



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 08:15 PM UTC

PDB ID : 8IRD / pdb\_00008ird  
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)  
with a 20-nanosecond delay  
Authors : Li, H.; Suga, M.; Shen, J.R.  
Deposited on : 2023-03-17  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.48.1

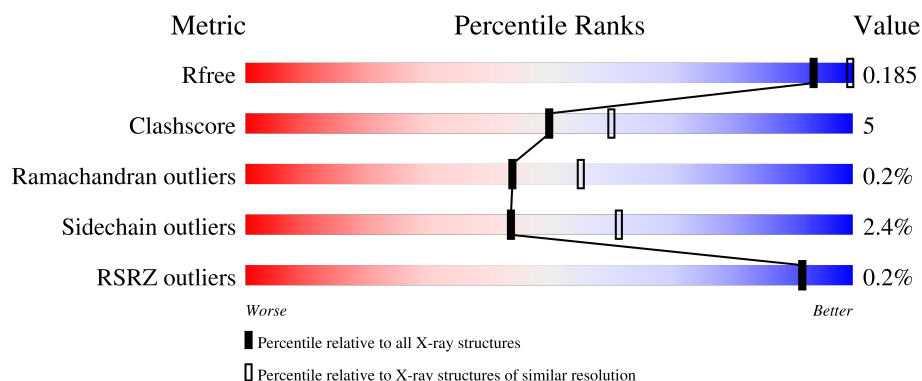
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 164625                      | 5963 (2.30-2.30)                                      |
| Clashscore            | 180529                      | 6698 (2.30-2.30)                                      |
| Ramachandran outliers | 177936                      | 6640 (2.30-2.30)                                      |
| Sidechain outliers    | 177891                      | 6640 (2.30-2.30)                                      |
| RSRZ outliers         | 164620                      | 5963 (2.30-2.30)                                      |

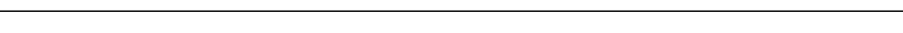
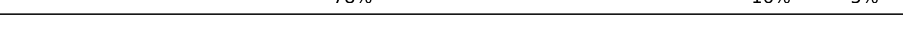
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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>90%</div> <div>7%</div> <div>.</div> </div>  |
| 1   | a     | 344    | <div> <div>85%</div> <div>11%</div> <div>.</div> </div> |
| 2   | B     | 505    | <div> <div>91%</div> <div>9%</div> </div>               |
| 2   | b     | 505    | <div> <div>90%</div> <div>8%</div> <div>.</div> </div>  |
| 3   | C     | 455    | <div> <div>91%</div> <div>7%</div> <div>.</div> </div>  |

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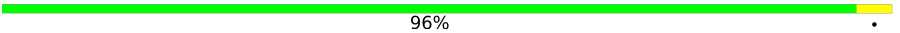


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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 3   | c     | 455    |  89% 10% .      |
| 4   | D     | 342    |  90% 10%        |
| 4   | d     | 342    |  92% 8%         |
| 5   | E     | 84     |  79% 18% .      |
| 5   | e     | 84     |  86% 8% 6%      |
| 6   | F     | 44     |  68% 9% 23%     |
| 6   | f     | 44     |  64% 7% 30%     |
| 7   | H     | 65     |  94% 5% .       |
| 7   | h     | 65     |  83% 14% . .    |
| 8   | I     | 38     |  76% 21% .      |
| 8   | i     | 38     |  87% 13%        |
| 9   | J     | 39     |  77% 21% .      |
| 9   | j     | 39     |  92% 8%       |
| 10  | K     | 37     |  81% 16% .    |
| 10  | k     | 37     |  78% 16% 5%   |
| 11  | L     | 37     |  92% 5% .     |
| 11  | l     | 37     |  81% 16% .    |
| 12  | M     | 36     |  78% 8% 6% 8% |
| 12  | m     | 36     |  78% 14% . 6% |
| 13  | O     | 244    |  84% 16%      |
| 13  | o     | 244    |  89% 10%      |
| 14  | T     | 32     |  75% 16% . 6% |
| 14  | t     | 32     |  72% 22% 6%   |
| 15  | U     | 104    |  85% 8% 8%    |
| 15  | u     | 104    |  87% 6% . 7%  |

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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 16  | V     | 137    |  96% .      |
| 16  | v     | 137    |  90% 10%    |
| 17  | X     | 40     |  88% 8% 5%  |
| 17  | x     | 40     |  90% 5% 5%  |
| 18  | Y     | 30     |  80% 17% .  |
| 18  | y     | 30     |  60% 37% .  |
| 19  | Z     | 62     |  85% 13% .  |
| 19  | z     | 62     |  74% 24% .  |
| 20  | R     | 34     |  3% 71% 29% |

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 |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 23  | CLA  | A     | 404[A] | X         | -        | -       | -                |
| 23  | CLA  | A     | 404[B] | X         | -        | -       | -                |
| 23  | CLA  | A     | 405[A] | X         | -        | -       | -                |
| 23  | CLA  | A     | 405[B] | X         | -        | -       | -                |
| 23  | CLA  | A     | 407    | X         | -        | -       | -                |
| 23  | CLA  | B     | 601    | X         | -        | -       | -                |
| 23  | CLA  | B     | 602    | X         | -        | -       | -                |
| 23  | CLA  | B     | 603    | X         | -        | -       | -                |
| 23  | CLA  | B     | 604    | X         | -        | -       | -                |
| 23  | CLA  | B     | 605    | X         | -        | -       | -                |
| 23  | CLA  | B     | 606    | X         | -        | -       | -                |
| 23  | CLA  | B     | 607    | X         | -        | -       | -                |
| 23  | CLA  | B     | 609    | X         | -        | -       | -                |
| 23  | CLA  | B     | 610    | X         | -        | -       | -                |
| 23  | CLA  | B     | 611    | X         | -        | -       | -                |
| 23  | CLA  | B     | 612    | X         | -        | -       | -                |
| 23  | CLA  | B     | 613    | X         | -        | -       | -                |
| 23  | CLA  | B     | 614    | X         | -        | -       | -                |
| 23  | CLA  | B     | 615    | X         | -        | -       | -                |
| 23  | CLA  | B     | 616    | X         | -        | -       | -                |
| 23  | CLA  | C     | 502    | X         | -        | -       | -                |
| 23  | CLA  | C     | 503    | X         | -        | -       | -                |

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| Mol | Type | Chain | Res    | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 23  | CLA  | C     | 505    | X         | -        | -       | -                |
| 23  | CLA  | C     | 506    | X         | -        | -       | -                |
| 23  | CLA  | C     | 507    | X         | -        | -       | -                |
| 23  | CLA  | C     | 508    | X         | -        | -       | -                |
| 23  | CLA  | C     | 509    | X         | -        | -       | -                |
| 23  | CLA  | C     | 510    | X         | -        | -       | -                |
| 23  | CLA  | C     | 511    | X         | -        | -       | -                |
| 23  | CLA  | C     | 512    | X         | -        | -       | -                |
| 23  | CLA  | C     | 513    | X         | -        | -       | -                |
| 23  | CLA  | C     | 514    | X         | -        | -       | -                |
| 23  | CLA  | D     | 403[A] | X         | -        | -       | -                |
| 23  | CLA  | D     | 403[B] | X         | -        | -       | -                |
| 23  | CLA  | D     | 404    | X         | -        | -       | -                |
| 23  | CLA  | a     | 404[A] | X         | -        | -       | -                |
| 23  | CLA  | a     | 404[B] | X         | -        | -       | -                |
| 23  | CLA  | a     | 407    | X         | -        | -       | -                |
| 23  | CLA  | b     | 601    | X         | -        | -       | -                |
| 23  | CLA  | b     | 602    | X         | -        | -       | -                |
| 23  | CLA  | b     | 603    | X         | -        | -       | -                |
| 23  | CLA  | b     | 604    | X         | -        | -       | -                |
| 23  | CLA  | b     | 605    | X         | -        | -       | -                |
| 23  | CLA  | b     | 606    | X         | -        | -       | -                |
| 23  | CLA  | b     | 607    | X         | -        | -       | -                |
| 23  | CLA  | b     | 609    | X         | -        | -       | -                |
| 23  | CLA  | b     | 610    | X         | -        | -       | -                |
| 23  | CLA  | b     | 611    | X         | -        | -       | -                |
| 23  | CLA  | b     | 612    | X         | -        | -       | -                |
| 23  | CLA  | b     | 613    | X         | -        | -       | -                |
| 23  | CLA  | b     | 614    | X         | -        | -       | -                |
| 23  | CLA  | b     | 615    | X         | -        | -       | -                |
| 23  | CLA  | b     | 616    | X         | -        | -       | -                |
| 23  | CLA  | c     | 502    | X         | -        | -       | -                |
| 23  | CLA  | c     | 503    | X         | -        | -       | -                |
| 23  | CLA  | c     | 504    | X         | -        | -       | -                |
| 23  | CLA  | c     | 505    | X         | -        | -       | -                |
| 23  | CLA  | c     | 506    | X         | -        | -       | -                |
| 23  | CLA  | c     | 507    | X         | -        | -       | -                |
| 23  | CLA  | c     | 508    | X         | -        | -       | -                |
| 23  | CLA  | c     | 509    | X         | -        | -       | -                |
| 23  | CLA  | c     | 510    | X         | -        | -       | -                |
| 23  | CLA  | c     | 511    | X         | -        | -       | -                |
| 23  | CLA  | c     | 512    | X         | -        | -       | -                |

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| Mol | Type | Chain | Res    | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 23  | CLA  | c     | 513    | X         | -        | -       | -                |
| 23  | CLA  | d     | 402[A] | X         | -        | -       | -                |
| 23  | CLA  | d     | 402[B] | X         | -        | -       | -                |
| 23  | CLA  | d     | 403[A] | X         | -        | -       | -                |
| 23  | CLA  | d     | 403[B] | X         | -        | -       | -                |
| 23  | CLA  | d     | 404    | X         | -        | -       | -                |
| 26  | GOL  | D     | 402    | -         | -        | X       | -                |
| 26  | GOL  | D     | 413    | -         | X        | -       | -                |

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62600 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       | 222     | 0     |
|     |       |          | 4338  | 2836 | 717 | 760 | 25 |         |         |       |
| 1   | a     | 334      | Total | C    | N   | O   | S  | 0       | 221     | 0     |
|     |       |          | 4330  | 2830 | 716 | 759 | 25 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 504      | Total | C    | N   | O   | S  | 0       | 20      | 0     |
|     |       |          | 4146  | 2721 | 692 | 720 | 13 |         |         |       |
| 2   | b     | 504      | Total | C    | N   | O   | S  | 0       | 19      | 0     |
|     |       |          | 4134  | 2718 | 687 | 716 | 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       | 97      | 0     |
|     |       |          | 4260  | 2788 | 713 | 741 | 18 |         |         |       |
| 3   | c     | 455      | Total | C    | N   | O   | S  | 0       | 100     | 0     |
|     |       |          | 4308  | 2821 | 719 | 750 | 18 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 342      | Total | C    | N   | O   | S  | 0       | 114     | 0     |
|     |       |          | 3620  | 2387 | 596 | 622 | 15 |         |         |       |
| 4   | d     | 341      | Total | C    | N   | O   | S  | 0       | 116     | 0     |
|     |       |          | 3628  | 2391 | 599 | 623 | 15 |         |         |       |

- 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       | 0       | 0     |
|     |       |          | 662   | 432 | 107 | 123 |  |         |         |       |
| 5   | e     | 79       | Total | C   | N   | O   |  | 0       | 2       | 0     |
|     |       |          | 670   | 439 | 110 | 121 |  |         |         |       |

- 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     | 31       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 261   | 179 | 43 | 38 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | H     | 64       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 506   | 339 | 81 | 84 | 2 |         |         |       |
| 7   | h     | 64       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 517   | 345 | 85 | 85 | 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     |
|     |       |          | 277   | 185 | 43 | 48 | 1 |         |         |       |

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 11  | L     | 36       | Total | C   | N  | O  | 0       | 2       | 0     |
|     |       |          | 311   | 207 | 49 | 55 |         |         |       |
| 11  | l     | 36       | Total | C   | N  | O  | 0       | 2       | 0     |
|     |       |          | 311   | 207 | 49 | 55 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | M     | 33       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 268   | 179 | 39 | 49 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | m     | 34       | Total | C   | N  | O  | S | 0       | 2       | 0     |
|     |       |          | 286   | 190 | 43 | 52 | 1 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | O     | 243      | Total | C    | N   | O   | S | 0       | 10      | 0     |
|     |       |          | 1958  | 1221 | 335 | 398 | 4 |         |         |       |
| 13  | o     | 243      | Total | C    | N   | O   | S | 0       | 8       | 0     |
|     |       |          | 1933  | 1207 | 330 | 392 | 4 |         |         |       |

- 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       | 6       | 0     |
|     |       |          | 311   | 213 | 48 | 48 | 2 |         |         |       |
| 14  | t     | 30       | Total | C   | N  | O  | S | 0       | 5       | 0     |
|     |       |          | 302   | 208 | 47 | 45 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 15  | U     | 96       | Total | C   | N   | O   |  | 0       | 4       | 0     |
|     |       |          | 800   | 508 | 133 | 159 |  |         |         |       |
| 15  | u     | 97       | Total | C   | N   | O   |  | 0       | 4       | 0     |
|     |       |          | 807   | 513 | 134 | 160 |  |         |         |       |

- 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       | 6       | 0     |
|     |       |          | 1120  | 711 | 185 | 220 | 4 |         |         |       |
| 16  | v     | 137      | Total | C   | N   | O   | S | 0       | 6       | 0     |
|     |       |          | 1117  | 712 | 185 | 216 | 4 |         |         |       |

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



| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17  | X     | 38       | Total | C   | N  | O  | 0       | 1       | 0     |
|     |       |          | 289   | 194 | 46 | 49 |         |         |       |
| 17  | x     | 38       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 281   | 188 | 45 | 48 |         |         |       |

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18  | Y     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 215   | 142 | 37 | 33 | 3 |         |         |       |
| 18  | y     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 215   | 142 | 37 | 33 | 3 |         |         |       |

- 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     | 34       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 273   | 186 | 47 | 40 |         |         |       |

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

| 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) (labeled as "Ligand of Interest" by depositor).

