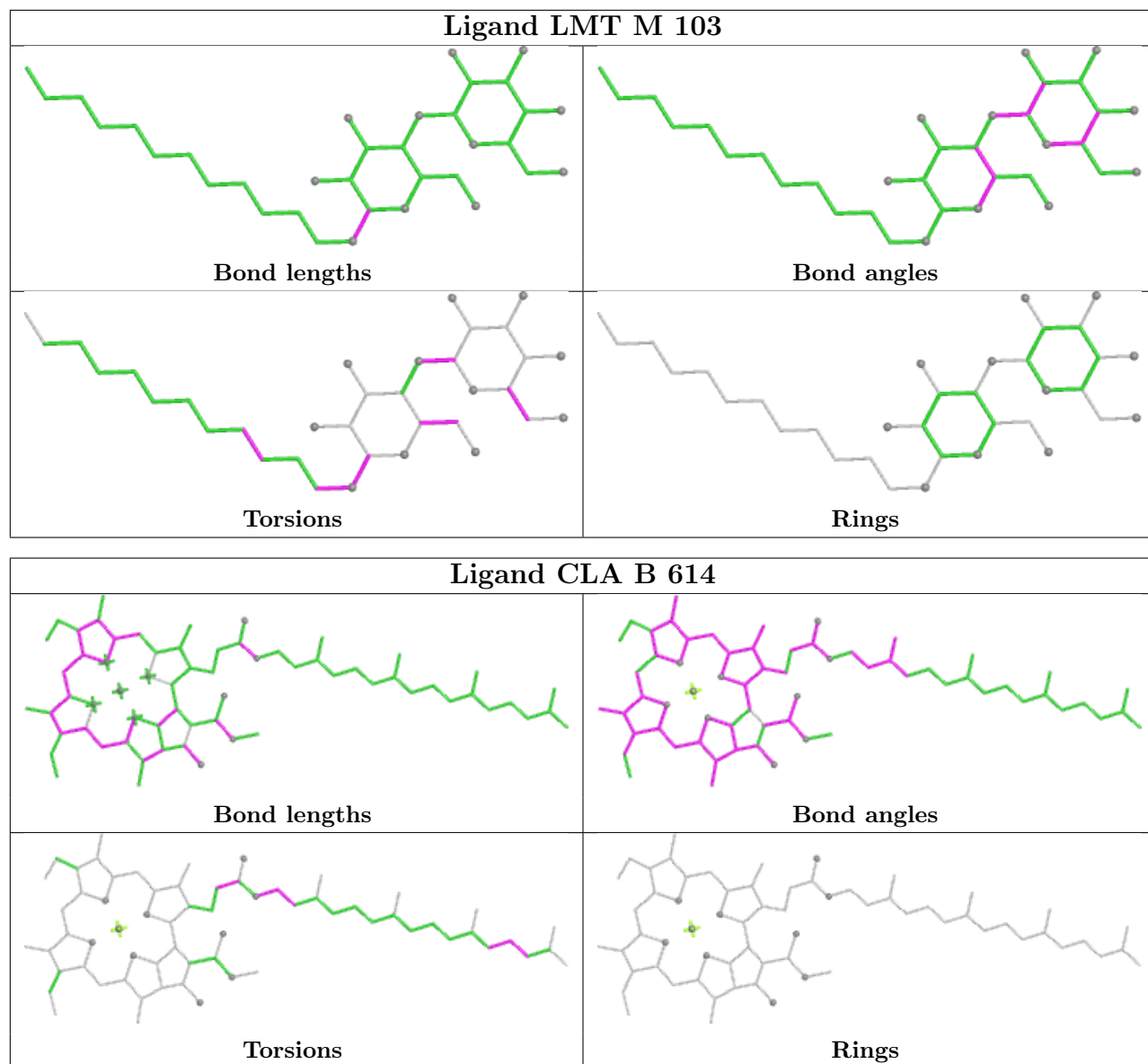


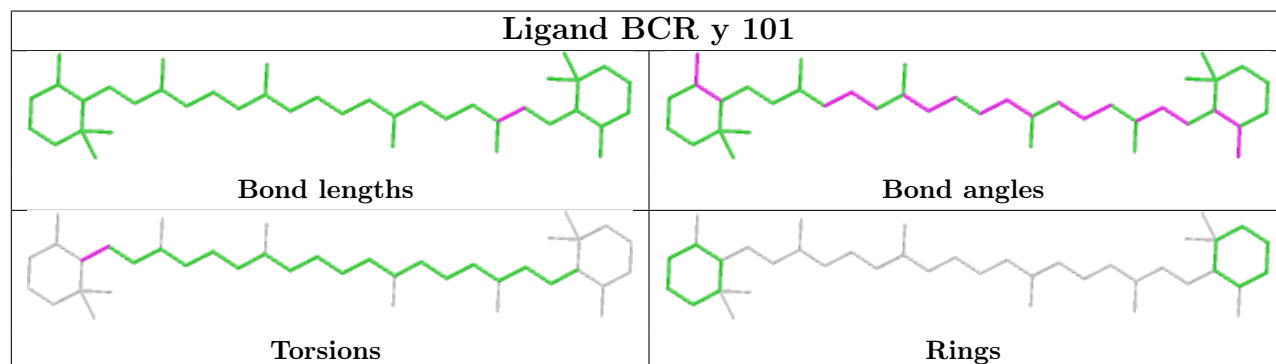
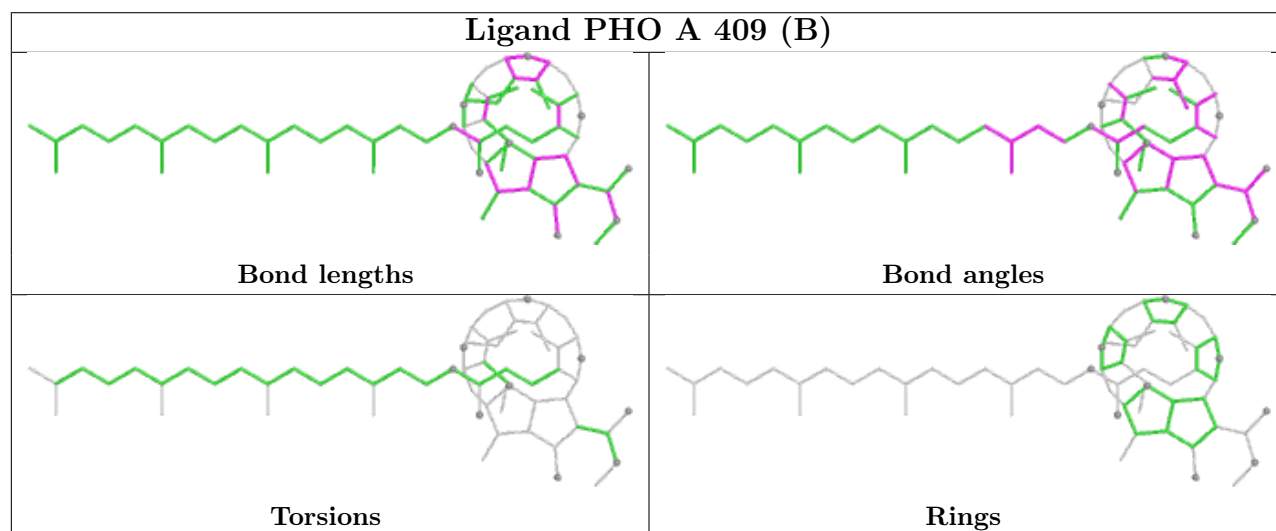
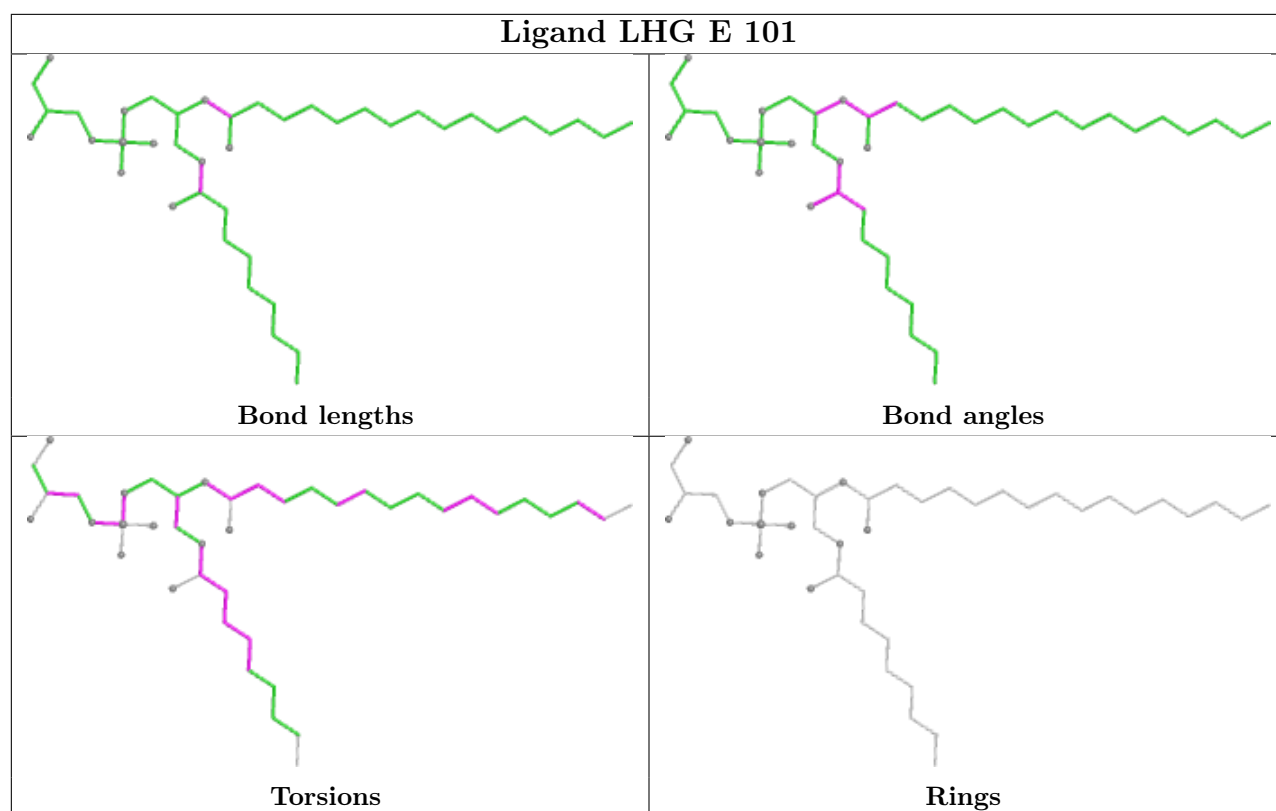
## Ligand LHG e 102

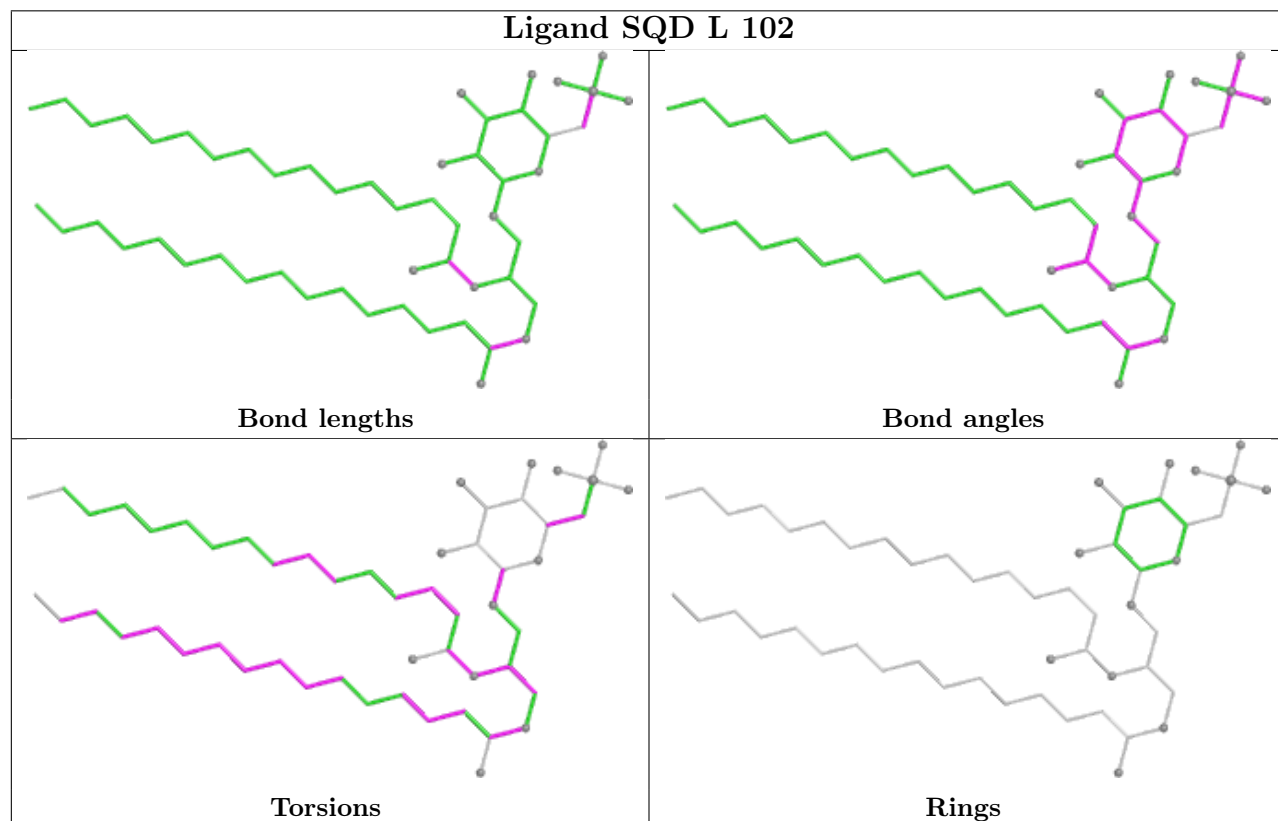
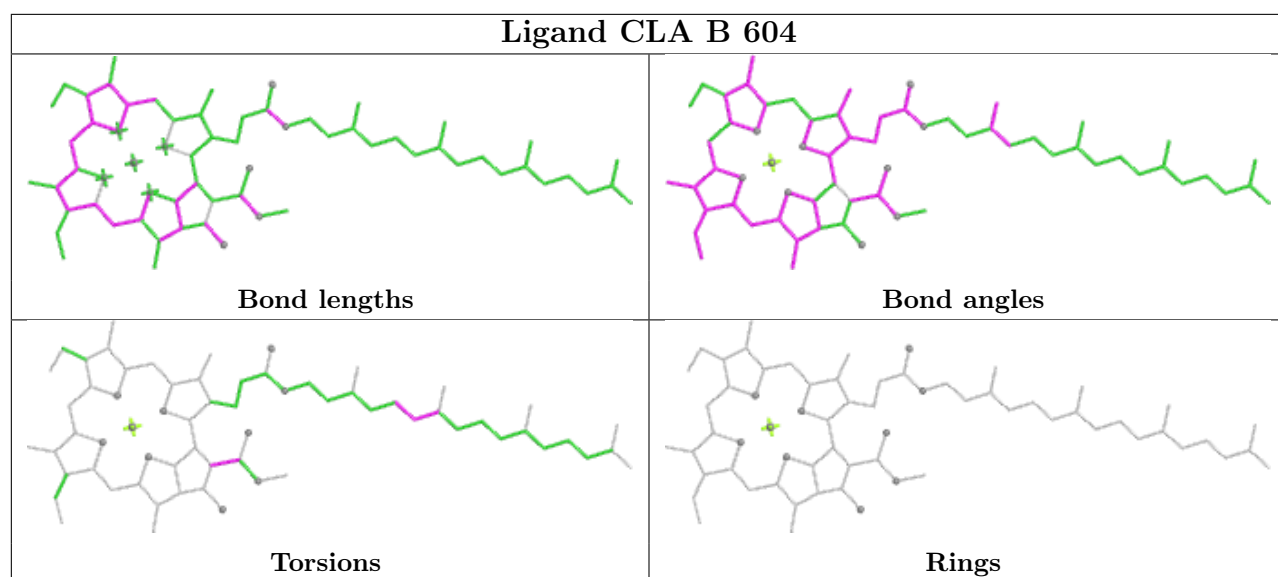


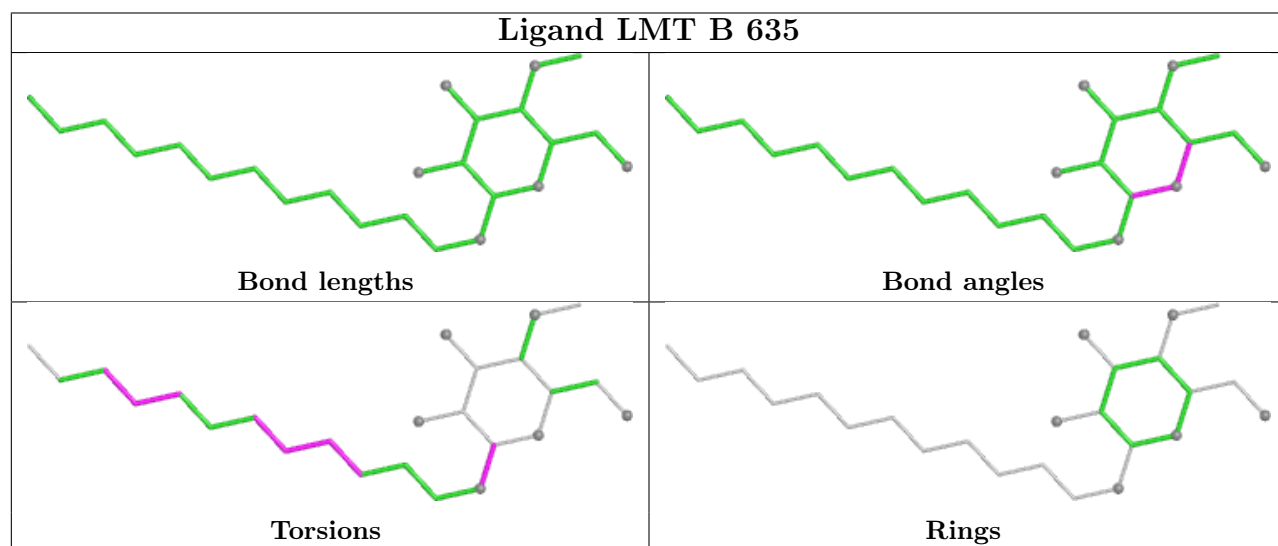
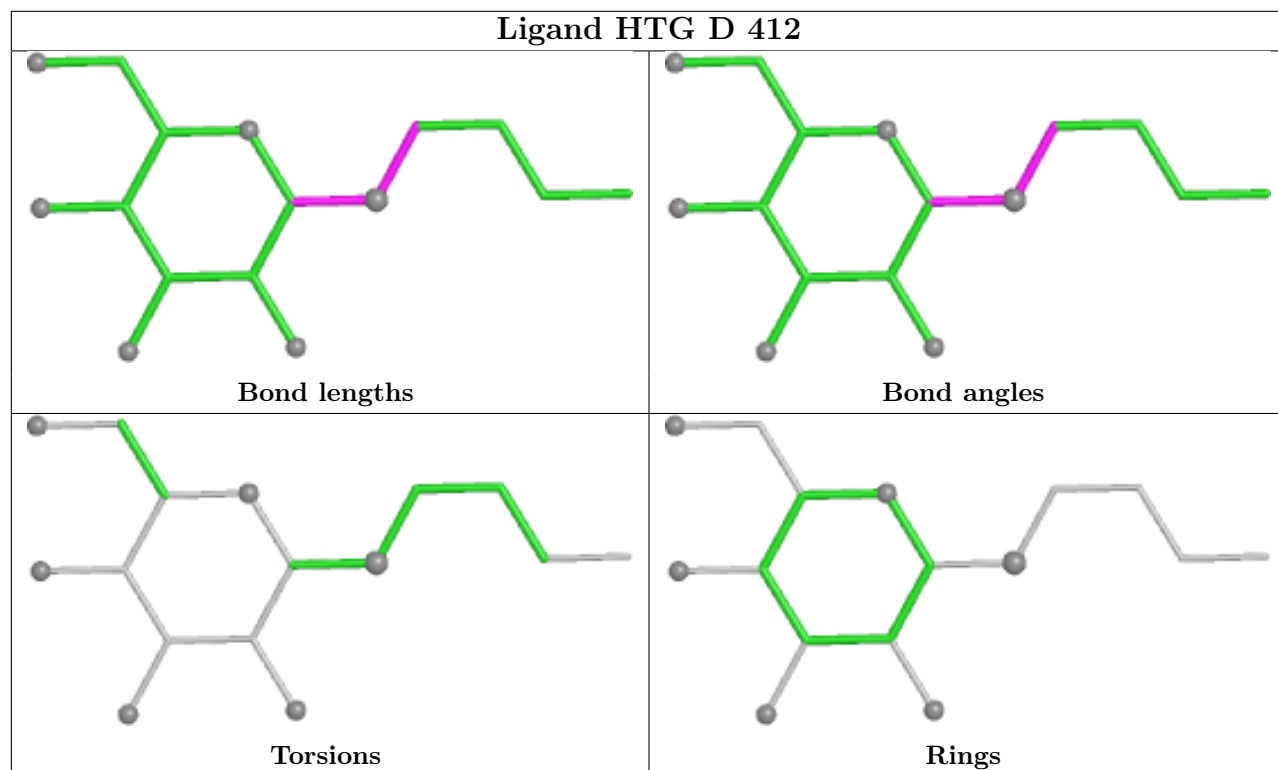


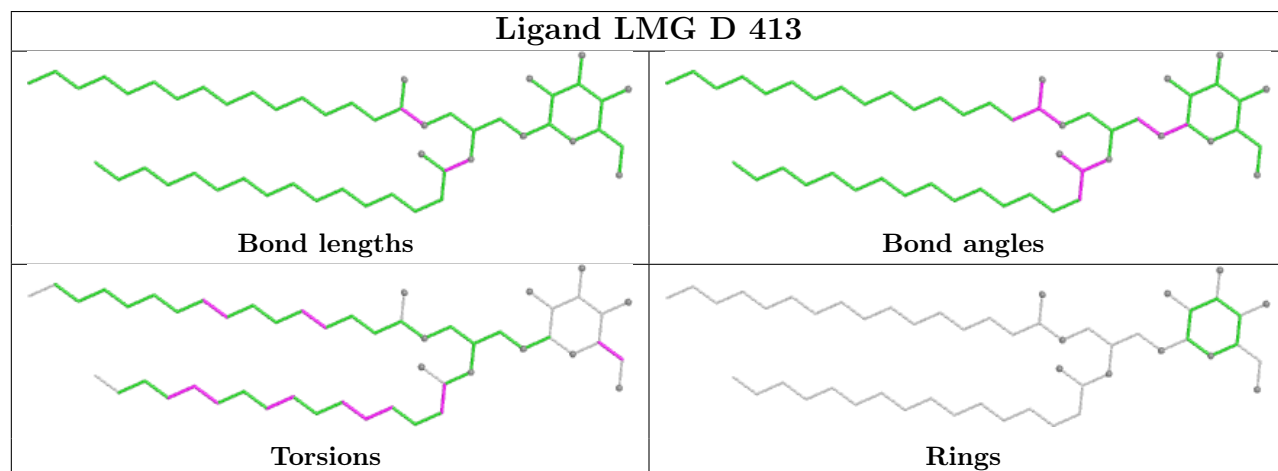
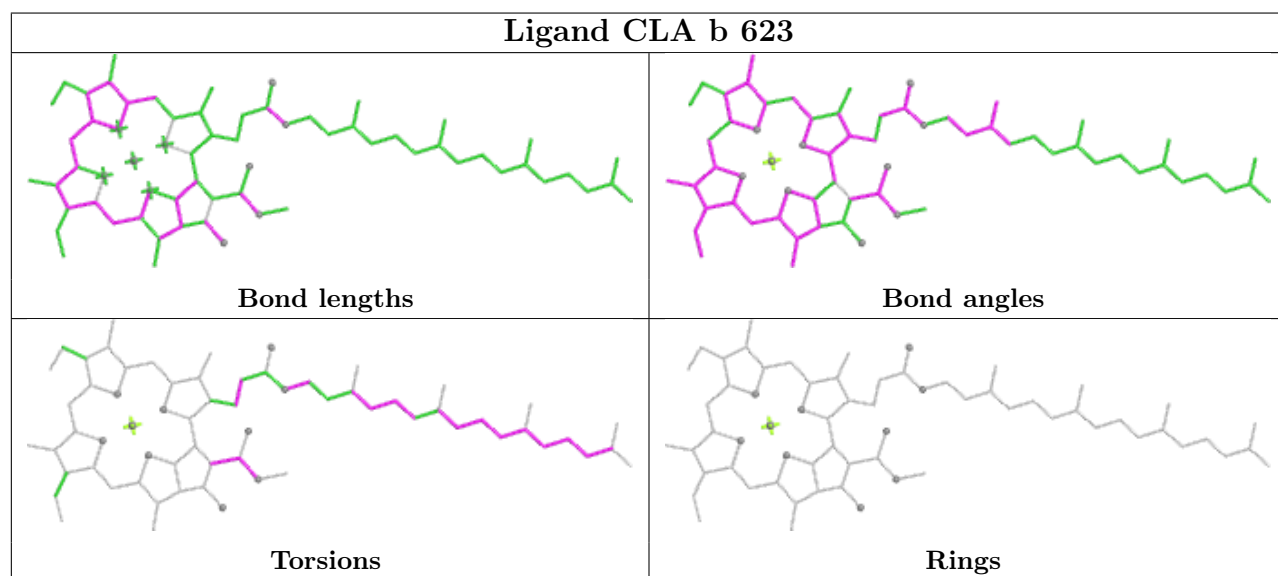
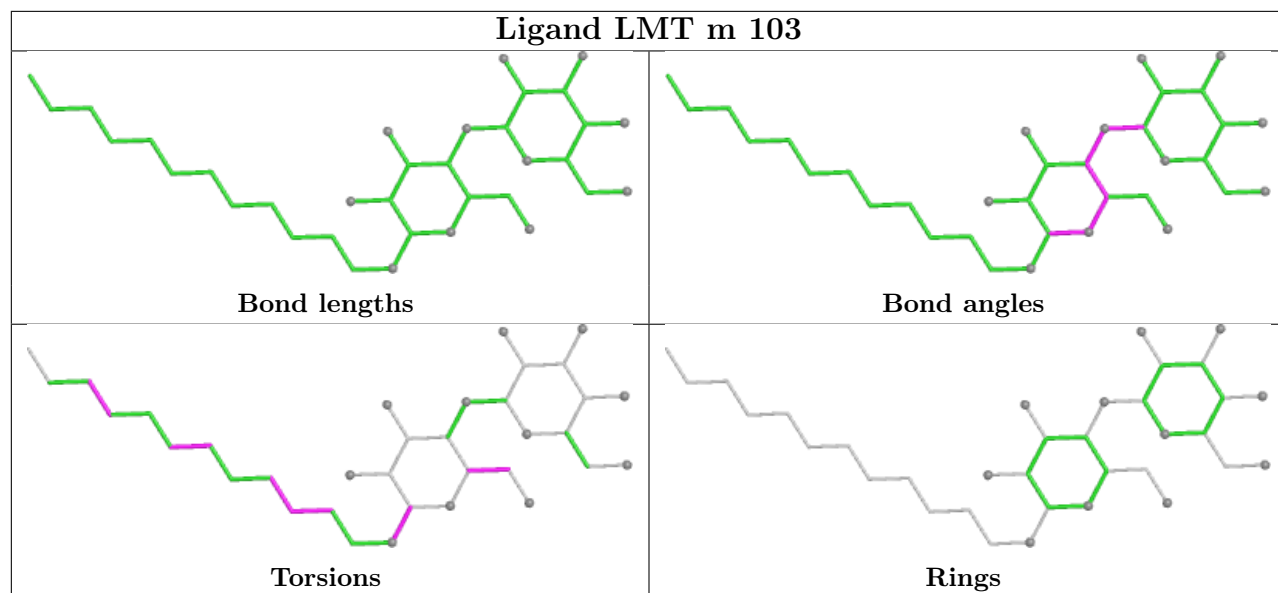


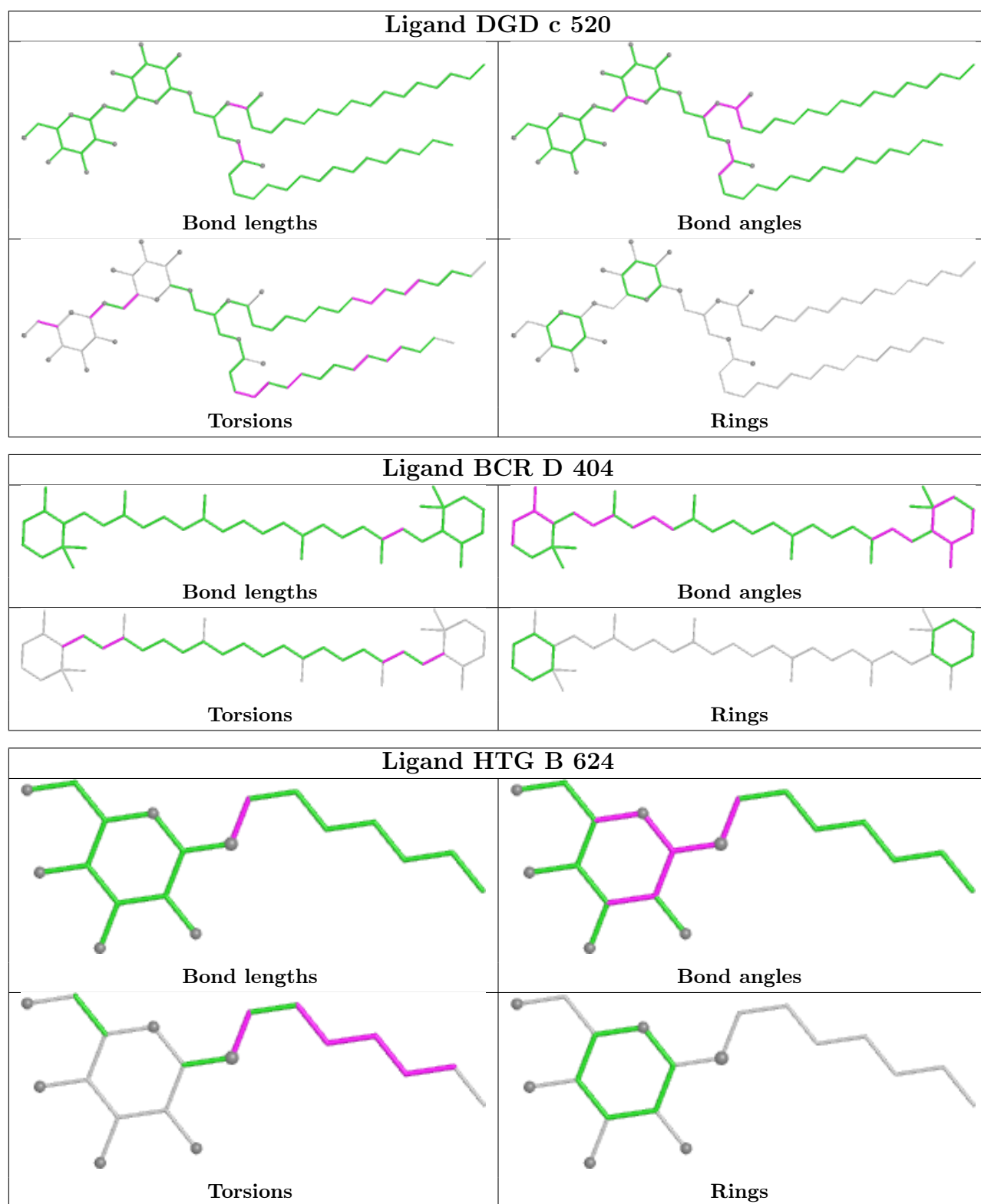




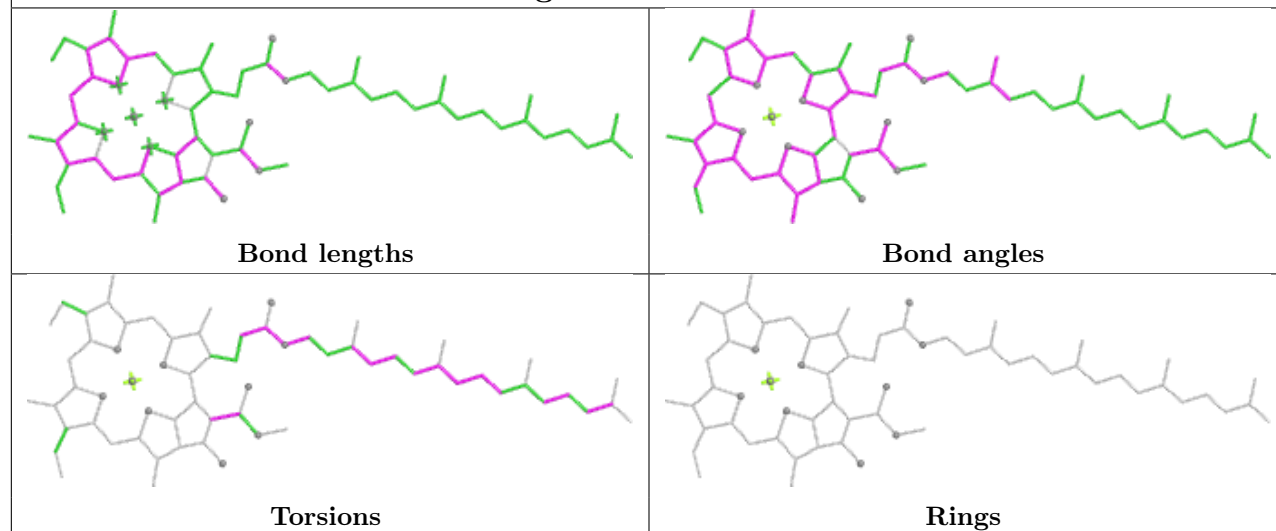




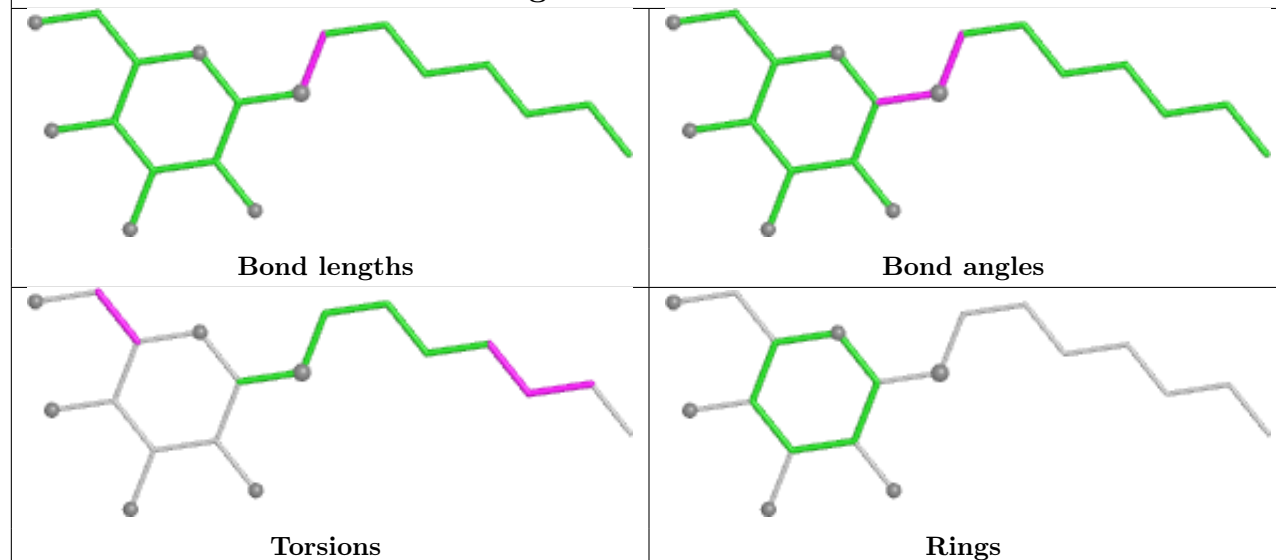




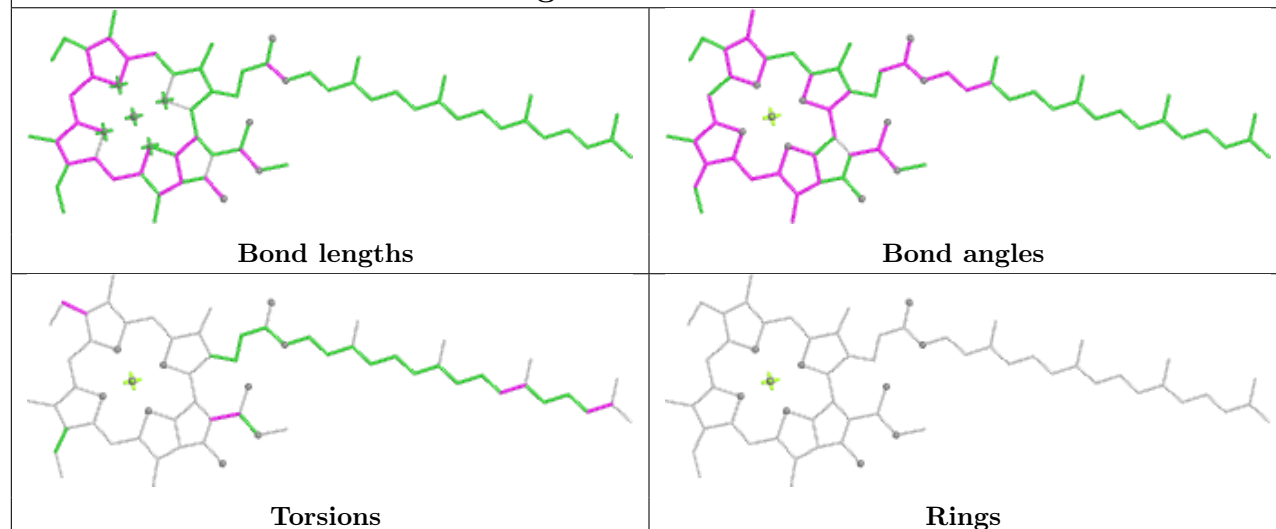
## Ligand CLA b 610



## Ligand HTG B 623

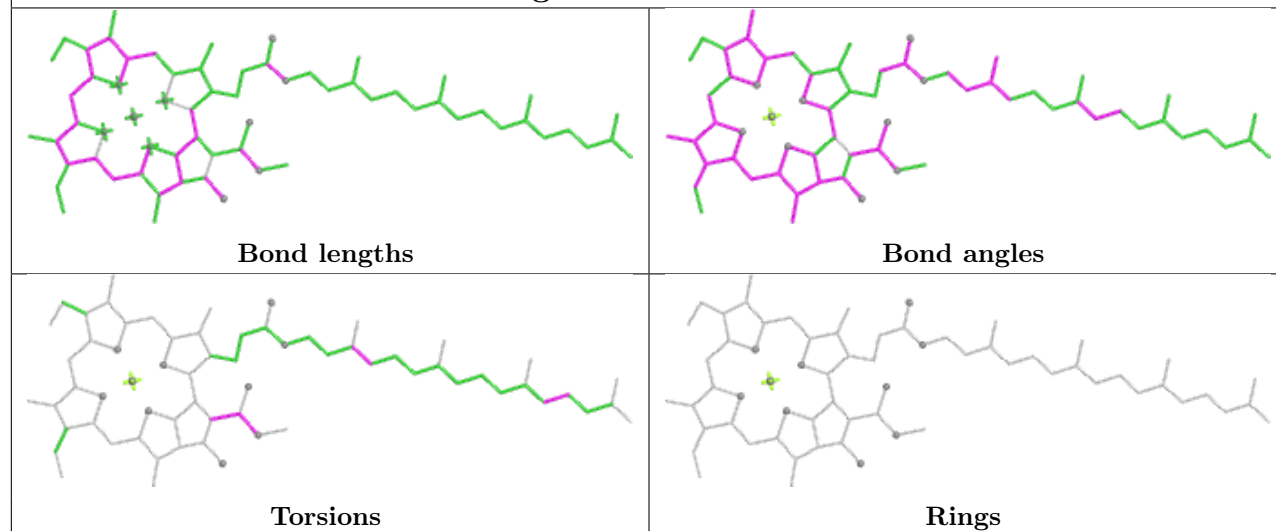


## Ligand CLA c 507

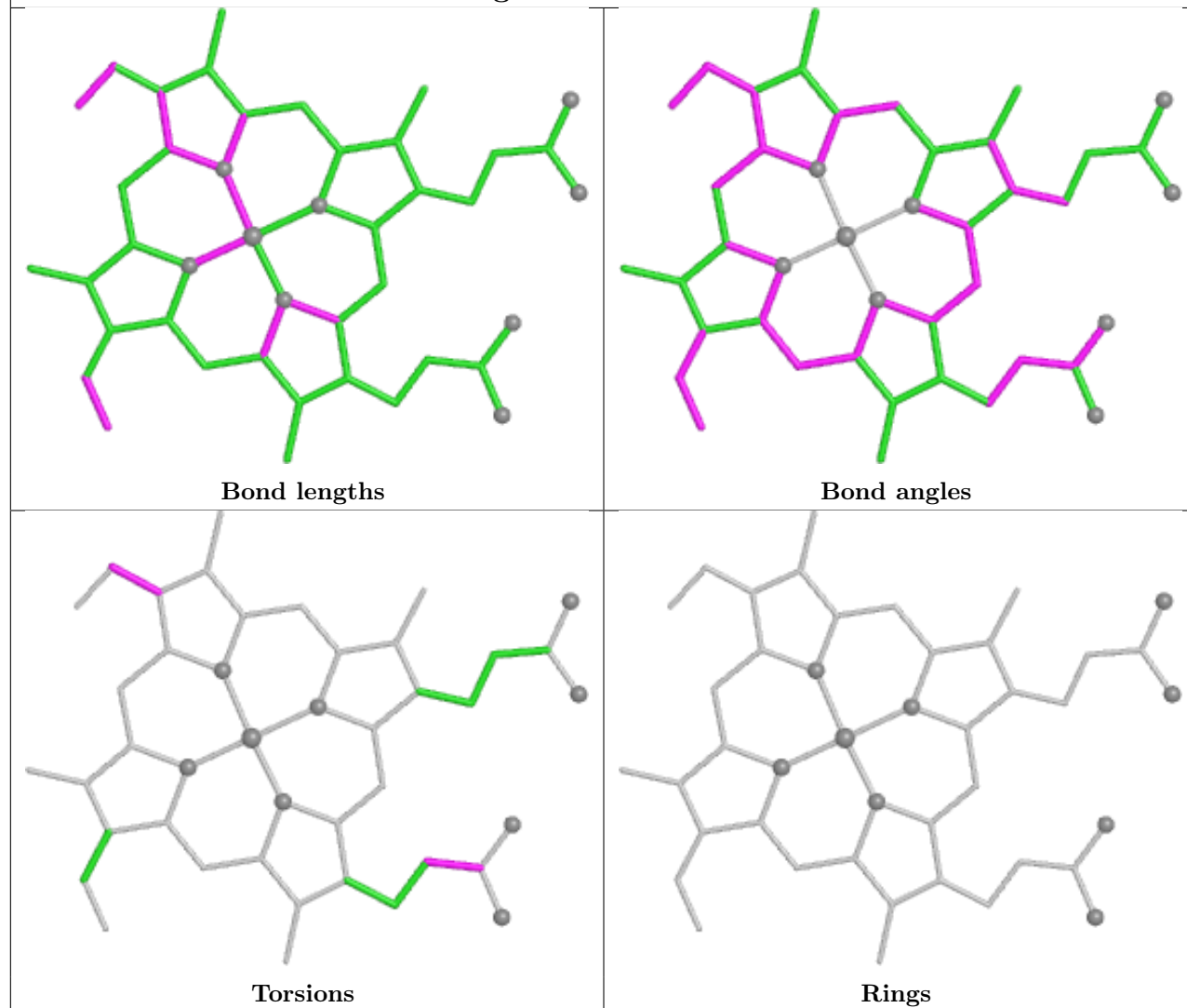


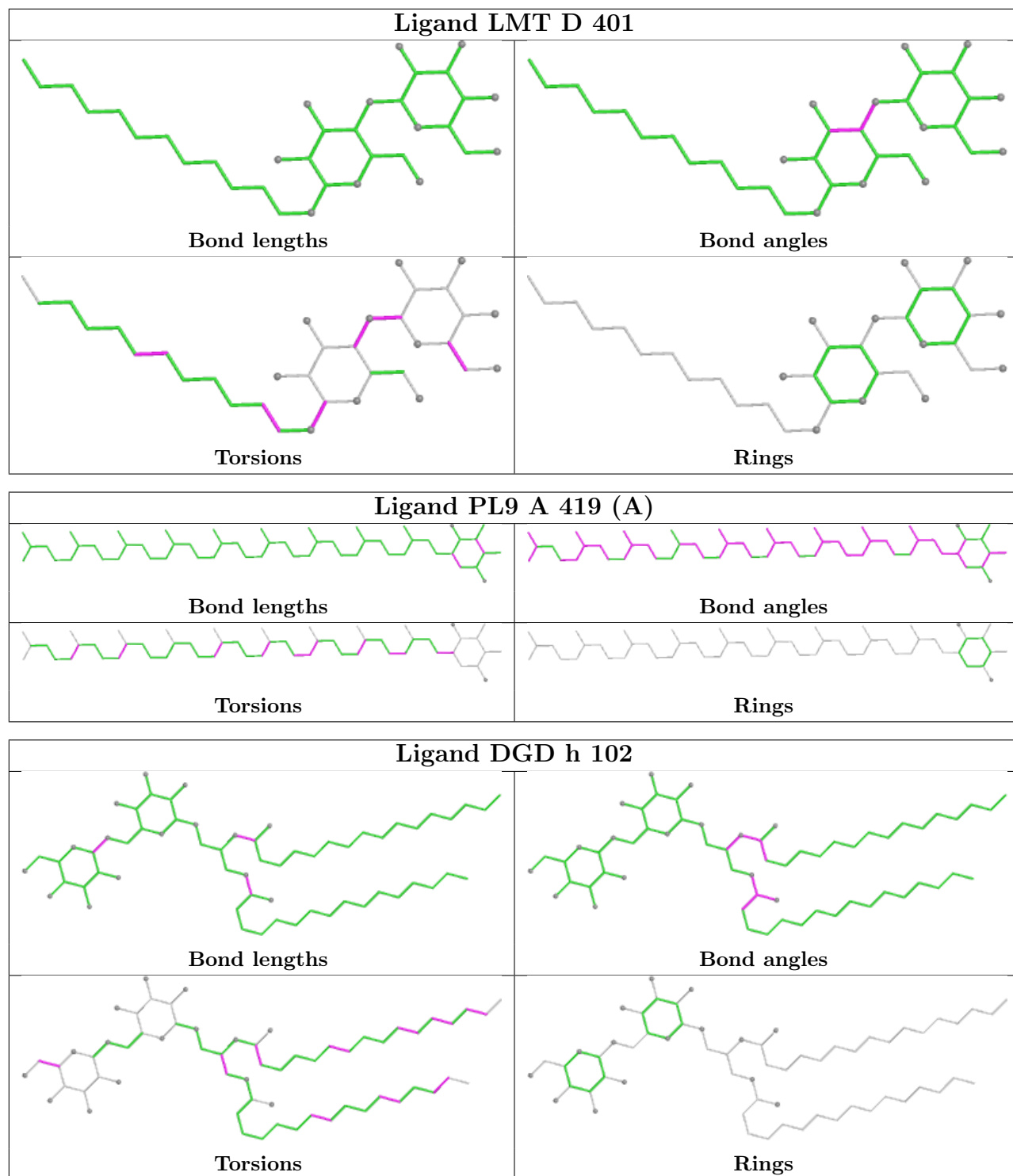


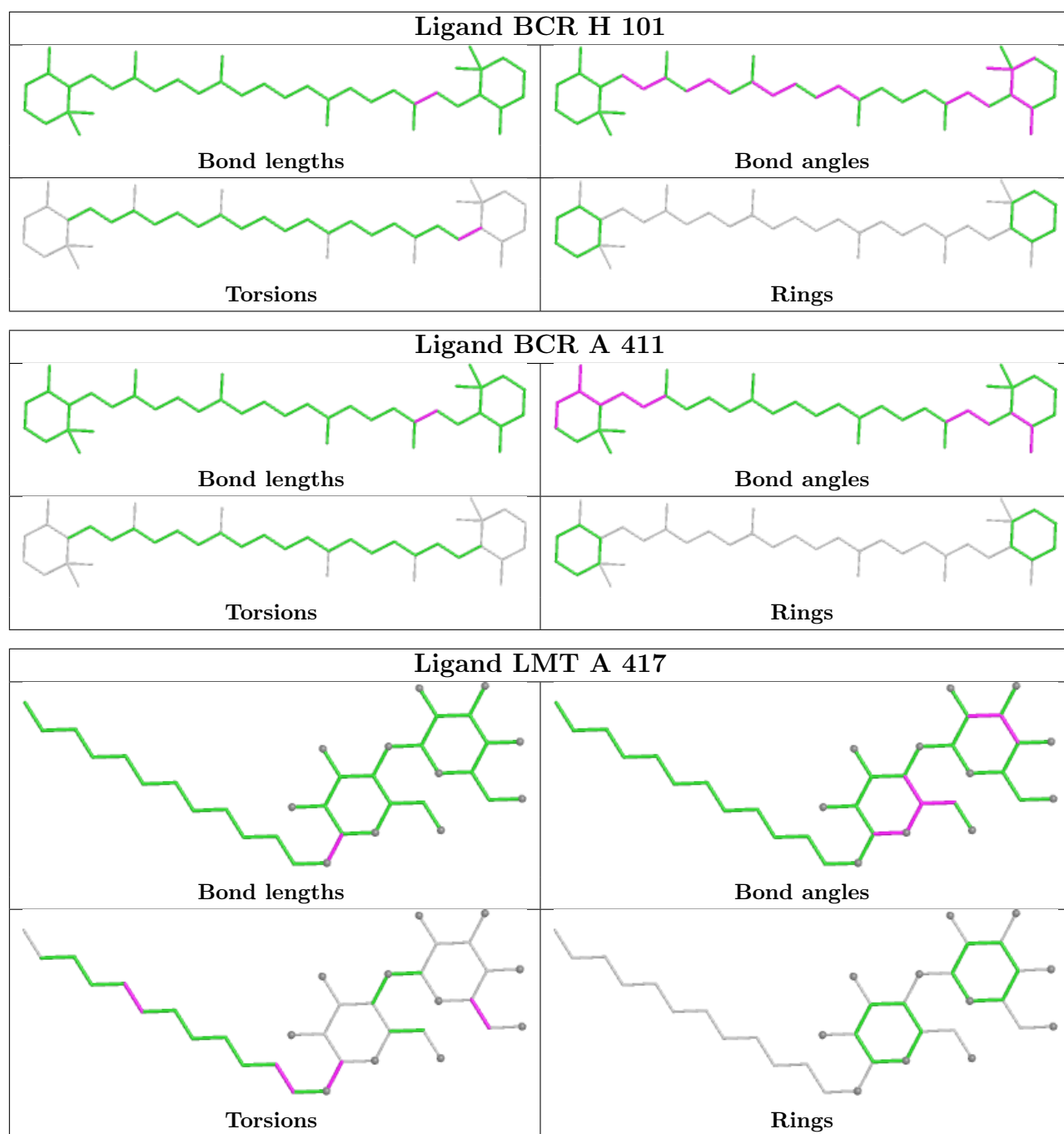
## Ligand CLA B 605

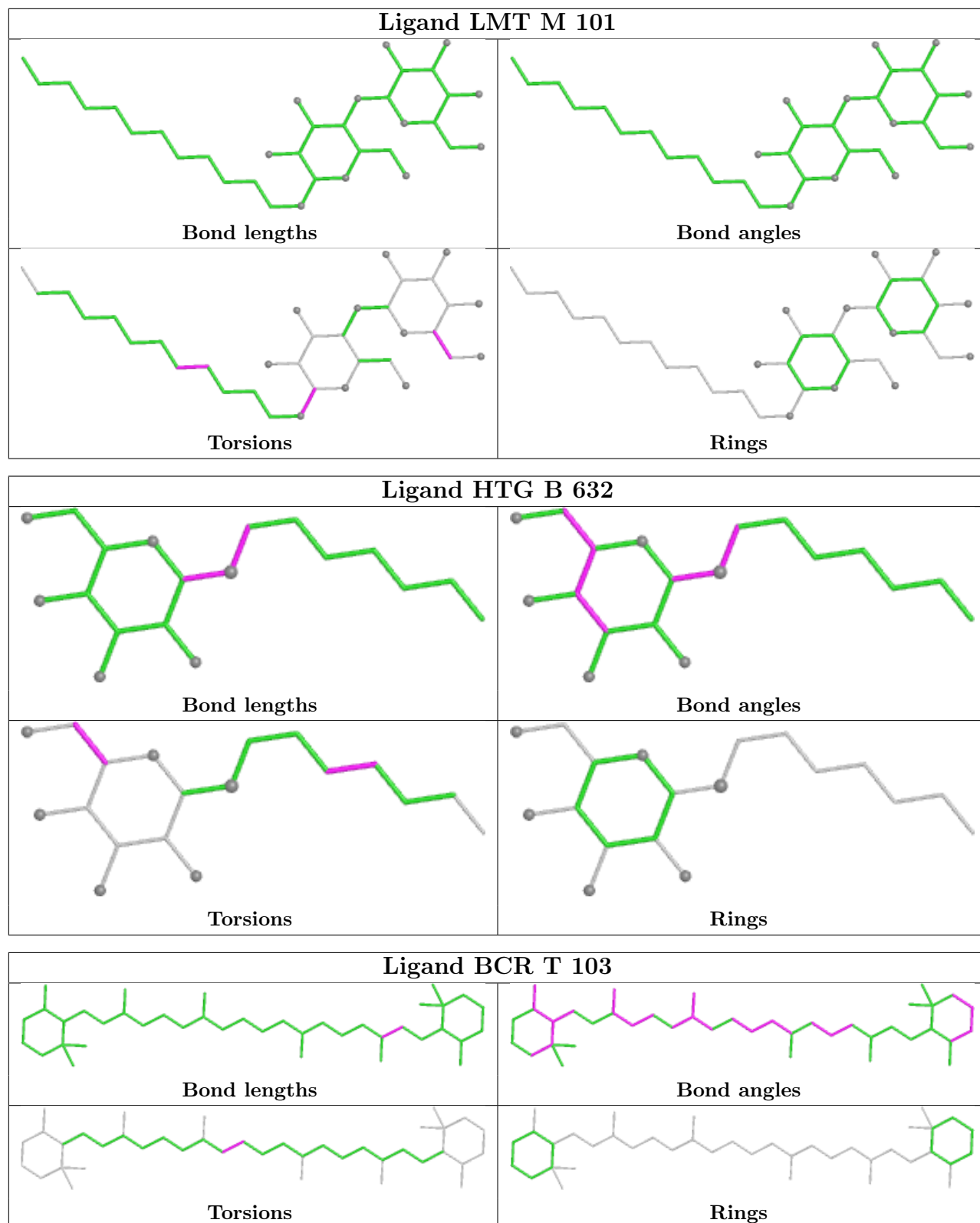


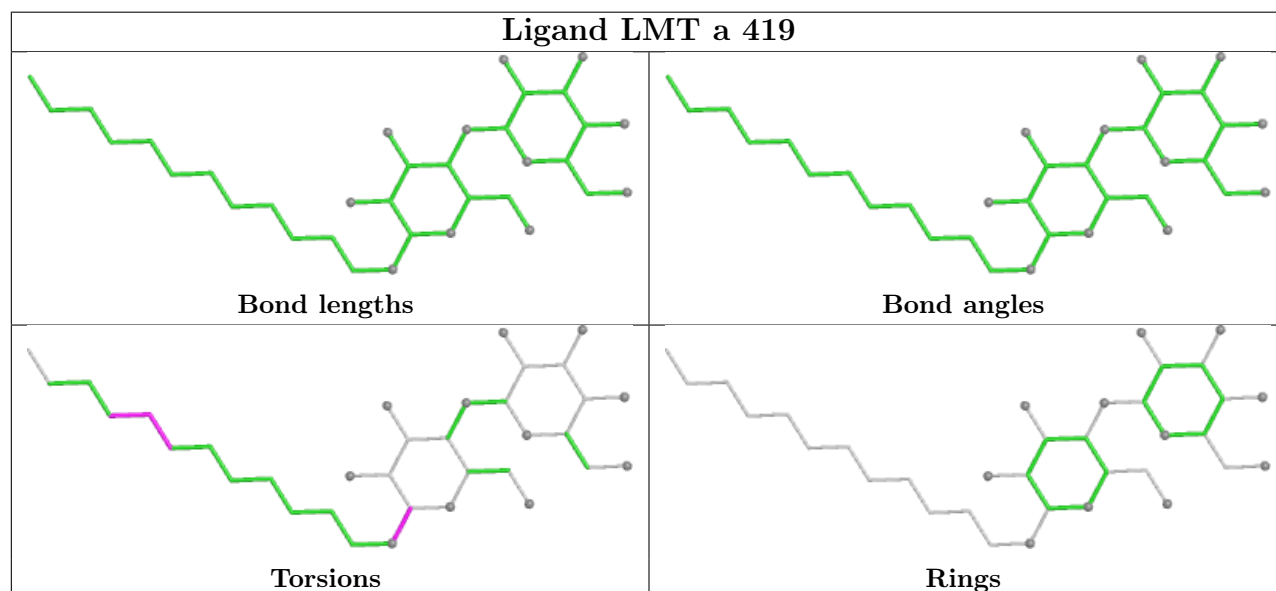
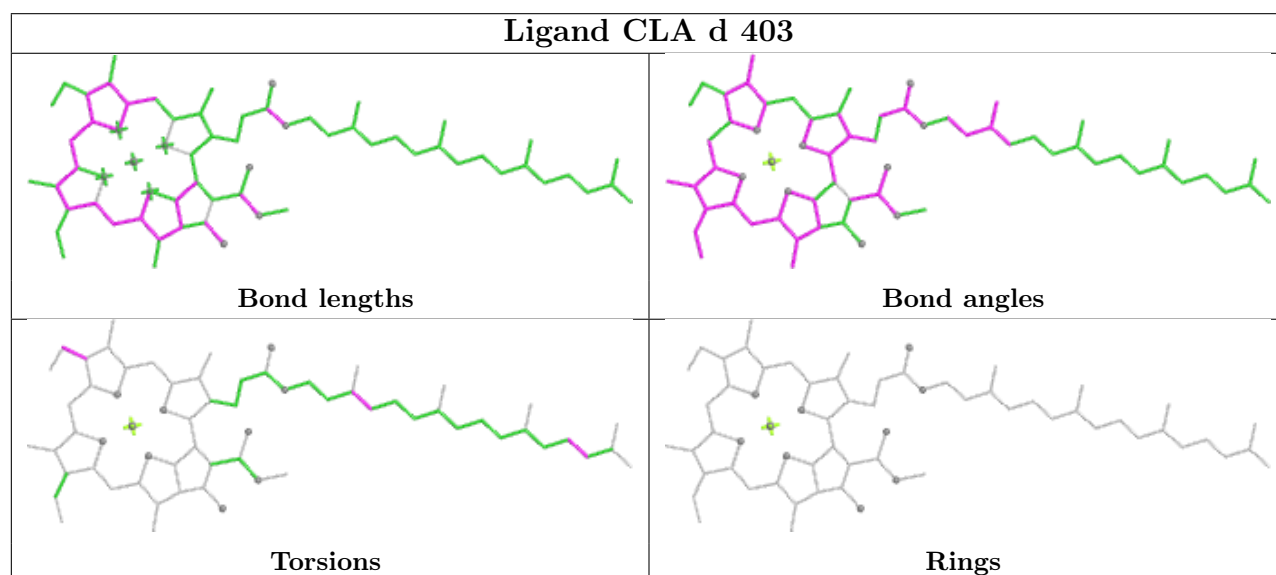
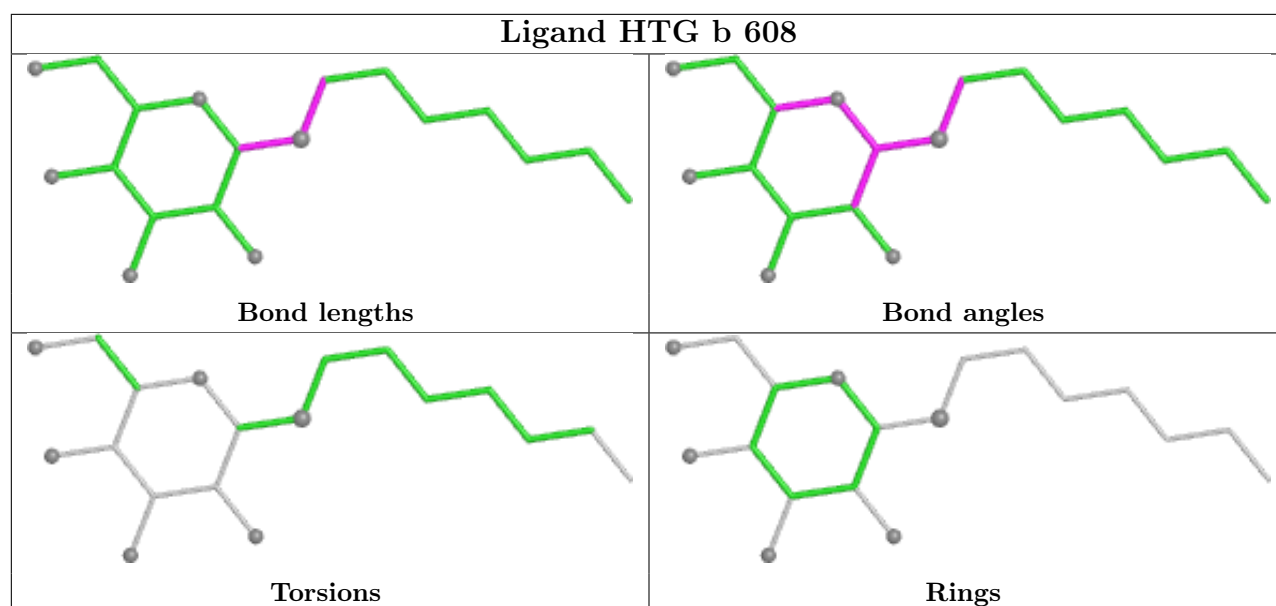
## Ligand HEC V 205



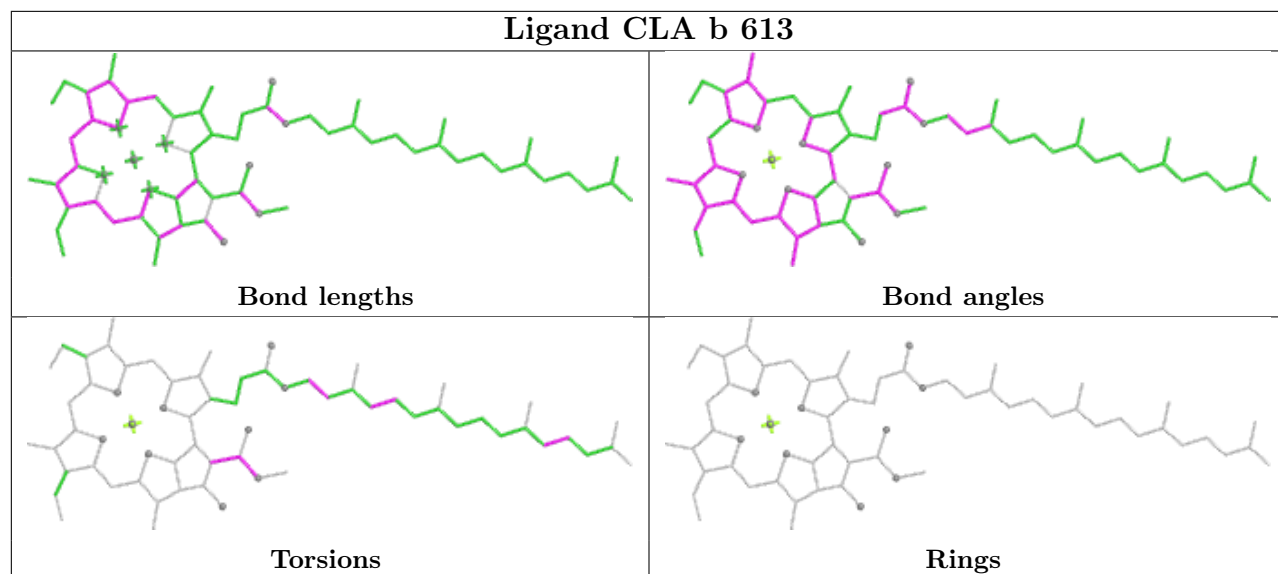




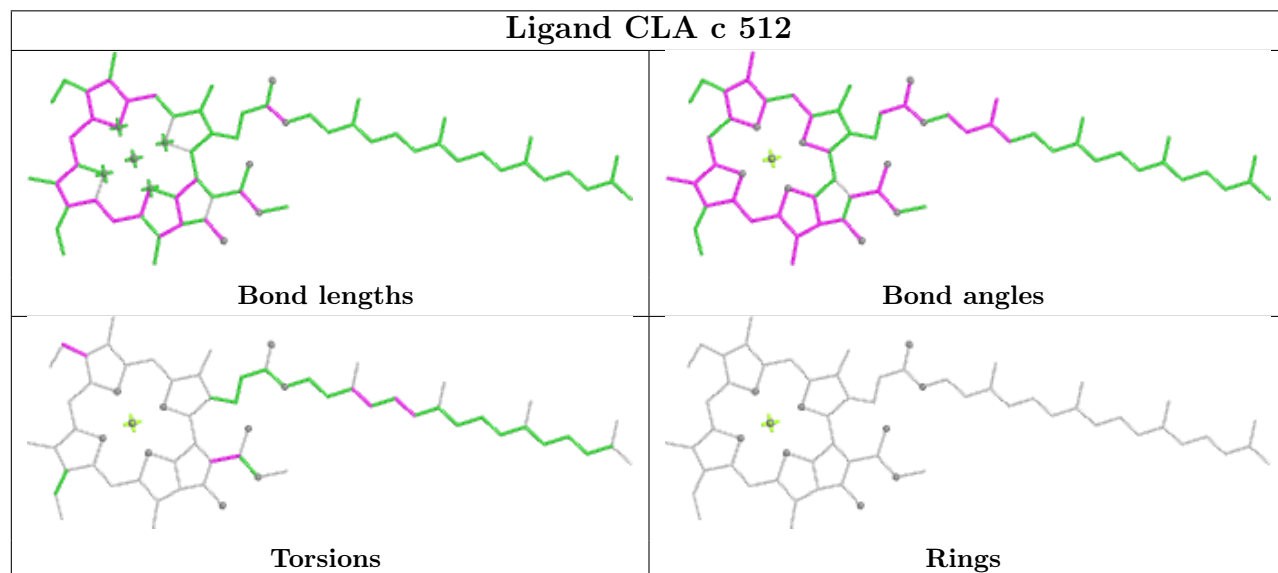




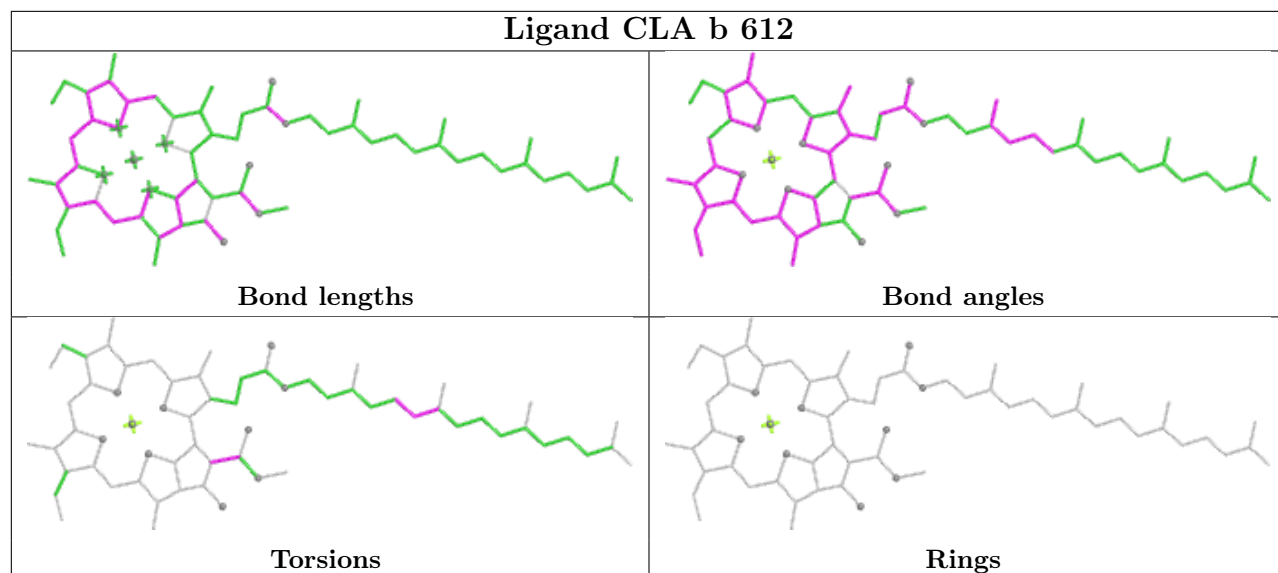
## Ligand CLA b 613



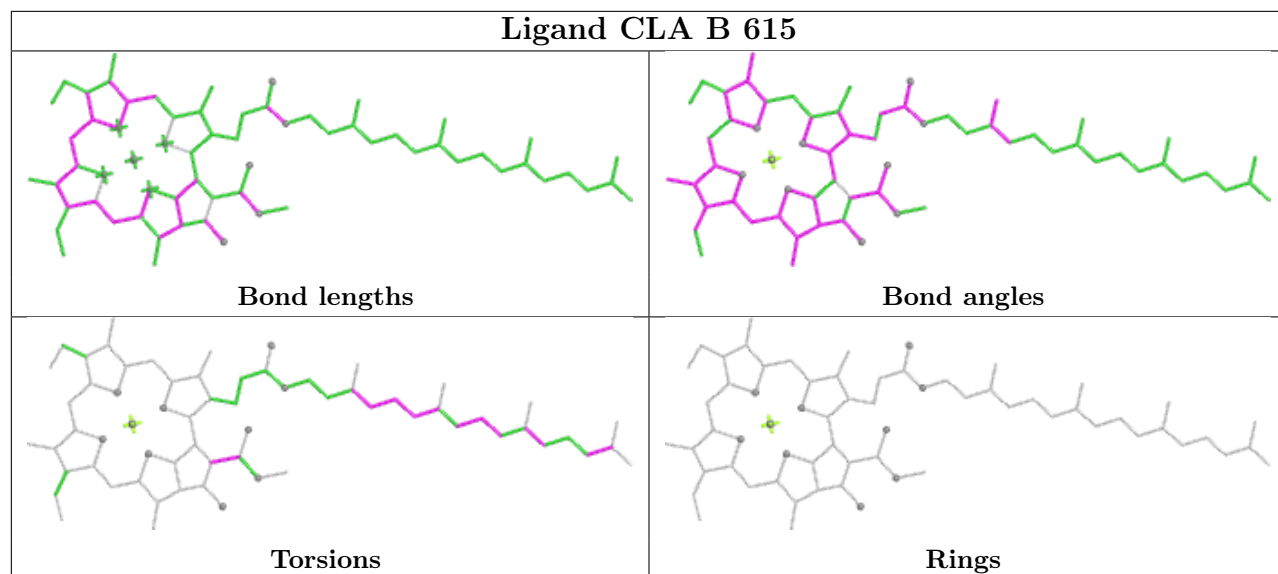
## Ligand CLA c 512



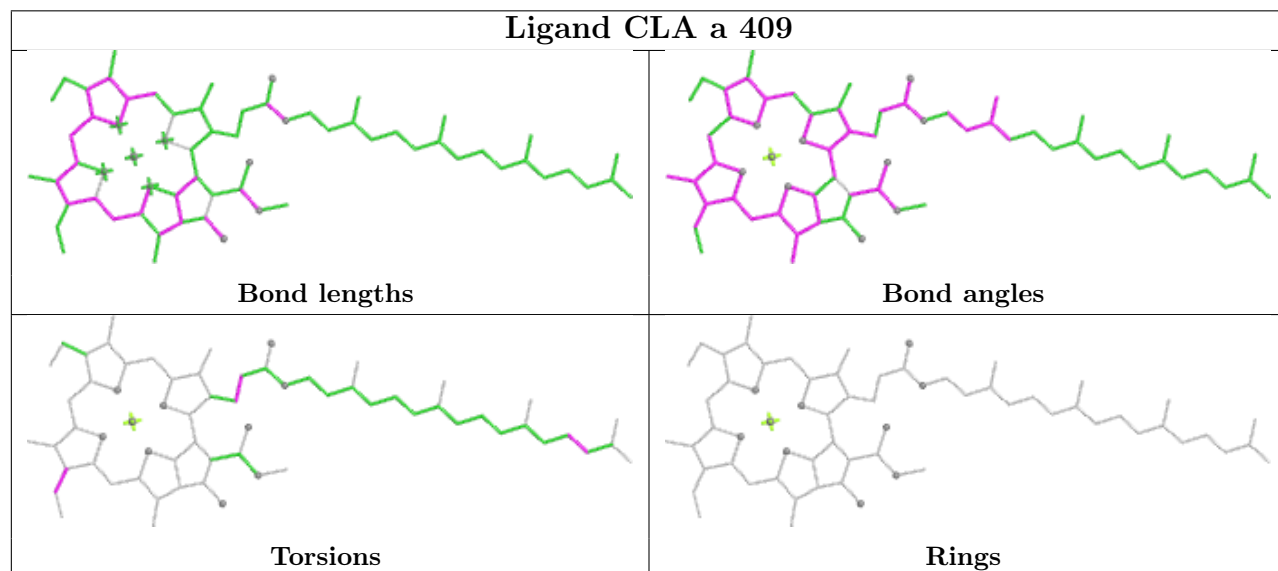
## Ligand CLA b 612



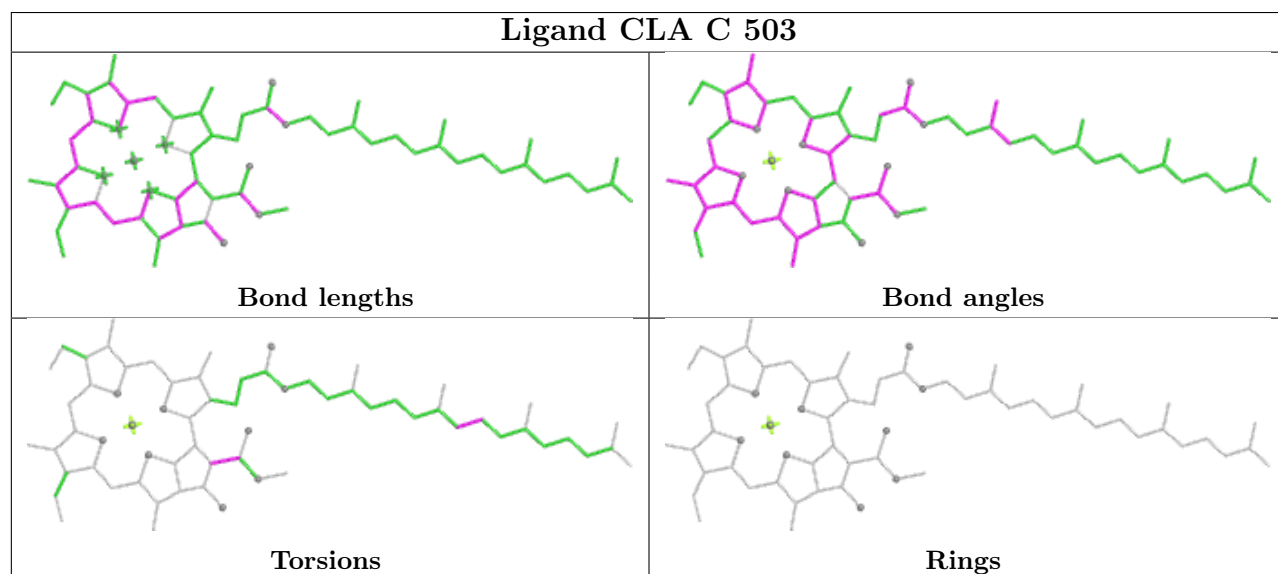
## Ligand CLA B 615



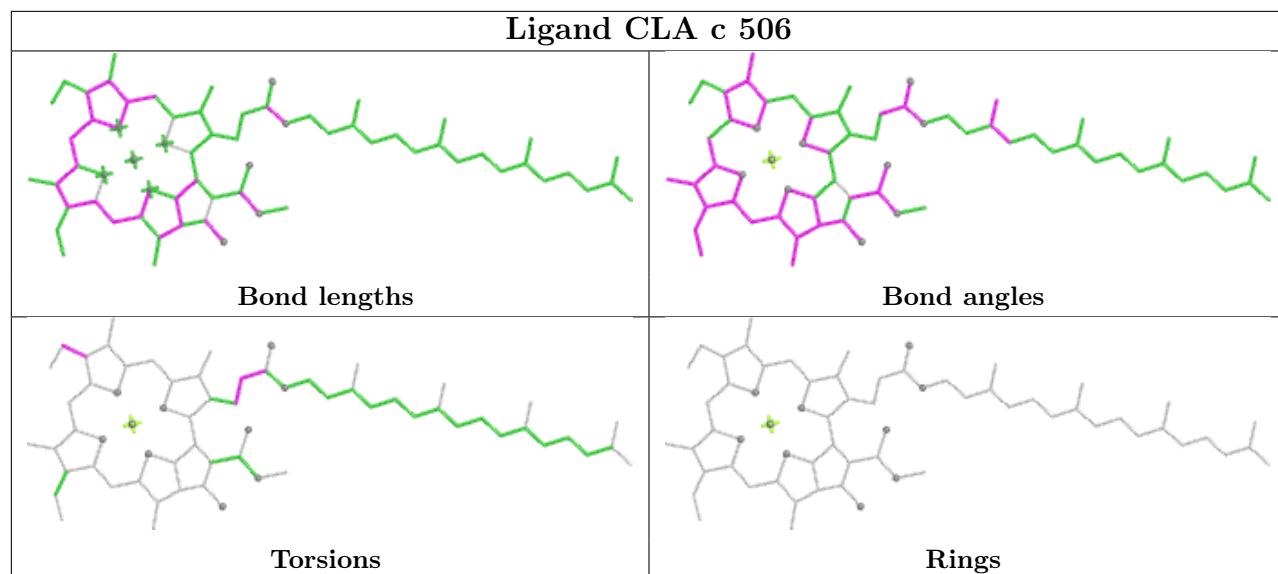
## Ligand CLA a 409



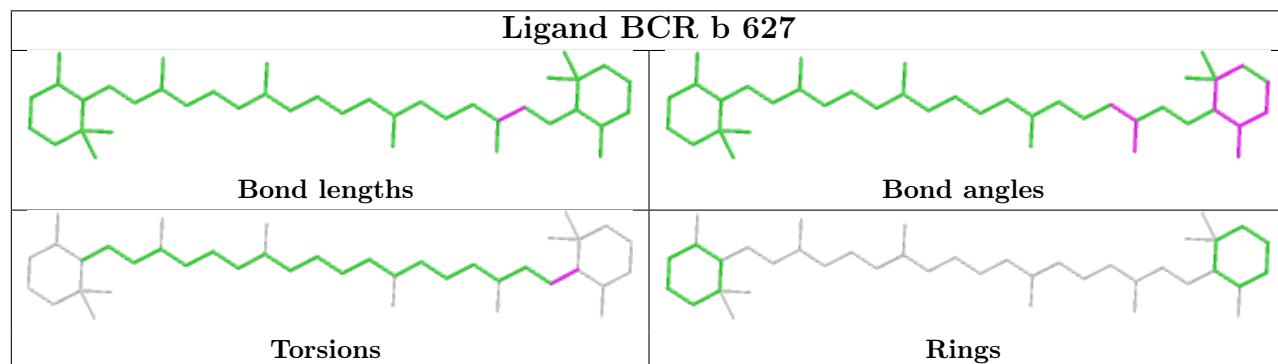
## Ligand CLA C 503



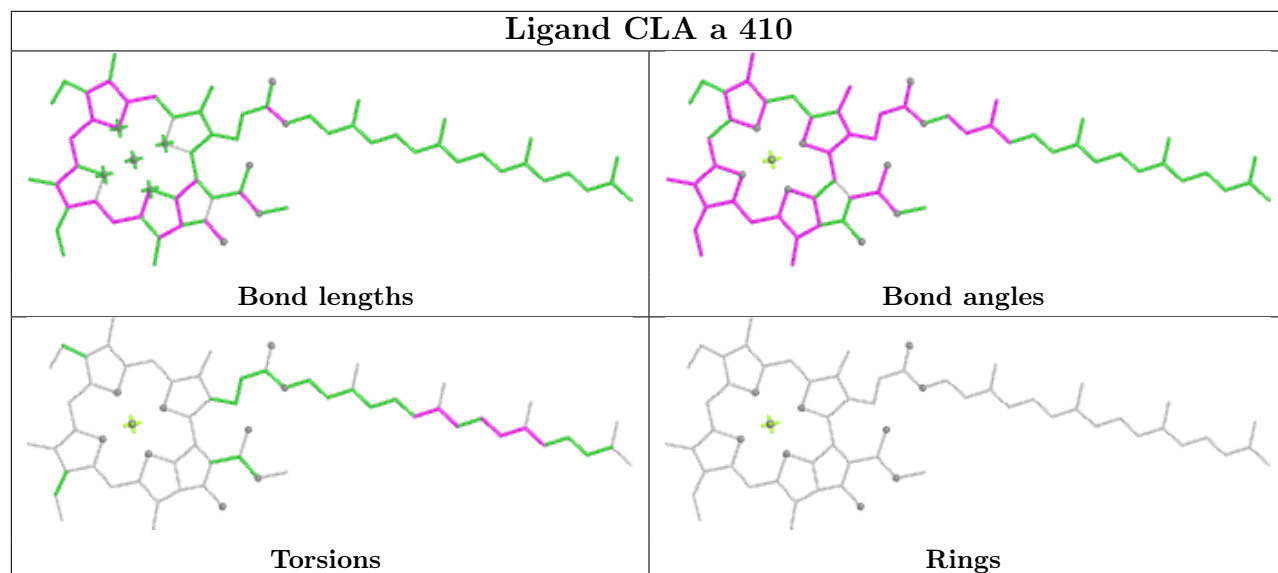
## Ligand CLA c 506



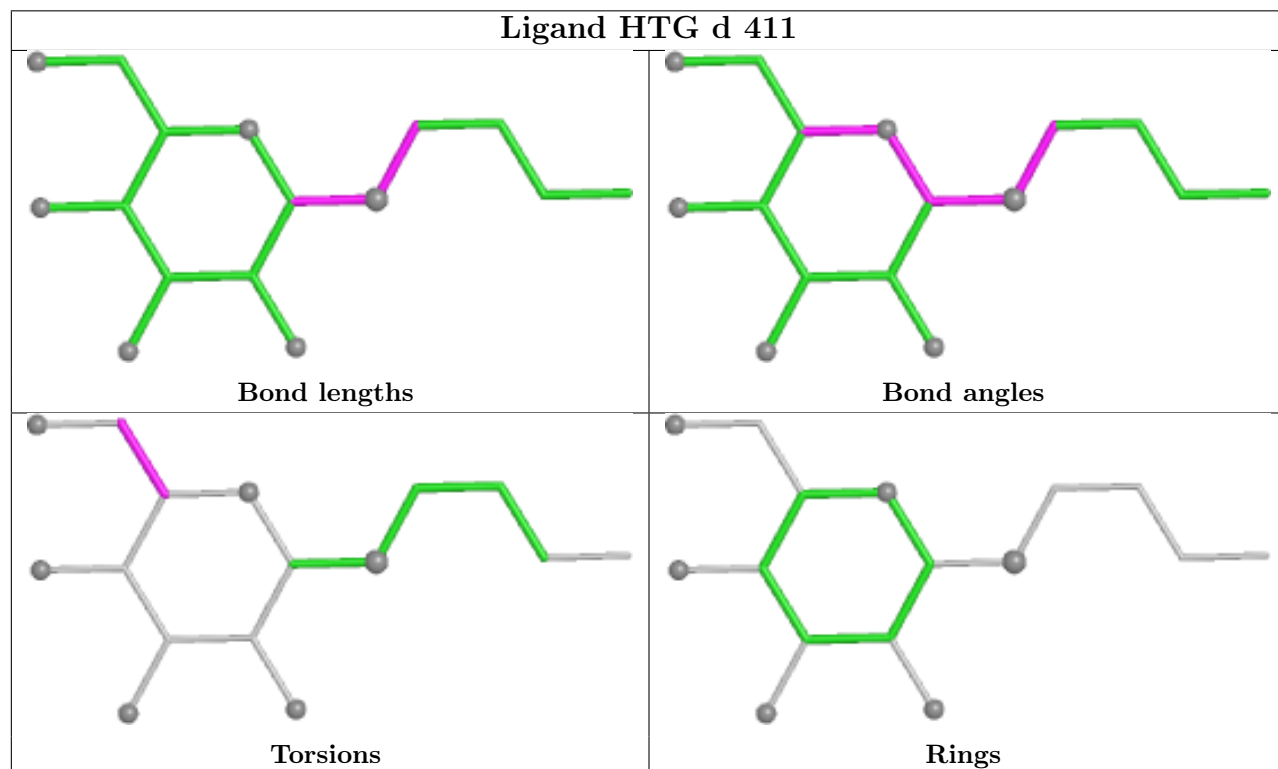
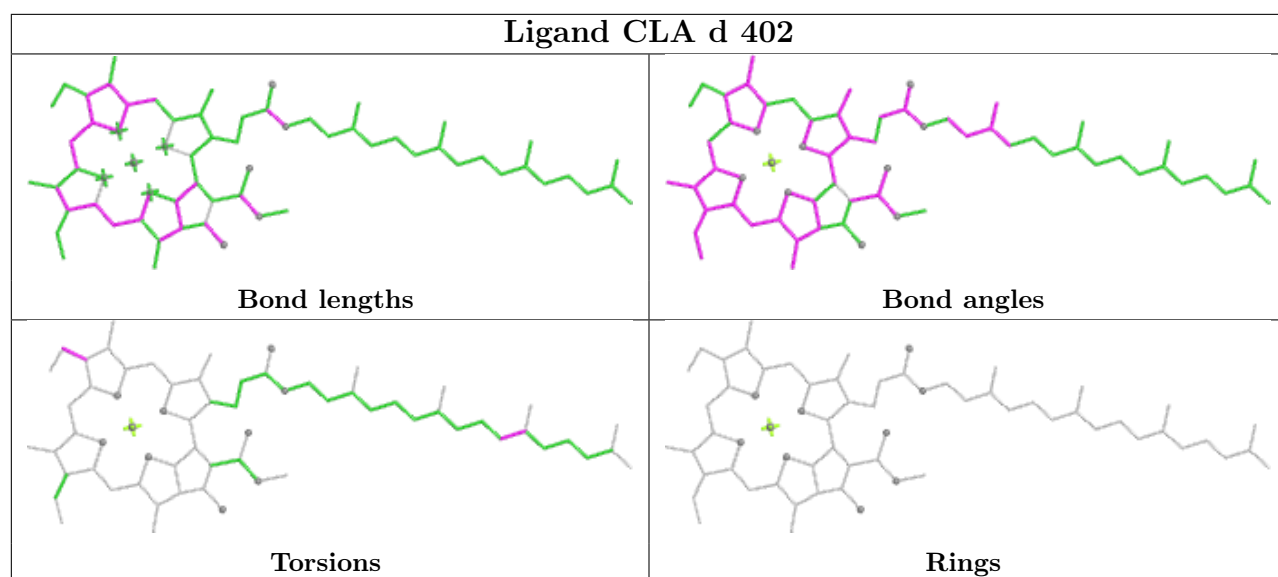
## Ligand BCR b 627