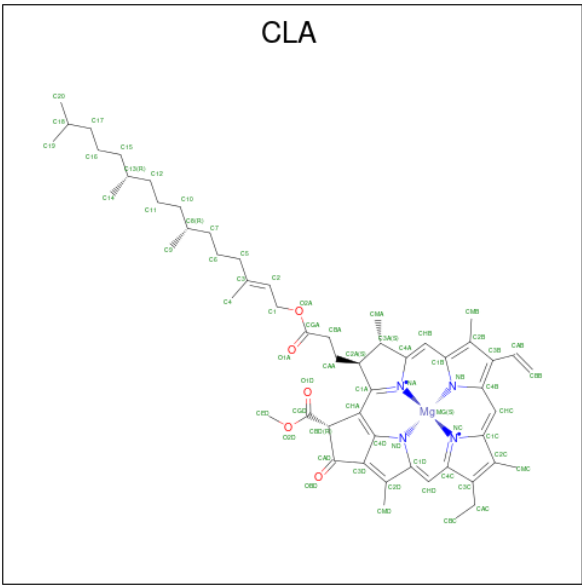
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22  | A     | 2        | Total | Cl | 0       | 2       |
|     |       |          | 4     | 4  |         |         |

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |     |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|----|---|----|---------|---------|
| 23  | A     | 1        | Total | C   | Mg | N | O  | 0       | 1       |
|     |       |          | 130   | 110 | 2  | 8 | 10 |         |         |
| 23  | A     | 1        | Total | C   | Mg | N | O  | 0       | 1       |
|     |       |          | 130   | 110 | 2  | 8 | 10 |         |         |
| 23  | A     | 1        | Total | C   | Mg | N | O  | 0       | 1       |
|     |       |          | 130   | 110 | 2  | 8 | 10 |         |         |
| 23  | A     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | B     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | B     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | B     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | B     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | B     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |

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

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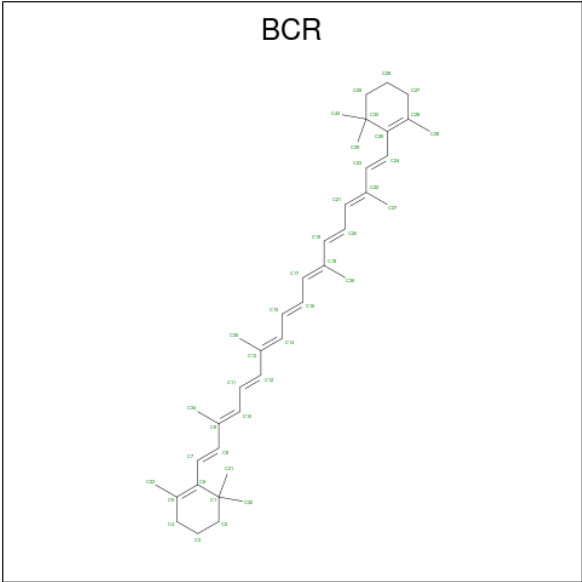
| Mol | Chain | Residues | Atoms        |          |         |        |         | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|--------|---------|---------|---------|
| 23  | C     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | C     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | D     | 1        | Total<br>130 | C<br>110 | Mg<br>2 | N<br>8 | O<br>10 | 0       | 1       |
| 23  | D     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | a     | 1        | Total<br>130 | C<br>110 | Mg<br>2 | N<br>8 | O<br>10 | 0       | 1       |
| 23  | a     | 1        | Total<br>130 | C<br>110 | Mg<br>2 | N<br>8 | O<br>10 | 0       | 1       |
| 23  | a     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |
| 23  | b     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0       |

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| Mol | Chain | Residues | Atoms |     |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|----|---|----|---------|---------|
| 23  | b     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | b     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | c     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
| 23  | d     | 1        | Total | C   | Mg | N | O  | 0       | 1       |
|     |       |          | 130   | 110 | 2  | 8 | 10 |         |         |
| 23  | d     | 1        | Total | C   | Mg | N | O  | 0       | 1       |
|     |       |          | 130   | 110 | 2  | 8 | 10 |         |         |
| 23  | d     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |

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



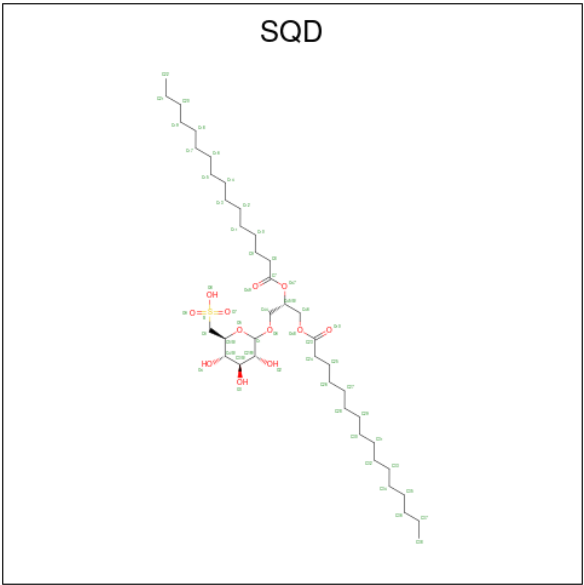
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 24  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | D     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | T     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | a     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | b     | 1        | Total C<br>40 40 | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 24  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | d     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | h     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | k     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | t     | 1        | Total C<br>40 40 | 0       | 0       |
| 24  | y     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



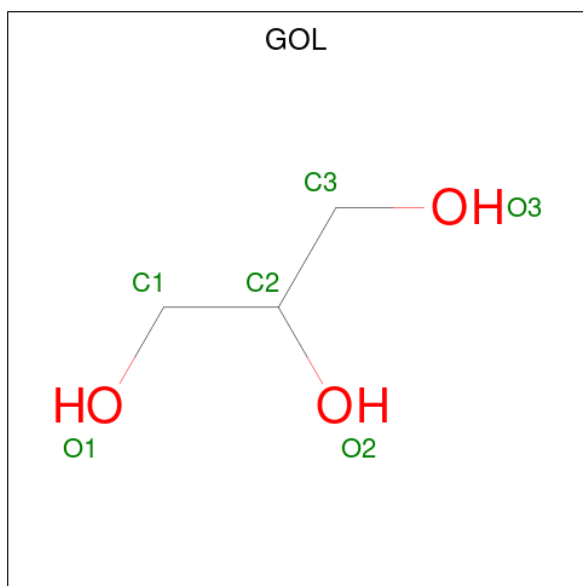
| Mol | Chain | Residues | Atoms                      | ZeroOcc | AltConf |
|-----|-------|----------|----------------------------|---------|---------|
| 25  | A     | 1        | Total C O S<br>108 82 24 2 | 0       | 1       |
| 25  | A     | 1        | Total C O S<br>54 41 12 1  | 0       | 0       |
| 25  | X     | 1        | Total C O S<br>43 30 12 1  | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 25  | a     | 1        | Total | C  | O  | S | 0       | 1       |
|     |       |          | 108   | 82 | 24 | 2 |         |         |
| 25  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 25  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 25  | f     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |
| 25  | l     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |

- Molecule 26 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 26  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | C     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |
| 26  | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

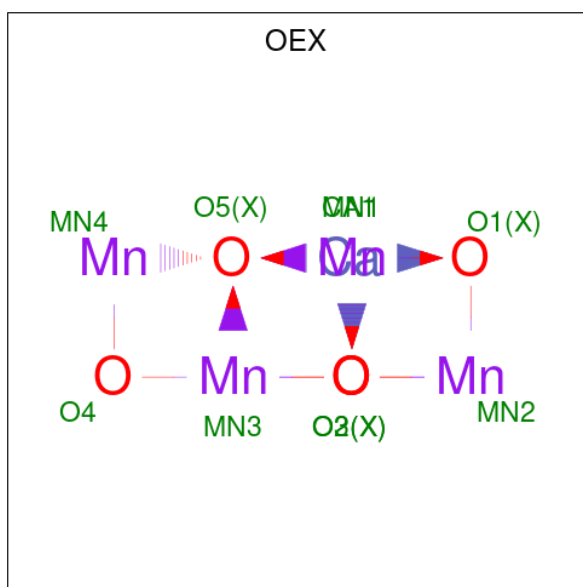
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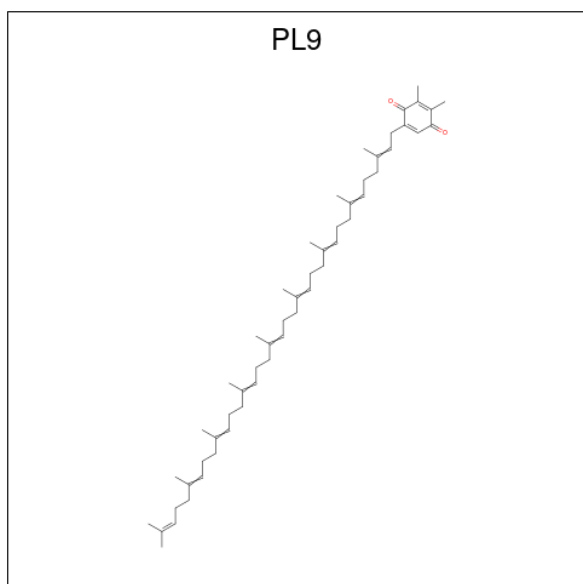
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 26  | O     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | O     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | V     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |
| 26  | a     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | a     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | a     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | b     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | b     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | c     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |
| 26  | c     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | d     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | l     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |
| 26  | o     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | o     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 26  | v     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |

- Molecule 27 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 27  | A     | 1        | Total | Ca | Mn | O  | 0       | 1       |
|     |       |          | 20    | 2  | 8  | 10 |         |         |
| 27  | a     | 1        | Total | Ca | Mn | O  | 0       | 1       |
|     |       |          | 20    | 2  | 8  | 10 |         |         |

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

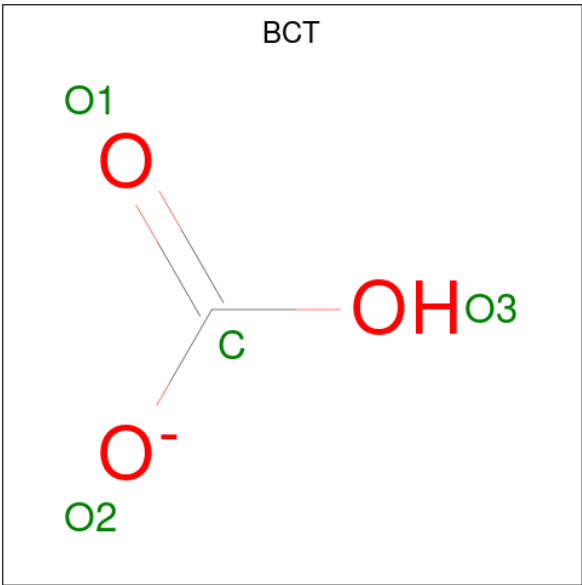


| Mol | Chain | Residues | Atoms |     |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---|---------|---------|
| 28  | A     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |
| 28  | D     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |
| 28  | a     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |
| 28  | d     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

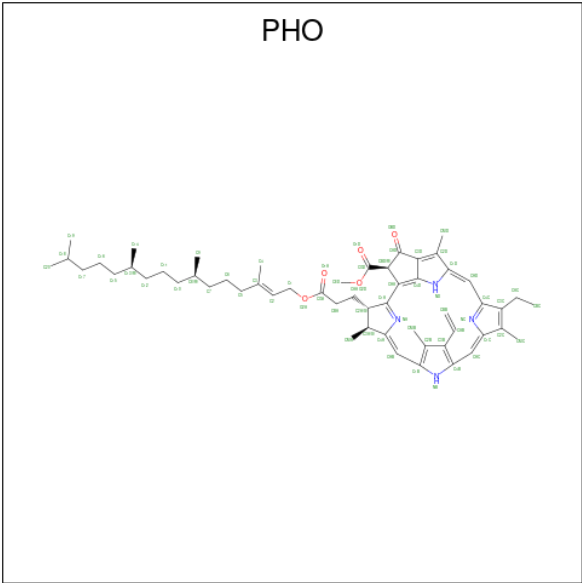
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 29  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 28    | 23 | 5  |         |         |
| 29  | B     | 2        | Total | C  | O  | 0       | 0       |
|     |       |          | 73    | 63 | 10 |         |         |
| 29  | D     | 2        | Total | C  | O  | 0       | 0       |
|     |       |          | 57    | 51 | 6  |         |         |
| 29  | I     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 40    | 35 | 5  |         |         |
| 29  | J     | 1        | Total | C  |    | 0       | 0       |
|     |       |          | 10    | 10 |    |         |         |
| 29  | K     | 1        | Total | C  | O  | 0       | 1       |
|     |       |          | 68    | 58 | 10 |         |         |
| 29  | X     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 18    | 16 | 2  |         |         |
| 29  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 30    | 25 | 5  |         |         |
| 29  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 28 | 5  |         |         |
| 29  | c     | 1        | Total | C  | O  | 0       | 1       |
|     |       |          | 64    | 54 | 10 |         |         |
| 29  | d     | 3        | Total | C  | O  | 0       | 0       |
|     |       |          | 71    | 63 | 8  |         |         |
| 29  | j     | 1        | Total | C  |    | 0       | 0       |
|     |       |          | 10    | 10 |    |         |         |
| 29  | l     | 1        | Total | C  |    | 0       | 0       |
|     |       |          | 10    | 10 |    |         |         |
| 29  | m     | 1        | Total | C  |    | 0       | 0       |
|     |       |          | 10    | 10 |    |         |         |

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 30  | A     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 8     | 2 | 6 |         |         |
| 30  | d     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 8     | 2 | 6 |         |         |

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



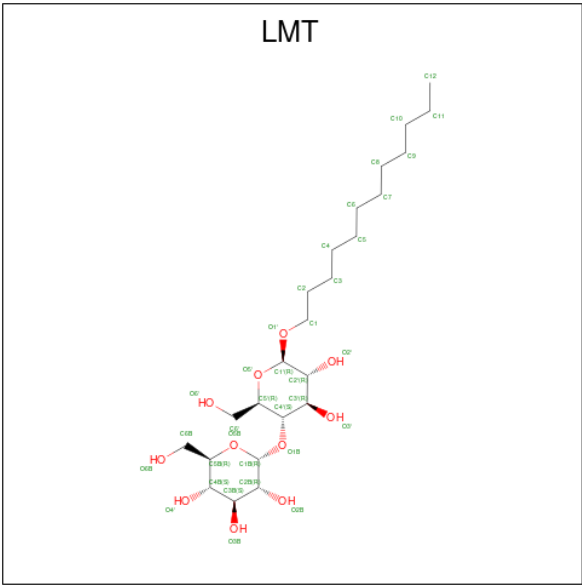
| Mol | Chain | Residues | Atoms |     |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---|----|---------|---------|
| 31  | A     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |
| 31  | D     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |

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| Mol | Chain | Residues | Atoms |     |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---|----|---------|---------|
| 31  | a     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |
| 31  | a     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