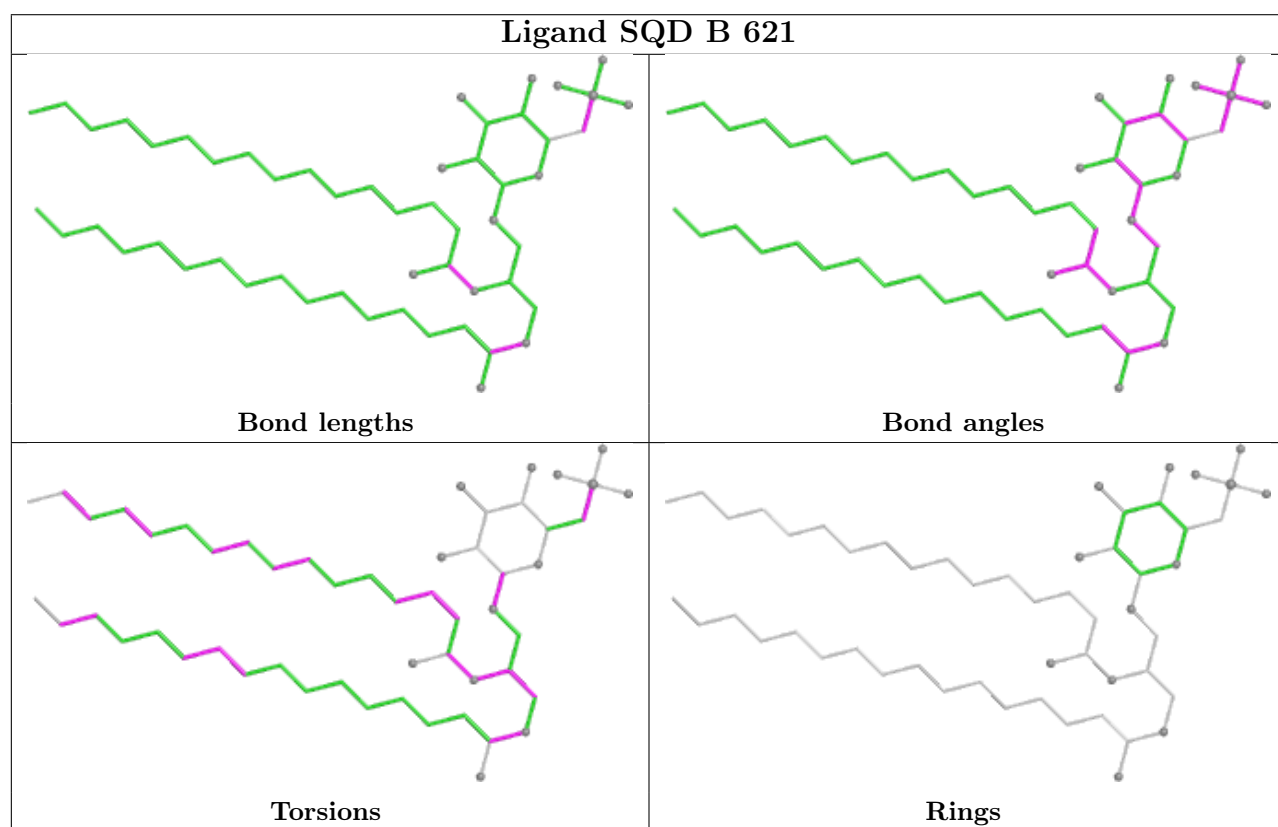
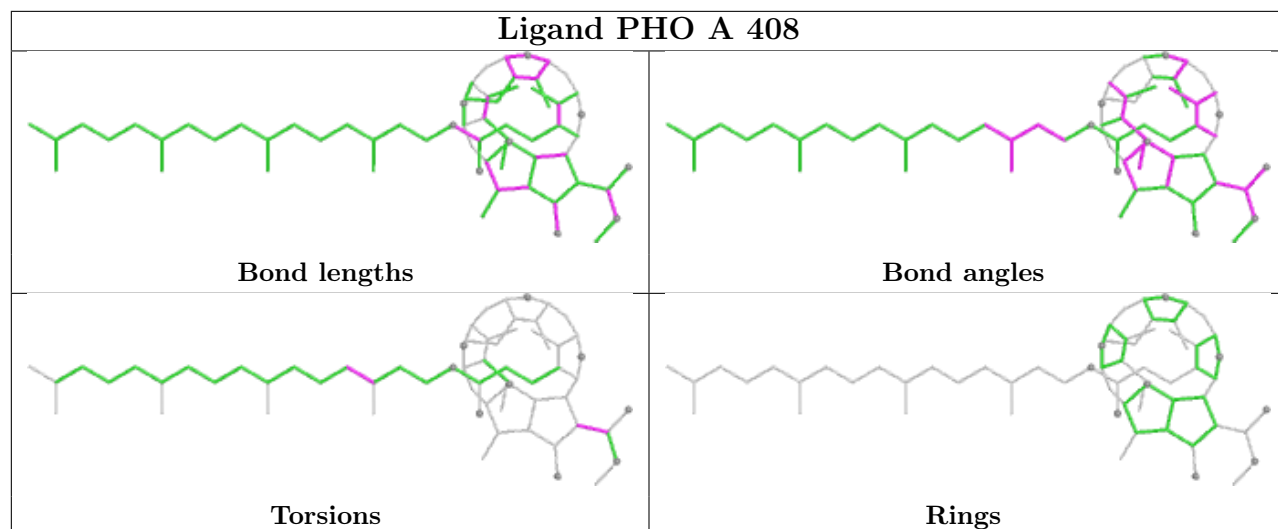


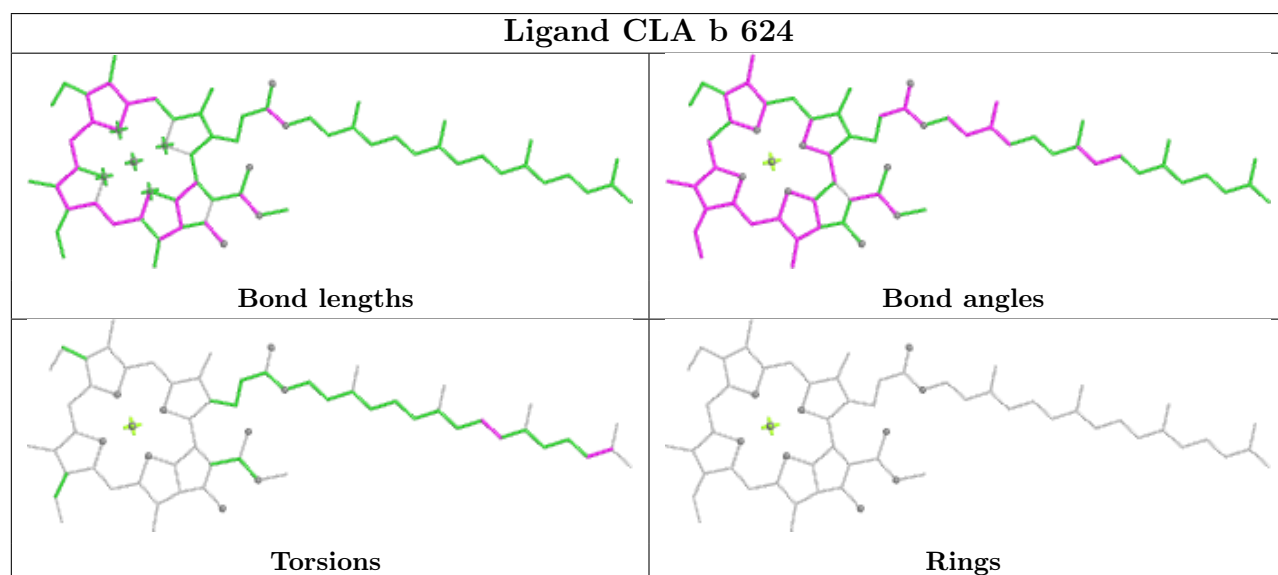
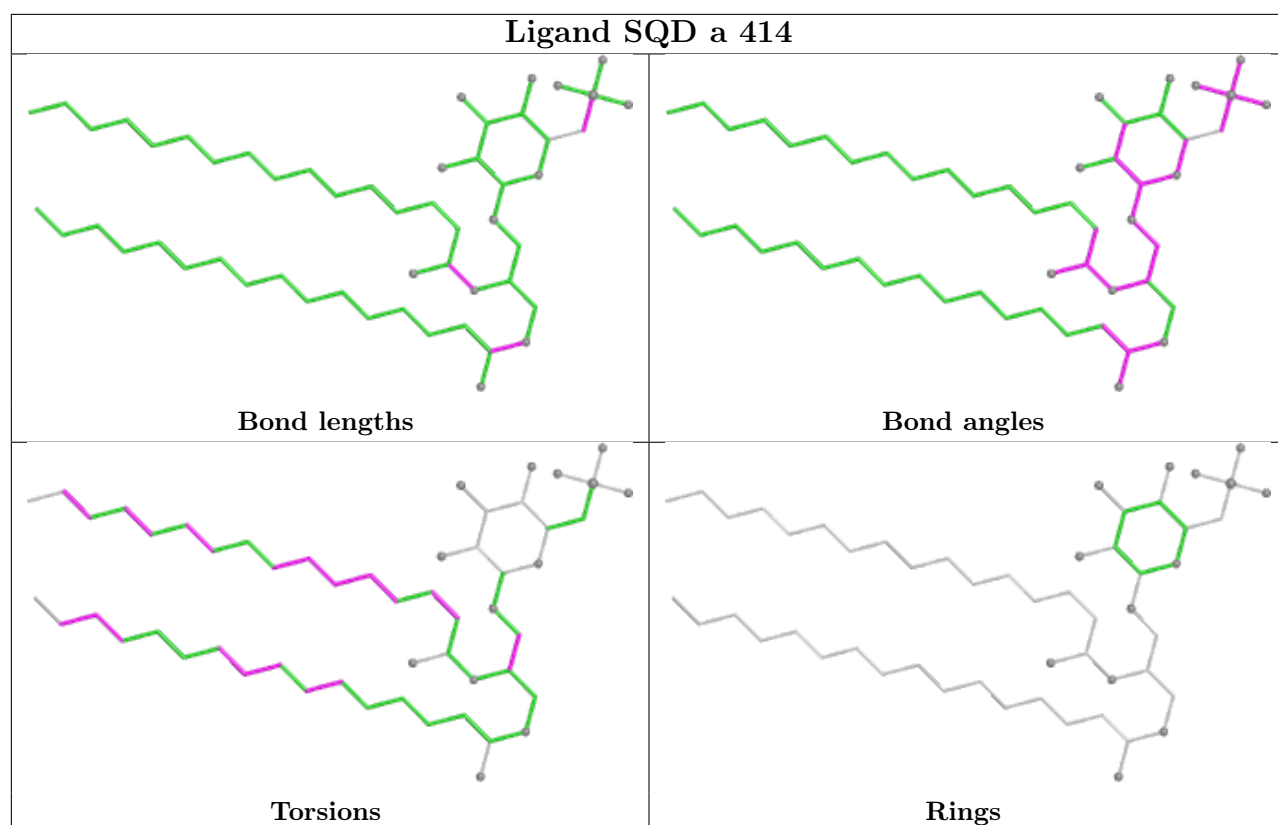
## Ligand CLA a 410

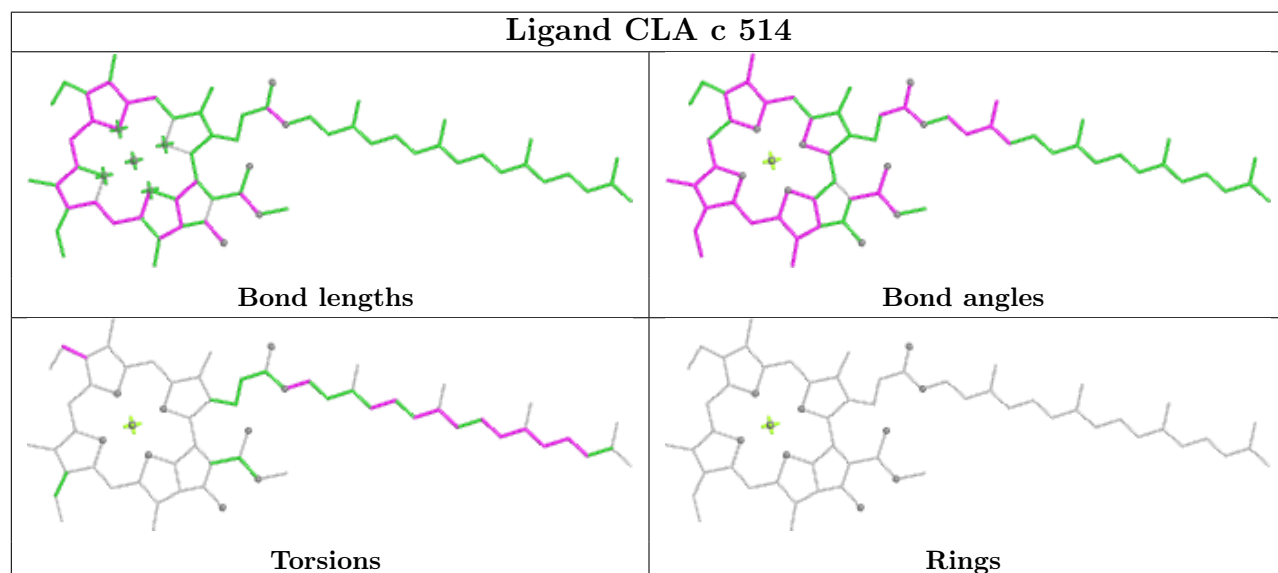
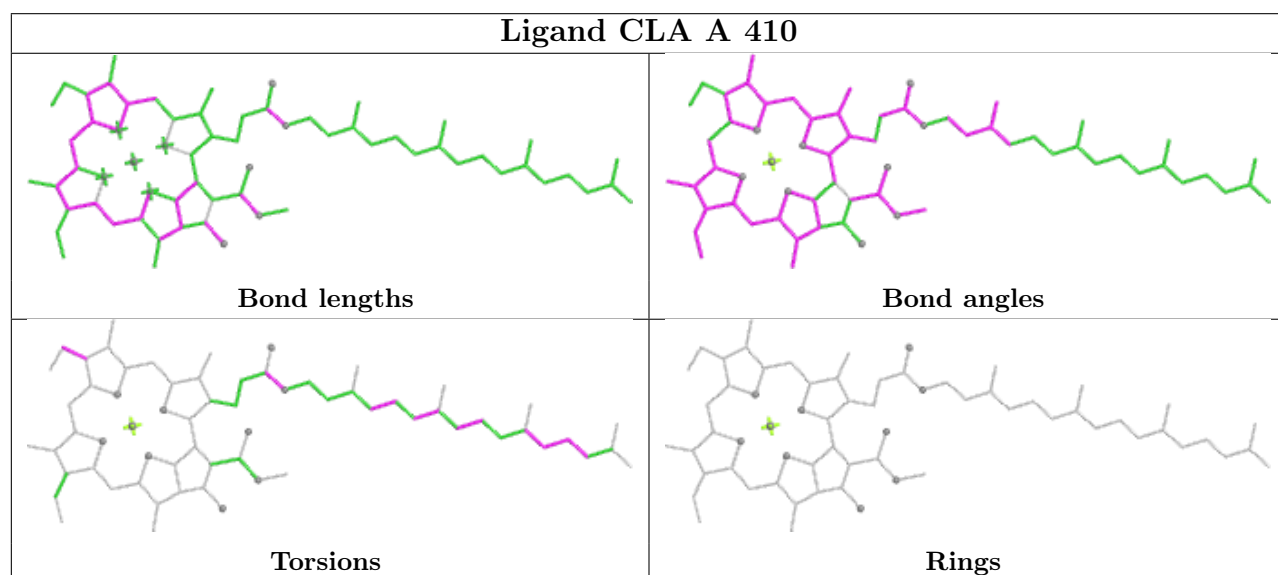
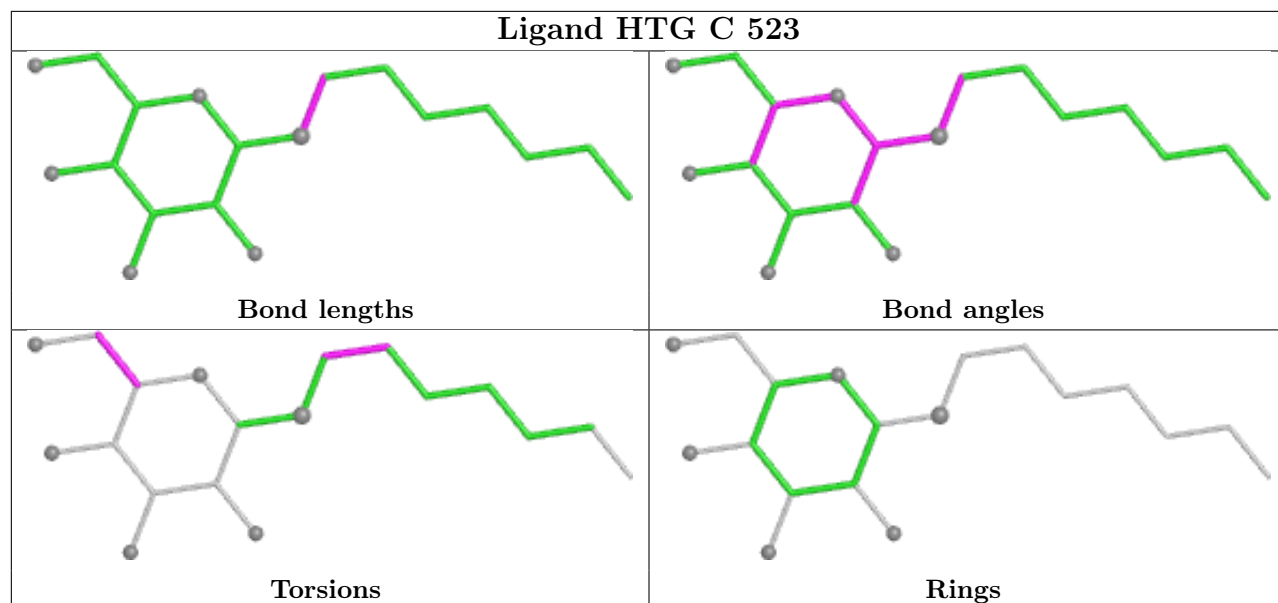


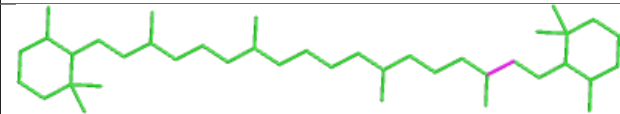
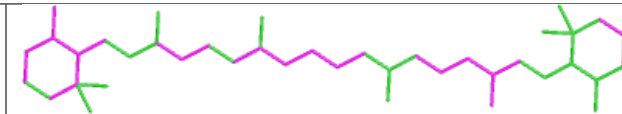
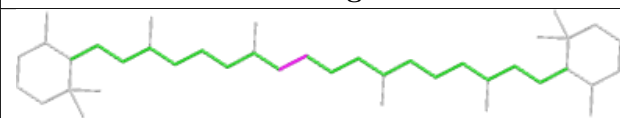
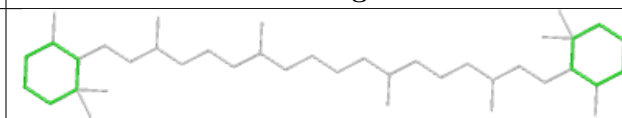
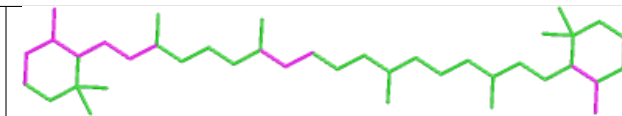
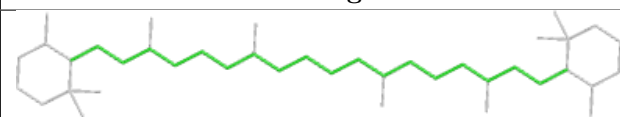
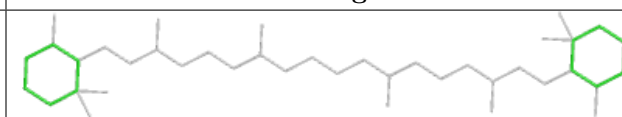
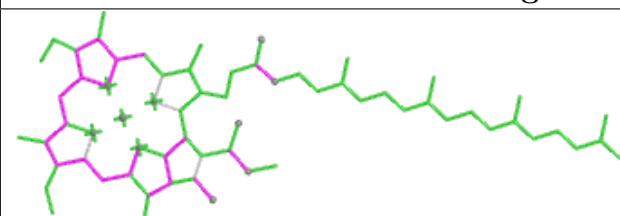
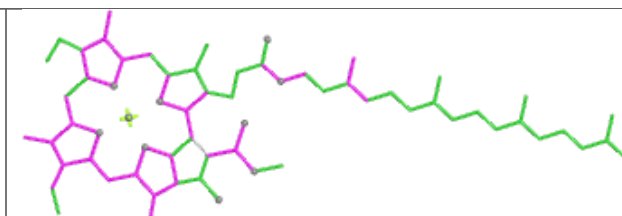
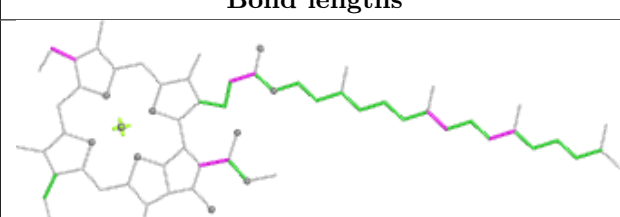
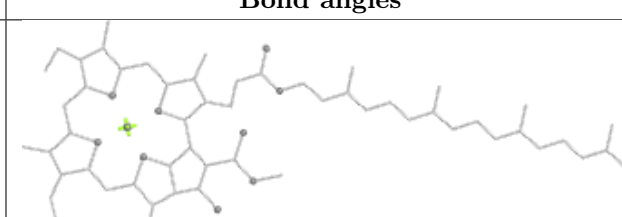
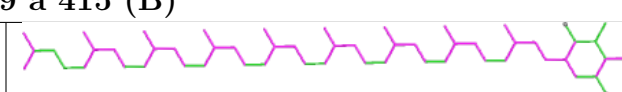
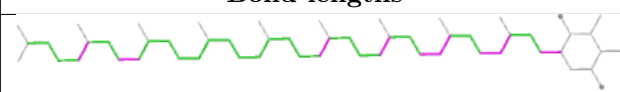
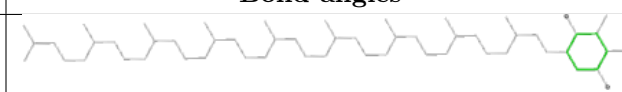


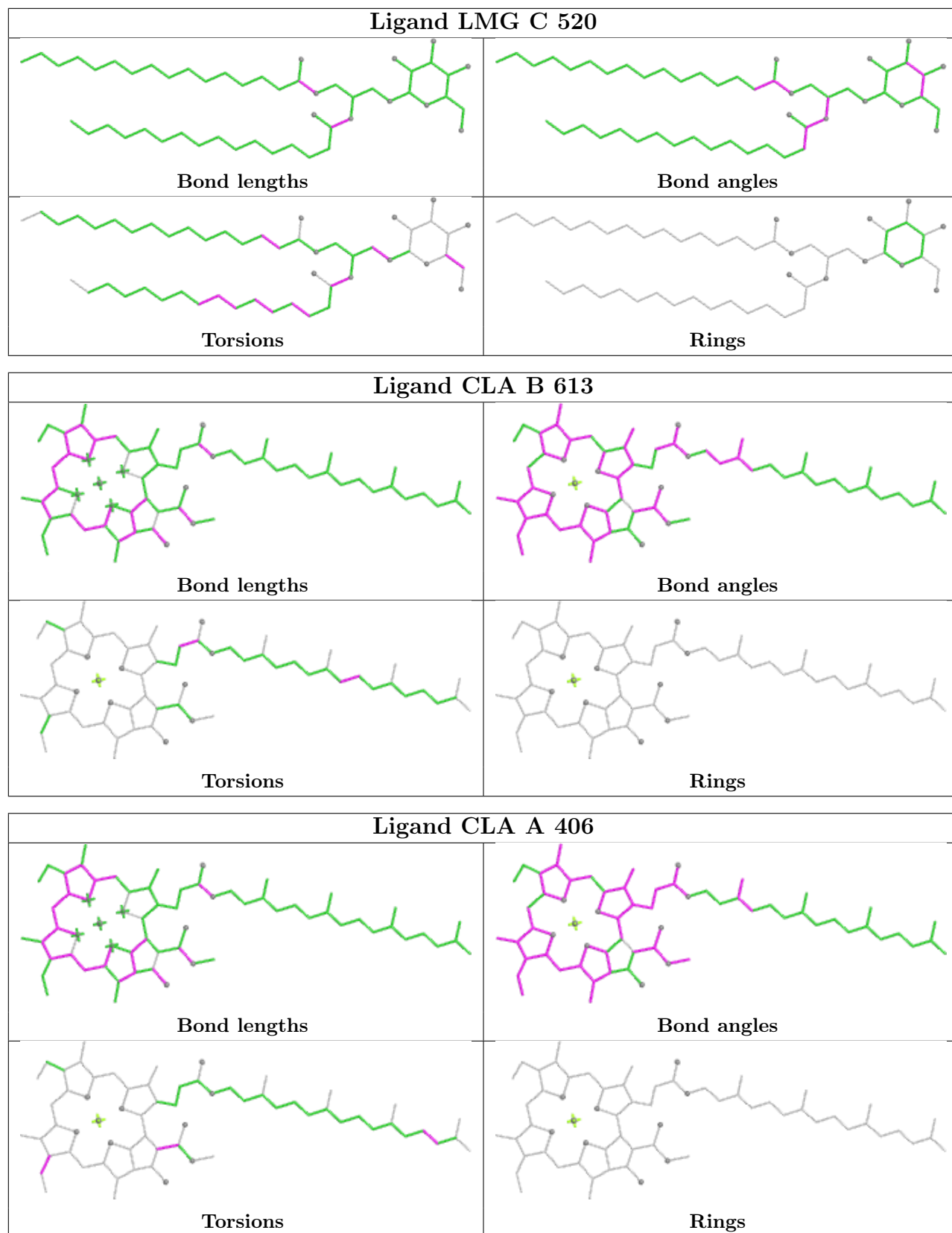


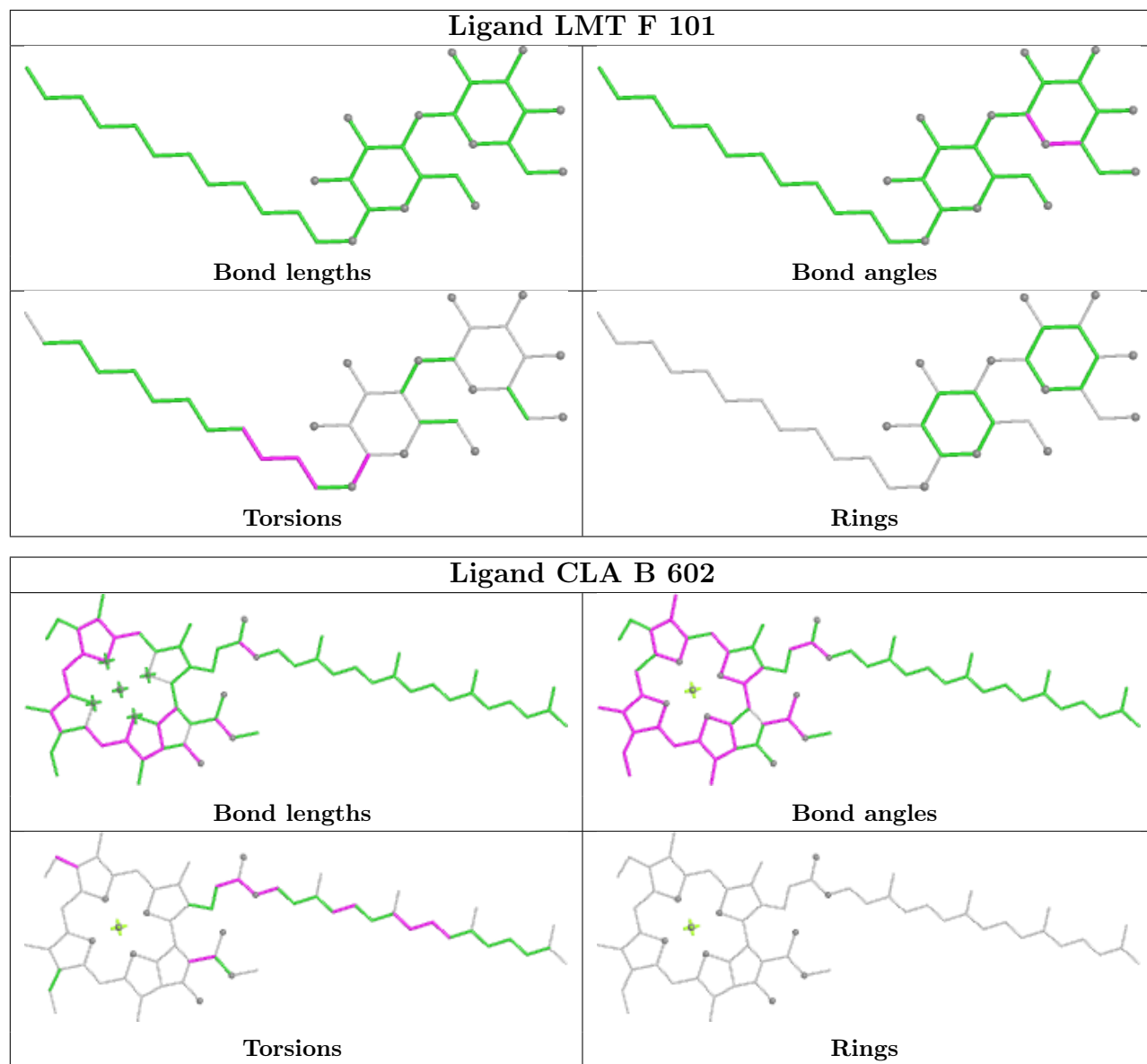


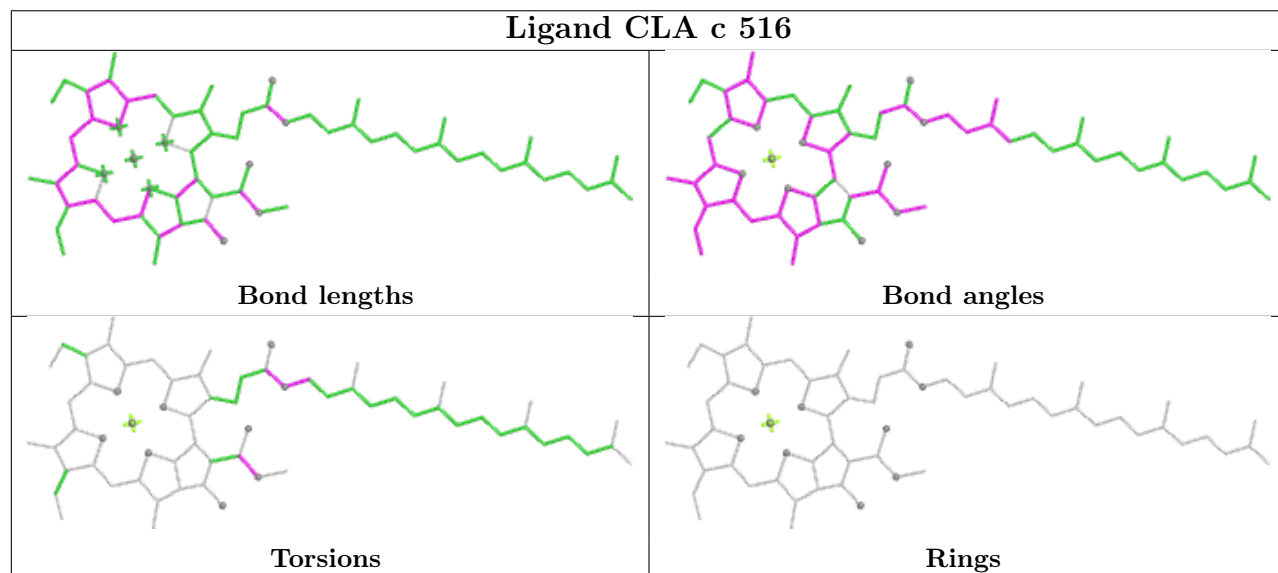
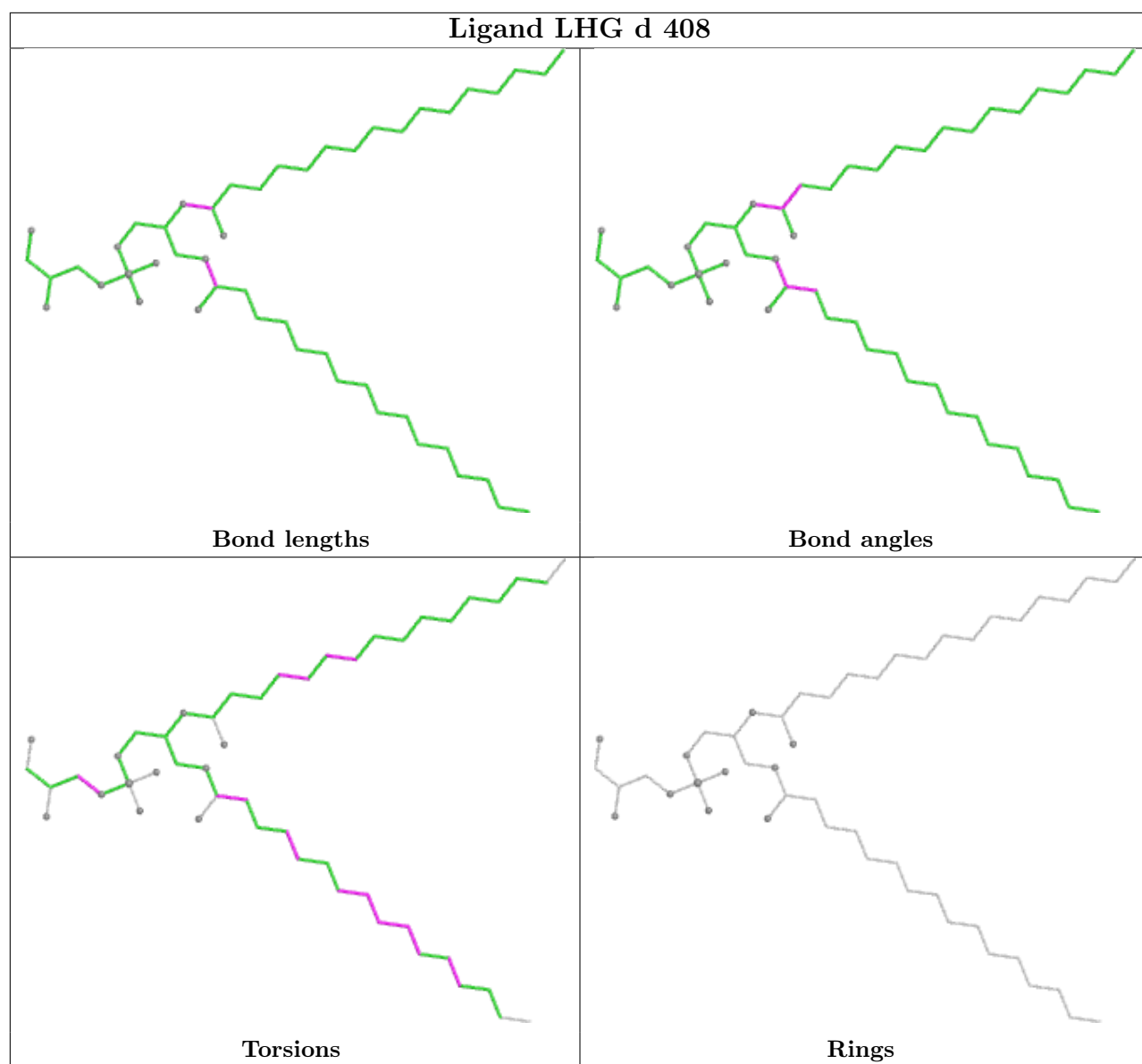




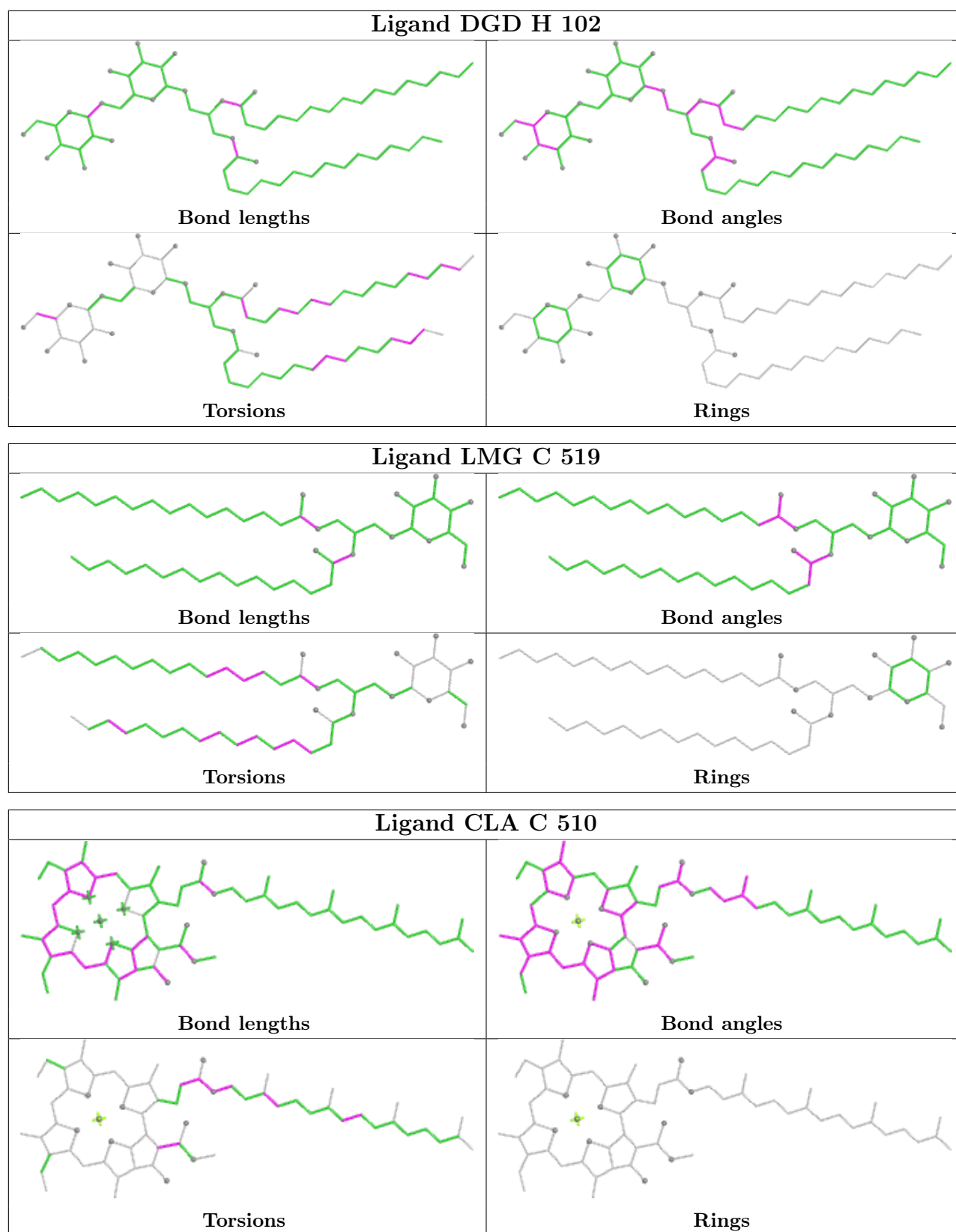
| Ligand BCR t 101                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|    |    |
| Torsions                                                                            | Rings                                                                                |
| Ligand BCR a 413                                                                    |                                                                                      |
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|    |    |
| Torsions                                                                            | Rings                                                                                |
| Ligand CLA C 505                                                                    |                                                                                      |
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |
| Ligand PL9 a 415 (B)                                                                |                                                                                      |
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

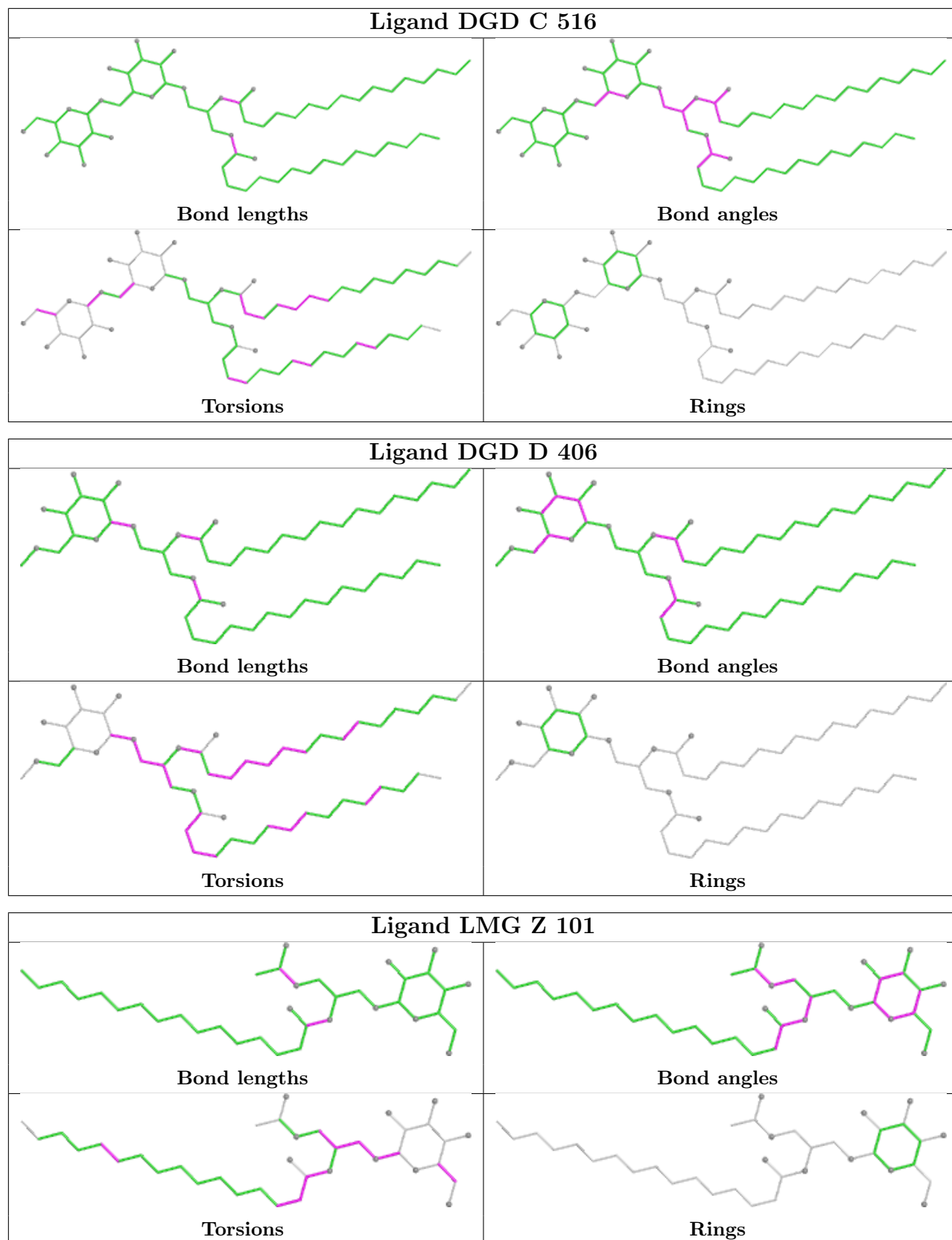


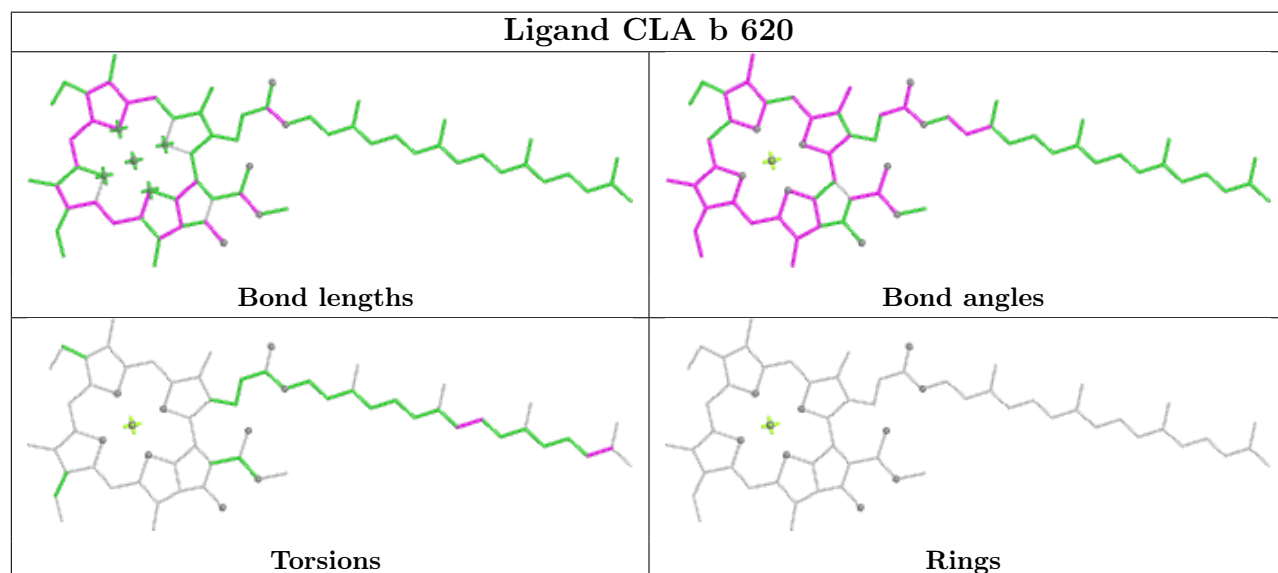
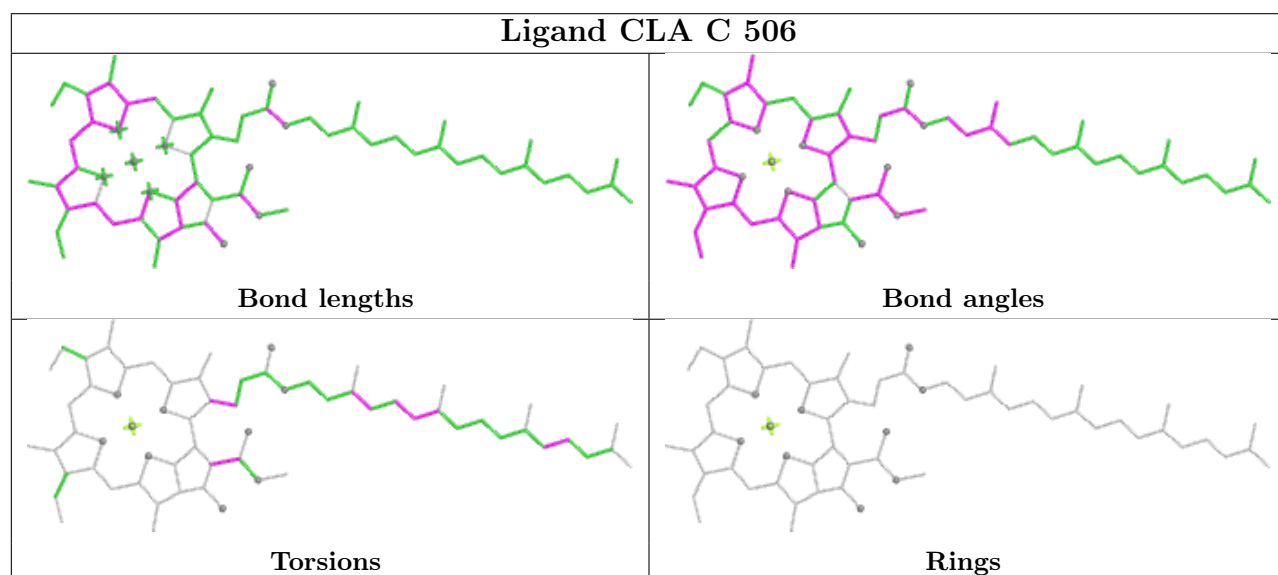
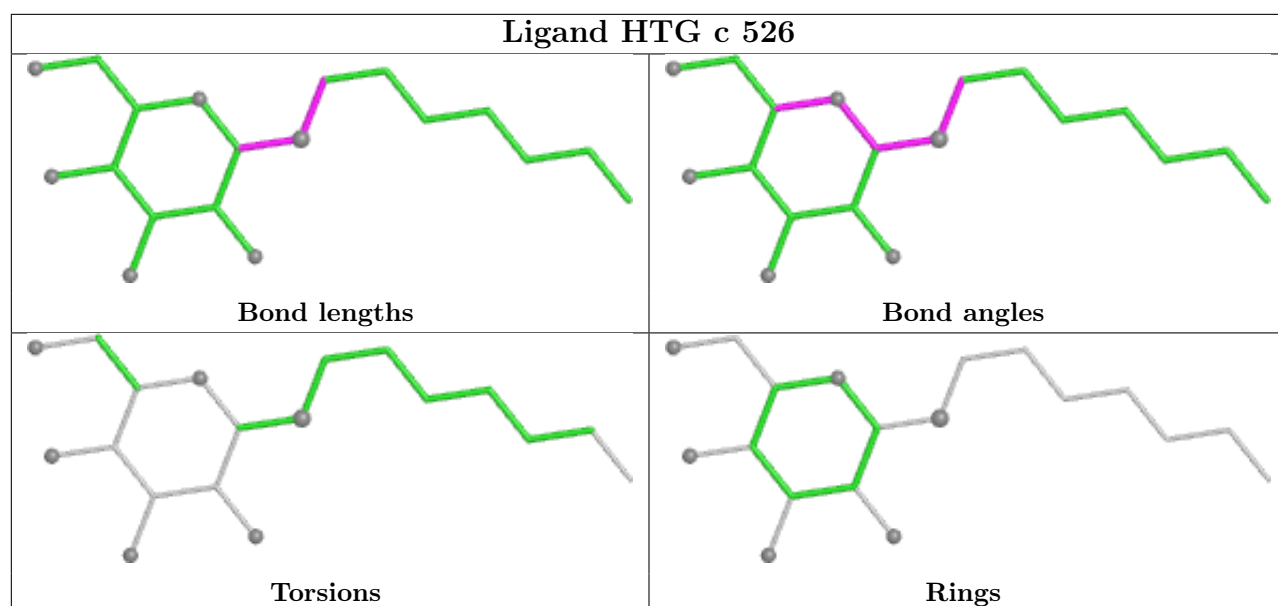


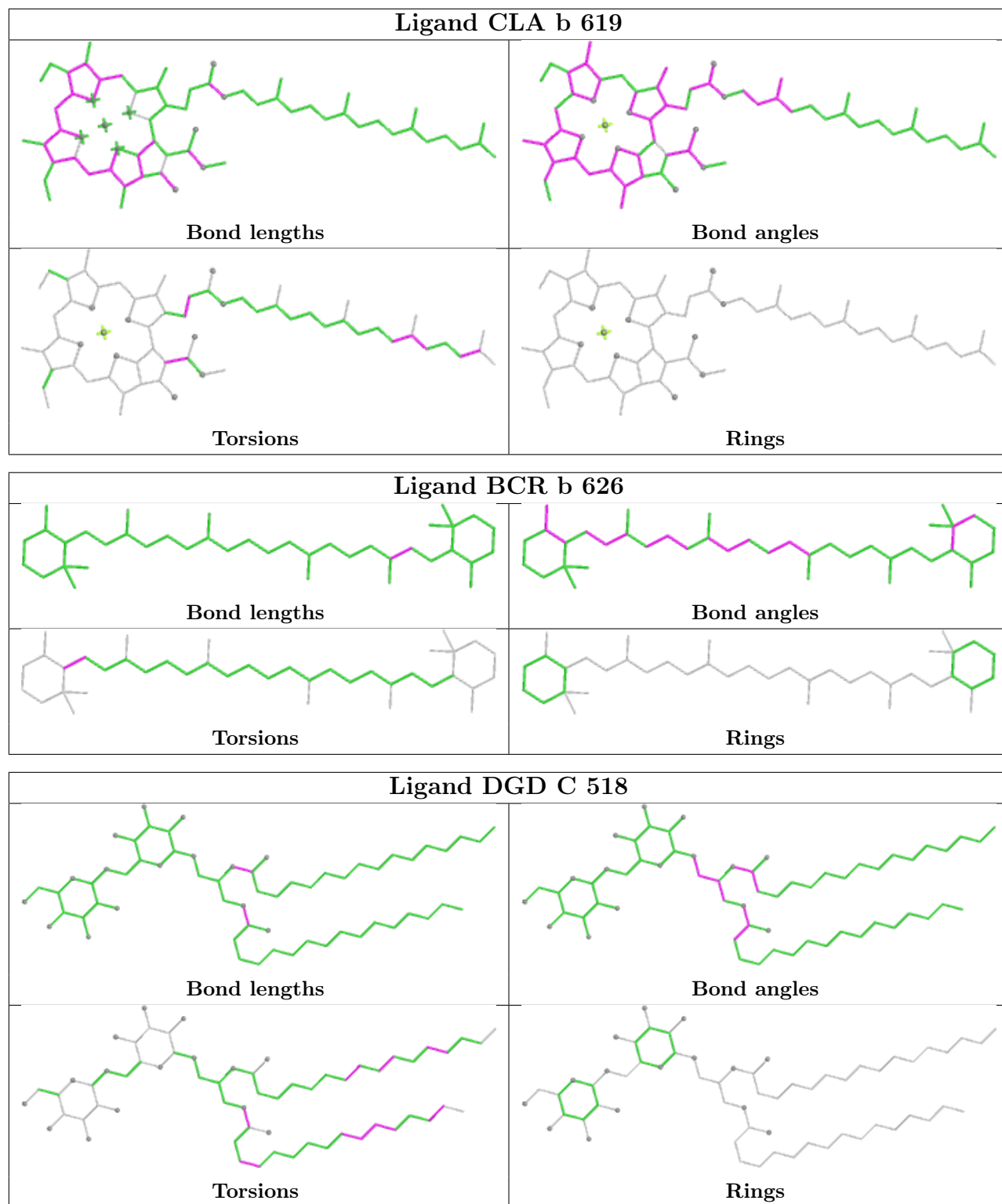


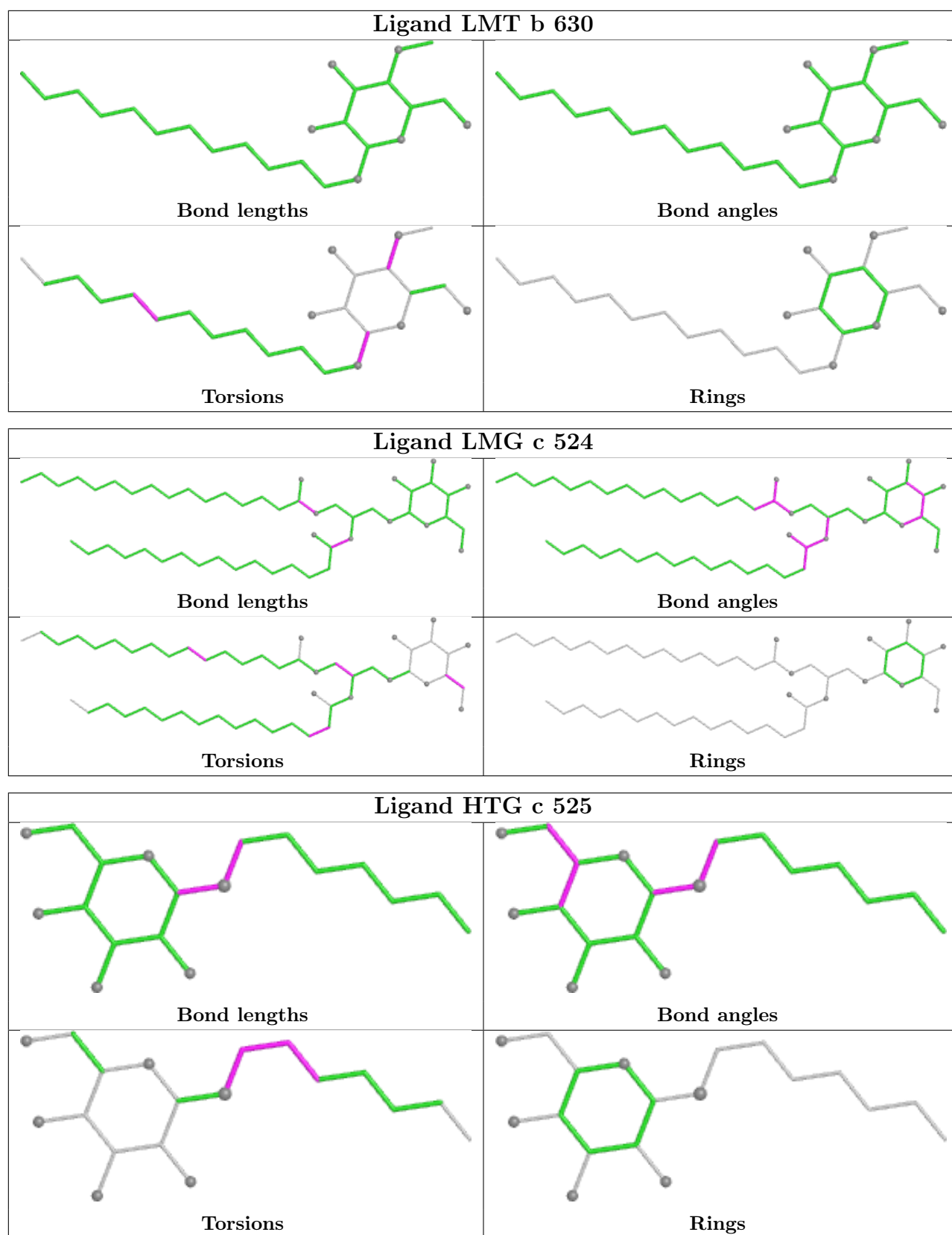


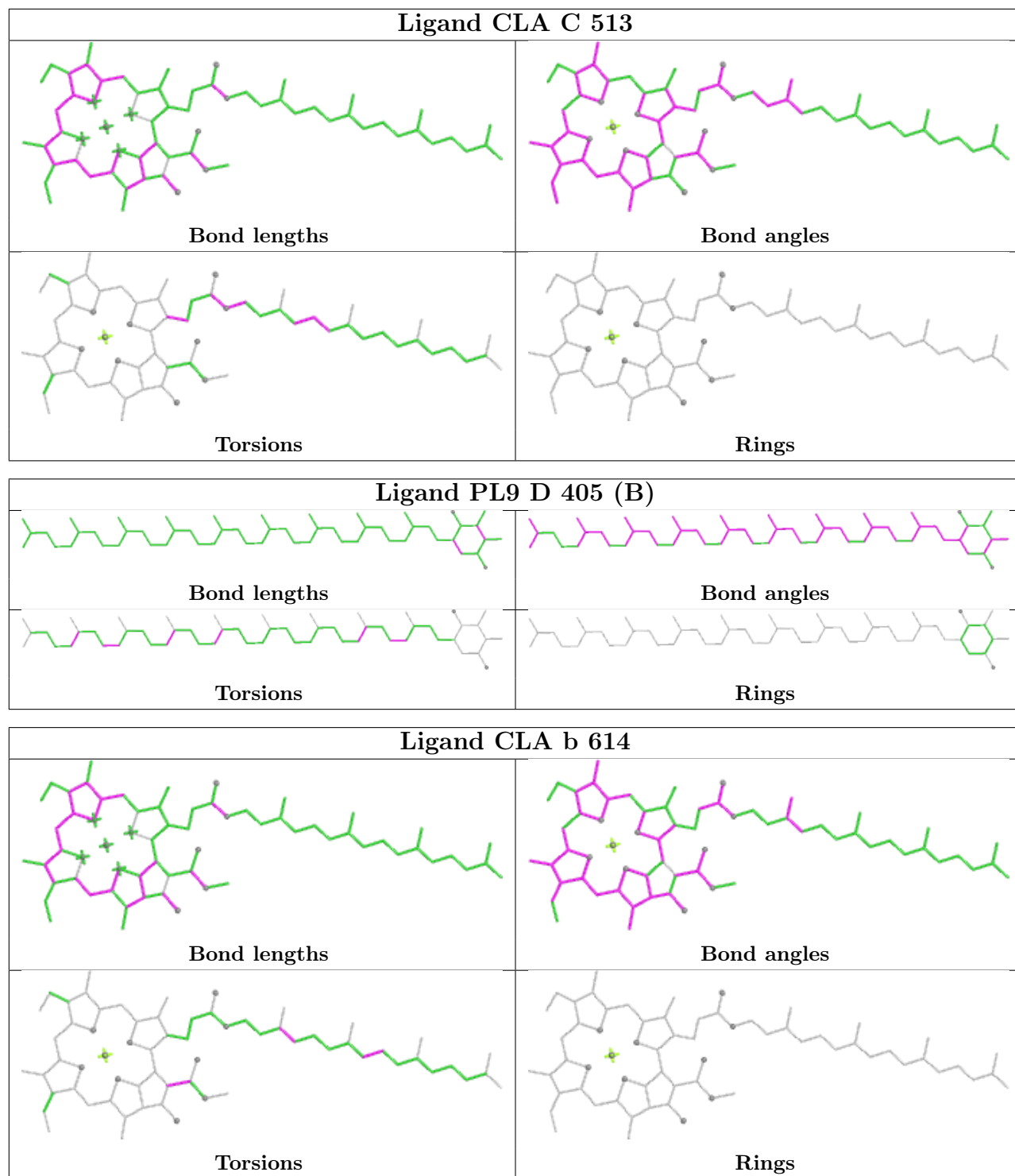


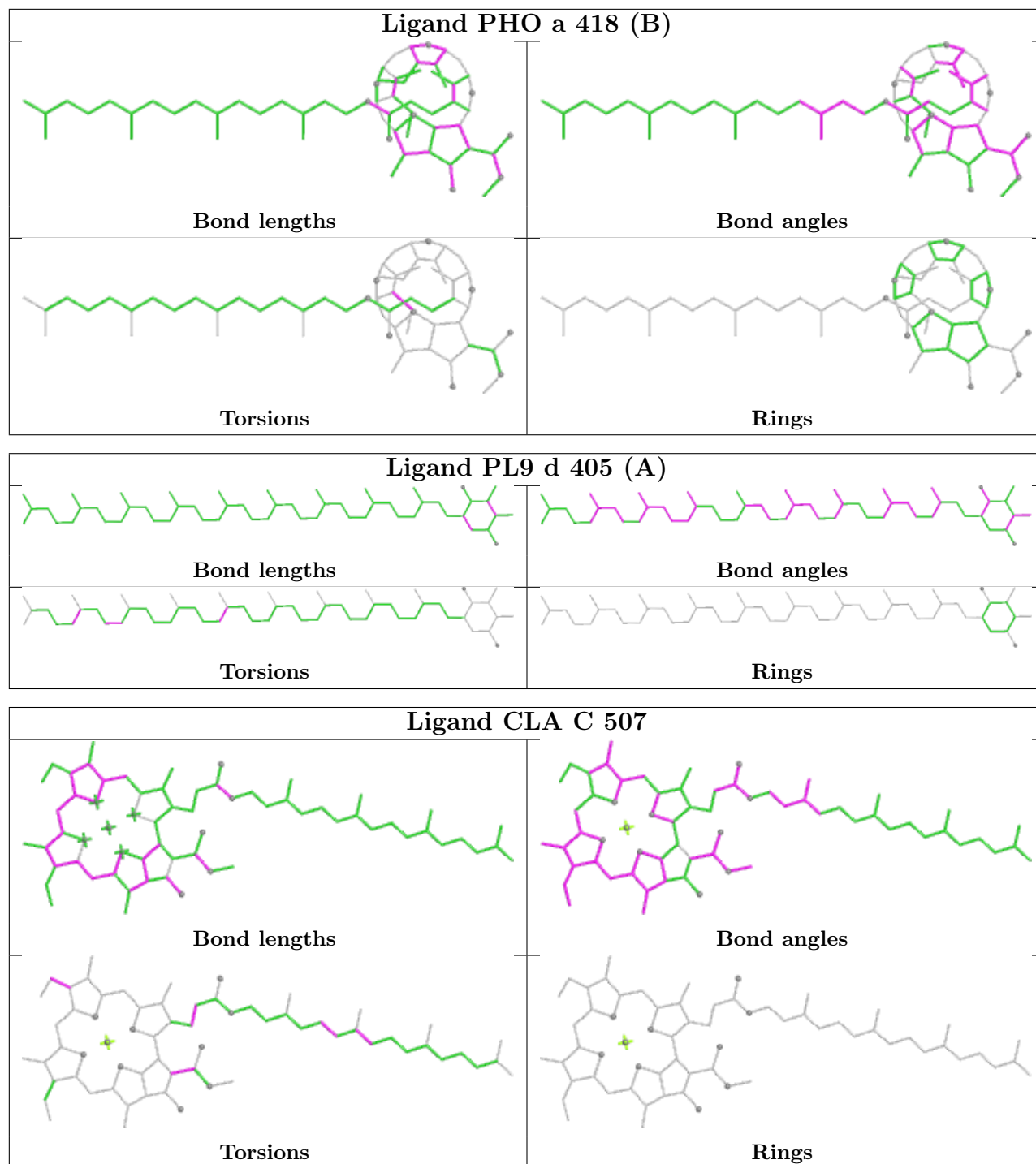


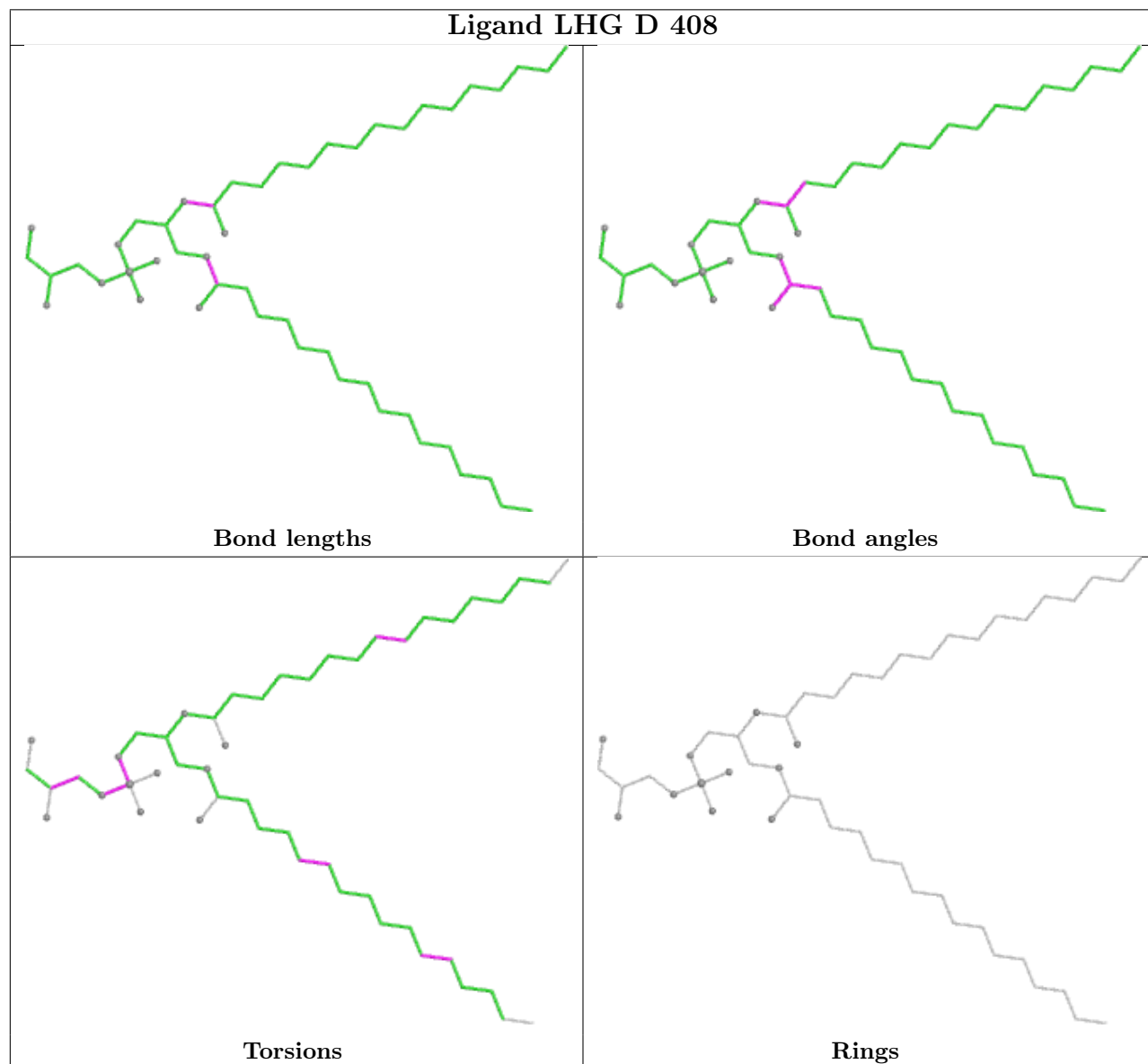
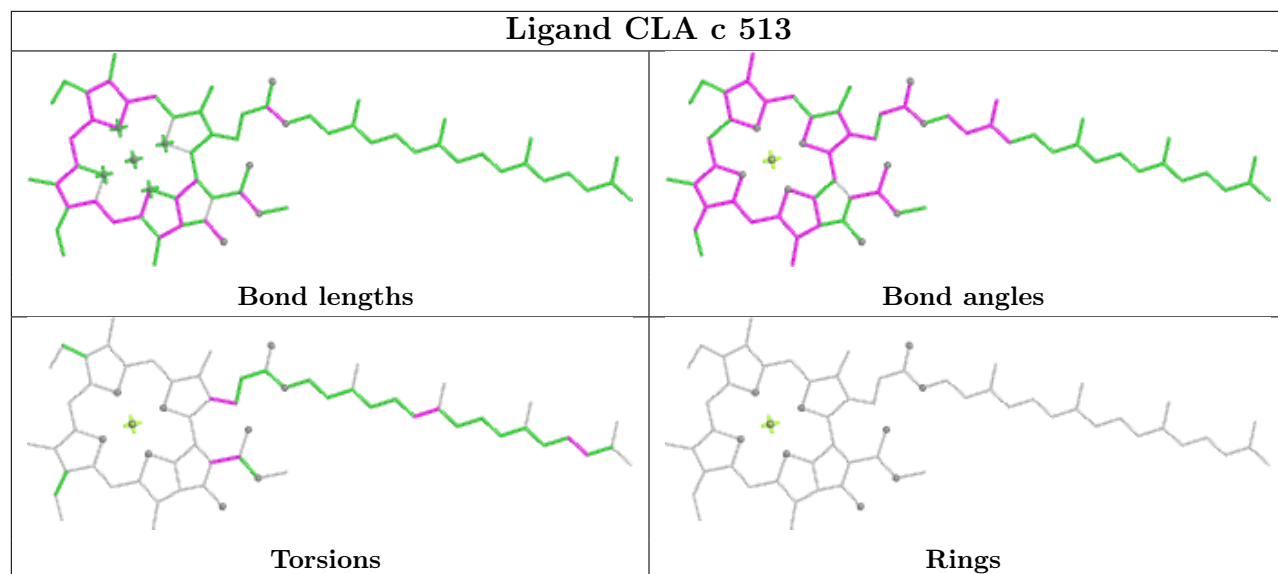




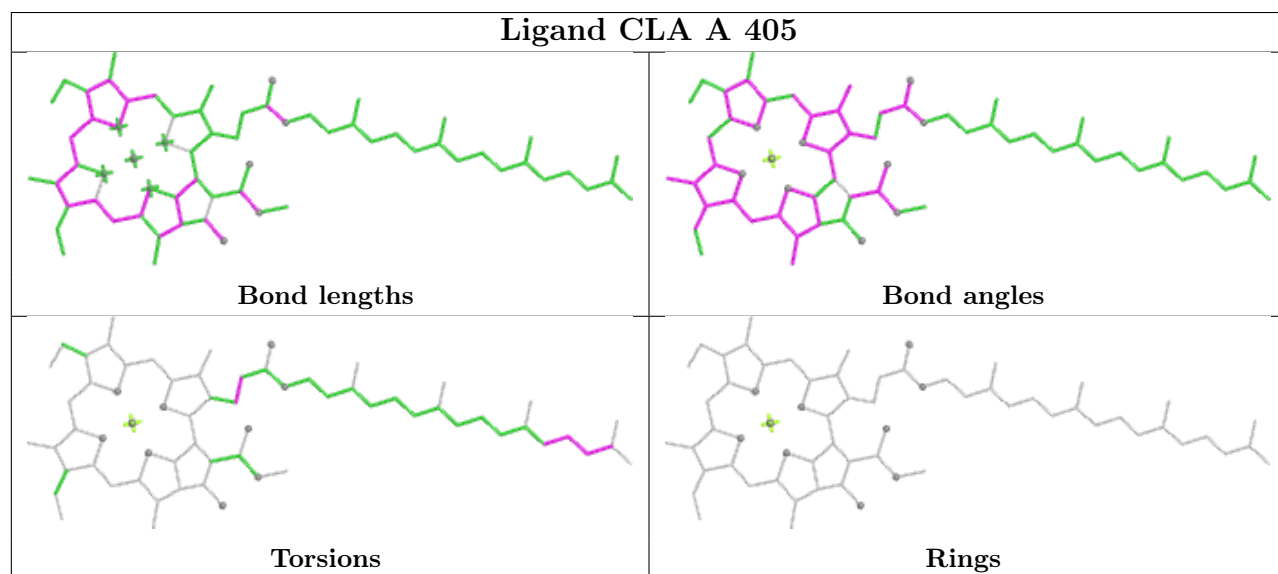
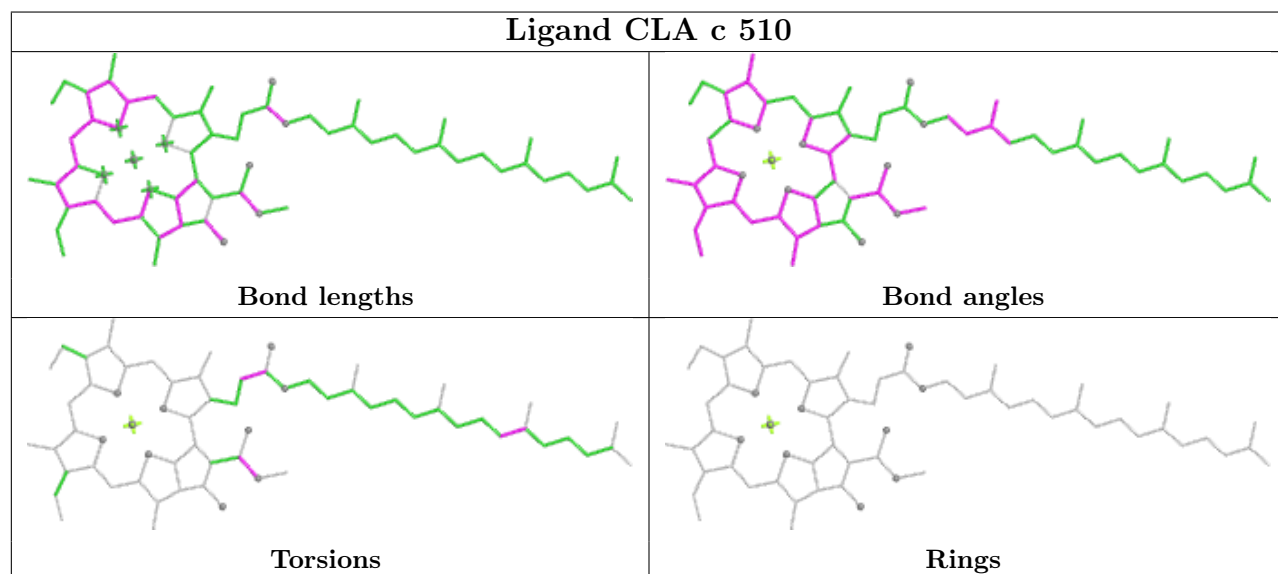
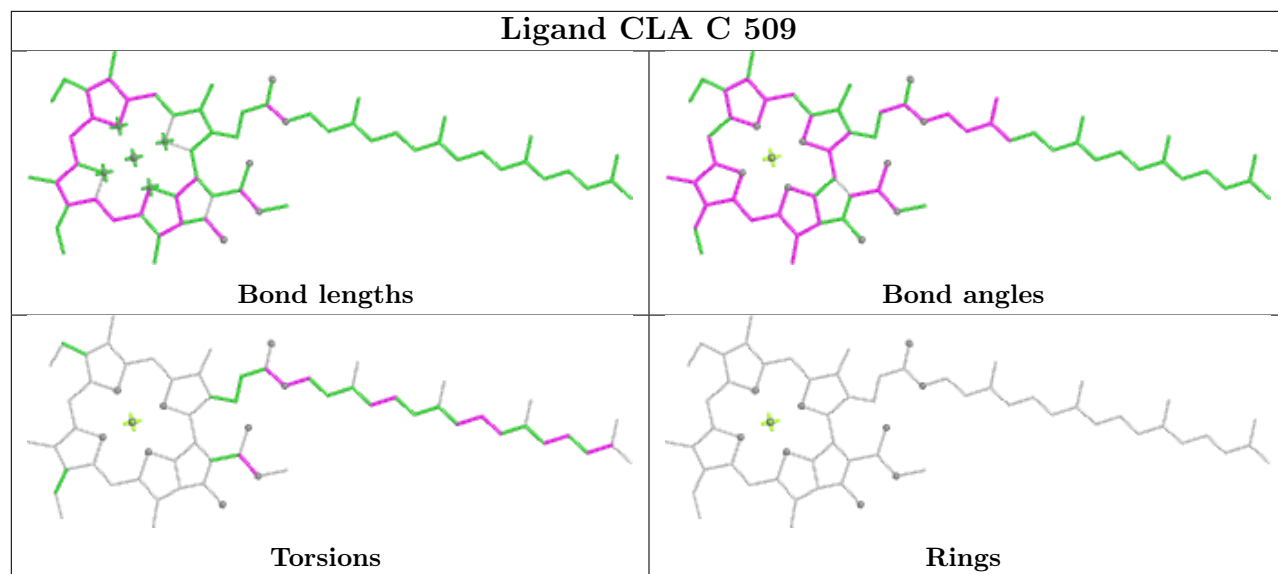




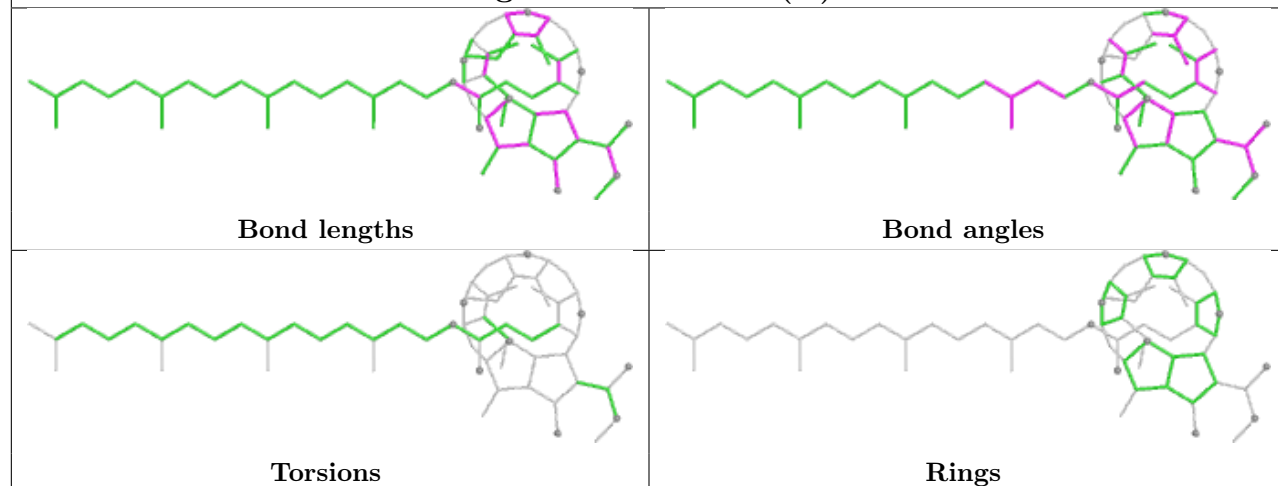




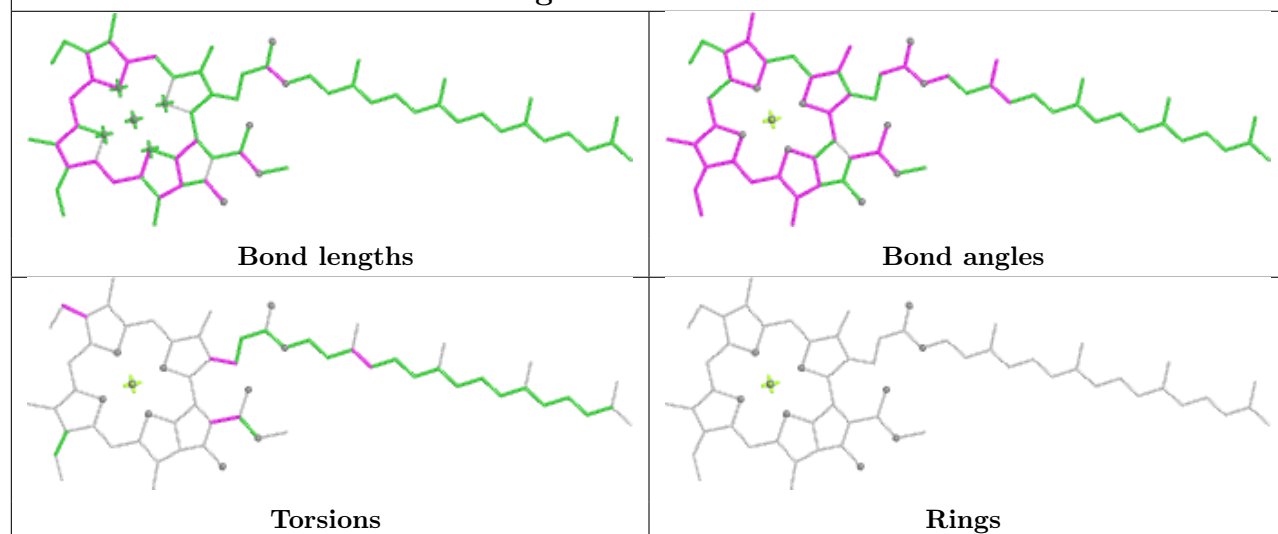




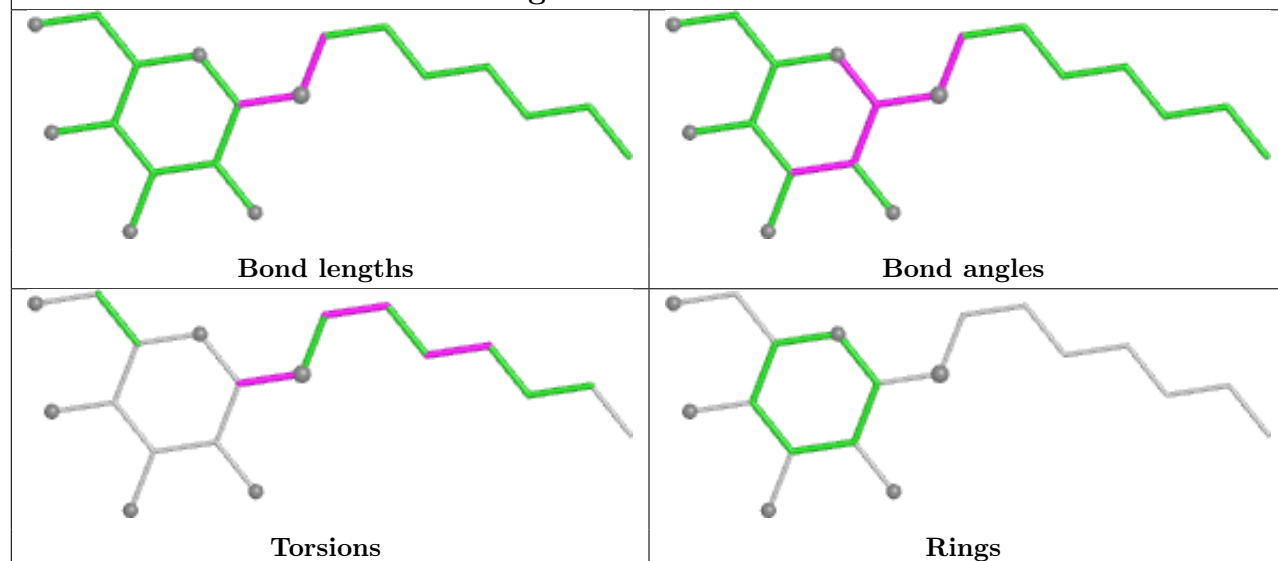
## Ligand PHO A 409 (A)

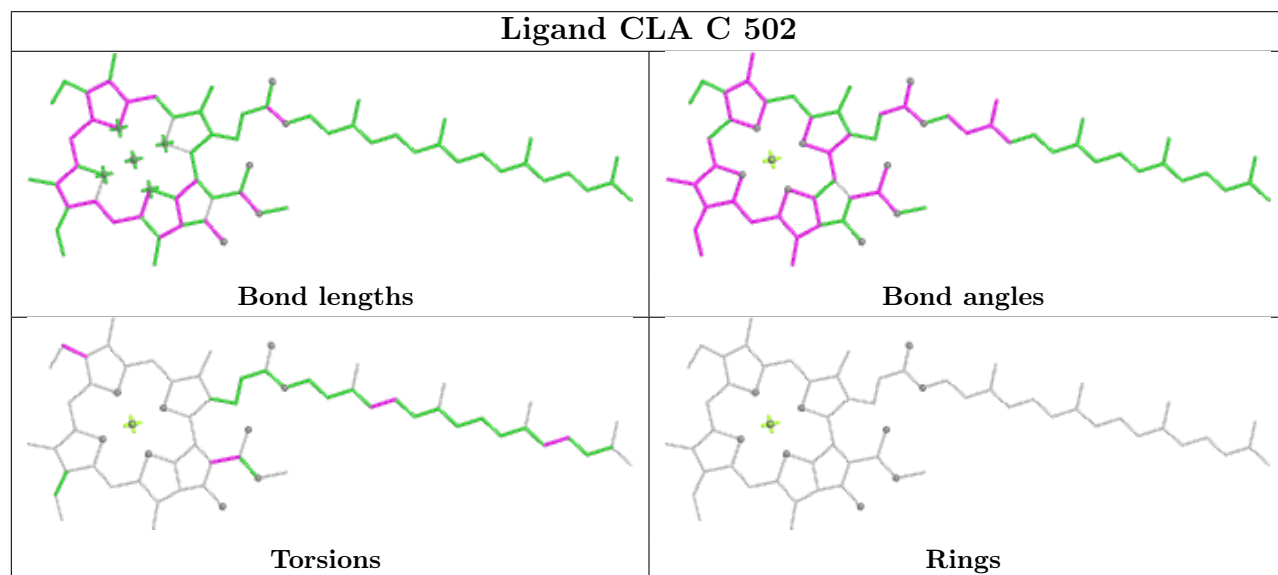
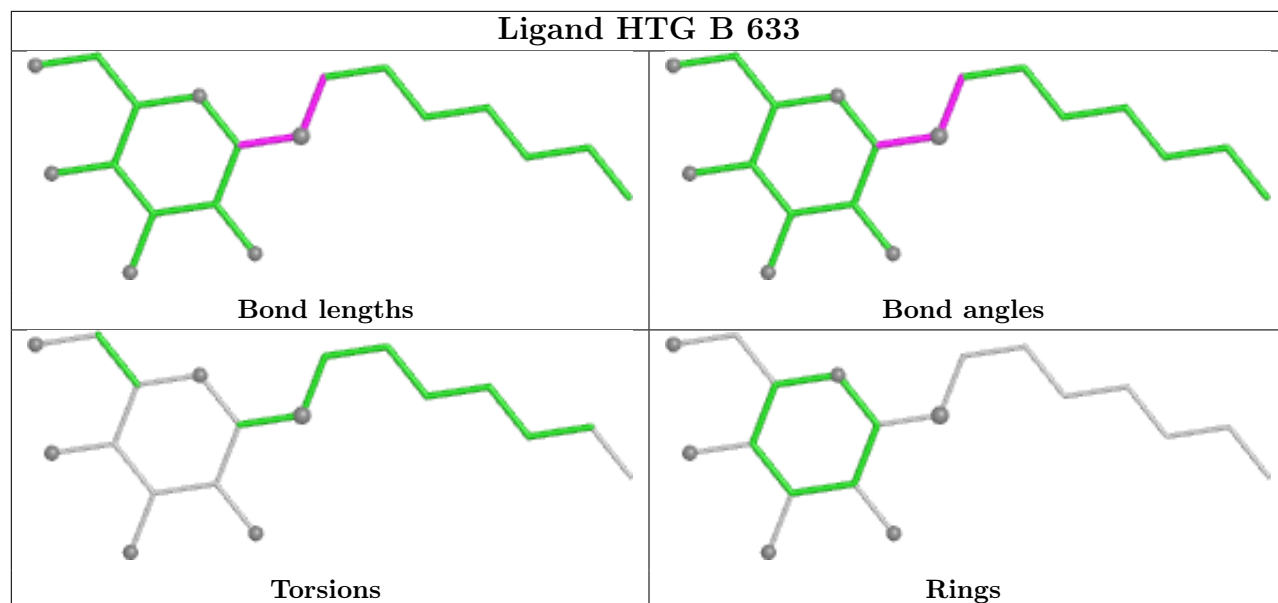


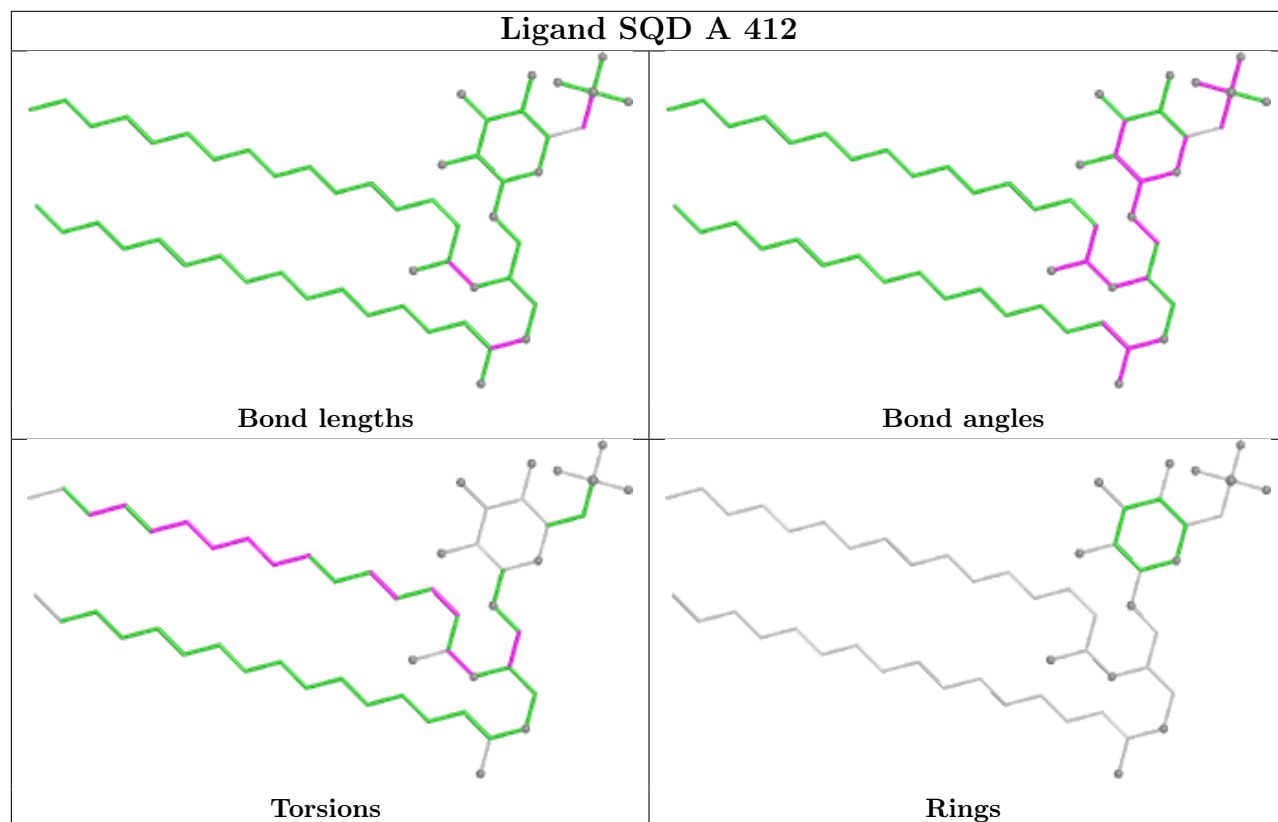
## Ligand CLA b 618

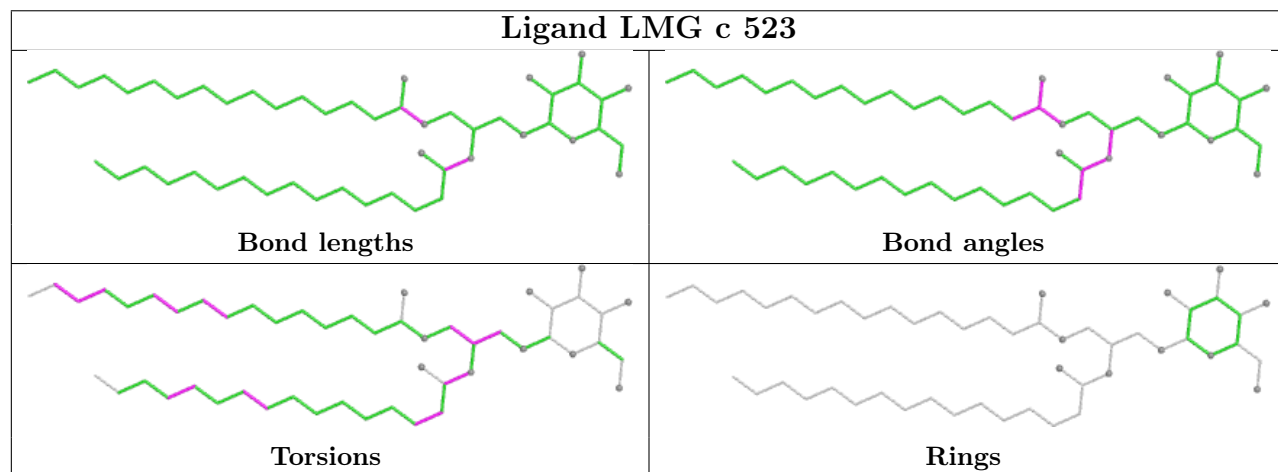
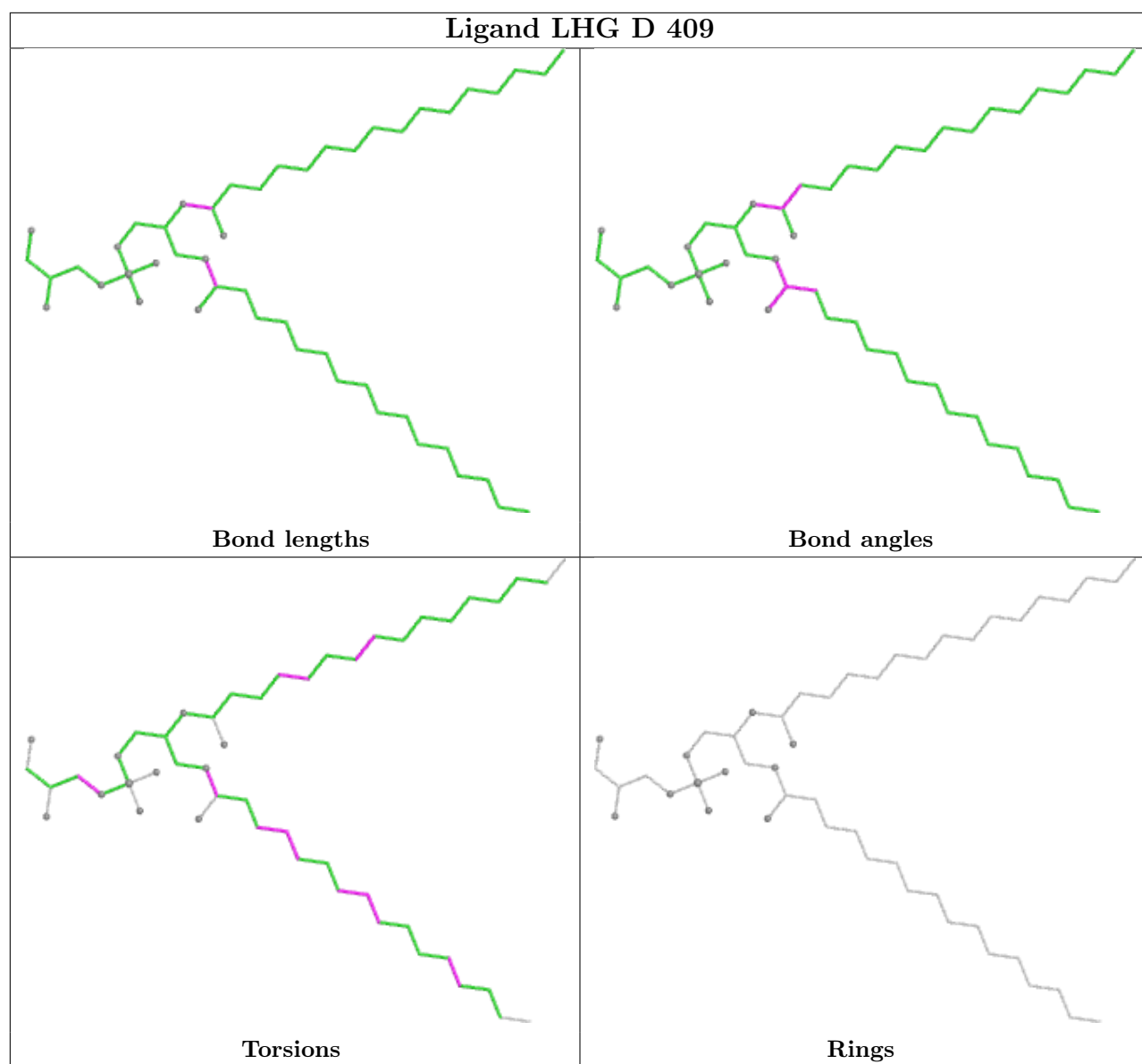


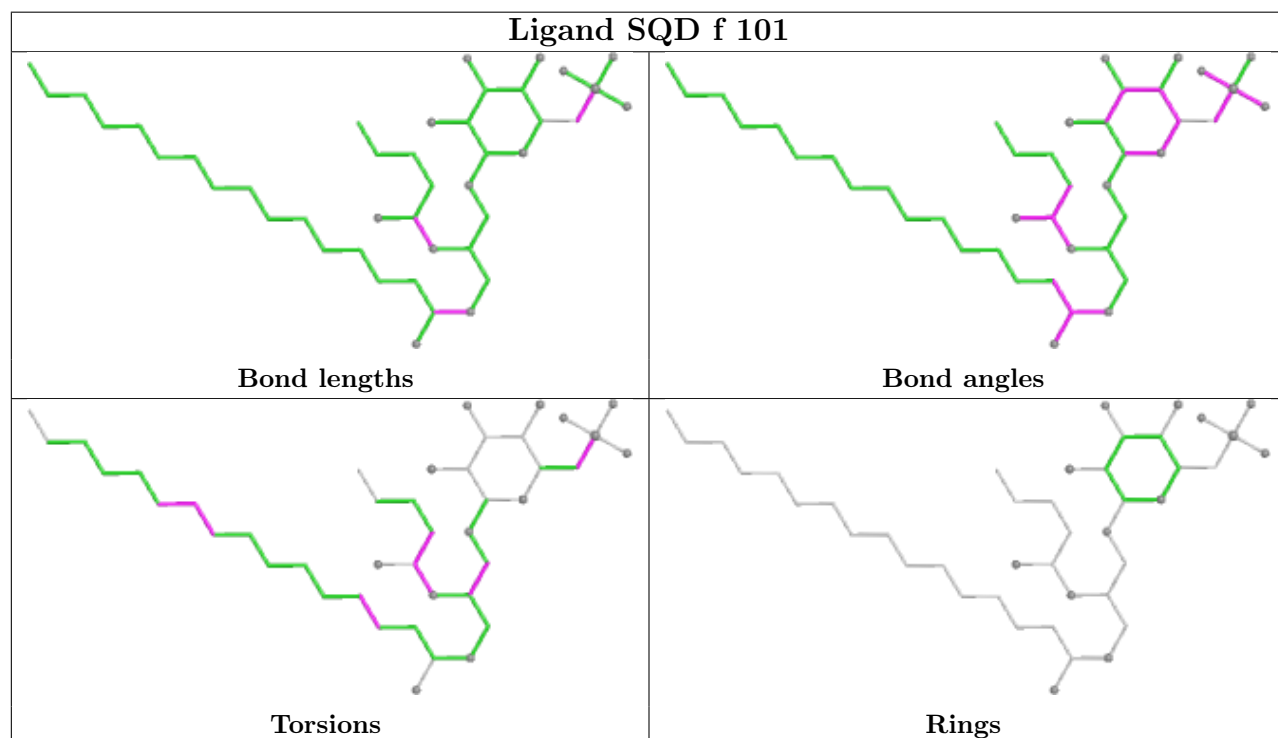
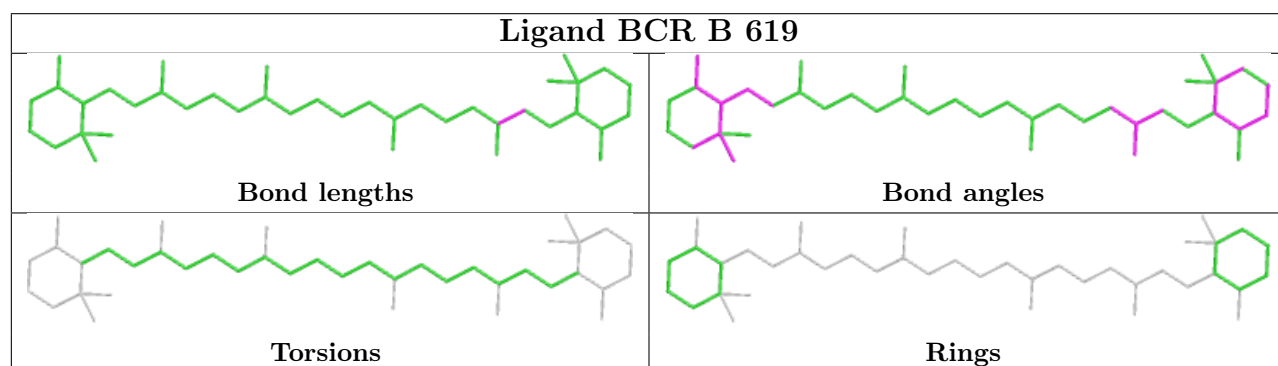
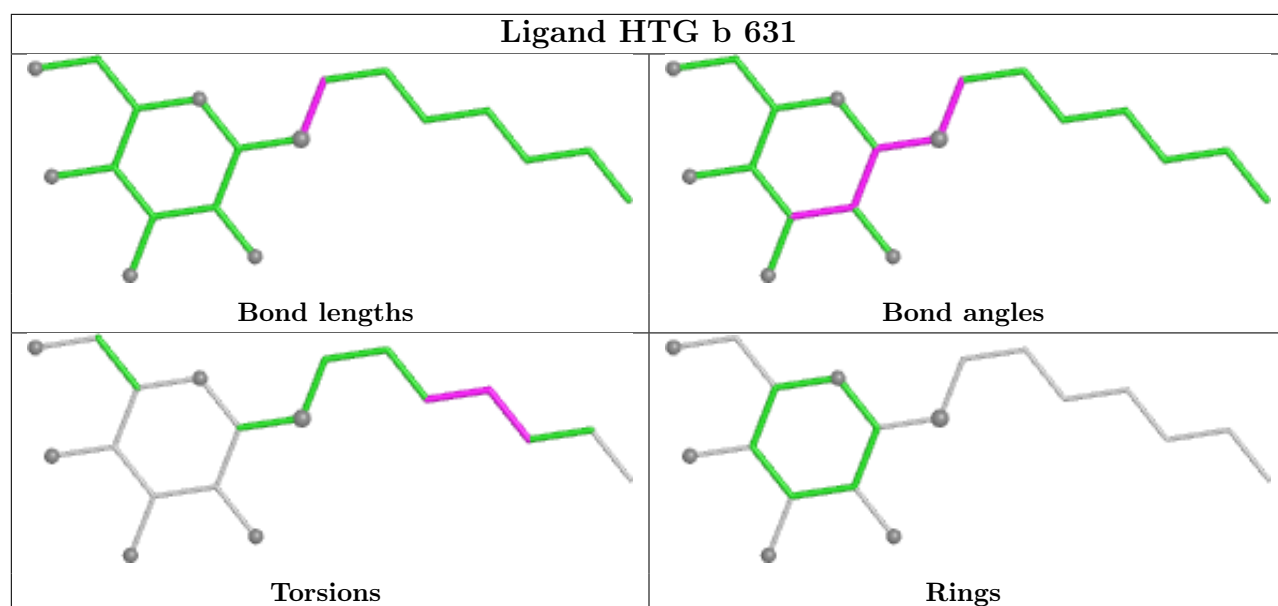
## Ligand HTG V 206

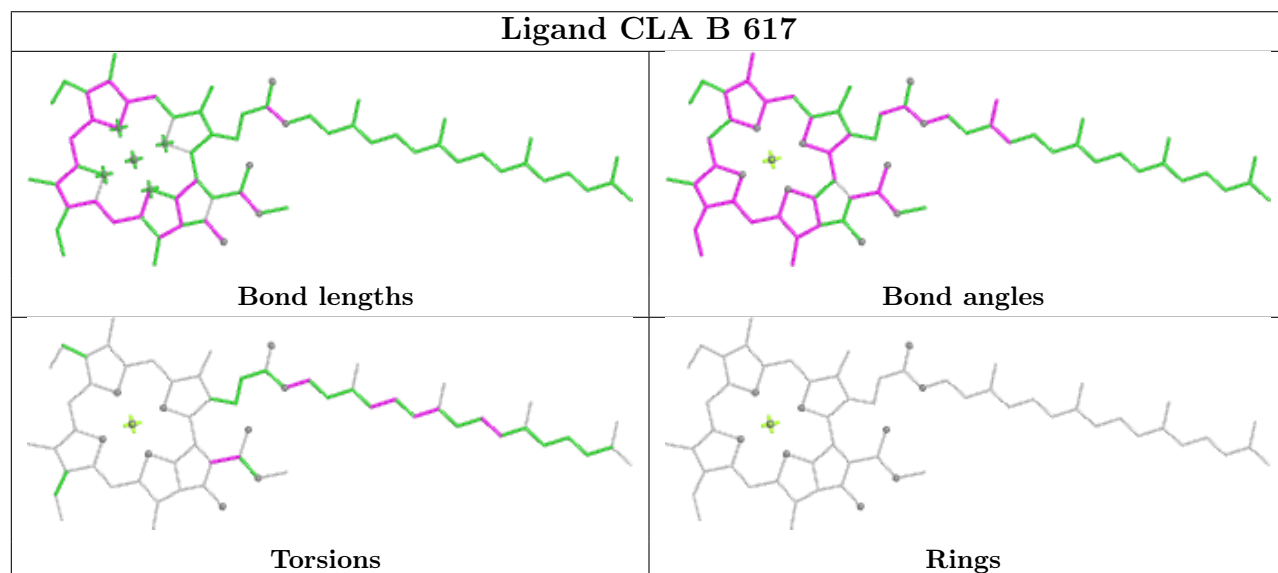
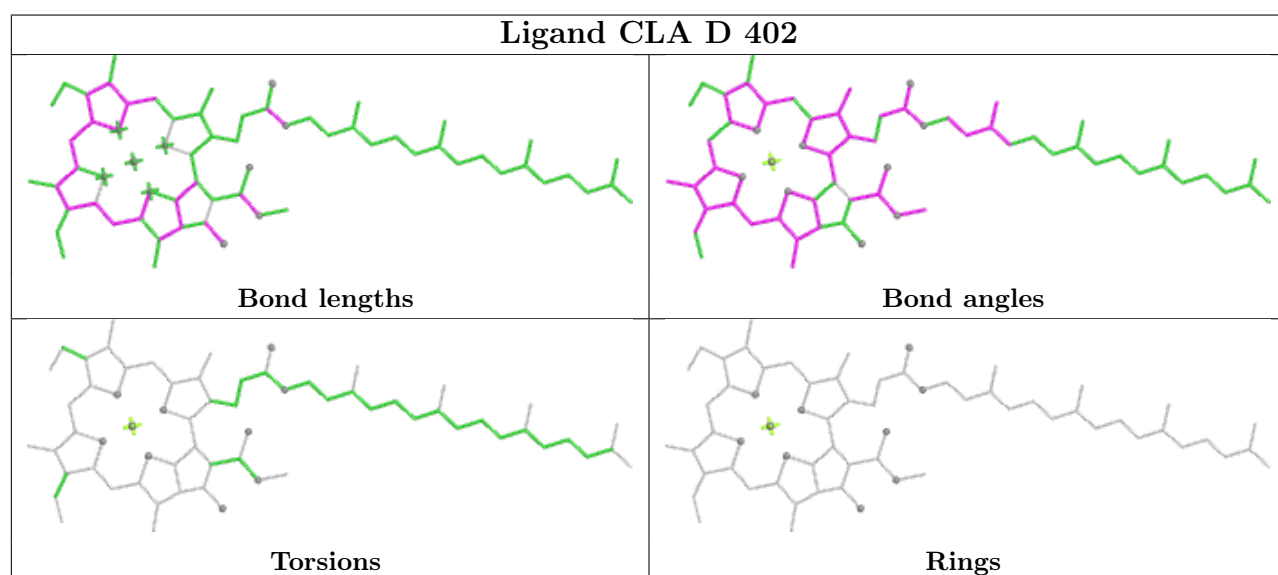
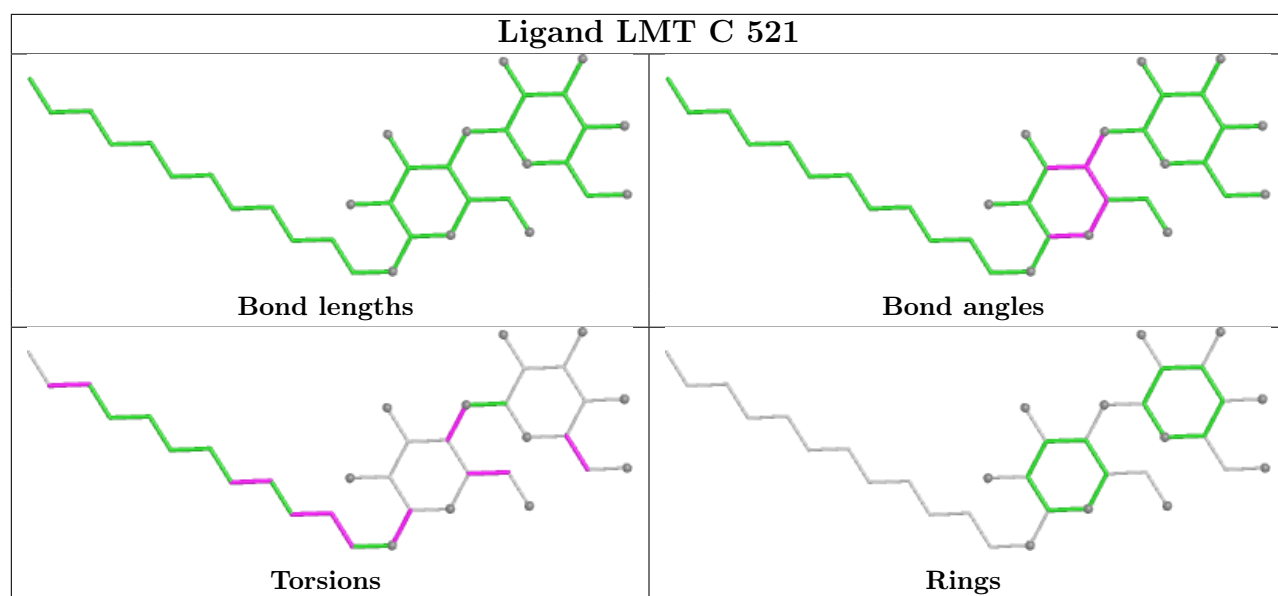




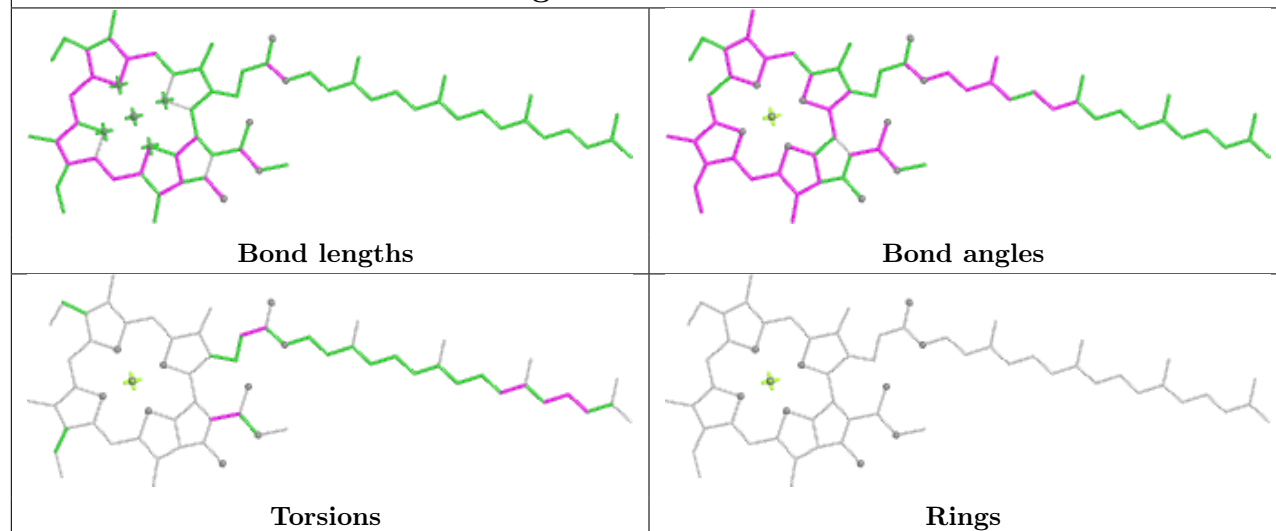




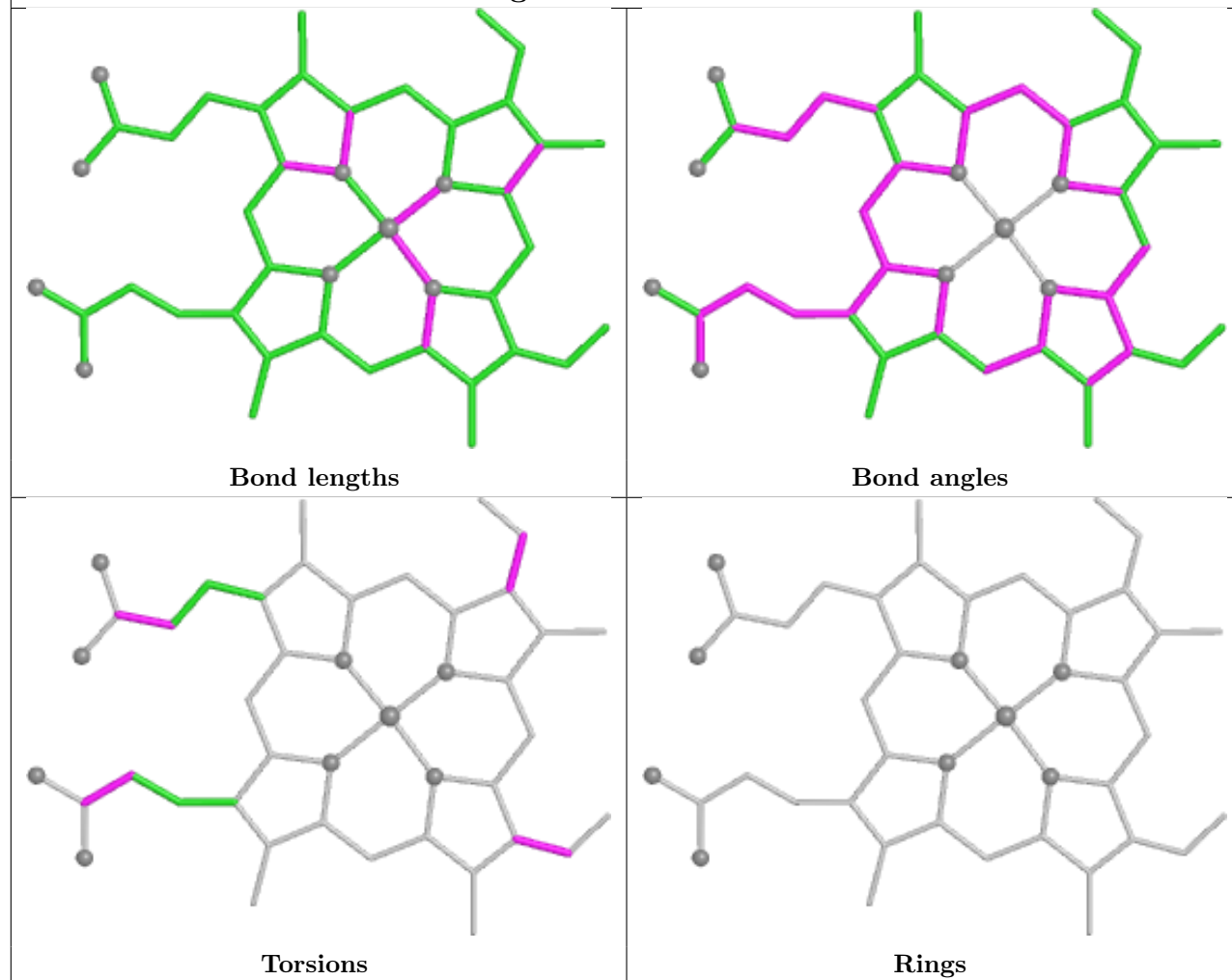




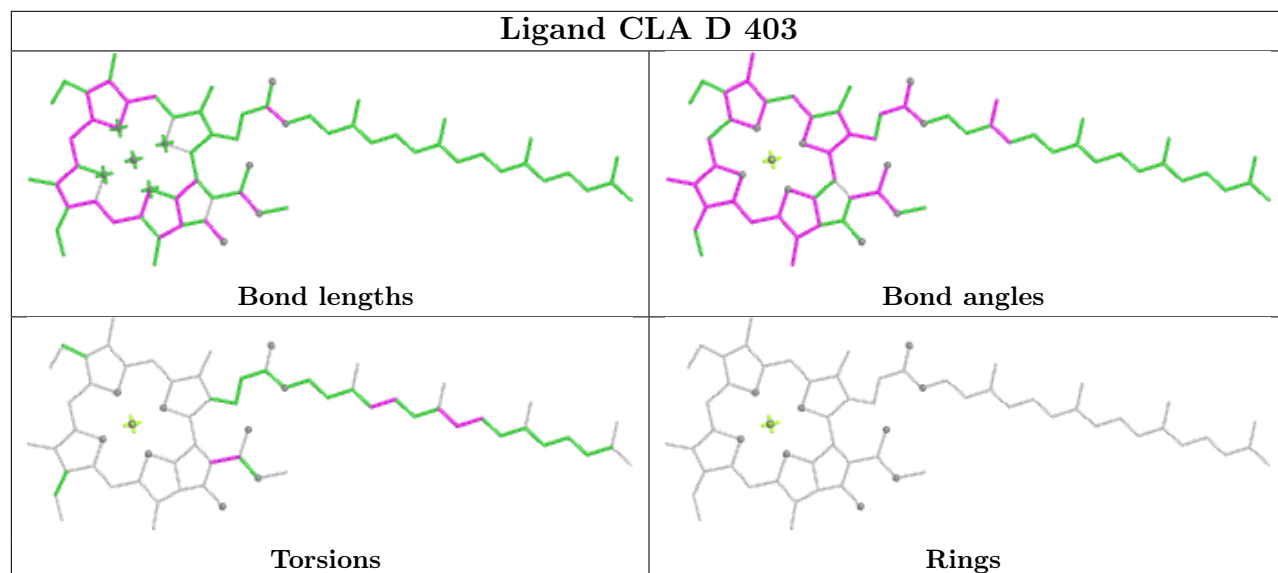
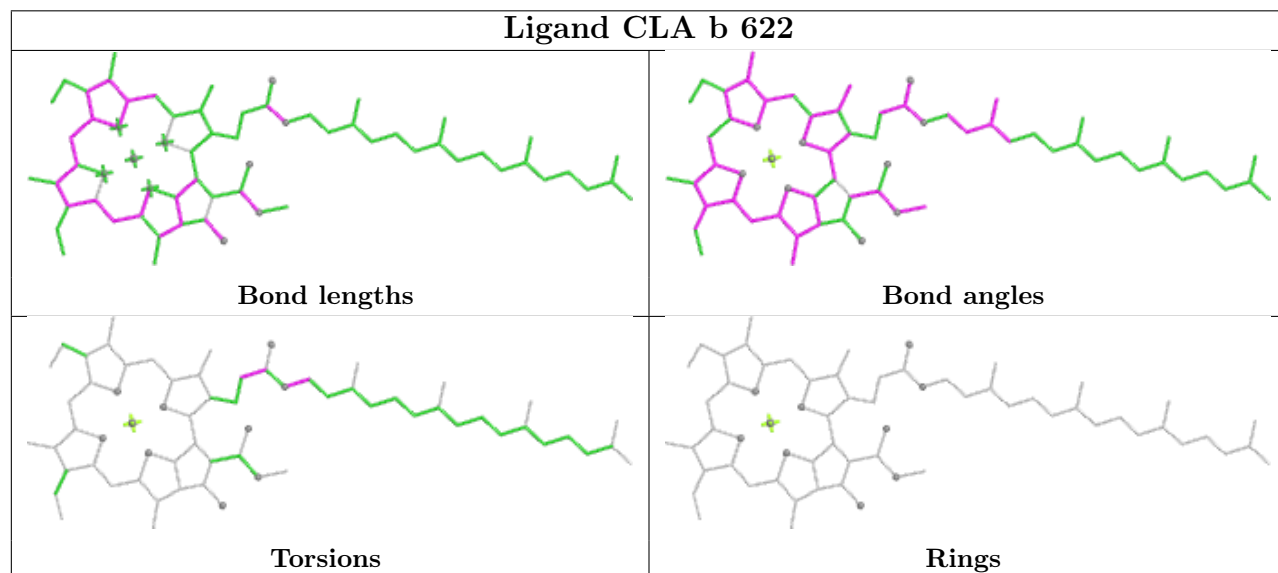
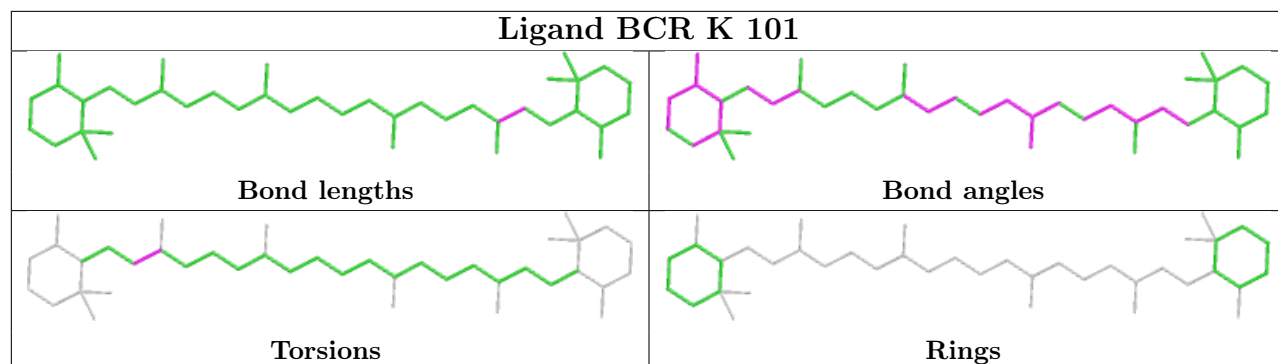
## Ligand CLA C 501



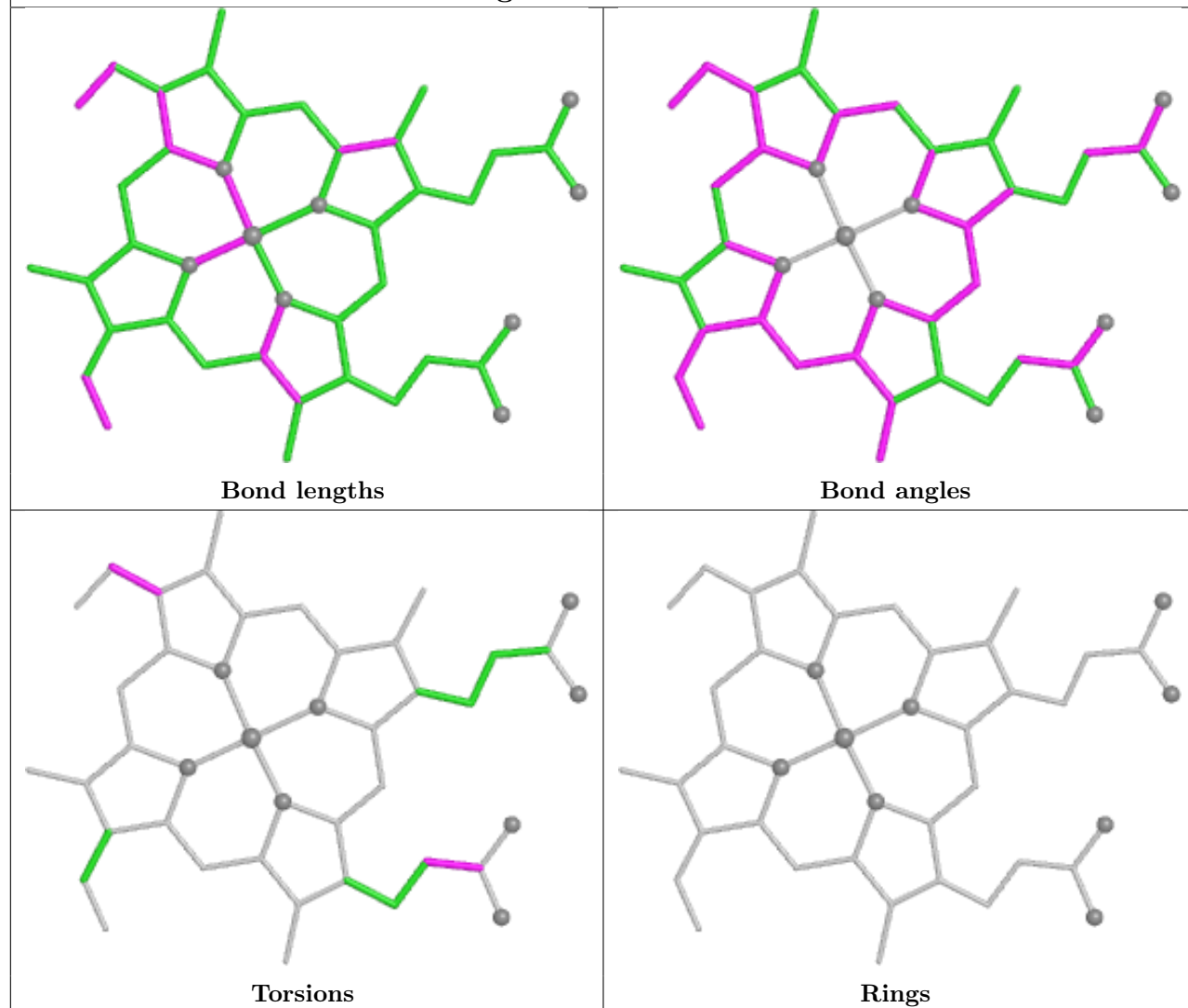
## Ligand HEM F 102



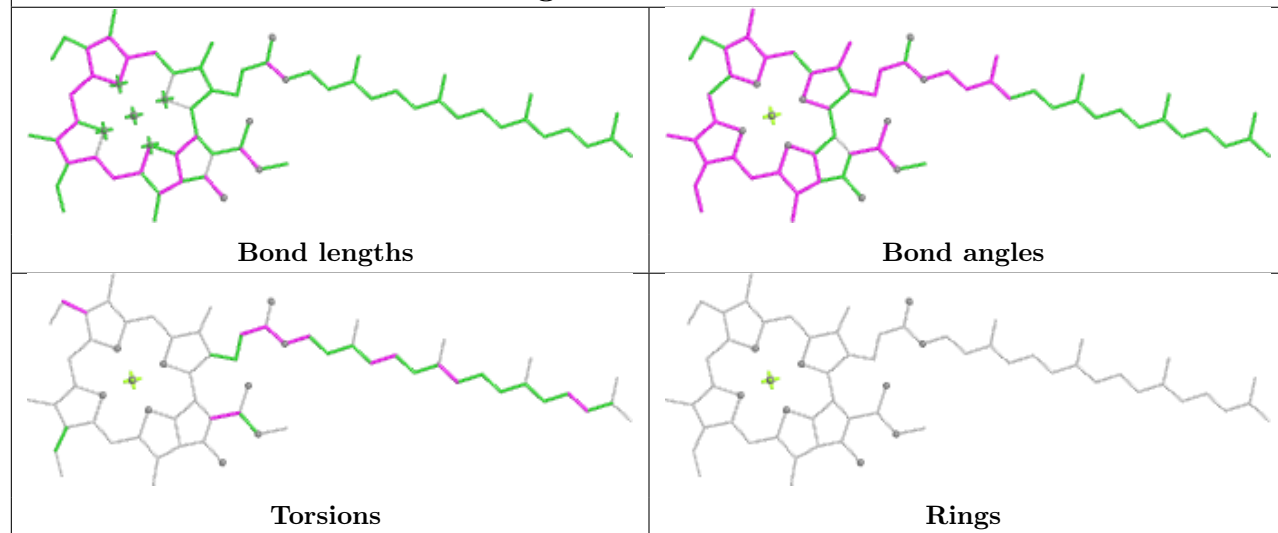


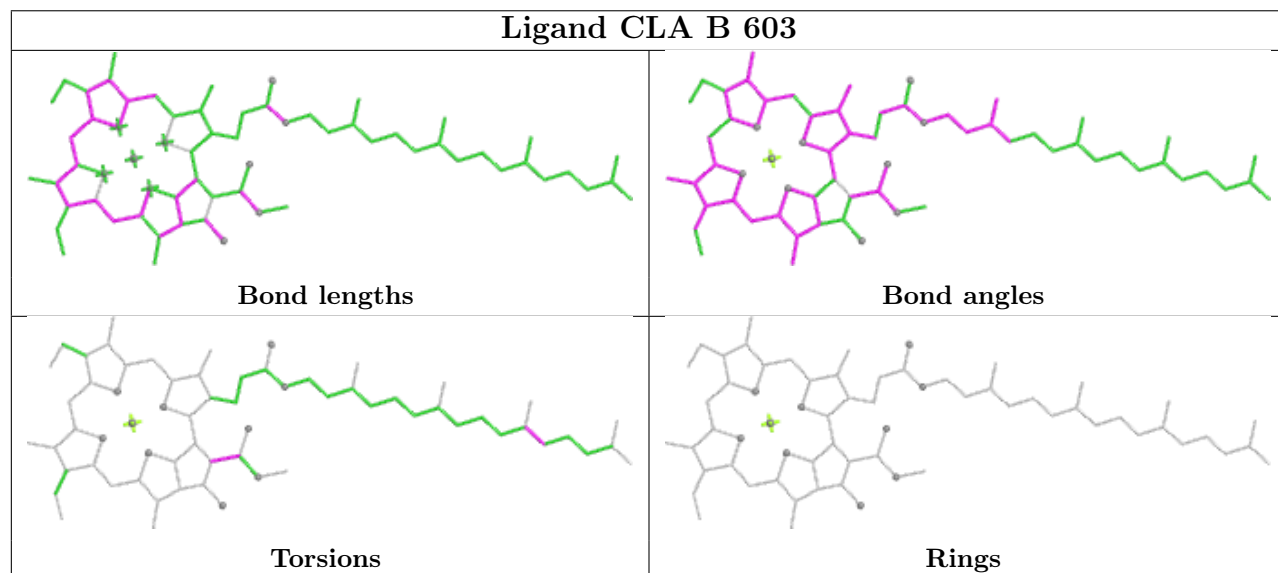
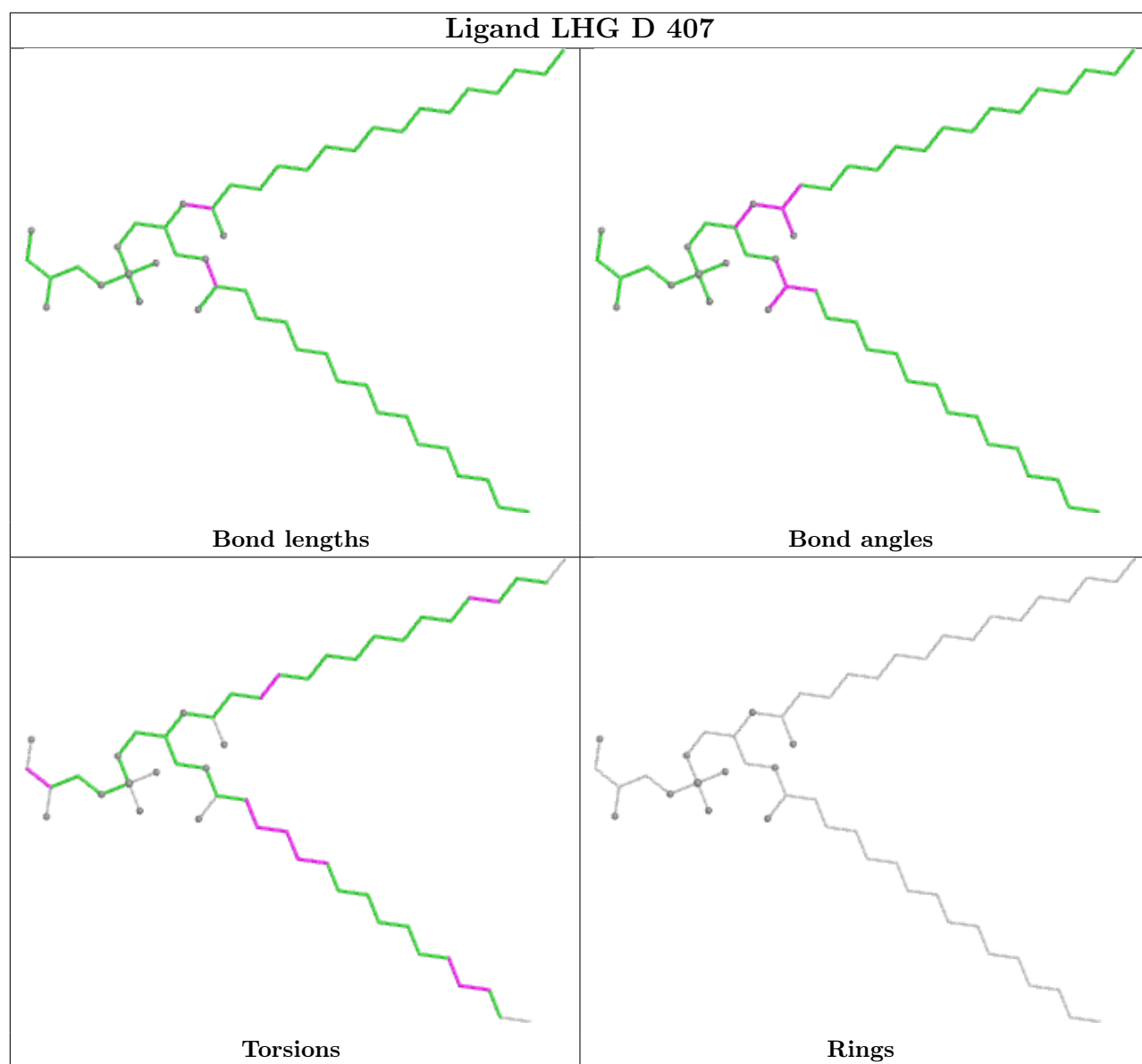