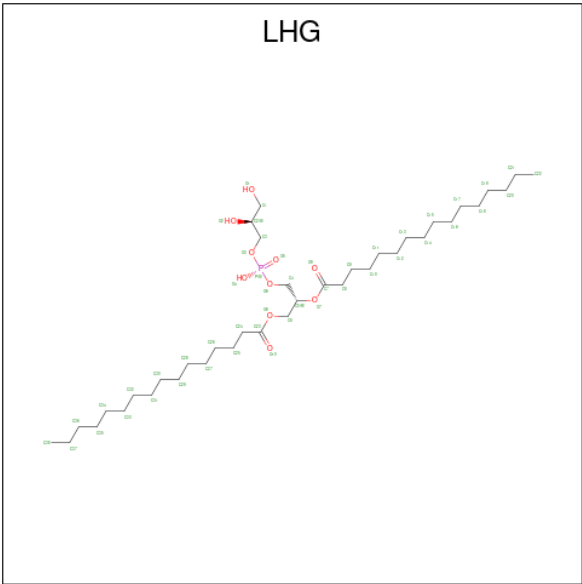
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 32  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 25    | 19 | 6  |         |         |
| 32  | F     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | T     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 32  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 25    | 19 | 6  |         |         |
| 32  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 25    | 19 | 6  |         |         |
| 32  | e     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | t     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 26    | 19 | 7  |         |         |

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



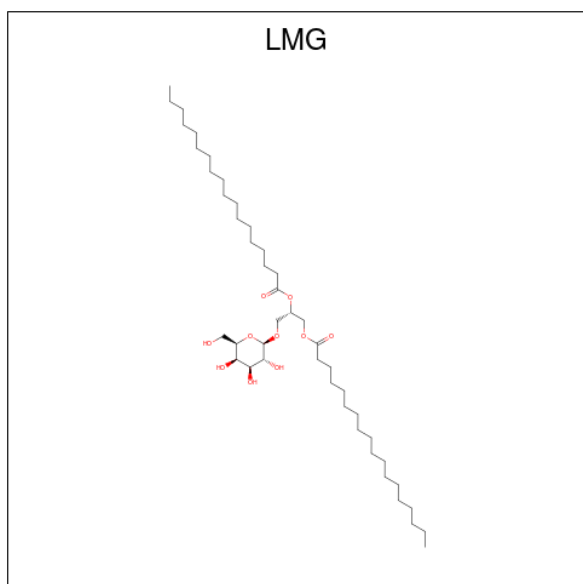
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 33  | A     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 98    | 76 | 20 | 2 |         |         |
| 33  | D     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 98    | 76 | 20 | 2 |         |         |
| 33  | D     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 98    | 76 | 20 | 2 |         |         |
| 33  | E     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 84    | 62 | 20 | 2 |         |         |
| 33  | L     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 98    | 76 | 20 | 2 |         |         |
| 33  | a     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 84    | 62 | 20 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 33  | b     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 98    | 76 | 20 | 2 |         |         |
| 33  | d     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 98    | 76 | 20 | 2 |         |         |
| 33  | d     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 98    | 76 | 20 | 2 |         |         |
| 33  | d     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 98    | 76 | 20 | 2 |         |         |

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



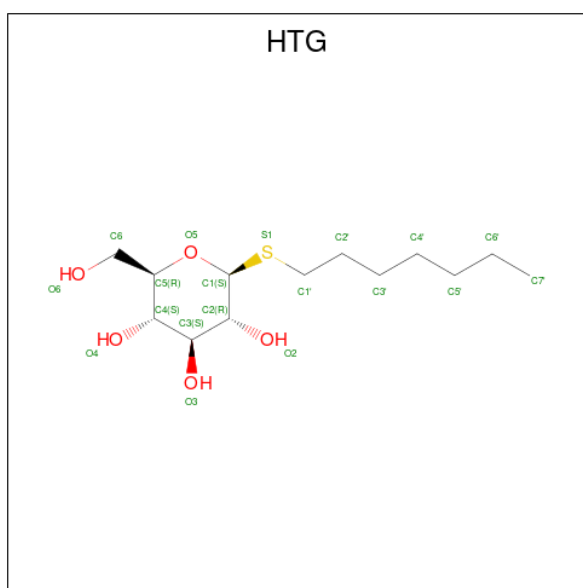
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 34  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 34  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 34  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 34  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 34  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 34  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 34  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 34  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 34  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 34  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 34  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 37    | 27 | 10 |         |         |
| 34  | z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 39    | 29 | 10 |         |         |

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



| 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  | 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 |   | 0       | 0       |
|     |       |          | 11    | 6  | 5 |   |         |         |
| 35  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |

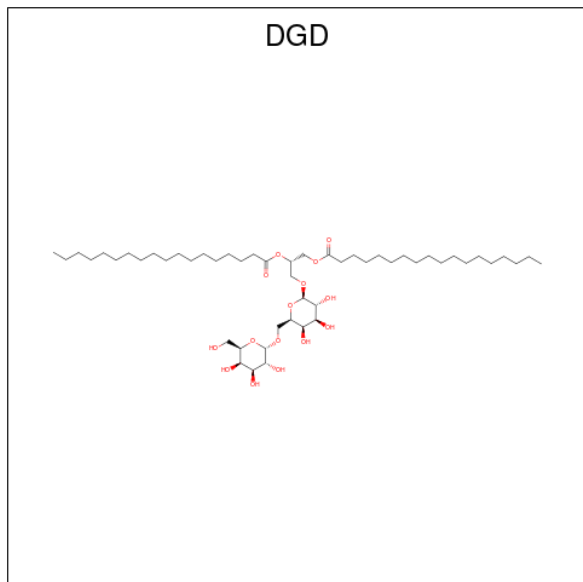
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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 35  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | b     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 5 | 1 |         |         |
| 35  | 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  | o     | 1        | Total | C  | O | S | 0       | 0       |
|     |       |          | 19    | 13 | 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       | 1       |
|     |       |          | 124   | 94 | 30 |  |         |         |
| 36  | C     | 1        | Total | C  | O  |  | 0       | 1       |
|     |       |          | 124   | 94 | 30 |  |         |         |
| 36  | C     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 36  | H     | 1        | Total | C  | O  |  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |  |         |         |
| 36  | c     | 1        | Total | C  | O  |  | 0       | 1       |
|     |       |          | 124   | 94 | 30 |  |         |         |
| 36  | c     | 1        | Total | C  | O  |  | 0       | 1       |
|     |       |          | 124   | 94 | 30 |  |         |         |

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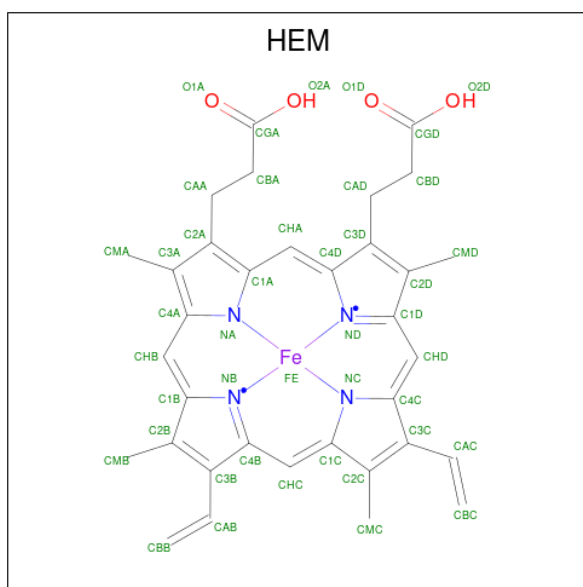
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| Mol | Chain | Residues | Atoms       |         |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|---------|
| 36  | c     | 1        | Total<br>62 | C<br>47 | O<br>15 | 0       | 0       |
| 36  | h     | 1        | Total<br>62 | C<br>47 | O<br>15 | 0       | 0       |

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 37  | C     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 37  | F     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 37  | O     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 37  | c     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 37  | f     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 37  | o     | 1        | Total Ca<br>1 1 | 0       | 0       |

- 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 |

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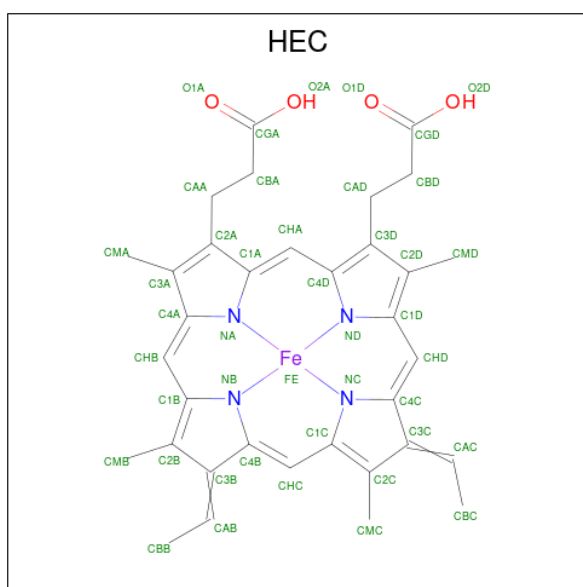
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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 38  | f     | 1        | Total | C  | Fe | N | O       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 41 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 41  | A     | 133      | Total | O   | 0       | 83      |
|     |       |          | 215   | 215 |         |         |
| 41  | B     | 190      | Total | O   | 0       | 3       |
|     |       |          | 193   | 193 |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 41  | C     | 165      | Total<br>202 | O<br>202 | 0       | 37      |
| 41  | D     | 127      | Total<br>162 | O<br>162 | 0       | 35      |
| 41  | E     | 15       | Total<br>15  | O<br>15  | 0       | 0       |
| 41  | F     | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 41  | H     | 23       | Total<br>23  | O<br>23  | 0       | 0       |
| 41  | I     | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 41  | J     | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 41  | K     | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 41  | L     | 7        | Total<br>8   | O<br>8   | 0       | 1       |
| 41  | M     | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 41  | O     | 102      | Total<br>106 | O<br>106 | 0       | 4       |
| 41  | T     | 10       | Total<br>13  | O<br>13  | 0       | 3       |
| 41  | U     | 47       | Total<br>49  | O<br>49  | 0       | 2       |
| 41  | V     | 80       | Total<br>82  | O<br>82  | 0       | 2       |
| 41  | X     | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 41  | a     | 129      | Total<br>207 | O<br>207 | 0       | 79      |
| 41  | b     | 206      | Total<br>209 | O<br>209 | 0       | 3       |
| 41  | c     | 159      | Total<br>192 | O<br>192 | 0       | 33      |
| 41  | d     | 118      | Total<br>152 | O<br>152 | 0       | 34      |
| 41  | e     | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 41  | f     | 3        | Total<br>3   | O<br>3   | 0       | 0       |

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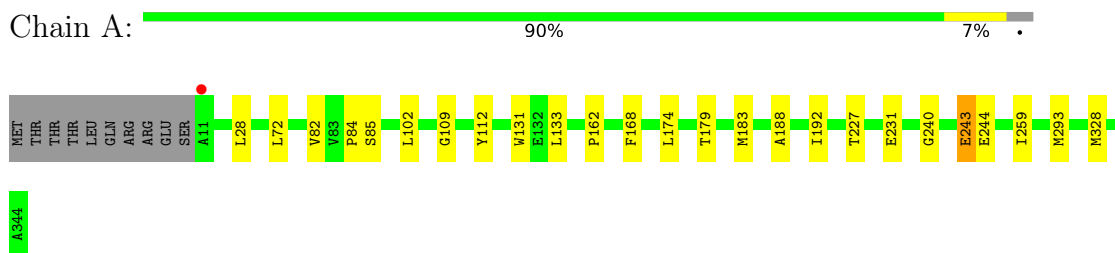
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 41  | h     | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 41  | i     | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 41  | j     | 1        | Total<br>1  | O<br>1  | 0       | 0       |
| 41  | k     | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 41  | l     | 7        | Total<br>8  | O<br>8  | 0       | 1       |
| 41  | m     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 41  | o     | 95       | Total<br>99 | O<br>99 | 0       | 4       |
| 41  | t     | 8        | Total<br>11 | O<br>11 | 0       | 3       |
| 41  | u     | 50       | Total<br>51 | O<br>51 | 0       | 1       |
| 41  | v     | 58       | Total<br>61 | O<br>61 | 0       | 3       |
| 41  | x     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 41  | y     | 2        | Total<br>2  | O<br>2  | 0       | 0       |

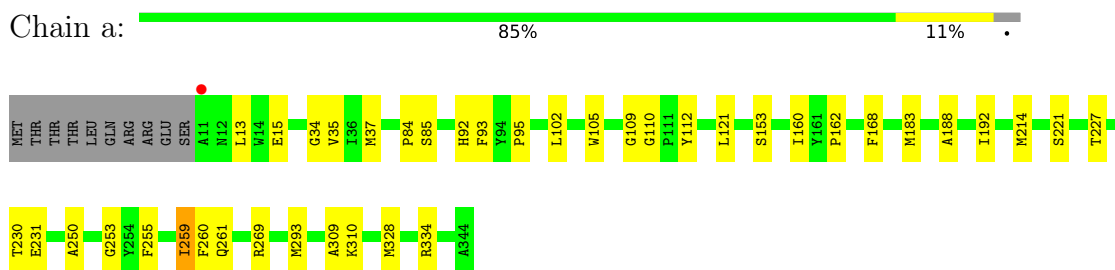
### 3 Residue-property plots [i](#)

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

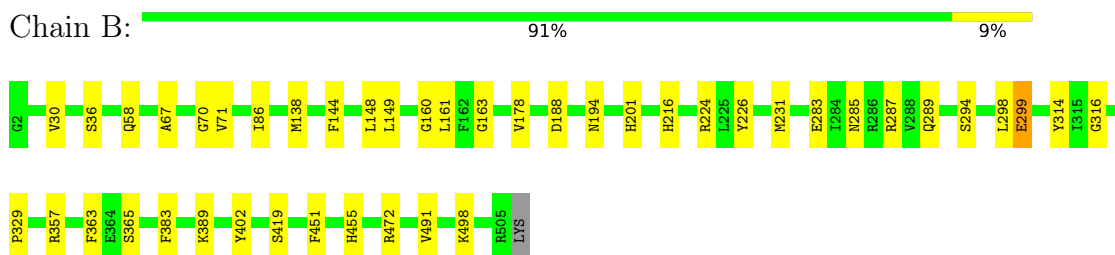
- Molecule 1: Photosystem II protein D1



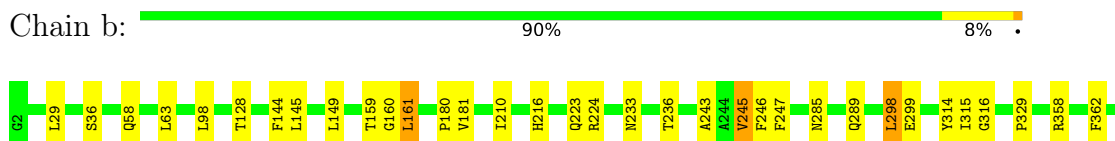
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



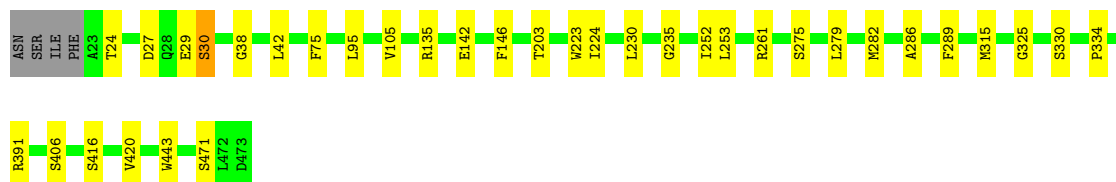
- Molecule 2: Photosystem II CP47 reaction center protein





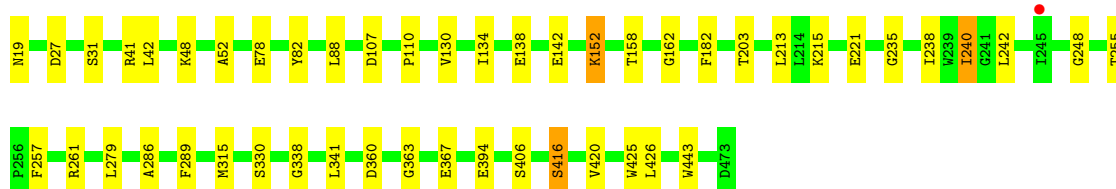
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91% 7% .



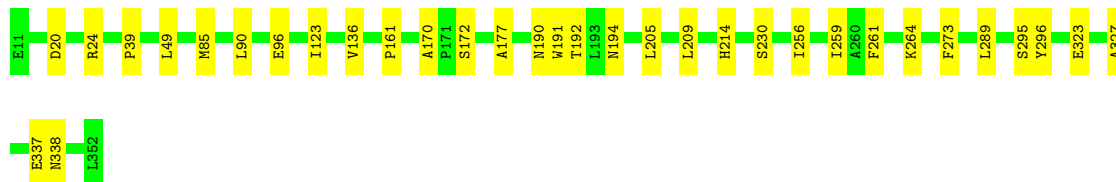
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 10% .



- Molecule 4: Photosystem II D2 protein

Chain D: 90% 10%



- Molecule 4: Photosystem II D2 protein

Chain d: 92% 8%

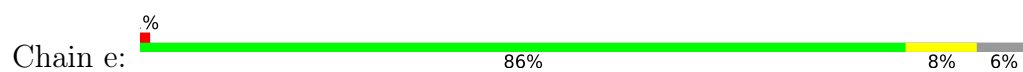


- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 79% 18% .



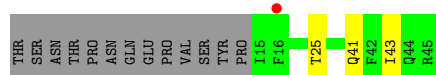
- Molecule 5: Cytochrome b559 subunit alpha



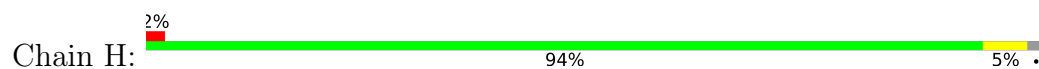
- Molecule 6: Cytochrome b559 subunit beta



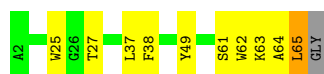
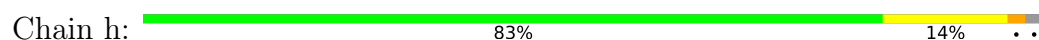
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



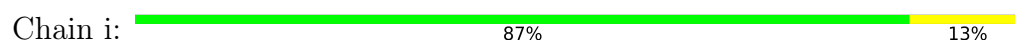
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



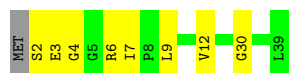
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



Chain J:  77% 21% .



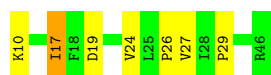
- Molecule 9: Photosystem II reaction center protein J

Chain j:  92% 8%



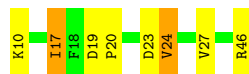
- Molecule 10: Photosystem II reaction center protein K

Chain K:  81% 16% .



- Molecule 10: Photosystem II reaction center protein K

Chain k:  78% 16% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  92% 5% .



- Molecule 11: Photosystem II reaction center protein L

Chain l:  81% 16% .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 8% 6% 8%



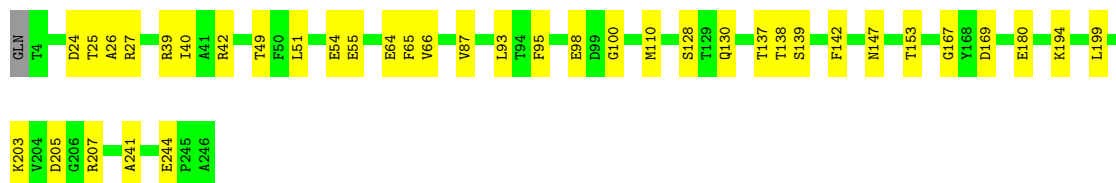
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 14% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  84% 16%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  89% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  75% 16% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 72% 22% 6%



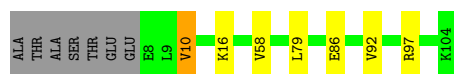
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 8% 8%

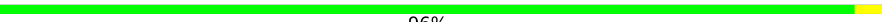


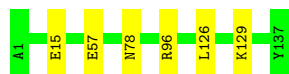
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  87% 6% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



- Molecule 16: Cytochrome c-550

Chain v:  90% 10%



- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  90% 5% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  80% 17% .



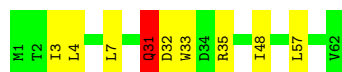
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  60% 37% .

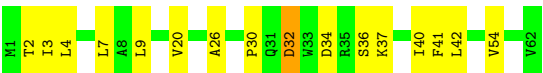


- Molecule 19: Photosystem II reaction center protein Z

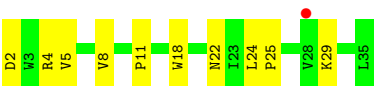
Chain Z:  85% 13% .



- 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, $\alpha$ , $\beta$ , $\gamma$                | 125.77Å 231.76Å 288.58Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 19.99 – 2.30<br>19.99 – 2.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (19.99-2.30)<br>99.7 (19.99-2.30)                     | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.70 (at 2.30Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.19.2_4158: ???)                                   | Depositor        |
| R, $R_{free}$                                                           | 0.142 , 0.183<br>0.143 , 0.185                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 18693 reflections (2.29%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 50.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.494                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 72.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.98                                                        | EDS              |
| Total number of atoms                                                   | 62600                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 63.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BCR, LHG, BCT, DGD, FE2, UNL, HTG, CL, GOL, SQD, CLA, PL9, LMG, FME, OEX, LMT, MG, HEM, PHO, HEC