## Ligand HEC v 205

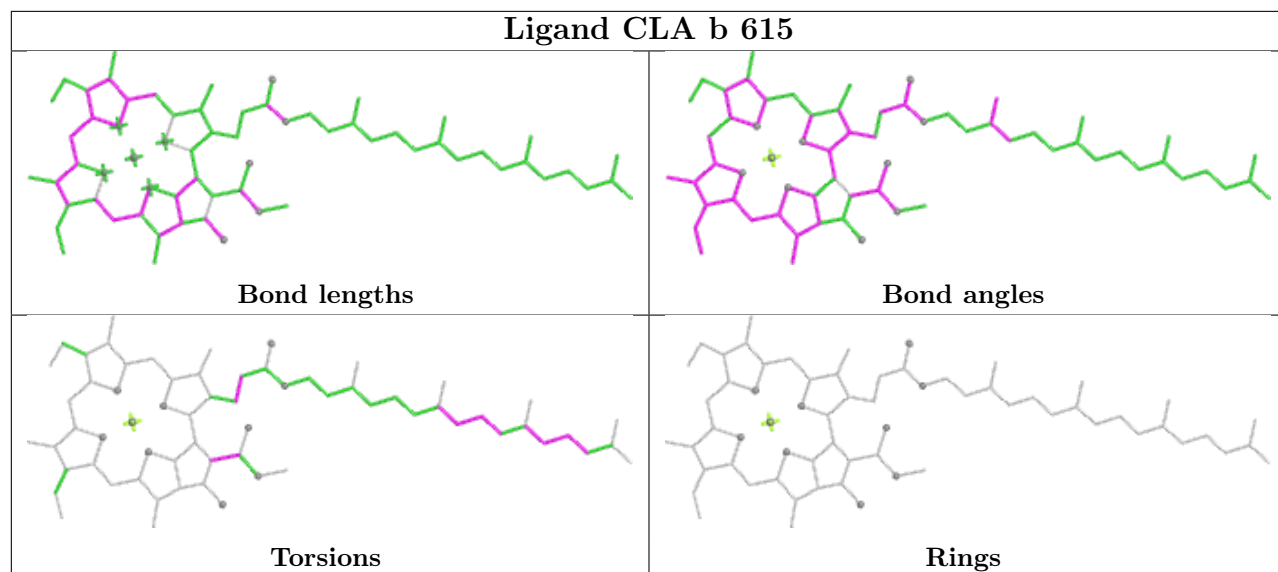


## Ligand CLA c 517

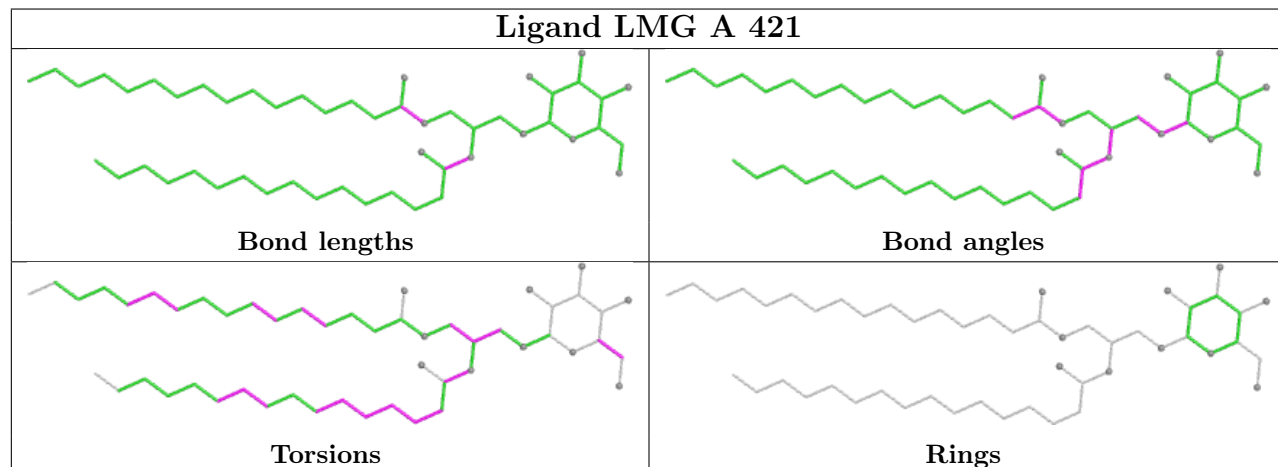




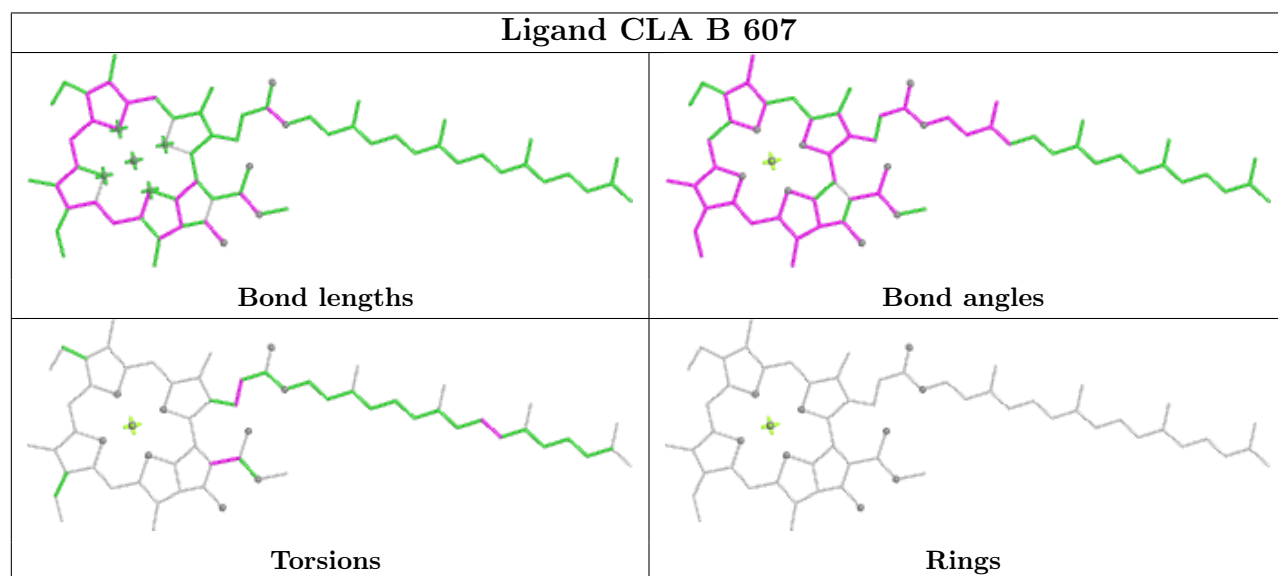
## Ligand CLA b 615

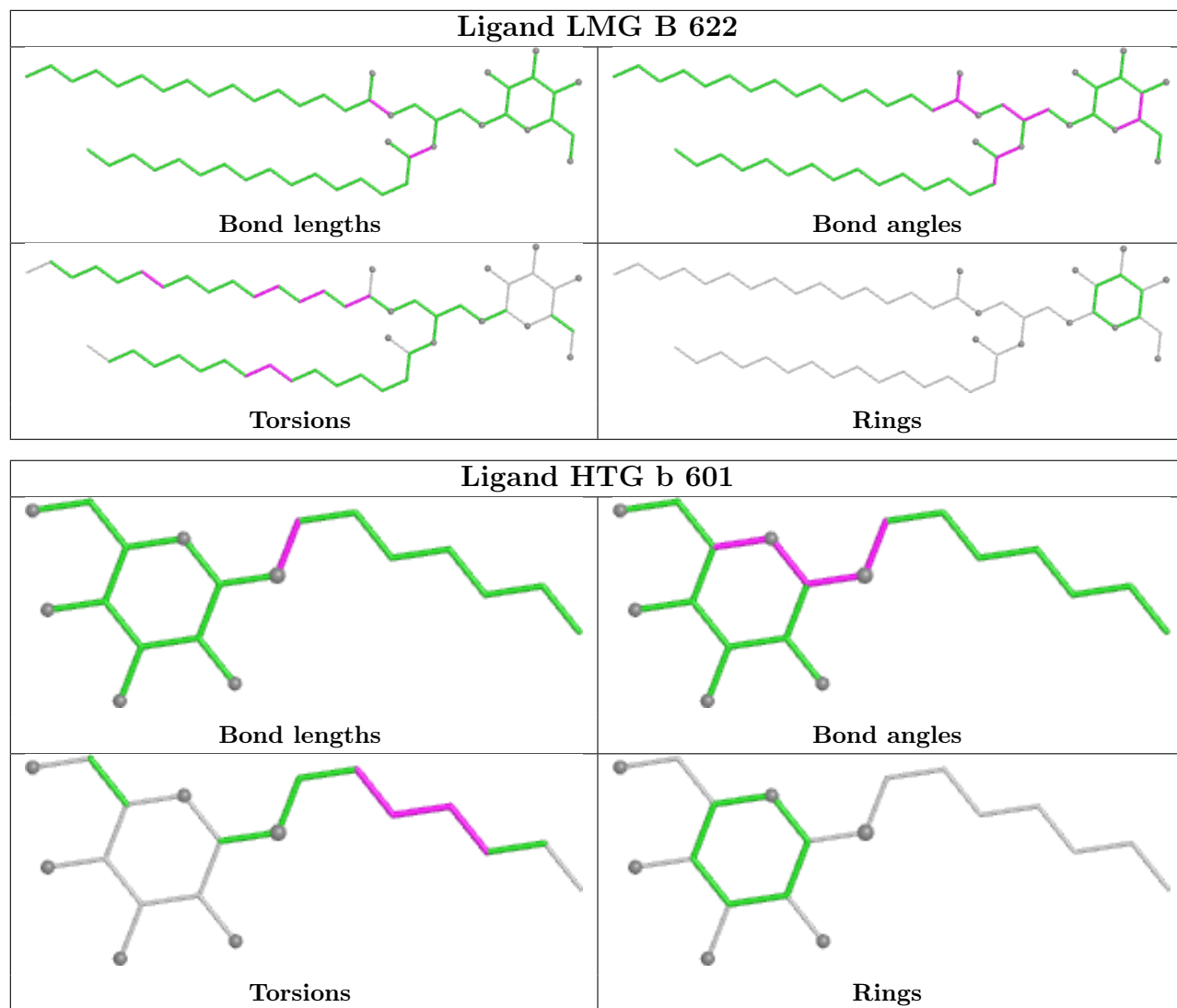


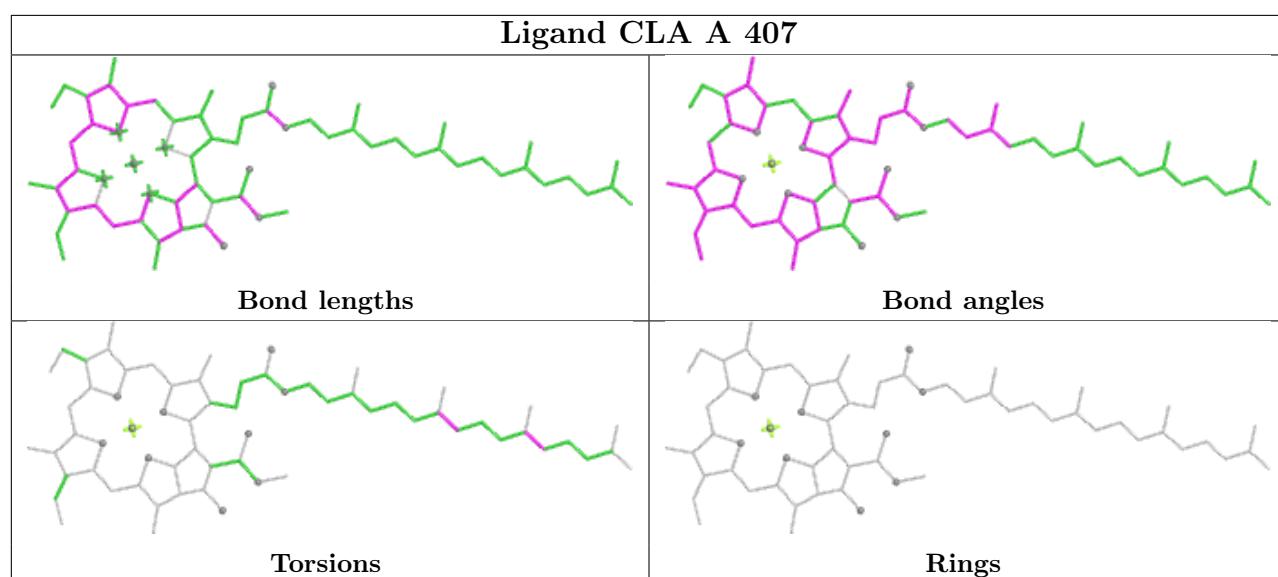
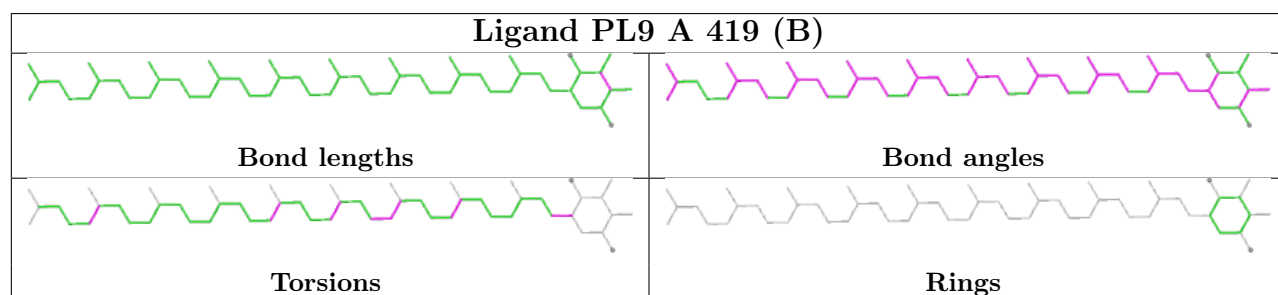
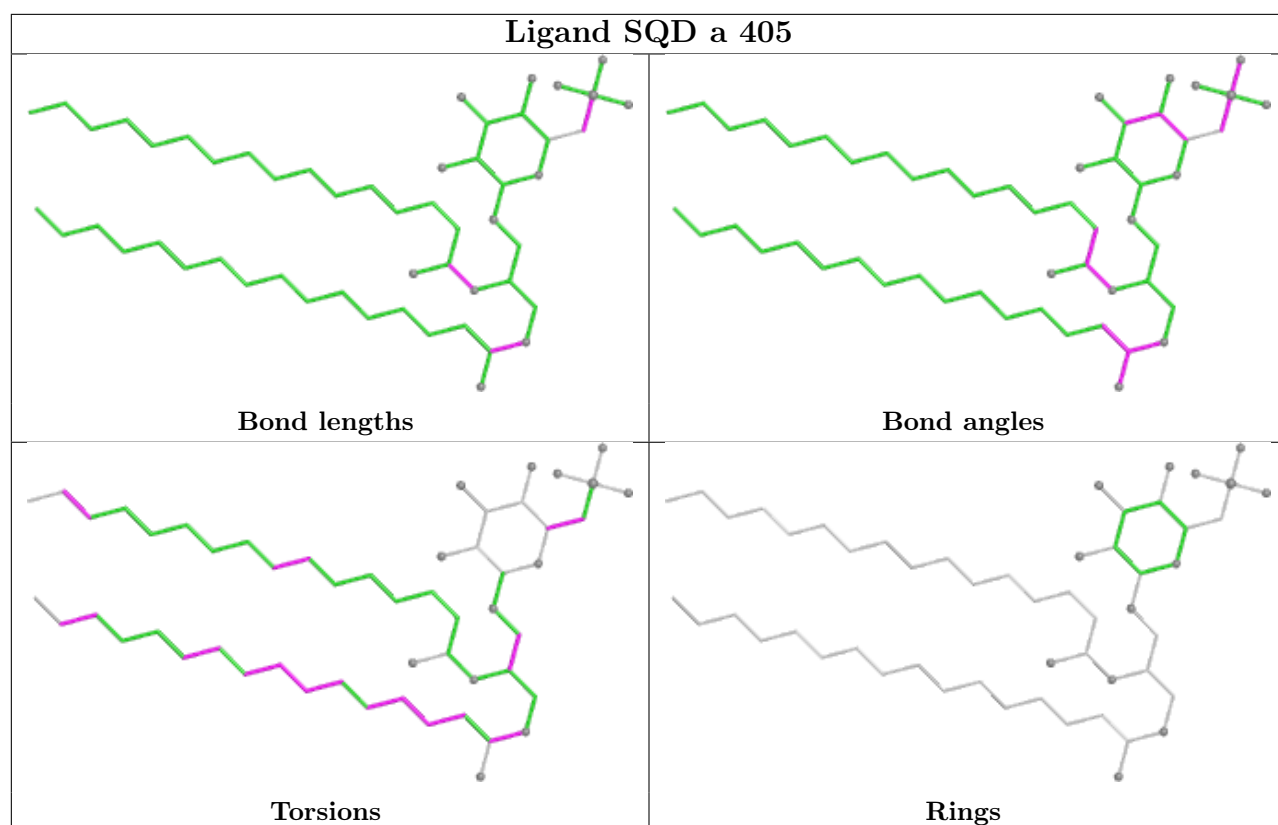
## Ligand LMG A 421

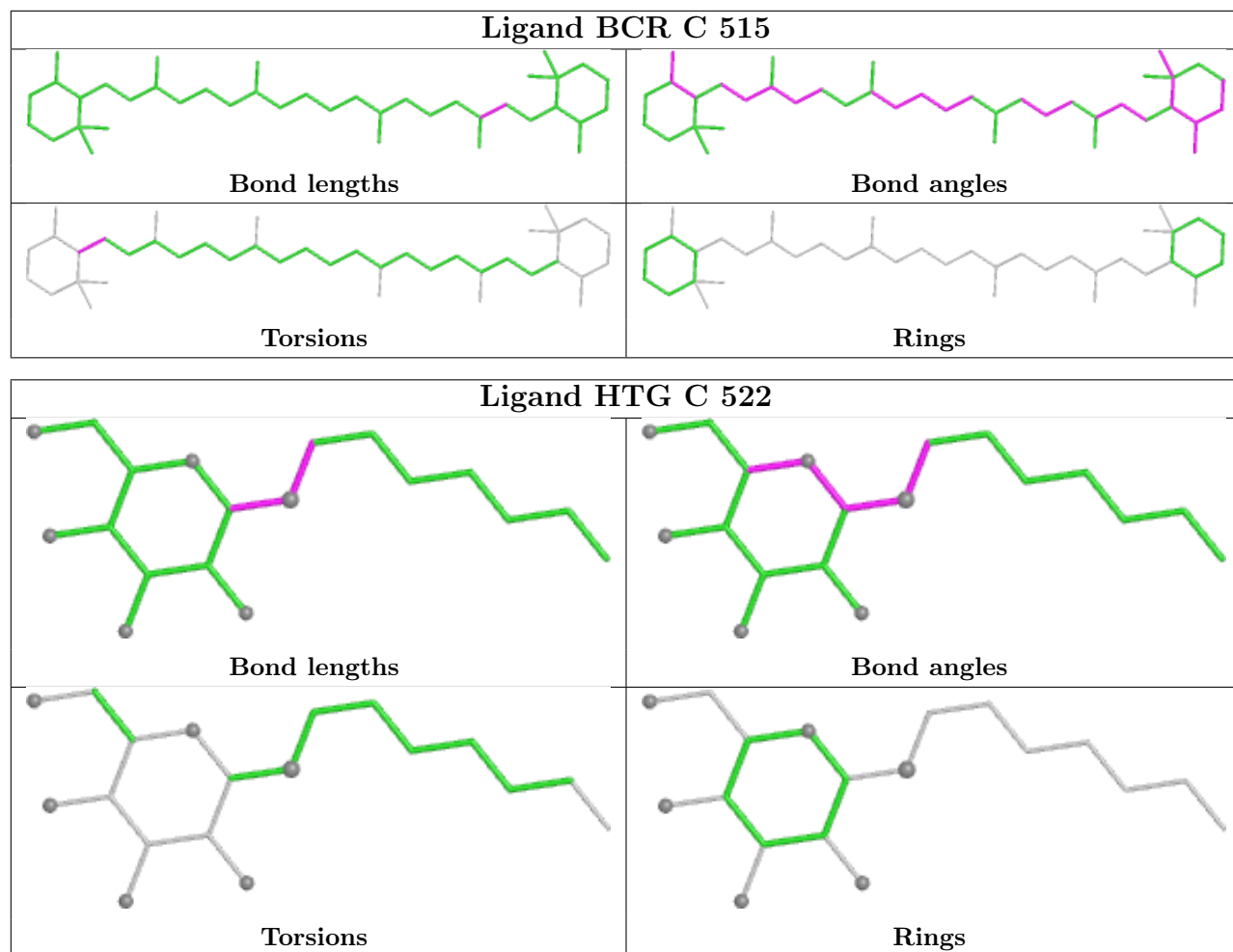


## Ligand CLA B 607

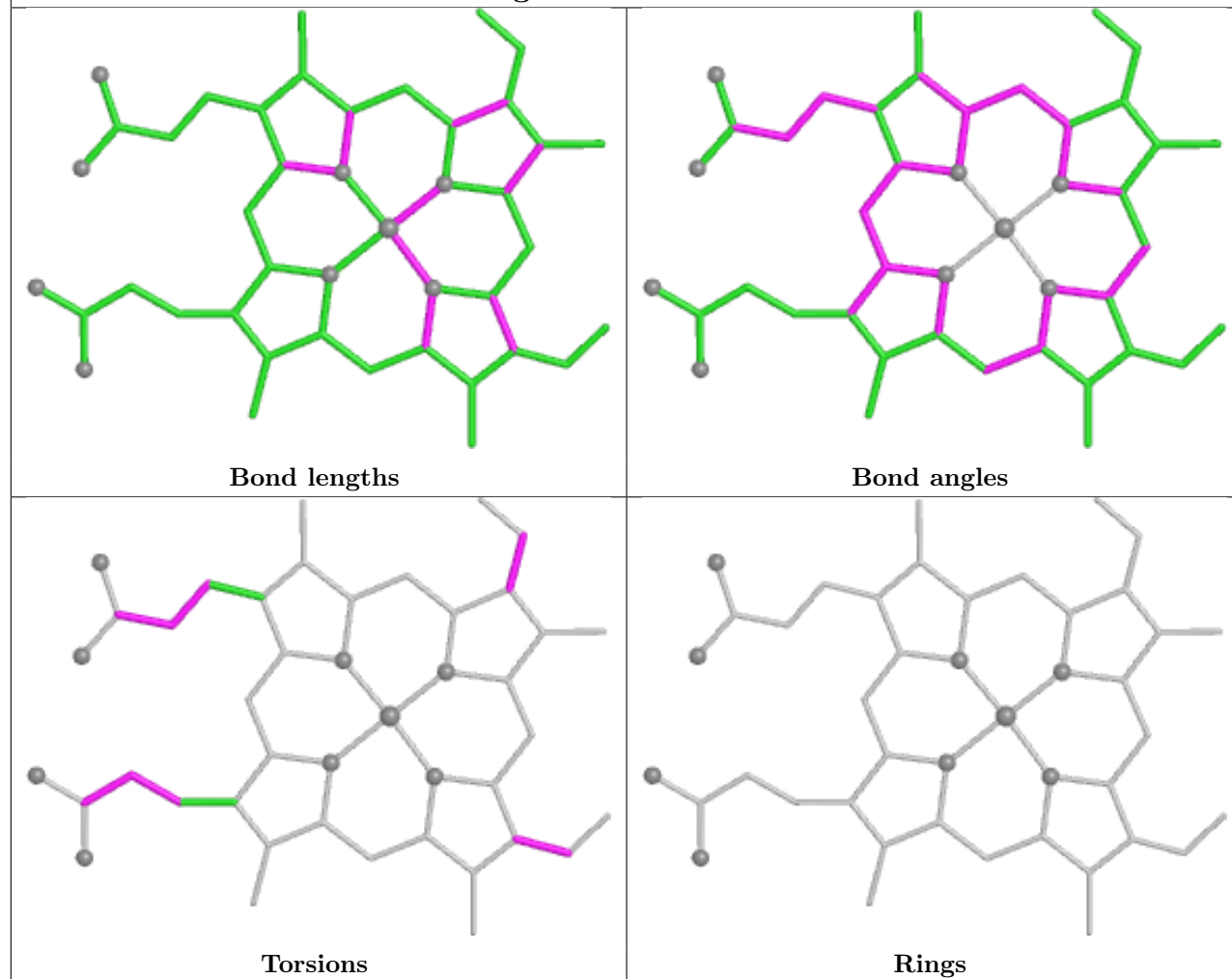




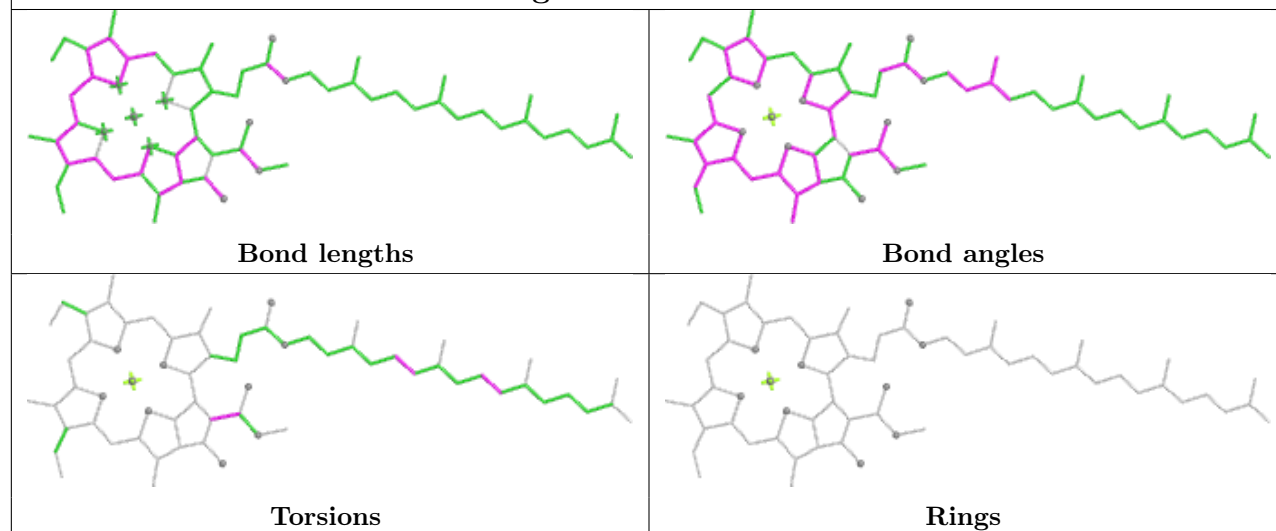




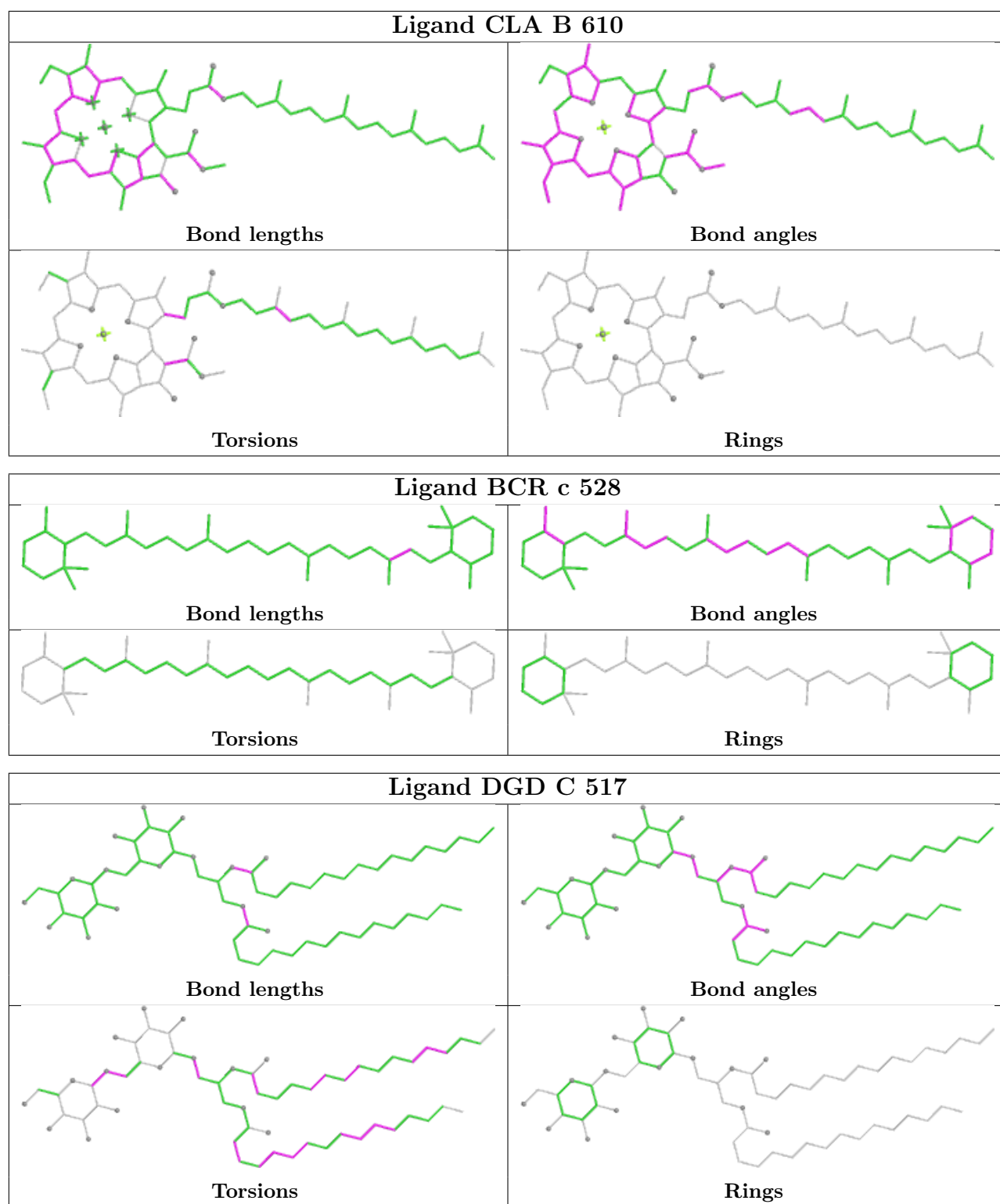
## Ligand HEM e 103

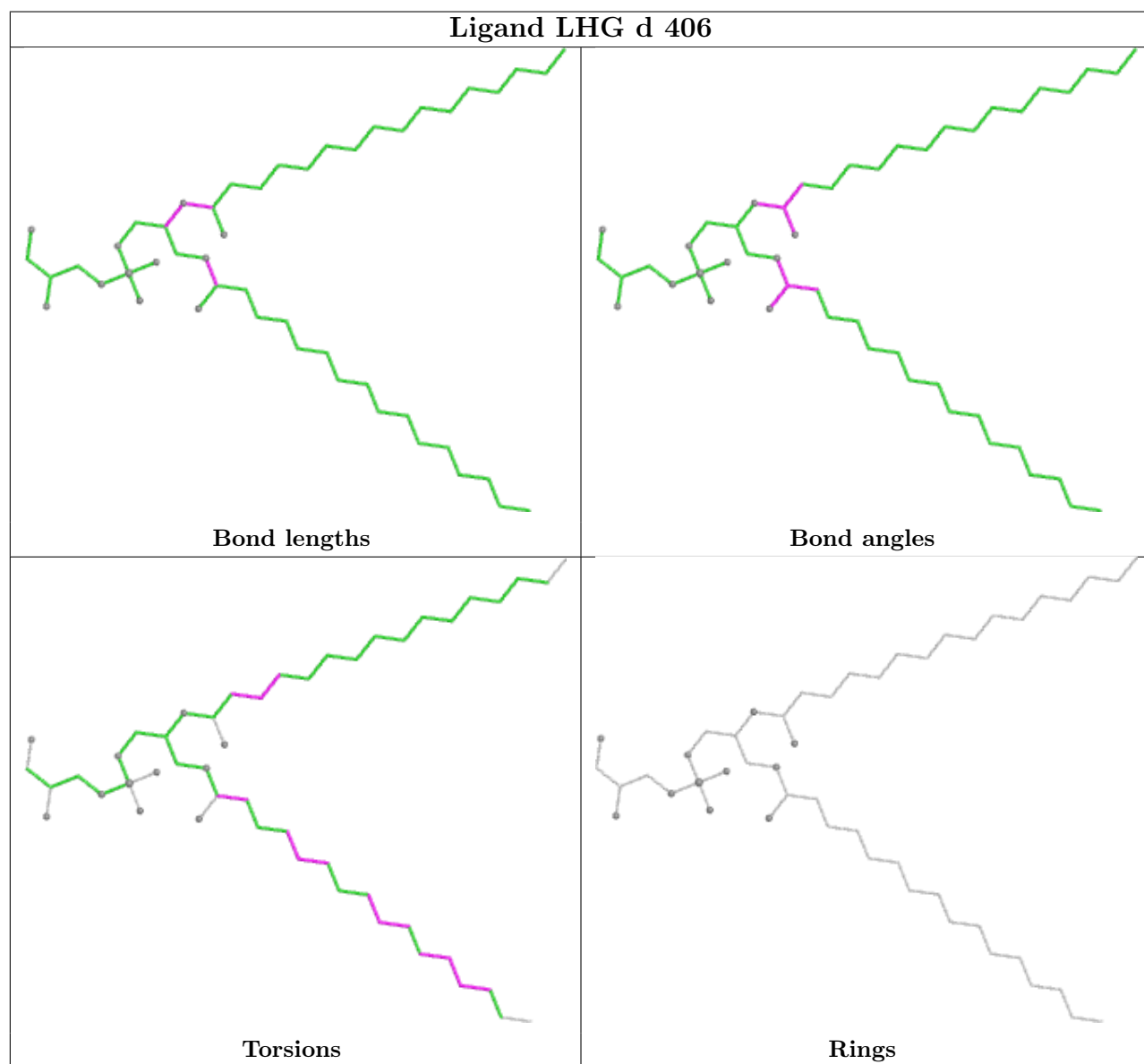
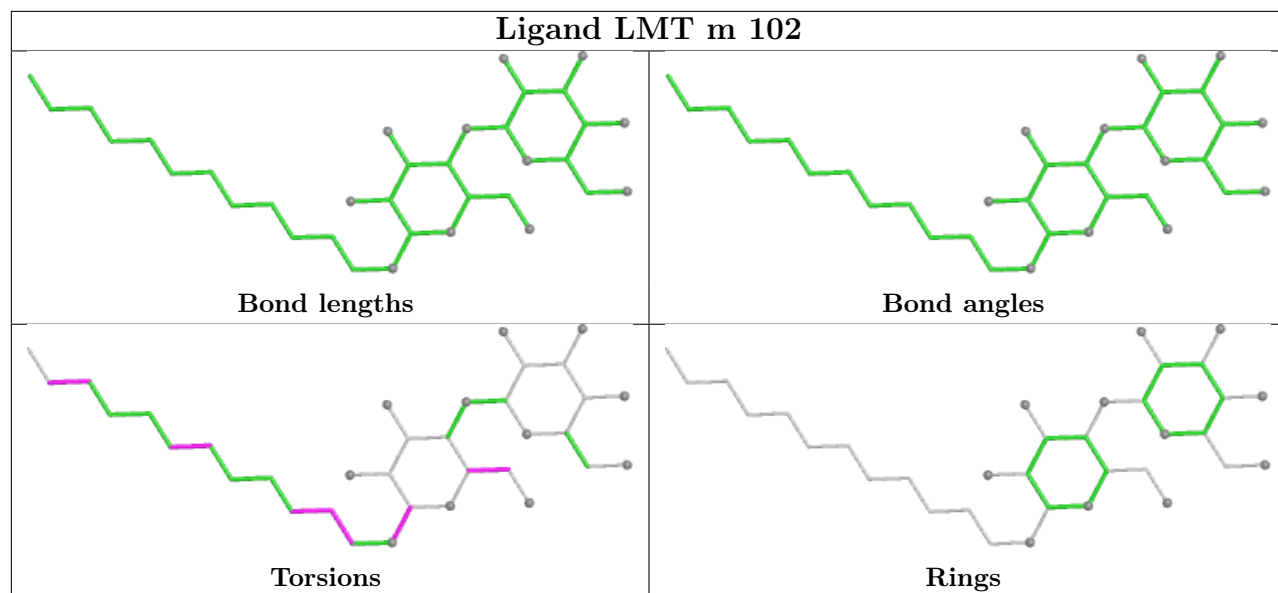


## Ligand CLA C 508

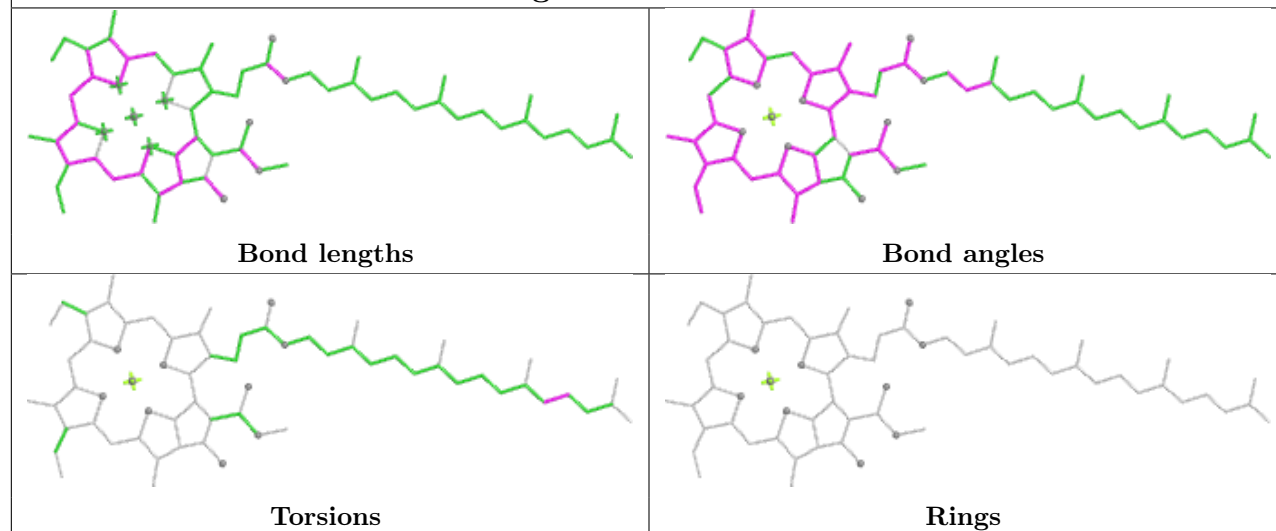




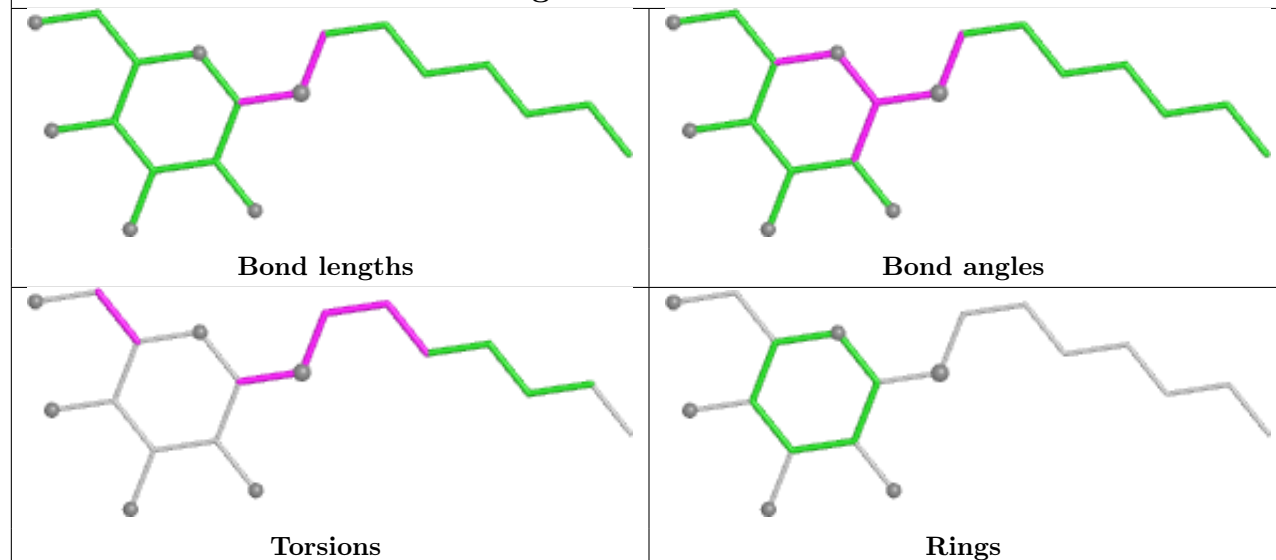




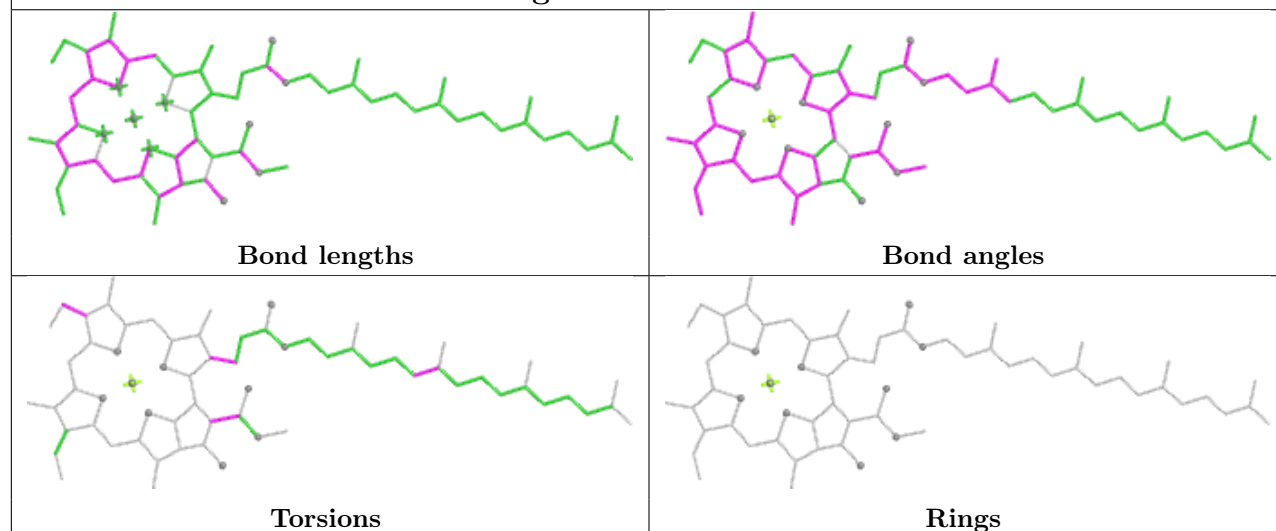
## Ligand CLA B 609

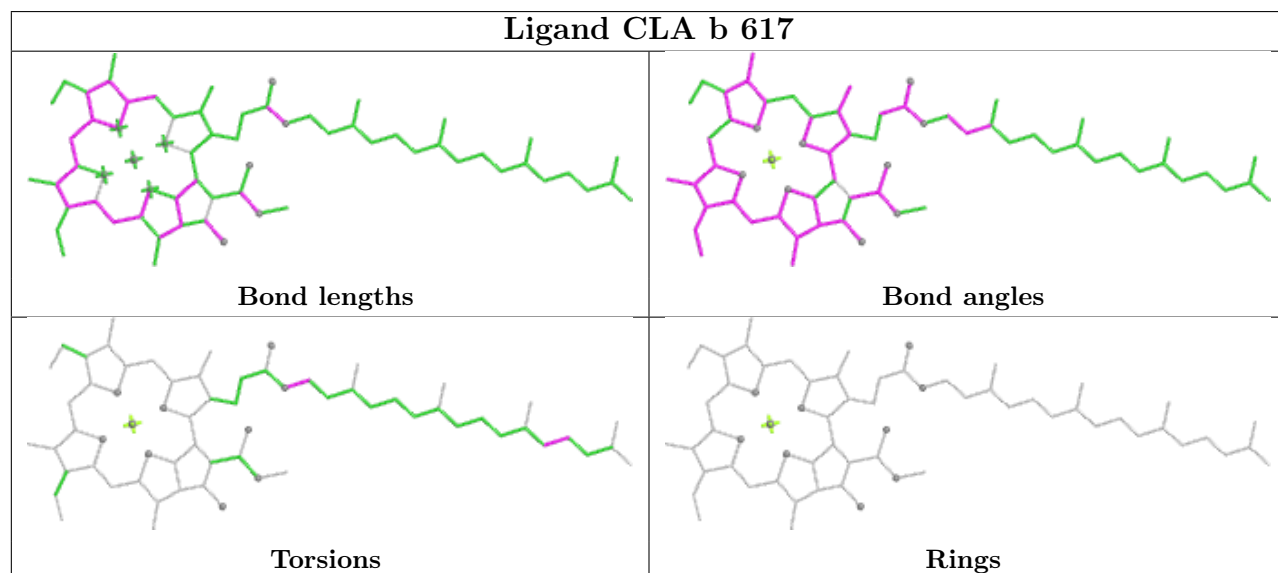
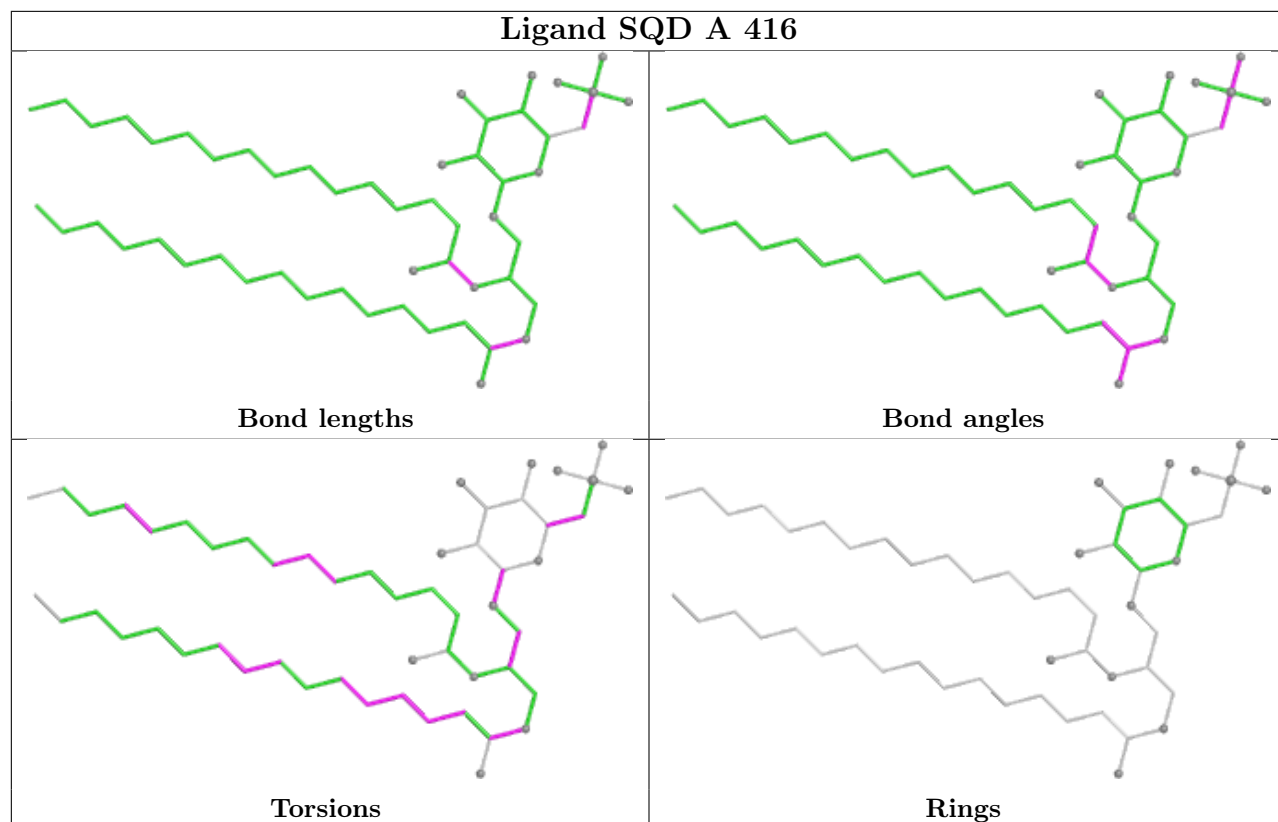


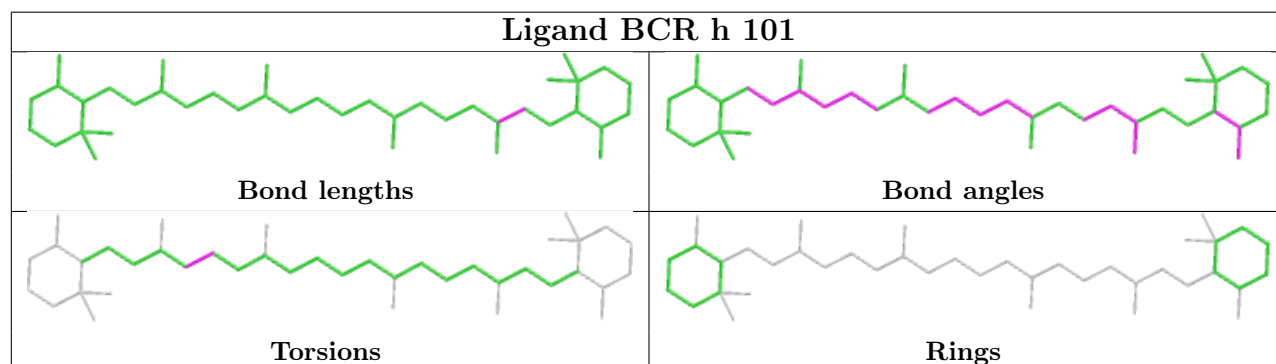
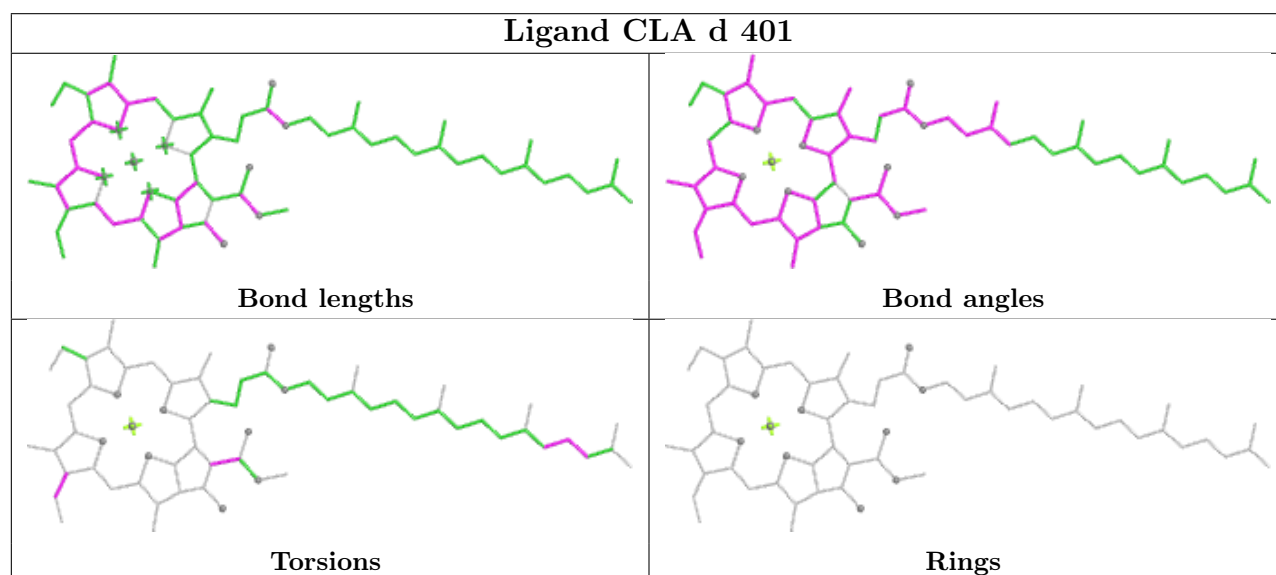
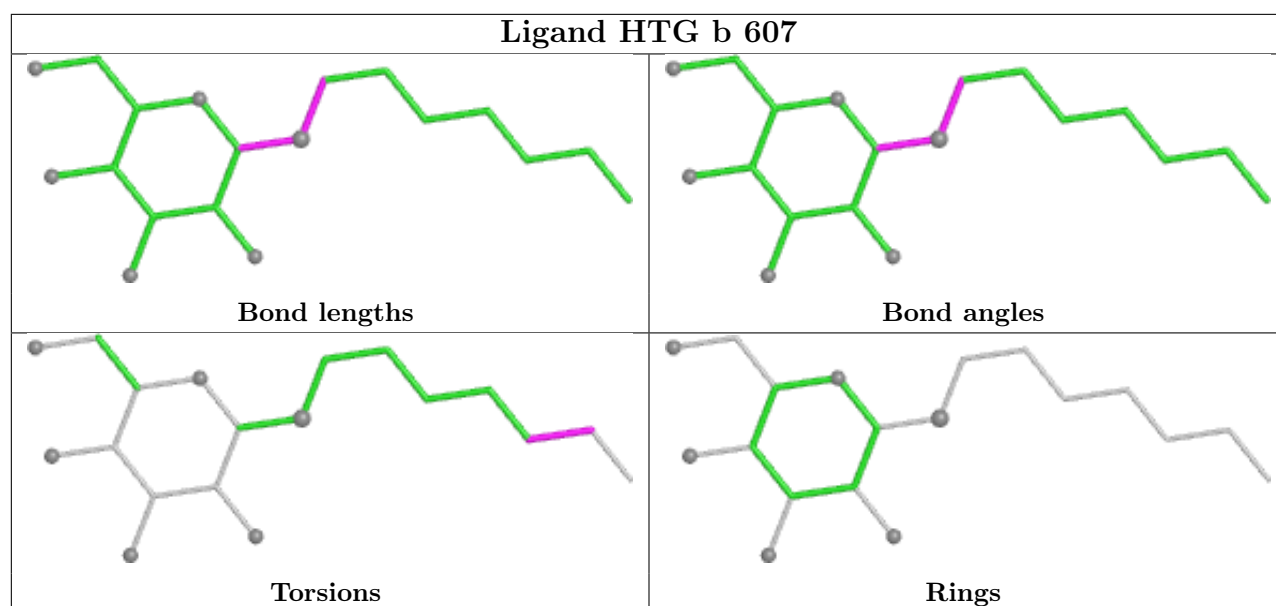
## Ligand HTG b 632

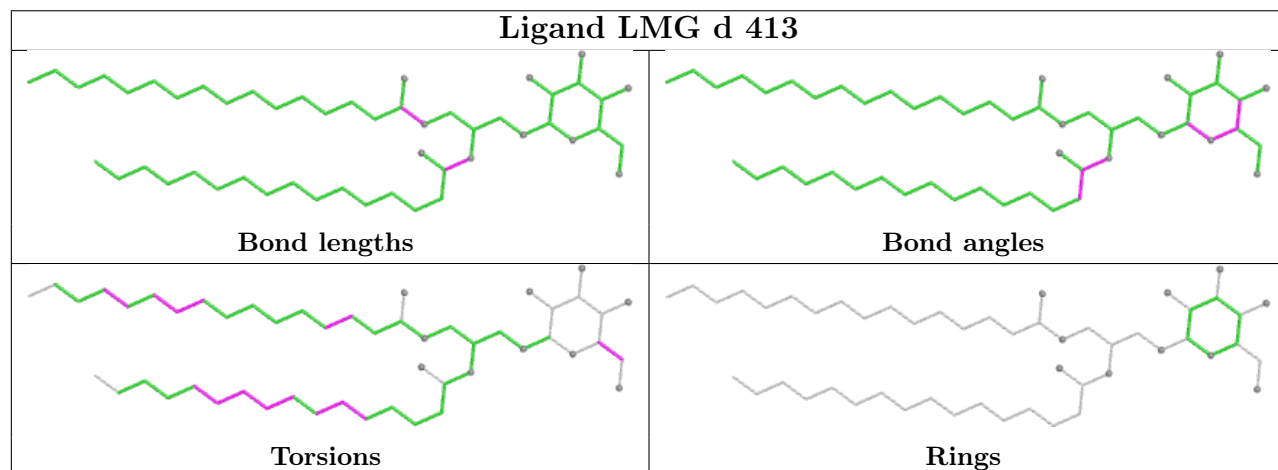
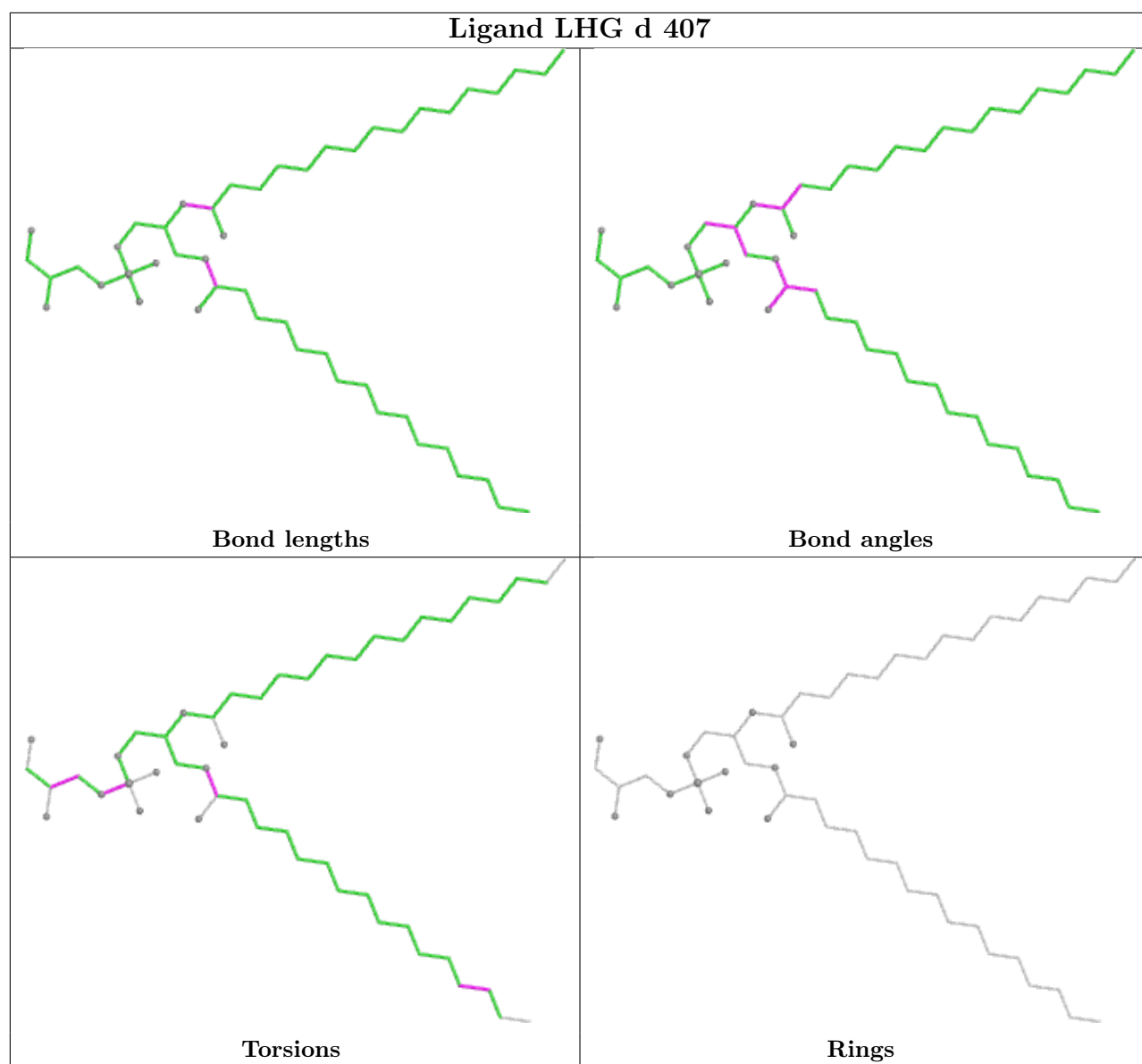


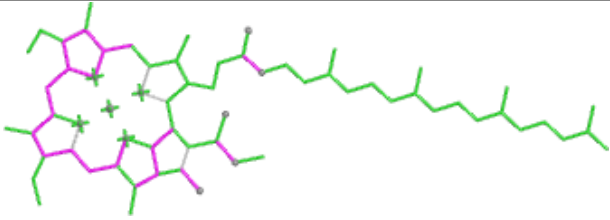
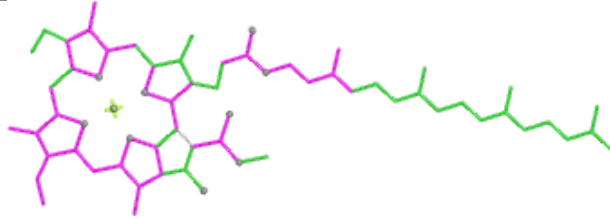
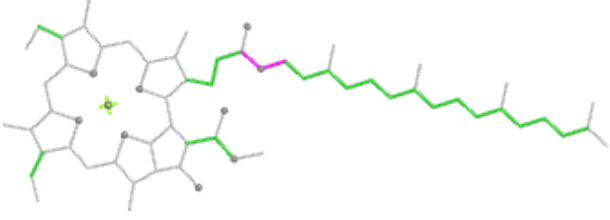
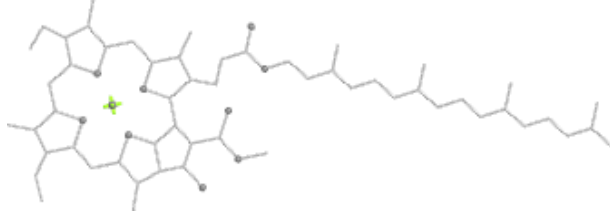
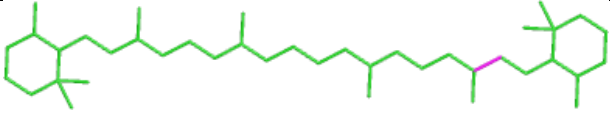
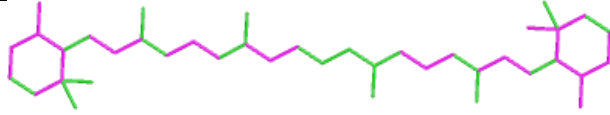
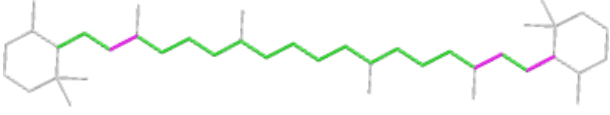
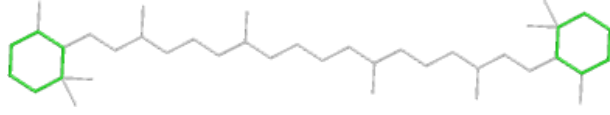
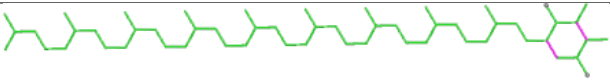
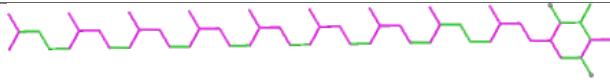
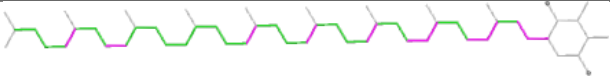
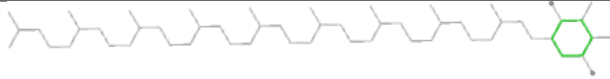
## Ligand CLA B 608

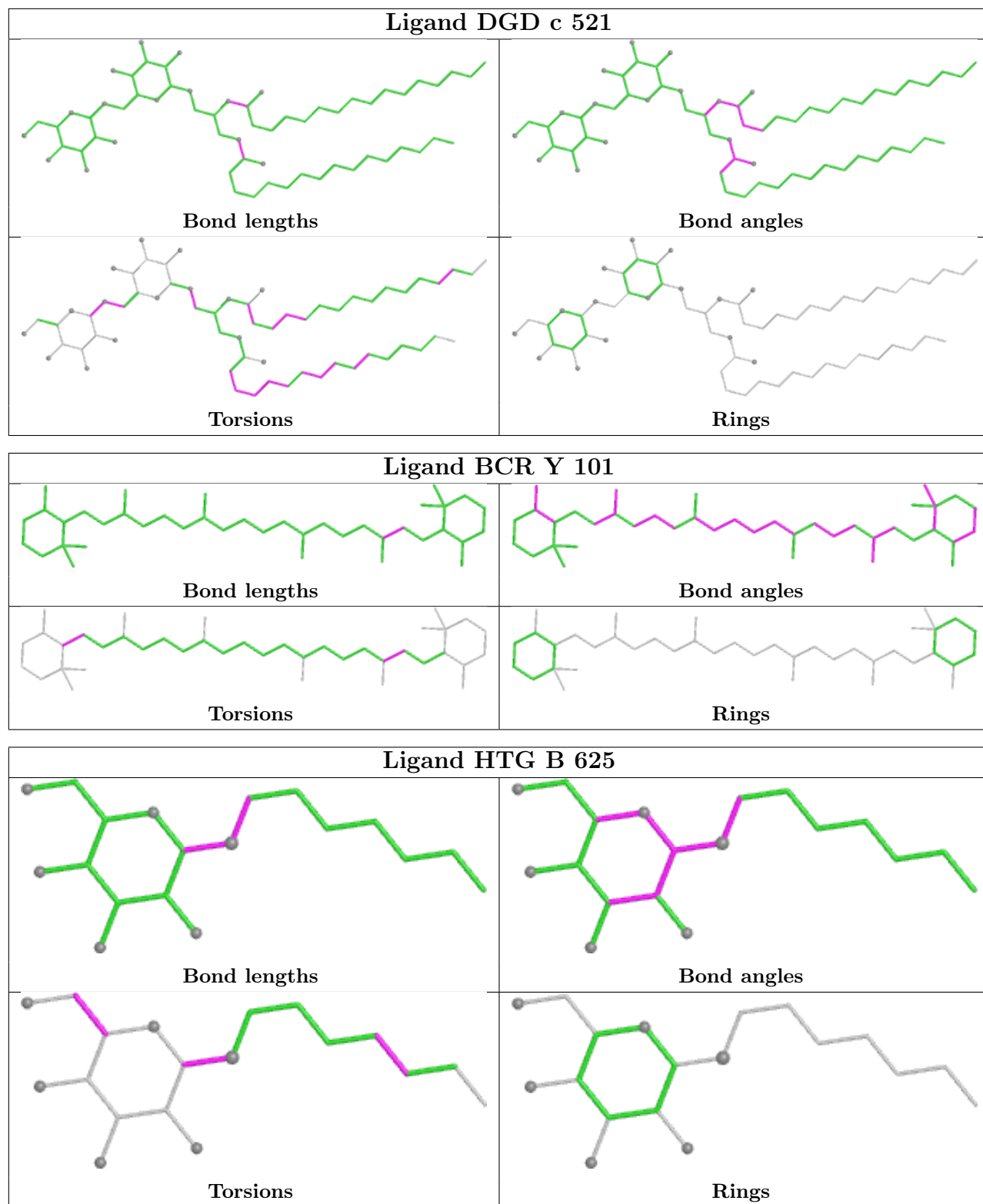




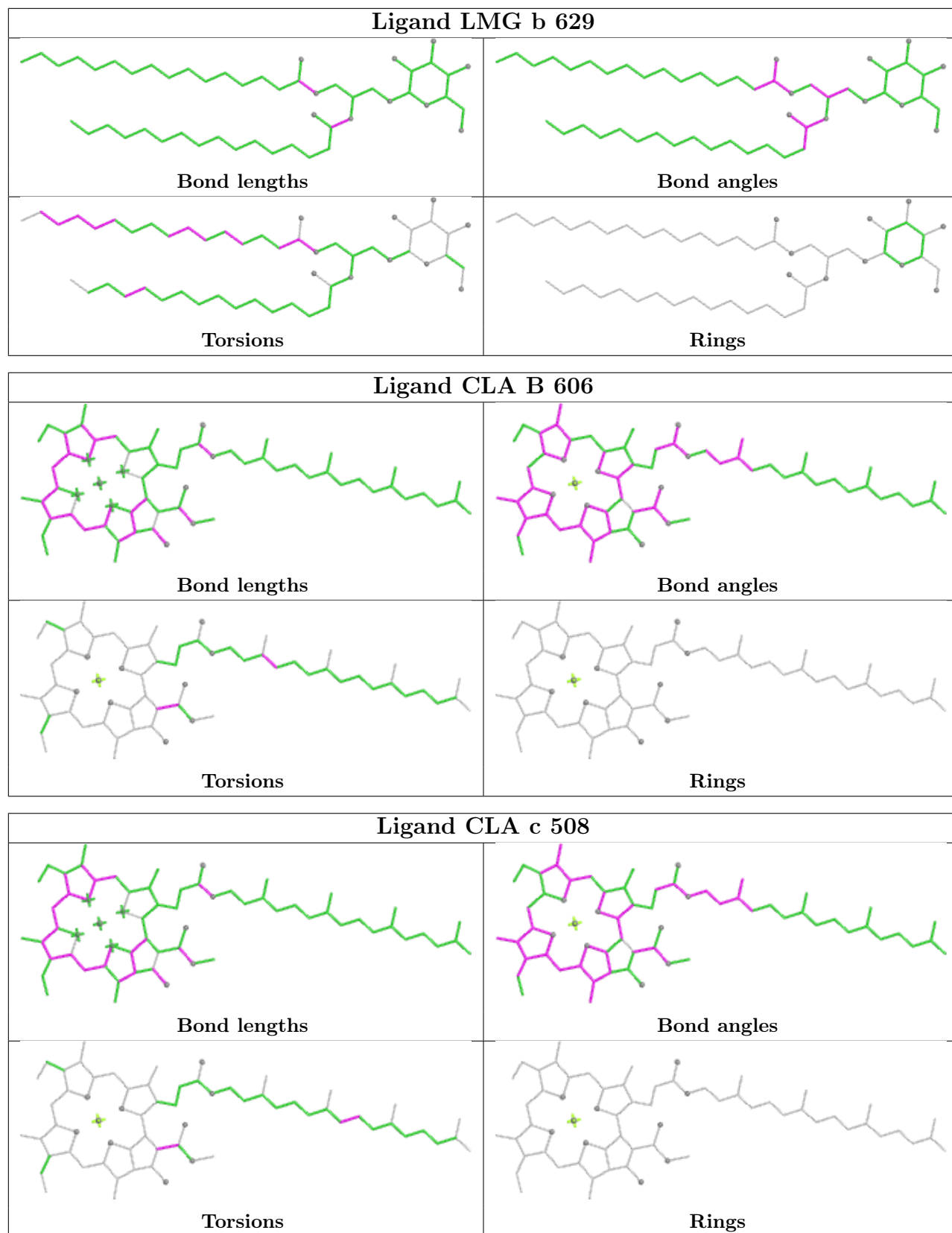


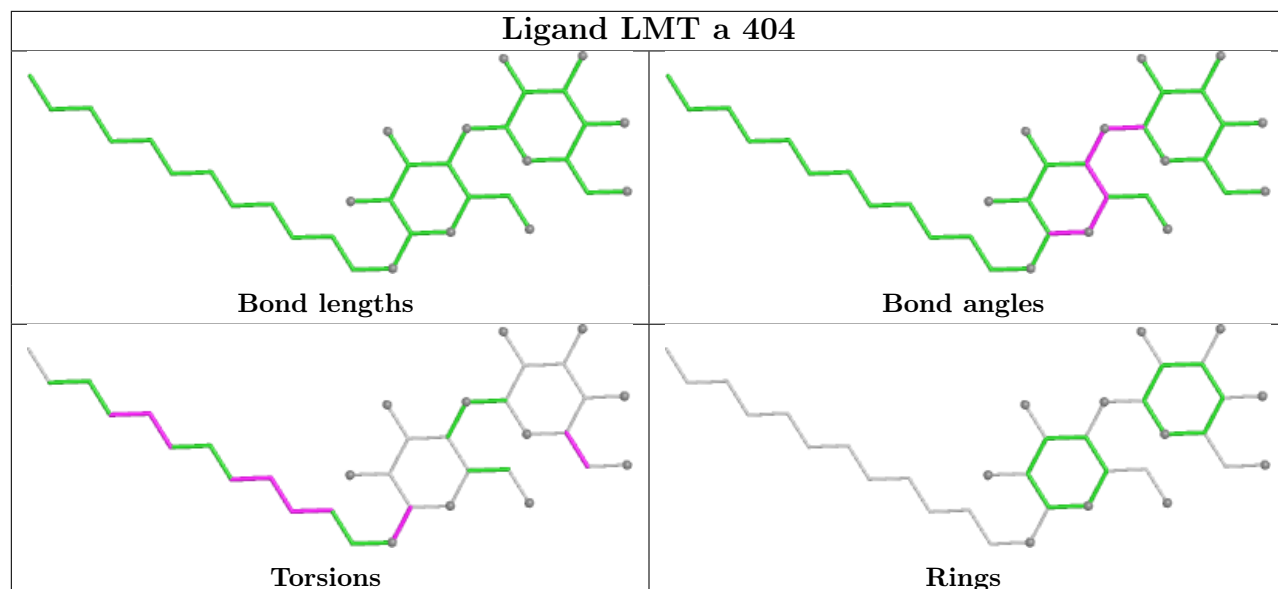
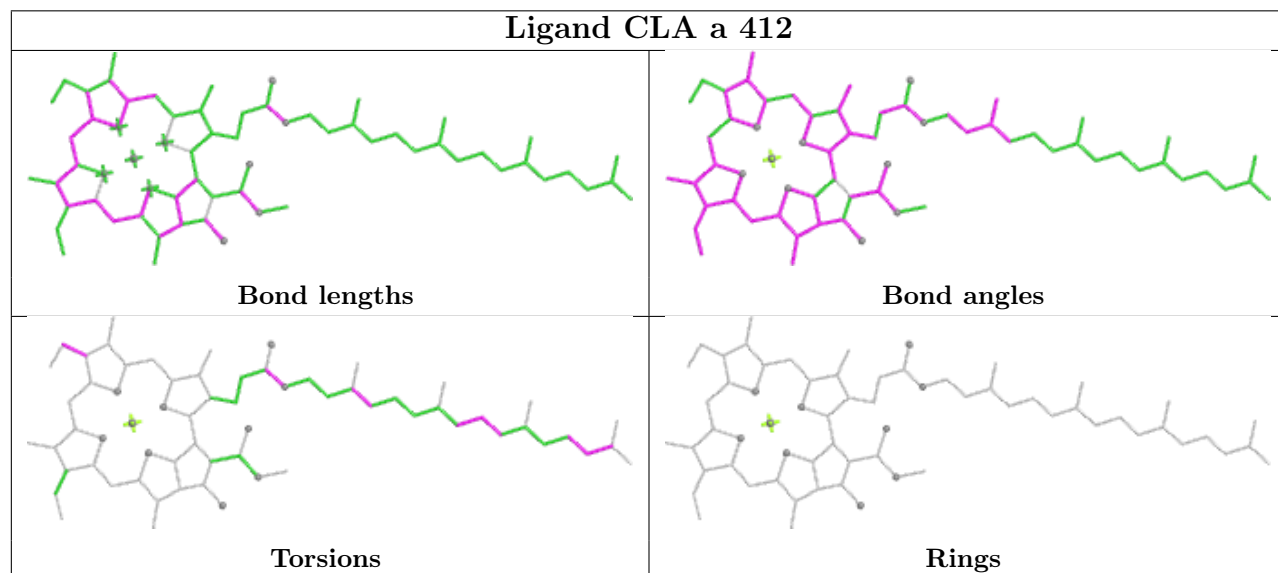
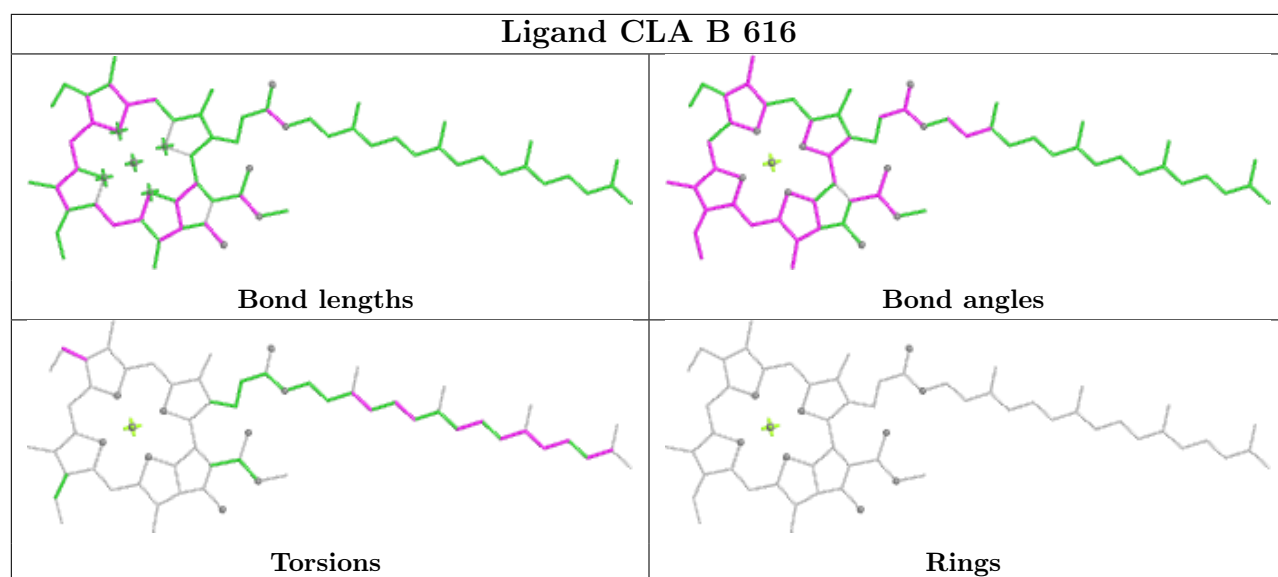


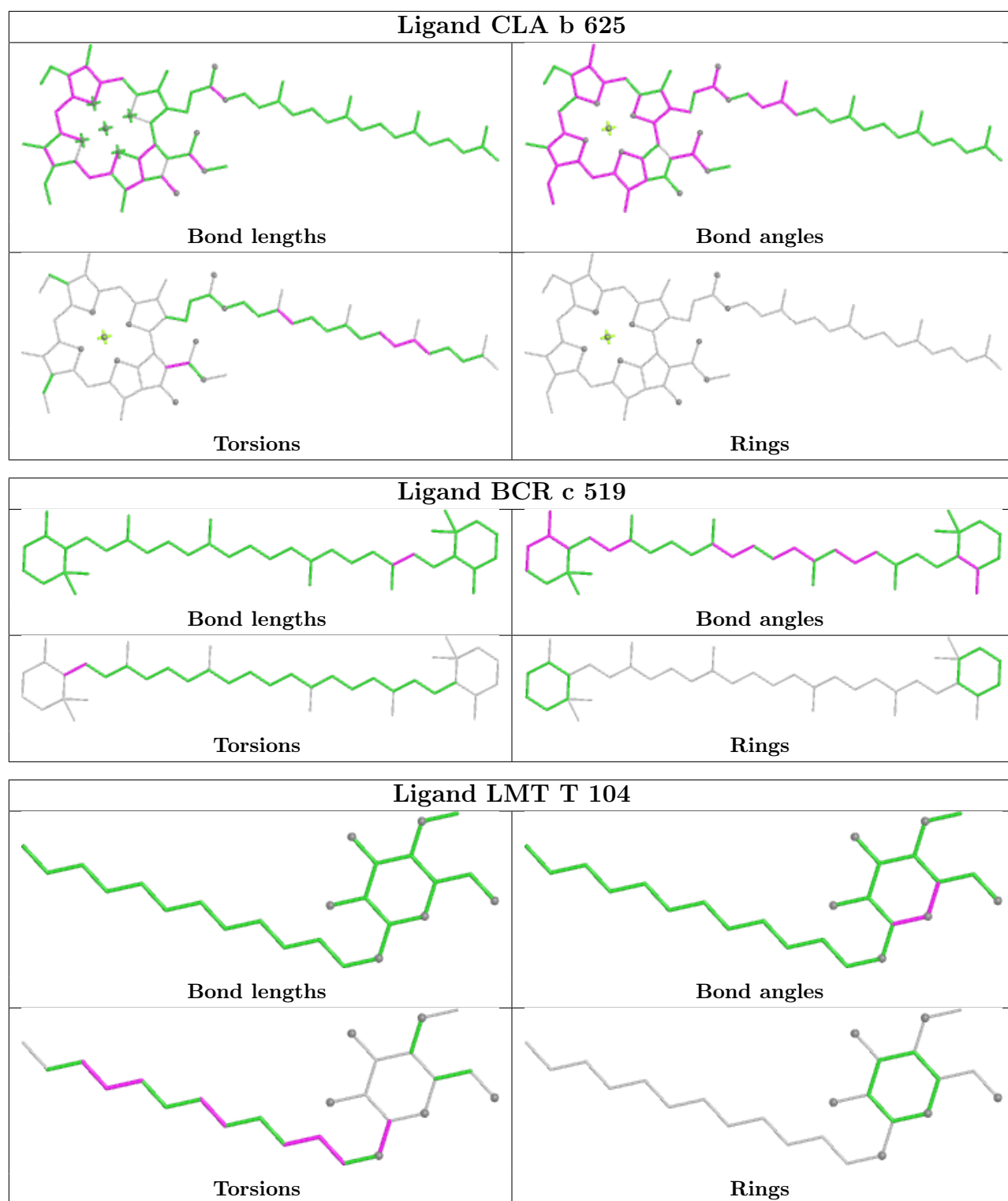
| Ligand CLA C 511                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR d 404                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand PL9 a 415 (A)                                                                                    |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