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     | 0.26         | 0/4478      | 0.42        | 0/6098      |
| 1   | a     | 0.24         | 0/4470      | 0.40        | 0/6087      |
| 2   | B     | 0.37         | 0/4293      | 0.50        | 0/5851      |
| 2   | b     | 0.33         | 0/4285      | 0.49        | 0/5841      |
| 3   | C     | 0.29         | 0/4404      | 0.43        | 0/5997      |
| 3   | c     | 0.28         | 0/4459      | 0.43        | 0/6071      |
| 4   | D     | 0.33         | 0/3741      | 0.46        | 0/5095      |
| 4   | d     | 0.30         | 0/3749      | 0.46        | 0/5106      |
| 5   | E     | 0.35         | 0/681       | 0.53        | 0/928       |
| 5   | e     | 0.31         | 0/690       | 0.49        | 0/939       |
| 6   | F     | 0.32         | 0/284       | 0.45        | 0/387       |
| 6   | f     | 0.29         | 0/269       | 0.43        | 0/365       |
| 7   | H     | 0.33         | 0/519       | 0.50        | 0/708       |
| 7   | h     | 0.30         | 0/530       | 0.49        | 0/722       |
| 8   | I     | 0.31         | 0/311       | 0.44        | 0/419       |
| 8   | i     | 0.35         | 0/311       | 0.51        | 0/419       |
| 9   | J     | 0.34         | 0/278       | 0.41        | 0/376       |
| 9   | j     | 0.28         | 0/283       | 0.42        | 0/383       |
| 10  | K     | 0.32         | 0/303       | 0.48        | 0/416       |
| 10  | k     | 0.32         | 0/303       | 0.46        | 0/416       |
| 11  | L     | 0.38         | 0/318       | 0.47        | 0/433       |
| 11  | l     | 0.38         | 0/318       | 0.45        | 0/433       |
| 12  | M     | 0.40         | 0/261       | 0.51        | 0/357       |
| 12  | m     | 0.36         | 0/279       | 0.48        | 0/380       |
| 13  | O     | 0.35         | 0/1991      | 0.51        | 0/2698      |
| 13  | o     | 0.34         | 0/1966      | 0.52        | 0/2665      |
| 14  | T     | 0.36         | 0/310       | 0.43        | 0/419       |
| 14  | t     | 0.33         | 0/301       | 0.43        | 0/406       |
| 15  | U     | 0.37         | 0/811       | 0.54        | 0/1095      |
| 15  | u     | 0.36         | 0/818       | 0.57        | 0/1105      |
| 16  | V     | 0.35         | 0/1142      | 0.48        | 0/1545      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 16  | v     | 0.31         | 0/1139  | 0.47        | 0/1542  |
| 17  | X     | 0.25         | 0/292   | 0.38        | 0/395   |
| 17  | x     | 0.28         | 0/284   | 0.39        | 0/384   |
| 18  | Y     | 0.25         | 0/216   | 0.43        | 0/289   |
| 18  | y     | 0.25         | 0/216   | 0.41        | 0/289   |
| 19  | Z     | 0.24         | 0/490   | 0.39        | 0/669   |
| 19  | z     | 0.23         | 0/490   | 0.42        | 0/669   |
| 20  | R     | 0.25         | 0/279   | 0.35        | 0/383   |
| All | All   | 0.31         | 0/50562 | 0.46        | 0/68780 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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     | 4338  | 0        | 4142     | 23      | 0            |
| 1   | a     | 4330  | 0        | 4132     | 39      | 0            |
| 2   | B     | 4146  | 0        | 3983     | 32      | 0            |
| 2   | b     | 4134  | 0        | 3976     | 41      | 0            |
| 3   | C     | 4260  | 0        | 4123     | 24      | 0            |
| 3   | c     | 4308  | 0        | 4172     | 36      | 0            |
| 4   | D     | 3620  | 0        | 3484     | 33      | 0            |
| 4   | d     | 3628  | 0        | 3490     | 22      | 0            |
| 5   | E     | 662   | 0        | 648      | 12      | 0            |
| 5   | e     | 670   | 0        | 655      | 5       | 0            |
| 6   | F     | 275   | 0        | 282      | 3       | 0            |
| 6   | f     | 261   | 0        | 269      | 4       | 0            |
| 7   | H     | 506   | 0        | 529      | 2       | 0            |
| 7   | h     | 517   | 0        | 541      | 7       | 0            |
| 8   | I     | 314   | 0        | 328      | 5       | 0            |
| 8   | i     | 314   | 0        | 328      | 2       | 0            |
| 9   | J     | 272   | 0        | 279      | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | j     | 277   | 0        | 284      | 2       | 0            |
| 10  | K     | 293   | 0        | 305      | 3       | 0            |
| 10  | k     | 293   | 0        | 305      | 6       | 0            |
| 11  | L     | 311   | 0        | 320      | 3       | 0            |
| 11  | l     | 311   | 0        | 320      | 5       | 0            |
| 12  | M     | 268   | 0        | 285      | 7       | 0            |
| 12  | m     | 286   | 0        | 305      | 8       | 0            |
| 13  | O     | 1958  | 0        | 1920     | 23      | 0            |
| 13  | o     | 1933  | 0        | 1900     | 13      | 0            |
| 14  | T     | 311   | 0        | 318      | 3       | 0            |
| 14  | t     | 302   | 0        | 311      | 6       | 0            |
| 15  | U     | 800   | 0        | 796      | 4       | 0            |
| 15  | u     | 807   | 0        | 805      | 4       | 0            |
| 16  | V     | 1120  | 0        | 1122     | 3       | 0            |
| 16  | v     | 1117  | 0        | 1131     | 11      | 0            |
| 17  | X     | 289   | 0        | 322      | 3       | 0            |
| 17  | x     | 281   | 0        | 312      | 2       | 0            |
| 18  | Y     | 215   | 0        | 246      | 3       | 0            |
| 18  | y     | 215   | 0        | 246      | 6       | 0            |
| 19  | Z     | 479   | 0        | 516      | 7       | 0            |
| 19  | z     | 479   | 0        | 516      | 5       | 0            |
| 20  | R     | 273   | 0        | 305      | 4       | 0            |
| 21  | A     | 2     | 0        | 0        | 0       | 0            |
| 21  | a     | 2     | 0        | 0        | 0       | 0            |
| 22  | A     | 4     | 0        | 0        | 0       | 0            |
| 22  | a     | 4     | 0        | 0        | 0       | 0            |
| 23  | A     | 455   | 0        | 504      | 18      | 0            |
| 23  | B     | 1040  | 0        | 1152     | 26      | 0            |
| 23  | C     | 845   | 0        | 936      | 30      | 0            |
| 23  | D     | 195   | 0        | 216      | 9       | 0            |
| 23  | a     | 325   | 0        | 360      | 22      | 0            |
| 23  | b     | 1040  | 0        | 1152     | 29      | 0            |
| 23  | c     | 845   | 0        | 936      | 45      | 0            |
| 23  | d     | 325   | 0        | 360      | 15      | 0            |
| 24  | A     | 40    | 0        | 56       | 1       | 0            |
| 24  | B     | 120   | 0        | 168      | 5       | 0            |
| 24  | C     | 80    | 0        | 112      | 1       | 0            |
| 24  | D     | 40    | 0        | 56       | 1       | 0            |
| 24  | H     | 40    | 0        | 56       | 1       | 0            |
| 24  | K     | 40    | 0        | 56       | 1       | 0            |
| 24  | T     | 40    | 0        | 56       | 5       | 0            |
| 24  | Y     | 40    | 0        | 56       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | a     | 40    | 0        | 56       | 1       | 0            |
| 24  | b     | 120   | 0        | 168      | 8       | 0            |
| 24  | c     | 80    | 0        | 112      | 3       | 0            |
| 24  | d     | 40    | 0        | 56       | 2       | 0            |
| 24  | h     | 40    | 0        | 56       | 5       | 0            |
| 24  | k     | 40    | 0        | 56       | 1       | 0            |
| 24  | t     | 40    | 0        | 56       | 7       | 0            |
| 24  | y     | 40    | 0        | 56       | 1       | 0            |
| 25  | A     | 162   | 0        | 234      | 3       | 0            |
| 25  | X     | 43    | 0        | 53       | 1       | 0            |
| 25  | a     | 162   | 0        | 233      | 10      | 0            |
| 25  | b     | 54    | 0        | 78       | 2       | 0            |
| 25  | f     | 43    | 0        | 53       | 1       | 0            |
| 25  | l     | 54    | 0        | 78       | 2       | 0            |
| 26  | A     | 6     | 0        | 8        | 0       | 0            |
| 26  | B     | 12    | 0        | 16       | 2       | 0            |
| 26  | C     | 12    | 0        | 16       | 0       | 0            |
| 26  | D     | 12    | 0        | 16       | 7       | 0            |
| 26  | O     | 12    | 0        | 16       | 3       | 0            |
| 26  | V     | 12    | 0        | 16       | 0       | 0            |
| 26  | a     | 18    | 0        | 24       | 5       | 0            |
| 26  | b     | 12    | 0        | 16       | 2       | 0            |
| 26  | c     | 18    | 0        | 24       | 0       | 0            |
| 26  | d     | 6     | 0        | 8        | 0       | 0            |
| 26  | l     | 12    | 0        | 16       | 2       | 0            |
| 26  | o     | 12    | 0        | 16       | 0       | 0            |
| 26  | v     | 12    | 0        | 16       | 3       | 0            |
| 27  | A     | 20    | 0        | 0        | 0       | 0            |
| 27  | a     | 20    | 0        | 0        | 0       | 0            |
| 28  | A     | 110   | 0        | 160      | 21      | 0            |
| 28  | D     | 110   | 0        | 160      | 2       | 0            |
| 28  | a     | 110   | 0        | 160      | 8       | 0            |
| 28  | d     | 110   | 0        | 160      | 0       | 0            |
| 29  | A     | 28    | 0        | 0        | 0       | 0            |
| 29  | B     | 73    | 0        | 0        | 0       | 0            |
| 29  | D     | 57    | 0        | 0        | 0       | 0            |
| 29  | I     | 40    | 0        | 0        | 0       | 0            |
| 29  | J     | 10    | 0        | 0        | 0       | 0            |
| 29  | K     | 68    | 0        | 0        | 0       | 0            |
| 29  | X     | 18    | 0        | 0        | 0       | 0            |
| 29  | a     | 30    | 0        | 0        | 1       | 0            |
| 29  | b     | 33    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | c     | 64    | 0        | 0        | 0       | 0            |
| 29  | d     | 71    | 0        | 0        | 0       | 0            |
| 29  | j     | 10    | 0        | 0        | 0       | 0            |
| 29  | l     | 10    | 0        | 0        | 0       | 0            |
| 29  | m     | 10    | 0        | 0        | 0       | 0            |
| 30  | A     | 8     | 0        | 0        | 0       | 0            |
| 30  | d     | 8     | 0        | 0        | 0       | 0            |
| 31  | A     | 128   | 0        | 148      | 2       | 0            |
| 31  | D     | 128   | 0        | 148      | 3       | 0            |
| 31  | a     | 256   | 0        | 296      | 4       | 0            |
| 32  | A     | 70    | 0        | 91       | 2       | 0            |
| 32  | B     | 95    | 0        | 127      | 3       | 0            |
| 32  | F     | 35    | 0        | 46       | 0       | 0            |
| 32  | M     | 35    | 0        | 45       | 2       | 0            |
| 32  | T     | 35    | 0        | 46       | 0       | 0            |
| 32  | a     | 35    | 0        | 46       | 1       | 0            |
| 32  | b     | 50    | 0        | 70       | 1       | 0            |
| 32  | e     | 35    | 0        | 46       | 1       | 0            |
| 32  | m     | 35    | 0        | 46       | 2       | 0            |
| 32  | t     | 26    | 0        | 34       | 3       | 0            |
| 33  | A     | 98    | 0        | 148      | 2       | 0            |
| 33  | D     | 196   | 0        | 296      | 11      | 0            |
| 33  | E     | 84    | 0        | 114      | 6       | 0            |
| 33  | L     | 98    | 0        | 148      | 1       | 0            |
| 33  | a     | 84    | 0        | 114      | 8       | 0            |
| 33  | b     | 98    | 0        | 148      | 0       | 0            |
| 33  | d     | 294   | 0        | 444      | 22      | 0            |
| 34  | B     | 51    | 0        | 72       | 2       | 0            |
| 34  | C     | 153   | 0        | 216      | 3       | 0            |
| 34  | D     | 51    | 0        | 72       | 0       | 0            |
| 34  | Z     | 37    | 0        | 44       | 3       | 0            |
| 34  | c     | 153   | 0        | 216      | 3       | 0            |
| 34  | d     | 51    | 0        | 72       | 3       | 0            |
| 34  | m     | 51    | 0        | 72       | 0       | 0            |
| 34  | z     | 39    | 0        | 48       | 2       | 0            |
| 35  | B     | 38    | 0        | 52       | 2       | 0            |
| 35  | C     | 19    | 0        | 26       | 0       | 0            |
| 35  | D     | 16    | 0        | 17       | 0       | 0            |
| 35  | V     | 11    | 0        | 10       | 0       | 0            |
| 35  | b     | 57    | 0        | 78       | 3       | 0            |
| 35  | c     | 19    | 0        | 26       | 1       | 0            |
| 35  | d     | 16    | 0        | 17       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | o     | 19    | 0        | 26       | 1       | 0            |
| 36  | C     | 310   | 0        | 410      | 6       | 0            |
| 36  | H     | 62    | 0        | 82       | 1       | 0            |
| 36  | c     | 310   | 0        | 410      | 10      | 0            |
| 36  | h     | 62    | 0        | 82       | 2       | 0            |
| 37  | C     | 1     | 0        | 0        | 0       | 0            |
| 37  | F     | 1     | 0        | 0        | 0       | 0            |
| 37  | O     | 1     | 0        | 0        | 0       | 0            |
| 37  | c     | 2     | 0        | 0        | 0       | 0            |
| 37  | f     | 1     | 0        | 0        | 0       | 0            |
| 37  | o     | 1     | 0        | 0        | 0       | 0            |
| 38  | F     | 43    | 0        | 30       | 1       | 0            |
| 38  | f     | 43    | 0        | 30       | 0       | 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     | 215   | 0        | 0        | 1       | 0            |
| 41  | B     | 193   | 0        | 0        | 2       | 0            |
| 41  | C     | 202   | 0        | 0        | 1       | 0            |
| 41  | D     | 162   | 0        | 0        | 4       | 0            |
| 41  | E     | 15    | 0        | 0        | 0       | 0            |
| 41  | F     | 6     | 0        | 0        | 0       | 0            |
| 41  | H     | 23    | 0        | 0        | 0       | 0            |
| 41  | I     | 6     | 0        | 0        | 0       | 0            |
| 41  | J     | 7     | 0        | 0        | 1       | 0            |
| 41  | K     | 6     | 0        | 0        | 0       | 0            |
| 41  | L     | 8     | 0        | 0        | 0       | 0            |
| 41  | M     | 5     | 0        | 0        | 0       | 0            |
| 41  | O     | 106   | 0        | 0        | 0       | 0            |
| 41  | T     | 13    | 0        | 0        | 0       | 0            |
| 41  | U     | 49    | 0        | 0        | 0       | 0            |
| 41  | V     | 82    | 0        | 0        | 0       | 0            |
| 41  | X     | 8     | 0        | 0        | 0       | 0            |
| 41  | a     | 207   | 0        | 0        | 3       | 0            |
| 41  | b     | 209   | 0        | 0        | 0       | 0            |
| 41  | c     | 192   | 0        | 0        | 3       | 0            |
| 41  | d     | 152   | 0        | 0        | 0       | 0            |
| 41  | e     | 9     | 0        | 0        | 0       | 0            |
| 41  | f     | 3     | 0        | 0        | 0       | 0            |
| 41  | h     | 18    | 0        | 0        | 0       | 0            |
| 41  | i     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41  | j     | 1     | 0        | 0        | 0       | 0            |
| 41  | k     | 3     | 0        | 0        | 0       | 0            |
| 41  | l     | 8     | 0        | 0        | 0       | 0            |
| 41  | m     | 12    | 0        | 0        | 0       | 0            |
| 41  | o     | 99    | 0        | 0        | 0       | 0            |
| 41  | t     | 11    | 0        | 0        | 1       | 0            |
| 41  | u     | 51    | 0        | 0        | 1       | 0            |
| 41  | v     | 61    | 0        | 0        | 0       | 0            |
| 41  | x     | 6     | 0        | 0        | 0       | 0            |
| 41  | y     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 62600 | 0        | 61445    | 629     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (629) 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) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:B:604:CLA:H42     | 23:B:605:CLA:H2      | 1.44                     | 0.95              |
| 1:a:250[A]:ALA:HA    | 2:b:491[A]:VAL:HG11  | 1.51                     | 0.93              |
| 1:a:250[B]:ALA:HA    | 2:b:491[B]:VAL:HG11  | 1.53                     | 0.91              |
| 26:D:402:GOL:H11     | 12:M:1:FME:HG2       | 1.57                     | 0.86              |
| 23:d:402[B]:CLA:HHC  | 23:d:402[B]:CLA:HBB1 | 1.64                     | 0.80              |
| 4:d:192[A]:THR:HG23  | 23:d:403[A]:CLA:HBC2 | 1.66                     | 0.77              |
| 23:B:601:CLA:H12     | 23:B:601:CLA:H71     | 1.65                     | 0.77              |
| 23:b:605:CLA:HHC     | 23:b:605:CLA:HBB1    | 1.67                     | 0.77              |
| 23:c:504:CLA:HBB1    | 23:c:513:CLA:H41     | 1.66                     | 0.77              |
| 23:A:406[A]:CLA:H152 | 28:A:413[A]:PL9:H252 | 1.67                     | 0.76              |
| 23:A:406[B]:CLA:H152 | 28:A:413[B]:PL9:H252 | 1.68                     | 0.76              |
| 23:C:502:CLA:H193    | 23:C:508:CLA:HBB1    | 1.68                     | 0.75              |
| 4:d:192[B]:THR:HG23  | 23:d:403[B]:CLA:HBC2 | 1.69                     | 0.75              |
| 23:C:506:CLA:HHC     | 23:C:506:CLA:HBB1    | 1.69                     | 0.74              |
| 23:C:504:CLA:HBB1    | 23:C:513:CLA:H41     | 1.69                     | 0.74              |
| 4:D:85:MET:HE1       | 4:D:96:GLU:HG2       | 1.71                     | 0.71              |
| 23:a:407:CLA:H192    | 23:c:506:CLA:H142    | 1.74                     | 0.70              |
| 23:A:407:CLA:H193    | 23:C:507:CLA:H101    | 1.74                     | 0.69              |
| 1:a:253[A]:GLY:HA3   | 2:b:491[A]:VAL:HG12  | 1.75                     | 0.69              |
| 1:a:253[B]:GLY:HA3   | 2:b:491[B]:VAL:HG12  | 1.75                     | 0.69              |
| 23:C:514:CLA:H202    | 34:C:521:LMG:H402    | 1.74                     | 0.69              |
| 32:B:627:LMT:H52     | 35:o:301:HTG:H4'1    | 1.76                     | 0.68              |
| 2:b:98:LEU:HB2       | 35:b:622:HTG:H7'1    | 1.74                     | 0.68              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:B:226:TYR:HA       | 2:B:231:MET:HG3      | 1.74                     | 0.68              |
| 23:c:512:CLA:H191    | 34:z:101:LMG:H241    | 1.75                     | 0.68              |
| 33:D:408[A]:LHG:H382 | 33:D:408[A]:LHG:H112 | 1.76                     | 0.68              |
| 4:D:85:MET:HE2       | 4:D:90:LEU:HD21      | 1.77                     | 0.66              |
| 23:a:407:CLA:H152    | 23:c:507:CLA:H142    | 1.76                     | 0.66              |
| 3:c:134[B]:ILE:HD13  | 23:c:512:CLA:H43     | 1.78                     | 0.66              |
| 23:c:503:CLA:H61     | 23:c:513:CLA:H42     | 1.77                     | 0.66              |
| 32:B:629:LMT:H6E     | 32:t:101:LMT:H6D     | 1.76                     | 0.65              |
| 19:z:32:ASP:O        | 19:z:36:SER:OG       | 2.12                     | 0.65              |
| 12:M:33:GLN:HB2      | 12:m:33:GLN:HG3      | 1.78                     | 0.65              |
| 3:c:213:LEU:HD13     | 23:c:507:CLA:H202    | 1.79                     | 0.65              |
| 23:d:402[A]:CLA:HHC  | 23:d:402[A]:CLA:HBB1 | 1.80                     | 0.64              |
| 2:b:482[A]:ILE:HD12  | 2:b:486[A]:LEU:HD12  | 1.80                     | 0.64              |
| 28:A:413[A]:PL9:H262 | 33:E:101[A]:LHG:H223 | 1.80                     | 0.63              |
| 23:B:615:CLA:HHC     | 23:B:615:CLA:HBB1    | 1.80                     | 0.63              |
| 1:a:192[B]:ILE:HG13  | 1:a:293[B]:MET:HE1   | 1.80                     | 0.63              |
| 2:b:482[B]:ILE:HD12  | 2:b:486[B]:LEU:HD12  | 1.80                     | 0.63              |
| 25:a:409[A]:SQD:H152 | 33:d:408[A]:LHG:H172 | 1.82                     | 0.62              |
| 19:z:9:LEU:HD13      | 19:z:54:VAL:HG11     | 1.81                     | 0.62              |
| 23:b:601:CLA:H72     | 23:b:601:CLA:H2      | 1.81                     | 0.62              |
| 23:C:507:CLA:H142    | 36:C:517[B]:DGD:HAF2 | 1.80                     | 0.62              |
| 13:O:66:VAL:HG21     | 13:O:110:MET:HE3     | 1.82                     | 0.62              |
| 23:b:610:CLA:HHC     | 23:b:610:CLA:HBB1    | 1.81                     | 0.62              |
| 23:C:507:CLA:H142    | 36:C:517[A]:DGD:HAF2 | 1.81                     | 0.62              |
| 23:c:506:CLA:CMD     | 23:c:508:CLA:HAB     | 2.30                     | 0.61              |
| 16:v:134[B]:LYS:HE2  | 26:v:202[B]:GOL:H32  | 1.81                     | 0.61              |
| 10:k:17:ILE:HD13     | 10:k:17:ILE:H        | 1.64                     | 0.61              |
| 4:d:85:MET:HE1       | 4:d:96:GLU:HG2       | 1.82                     | 0.61              |
| 26:D:402:GOL:H31     | 12:M:1:FME:HE3       | 1.82                     | 0.60              |
| 3:C:261:ARG:NH1      | 8:I:38:GLU:OE2       | 2.35                     | 0.60              |
| 23:B:616:CLA:HED2    | 23:B:616:CLA:H43     | 1.82                     | 0.60              |
| 3:c:88:LEU:HD13      | 23:c:504:CLA:HED3    | 1.84                     | 0.60              |
| 28:A:413[B]:PL9:H262 | 33:E:101[B]:LHG:H223 | 1.83                     | 0.60              |
| 23:B:615:CLA:H2      | 23:B:616:CLA:HBB2    | 1.84                     | 0.60              |
| 10:K:17:ILE:H        | 10:K:17:ILE:HD13     | 1.66                     | 0.59              |
| 25:a:409[A]:SQD:H141 | 33:d:408[A]:LHG:H152 | 1.84                     | 0.59              |
| 3:c:261:ARG:NH1      | 8:i:38:GLU:OE2       | 2.36                     | 0.59              |
| 24:b:619:BCR:H331    | 24:b:619:BCR:HC8     | 1.84                     | 0.59              |
| 36:c:519:DGD:HBH2    | 33:d:408[A]:LHG:H211 | 1.86                     | 0.58              |
| 34:z:101:LMG:H302    | 34:z:101:LMG:H141    | 1.85                     | 0.58              |
| 24:y:101:BCR:H321    | 24:y:101:BCR:HC8     | 1.85                     | 0.58              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 33:D:408[B]:LHG:H112 | 33:D:408[B]:LHG:H382 | 1.86                     | 0.58              |
| 23:C:506:CLA:CMD     | 23:C:508:CLA:HAB     | 2.33                     | 0.57              |
| 1:a:84[B]:PRO:HA     | 1:a:112[B]:TYR:CG    | 2.39                     | 0.57              |
| 3:c:338[B]:GLY:HA3   | 3:c:341[B]:LEU:O     | 2.05                     | 0.57              |
| 23:c:506:CLA:HHC     | 23:c:506:CLA:HBB1    | 1.85                     | 0.57              |
| 12:M:32:GLN:HG2      | 32:m:103:LMT:H6'2    | 1.86                     | 0.57              |
| 4:D:192[A]:THR:HG23  | 23:D:403[A]:CLA:HBC2 | 1.87                     | 0.57              |
| 1:a:15:GLU:HB2       | 32:a:416:LMT:H6'2    | 1.86                     | 0.57              |
| 24:Y:101:BCR:H321    | 24:Y:101:BCR:HC8     | 1.87                     | 0.57              |
| 26:a:417:GOL:H32     | 12:m:1:FME:HG3       | 1.85                     | 0.57              |
| 23:b:606:CLA:H72     | 24:b:619:BCR:HC7     | 1.86                     | 0.57              |
| 23:b:616:CLA:HHC     | 23:b:616:CLA:HBB1    | 1.86                     | 0.57              |
| 23:a:405[A]:CLA:H191 | 33:a:419[A]:LHG:H111 | 1.85                     | 0.57              |
| 1:a:221[B]:SER:HB2   | 4:d:139[B]:ARG:O     | 2.04                     | 0.57              |
| 26:a:418:GOL:O2      | 41:a:501:HOH:O       | 2.10                     | 0.57              |
| 31:A:416[B]:PHO:H3A  | 23:D:403[B]:CLA:H142 | 1.88                     | 0.56              |
| 35:B:623:HTG:H61     | 1:a:102:LEU:HD12     | 1.87                     | 0.56              |
| 10:K:24:VAL:HG13     | 18:Y:25:ILE:HD13     | 1.86                     | 0.56              |
| 23:c:502:CLA:C4D     | 23:c:504:CLA:H2      | 2.35                     | 0.56              |
| 1:A:84[B]:PRO:HA     | 1:A:112[B]:TYR:CG    | 2.40                     | 0.56              |
| 36:c:517[A]:DGD:HG11 | 41:c:606[A]:HOH:O    | 2.06                     | 0.56              |
| 26:a:418:GOL:O3      | 14:t:2:GLU:OE1       | 2.24                     | 0.55              |
| 23:a:405[B]:CLA:H203 | 34:d:412:LMG:H412    | 1.88                     | 0.55              |
| 3:c:82:TYR:OH        | 3:c:394[A]:GLU:OE2   | 2.24                     | 0.55              |
| 2:b:216:HIS:HE1      | 23:b:609:CLA:C1A     | 2.19                     | 0.55              |
| 2:B:498:LYS:HE3      | 4:D:20:ASP:HA        | 1.87                     | 0.55              |
| 23:c:514:CLA:HBB1    | 24:c:515:BCR:H24C    | 1.88                     | 0.55              |
| 24:B:618:BCR:H363    | 24:t:102:BCR:H19C    | 1.88                     | 0.55              |
| 26:a:418:GOL:H11     | 12:m:1:FME:HE3       | 1.88                     | 0.55              |
| 13:o:92:SER:HB3      | 13:o:131:PRO:HA      | 1.88                     | 0.55              |
| 17:X:31:ILE:HD11     | 25:X:101:SQD:H102    | 1.88                     | 0.55              |
| 19:Z:32:ASP:OD2      | 19:Z:35:ARG:HB3      | 2.07                     | 0.55              |
| 2:B:224:ARG:HD3      | 7:H:25:TRP:CE2       | 2.41                     | 0.55              |
| 1:A:227[B]:THR:HB    | 1:A:231:GLU:HG3      | 1.89                     | 0.54              |
| 2:B:357[B]:ARG:NH2   | 4:D:337:GLU:O        | 2.35                     | 0.54              |
| 24:b:619:BCR:H331    | 24:b:619:BCR:C8      | 2.37                     | 0.54              |
| 15:U:86[B]:GLU:H     | 15:U:86[B]:GLU:CD    | 2.15                     | 0.54              |
| 1:a:183[A]:MET:HA    | 23:a:404[A]:CLA:HMD1 | 1.89                     | 0.54              |
| 25:a:409[B]:SQD:H141 | 33:d:408[B]:LHG:H152 | 1.88                     | 0.54              |
| 16:v:134[A]:LYS:HE2  | 26:v:202[A]:GOL:H32  | 1.88                     | 0.54              |
| 2:b:285:ASN:O        | 2:b:289:GLN:HG2      | 2.07                     | 0.54              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 33:D:408[A]:LHG:H382 | 33:D:408[A]:LHG:H132 | 1.89                     | 0.54              |
| 13:O:42:ARG:HH12     | 26:O:302:GOL:H12     | 1.71                     | 0.54              |
| 23:C:509:CLA:HBC3    | 23:C:511:CLA:H71     | 1.89                     | 0.54              |
| 3:c:279:LEU:HD22     | 23:c:510:CLA:HED2    | 1.90                     | 0.54              |
| 23:B:613:CLA:HBB1    | 23:B:613:CLA:HMB1    | 1.88                     | 0.54              |
| 3:C:252:ILE:HG22     | 3:C:253:LEU:HD23     | 1.90                     | 0.54              |
| 23:a:405[A]:CLA:H203 | 34:d:412:LMG:H412    | 1.90                     | 0.54              |
| 3:c:406:SER:HA       | 3:c:420[B]:VAL:HG23  | 1.90                     | 0.54              |
| 28:A:413[A]:PL9:H253 | 23:D:403[A]:CLA:H141 | 1.89                     | 0.54              |
| 5:E:27:ILE:HD11      | 38:F:102:HEM:HBC2    | 1.89                     | 0.54              |
| 2:B:216:HIS:HE1      | 23:B:609:CLA:C1A     | 2.20                     | 0.53              |
| 1:a:214[B]:MET:HB3   | 28:a:413[B]:PL9:H103 | 1.90                     | 0.53              |
| 33:d:407[B]:LHG:HC62 | 11:l:15[B]:THR:HG23  | 1.91                     | 0.53              |
| 1:a:192[A]:ILE:HG13  | 1:a:293[A]:MET:HE1   | 1.90                     | 0.53              |
| 23:A:404[B]:CLA:HBB1 | 23:D:403[B]:CLA:C4B  | 2.14                     | 0.53              |
| 23:C:502:CLA:C3D     | 23:C:504:CLA:H2      | 2.39                     | 0.53              |
| 13:O:169:ASP:OD1     | 26:O:303:GOL:H12     | 2.09                     | 0.53              |
| 3:C:42:LEU:HD21      | 23:C:512:CLA:H2A     | 1.91                     | 0.53              |
| 4:D:205[B]:LEU:HD13  | 31:D:401[B]:PHO:HAB  | 1.89                     | 0.53              |
| 23:B:606:CLA:H202    | 25:a:411:SQD:H302    | 1.91                     | 0.53              |
| 23:b:609:CLA:HMD1    | 7:h:27:THR:HB        | 1.90                     | 0.53              |
| 23:c:511:CLA:HBB1    | 23:c:511:CLA:HMB1    | 1.91                     | 0.52              |
| 26:D:402:GOL:O2      | 41:D:501:HOH:O       | 2.19                     | 0.52              |
| 16:v:78:ASN:OD1      | 16:v:96:ARG:NH1      | 2.35                     | 0.52              |
| 5:E:57:ALA:HB3       | 5:E:60:GLN:HG2       | 1.91                     | 0.52              |
| 1:a:188[B]:ALA:HB2   | 1:a:328[B]:MET:HB2   | 1.91                     | 0.52              |