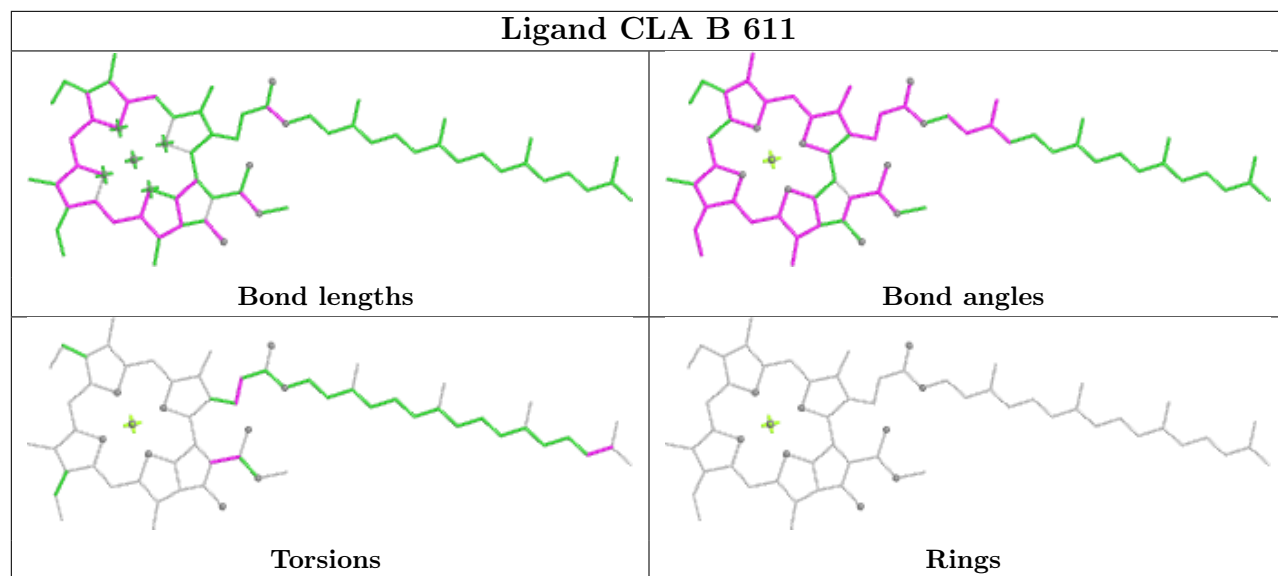












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|----------------|--------|--------------|-----------------------|----------|
| 1   | A     | 334/344 (97%)  | -0.70  | 0 100 100    | 16, 37, 62, 117       | 53 (15%) |
| 1   | a     | 334/344 (97%)  | -0.66  | 4 (1%) 76 79 | 17, 38, 70, 152       | 55 (16%) |
| 2   | B     | 504/505 (99%)  | -0.63  | 2 (0%) 88 90 | 23, 43, 77, 123       | 10 (1%)  |
| 2   | b     | 503/505 (99%)  | -0.54  | 6 (1%) 76 79 | 26, 43, 78, 180       | 12 (2%)  |
| 3   | C     | 451/455 (99%)  | -0.52  | 0 100 100    | 17, 51, 70, 116       | 7 (1%)   |
| 3   | c     | 455/455 (100%) | -0.52  | 0 100 100    | 19, 53, 70, 115       | 13 (2%)  |
| 4   | D     | 341/342 (99%)  | -0.74  | 0 100 100    | 18, 39, 61, 131       | 16 (4%)  |
| 4   | d     | 341/342 (99%)  | -0.72  | 1 (0%) 90 91 | 19, 41, 60, 122       | 16 (4%)  |
| 5   | E     | 81/84 (96%)    | -0.09  | 1 (1%) 76 79 | 32, 63, 94, 130       | 2 (2%)   |
| 5   | e     | 81/84 (96%)    | -0.00  | 2 (2%) 58 62 | 36, 64, 115, 176      | 2 (2%)   |
| 6   | F     | 34/44 (77%)    | -0.18  | 0 100 100    | 46, 56, 90, 105       | 0        |
| 6   | f     | 32/44 (72%)    | -0.15  | 1 (3%) 51 55 | 47, 57, 116, 141      | 0        |
| 7   | H     | 65/65 (100%)   | -0.31  | 2 (3%) 51 55 | 35, 52, 72, 150       | 1 (1%)   |
| 7   | h     | 65/65 (100%)   | -0.39  | 2 (3%) 51 55 | 42, 55, 75, 163       | 0        |
| 8   | I     | 37/38 (97%)    | -0.26  | 0 100 100    | 43, 54, 108, 151      | 0        |
| 8   | i     | 37/38 (97%)    | -0.23  | 1 (2%) 56 60 | 42, 52, 98, 131       | 0        |
| 9   | J     | 38/39 (97%)    | 0.09   | 2 (5%) 32 36 | 46, 61, 135, 169      | 0        |
| 9   | j     | 39/39 (100%)   | -0.05  | 1 (2%) 57 61 | 47, 61, 131, 171      | 0        |
| 10  | K     | 37/37 (100%)   | -0.29  | 0 100 100    | 51, 61, 77, 101       | 0        |
| 10  | k     | 37/37 (100%)   | -0.32  | 0 100 100    | 52, 61, 77, 102       | 0        |
| 11  | L     | 37/37 (100%)   | -0.72  | 0 100 100    | 18, 35, 100, 120      | 1 (2%)   |
| 11  | l     | 37/37 (100%)   | -0.65  | 0 100 100    | 22, 35, 99, 120       | 1 (2%)   |
| 12  | M     | 33/36 (91%)    | -0.72  | 0 100 100    | 22, 37, 63, 113       | 1 (3%)   |
| 12  | m     | 33/36 (91%)    | -0.67  | 0 100 100    | 32, 38, 68, 114       | 0        |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|-----------------|--------|---------------|-----------------------|----------|
| 13  | O     | 243/244 (99%)   | -0.57  | 2 (0%) 82 84  | 24, 48, 91, 137       | 8 (3%)   |
| 13  | o     | 243/244 (99%)   | -0.48  | 2 (0%) 82 84  | 27, 50, 104, 170      | 5 (2%)   |
| 14  | T     | 29/32 (90%)     | -0.74  | 1 (3%) 48 52  | 31, 37, 64, 133       | 1 (3%)   |
| 14  | t     | 29/32 (90%)     | -0.67  | 1 (3%) 48 52  | 29, 37, 64, 133       | 1 (3%)   |
| 15  | U     | 97/104 (93%)    | -0.65  | 0 100 100     | 37, 48, 77, 116       | 0        |
| 15  | u     | 97/104 (93%)    | -0.64  | 0 100 100     | 39, 49, 71, 116       | 0        |
| 16  | V     | 137/137 (100%)  | -0.54  | 0 100 100     | 20, 49, 78, 116       | 2 (1%)   |
| 16  | v     | 137/137 (100%)  | -0.54  | 1 (0%) 84 85  | 21, 55, 84, 118       | 1 (0%)   |
| 17  | Y     | 29/30 (96%)     | 0.76   | 3 (10%) 12 13 | 66, 80, 141, 149      | 0        |
| 17  | y     | 29/30 (96%)     | 0.42   | 3 (10%) 12 13 | 66, 81, 142, 149      | 0        |
| 18  | X     | 39/40 (97%)     | 0.09   | 1 (2%) 57 61  | 51, 61, 115, 136      | 0        |
| 18  | x     | 38/40 (95%)     | 0.19   | 2 (5%) 32 36  | 53, 62, 116, 137      | 0        |
| 19  | Z     | 62/62 (100%)    | 0.28   | 4 (6%) 25 28  | 66, 78, 125, 165      | 0        |
| 19  | z     | 62/62 (100%)    | 0.44   | 3 (4%) 35 40  | 68, 80, 126, 166      | 0        |
| 20  | R     | 18/34 (52%)     | 2.74   | 12 (66%) 0 0  | 106, 137, 176, 178    | 0        |
| All | All   | 5275/5384 (97%) | -0.50  | 60 (1%) 78 80 | 16, 47, 90, 180       | 208 (3%) |

All (60) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 20  | R     | 15  | ALA  | 5.2  |
| 20  | R     | 3   | TRP  | 4.3  |
| 19  | z     | 3   | ILE  | 4.0  |
| 2   | b     | 499 | VAL  | 3.9  |
| 20  | R     | 13  | LEU  | 3.9  |
| 7   | h     | 65  | LEU  | 3.8  |
| 18  | x     | 2   | THR  | 3.8  |
| 20  | R     | 9   | LEU  | 3.7  |
| 20  | R     | 5   | VAL  | 3.5  |
| 5   | e     | 5   | THR  | 3.5  |
| 7   | H     | 66  | GLY  | 3.4  |
| 2   | b     | 495 | PHE  | 3.4  |
| 20  | R     | 12  | VAL  | 3.4  |
| 2   | B     | 479 | PHE  | 3.3  |
| 17  | Y     | 18  | VAL  | 3.2  |
| 2   | b     | 486 | LEU  | 3.2  |
| 7   | H     | 65  | LEU  | 3.2  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 20  | R     | 10     | LEU  | 3.2  |
| 20  | R     | 14     | LEU  | 3.1  |
| 20  | R     | 6      | LEU  | 3.1  |
| 2   | B     | 495    | PHE  | 3.0  |
| 5   | e     | 4      | THR  | 3.0  |
| 14  | t     | 30     | THR  | 3.0  |
| 17  | y     | 18     | VAL  | 2.9  |
| 13  | o     | 58     | ASN  | 2.8  |
| 17  | Y     | 20     | ALA  | 2.8  |
| 20  | R     | 16     | ALA  | 2.8  |
| 2   | b     | 502    | VAL  | 2.8  |
| 20  | R     | 18     | TRP  | 2.8  |
| 19  | Z     | 3      | ILE  | 2.8  |
| 19  | Z     | 61     | VAL  | 2.7  |
| 5   | E     | 4      | THR  | 2.7  |
| 18  | x     | 37     | VAL  | 2.7  |
| 9   | j     | 1      | MET  | 2.6  |
| 20  | R     | 7      | VAL  | 2.6  |
| 17  | y     | 20     | ALA  | 2.6  |
| 1   | a     | 11     | ALA  | 2.6  |
| 17  | y     | 19     | ILE  | 2.6  |
| 7   | h     | 66     | GLY  | 2.6  |
| 19  | Z     | 33     | TRP  | 2.5  |
| 9   | J     | 2      | SER  | 2.5  |
| 17  | Y     | 19     | ILE  | 2.5  |
| 6   | f     | 14     | PRO  | 2.4  |
| 2   | b     | 493    | TRP  | 2.4  |
| 1   | a     | 263    | ALA  | 2.4  |
| 8   | i     | 37     | LEU  | 2.4  |
| 18  | X     | 37     | VAL  | 2.4  |
| 19  | Z     | 62     | VAL  | 2.4  |
| 13  | o     | 4      | THR  | 2.4  |
| 1   | a     | 260    | PHE  | 2.3  |
| 19  | z     | 62     | VAL  | 2.3  |
| 13  | O     | 4      | THR  | 2.2  |
| 19  | z     | 5      | PHE  | 2.2  |
| 16  | v     | 106    | ASN  | 2.1  |
| 14  | T     | 30     | THR  | 2.1  |
| 1   | a     | 248[A] | ILE  | 2.1  |
| 4   | d     | 12     | ARG  | 2.1  |
| 9   | J     | 5      | GLY  | 2.0  |
| 2   | b     | 479    | PHE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13  | O     | 56  | PRO  | 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 14  | FME  | T     | 1   | 10/11 | 0.96 | 0.06 | 35,38,64,74                | 0     |
| 12  | FME  | m     | 1   | 10/11 | 0.96 | 0.08 | 34,43,98,115               | 0     |
| 8   | FME  | I     | 1   | 10/11 | 0.97 | 0.07 | 37,45,52,53                | 0     |
| 8   | FME  | i     | 1   | 10/11 | 0.97 | 0.06 | 41,51,56,58                | 0     |
| 12  | FME  | M     | 1   | 10/11 | 0.97 | 0.07 | 31,47,81,85                | 0     |
| 14  | FME  | t     | 1   | 10/11 | 0.97 | 0.05 | 28,38,44,87                | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 36  | DGD  | e     | 101 | 62/66 | 0.69 | 0.16 | 70,118,175,181             | 0     |
| 36  | DGD  | D     | 406 | 52/66 | 0.70 | 0.15 | 65,108,147,157             | 0     |
| 37  | LHG  | e     | 102 | 42/49 | 0.70 | 0.13 | 69,134,167,172             | 0     |
| 29  | LMT  | F     | 101 | 35/35 | 0.73 | 0.15 | 86,125,152,156             | 0     |
| 34  | CA   | b     | 609 | 1/1   | 0.75 | 0.12 | 134,134,134,134            | 0     |
| 29  | LMT  | b     | 630 | 25/35 | 0.75 | 0.14 | 72,92,147,149              | 0     |
| 29  | LMT  | C     | 521 | 35/35 | 0.76 | 0.14 | 90,123,152,162             | 0     |
| 32  | UNL  | M     | 102 | 10/-  | 0.76 | 0.12 | 47,64,75,75                | 0     |
| 29  | LMT  | a     | 419 | 35/35 | 0.77 | 0.14 | 87,111,130,134             | 0     |
| 32  | UNL  | a     | 403 | 30/-  | 0.77 | 0.14 | 69,91,126,131              | 0     |
| 27  | SQD  | f     | 101 | 43/54 | 0.77 | 0.14 | 86,120,144,145             | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 32  | UNL  | m     | 101    | 10/-  | 0.78 | 0.15 | 49,60,85,88                 | 0     |
| 35  | HTG  | D     | 412    | 16/19 | 0.79 | 0.14 | 75,142,157,157              | 0     |
| 32  | UNL  | j     | 101    | 10/-  | 0.79 | 0.14 | 70,82,96,99                 | 0     |
| 28  | GOL  | V     | 201    | 6/6   | 0.79 | 0.14 | 64,77,86,93                 | 0     |
| 29  | LMT  | f     | 102    | 35/35 | 0.79 | 0.13 | 72,121,149,154              | 0     |
| 29  | LMT  | M     | 103    | 35/35 | 0.80 | 0.14 | 41,102,141,150              | 0     |
| 32  | UNL  | A     | 420    | 28/-  | 0.80 | 0.14 | 61,86,104,106               | 0     |
| 35  | HTG  | c     | 526    | 19/19 | 0.80 | 0.12 | 66,105,123,137              | 0     |
| 32  | UNL  | C     | 527    | 34/-  | 0.81 | 0.13 | 73,108,129,134              | 0     |
| 32  | UNL  | I     | 101    | 40/-  | 0.81 | 0.14 | 41,84,142,153               | 0     |
| 29  | LMT  | A     | 417    | 35/35 | 0.82 | 0.12 | 40,80,108,129               | 0     |
| 35  | HTG  | V     | 206    | 19/19 | 0.82 | 0.12 | 66,94,116,209               | 0     |
| 32  | UNL  | J     | 101    | 10/-  | 0.82 | 0.13 | 47,72,89,101                | 0     |
| 33  | LMG  | C     | 520    | 51/55 | 0.82 | 0.12 | 56,109,125,129              | 0     |
| 32  | UNL  | i     | 101    | 40/-  | 0.82 | 0.13 | 48,78,138,141               | 0     |
| 37  | LHG  | E     | 101    | 42/49 | 0.82 | 0.12 | 67,101,123,128              | 0     |
| 35  | HTG  | B     | 625    | 19/19 | 0.82 | 0.11 | 70,112,141,147              | 0     |
| 35  | HTG  | b     | 608    | 19/19 | 0.83 | 0.12 | 56,108,148,148              | 0     |
| 29  | LMT  | D     | 401    | 35/35 | 0.83 | 0.12 | 67,118,146,155              | 0     |
| 32  | UNL  | D     | 411    | 40/-  | 0.83 | 0.12 | 52,79,130,139               | 0     |
| 35  | HTG  | d     | 411    | 16/19 | 0.84 | 0.11 | 65,109,124,127              | 0     |
| 28  | GOL  | c     | 503    | 6/6   | 0.84 | 0.17 | 76,80,97,101                | 0     |
| 32  | UNL  | b     | 633    | 33/-  | 0.84 | 0.14 | 50,94,155,158               | 0     |
| 32  | UNL  | c     | 527    | 32/-  | 0.84 | 0.13 | 67,100,136,144              | 0     |
| 35  | HTG  | B     | 633    | 19/19 | 0.84 | 0.11 | 56,109,139,175              | 0     |
| 33  | LMG  | z     | 101    | 39/55 | 0.85 | 0.13 | 67,115,138,158              | 0     |
| 34  | CA   | B     | 601    | 1/1   | 0.85 | 0.08 | 130,130,130,130             | 0     |
| 31  | PL9  | A     | 419[A] | 55/55 | 0.85 | 0.14 | 68,94,108,110               | 55    |
| 31  | PL9  | A     | 419[B] | 55/55 | 0.85 | 0.14 | 69,94,108,111               | 55    |
| 31  | PL9  | a     | 415[A] | 55/55 | 0.85 | 0.15 | 75,104,117,119              | 55    |
| 31  | PL9  | a     | 415[B] | 55/55 | 0.85 | 0.15 | 73,103,117,120              | 55    |
| 29  | LMT  | a     | 404    | 35/35 | 0.85 | 0.12 | 47,82,112,131               | 0     |
| 32  | UNL  | d     | 410    | 36/-  | 0.85 | 0.11 | 51,76,129,142               | 0     |
| 32  | UNL  | B     | 634    | 33/-  | 0.85 | 0.14 | 56,87,134,138               | 0     |
| 27  | SQD  | B     | 621    | 54/54 | 0.85 | 0.12 | 51,88,147,155               | 0     |
| 28  | GOL  | O     | 301    | 6/6   | 0.85 | 0.10 | 64,79,82,85                 | 0     |
| 27  | SQD  | F     | 103    | 43/54 | 0.85 | 0.11 | 76,102,119,129              | 0     |
| 33  | LMG  | Z     | 101    | 37/55 | 0.85 | 0.14 | 54,111,132,135              | 0     |
| 33  | LMG  | c     | 524    | 51/55 | 0.85 | 0.11 | 49,106,129,132              | 0     |
| 35  | HTG  | C     | 523    | 19/19 | 0.86 | 0.10 | 79,91,124,126               | 0     |
| 27  | SQD  | a     | 405    | 54/54 | 0.86 | 0.10 | 47,77,116,122               | 0     |
| 35  | HTG  | b     | 632    | 19/19 | 0.86 | 0.11 | 66,118,148,149              | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 28  | GOL  | C     | 524    | 6/6   | 0.87 | 0.12 | 59,63,76,80                 | 0     |
| 27  | SQD  | A     | 416    | 54/54 | 0.87 | 0.11 | 52,73,111,128               | 0     |
| 35  | HTG  | B     | 624    | 19/19 | 0.87 | 0.12 | 48,64,89,93                 | 0     |
| 29  | LMT  | B     | 635    | 25/35 | 0.87 | 0.12 | 40,80,134,138               | 0     |
| 28  | GOL  | T     | 102    | 6/6   | 0.87 | 0.13 | 94,108,113,115              | 0     |
| 27  | SQD  | L     | 102    | 54/54 | 0.87 | 0.10 | 50,77,123,141               | 0     |
| 29  | LMT  | m     | 103    | 35/35 | 0.87 | 0.11 | 40,96,125,132               | 0     |
| 28  | GOL  | a     | 402    | 6/6   | 0.87 | 0.12 | 70,93,94,94                 | 0     |
| 34  | CA   | f     | 103    | 1/1   | 0.88 | 0.07 | 106,106,106,106             | 0     |
| 28  | GOL  | v     | 201    | 6/6   | 0.89 | 0.12 | 68,88,90,92                 | 0     |
| 29  | LMT  | T     | 104    | 25/35 | 0.89 | 0.12 | 37,79,133,138               | 0     |
| 35  | HTG  | C     | 522    | 19/19 | 0.89 | 0.09 | 72,85,101,107               | 0     |
| 35  | HTG  | b     | 631    | 19/19 | 0.89 | 0.12 | 56,71,84,96                 | 0     |
| 28  | GOL  | T     | 101    | 6/6   | 0.89 | 0.14 | 58,74,93,97                 | 0     |
| 35  | HTG  | c     | 525    | 19/19 | 0.89 | 0.09 | 87,92,102,120               | 0     |
| 28  | GOL  | A     | 415    | 6/6   | 0.90 | 0.11 | 52,75,79,82                 | 0     |
| 33  | LMG  | c     | 523    | 51/55 | 0.90 | 0.10 | 48,86,111,115               | 0     |
| 28  | GOL  | B     | 630    | 6/6   | 0.90 | 0.12 | 48,59,72,76                 | 0     |
| 22  | CL   | U     | 201    | 1/1   | 0.90 | 0.11 | 92,92,92,92                 | 0     |
| 28  | GOL  | t     | 102    | 6/6   | 0.90 | 0.14 | 51,80,90,96                 | 0     |
| 33  | LMG  | A     | 421    | 51/55 | 0.90 | 0.09 | 57,82,106,115               | 0     |
| 33  | LMG  | C     | 519    | 51/55 | 0.90 | 0.10 | 49,83,108,117               | 0     |
| 29  | LMT  | m     | 102    | 35/35 | 0.90 | 0.09 | 42,81,100,107               | 0     |
| 33  | LMG  | c     | 501    | 51/55 | 0.91 | 0.10 | 57,79,98,99                 | 0     |
| 28  | GOL  | B     | 626    | 6/6   | 0.91 | 0.10 | 44,54,59,80                 | 0     |
| 28  | GOL  | b     | 606    | 6/6   | 0.91 | 0.10 | 64,79,86,86                 | 0     |
| 29  | LMT  | M     | 101    | 35/35 | 0.91 | 0.09 | 41,80,99,100                | 0     |
| 38  | HEM  | F     | 102    | 43/43 | 0.91 | 0.09 | 44,66,89,137                | 0     |
| 28  | GOL  | v     | 202    | 6/6   | 0.92 | 0.10 | 70,79,96,112                | 0     |
| 23  | BCT  | a     | 417[A] | 4/4   | 0.92 | 0.08 | 59,60,62,70                 | 4     |
| 32  | UNL  | X     | 101    | 18/-  | 0.92 | 0.10 | 54,73,97,100                | 0     |
| 28  | GOL  | B     | 636    | 6/6   | 0.92 | 0.08 | 48,56,62,62                 | 0     |
| 28  | GOL  | b     | 605    | 6/6   | 0.92 | 0.14 | 70,80,101,103               | 0     |
| 23  | BCT  | a     | 417[B] | 4/4   | 0.92 | 0.08 | 50,59,61,66                 | 4     |
| 24  | CLA  | c     | 518    | 65/65 | 0.92 | 0.09 | 56,80,99,108                | 0     |
| 32  | UNL  | d     | 412    | 18/-  | 0.92 | 0.10 | 60,72,112,113               | 0     |
| 27  | SQD  | A     | 412    | 54/54 | 0.92 | 0.09 | 45,78,95,98                 | 0     |
| 28  | GOL  | B     | 628    | 6/6   | 0.92 | 0.10 | 54,73,79,84                 | 0     |
| 24  | CLA  | C     | 506    | 65/65 | 0.93 | 0.08 | 46,62,105,114               | 0     |
| 28  | GOL  | A     | 414    | 6/6   | 0.93 | 0.12 | 49,59,62,64                 | 0     |
| 24  | CLA  | C     | 513    | 65/65 | 0.93 | 0.08 | 52,66,102,109               | 0     |
| 28  | GOL  | A     | 422    | 6/6   | 0.93 | 0.07 | 68,73,74,82                 | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 24  | CLA  | b     | 610    | 65/65 | 0.93 | 0.09 | 44,68,104,134               | 0     |
| 35  | HTG  | B     | 632    | 19/19 | 0.93 | 0.08 | 45,72,101,109               | 0     |
| 24  | CLA  | B     | 602    | 65/65 | 0.93 | 0.09 | 41,62,95,124                | 0     |
| 32  | UNL  | d     | 409    | 17/-  | 0.93 | 0.10 | 47,69,97,101                | 0     |
| 37  | LHG  | D     | 409    | 49/49 | 0.93 | 0.10 | 39,55,116,129               | 0     |
| 28  | GOL  | a     | 420    | 6/6   | 0.93 | 0.09 | 78,80,91,92                 | 0     |
| 26  | BCR  | C     | 514    | 40/40 | 0.93 | 0.08 | 49,67,81,84                 | 0     |
| 26  | BCR  | y     | 101    | 40/40 | 0.93 | 0.08 | 43,63,72,80                 | 0     |
| 33  | LMG  | B     | 622    | 51/55 | 0.94 | 0.07 | 33,50,74,90                 | 0     |
| 26  | BCR  | t     | 101    | 40/40 | 0.94 | 0.06 | 34,47,64,65                 | 0     |
| 28  | GOL  | A     | 413    | 6/6   | 0.94 | 0.09 | 45,49,54,58                 | 0     |
| 33  | LMG  | D     | 413    | 51/55 | 0.94 | 0.09 | 38,60,105,128               | 0     |
| 24  | CLA  | C     | 504    | 65/65 | 0.94 | 0.07 | 34,47,81,94                 | 0     |
| 33  | LMG  | b     | 629    | 51/55 | 0.94 | 0.08 | 42,51,72,94                 | 0     |
| 24  | CLA  | b     | 615    | 65/65 | 0.94 | 0.07 | 32,44,88,106                | 0     |
| 23  | BCT  | A     | 404[B] | 4/4   | 0.94 | 0.08 | 47,48,62,72                 | 4     |
| 23  | BCT  | A     | 404[A] | 4/4   | 0.94 | 0.08 | 47,55,60,72                 | 4     |
| 33  | LMG  | d     | 413    | 51/55 | 0.94 | 0.08 | 45,58,100,110               | 0     |
| 28  | GOL  | B     | 627    | 6/6   | 0.94 | 0.11 | 52,62,79,94                 | 0     |
| 36  | DGD  | C     | 517    | 62/66 | 0.94 | 0.07 | 42,54,96,112                | 0     |
| 26  | BCR  | D     | 404    | 40/40 | 0.94 | 0.07 | 41,50,92,105                | 0     |
| 26  | BCR  | c     | 528    | 40/40 | 0.94 | 0.08 | 60,73,83,85                 | 0     |
| 37  | LHG  | D     | 407    | 49/49 | 0.94 | 0.08 | 31,49,62,73                 | 0     |
| 28  | GOL  | o     | 301    | 6/6   | 0.94 | 0.09 | 65,78,89,107                | 0     |
| 32  | UNL  | D     | 410    | 17/-  | 0.94 | 0.08 | 40,70,83,89                 | 0     |
| 26  | BCR  | d     | 404    | 40/40 | 0.94 | 0.07 | 40,52,79,83                 | 0     |
| 27  | SQD  | a     | 414    | 54/54 | 0.94 | 0.09 | 57,80,103,109               | 0     |
| 34  | CA   | F     | 104    | 1/1   | 0.95 | 0.04 | 84,84,84,84                 | 0     |
| 26  | BCR  | h     | 101    | 40/40 | 0.95 | 0.06 | 38,55,66,68                 | 0     |
| 28  | GOL  | B     | 631    | 6/6   | 0.95 | 0.10 | 43,76,84,87                 | 0     |
| 26  | BCR  | k     | 101    | 40/40 | 0.95 | 0.07 | 44,59,73,75                 | 0     |
| 24  | CLA  | b     | 623    | 65/65 | 0.95 | 0.07 | 26,40,88,115                | 0     |
| 24  | CLA  | b     | 625    | 65/65 | 0.95 | 0.08 | 35,52,101,109               | 0     |
| 24  | CLA  | c     | 508    | 65/65 | 0.95 | 0.07 | 41,52,62,86                 | 0     |
| 24  | CLA  | c     | 511    | 65/65 | 0.95 | 0.07 | 43,63,91,107                | 0     |
| 24  | CLA  | c     | 512    | 65/65 | 0.95 | 0.07 | 42,54,67,72                 | 0     |
| 24  | CLA  | c     | 517    | 65/65 | 0.95 | 0.06 | 49,63,82,86                 | 0     |
| 24  | CLA  | C     | 512    | 65/65 | 0.95 | 0.07 | 48,64,81,92                 | 0     |
| 28  | GOL  | b     | 602    | 6/6   | 0.95 | 0.09 | 56,58,65,89                 | 0     |
| 26  | BCR  | A     | 411    | 40/40 | 0.95 | 0.06 | 28,39,46,48                 | 0     |
| 24  | CLA  | B     | 615    | 65/65 | 0.95 | 0.07 | 26,40,90,99                 | 0     |
| 24  | CLA  | C     | 505    | 65/65 | 0.95 | 0.07 | 38,47,68,78                 | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 26  | BCR  | H     | 101    | 40/40 | 0.95 | 0.06 | 35,51,65,67                 | 0     |
| 31  | PL9  | d     | 405[A] | 55/55 | 0.95 | 0.06 | 27,37,46,57                 | 55    |
| 36  | DGD  | C     | 516    | 62/66 | 0.95 | 0.07 | 33,47,88,96                 | 0     |
| 31  | PL9  | d     | 405[B] | 55/55 | 0.95 | 0.06 | 24,38,46,57                 | 55    |
| 26  | BCR  | K     | 101    | 40/40 | 0.95 | 0.07 | 43,57,65,68                 | 0     |
| 36  | DGD  | H     | 102    | 62/66 | 0.95 | 0.07 | 35,48,66,78                 | 0     |
| 36  | DGD  | c     | 521    | 62/66 | 0.95 | 0.07 | 41,52,105,128               | 0     |
| 36  | DGD  | c     | 522    | 62/66 | 0.95 | 0.07 | 38,52,87,96                 | 0     |
| 26  | BCR  | T     | 103    | 40/40 | 0.95 | 0.06 | 31,46,61,62                 | 0     |
| 26  | BCR  | Y     | 101    | 40/40 | 0.95 | 0.06 | 47,60,71,80                 | 0     |
| 28  | GOL  | v     | 203    | 6/6   | 0.95 | 0.10 | 48,49,57,59                 | 0     |
| 26  | BCR  | b     | 627    | 40/40 | 0.95 | 0.06 | 31,42,60,67                 | 0     |
| 37  | LHG  | d     | 408    | 49/49 | 0.95 | 0.09 | 34,53,104,109               | 0     |
| 24  | CLA  | B     | 617    | 65/65 | 0.95 | 0.09 | 36,49,116,118               | 0     |
| 24  | CLA  | b     | 618    | 65/65 | 0.95 | 0.06 | 37,49,58,71                 | 0     |
| 24  | CLA  | c     | 510    | 65/65 | 0.96 | 0.06 | 36,48,67,78                 | 0     |
| 24  | CLA  | C     | 508    | 65/65 | 0.96 | 0.06 | 36,48,114,125               | 0     |
| 24  | CLA  | C     | 509    | 65/65 | 0.96 | 0.07 | 43,55,74,81                 | 0     |
| 24  | CLA  | c     | 513    | 65/65 | 0.96 | 0.07 | 35,48,113,129               | 0     |
| 24  | CLA  | c     | 515    | 65/65 | 0.96 | 0.06 | 39,52,65,71                 | 0     |
| 24  | CLA  | c     | 516    | 65/65 | 0.96 | 0.07 | 43,55,75,88                 | 0     |
| 24  | CLA  | C     | 510    | 65/65 | 0.96 | 0.06 | 39,51,62,71                 | 0     |
| 24  | CLA  | C     | 511    | 65/65 | 0.96 | 0.07 | 41,58,69,83                 | 0     |
| 24  | CLA  | d     | 403    | 65/65 | 0.96 | 0.07 | 41,51,103,111               | 0     |
| 25  | PHO  | a     | 418[A] | 64/64 | 0.96 | 0.05 | 28,41,47,50                 | 64    |
| 25  | PHO  | a     | 418[B] | 64/64 | 0.96 | 0.05 | 28,41,48,51                 | 64    |
| 28  | GOL  | B     | 629    | 6/6   | 0.96 | 0.09 | 50,52,55,60                 | 0     |
| 24  | CLA  | A     | 410    | 65/65 | 0.96 | 0.07 | 30,45,122,130               | 0     |
| 31  | PL9  | D     | 405[A] | 55/55 | 0.96 | 0.05 | 26,37,44,57                 | 55    |
| 31  | PL9  | D     | 405[B] | 55/55 | 0.96 | 0.05 | 28,36,45,62                 | 55    |
| 26  | BCR  | B     | 619    | 40/40 | 0.96 | 0.05 | 27,40,56,63                 | 0     |
| 26  | BCR  | B     | 620    | 40/40 | 0.96 | 0.06 | 35,46,58,60                 | 0     |
| 24  | CLA  | A     | 407    | 65/65 | 0.96 | 0.06 | 28,39,101,116               | 0     |
| 26  | BCR  | C     | 515    | 40/40 | 0.96 | 0.06 | 39,54,63,65                 | 0     |
| 24  | CLA  | D     | 403    | 65/65 | 0.96 | 0.07 | 38,51,101,119               | 0     |
| 24  | CLA  | a     | 412    | 65/65 | 0.96 | 0.08 | 31,46,114,124               | 0     |
| 35  | HTG  | b     | 601    | 19/19 | 0.96 | 0.07 | 40,47,70,71                 | 0     |
| 35  | HTG  | b     | 607    | 19/19 | 0.96 | 0.06 | 47,71,80,81                 | 0     |
| 24  | CLA  | C     | 501    | 65/65 | 0.96 | 0.06 | 38,50,73,81                 | 0     |
| 28  | GOL  | V     | 202    | 6/6   | 0.96 | 0.07 | 39,47,52,62                 | 0     |
| 28  | GOL  | V     | 203    | 6/6   | 0.96 | 0.08 | 54,59,59,63                 | 0     |
| 28  | GOL  | V     | 204    | 6/6   | 0.96 | 0.08 | 72,78,80,89                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 24  | CLA  | C     | 503 | 65/65 | 0.96 | 0.06 | 40,50,61,64                 | 0     |
| 24  | CLA  | b     | 616 | 65/65 | 0.96 | 0.05 | 24,35,44,54                 | 0     |
| 24  | CLA  | B     | 607 | 65/65 | 0.96 | 0.07 | 32,44,93,103                | 0     |
| 28  | GOL  | b     | 604 | 6/6   | 0.96 | 0.07 | 58,63,68,86                 | 0     |
| 36  | DGD  | C     | 518 | 62/66 | 0.96 | 0.06 | 35,51,74,87                 | 0     |
| 26  | BCR  | c     | 519 | 40/40 | 0.96 | 0.06 | 39,54,66,70                 | 0     |
| 24  | CLA  | b     | 619 | 65/65 | 0.96 | 0.06 | 36,45,53,62                 | 0     |
| 36  | DGD  | c     | 520 | 62/66 | 0.96 | 0.07 | 36,48,94,107                | 0     |
| 24  | CLA  | b     | 620 | 65/65 | 0.96 | 0.06 | 29,39,49,55                 | 0     |
| 24  | CLA  | b     | 622 | 65/65 | 0.96 | 0.06 | 27,39,56,62                 | 0     |
| 24  | CLA  | B     | 611 | 65/65 | 0.96 | 0.06 | 36,46,54,69                 | 0     |
| 36  | DGD  | h     | 102 | 62/66 | 0.96 | 0.06 | 39,50,67,79                 | 0     |
| 24  | CLA  | b     | 624 | 65/65 | 0.96 | 0.05 | 33,46,62,70                 | 0     |
| 24  | CLA  | B     | 614 | 65/65 | 0.96 | 0.06 | 27,36,66,74                 | 0     |
| 24  | CLA  | c     | 506 | 65/65 | 0.96 | 0.06 | 41,55,65,70                 | 0     |
| 37  | LHG  | d     | 406 | 49/49 | 0.96 | 0.07 | 37,51,59,74                 | 0     |
| 24  | CLA  | c     | 507 | 65/65 | 0.96 | 0.06 | 40,51,66,73                 | 0     |
| 24  | CLA  | C     | 507 | 65/65 | 0.96 | 0.07 | 41,56,68,70                 | 0     |
| 24  | CLA  | c     | 509 | 65/65 | 0.96 | 0.06 | 38,53,74,79                 | 0     |
| 25  | PHO  | a     | 411 | 64/64 | 0.97 | 0.04 | 28,36,41,47                 | 0     |
| 24  | CLA  | B     | 613 | 65/65 | 0.97 | 0.05 | 27,37,46,54                 | 0     |
| 24  | CLA  | A     | 406 | 65/65 | 0.97 | 0.04 | 25,32,42,51                 | 0     |
| 24  | CLA  | b     | 621 | 65/65 | 0.97 | 0.05 | 28,40,49,52                 | 0     |
| 24  | CLA  | B     | 603 | 65/65 | 0.97 | 0.05 | 35,43,50,53                 | 0     |
| 24  | CLA  | B     | 616 | 65/65 | 0.97 | 0.06 | 34,45,65,77                 | 0     |
| 24  | CLA  | B     | 604 | 65/65 | 0.97 | 0.05 | 34,43,49,63                 | 0     |
| 22  | CL   | v     | 204 | 1/1   | 0.97 | 0.07 | 95,95,95,95                 | 0     |
| 24  | CLA  | C     | 502 | 65/65 | 0.97 | 0.05 | 36,46,61,78                 | 0     |
| 24  | CLA  | a     | 409 | 65/65 | 0.97 | 0.05 | 27,35,49,58                 | 0     |
| 24  | CLA  | a     | 410 | 65/65 | 0.97 | 0.06 | 31,41,105,114               | 0     |
| 24  | CLA  | B     | 608 | 65/65 | 0.97 | 0.05 | 24,35,47,52                 | 0     |
| 24  | CLA  | B     | 609 | 65/65 | 0.97 | 0.05 | 35,43,56,60                 | 0     |
| 26  | BCR  | a     | 413 | 40/40 | 0.97 | 0.04 | 28,39,48,56                 | 0     |
| 26  | BCR  | b     | 626 | 40/40 | 0.97 | 0.04 | 32,41,47,49                 | 0     |
| 24  | CLA  | b     | 611 | 65/65 | 0.97 | 0.06 | 32,46,52,57                 | 0     |
| 26  | BCR  | b     | 628 | 40/40 | 0.97 | 0.05 | 35,50,62,66                 | 0     |
| 24  | CLA  | b     | 612 | 65/65 | 0.97 | 0.05 | 33,44,54,59                 | 0     |
| 24  | CLA  | b     | 613 | 65/65 | 0.97 | 0.05 | 27,38,73,79                 | 0     |
| 24  | CLA  | c     | 514 | 65/65 | 0.97 | 0.07 | 43,54,74,85                 | 0     |
| 24  | CLA  | b     | 614 | 65/65 | 0.97 | 0.06 | 28,39,52,55                 | 0     |
| 24  | CLA  | B     | 610 | 65/65 | 0.97 | 0.05 | 34,46,55,64                 | 0     |
| 28  | GOL  | a     | 401 | 6/6   | 0.97 | 0.08 | 49,63,68,76                 | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 24  | CLA  | A     | 405    | 65/65 | 0.97 | 0.05 | 25,33,45,67                 | 0     |
| 24  | CLA  | b     | 617    | 65/65 | 0.97 | 0.05 | 32,45,53,60                 | 0     |
| 24  | CLA  | d     | 401    | 65/65 | 0.97 | 0.04 | 26,33,43,52                 | 0     |
| 37  | LHG  | D     | 408    | 49/49 | 0.97 | 0.06 | 33,43,61,89                 | 0     |
| 28  | GOL  | b     | 603    | 6/6   | 0.97 | 0.06 | 45,63,75,80                 | 0     |
| 24  | CLA  | B     | 612    | 65/65 | 0.97 | 0.05 | 26,38,50,57                 | 0     |
| 37  | LHG  | L     | 101    | 49/49 | 0.97 | 0.06 | 33,45,56,59                 | 0     |
| 37  | LHG  | b     | 634    | 49/49 | 0.97 | 0.06 | 36,45,58,64                 | 0     |
| 25  | PHO  | A     | 408    | 64/64 | 0.97 | 0.05 | 28,34,40,40                 | 0     |
| 25  | PHO  | A     | 409[A] | 64/64 | 0.97 | 0.05 | 33,40,47,49                 | 64    |
| 35  | HTG  | B     | 623    | 19/19 | 0.97 | 0.07 | 40,56,72,76                 | 0     |
| 25  | PHO  | A     | 409[B] | 64/64 | 0.97 | 0.05 | 27,40,48,49                 | 64    |
| 38  | HEM  | e     | 103    | 43/43 | 0.97 | 0.10 | 55,81,121,150               | 0     |
| 22  | CL   | A     | 403[B] | 1/1   | 0.98 | 0.08 | 35,35,35,35                 | 1     |
| 26  | BCR  | B     | 618    | 40/40 | 0.98 | 0.04 | 27,39,46,48                 | 0     |
| 22  | CL   | A     | 403[A] | 1/1   | 0.98 | 0.08 | 33,33,33,33                 | 1     |
| 24  | CLA  | B     | 605    | 65/65 | 0.98 | 0.05 | 27,36,71,75                 | 0     |
| 24  | CLA  | B     | 606    | 65/65 | 0.98 | 0.05 | 29,39,54,58                 | 0     |
| 37  | LHG  | d     | 407    | 49/49 | 0.98 | 0.06 | 32,42,57,88                 | 0     |
| 24  | CLA  | d     | 402    | 65/65 | 0.98 | 0.05 | 26,36,60,71                 | 0     |
| 24  | CLA  | D     | 402    | 65/65 | 0.98 | 0.05 | 24,34,55,61                 | 0     |
| 28  | GOL  | c     | 502    | 6/6   | 0.98 | 0.05 | 38,44,46,48                 | 0     |
| 28  | GOL  | C     | 525    | 6/6   | 0.98 | 0.04 | 32,42,44,45                 | 0     |
| 39  | MG   | j     | 102    | 1/1   | 0.98 | 0.09 | 57,57,57,57                 | 0     |
| 30  | OEX  | A     | 418[A] | 10/10 | 0.99 | 0.03 | 30,36,43,56                 | 10    |
| 34  | CA   | C     | 526    | 1/1   | 0.99 | 0.07 | 70,70,70,70                 | 0     |
| 30  | OEX  | A     | 418[B] | 10/10 | 0.99 | 0.03 | 33,37,39,39                 | 10    |
| 22  | CL   | a     | 407[A] | 1/1   | 0.99 | 0.05 | 36,36,36,36                 | 1     |
| 34  | CA   | c     | 504    | 1/1   | 0.99 | 0.07 | 67,67,67,67                 | 0     |
| 34  | CA   | c     | 505    | 1/1   | 0.99 | 0.03 | 75,75,75,75                 | 0     |
| 22  | CL   | a     | 407[B] | 1/1   | 0.99 | 0.05 | 37,37,37,37                 | 1     |
| 39  | MG   | J     | 102    | 1/1   | 0.99 | 0.03 | 52,52,52,52                 | 0     |
| 34  | CA   | o     | 302    | 1/1   | 0.99 | 0.03 | 90,90,90,90                 | 0     |
| 40  | HEC  | V     | 205    | 43/43 | 0.99 | 0.05 | 34,40,51,56                 | 0     |
| 40  | HEC  | v     | 205    | 43/43 | 0.99 | 0.05 | 41,52,56,60                 | 0     |
| 22  | CL   | a     | 408[B] | 1/1   | 1.00 | 0.01 | 40,40,40,40                 | 1     |
| 22  | CL   | A     | 402[B] | 1/1   | 1.00 | 0.01 | 32,32,32,32                 | 1     |
| 21  | FE2  | A     | 401[A] | 1/1   | 1.00 | 0.01 | 47,47,47,47                 | 1     |
| 30  | OEX  | a     | 416[A] | 10/10 | 1.00 | 0.02 | 34,37,40,52                 | 10    |
| 30  | OEX  | a     | 416[B] | 10/10 | 1.00 | 0.02 | 32,38,43,46                 | 10    |
| 21  | FE2  | A     | 401[B] | 1/1   | 1.00 | 0.01 | 50,50,50,50                 | 1     |
| 34  | CA   | O     | 302    | 1/1   | 1.00 | 0.03 | 81,81,81,81                 | 0     |

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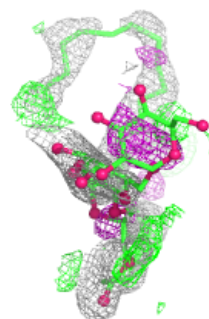
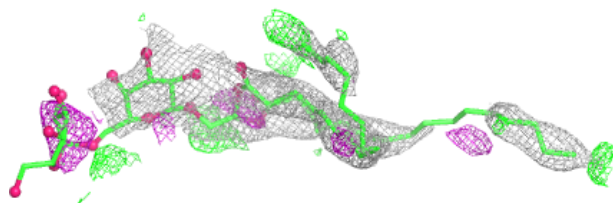
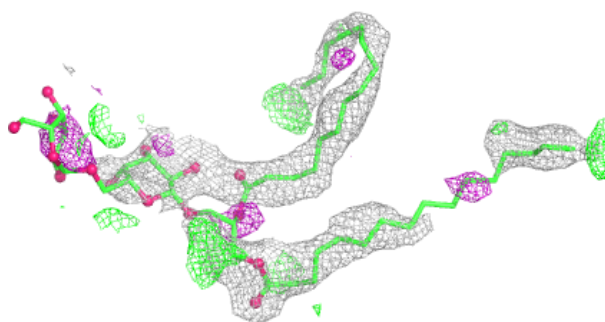
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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 21  | FE2  | a     | 406[A] | 1/1   | 1.00 | 0.02 | 48,48,48,48                 | 1     |
| 21  | FE2  | a     | 406[B] | 1/1   | 1.00 | 0.02 | 48,48,48,48                 | 1     |
| 22  | CL   | A     | 402[A] | 1/1   | 1.00 | 0.01 | 32,32,32,32                 | 1     |
| 22  | CL   | a     | 408[A] | 1/1   | 1.00 | 0.01 | 40,40,40,40                 | 1     |

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

**Electron density around DGD e 101:**

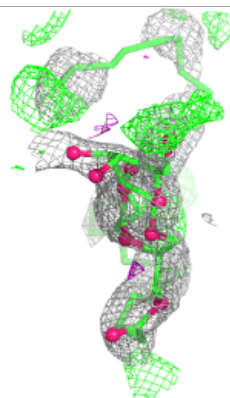
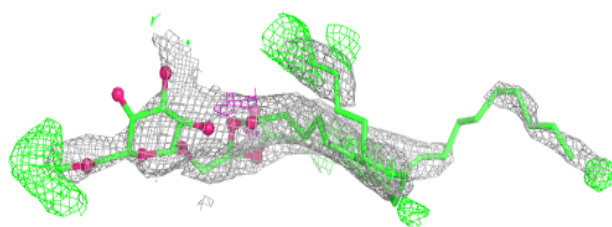
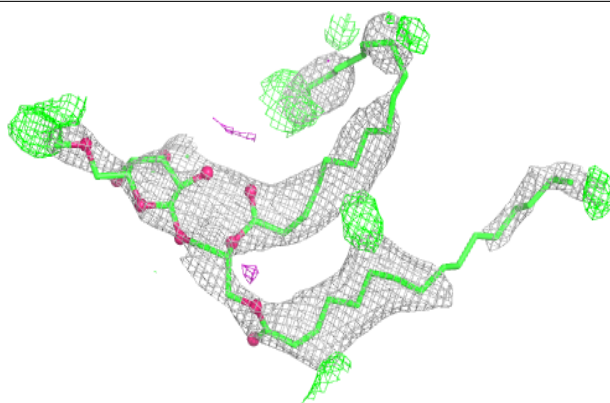
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



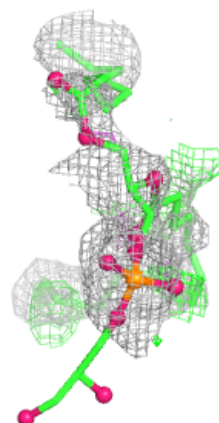
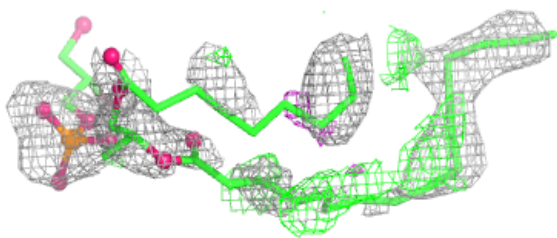
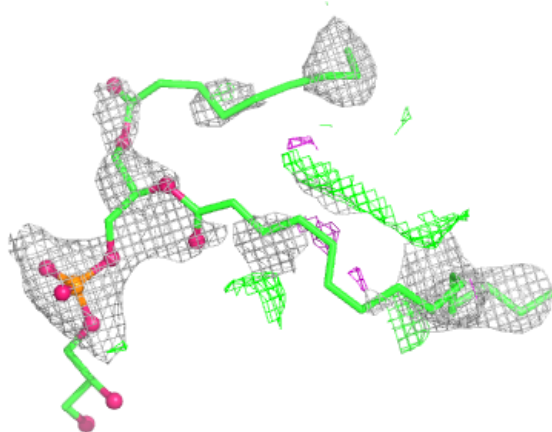


**Electron density around DGD D 406:**

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

**Electron density around LHG e 102:**

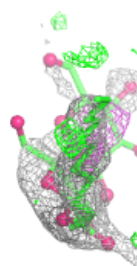
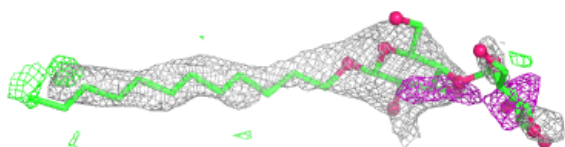
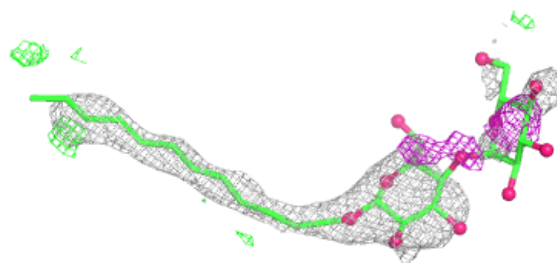
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



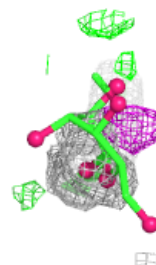
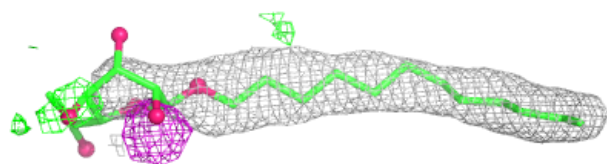
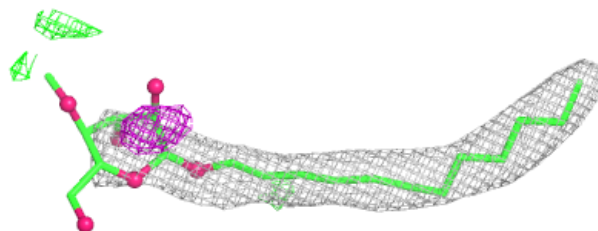


**Electron density around LMT F 101:**

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

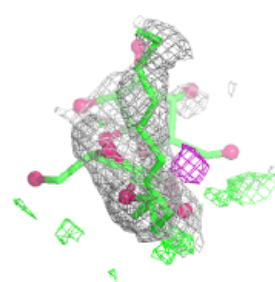
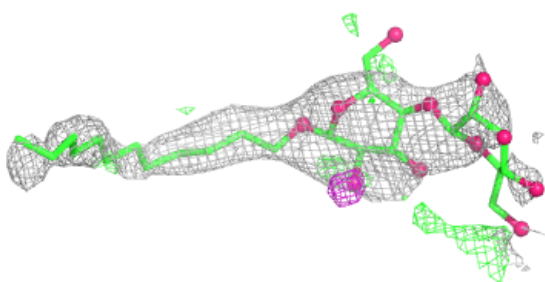
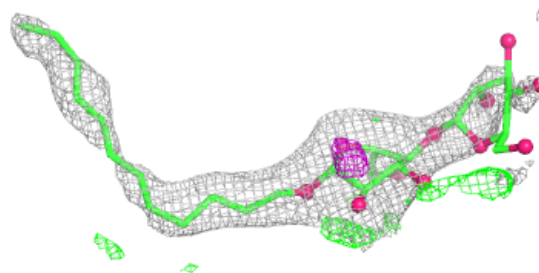
**Electron density around LMT b 630:**

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

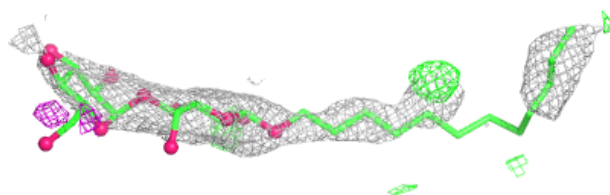
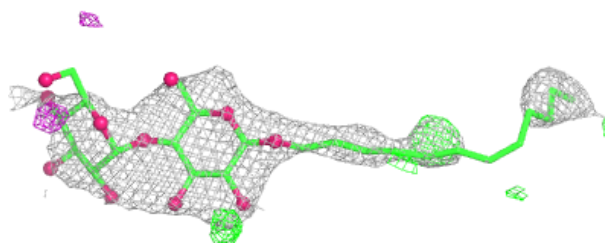


**Electron density around LMT C 521:**

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

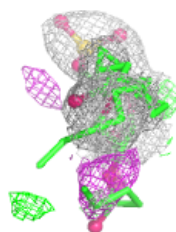
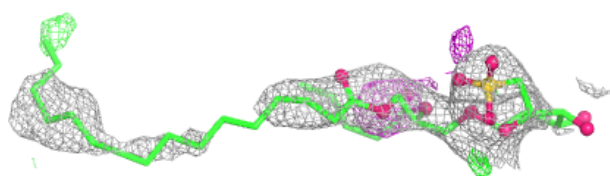
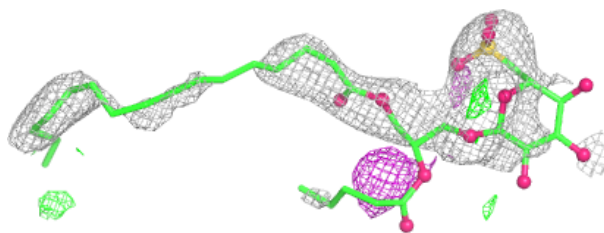
**Electron density around LMT a 419:**

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

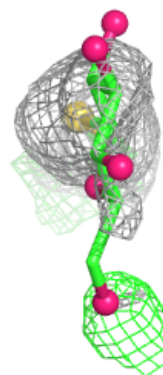
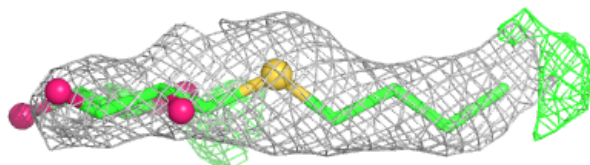
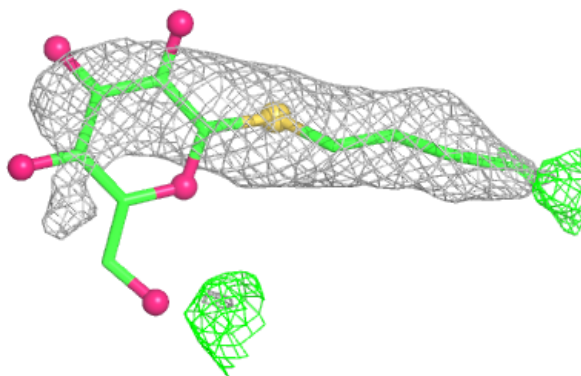


**Electron density around SQD f 101:**

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

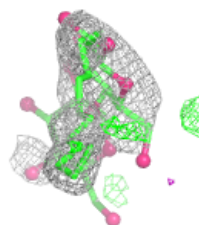
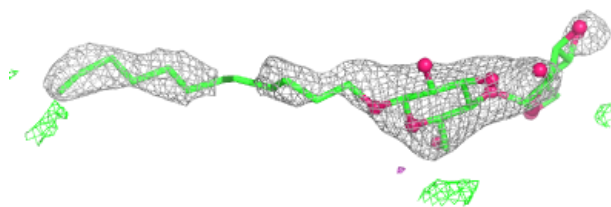
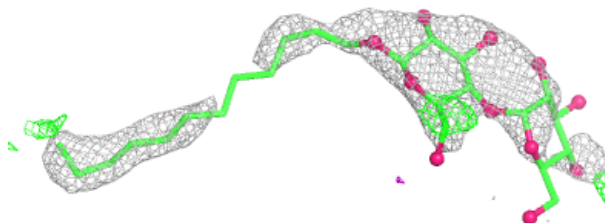
**Electron density around HTG D 412:**

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

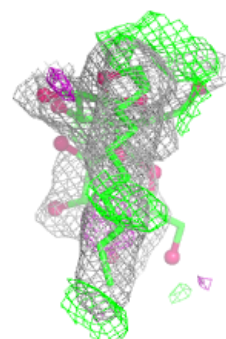
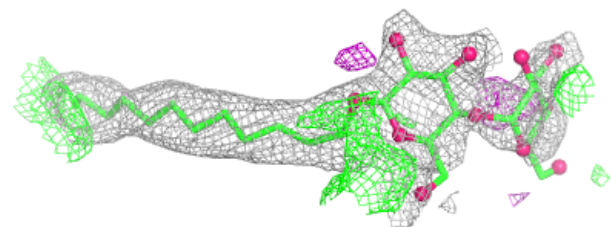
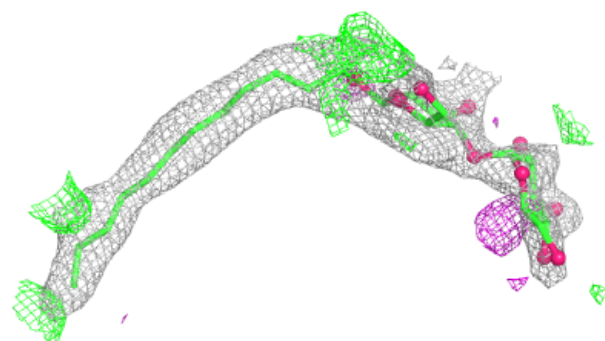


**Electron density around LMT f 102:**

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

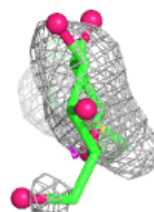
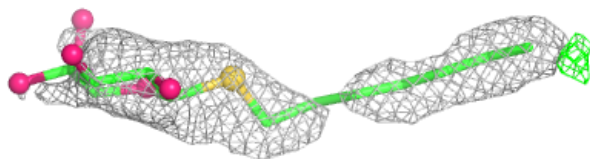
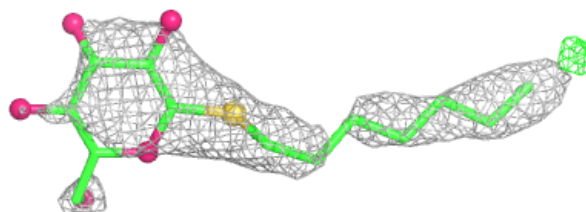
**Electron density around LMT M 103:**

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

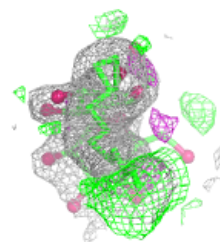
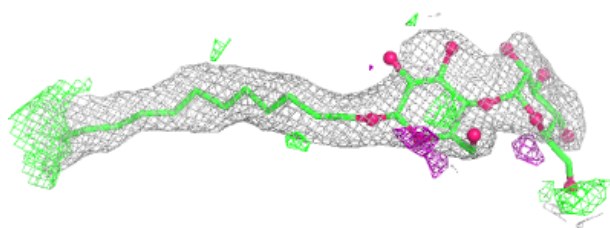
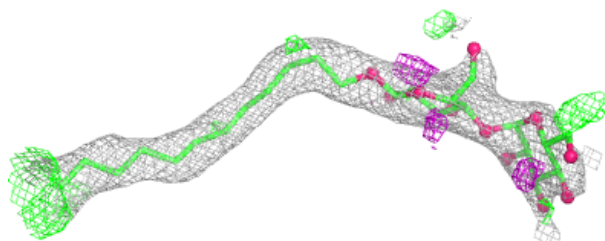


**Electron density around HTG c 526:**

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

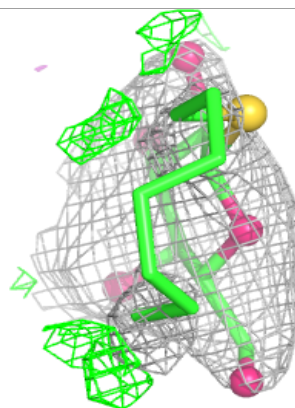
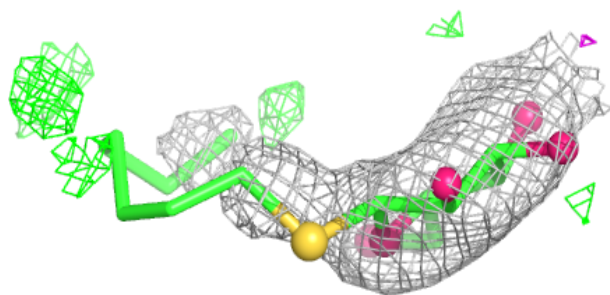
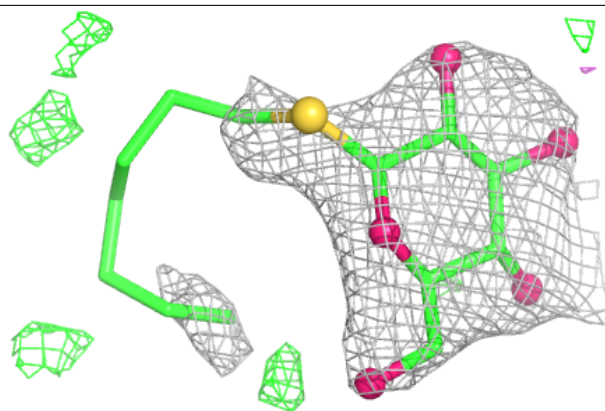
**Electron density around LMT A 417:**

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

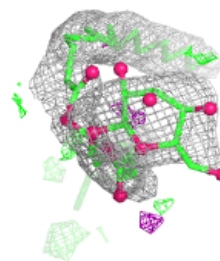
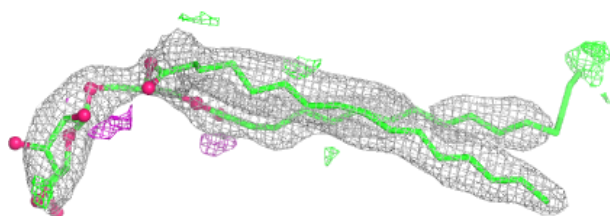
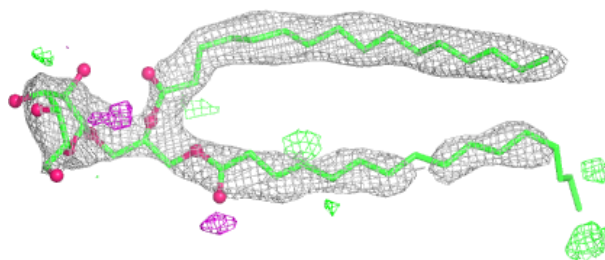


**Electron density around HTG V 206:**

$2mF_o-DF_c$  (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:**

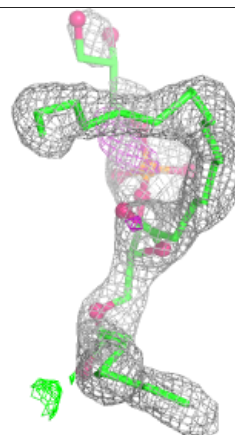
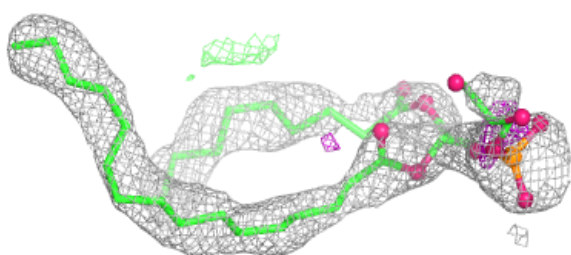
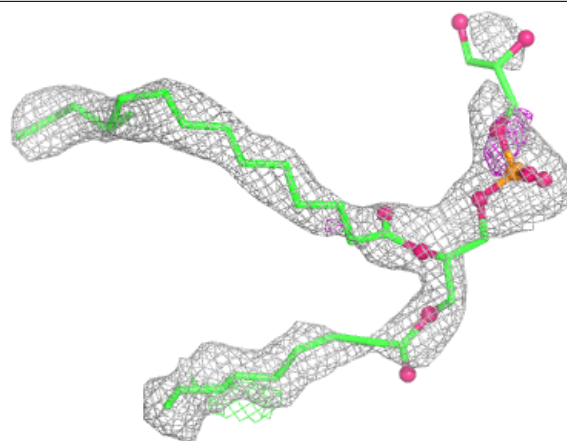
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





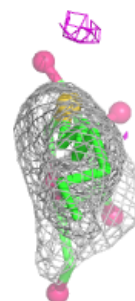
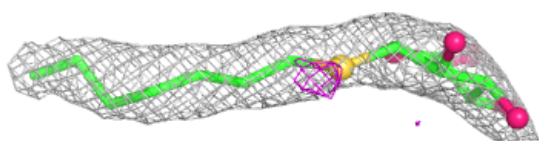
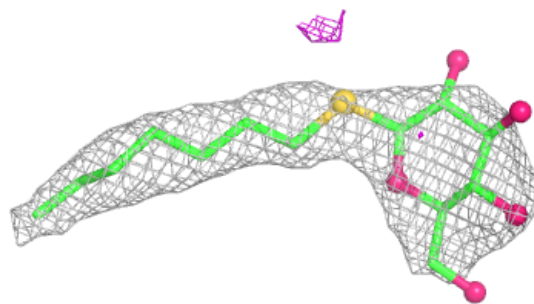
**Electron density around LHG E 101:**

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

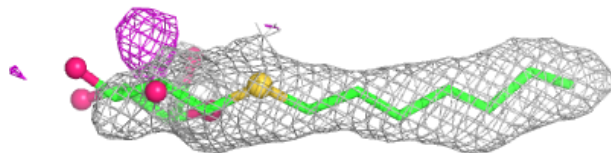
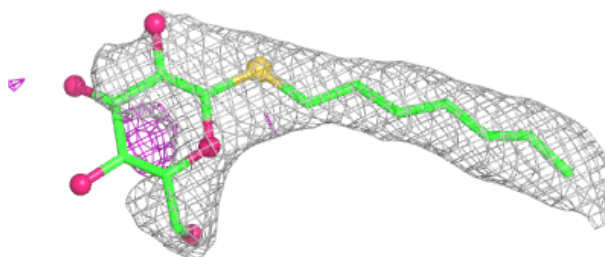


**Electron density around HTG B 625:**

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

**Electron density around HTG b 608:**

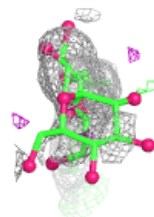
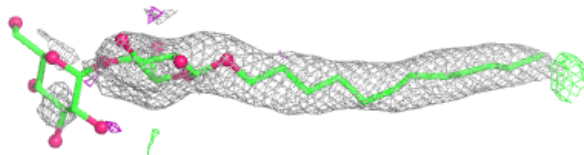
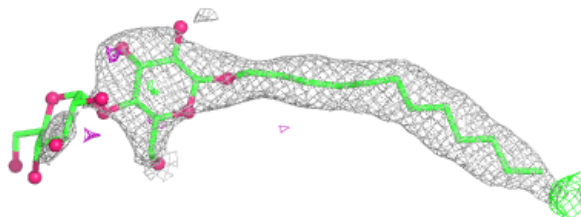
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



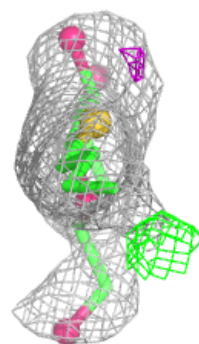
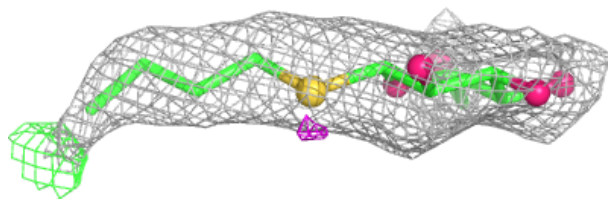
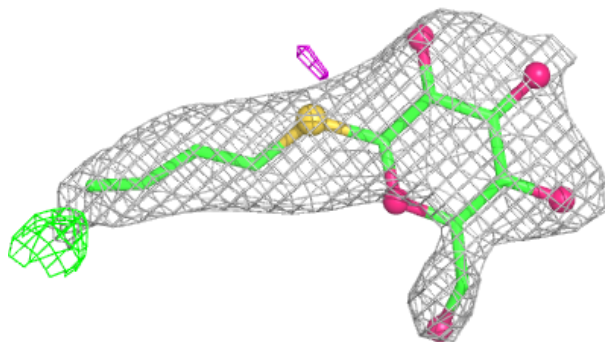


**Electron density around LMT D 401:**

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

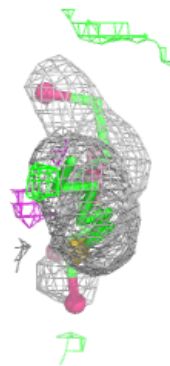
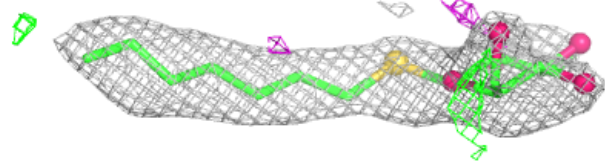
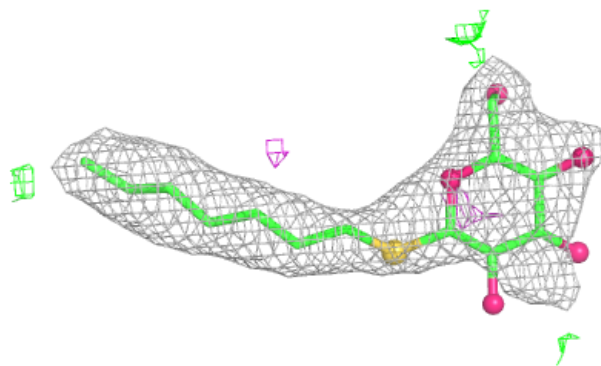
**Electron density around HTG d 411:**

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

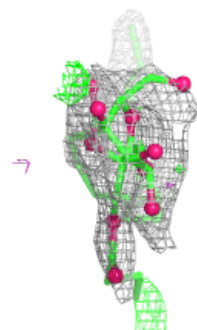
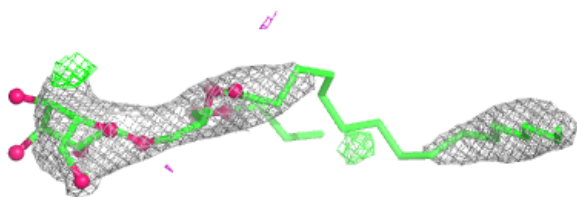


**Electron density around HTG B 633:**

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

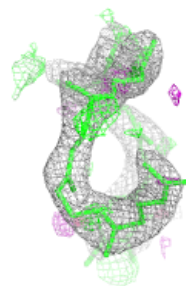
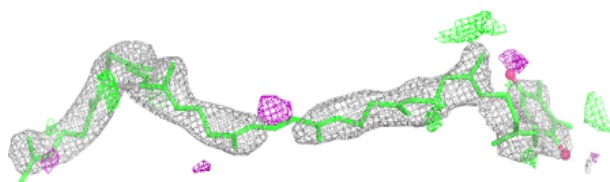
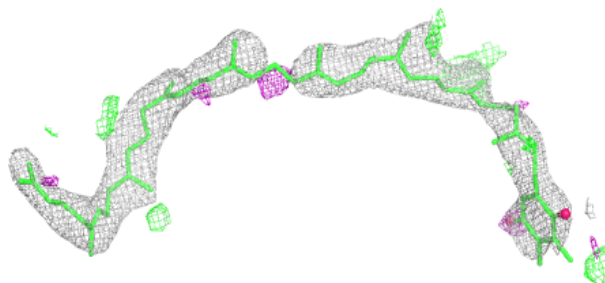
**Electron density around LMG z 101:**

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

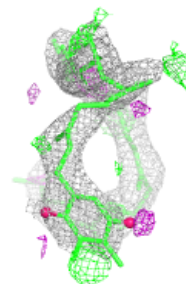
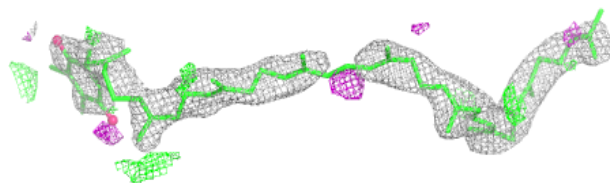
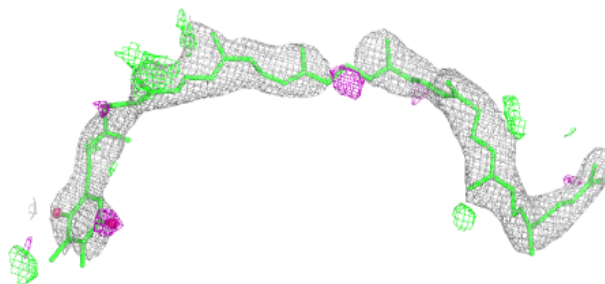


**Electron density around PL9 A 419 (A):**

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

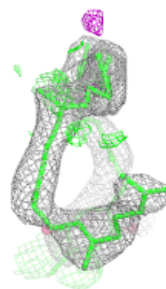
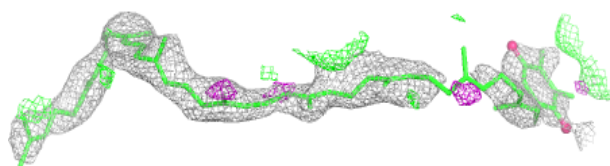
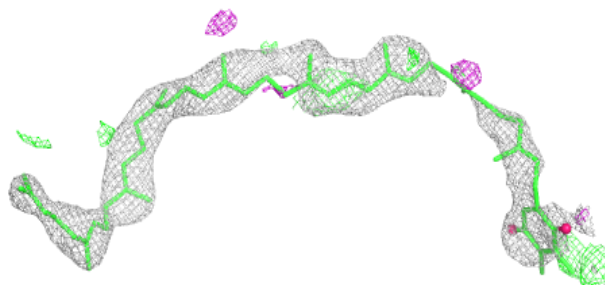
**Electron density around PL9 A 419 (B):**

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

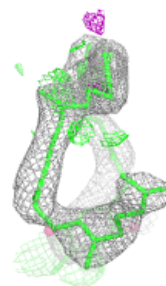
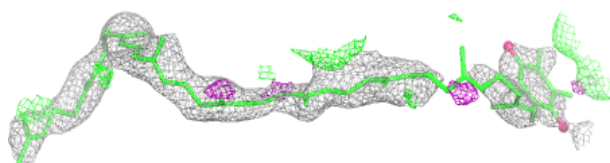
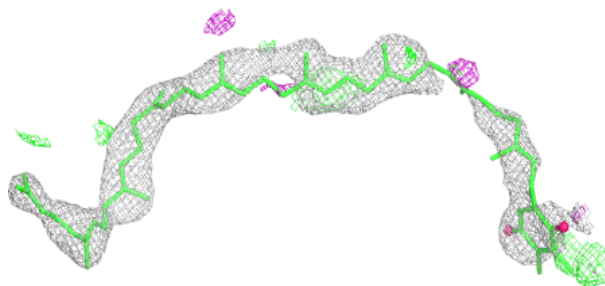


**Electron density around PL9 a 415 (A):**

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

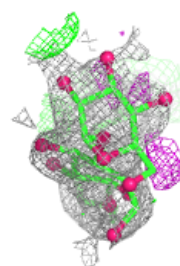
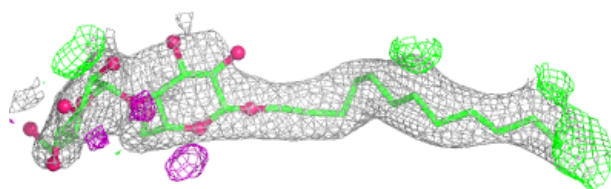
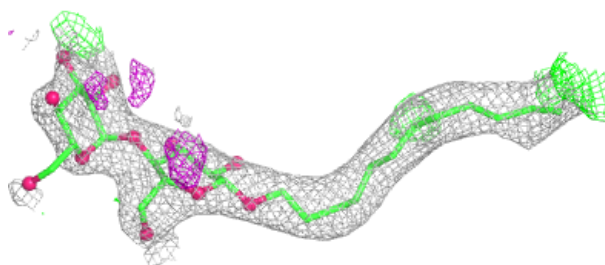
**Electron density around PL9 a 415 (B):**

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

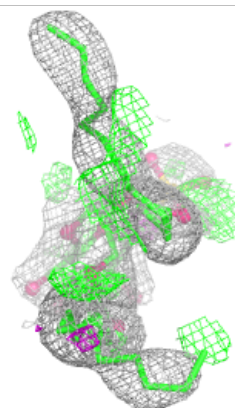
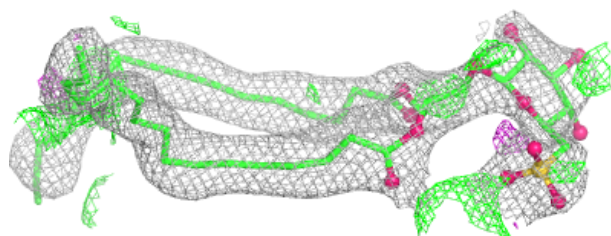
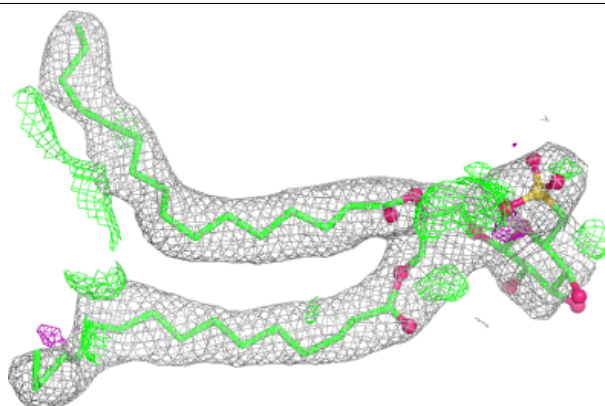


**Electron density around LMT a 404:**

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

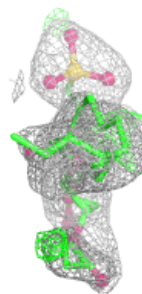
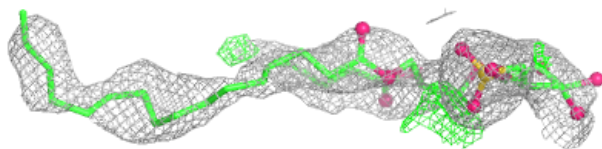
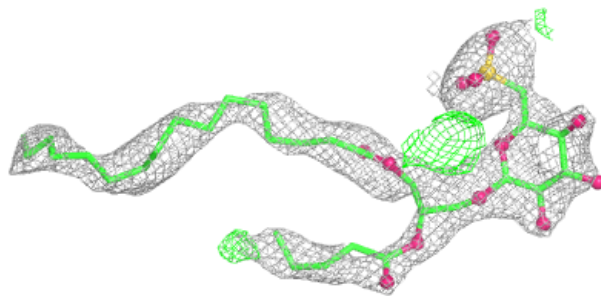
**Electron density around SQD B 621:**

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

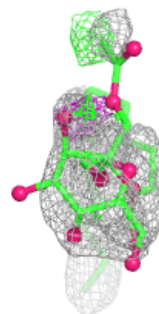
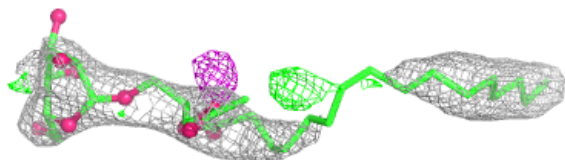
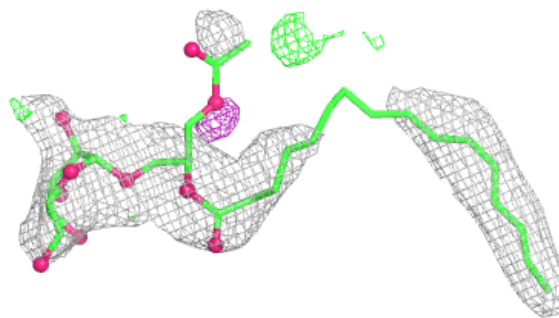


**Electron density around SQD F 103:**

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

**Electron density around LMG Z 101:**

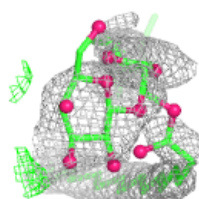
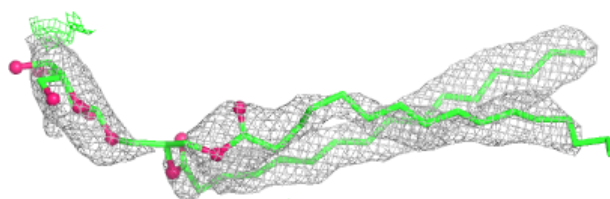
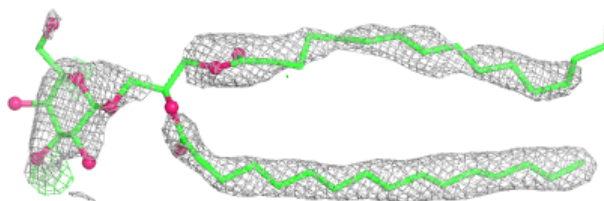
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



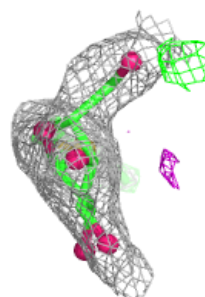
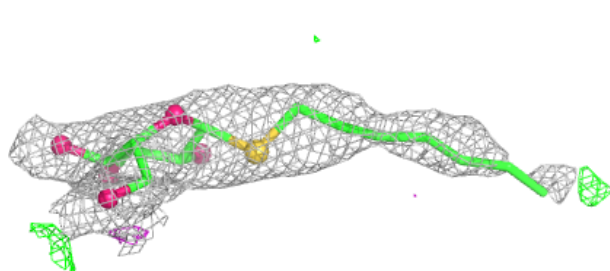
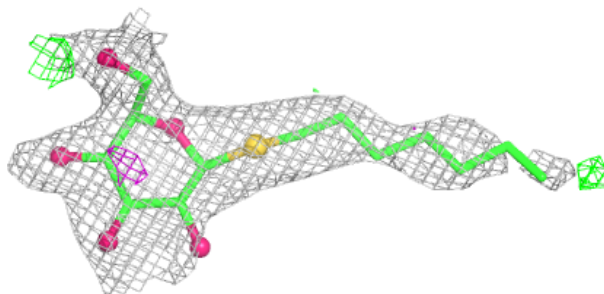


**Electron density around LMG c 524:**

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

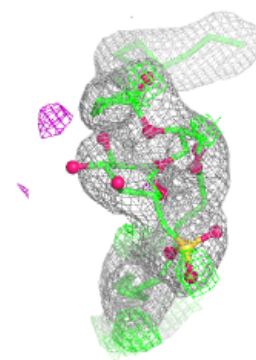
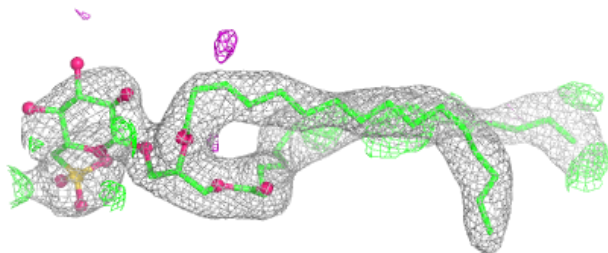
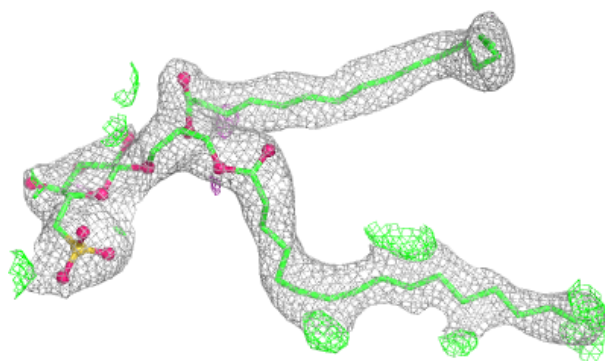
**Electron density around HTG C 523:**

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

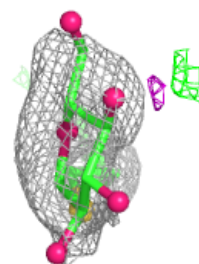
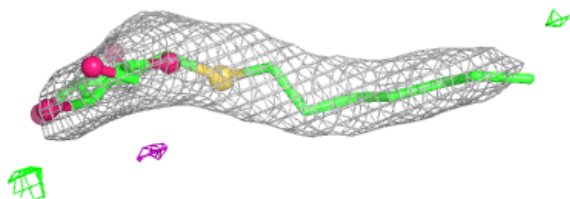
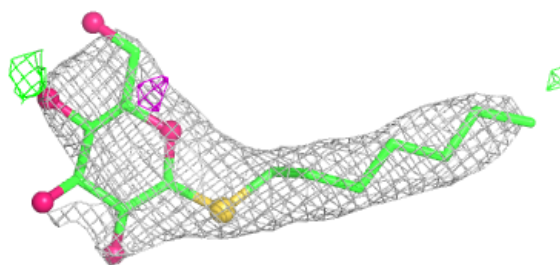


**Electron density around SQD a 405:**

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

**Electron density around HTG b 632:**

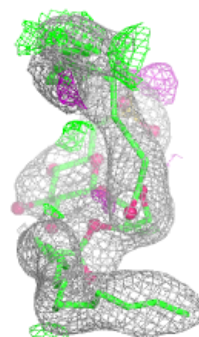
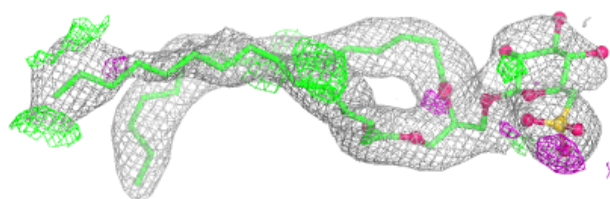
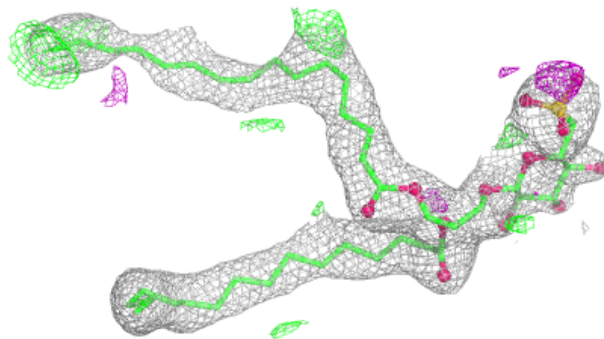
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



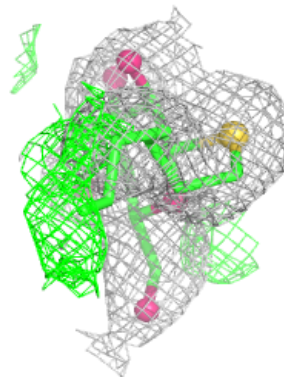
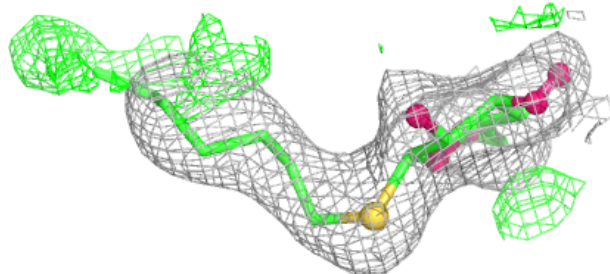
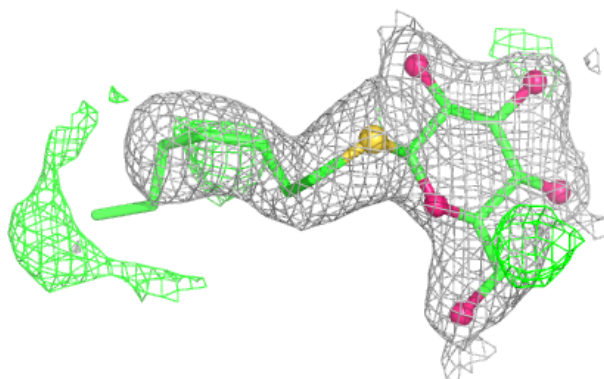


**Electron density around SQD A 416:**

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

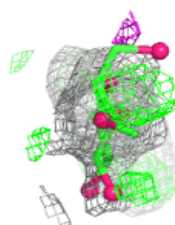
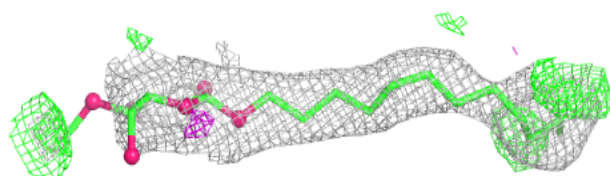
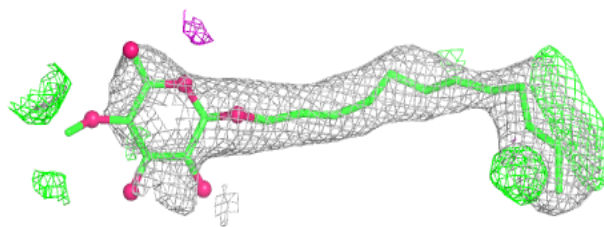
**Electron density around HTG B 624:**

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

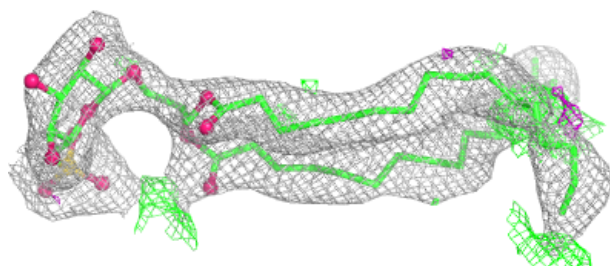
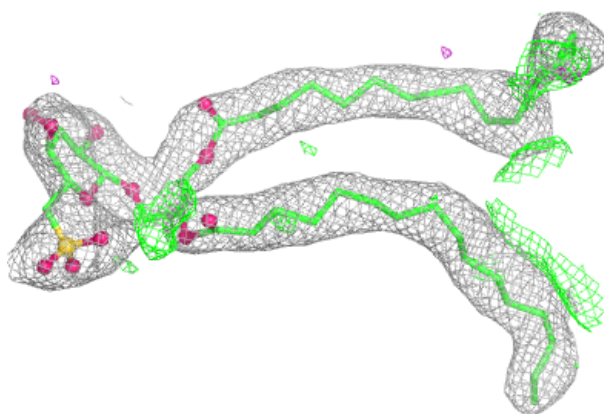


**Electron density around LMT B 635:**

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

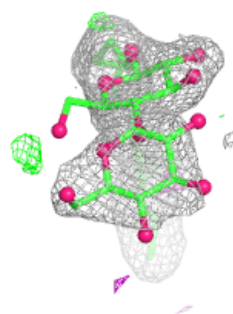
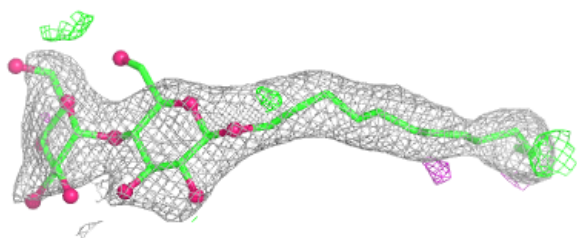
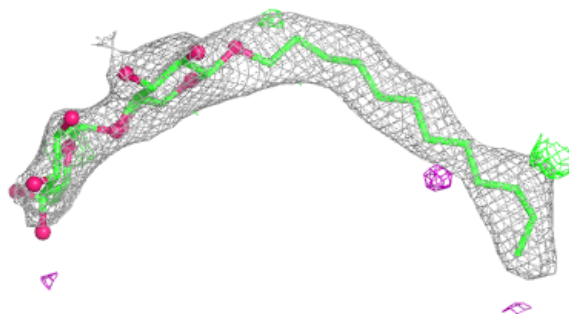
**Electron density around SQD L 102:**

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

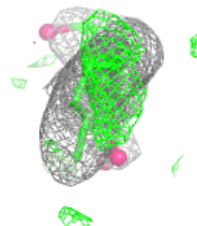
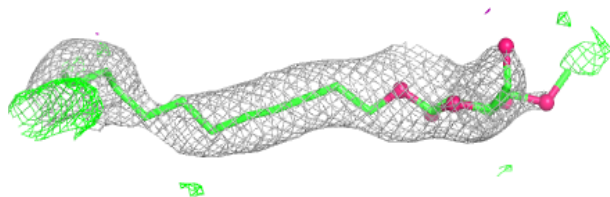
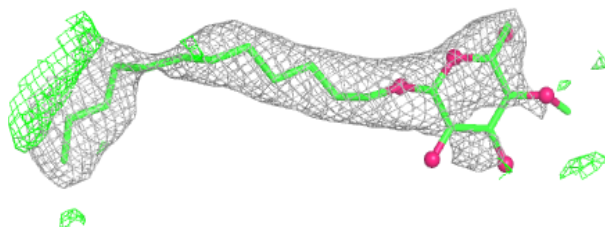


**Electron density around LMT m 103:**

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

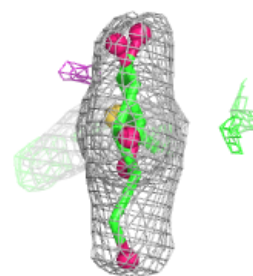
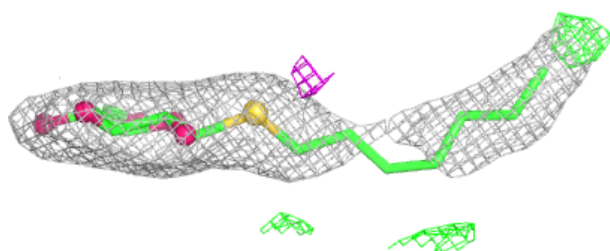
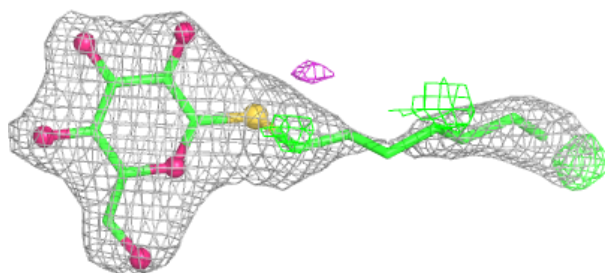
**Electron density around LMT T 104:**

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

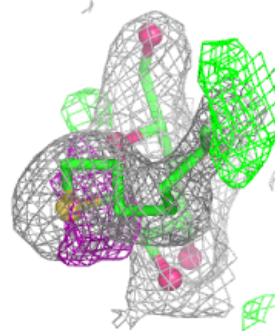
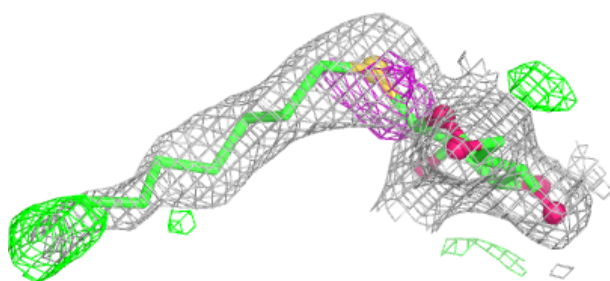
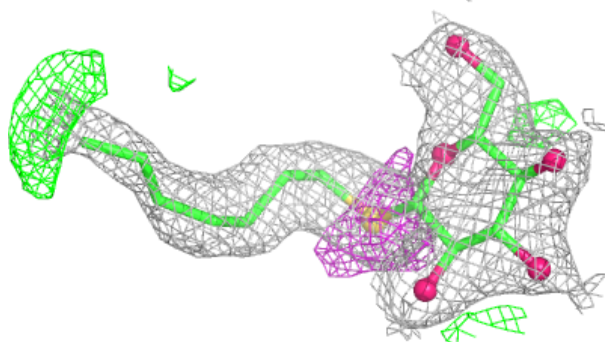


**Electron density around HTG C 522:**

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

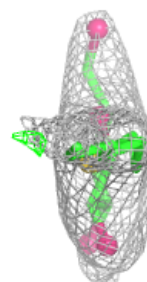
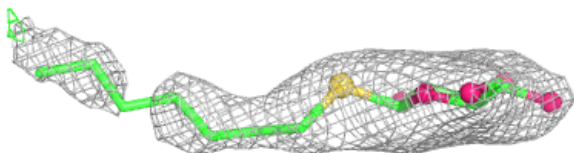
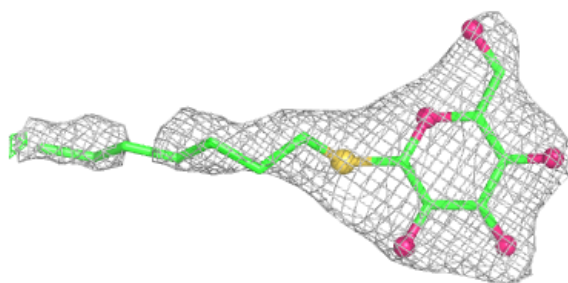
**Electron density around HTG b 631:**

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



**Electron density around HTG c 525:**

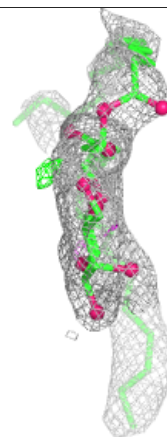
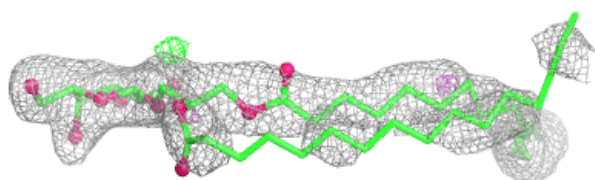
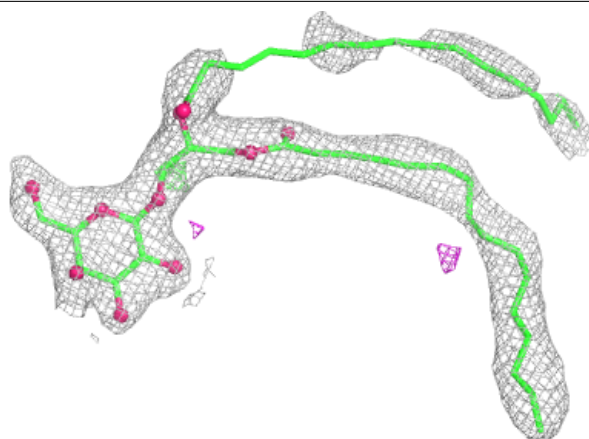
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



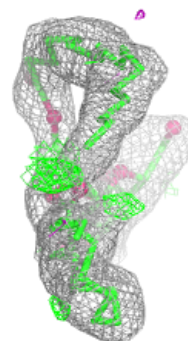
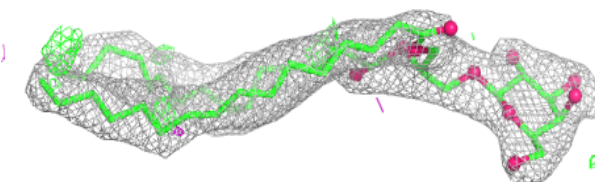
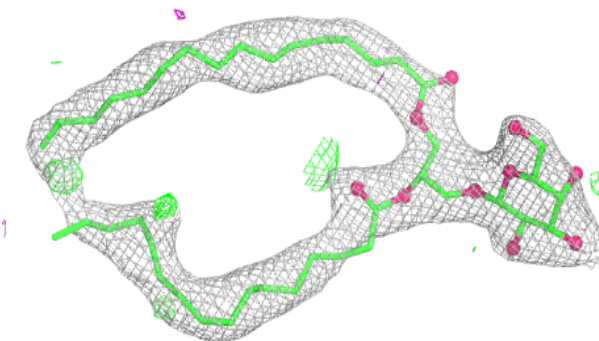


**Electron density around LMG c 523:**

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

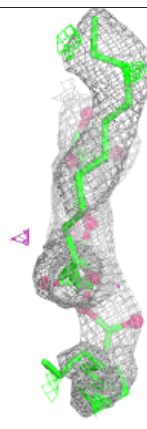
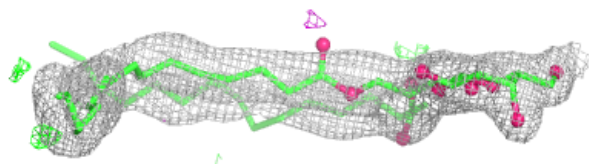
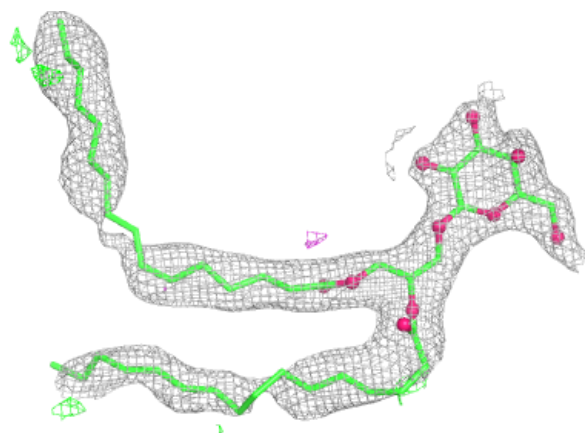
**Electron density around LMG A 421:**

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

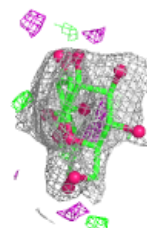
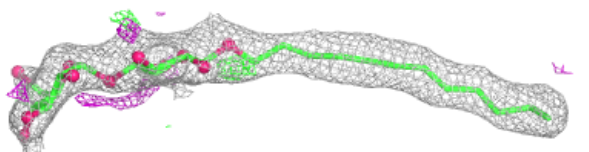
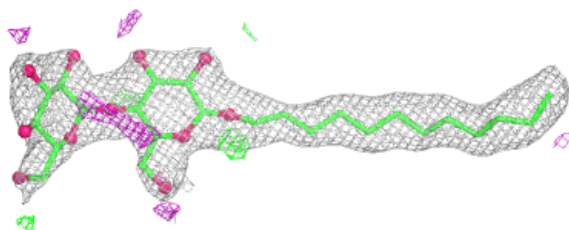


**Electron density around LMG C 519:**

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

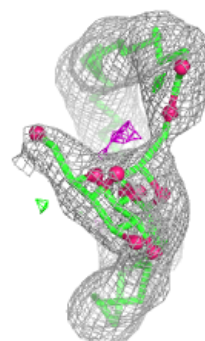
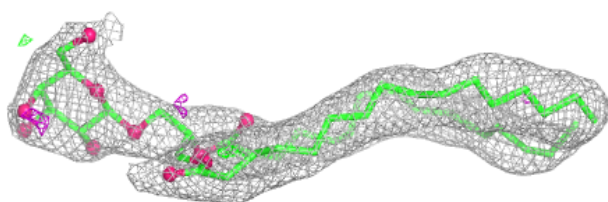
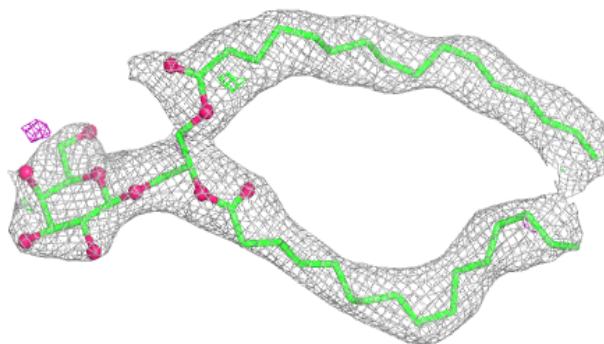
**Electron density around LMT m 102:**

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

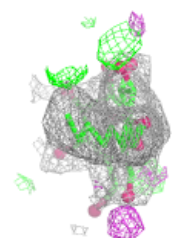
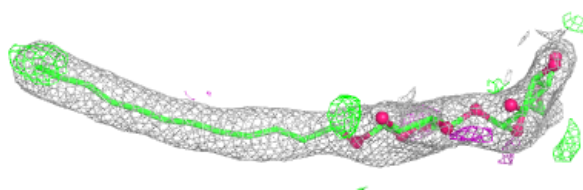
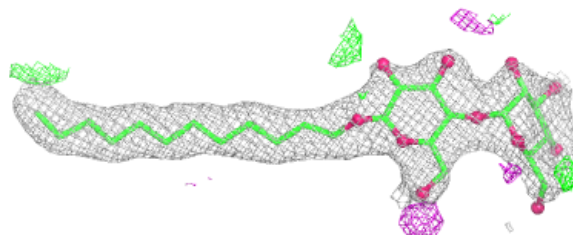


**Electron density around LMG c 501:**

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

**Electron density around LMT M 101:**

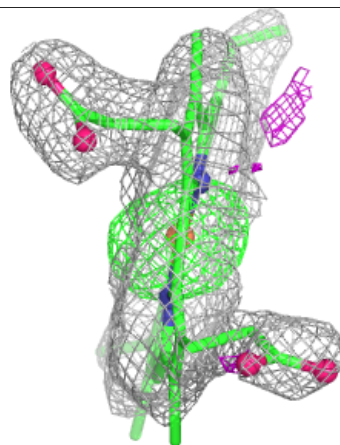
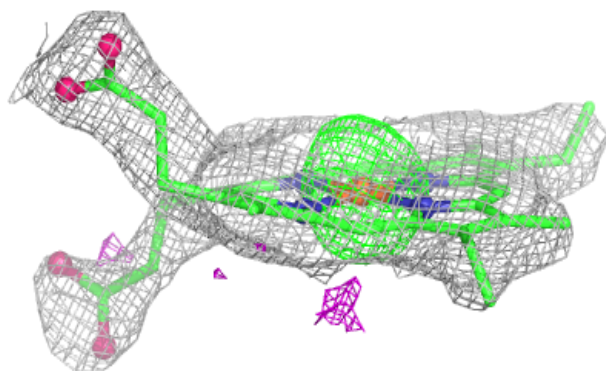
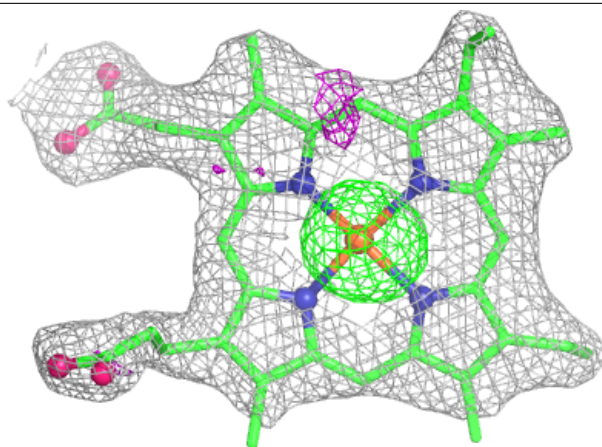
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



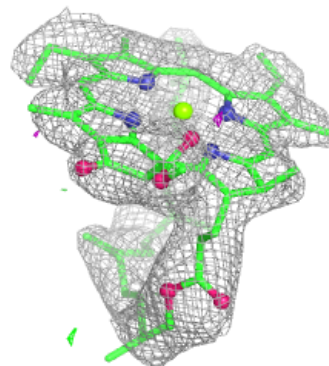
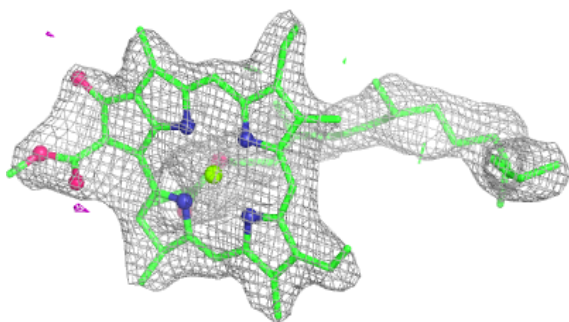
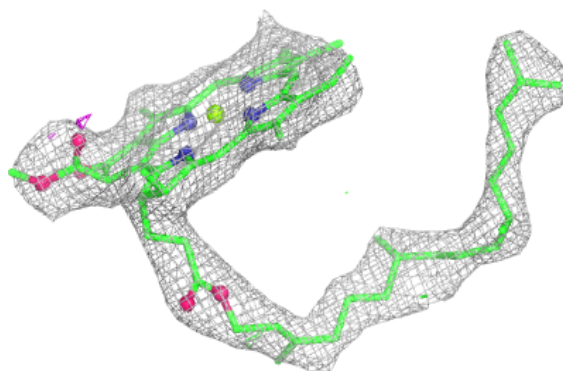


**Electron density around HEM F 102:**

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

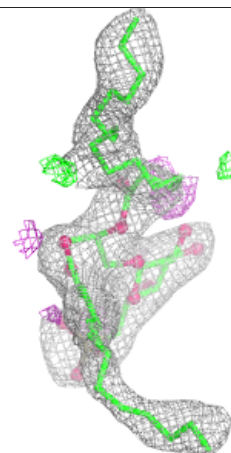
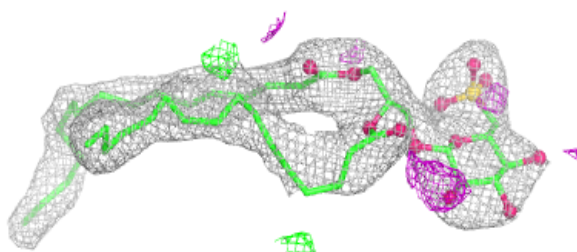
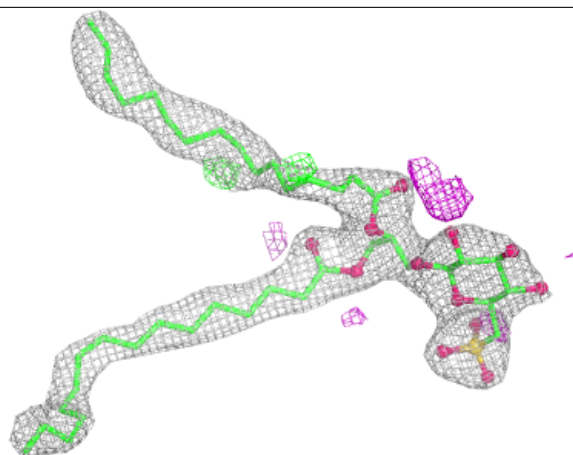
**Electron density around CLA c 518:**

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



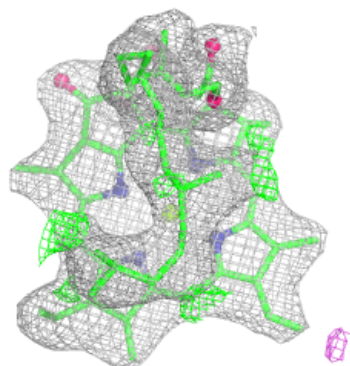
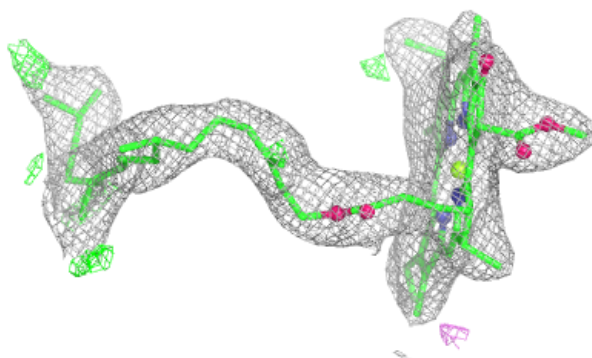
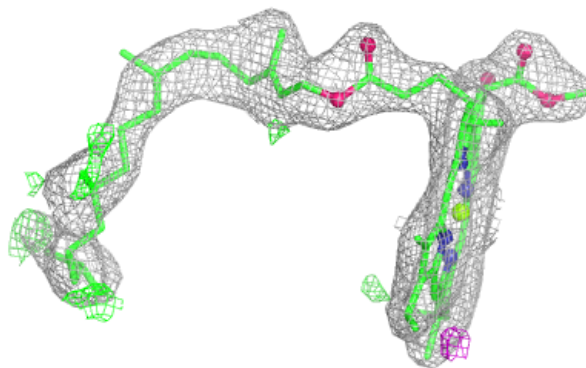
**Electron density around SQD A 412:**

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

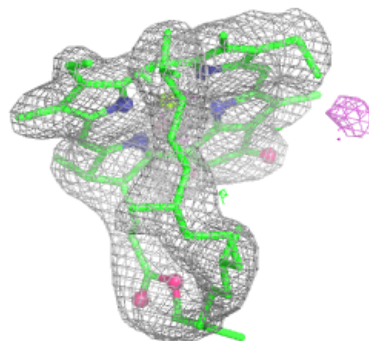
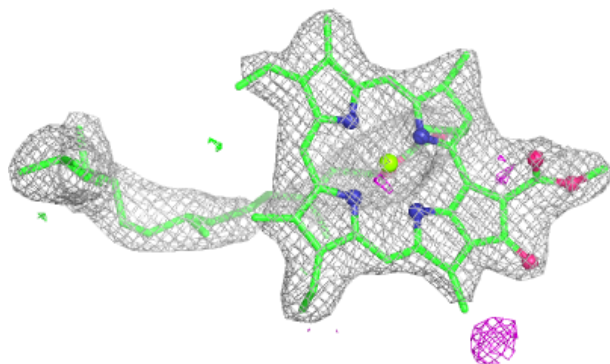
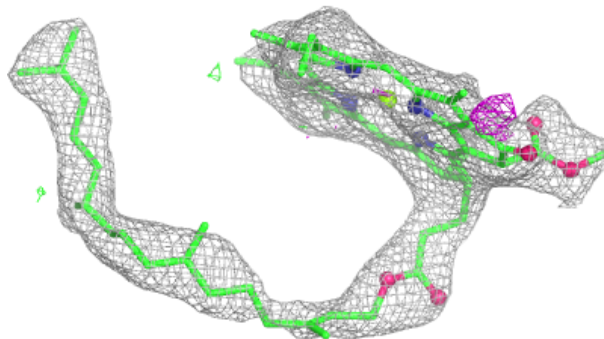


**Electron density around CLA C 506:**

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

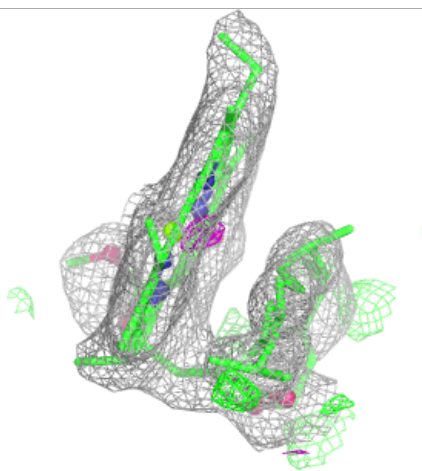
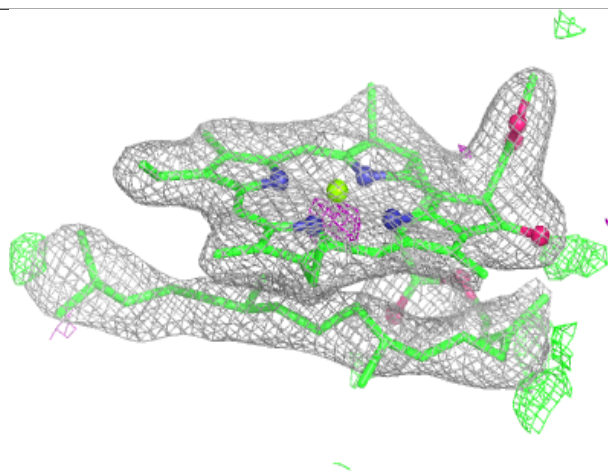
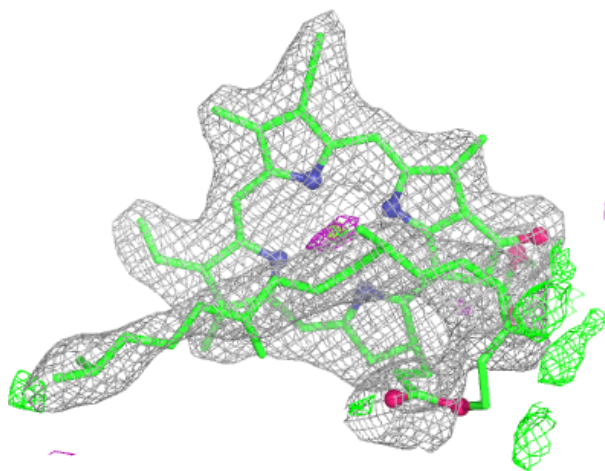
**Electron density around CLA C 513:**

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



**Electron density around CLA b 610:**

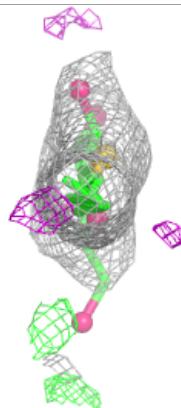
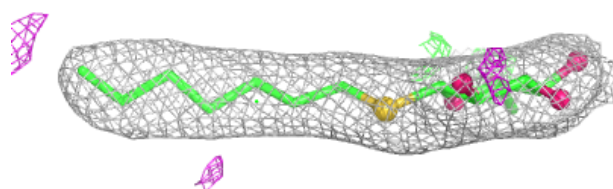
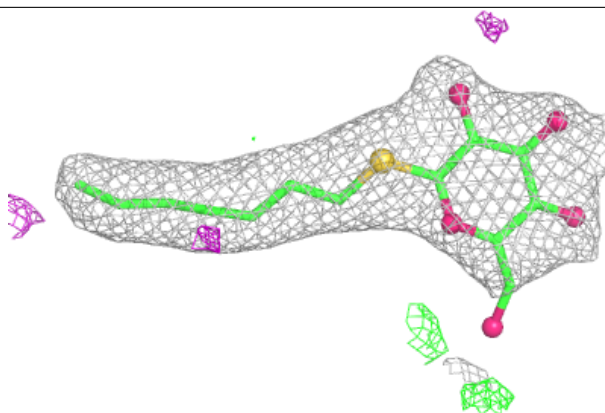
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



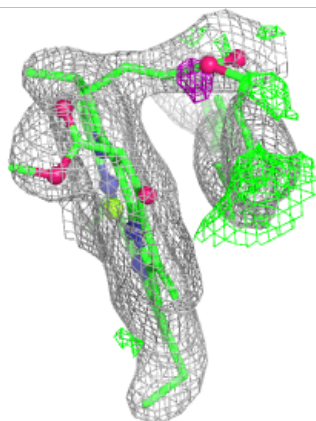
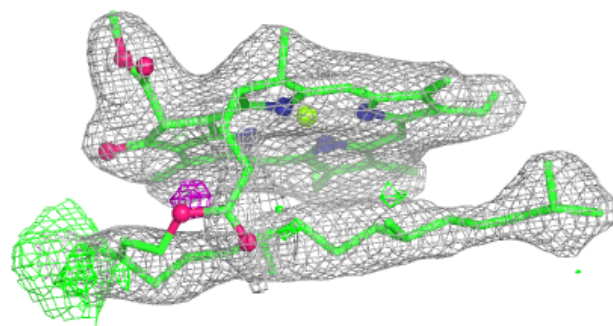
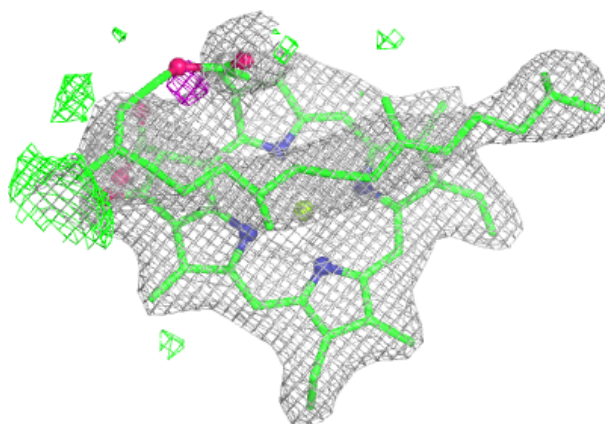


**Electron density around HTG B 632:**

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

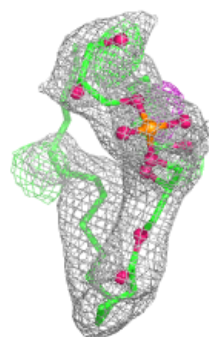
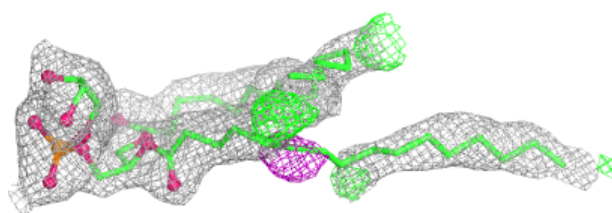
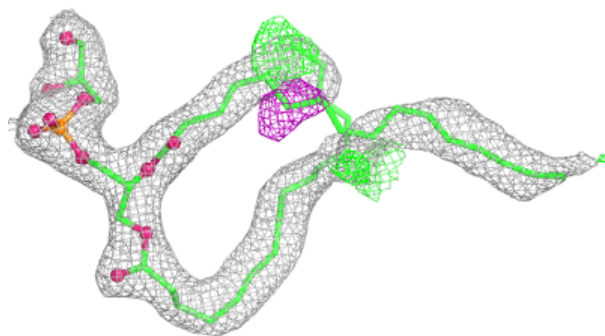
**Electron density around CLA B 602:**

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

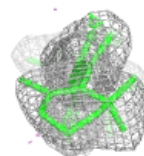
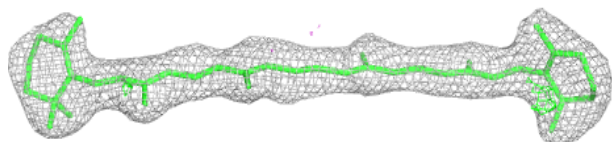
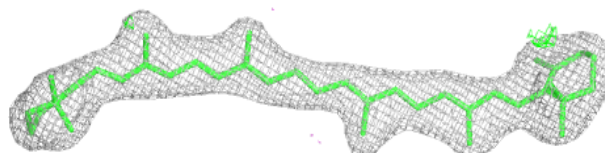


**Electron density around LHG D 409:**

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

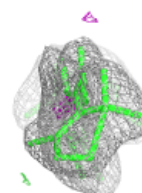
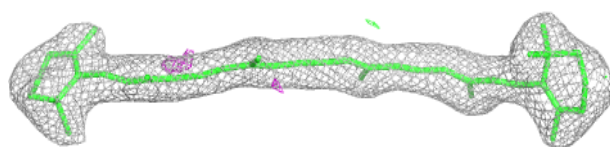
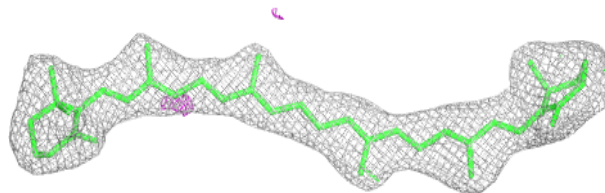
**Electron density around BCR C 514:**

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

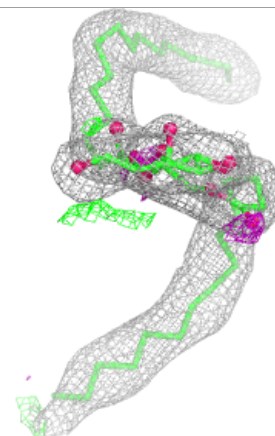
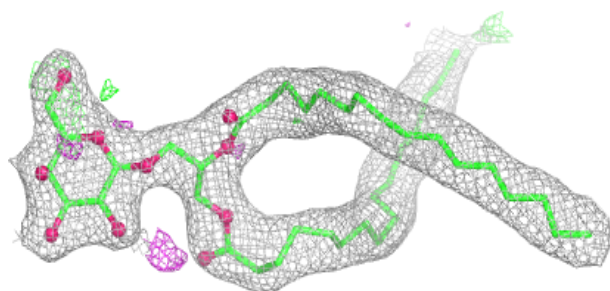
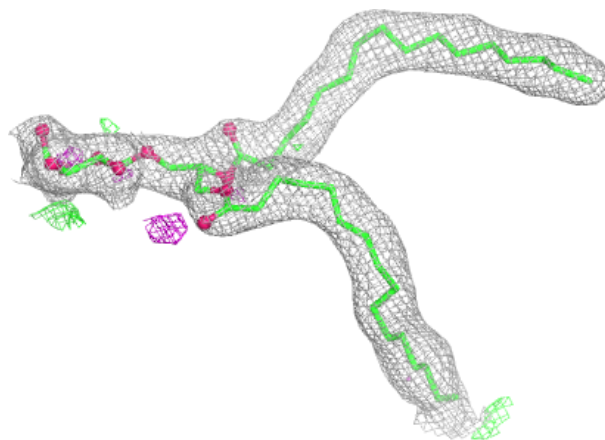


**Electron density around BCR y 101:**

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

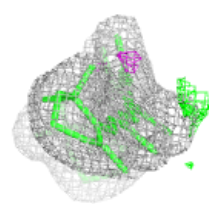
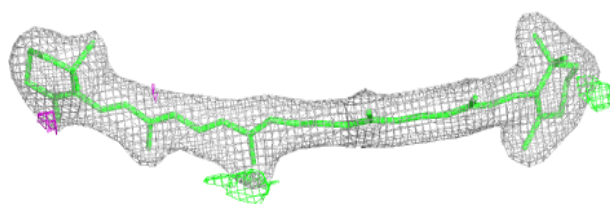
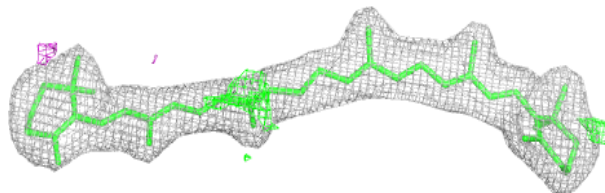
**Electron density around LMG B 622:**

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

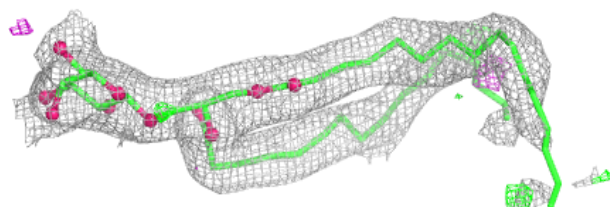
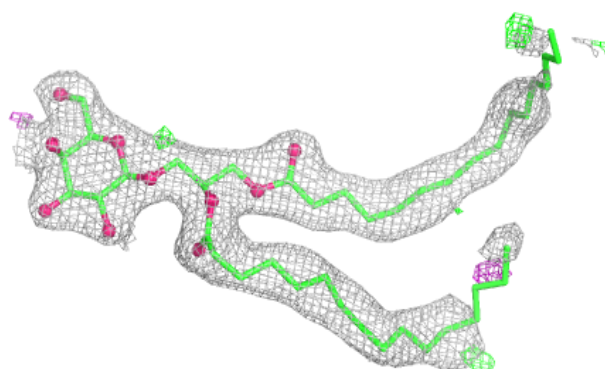


**Electron density around BCR t 101:**

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

**Electron density around LMG D 413:**

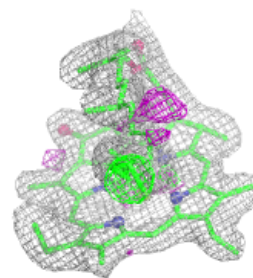
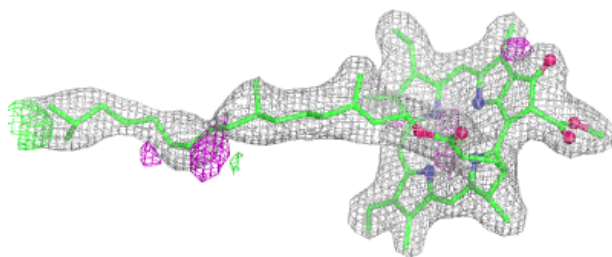
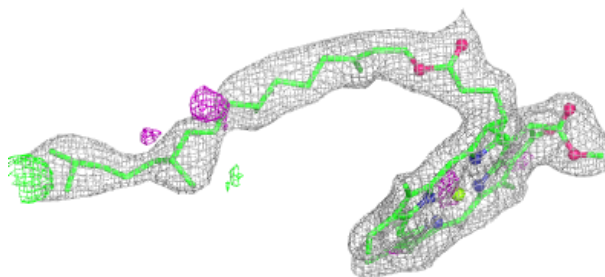
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



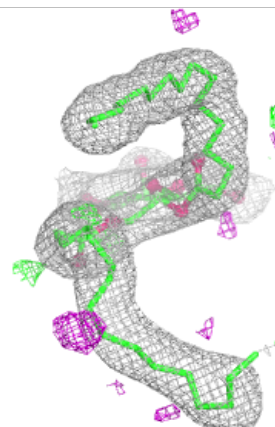
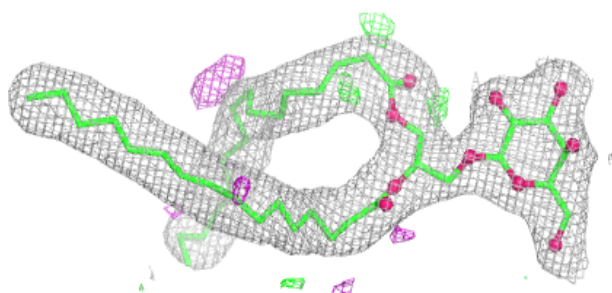
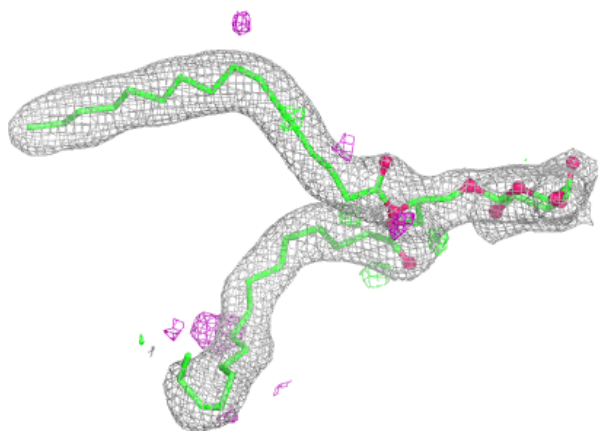


**Electron density around CLA C 504:**

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

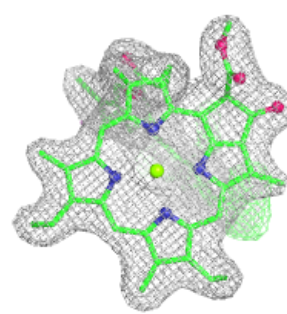
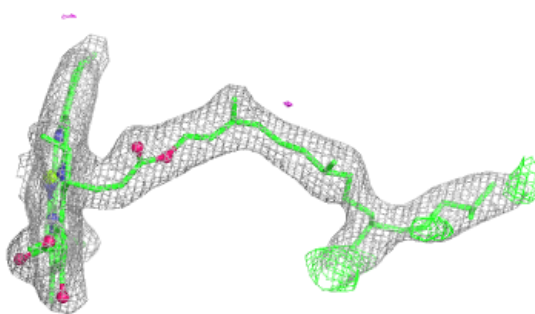
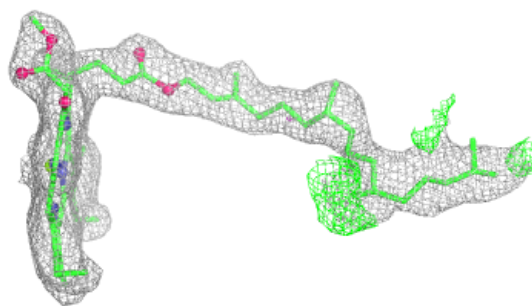
**Electron density around LMG b 629:**

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

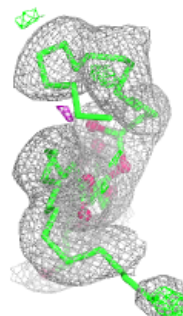
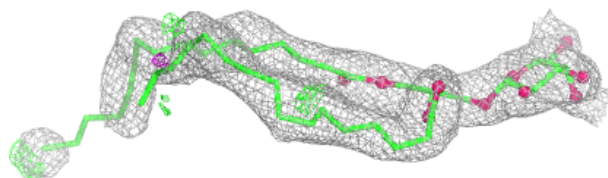
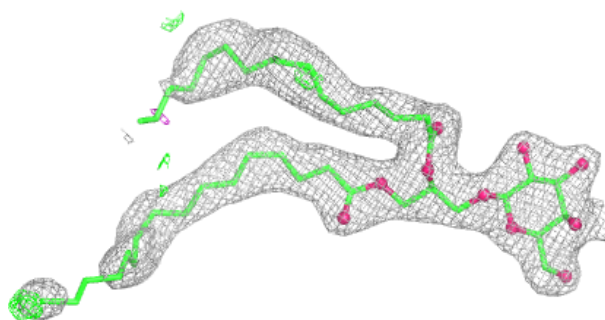


**Electron density around CLA b 615:**

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

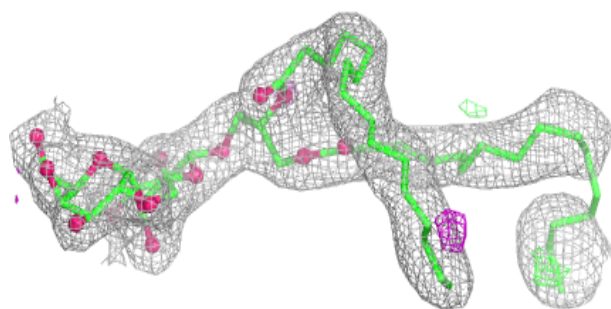
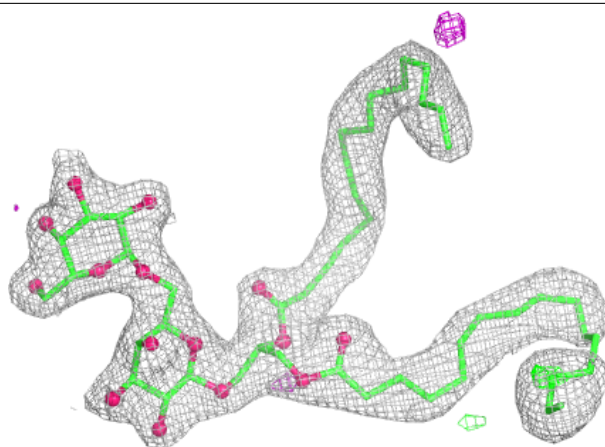
**Electron density around LMG d 413:**

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

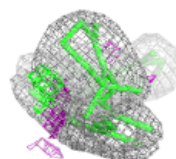
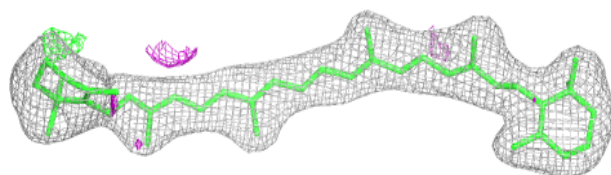
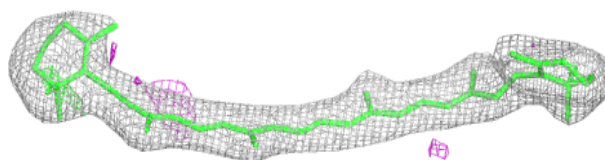


**Electron density around DGD C 517:**

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

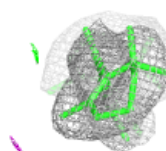
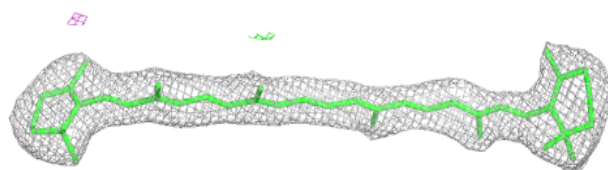
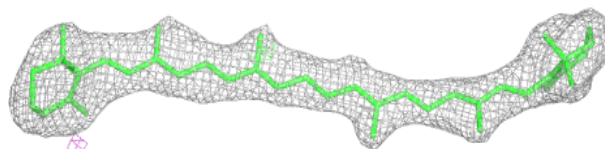
**Electron density around BCR D 404:**

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

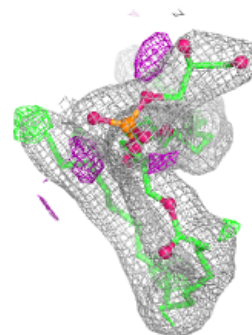
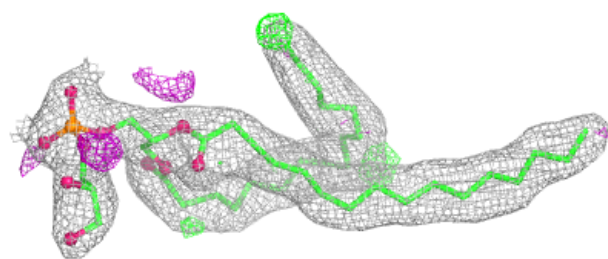
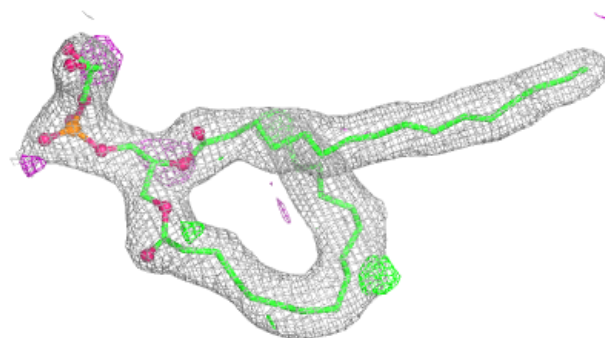


**Electron density around BCR c 528:**

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

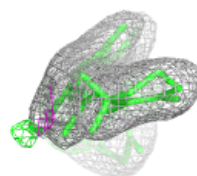
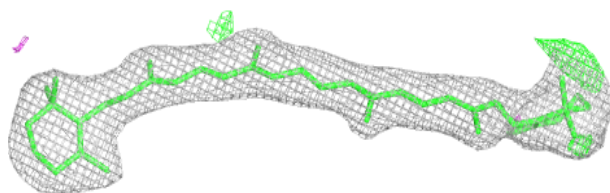
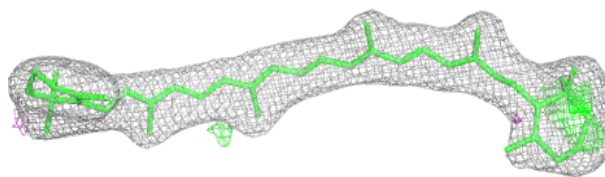
**Electron density around LHG D 407:**

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



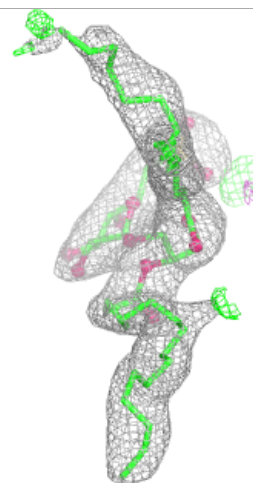
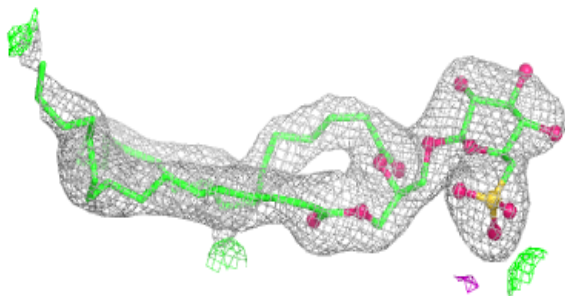
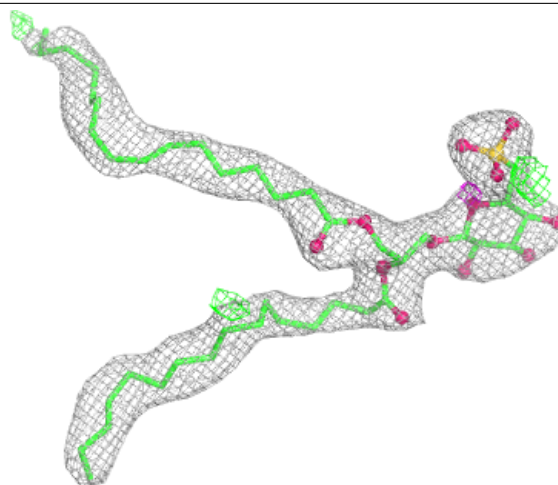
**Electron density around BCR d 404:**

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



**Electron density around SQD a 414:**

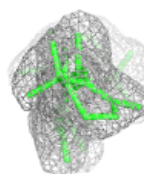
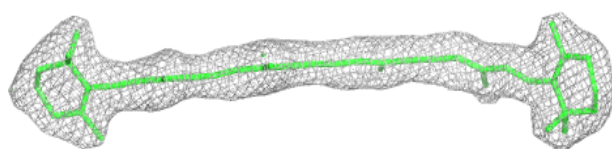
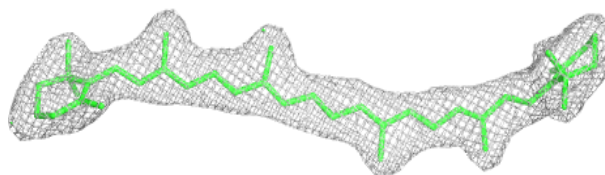
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



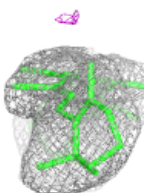
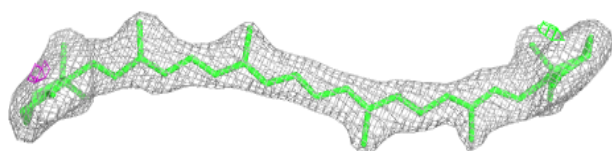
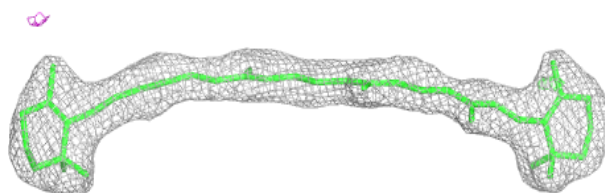


**Electron density around BCR h 101:**

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

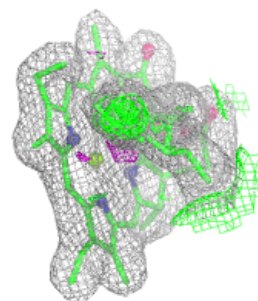
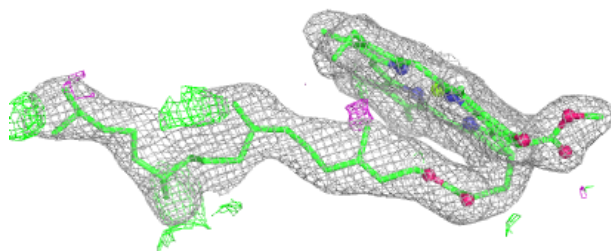
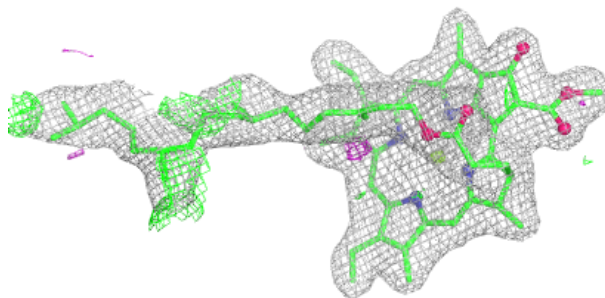
**Electron density around BCR k 101:**

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



**Electron density around CLA b 623:**

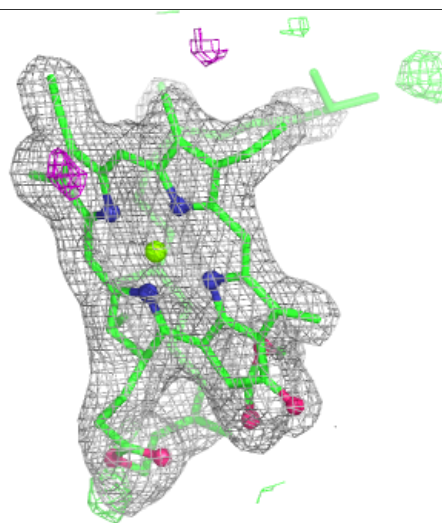
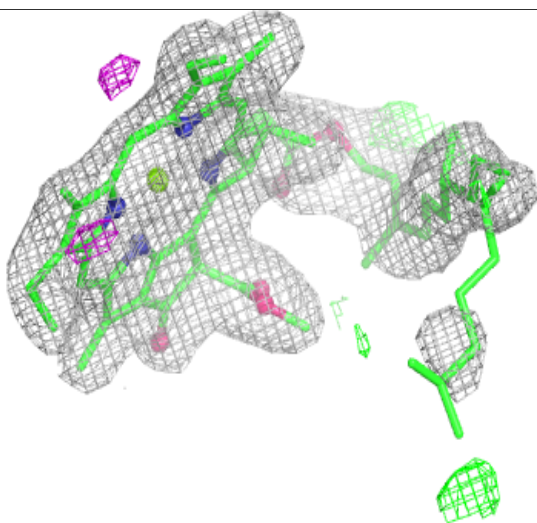
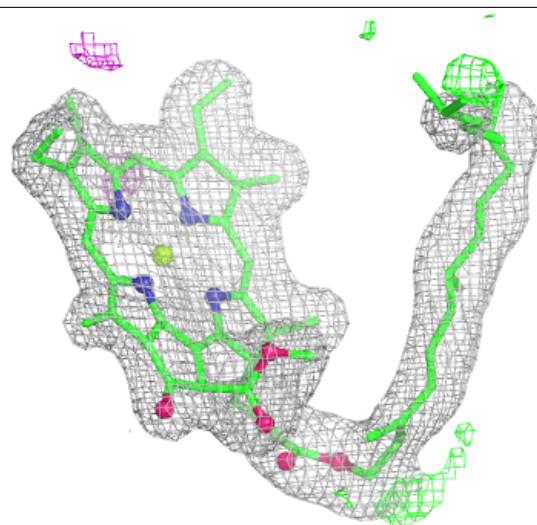
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





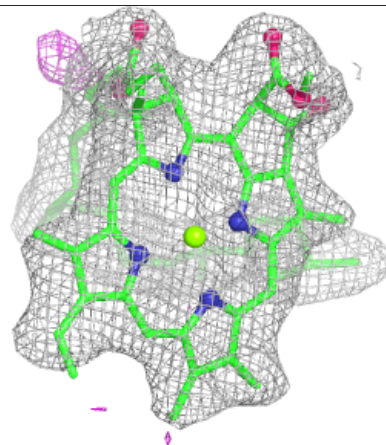
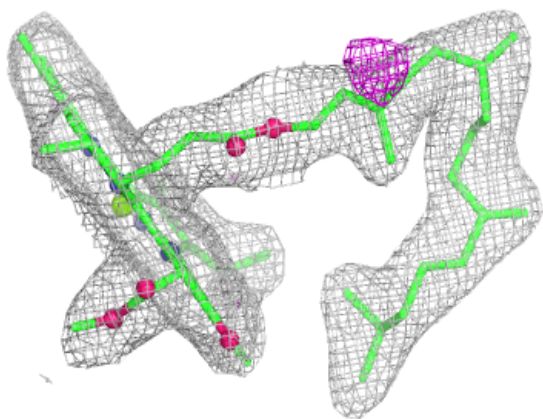
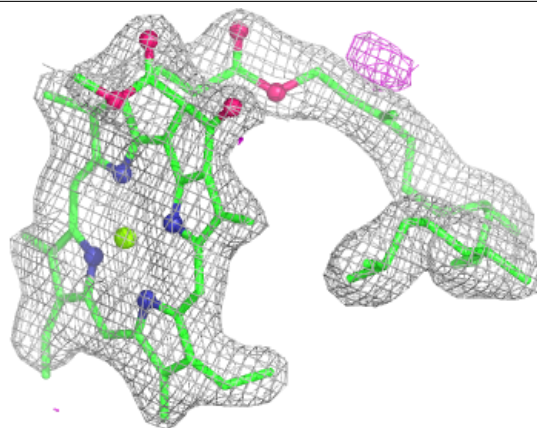
**Electron density around CLA b 625:**

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



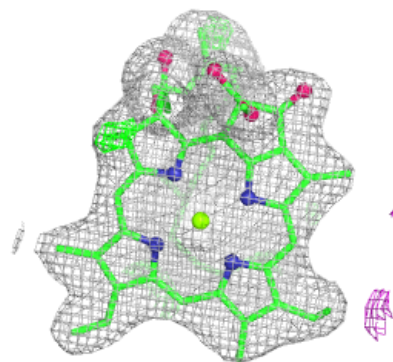
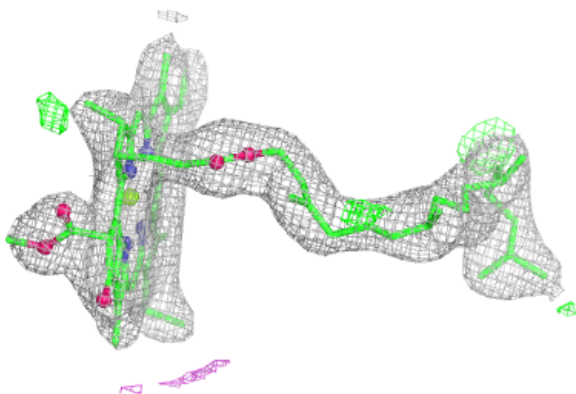
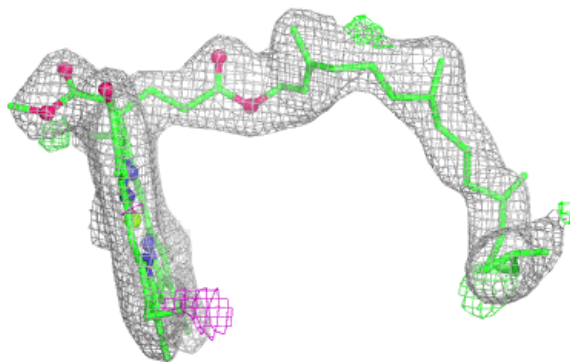
**Electron density around CLA c 508:**

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



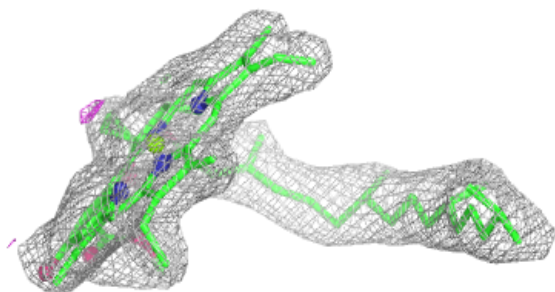
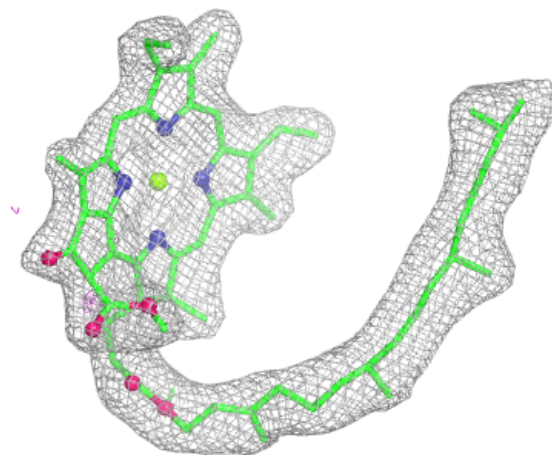
**Electron density around CLA c 511:**

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



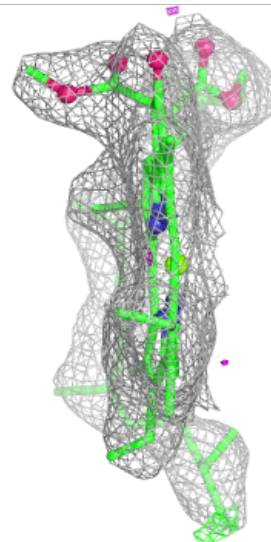
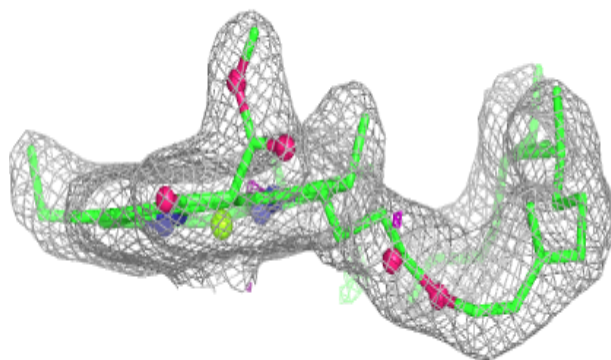
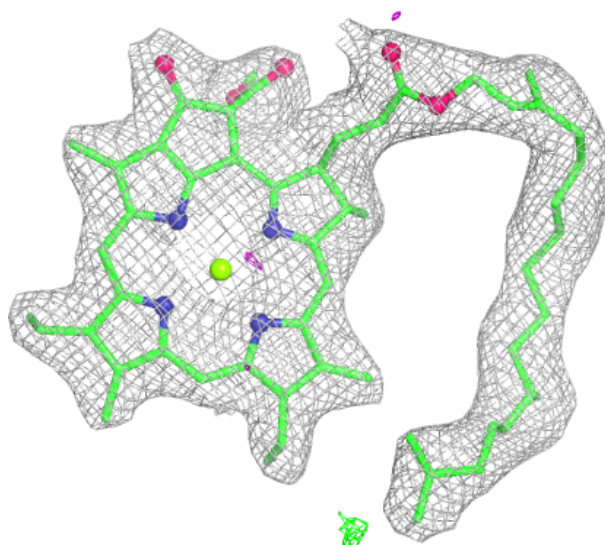
**Electron density around CLA c 512:**