| 3:c:286:ALA:HB2      | 23:c:503:CLA:HMD1    | 1.90                     | 0.52              |
| 2:b:29:LEU:HD23      | 25:b:620:SQD:H201    | 1.90                     | 0.52              |
| 24:C:515:BCR:H352    | 34:C:521:LMG:H352    | 1.91                     | 0.52              |
| 28:A:413[A]:PL9:H472 | 4:D:39:PRO:HD3       | 1.92                     | 0.52              |
| 28:A:413[B]:PL9:H472 | 4:D:39:PRO:HD3       | 1.92                     | 0.52              |
| 28:A:413[B]:PL9:H253 | 23:D:403[B]:CLA:H141 | 1.90                     | 0.52              |
| 2:b:379:ALA:HA       | 2:b:390:TYR:HB3      | 1.92                     | 0.52              |
| 3:C:325:GLY:O        | 15:U:51:LYS:NZ       | 2.38                     | 0.52              |
| 3:c:338[A]:GLY:HA3   | 3:c:341[A]:LEU:O     | 2.10                     | 0.52              |
| 23:a:404[B]:CLA:HBB1 | 23:d:403[B]:CLA:C4B  | 2.15                     | 0.52              |
| 1:A:84[A]:PRO:HA     | 1:A:112[A]:TYR:CG    | 2.44                     | 0.52              |
| 2:B:224:ARG:HD3      | 7:H:25:TRP:CD2       | 2.44                     | 0.52              |
| 2:b:233:ASN:O        | 2:b:236:THR:HG22     | 2.10                     | 0.52              |
| 25:l:101:SQD:H462    | 25:l:101:SQD:H1      | 1.91                     | 0.52              |
| 5:E:77:GLU:O         | 5:E:81:GLU:HG2       | 2.10                     | 0.51              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 3:c:41:ARG:NH1       | 23:c:512:CLA:HMD1    | 2.24                     | 0.51              |
| 18:y:20:ALA:O        | 18:y:24:MET:HG2      | 2.11                     | 0.51              |
| 33:A:418[A]:LHG:H361 | 23:B:613:CLA:H51     | 1.92                     | 0.51              |
| 2:B:357[A]:ARG:HH12  | 26:B:622:GOL:H32     | 1.75                     | 0.51              |
| 5:E:20:TRP:CD1       | 9:J:7:ILE:HD12       | 2.45                     | 0.51              |
| 13:O:42:ARG:O        | 13:O:241:ALA:HA      | 2.11                     | 0.51              |
| 29:a:414:UNL:O6      | 41:a:502:HOH:O       | 2.19                     | 0.51              |
| 3:c:42:LEU:HD21      | 23:c:512:CLA:H2A     | 1.92                     | 0.51              |
| 1:A:82[B]:VAL:HB     | 1:A:174[B]:LEU:HB2   | 1.93                     | 0.51              |
| 4:D:24:ARG:HD3       | 17:X:37:VAL:HG22     | 1.93                     | 0.51              |
| 33:d:408[B]:LHG:H342 | 33:d:408[B]:LHG:H151 | 1.93                     | 0.51              |
| 1:A:227[A]:THR:HB    | 1:A:231:GLU:HG3      | 1.92                     | 0.51              |
| 1:A:188[B]:ALA:HB2   | 1:A:328[B]:MET:HB2   | 1.93                     | 0.51              |
| 23:a:405[B]:CLA:H191 | 33:a:419[B]:LHG:H111 | 1.91                     | 0.51              |
| 4:d:85:MET:CE        | 4:d:96:GLU:HG2       | 2.40                     | 0.51              |
| 20:R:18:TRP:O        | 20:R:22:ASN:ND2      | 2.38                     | 0.51              |
| 5:E:73:LYS:NZ        | 5:E:77:GLU:OE2       | 2.42                     | 0.50              |
| 26:b:628:GOL:O3      | 26:b:628:GOL:O1      | 2.26                     | 0.50              |
| 4:D:323[A]:GLU:O     | 26:D:413:GOL:O2      | 2.29                     | 0.50              |
| 33:D:408[B]:LHG:H382 | 33:D:408[B]:LHG:H132 | 1.94                     | 0.50              |
| 2:b:145:LEU:HD22     | 23:b:604:CLA:H162    | 1.93                     | 0.50              |
| 10:k:23:ASP:OD2      | 18:y:21:GLN:NE2      | 2.45                     | 0.50              |
| 23:C:502:CLA:C4D     | 23:C:504:CLA:H2      | 2.41                     | 0.50              |
| 36:c:519:DGD:HBH2    | 33:d:408[B]:LHG:H211 | 1.93                     | 0.50              |
| 13:o:205:ASP:OD2     | 13:o:207:ARG:NH2     | 2.44                     | 0.50              |
| 15:u:10[A]:VAL:HG12  | 41:u:243:HOH:O       | 2.11                     | 0.50              |
| 32:e:101:LMT:H6'1    | 6:f:43:ILE:HG12      | 1.92                     | 0.50              |
| 1:A:183[B]:MET:HA    | 23:A:404[B]:CLA:HMD1 | 1.92                     | 0.50              |
| 16:v:126:LEU:HB3     | 16:v:129:LYS:HB2     | 1.93                     | 0.50              |
| 1:A:102:LEU:HD12     | 35:b:625:HTG:H61     | 1.94                     | 0.50              |
| 33:a:419[B]:LHG:HC31 | 5:e:9:PRO:HA         | 1.92                     | 0.50              |
| 4:D:191:TRP:CE3      | 4:D:289:LEU:HD11     | 2.47                     | 0.50              |
| 9:J:2:SER:N          | 41:J:201:HOH:O       | 2.44                     | 0.50              |
| 25:a:409[A]:SQD:H321 | 23:c:509:CLA:H102    | 1.93                     | 0.50              |
| 2:B:357[A]:ARG:HH12  | 26:B:622:GOL:C3      | 2.25                     | 0.49              |
| 12:M:20:VAL:HG22     | 12:m:20:VAL:HG11     | 1.93                     | 0.49              |
| 31:a:415[A]:PHO:HBC3 | 4:d:279:LEU:HD22     | 1.93                     | 0.49              |
| 18:y:31:ALA:O        | 18:y:35:ILE:HG13     | 2.11                     | 0.49              |
| 23:A:406[B]:CLA:HHC  | 23:A:406[B]:CLA:HBB1 | 1.94                     | 0.49              |
| 1:a:221[A]:SER:HB2   | 4:d:139[A]:ARG:O     | 2.12                     | 0.49              |
| 33:a:419[A]:LHG:HC31 | 5:e:9:PRO:HA         | 1.92                     | 0.49              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 4:D:192[B]:THR:HG23  | 23:D:403[B]:CLA:HBC2 | 1.93                     | 0.49              |
| 1:a:334[B]:ARG:NH2   | 41:a:504[B]:HOH:O    | 2.44                     | 0.49              |
| 23:a:404[A]:CLA:H201 | 33:d:407[A]:LHG:H161 | 1.95                     | 0.49              |
| 23:B:605:CLA:HHC     | 23:B:605:CLA:HBB1    | 1.95                     | 0.49              |
| 23:B:615:CLA:H2      | 23:B:616:CLA:CBB     | 2.42                     | 0.49              |
| 31:a:415[B]:PHO:HHD  | 31:a:415[B]:PHO:HBC2 | 1.95                     | 0.49              |
| 34:c:520:LMG:H181    | 10:k:27:VAL:HG11     | 1.95                     | 0.49              |
| 33:d:407[A]:LHG:HC62 | 11:l:15[A]:THR:HG23  | 1.95                     | 0.49              |
| 1:a:227[B]:THR:HB    | 1:a:231:GLU:HG3      | 1.95                     | 0.49              |
| 31:a:406[B]:PHO:HAB  | 4:d:205[B]:LEU:HD13  | 1.94                     | 0.49              |
| 3:C:95:LEU:HD21      | 23:C:502:CLA:OBD     | 2.13                     | 0.49              |
| 3:C:203:THR:O        | 3:C:235:GLY:HA3      | 2.12                     | 0.49              |
| 3:C:406:SER:HA       | 3:C:420[B]:VAL:HG23  | 1.95                     | 0.49              |
| 23:C:503:CLA:HBD     | 23:C:503:CLA:HAA1    | 1.94                     | 0.49              |
| 23:C:511:CLA:H112    | 23:C:511:CLA:H152    | 1.49                     | 0.49              |
| 2:B:36[B]:SER:OG     | 24:B:618:BCR:H362    | 2.13                     | 0.48              |
| 2:B:70:GLY:HA2       | 2:B:178:VAL:HG21     | 1.94                     | 0.48              |
| 5:E:9:PRO:HA         | 33:E:101[B]:LHG:HC31 | 1.95                     | 0.48              |
| 31:A:416[A]:PHO:H3A  | 23:D:403[A]:CLA:H142 | 1.94                     | 0.48              |
| 23:c:502:CLA:C3D     | 23:c:504:CLA:H2      | 2.43                     | 0.48              |
| 33:d:408[A]:LHG:C38  | 33:d:408[A]:LHG:H122 | 2.44                     | 0.48              |
| 23:b:604:CLA:H42     | 23:b:605:CLA:H2      | 1.96                     | 0.48              |
| 3:c:363:GLY:O        | 3:c:367:GLU:HG2      | 2.14                     | 0.48              |
| 7:h:38:PHE:HB2       | 24:h:101:BCR:C10     | 2.43                     | 0.48              |
| 3:c:78:GLU:OE2       | 16:v:106:ASN:ND2     | 2.47                     | 0.48              |
| 12:m:5[B]:GLN:H      | 12:m:5[B]:GLN:NE2    | 2.11                     | 0.48              |
| 24:h:101:BCR:H331    | 24:h:101:BCR:C8      | 2.44                     | 0.48              |
| 2:b:423:LYS:HA       | 2:b:423:LYS:HD3      | 1.72                     | 0.48              |
| 26:l:103[A]:GOL:H32  | 14:t:25:GLU:HB2      | 1.95                     | 0.48              |
| 4:D:123:ILE:HD11     | 36:H:102:DGD:HAH2    | 1.95                     | 0.48              |
| 23:A:405[B]:CLA:HHC  | 23:A:405[B]:CLA:HBB1 | 1.96                     | 0.48              |
| 10:K:26:PRO:O        | 10:K:29:PRO:HD2      | 2.14                     | 0.48              |
| 3:c:31:SER:CB        | 3:c:41:ARG:HG2       | 2.44                     | 0.48              |
| 36:c:518[B]:DGD:HAF1 | 36:c:518[B]:DGD:HA81 | 1.95                     | 0.48              |
| 2:B:299:GLU:HG3      | 2:B:402:TYR:HD1      | 1.79                     | 0.48              |
| 3:C:275:SER:HB3      | 23:C:510:CLA:HED3    | 1.95                     | 0.48              |
| 33:D:407[A]:LHG:HC62 | 11:L:15[A]:THR:HG23  | 1.96                     | 0.48              |
| 23:a:404[B]:CLA:H152 | 31:a:406[B]:PHO:H52  | 1.96                     | 0.48              |
| 28:a:413[B]:PL9:H171 | 28:a:413[B]:PL9:H151 | 1.52                     | 0.48              |
| 23:c:509:CLA:H18     | 36:c:518[A]:DGD:HAT2 | 1.95                     | 0.48              |
| 2:b:224:ARG:HD3      | 7:h:25:TRP:CE2       | 2.49                     | 0.47              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:b:607:CLA:H91     | 23:b:607:CLA:H112    | 1.60                     | 0.47              |
| 1:A:192[B]:ILE:HG13  | 1:A:293[B]:MET:HE1   | 1.96                     | 0.47              |
| 2:B:188:ASP:OD2      | 2:B:194:ASN:ND2      | 2.45                     | 0.47              |
| 4:D:172:SER:HB2      | 4:D:177:ALA:HB1      | 1.96                     | 0.47              |
| 24:T:102:BCR:H321    | 24:T:102:BCR:HC8     | 1.97                     | 0.47              |
| 28:A:413[B]:PL9:H322 | 28:A:413[B]:PL9:H301 | 1.72                     | 0.47              |
| 28:a:413[B]:PL9:H351 | 6:f:25:THR:OG1       | 2.15                     | 0.47              |
| 24:b:617:BCR:H24C    | 24:b:617:BCR:H371    | 1.69                     | 0.47              |
| 36:c:517[B]:DGD:HG11 | 41:c:606[B]:HOH:O    | 2.13                     | 0.47              |
| 1:a:84[A]:PRO:HA     | 1:a:112[A]:TYR:CG    | 2.49                     | 0.47              |
| 1:a:214[A]:MET:HE2   | 1:a:255[A]:PHE:CE1   | 2.50                     | 0.47              |
| 33:d:408[A]:LHG:H342 | 33:d:408[A]:LHG:H151 | 1.97                     | 0.47              |
| 36:h:102:DGD:HB62    | 36:h:102:DGD:HB32    | 1.71                     | 0.47              |
| 23:a:404[B]:CLA:HMC3 | 4:d:182:LEU:HD13     | 1.96                     | 0.47              |
| 33:d:408[A]:LHG:H302 | 33:d:408[A]:LHG:H332 | 1.67                     | 0.47              |
| 5:e:57:ALA:HB3       | 5:e:60:GLN:HG2       | 1.96                     | 0.47              |
| 1:A:240[B]:GLY:HA3   | 14:T:29[B]:ILE:HG23  | 1.97                     | 0.47              |
| 2:B:383:PHE:CZ       | 13:O:167:GLY:HA2     | 2.50                     | 0.47              |
| 23:B:610:CLA:H122    | 23:B:615:CLA:HAA1    | 1.96                     | 0.47              |
| 8:I:35:LYS:O         | 8:I:37:LEU:N         | 2.48                     | 0.47              |
| 16:v:41:HIS:HA       | 16:v:45[B]:ILE:O     | 2.15                     | 0.47              |
| 28:a:413[A]:PL9:H171 | 28:a:413[A]:PL9:H151 | 1.58                     | 0.47              |
| 24:t:102:BCR:HC7     | 24:t:102:BCR:H331    | 1.45                     | 0.47              |
| 25:a:409[B]:SQD:H152 | 33:d:408[B]:LHG:H172 | 1.97                     | 0.46              |
| 24:t:102:BCR:HC8     | 24:t:102:BCR:H321    | 1.97                     | 0.46              |
| 24:t:102:BCR:H382    | 24:t:102:BCR:H23C    | 1.97                     | 0.46              |
| 1:A:85[B]:SER:HA     | 1:A:109[B]:GLY:HA3   | 1.97                     | 0.46              |
| 1:A:133:LEU:HD23     | 4:D:256[B]:ILE:HG12  | 1.98                     | 0.46              |
| 1:A:192[A]:ILE:HG13  | 1:A:293[A]:MET:HE1   | 1.97                     | 0.46              |
| 1:A:231:GLU:HB3      | 41:B:877:HOH:O       | 2.16                     | 0.46              |
| 3:C:75:PHE:HZ        | 3:C:105:VAL:HG21     | 1.80                     | 0.46              |
| 5:E:9:PRO:HA         | 33:E:101[A]:LHG:HC31 | 1.97                     | 0.46              |
| 13:O:25:THR:O        | 13:O:27:ARG:N        | 2.47                     | 0.46              |
| 25:a:409[B]:SQD:H321 | 23:c:509:CLA:H102    | 1.97                     | 0.46              |
| 23:b:614:CLA:H112    | 23:b:614:CLA:H72     | 1.60                     | 0.46              |
| 10:k:24:VAL:HG21     | 18:y:25:ILE:HB       | 1.97                     | 0.46              |
| 2:B:149:LEU:HG       | 23:B:606:CLA:HBB2    | 1.97                     | 0.46              |
| 1:a:183[B]:MET:HA    | 23:a:404[B]:CLA:HMD1 | 1.97                     | 0.46              |
| 1:a:309:ALA:HB3      | 16:v:1:ALA:O         | 2.16                     | 0.46              |
| 13:o:58:ASN:HD22     | 13:o:61:GLN:HG3      | 1.80                     | 0.46              |
| 1:A:28:LEU:HD12      | 25:A:411:SQD:H121    | 1.98                     | 0.46              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:B:285:ASN:O        | 2:B:289:GLN:HG2      | 2.14                     | 0.46              |
| 4:d:191:TRP:CE3      | 4:d:289:LEU:HD11     | 2.50                     | 0.46              |
| 23:d:402[A]:CLA:HBA1 | 23:d:402[A]:CLA:C4A  | 2.45                     | 0.46              |
| 25:a:409[A]:SQD:H271 | 33:d:408[A]:LHG:H141 | 1.97                     | 0.46              |
| 28:a:413[A]:PL9:H351 | 6:f:25:THR:OG1       | 2.15                     | 0.46              |
| 25:b:620:SQD:H341    | 25:b:620:SQD:H311    | 1.58                     | 0.46              |
| 5:E:12:ASP:OD1       | 9:J:4:GLY:HA3        | 2.16                     | 0.46              |
| 33:d:408[B]:LHG:H331 | 33:d:408[B]:LHG:H361 | 1.60                     | 0.46              |
| 6:f:41:GLN:OE1       | 9:j:30:GLY:HA3       | 2.16                     | 0.46              |
| 25:A:409[B]:SQD:H152 | 25:A:409[B]:SQD:H122 | 1.71                     | 0.46              |
| 16:V:126:LEU:HB3     | 16:V:129:LYS:HB2     | 1.98                     | 0.46              |
| 33:d:408[A]:LHG:H331 | 33:d:408[A]:LHG:H361 | 1.46                     | 0.46              |
| 5:E:14:ILE:HD12      | 9:J:12:VAL:HG11      | 1.98                     | 0.46              |
| 3:c:48:LYS:HG3       | 3:c:138:GLU:HG3      | 1.98                     | 0.46              |
| 24:T:102:BCR:HC7     | 24:T:102:BCR:H331    | 1.64                     | 0.46              |