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



**Electron density around CLA c 517:**

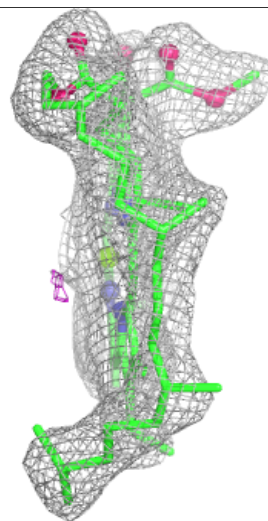
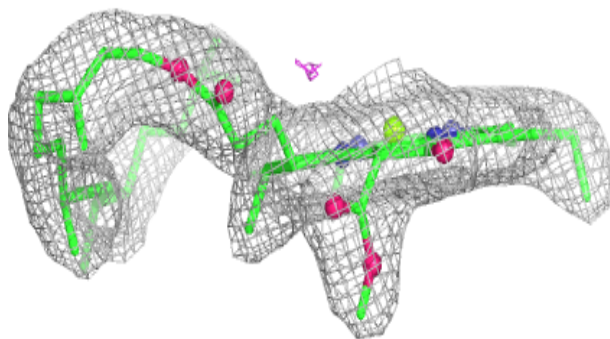
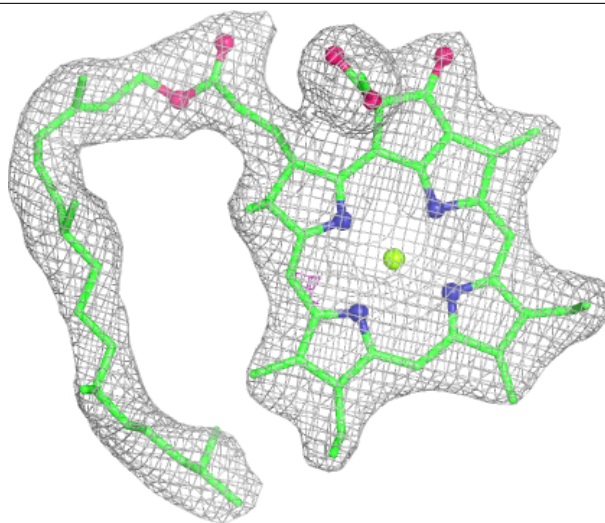
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





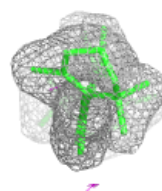
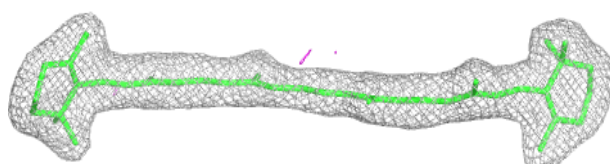
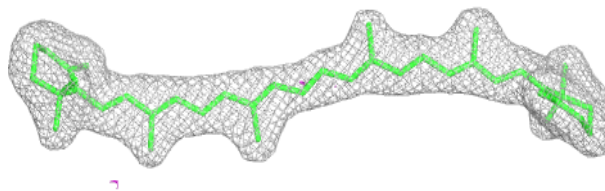
**Electron density around CLA C 512:**

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

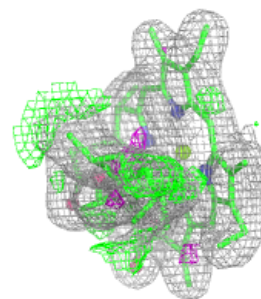
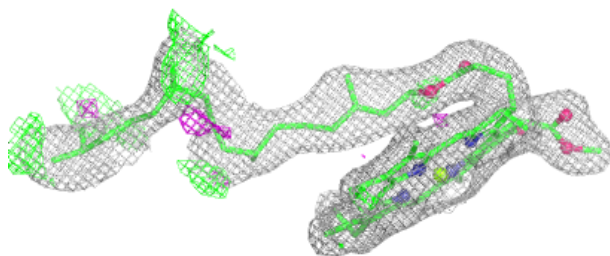
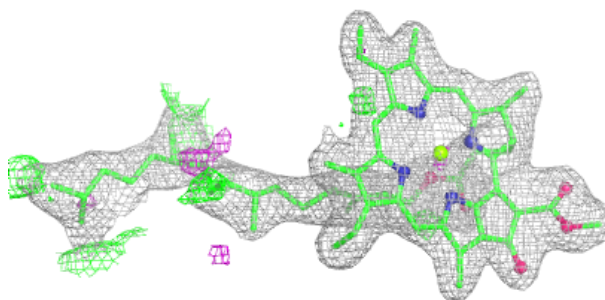


**Electron density around BCR A 411:**

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

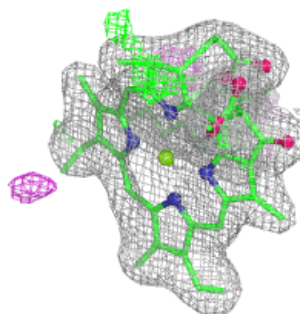
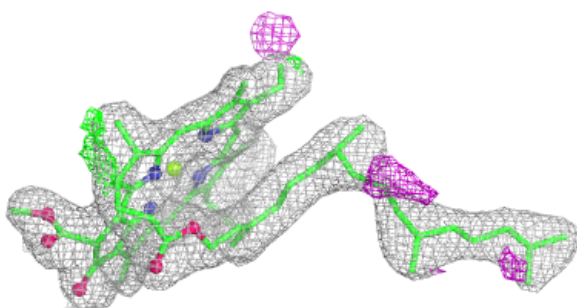
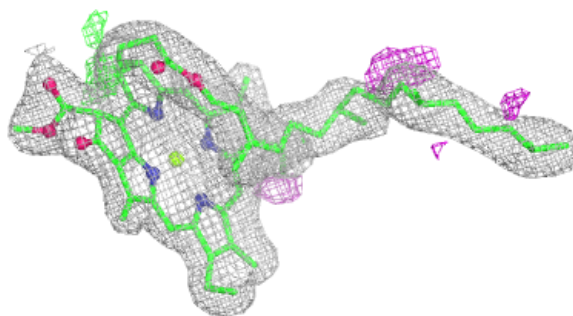
**Electron density around CLA B 615:**

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

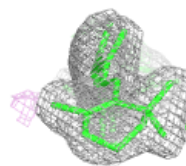
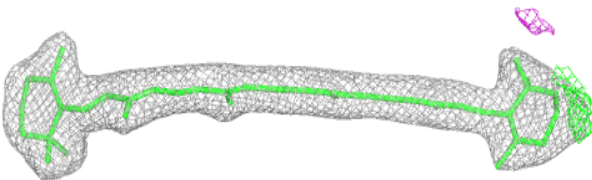
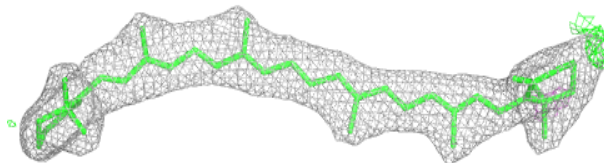


**Electron density around CLA C 505:**

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

**Electron density around BCR H 101:**

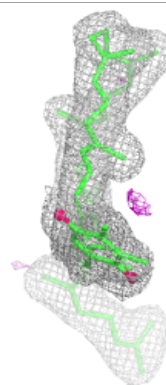
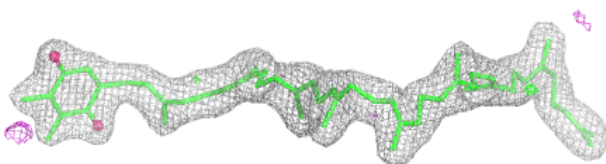
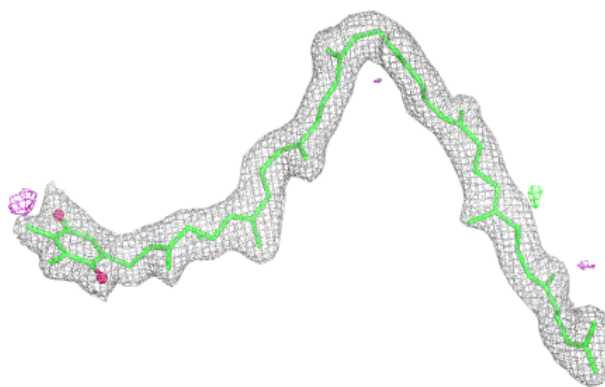
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



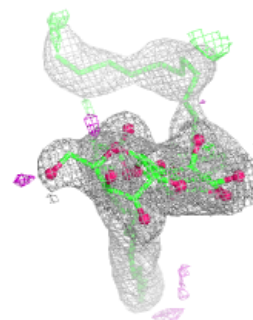
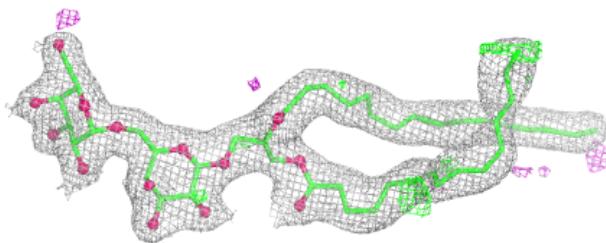
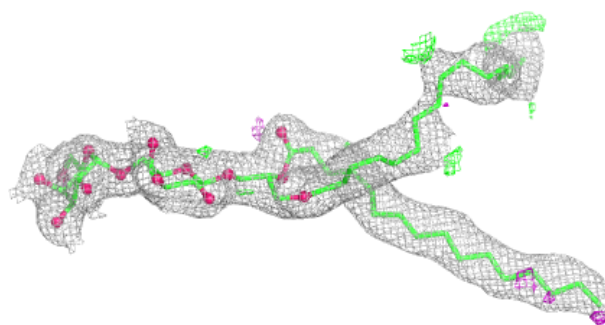


**Electron density around PL9 d 405 (A):**

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

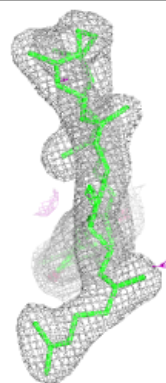
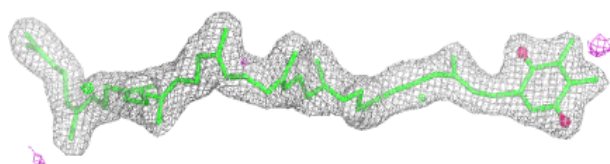
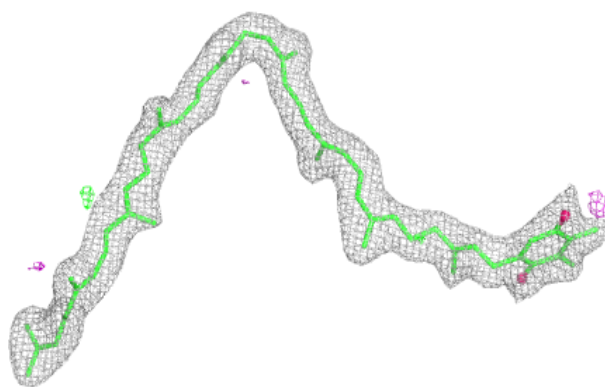
**Electron density around DGD C 516:**

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

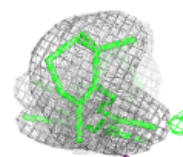
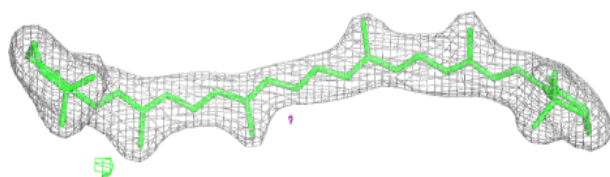
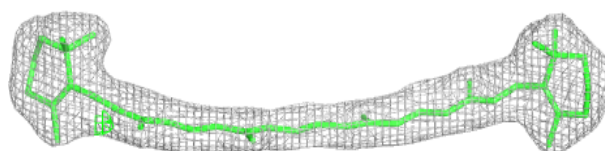


**Electron density around PL9 d 405 (B):**

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

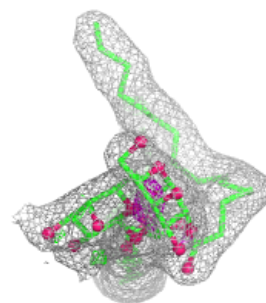
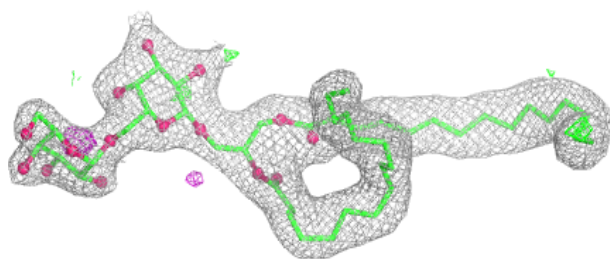
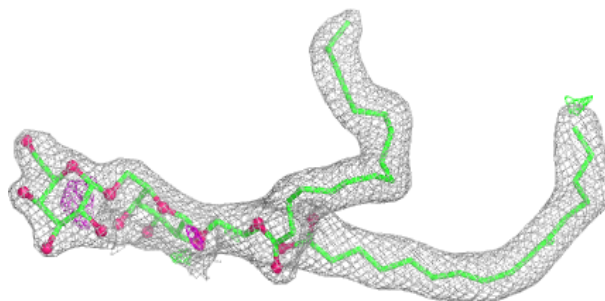
**Electron density around BCR K 101:**

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

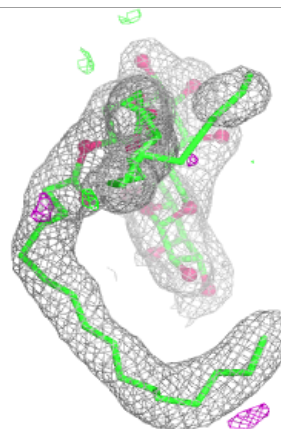
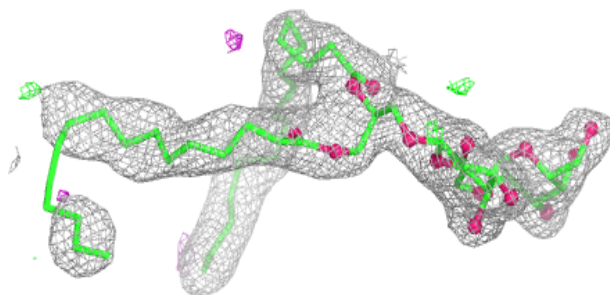
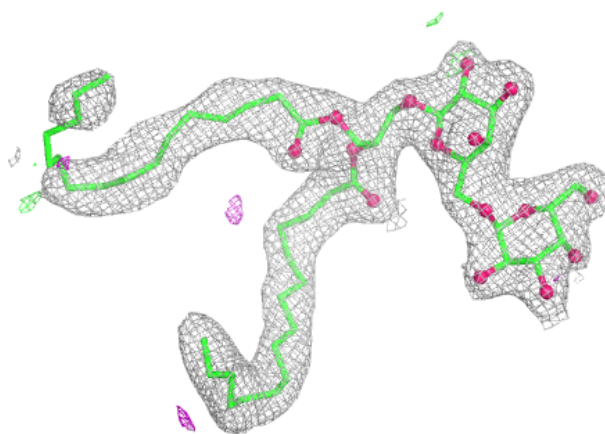


**Electron density around DGD H 102:**

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

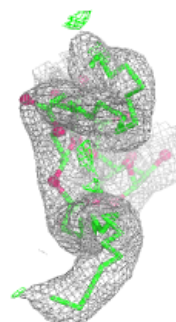
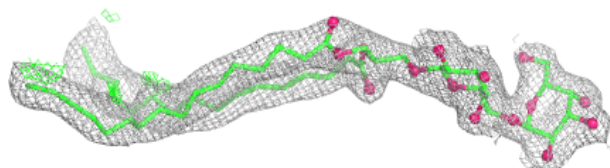
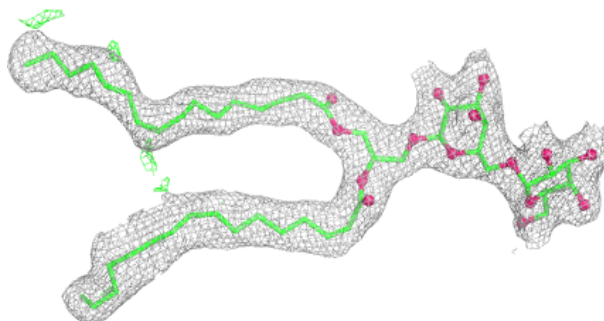
**Electron density around DGD c 521:**

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

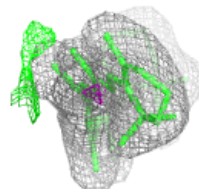
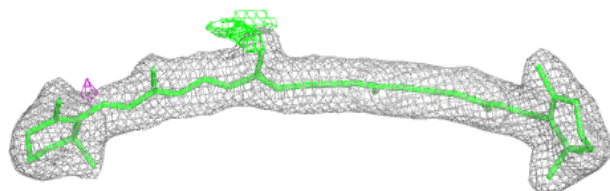
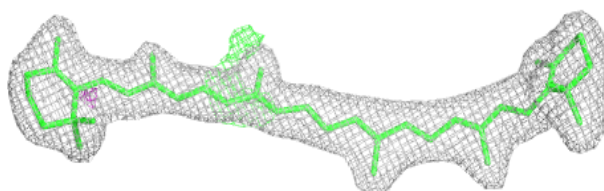


**Electron density around DGD c 522:**

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

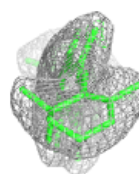
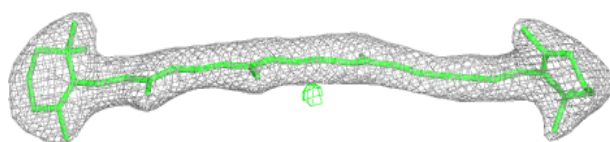
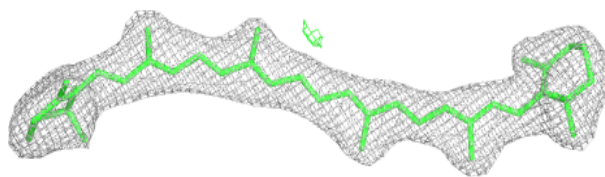
**Electron density around BCR T 103:**

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

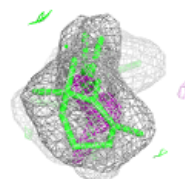
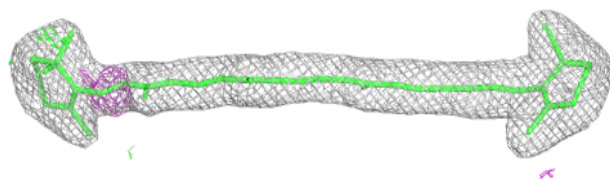
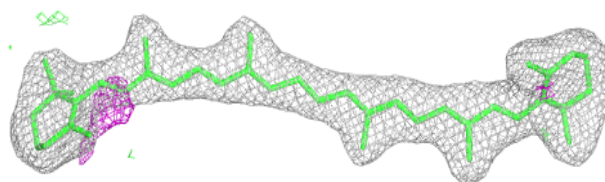


**Electron density around BCR Y 101:**

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

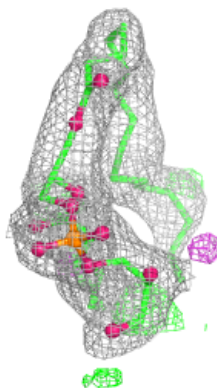
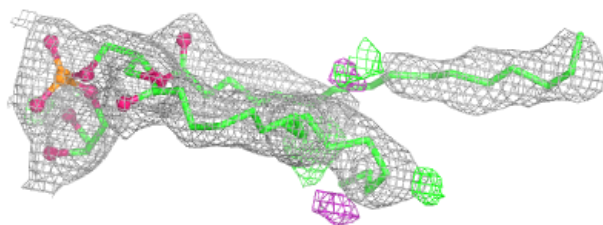
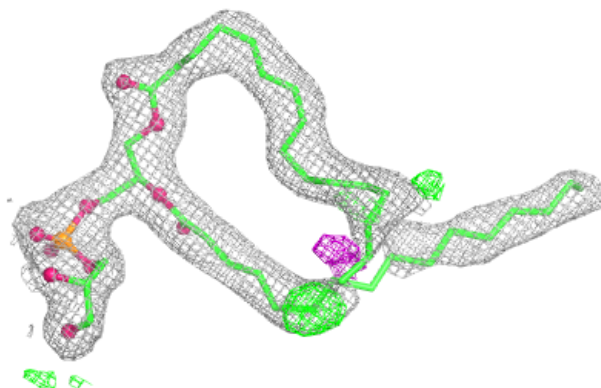
**Electron density around BCR b 627:**

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



**Electron density around LHG d 408:**

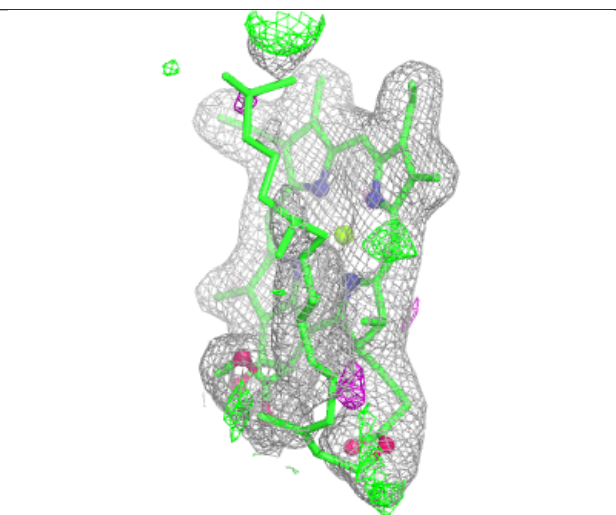
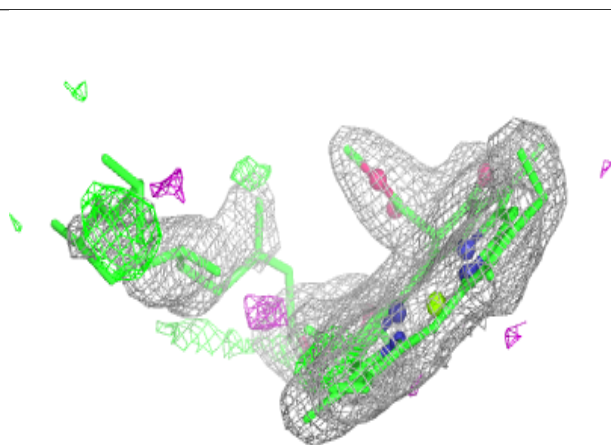
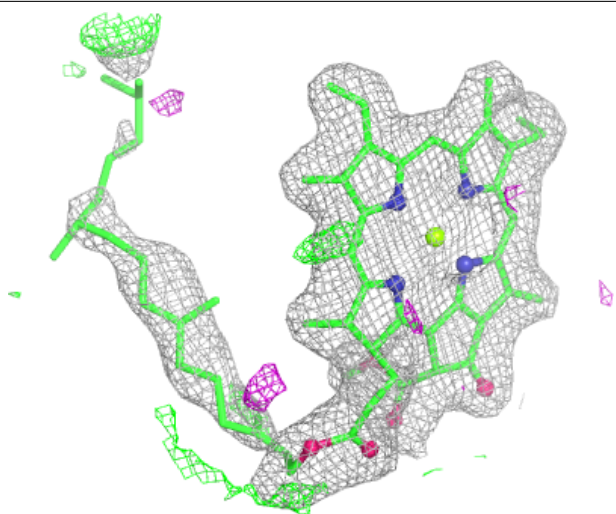
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





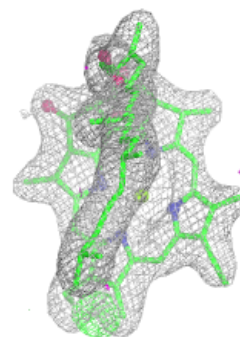
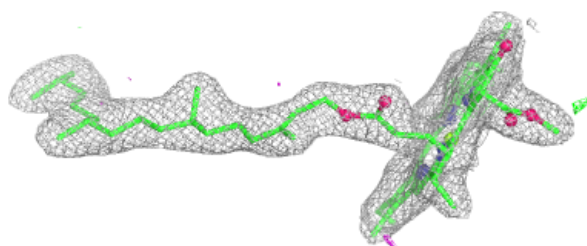
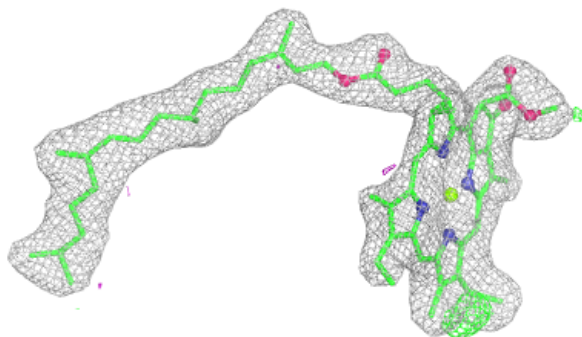
**Electron density around CLA B 617:**

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

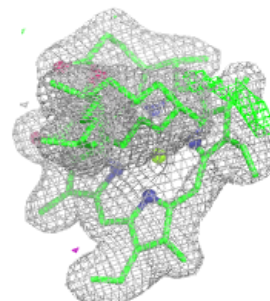
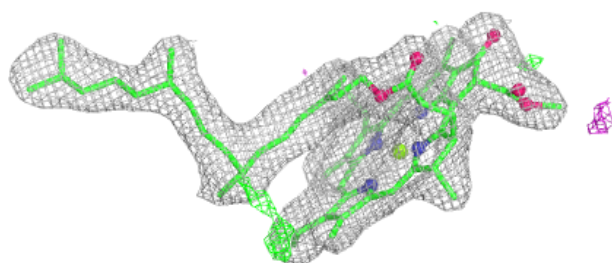
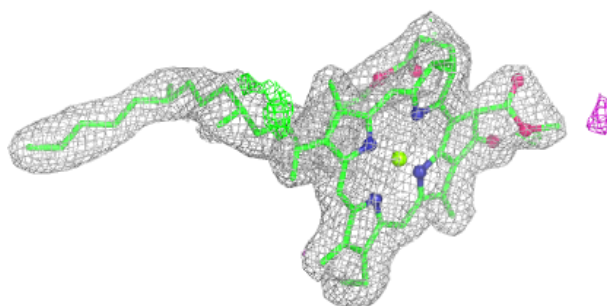


**Electron density around CLA b 618:**

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

**Electron density around CLA c 510:**

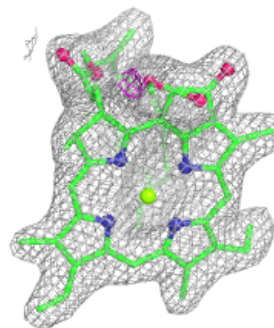
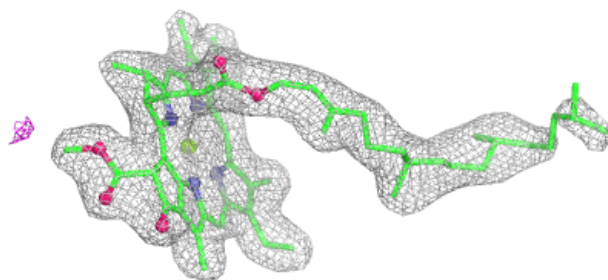
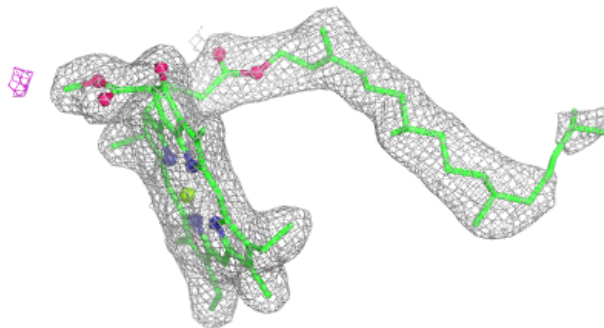
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





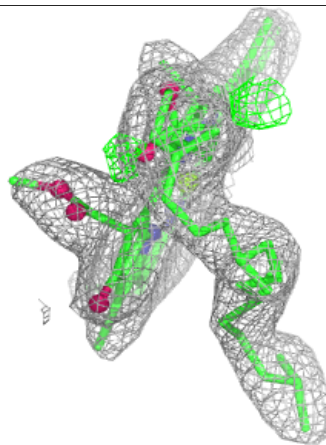
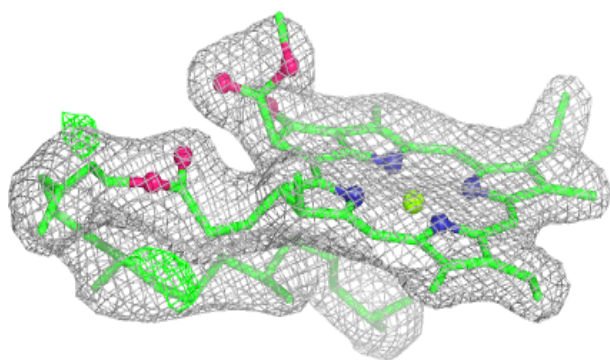
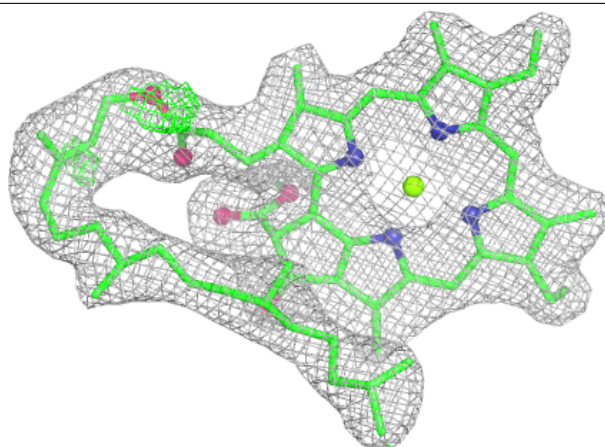
**Electron density around CLA C 508:**

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



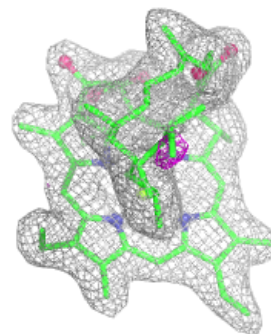
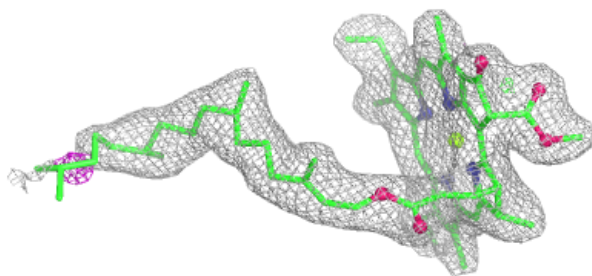
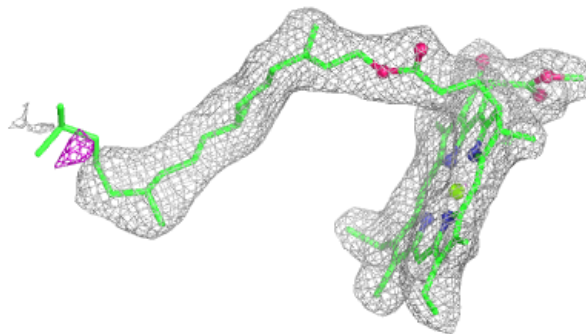
**Electron density around CLA C 509:**

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



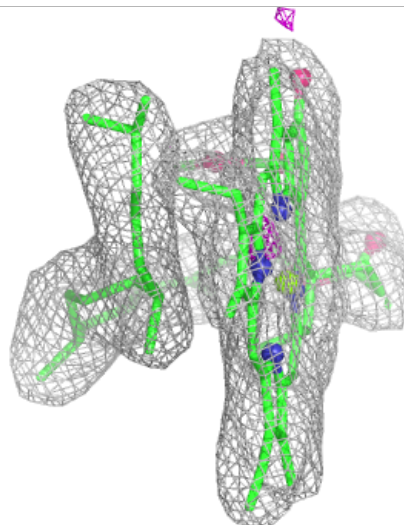
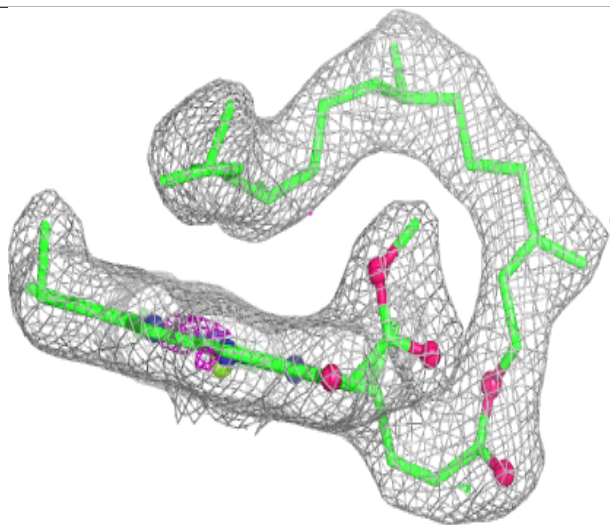
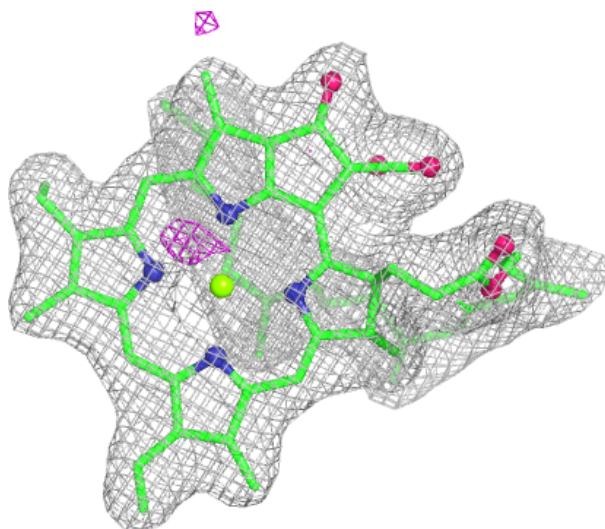
**Electron density around CLA c 513:**

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



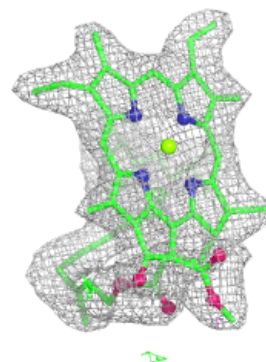
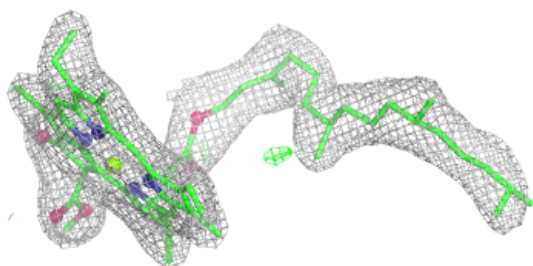
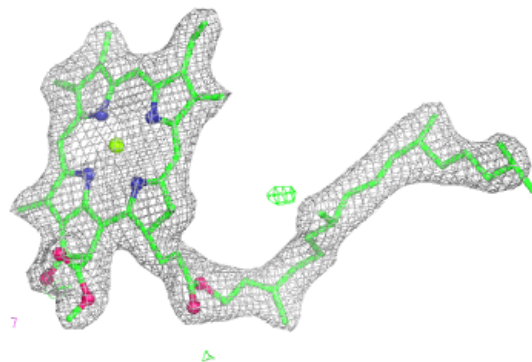
**Electron density around CLA c 515:**

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



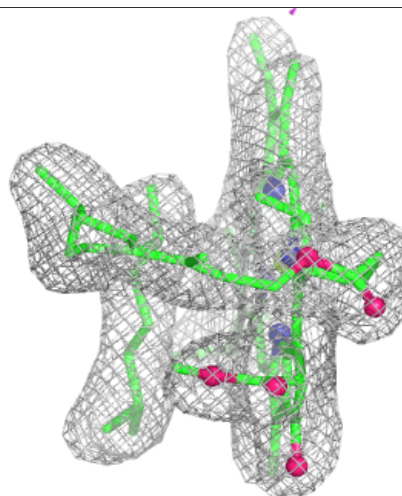
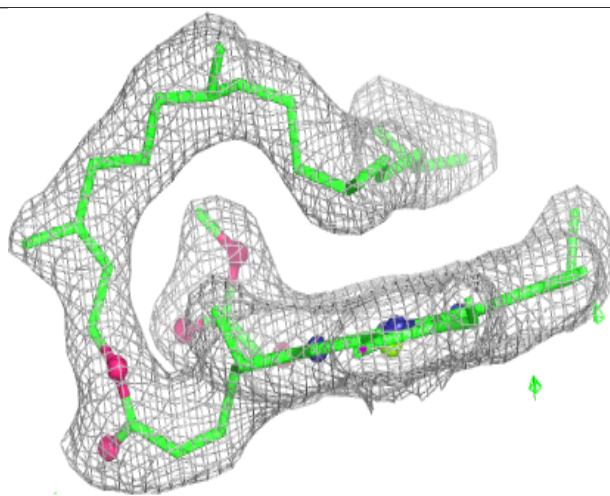
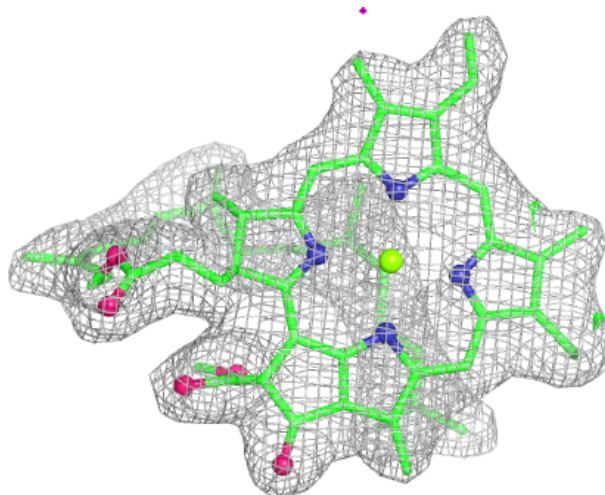
**Electron density around CLA c 516:**

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



**Electron density around CLA C 510:**

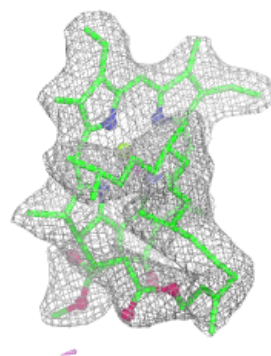
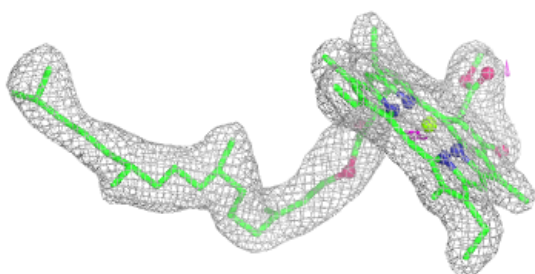
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



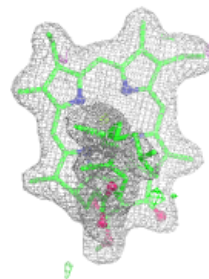
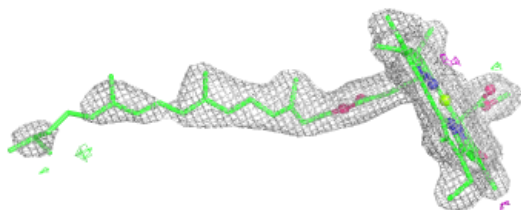
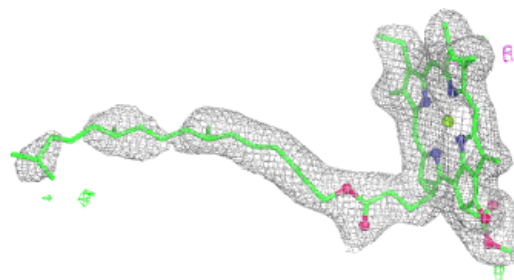


**Electron density around CLA C 511:**

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

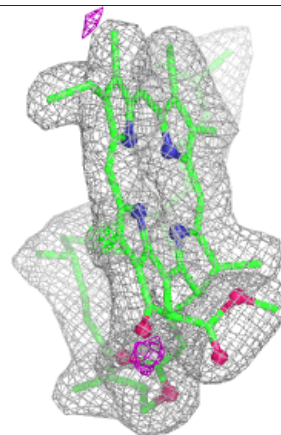
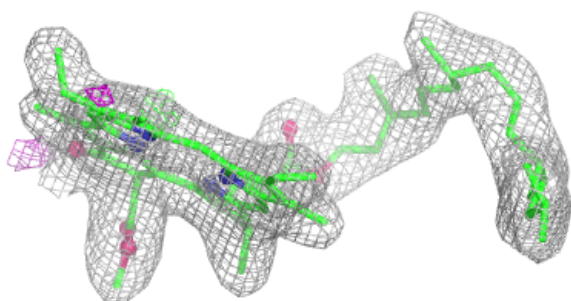
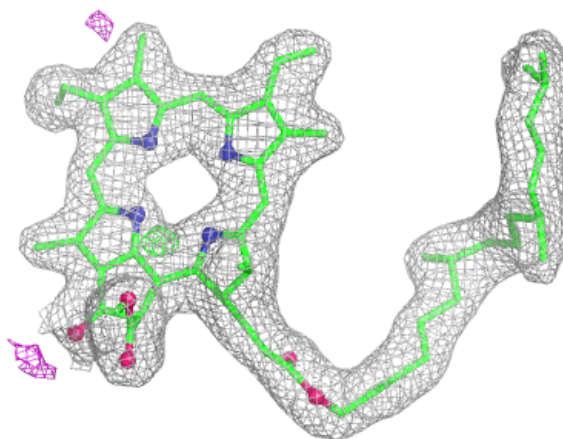
**Electron density around CLA d 403:**

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



**Electron density around PHO a 418 (A):**

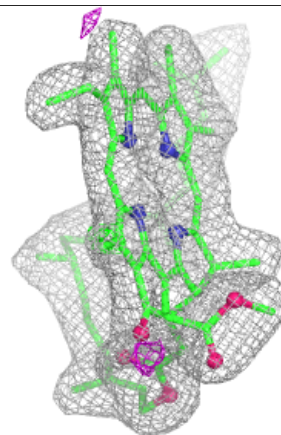
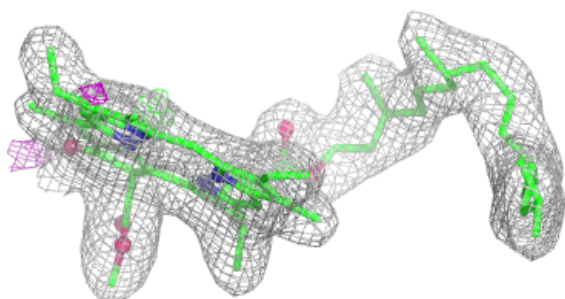
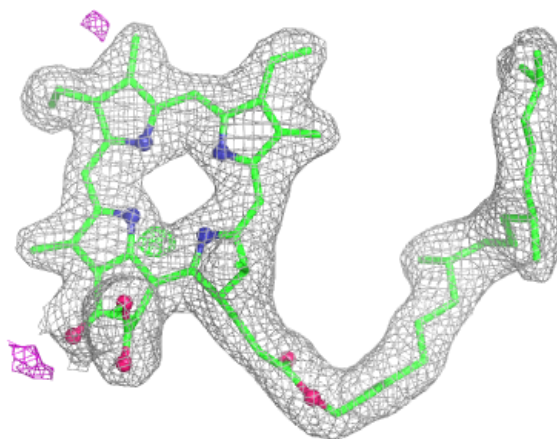
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





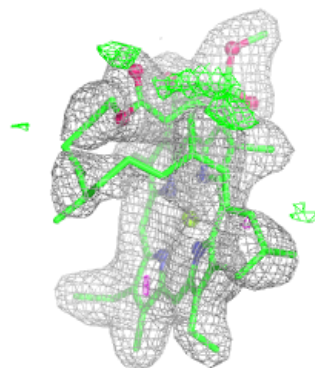
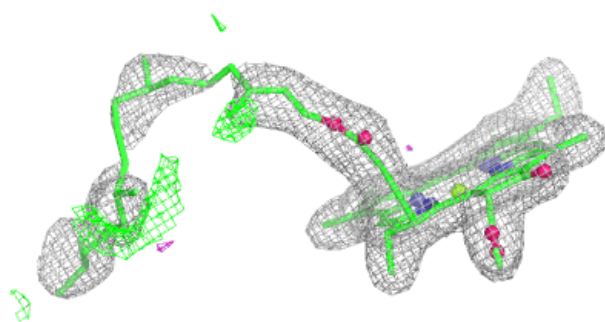
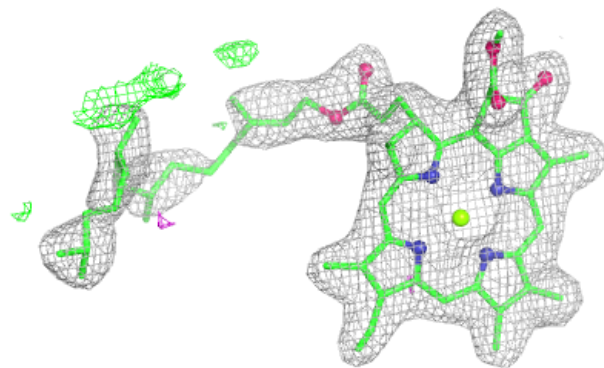
**Electron density around PHO a 418 (B):**

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

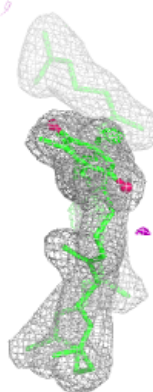
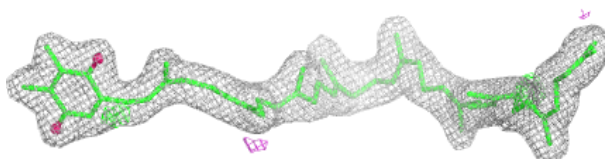
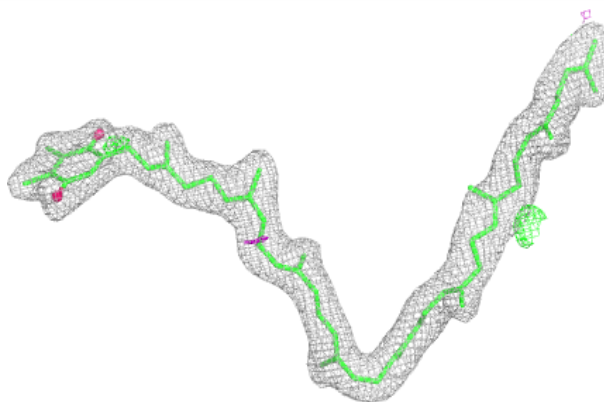


**Electron density around CLA A 410:**

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

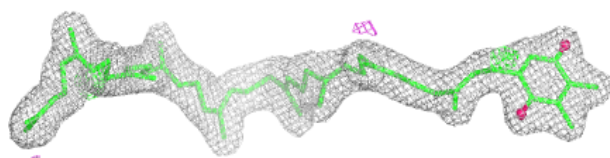
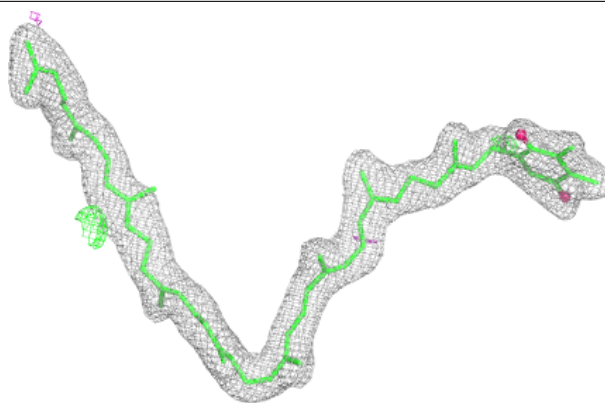
**Electron density around PL9 D 405 (A):**

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

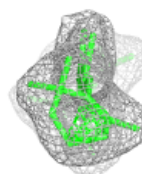
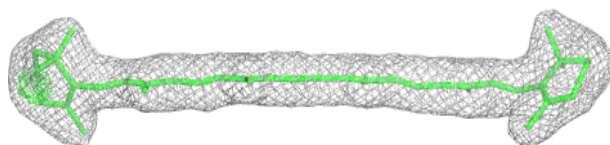
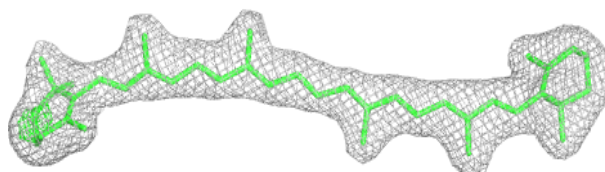


**Electron density around PL9 D 405 (B):**

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

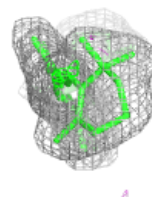
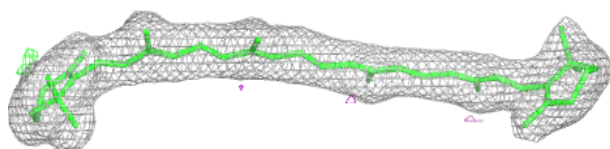
**Electron density around BCR B 619:**

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

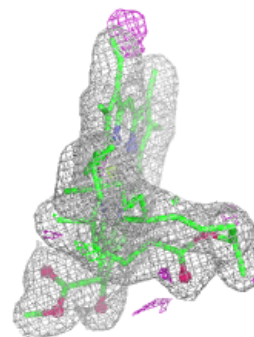
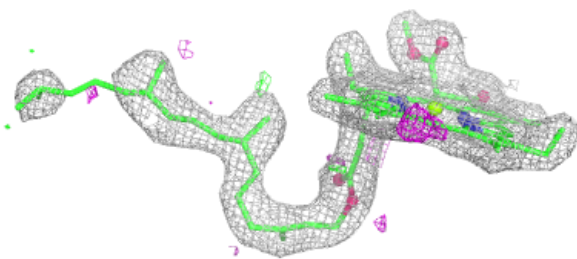
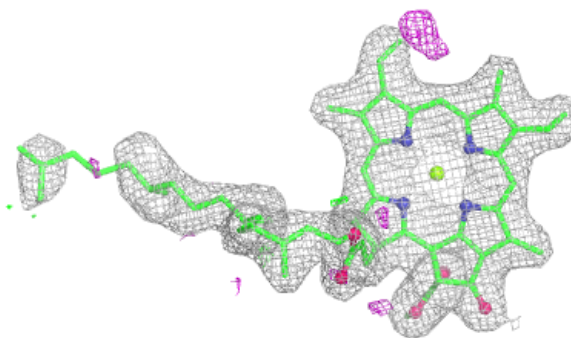


**Electron density around BCR B 620:**

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

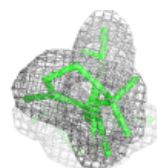
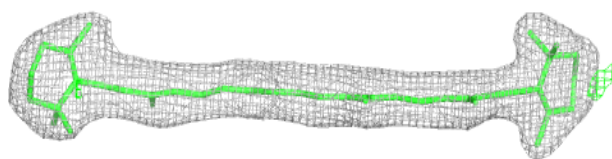
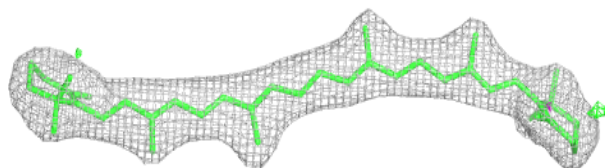
**Electron density around CLA A 407:**

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

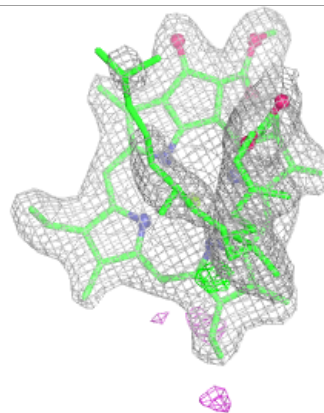
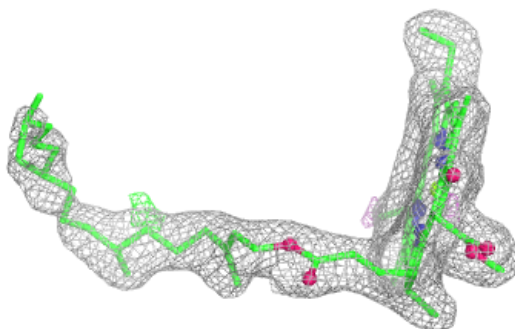
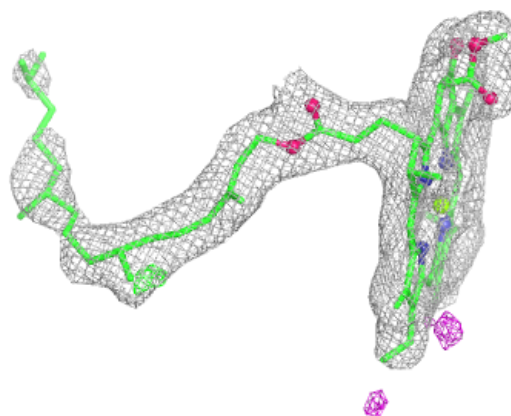


**Electron density around BCR C 515:**

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

**Electron density around CLA D 403:**

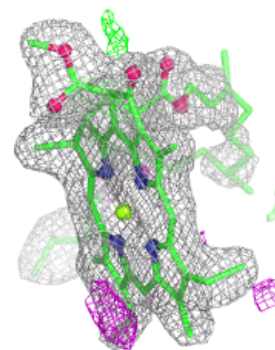
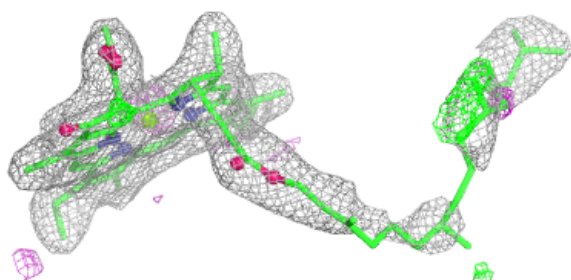
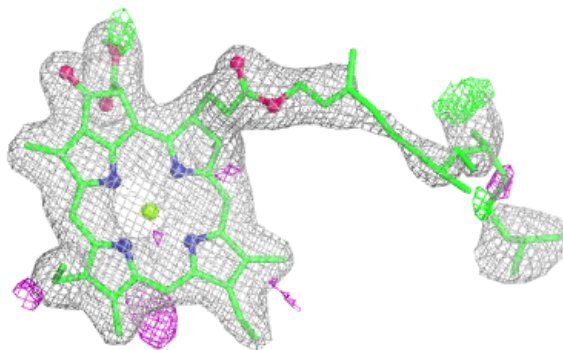
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



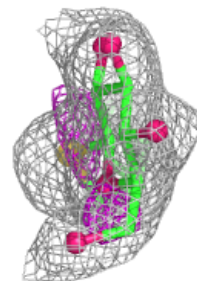
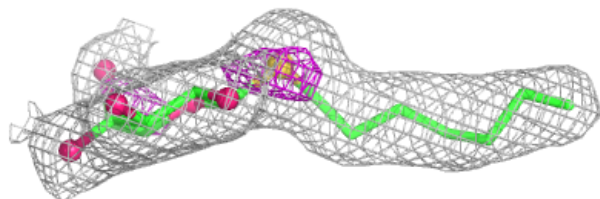
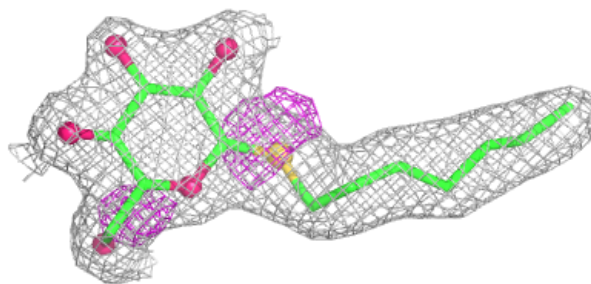


**Electron density around CLA a 412:**

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

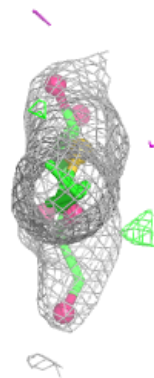
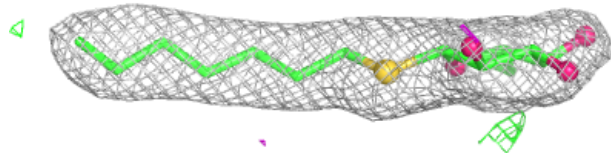
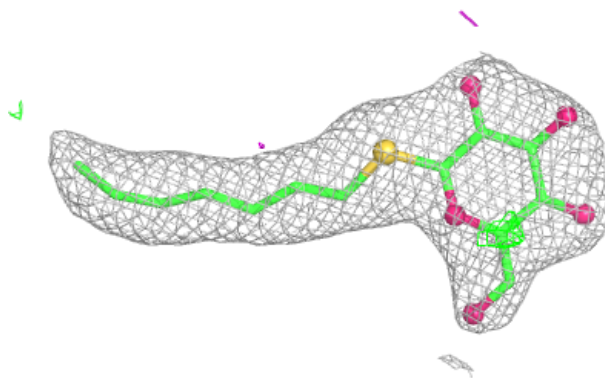
**Electron density around HTG b 601:**

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

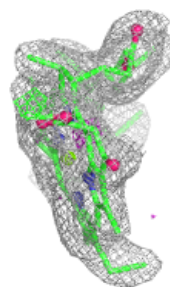
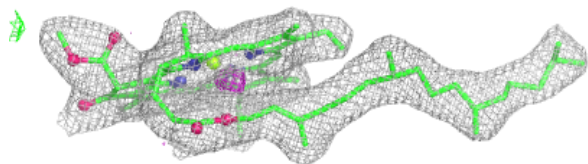
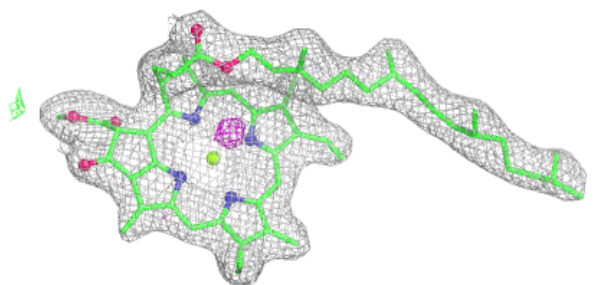


**Electron density around HTG b 607:**

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

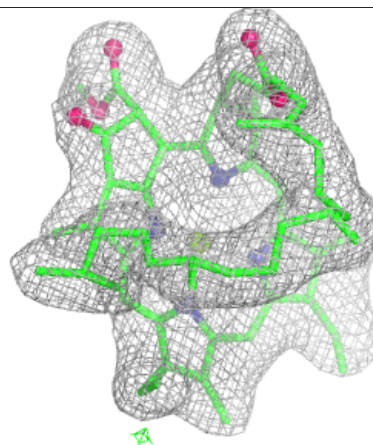
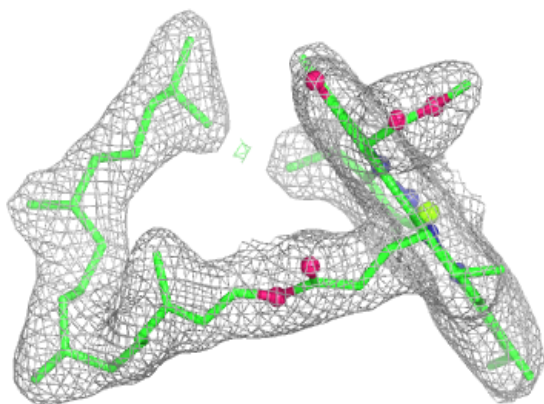
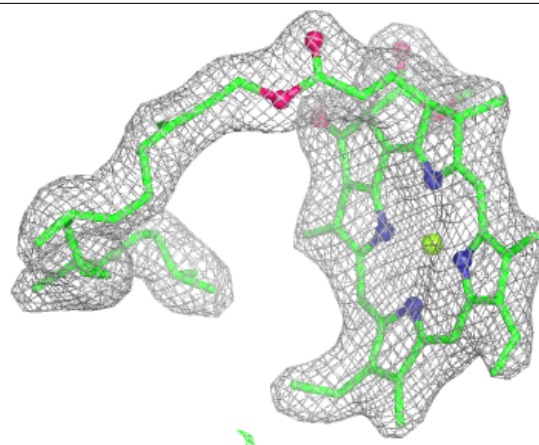
**Electron density around CLA C 501:**

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



**Electron density around CLA C 503:**

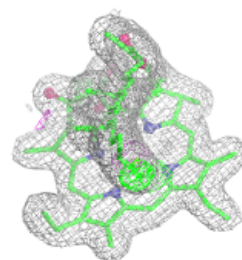
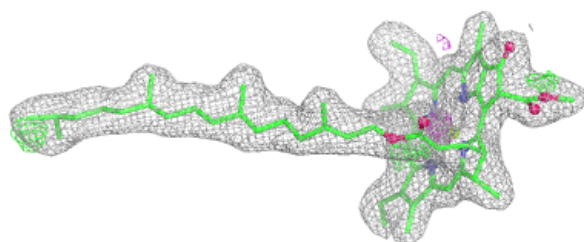
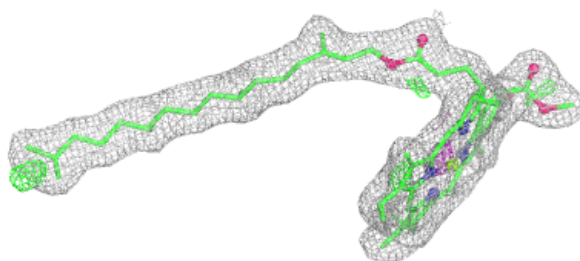
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



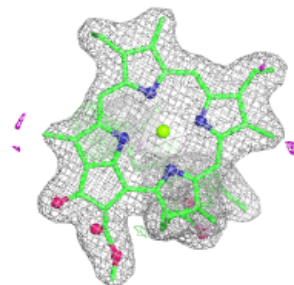
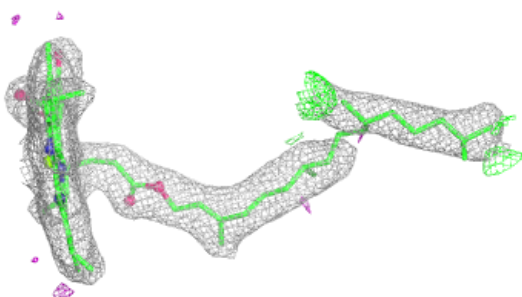
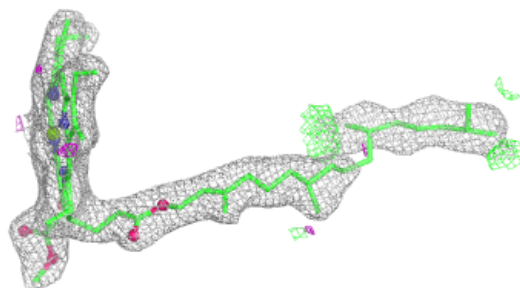


**Electron density around CLA b 616:**

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

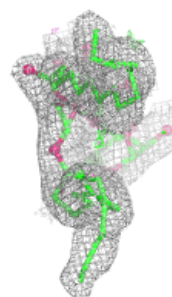
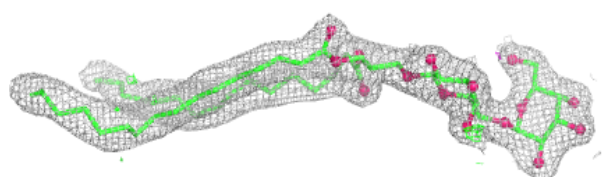
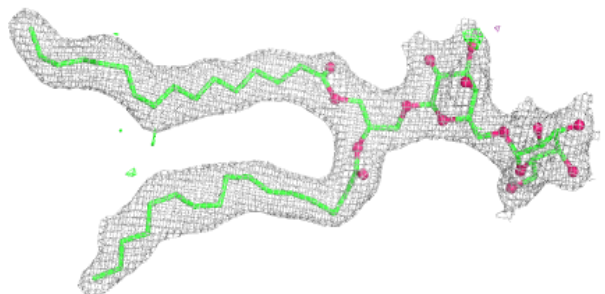
**Electron density around CLA B 607:**

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

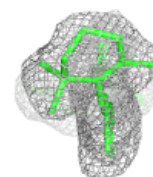
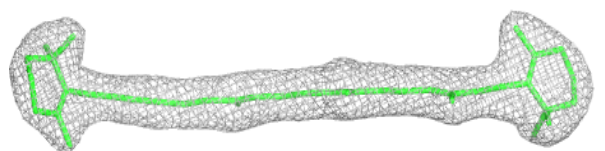
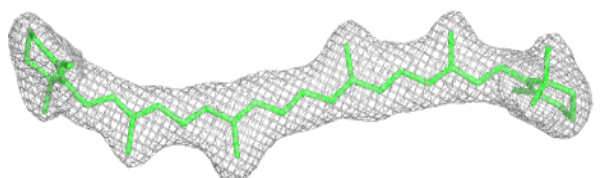


**Electron density around DGD C 518:**

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

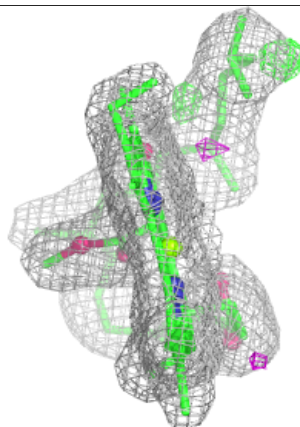
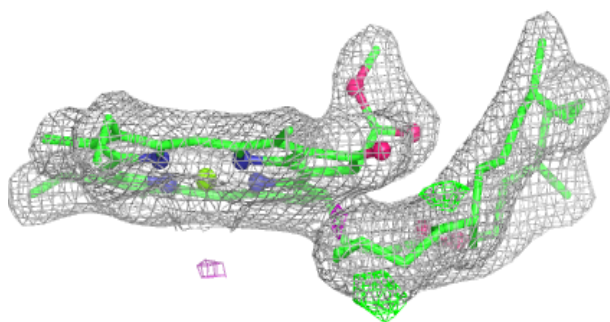
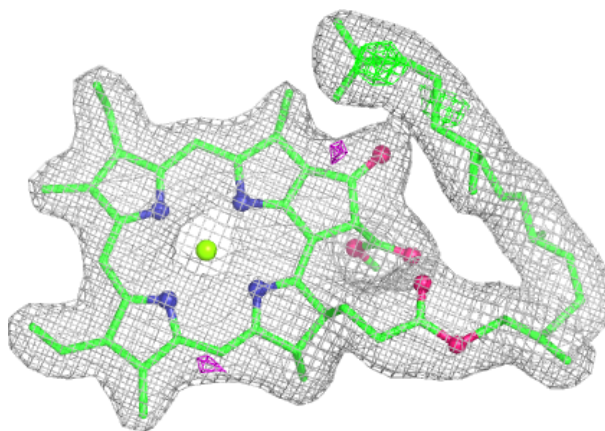
**Electron density around BCR c 519:**

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

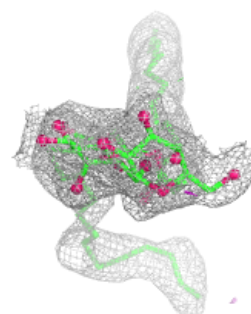
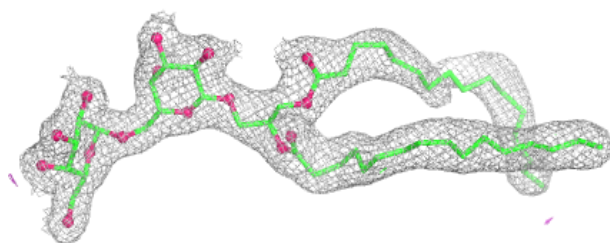
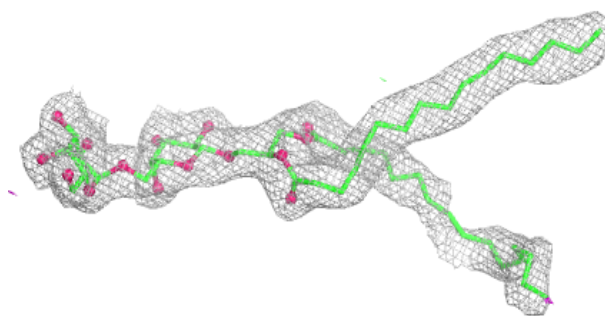


**Electron density around CLA b 619:**

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

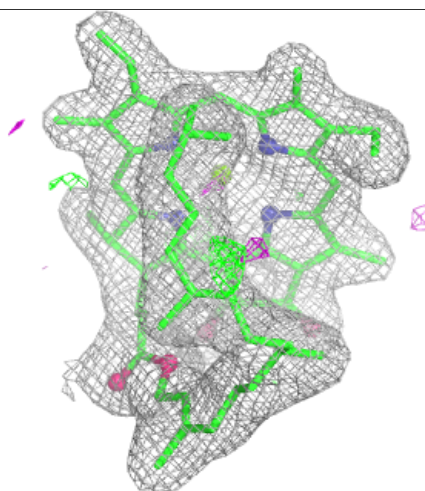
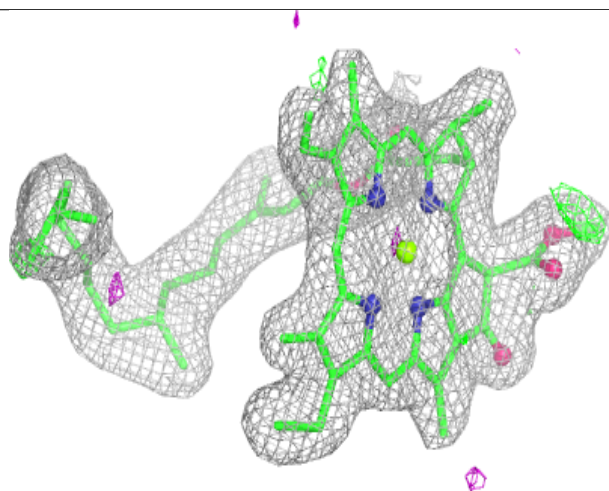
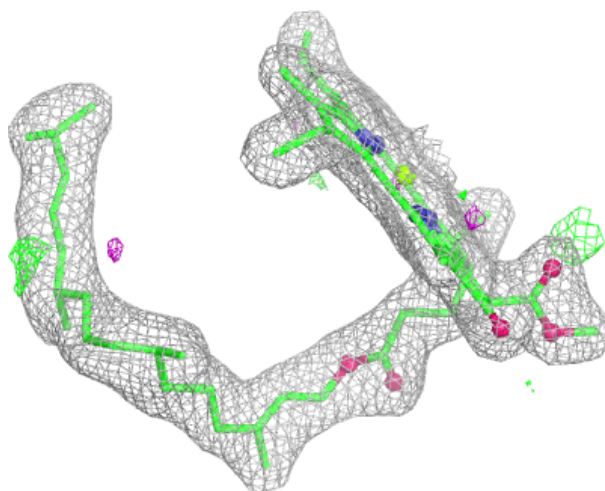
**Electron density around DGD c 520:**

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



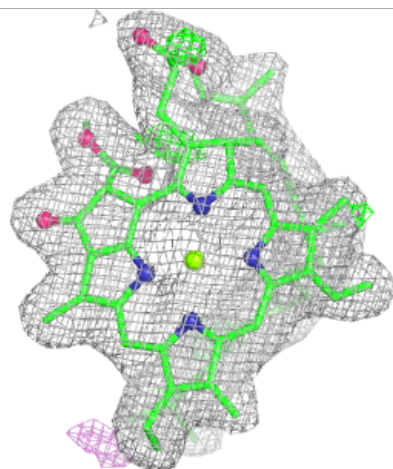
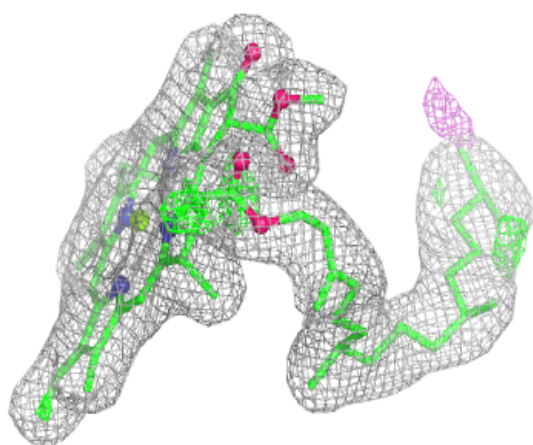
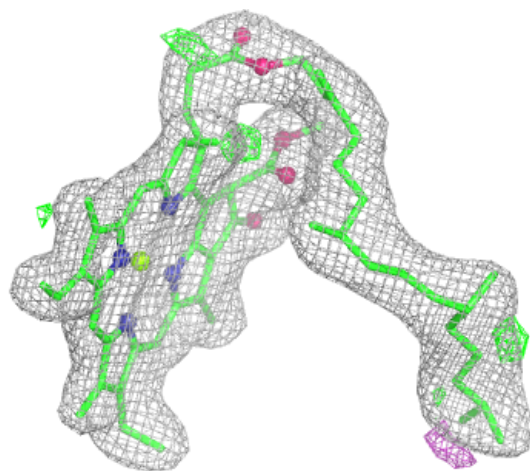
**Electron density around CLA b 620:**

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



**Electron density around CLA b 622:**

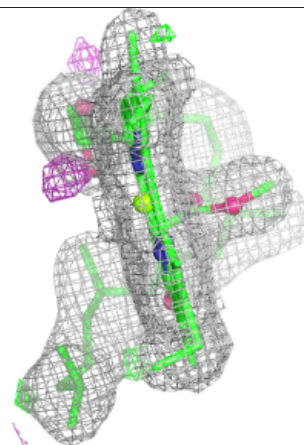
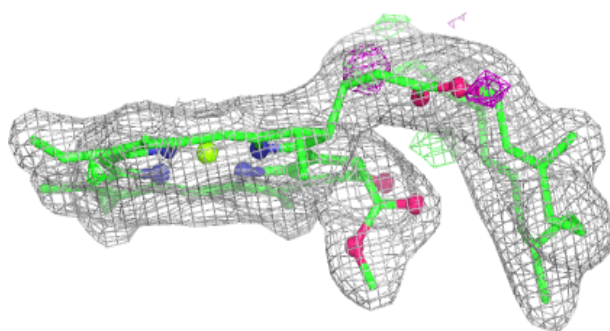
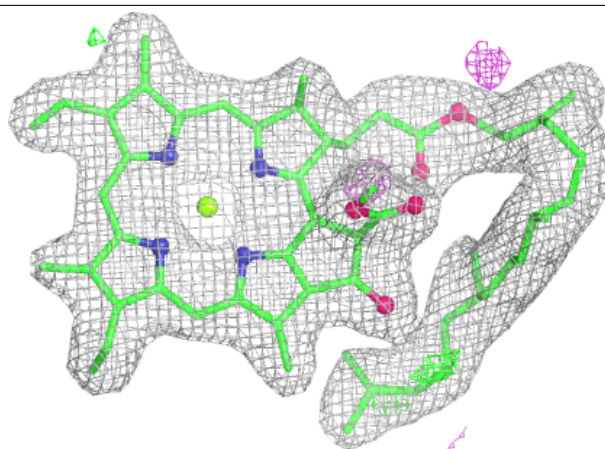
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



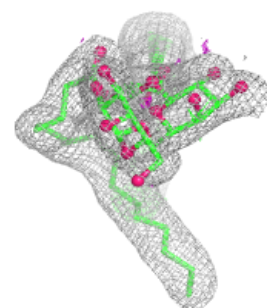
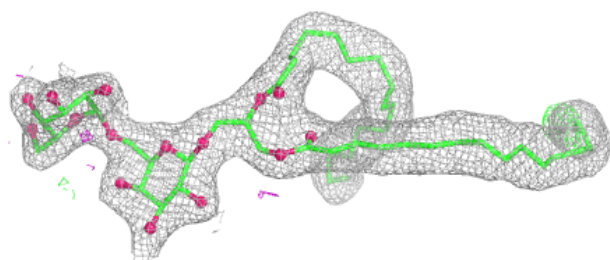
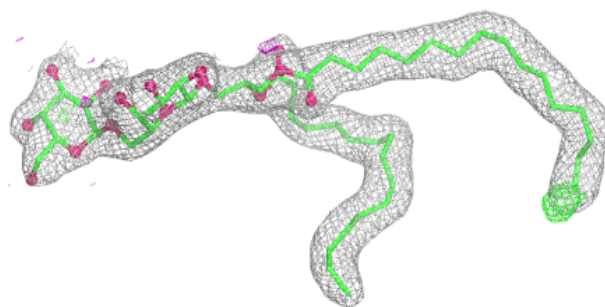


**Electron density around CLA B 611:**

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

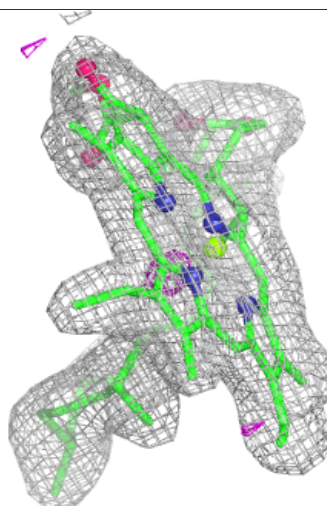
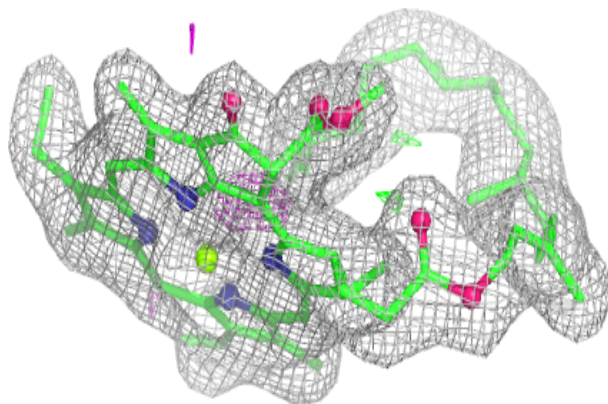
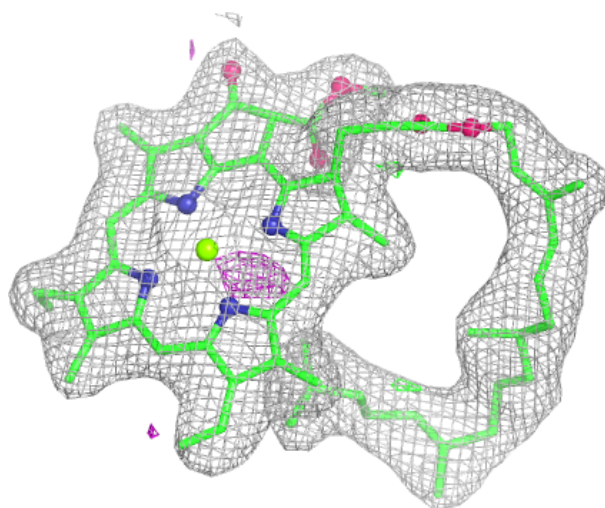
**Electron density around DGD h 102:**

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



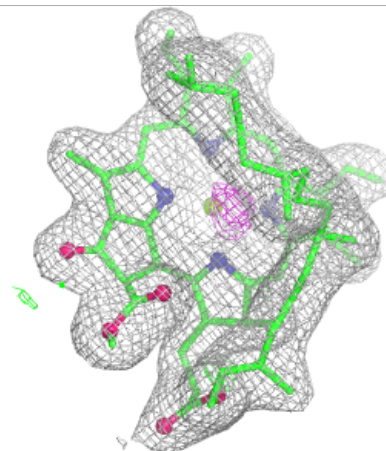
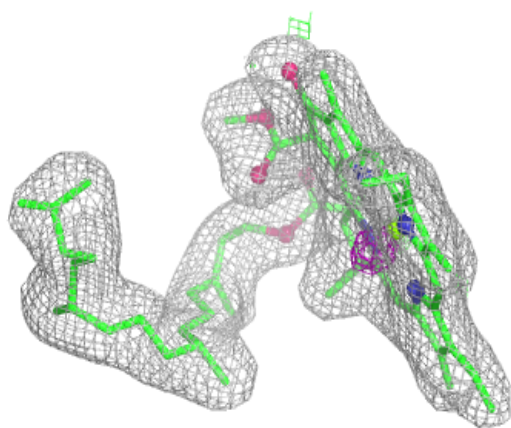
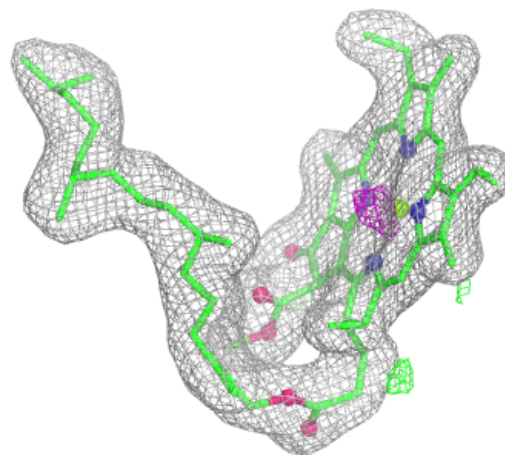
**Electron density around CLA b 624:**

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



**Electron density around CLA B 614:**

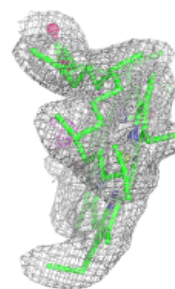
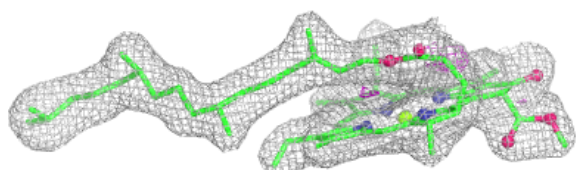
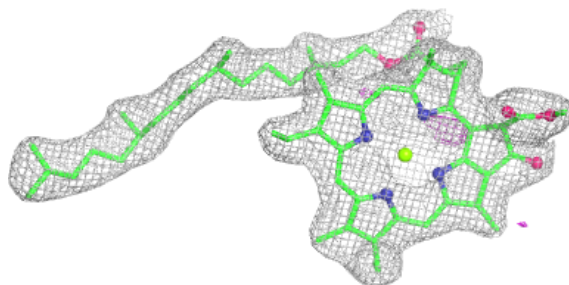
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



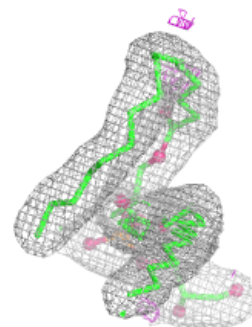
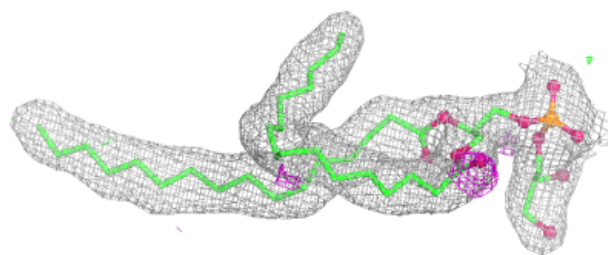
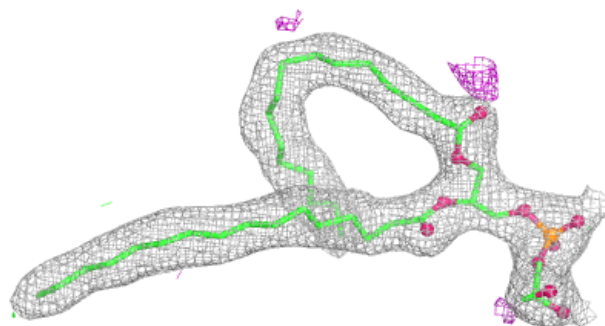


**Electron density around CLA c 506:**

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

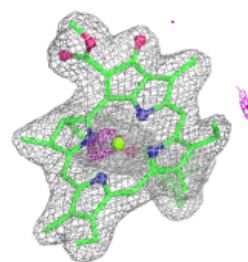
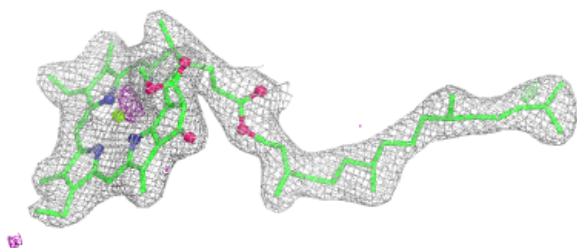
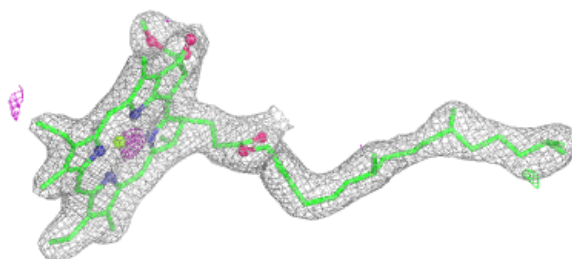
**Electron density around LHG d 406:**

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



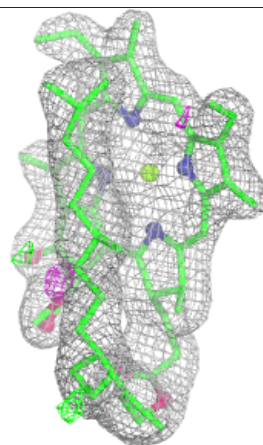
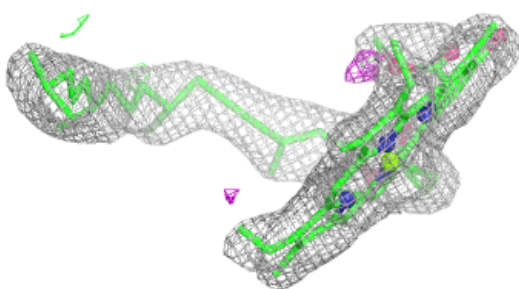
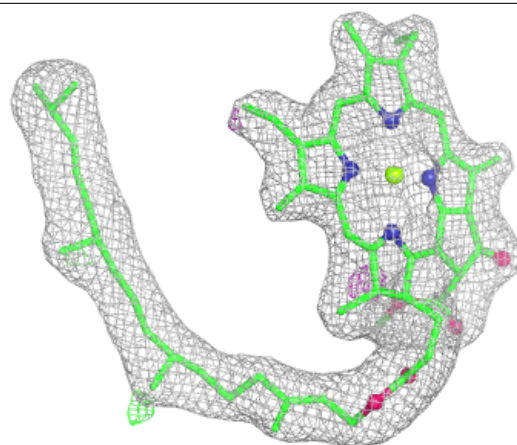
**Electron density around CLA c 507:**

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

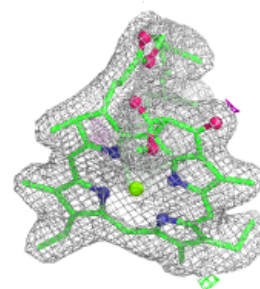
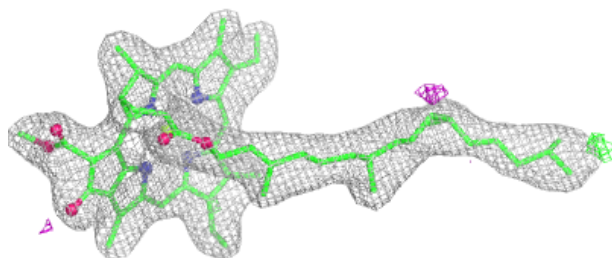
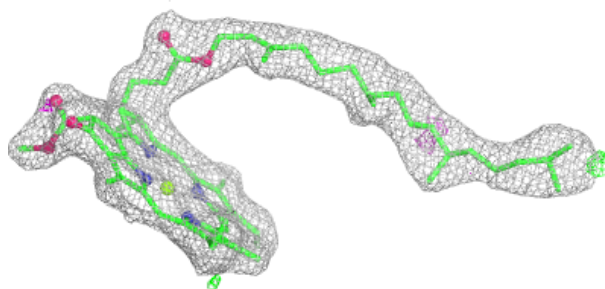


**Electron density around CLA C 507:**

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

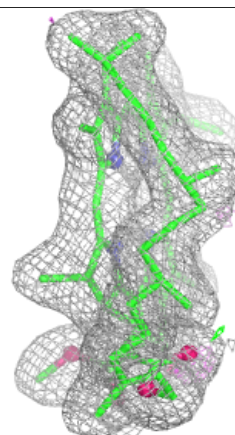
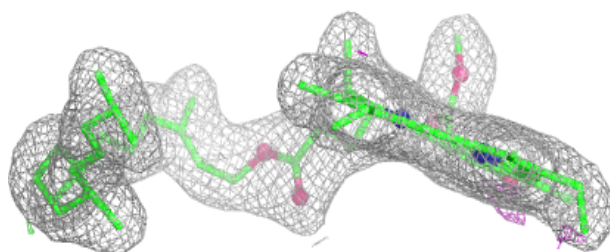
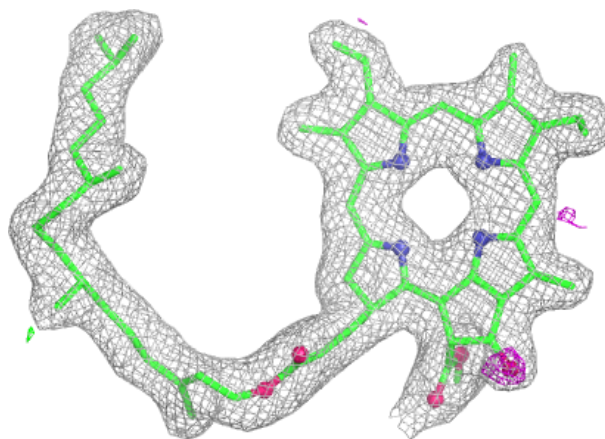
**Electron density around CLA c 509:**

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

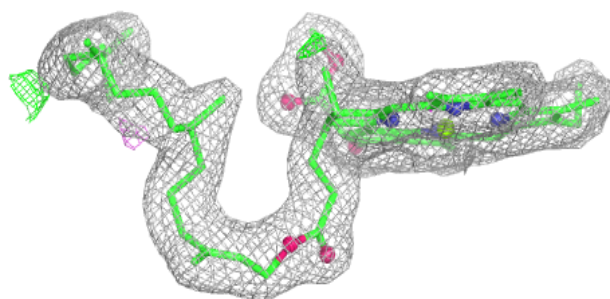
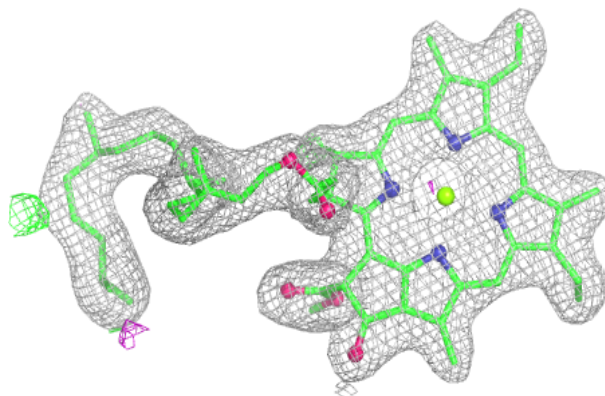


**Electron density around PHO a 411:**

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

**Electron density around CLA B 613:**

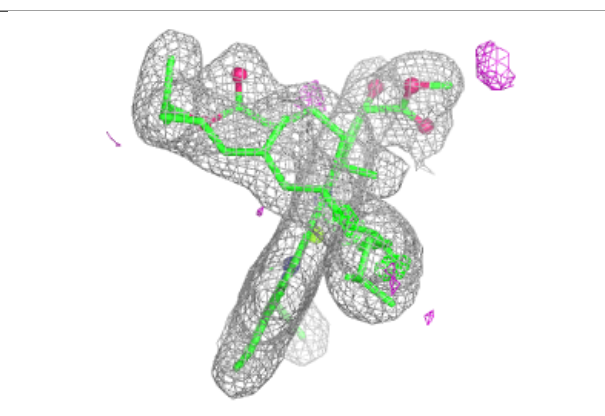
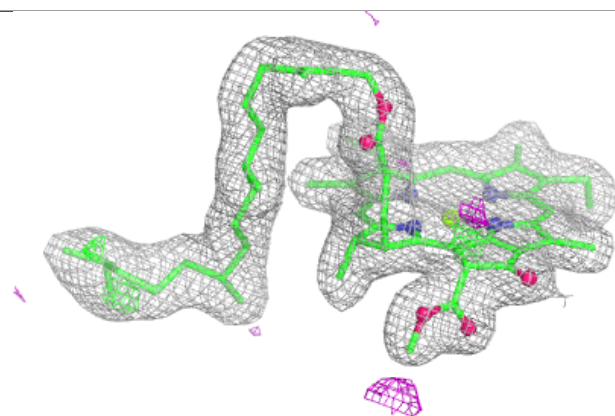
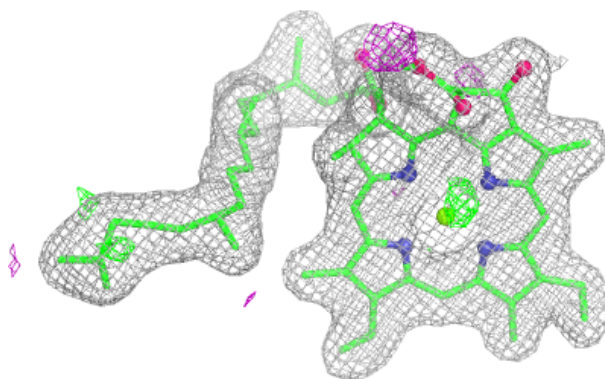
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



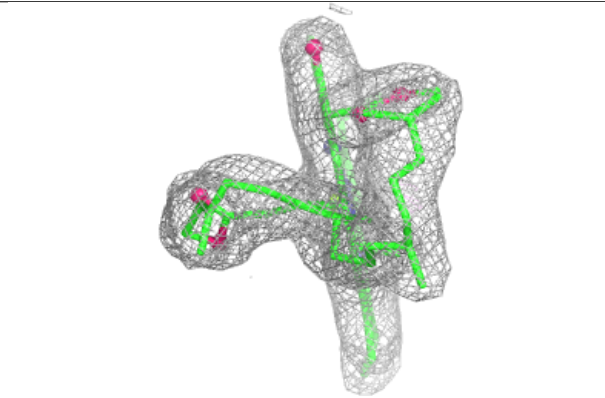
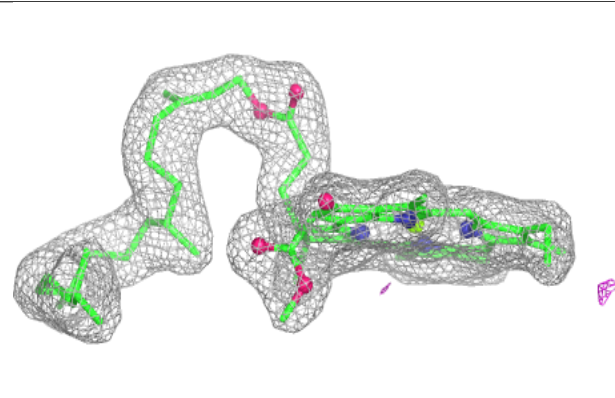
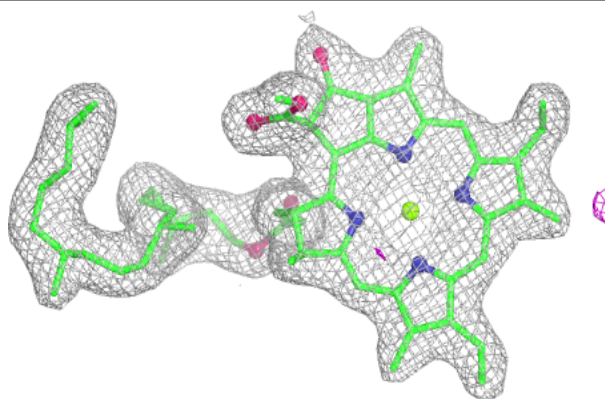


**Electron density around CLA A 406:**

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

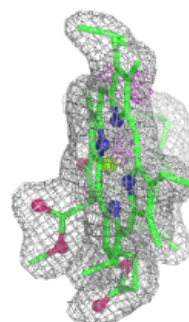
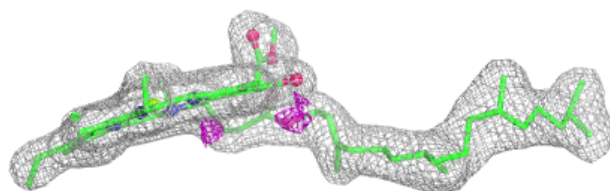
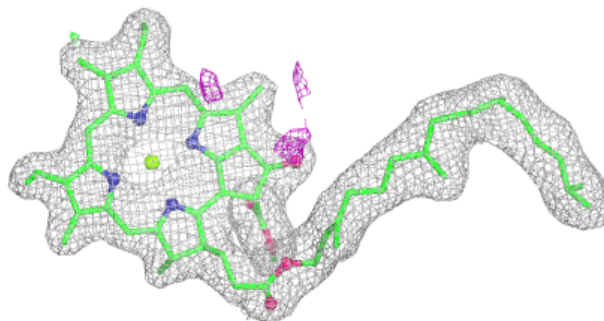
**Electron density around CLA b 621:**

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



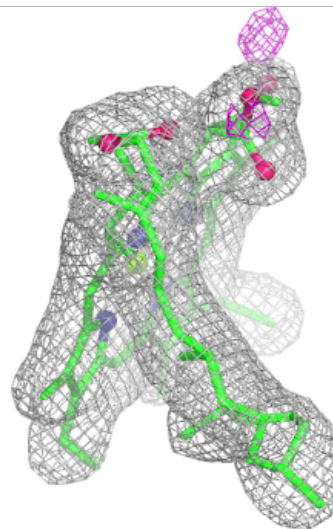
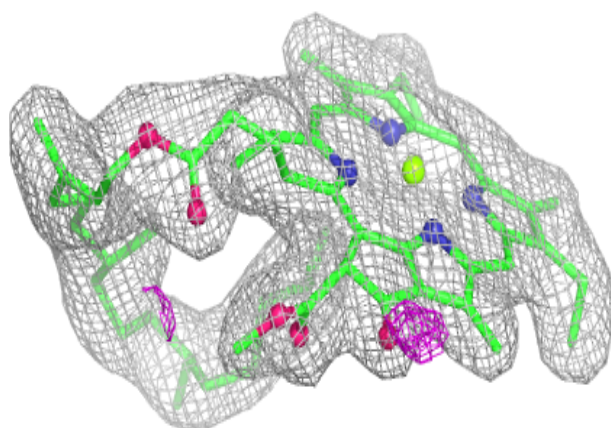
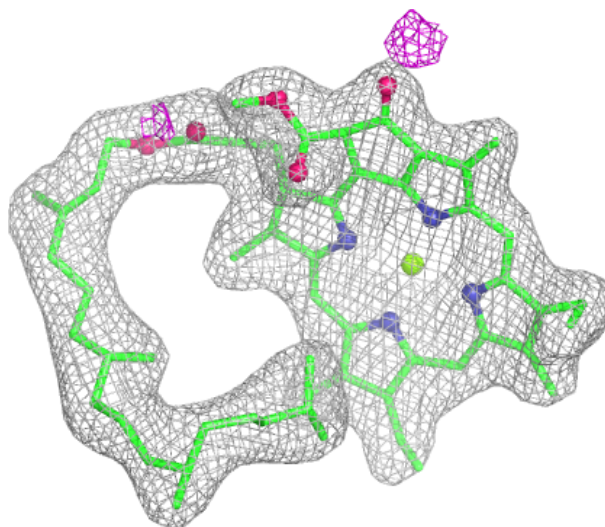
**Electron density around CLA B 603:**

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



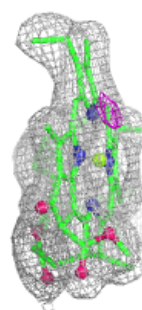
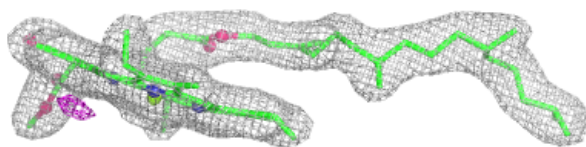
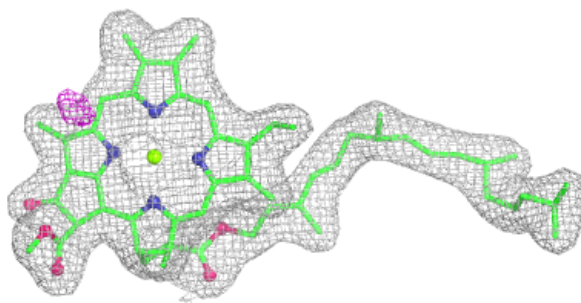
**Electron density around CLA B 616:**

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

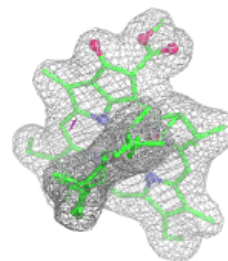
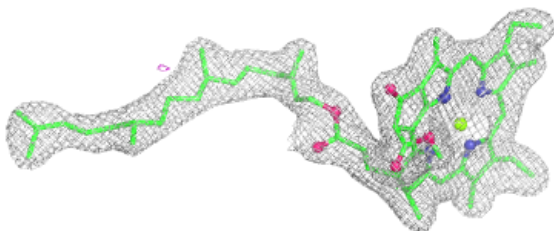
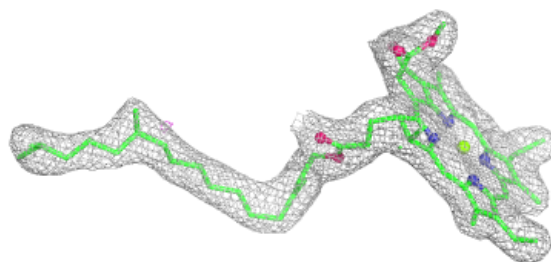


**Electron density around CLA B 604:**

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

**Electron density around CLA C 502:**

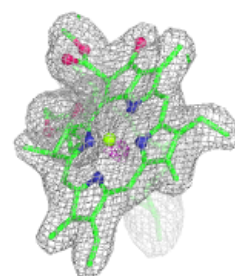
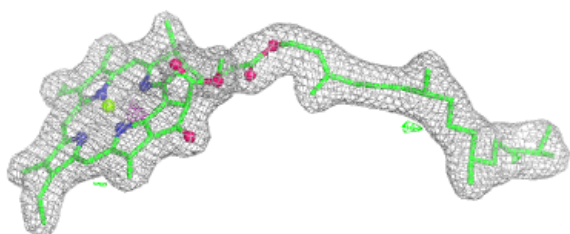
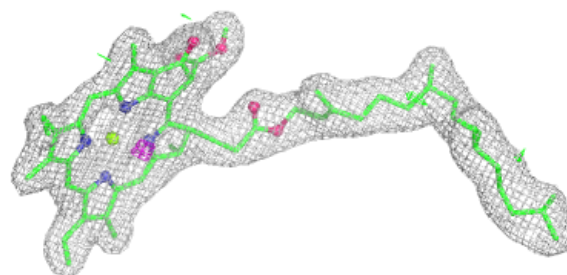
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



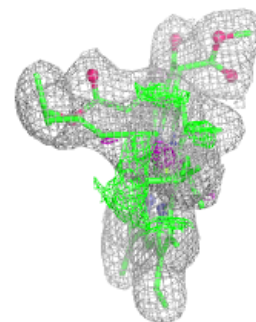
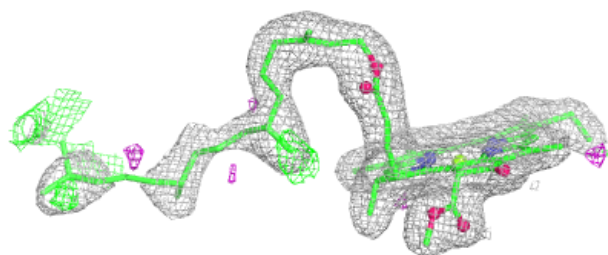
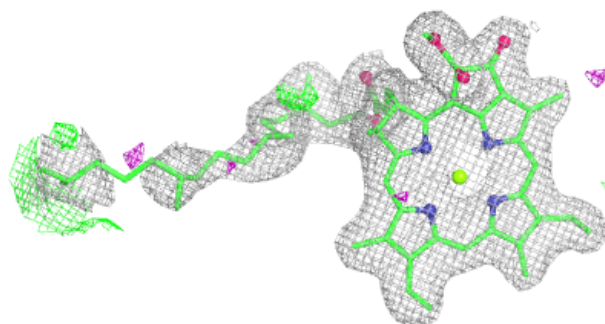


**Electron density around CLA a 409:**

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

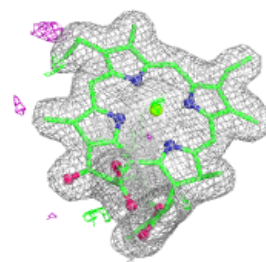
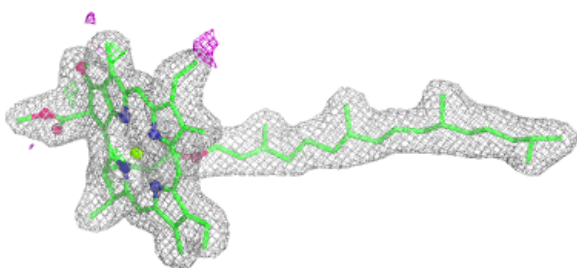
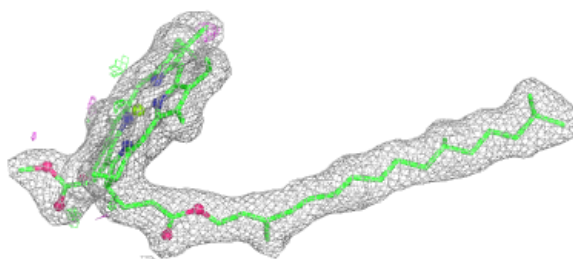
**Electron density around CLA a 410:**

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

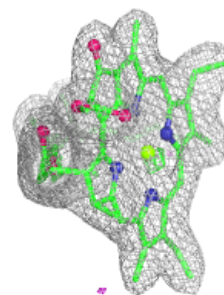
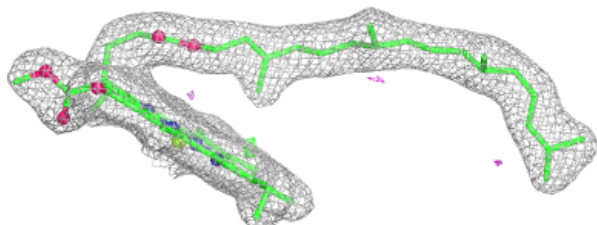
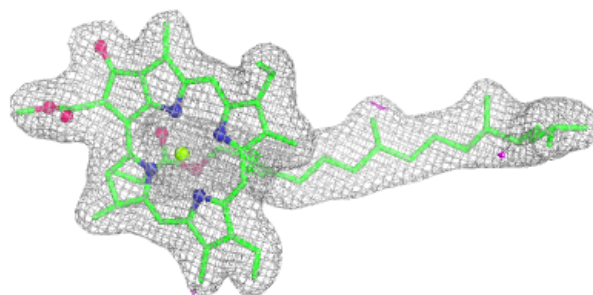


**Electron density around CLA B 608:**

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

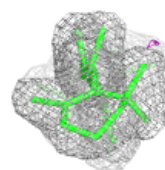
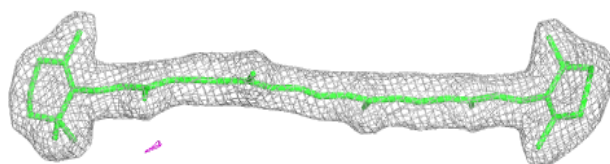
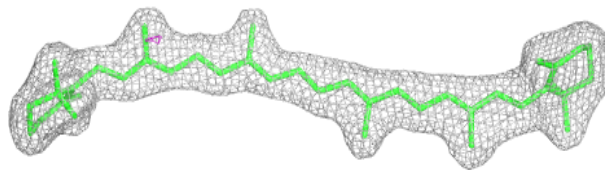
**Electron density around CLA B 609:**

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

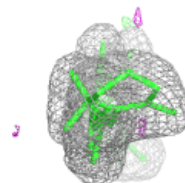
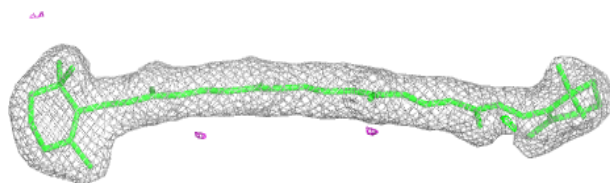
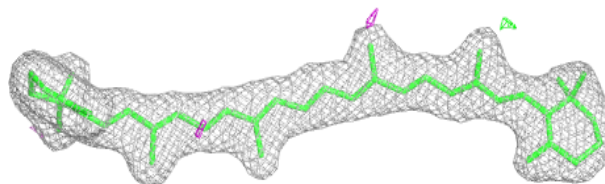


**Electron density around BCR a 413:**

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

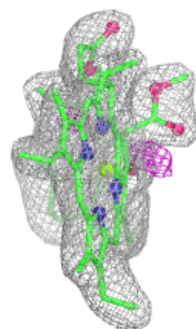
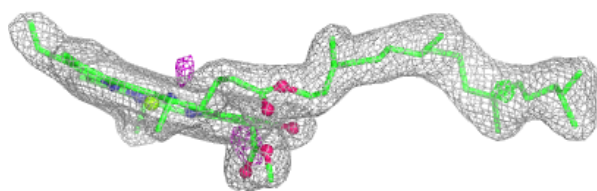
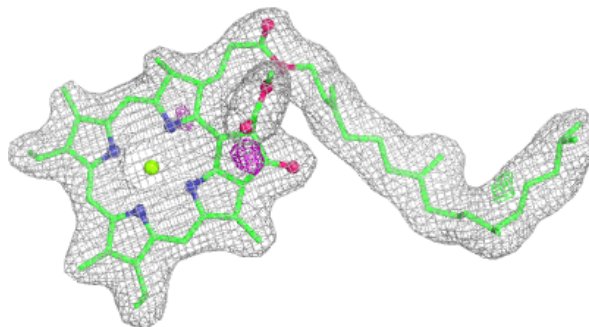
**Electron density around BCR b 626:**

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

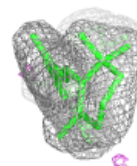
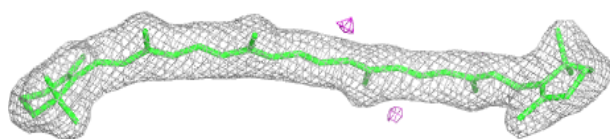
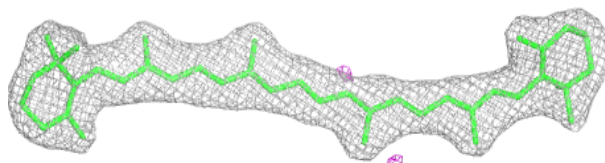


**Electron density around CLA b 611:**

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

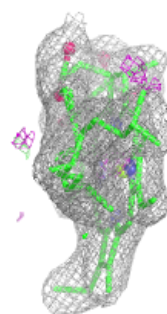
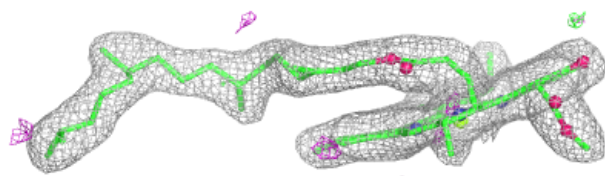
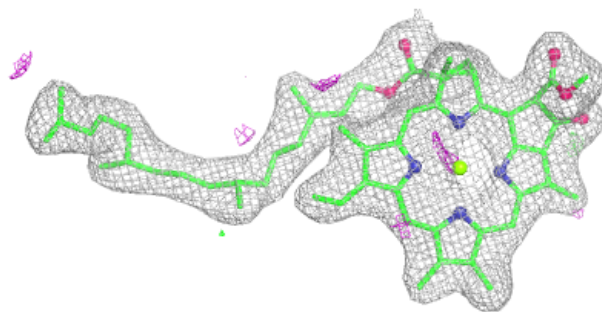
**Electron density around BCR b 628:**

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

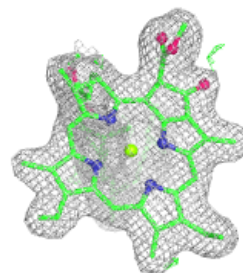
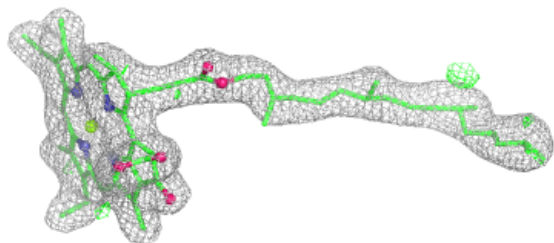
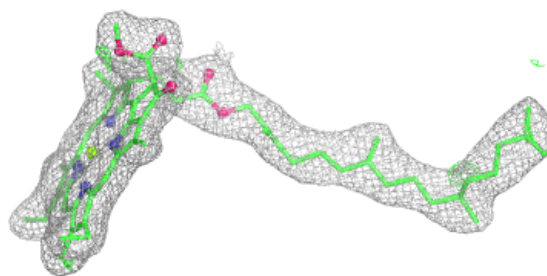


**Electron density around CLA b 612:**

$2mF_o-DF_c$  (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:**

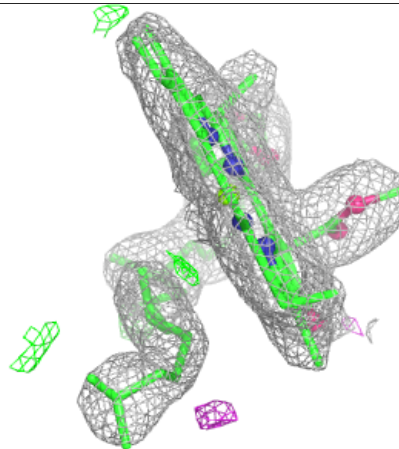
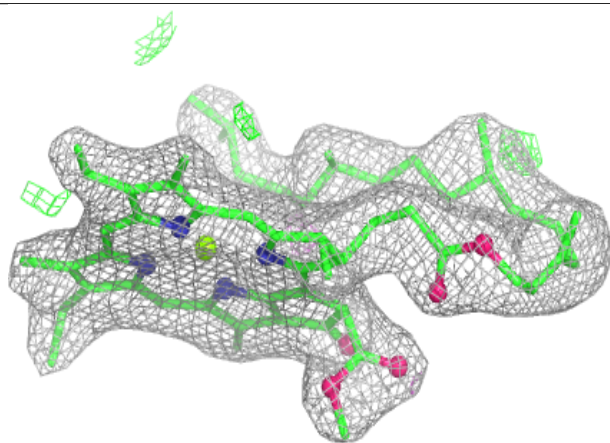
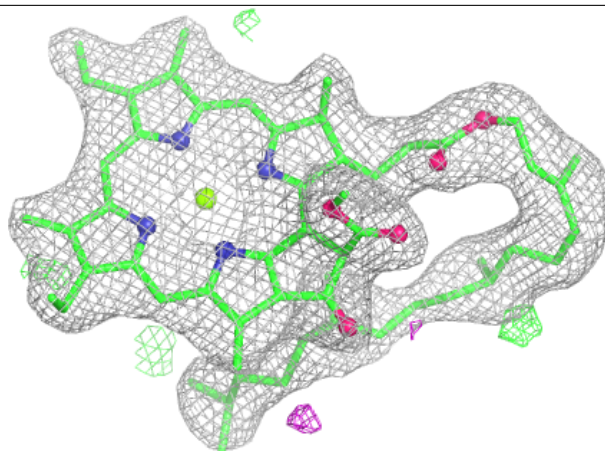
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





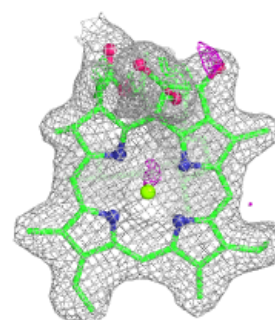
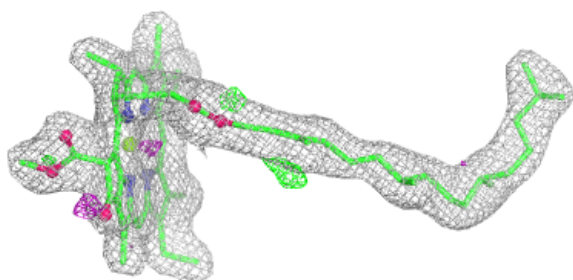
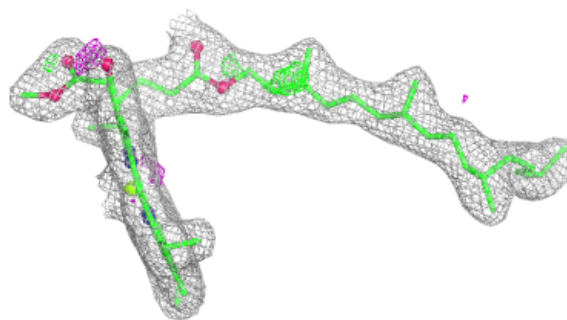
**Electron density around CLA c 514:**

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

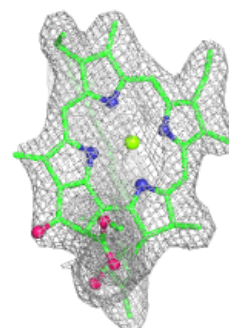
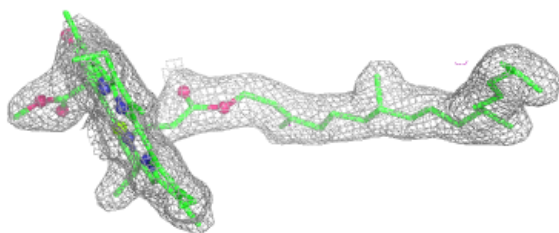
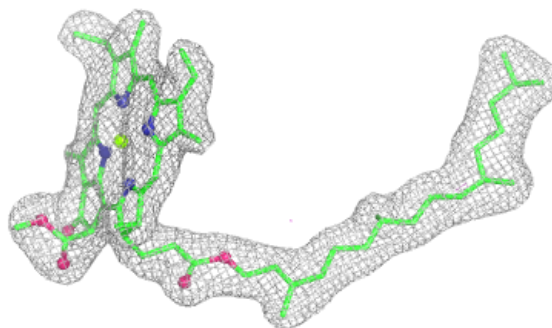


**Electron density around CLA b 614:**

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

**Electron density around CLA B 610:**

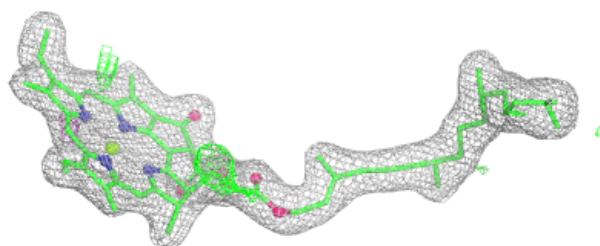
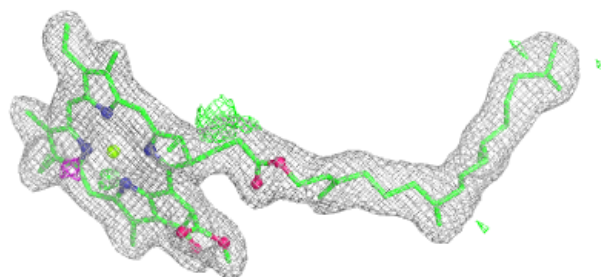
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



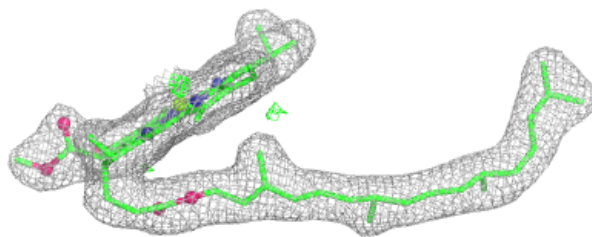
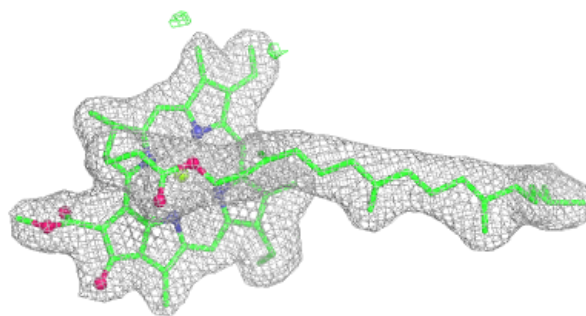


**Electron density around CLA A 405:**

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

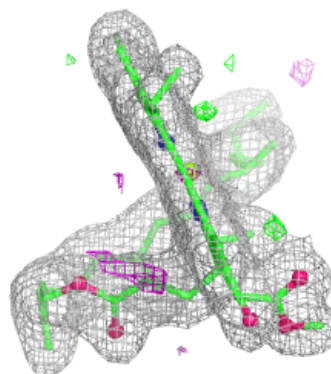
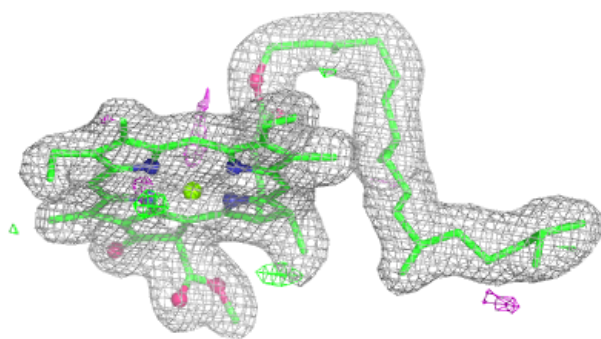
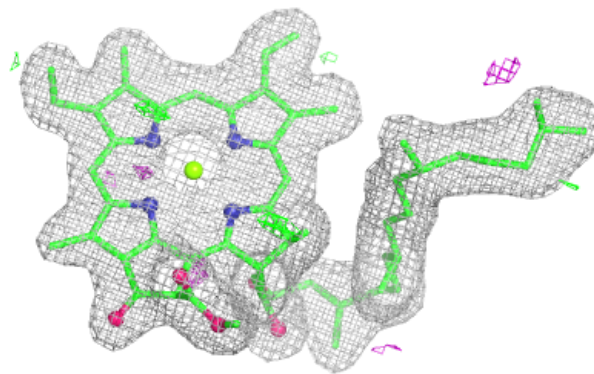
**Electron density around CLA b 617:**

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



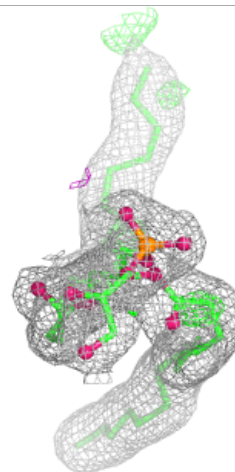
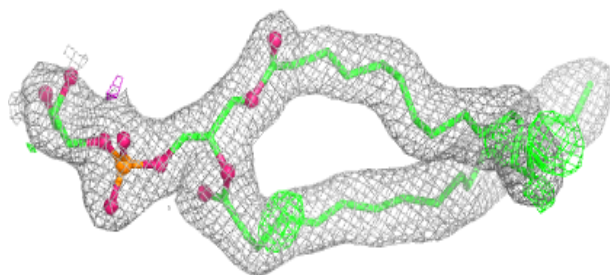
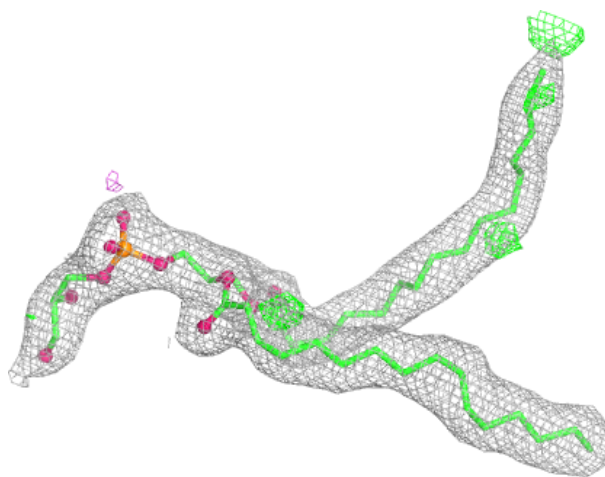
**Electron density around CLA d 401:**

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



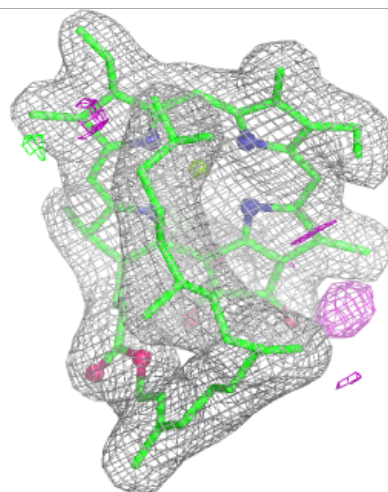
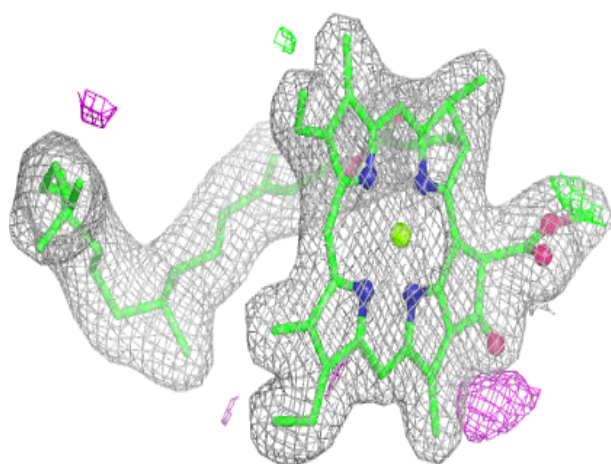
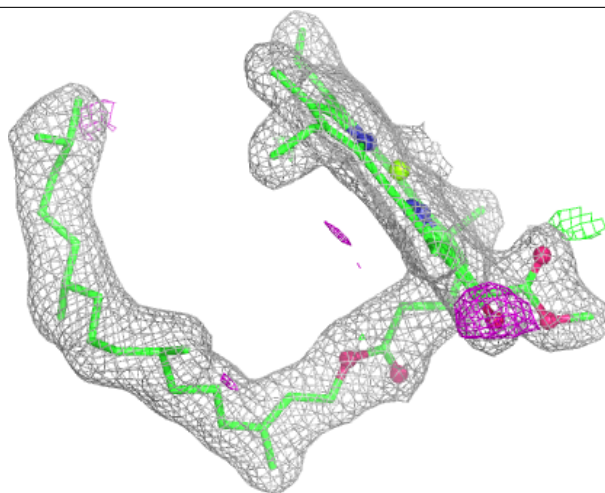
**Electron density around LHG D 408:**

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



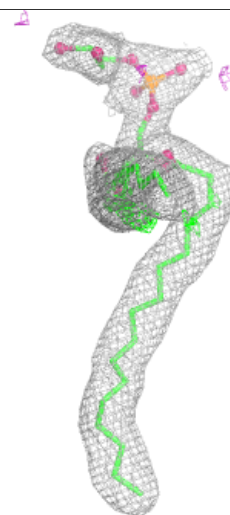
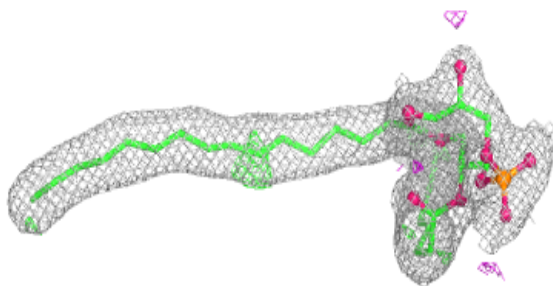
**Electron density around CLA B 612:**

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



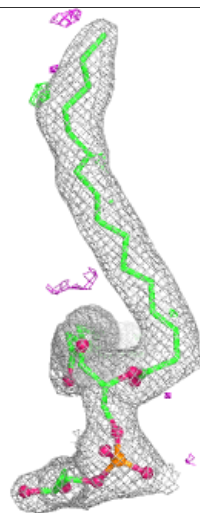
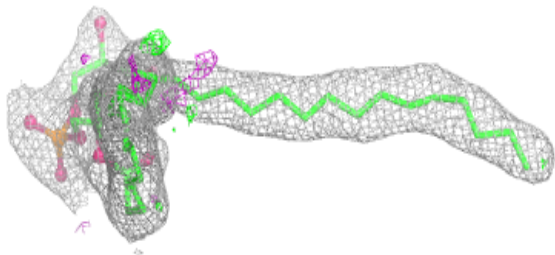
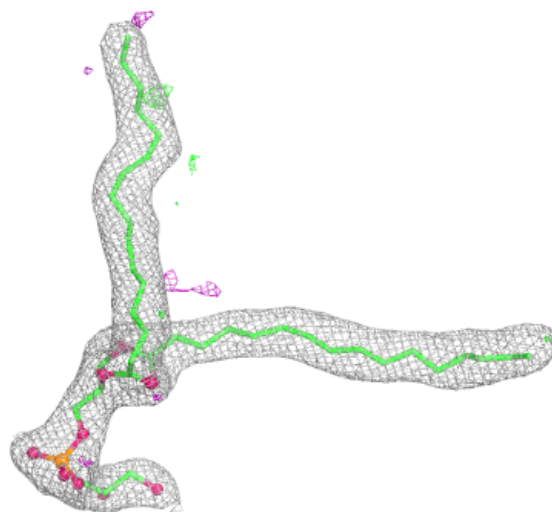
**Electron density around LHG L 101:**

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



**Electron density around LHG b 634:**

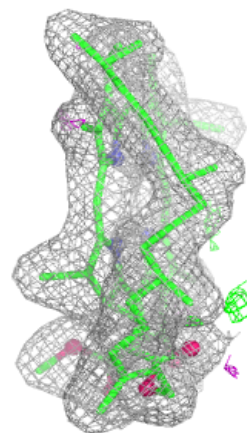
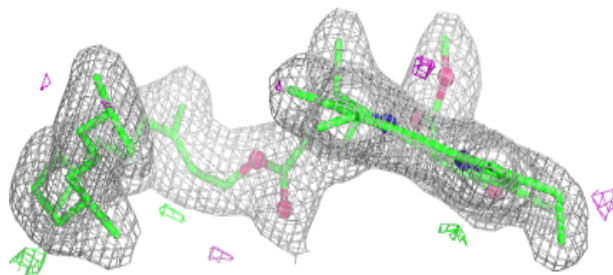
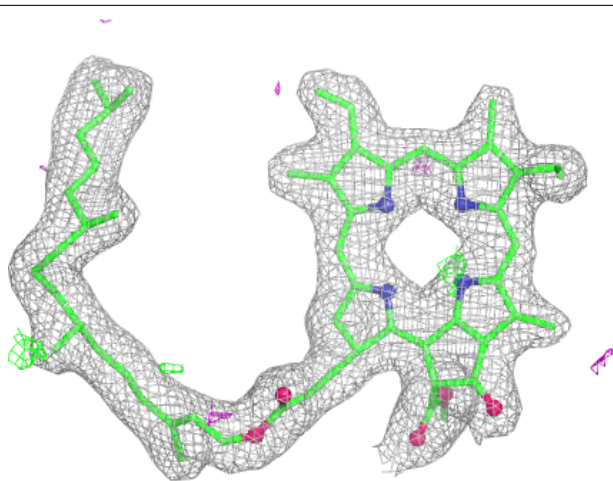
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PHO A 408:**

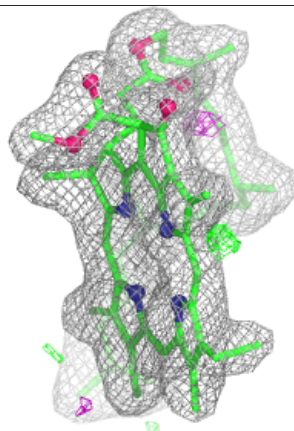
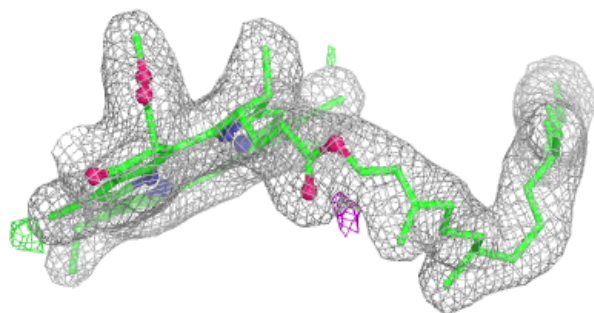
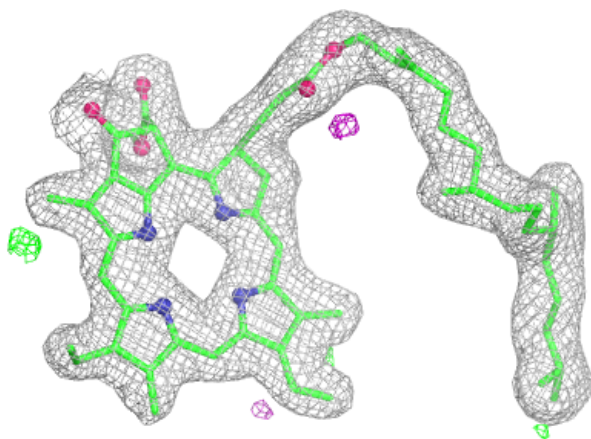
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



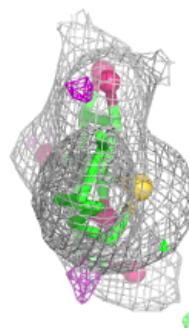
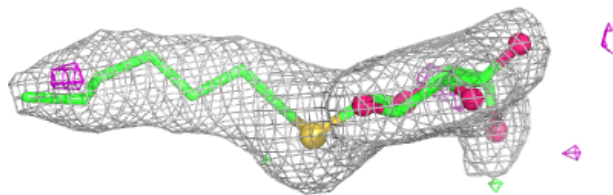
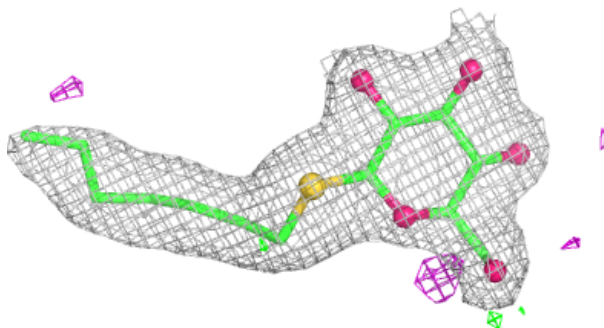


**Electron density around PHO A 409 (A):**

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

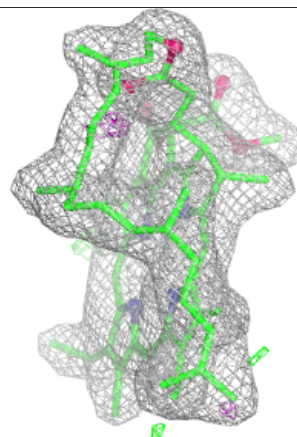
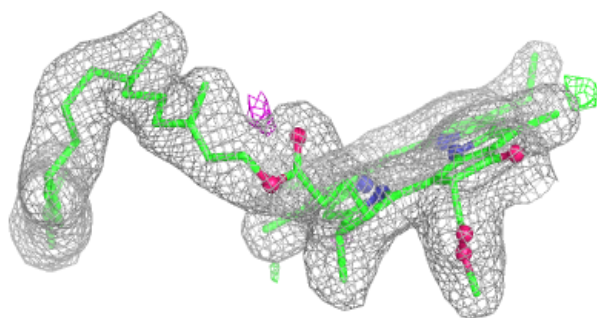
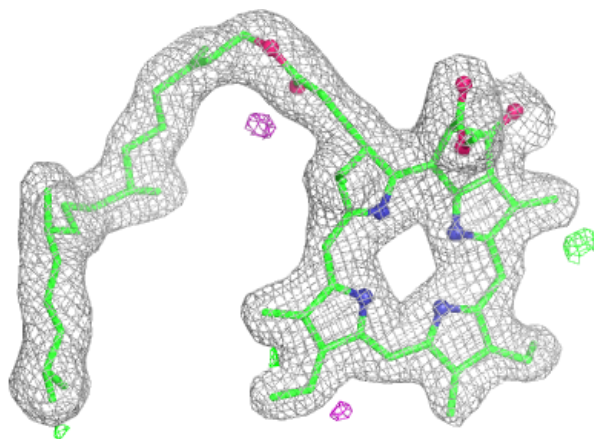
**Electron density around HTG B 623:**

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



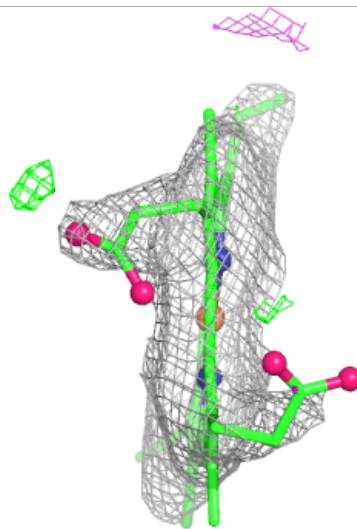
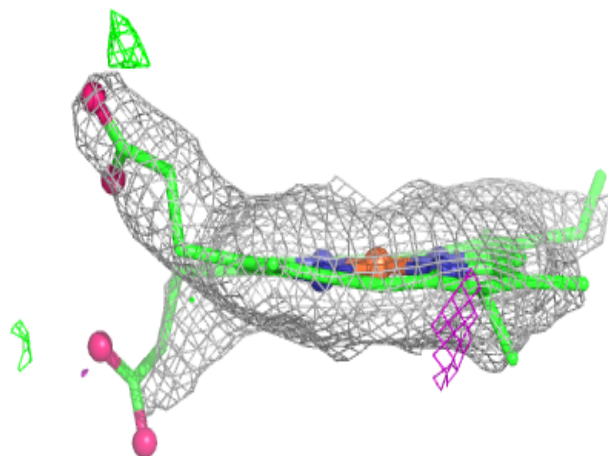
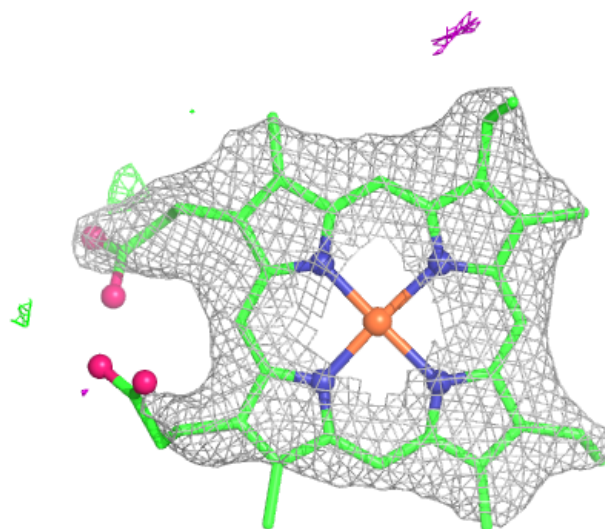
**Electron density around PHO A 409 (B):**

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



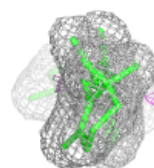
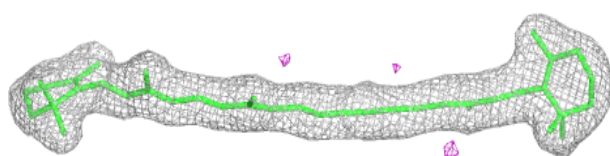
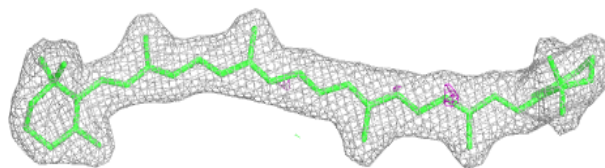
**Electron density around HEM e 103:**

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

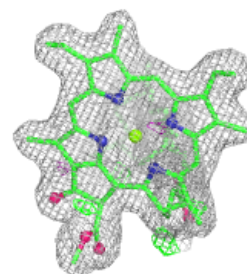
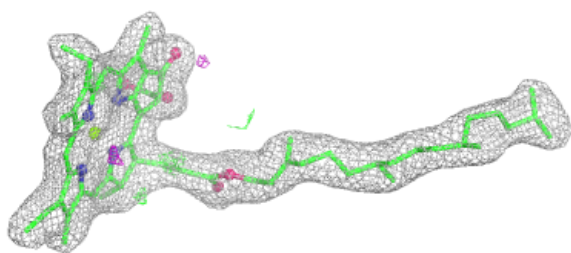
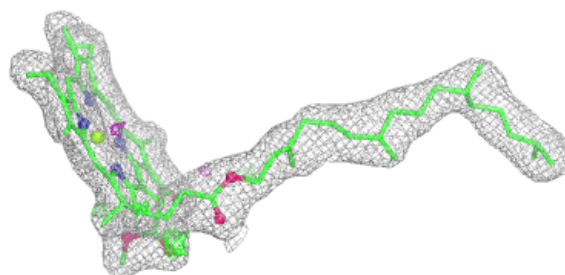


**Electron density around BCR B 618:**

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

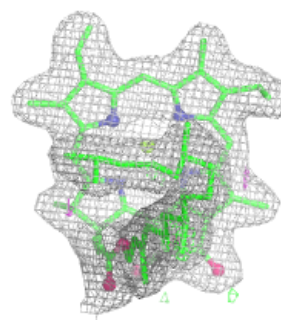
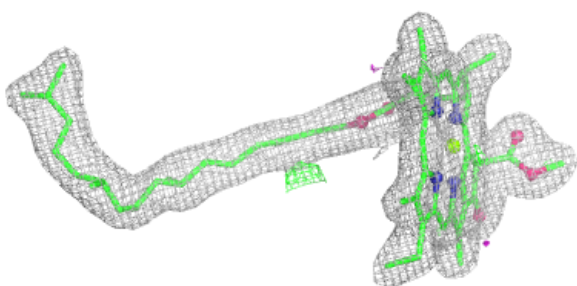
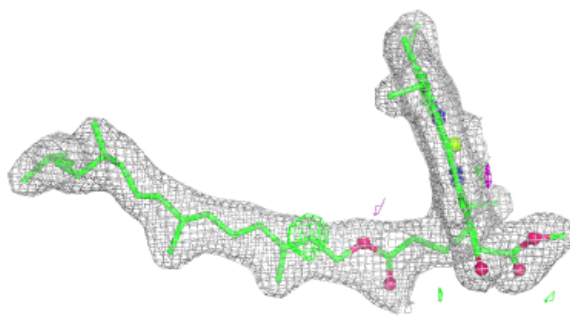
**Electron density around CLA B 605:**

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



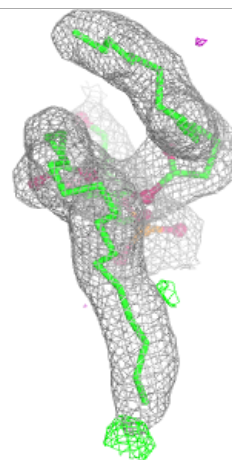
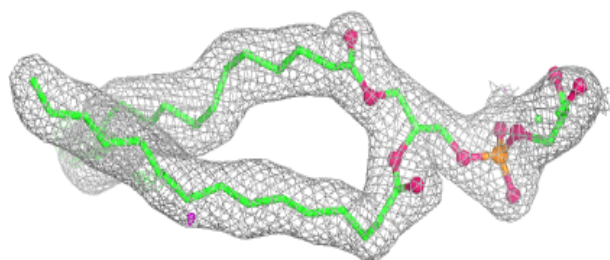
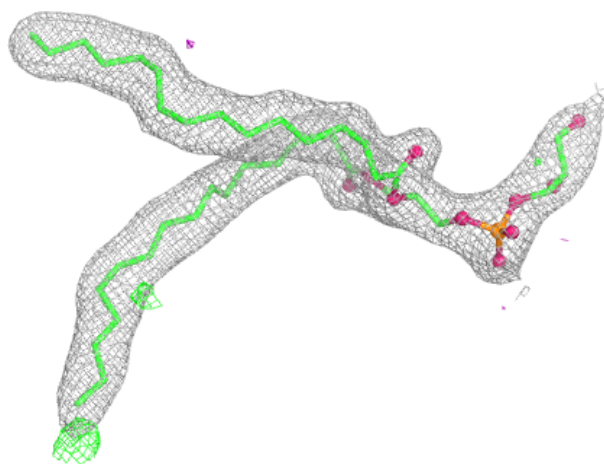
**Electron density around CLA B 606:**

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



**Electron density around LHG d 407:**

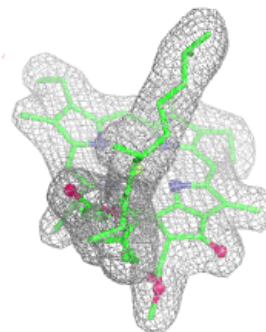
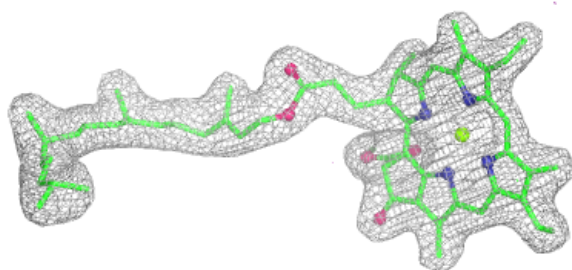
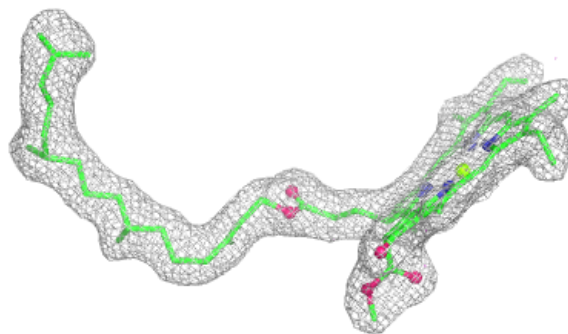
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



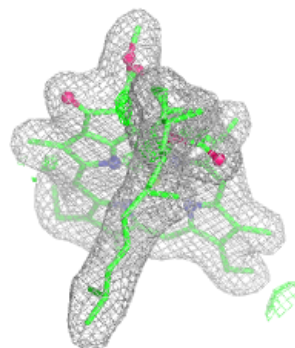
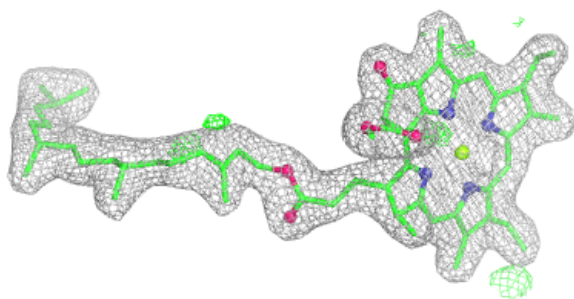
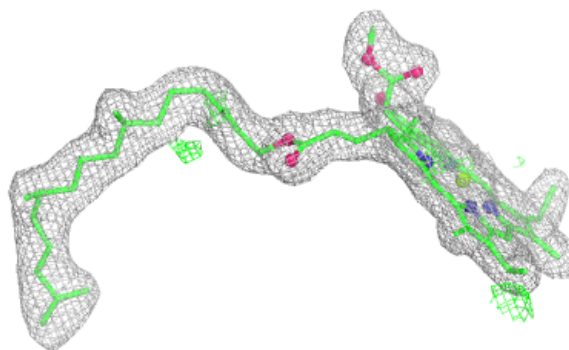


**Electron density around CLA d 402:**

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

**Electron density around CLA D 402:**

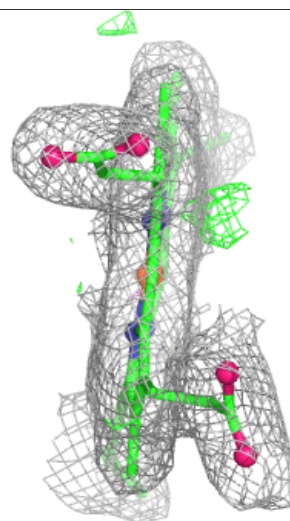
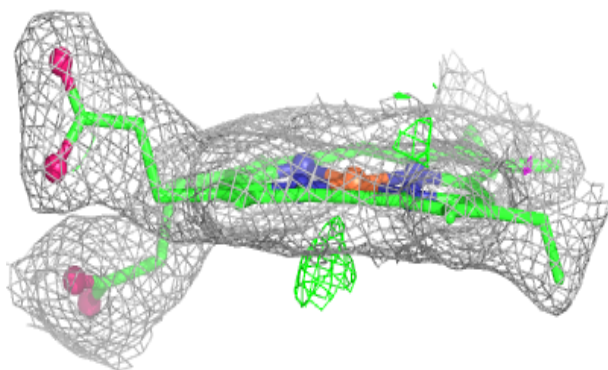
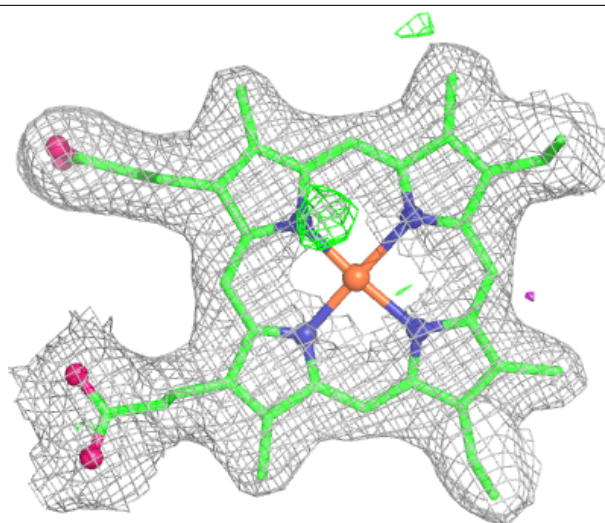
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





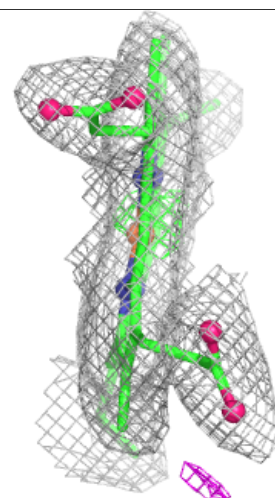
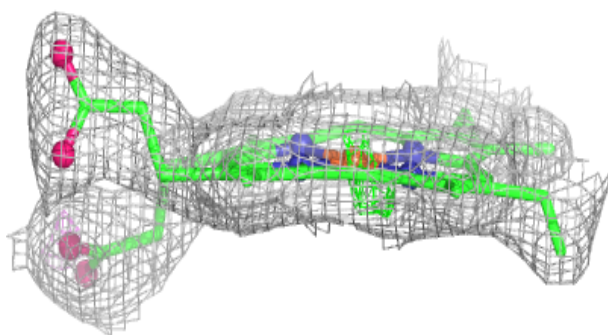
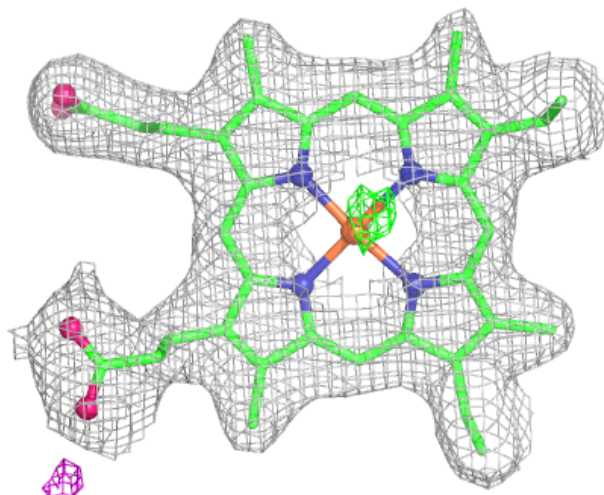
**Electron density around HEC V 205:**

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



**Electron density around HEC v 205:**

$2mF_o-DF_c$  (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.