| 23:b:616:CLA:H13     | 23:b:616:CLA:H102    | 1.77                     | 0.46              |
| 28:A:413[B]:PL9:H471 | 28:A:413[B]:PL9:H43  | 1.59                     | 0.45              |
| 33:A:418[A]:LHG:H171 | 23:B:613:CLA:H141    | 1.98                     | 0.45              |
| 4:D:264[A]:LYS:NZ    | 41:D:504[A]:HOH:O    | 2.49                     | 0.45              |
| 23:A:404[B]:CLA:H143 | 31:D:401[B]:PHO:H61  | 1.99                     | 0.45              |
| 1:a:188[A]:ALA:HB2   | 1:a:328[A]:MET:HB2   | 1.98                     | 0.45              |
| 33:d:408[B]:LHG:H122 | 33:d:408[B]:LHG:C38  | 2.46                     | 0.45              |
| 7:h:49:TYR:CG        | 36:h:102:DGD:HB22    | 2.52                     | 0.45              |
| 24:t:102:BCR:H11C    | 24:t:102:BCR:H341    | 1.85                     | 0.45              |
| 34:B:620:LMG:HC71    | 34:B:620:LMG:O9      | 2.16                     | 0.45              |
| 3:C:406:SER:HA       | 3:C:420[A]:VAL:HG23  | 1.98                     | 0.45              |
| 4:D:261[B]:PHE:CZ    | 33:D:407[B]:LHG:HC81 | 2.51                     | 0.45              |
| 6:F:41:GLN:OE1       | 9:J:30:GLY:HA3       | 2.16                     | 0.45              |
| 8:I:36:ASP:OD1       | 8:I:36:ASP:N         | 2.50                     | 0.45              |
| 12:m:5[B]:GLN:H      | 12:m:5[B]:GLN:CD     | 2.23                     | 0.45              |
| 24:B:619:BCR:H371    | 24:B:619:BCR:H24C    | 1.72                     | 0.45              |
| 2:b:159:THR:HA       | 2:b:181:VAL:O        | 2.17                     | 0.45              |
| 23:b:612:CLA:HBB1    | 23:b:612:CLA:HMB1    | 1.98                     | 0.45              |
| 3:c:443[A]:TRP:CE2   | 23:c:509:CLA:HMD2    | 2.52                     | 0.45              |
| 23:B:612:CLA:H61     | 23:B:612:CLA:H102    | 1.85                     | 0.45              |
| 23:C:507:CLA:H18     | 23:C:507:CLA:H152    | 1.52                     | 0.45              |
| 4:D:261[A]:PHE:CZ    | 33:D:407[A]:LHG:HC81 | 2.52                     | 0.45              |
| 2:b:36:SER:OG        | 24:b:618:BCR:H362    | 2.16                     | 0.45              |
| 3:C:146:PHE:HZ       | 23:C:513:CLA:HBB2    | 1.81                     | 0.45              |
| 4:D:85:MET:CE        | 4:D:96:GLU:HG2       | 2.42                     | 0.45              |
| 3:c:27:ASP:HB3       | 10:k:46:ARG:HG3      | 1.98                     | 0.45              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 13:O:142:PHE:HB2     | 13:O:199:LEU:HB2     | 1.99                     | 0.45              |
| 2:b:491[B]:VAL:HG13  | 4:d:136[B]:VAL:HG13  | 1.98                     | 0.45              |
| 3:c:182:PHE:HA       | 35:c:522:HTG:H61     | 1.98                     | 0.45              |
| 33:d:408[A]:LHG:H142 | 33:d:408[A]:LHG:H372 | 1.97                     | 0.45              |
| 13:o:216:GLU:CD      | 13:o:234:LYS:HD2     | 2.41                     | 0.45              |
| 23:A:405[B]:CLA:H203 | 23:A:405[B]:CLA:H162 | 1.83                     | 0.45              |
| 23:A:407:CLA:H61     | 23:A:407:CLA:H41     | 1.55                     | 0.45              |
| 28:A:413[B]:PL9:HC8  | 28:A:413[B]:PL9:H121 | 1.66                     | 0.45              |
| 3:C:286:ALA:HB2      | 23:C:503:CLA:HMD2    | 1.98                     | 0.45              |
| 36:C:518[B]:DGD:HAT1 | 36:C:519:DGD:HBE1    | 1.99                     | 0.45              |
| 4:D:273[B]:PHE:CE2   | 33:L:101[B]:LHG:H121 | 2.52                     | 0.45              |
| 1:a:153[B]:SER:CB    | 23:a:404[B]:CLA:H43  | 2.47                     | 0.45              |
| 23:c:506:CLA:H112    | 23:c:506:CLA:H72     | 1.70                     | 0.45              |
| 13:o:58:ASN:C        | 13:o:60:ARG:H        | 2.25                     | 0.45              |
| 4:D:190:ASN:HB2      | 4:D:296:TYR:CD1      | 2.52                     | 0.45              |
| 33:E:101[A]:LHG:H241 | 33:E:101[A]:LHG:HC61 | 1.83                     | 0.45              |
| 13:O:51:LEU:HB3      | 13:O:65:PHE:HB3      | 1.99                     | 0.45              |
| 3:c:215:LYS:HD3      | 3:c:221:GLU:O        | 2.16                     | 0.45              |
| 16:v:41:HIS:HA       | 16:v:45[A]:ILE:O     | 2.17                     | 0.45              |
| 19:Z:31:GLN:CD       | 19:Z:31:GLN:H        | 2.25                     | 0.45              |
| 23:B:613:CLA:H121    | 23:B:613:CLA:H162    | 1.78                     | 0.44              |
| 3:C:443[B]:TRP:CE2   | 23:C:509:CLA:HMD2    | 2.53                     | 0.44              |
| 1:a:227[A]:THR:HB    | 1:a:231:GLU:HG3      | 1.99                     | 0.44              |
| 2:b:383[A]:PHE:CZ    | 13:o:167:GLY:HA2     | 2.51                     | 0.44              |
| 23:c:510:CLA:H43     | 23:c:510:CLA:H12     | 1.86                     | 0.44              |
| 23:B:612:CLA:HBB1    | 23:B:612:CLA:HMB1    | 1.99                     | 0.44              |
| 3:C:391[B]:ARG:HA    | 3:C:391[B]:ARG:HD3   | 1.81                     | 0.44              |
| 2:b:216:HIS:CE1      | 23:b:609:CLA:NA      | 2.85                     | 0.44              |
| 3:c:203:THR:O        | 3:c:235:GLY:HA3      | 2.17                     | 0.44              |
| 4:d:126:MET:HE3      | 4:d:143[B]:ALA:O     | 2.17                     | 0.44              |
| 28:A:413[A]:PL9:H151 | 28:A:413[A]:PL9:H171 | 1.55                     | 0.44              |
| 28:A:413[A]:PL9:H322 | 28:A:413[A]:PL9:H301 | 1.76                     | 0.44              |
| 28:A:413[B]:PL9:HC8  | 28:A:413[B]:PL9:HC2  | 1.84                     | 0.44              |
| 4:D:230[A]:SER:HB2   | 41:D:566:HOH:O       | 2.16                     | 0.44              |
| 13:O:137:THR:C       | 13:O:139:SER:H       | 2.25                     | 0.44              |
| 15:U:58:VAL:HG12     | 15:U:79:LEU:HD22     | 1.98                     | 0.44              |
| 23:b:613:CLA:HBB1    | 23:b:613:CLA:HMB1    | 1.98                     | 0.44              |
| 3:c:134[B]:ILE:HD11  | 23:c:512:CLA:H71     | 1.98                     | 0.44              |
| 1:A:162[B]:PRO:HB3   | 1:A:168[B]:PHE:HA    | 2.00                     | 0.44              |
| 23:B:610:CLA:H162    | 23:B:612:CLA:O1A     | 2.18                     | 0.44              |
| 3:C:38:GLY:HA3       | 23:C:512:CLA:HMD2    | 1.98                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 3:c:130:VAL:O        | 3:c:134[A]:ILE:HG12  | 2.18                     | 0.44              |
| 34:c:501:LMG:H201    | 34:c:501:LMG:H172    | 1.80                     | 0.44              |
| 23:c:510:CLA:H91     | 23:c:510:CLA:H111    | 1.80                     | 0.44              |
| 9:j:6:ARG:NH1        | 9:j:6:ARG:HA         | 2.32                     | 0.44              |
| 1:A:131:TRP:CD2      | 1:A:131:TRP:C        | 2.94                     | 0.44              |
| 6:F:21:VAL:O         | 6:F:25:THR:HG23      | 2.17                     | 0.44              |
| 8:I:38:GLU:HG2       | 8:I:38:GLU:OXT       | 2.18                     | 0.44              |
| 1:a:214[A]:MET:HB3   | 28:a:413[A]:PL9:H103 | 1.98                     | 0.44              |
| 2:b:497:GLN:HB2      | 2:b:504:THR:HB       | 1.99                     | 0.44              |
| 23:b:609:CLA:NC      | 24:h:101:BCR:H332    | 2.33                     | 0.44              |
| 24:c:515:BCR:H15C    | 24:c:515:BCR:H351    | 1.83                     | 0.44              |
| 24:d:405:BCR:C8      | 24:d:405:BCR:H331    | 2.48                     | 0.44              |
| 13:O:39[B]:ARG:NH1   | 13:O:244:GLU:OE2     | 2.42                     | 0.44              |
| 23:b:615:CLA:H92     | 23:b:615:CLA:H61     | 1.64                     | 0.44              |
| 1:A:179[B]:THR:O     | 1:A:183[B]:MET:HG3   | 2.18                     | 0.44              |
| 7:h:62:TRP:O         | 7:h:65:LEU:HB2       | 2.17                     | 0.44              |
| 14:t:2:GLU:HG2       | 14:t:3:THR:N         | 2.33                     | 0.44              |
| 23:A:404[B]:CLA:CBD  | 23:A:405[B]:CLA:HAC2 | 2.48                     | 0.44              |
| 4:D:194:ASN:HA       | 4:D:295[B]:SER:OG    | 2.17                     | 0.44              |
| 4:D:327:ALA:HB2      | 26:D:413:GOL:H2      | 2.00                     | 0.44              |
| 24:T:102:BCR:H11C    | 24:T:102:BCR:H341    | 1.85                     | 0.44              |
| 3:c:52:ALA:HB2       | 23:c:512:CLA:HMA2    | 1.99                     | 0.44              |
| 23:d:404:CLA:H162    | 7:h:37:LEU:HD21      | 1.99                     | 0.44              |
| 23:A:404[B]:CLA:HBD  | 23:A:405[B]:CLA:HAC2 | 2.00                     | 0.43              |
| 28:A:413[B]:PL9:H171 | 28:A:413[B]:PL9:H151 | 1.52                     | 0.43              |
| 3:C:279:LEU:HD12     | 3:C:282:MET:HE3      | 1.99                     | 0.43              |
| 23:C:509:CLA:HBC2    | 33:D:408[B]:LHG:H351 | 2.00                     | 0.43              |
| 23:D:404:CLA:H3A     | 23:D:404:CLA:HBA1    | 1.84                     | 0.43              |
| 32:M:101:LMT:H6D     | 11:l:9:PRO:HA        | 2.00                     | 0.43              |
| 13:O:27:ARG:NH1      | 13:O:203:LYS:HG2     | 2.33                     | 0.43              |
| 25:a:409[B]:SQD:H302 | 23:c:509:CLA:H71     | 2.00                     | 0.43              |
| 28:a:413[A]:PL9:H28  | 33:a:419[A]:LHG:H222 | 1.99                     | 0.43              |
| 2:b:247:PHE:HB2      | 23:b:608:CLA:HBC1    | 1.99                     | 0.43              |
| 23:b:604:CLA:HBB1    | 23:b:607:CLA:HAB     | 2.00                     | 0.43              |
| 3:c:443[B]:TRP:CE2   | 23:c:509:CLA:HMD2    | 2.53                     | 0.43              |
| 34:d:412:LMG:H221    | 34:d:412:LMG:H191    | 1.68                     | 0.43              |
| 7:h:62:TRP:C         | 7:h:64:ALA:H         | 2.26                     | 0.43              |
| 24:t:102:BCR:HC8     | 24:t:102:BCR:H311    | 2.00                     | 0.43              |
| 2:B:363:PHE:HB3      | 2:B:365:SER:O        | 2.17                     | 0.43              |
| 23:B:614:CLA:H92     | 23:B:614:CLA:H61     | 1.75                     | 0.43              |
| 23:C:505:CLA:H41     | 23:C:505:CLA:H62     | 1.72                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 13:O:54:GLU:HG2      | 13:O:64:GLU:O        | 2.18                     | 0.43              |
| 1:a:259[A]:ILE:HG22  | 1:a:260[A]:PHE:CD1   | 2.53                     | 0.43              |
| 10:k:19:ASP:HB3      | 10:k:20:PRO:HD3      | 2.00                     | 0.43              |
| 15:u:58:VAL:HG12     | 15:u:79:LEU:HD22     | 2.00                     | 0.43              |
| 13:O:93:LEU:O        | 13:O:128:SER:HA      | 2.18                     | 0.43              |
| 23:a:405[B]:CLA:HMB2 | 23:d:403[B]:CLA:H122 | 2.00                     | 0.43              |
| 2:b:144:PHE:CE1      | 2:b:210:ILE:HG23     | 2.53                     | 0.43              |
| 3:c:152:LYS:HD2      | 41:c:746:HOH:O       | 2.18                     | 0.43              |
| 14:t:20:ALA:O        | 14:t:24[B]:ARG:HB3   | 2.19                     | 0.43              |
| 32:A:419:LMT:H6'2    | 32:A:419:LMT:O3'     | 2.18                     | 0.43              |
| 4:D:230[B]:SER:HB2   | 41:D:566:HOH:O       | 2.19                     | 0.43              |
| 1:a:269[B]:ARG:NE    | 4:d:222[B]:LEU:HD22  | 2.33                     | 0.43              |
| 23:a:404[B]:CLA:H203 | 23:a:404[B]:CLA:H162 | 1.85                     | 0.43              |
| 2:b:224:ARG:HH21     | 32:b:621:LMT:H1'     | 1.83                     | 0.43              |
| 28:A:413[A]:PL9:HC2  | 28:A:413[A]:PL9:HC8  | 1.71                     | 0.43              |
| 28:A:413[A]:PL9:H221 | 28:A:413[A]:PL9:H201 | 1.88                     | 0.43              |
| 2:B:160:GLY:HA2      | 2:B:163:GLY:O        | 2.17                     | 0.43              |
| 2:B:357[A]:ARG:HD2   | 41:B:779:HOH:O       | 2.18                     | 0.43              |
| 28:D:406[A]:PL9:H401 | 28:D:406[A]:PL9:H422 | 1.75                     | 0.43              |
| 5:E:18:ARG:H         | 9:J:2:SER:N          | 2.16                     | 0.43              |
| 1:a:34:GLY:HA2       | 1:a:37:MET:HB3       | 1.99                     | 0.43              |
| 2:b:314:TYR:CE2      | 2:b:316:GLY:HA3      | 2.54                     | 0.43              |
| 23:b:613:CLA:H172    | 24:b:618:BCR:H312    | 2.00                     | 0.43              |
| 34:c:521:LMG:H232    | 34:c:521:LMG:H391    | 2.00                     | 0.43              |
| 18:y:22:LEU:HA       | 18:y:25:ILE:HG22     | 1.99                     | 0.43              |
| 19:Z:33:TRP:HZ2      | 34:Z:101:LMG:HC61    | 1.84                     | 0.43              |
| 2:B:283:GLU:O        | 2:B:287:ARG:HG3      | 2.18                     | 0.43              |
| 5:E:56:TYR:HA        | 5:E:60:GLN:HE21      | 1.84                     | 0.43              |
| 1:a:121:LEU:HD11     | 23:c:506:CLA:H172    | 2.01                     | 0.43              |
| 1:a:160[B]:ILE:HD11  | 36:c:517[B]:DGD:HBT1 | 2.01                     | 0.43              |
| 2:b:383[B]:PHE:CZ    | 13:o:167:GLY:HA2     | 2.54                     | 0.43              |
| 23:c:505:CLA:ND      | 36:c:518[A]:DGD:HB32 | 2.34                     | 0.43              |
| 36:C:518[B]:DGD:HAE2 | 36:C:518[B]:DGD:HA81 | 1.91                     | 0.43              |
| 23:a:404[B]:CLA:H193 | 33:d:407[B]:LHG:H321 | 2.00                     | 0.43              |
| 26:a:417:GOL:H12     | 41:t:201:HOH:O       | 2.18                     | 0.43              |
| 25:A:409[A]:SQD:H122 | 25:A:409[A]:SQD:H152 | 1.52                     | 0.43              |
| 2:b:422:ARG:NH2      | 13:o:169:ASP:OD2     | 2.48                     | 0.43              |
| 24:B:619:BCR:H331    | 24:B:619:BCR:C8      | 2.48                     | 0.43              |
| 23:C:506:CLA:HAA1    | 23:C:506:CLA:HBD     | 2.01                     | 0.43              |
| 32:M:101:LMT:H6'2    | 12:m:32:GLN:HG2      | 2.01                     | 0.43              |
| 13:O:205:ASP:OD1     | 13:O:207:ARG:HG3     | 2.18                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:b:385:ARG:HG2      | 13:o:165:ALA:O       | 2.19                     | 0.43              |
| 23:c:513:CLA:H3A     | 23:c:513:CLA:HBA2    | 1.74                     | 0.43              |
| 23:c:513:CLA:H121    | 23:c:514:CLA:H142    | 2.01                     | 0.43              |
| 4:d:55:VAL:O         | 4:d:66:SER:HB3       | 2.19                     | 0.43              |
| 33:d:408[B]:LHG:H372 | 33:d:408[B]:LHG:H142 | 2.00                     | 0.43              |
| 13:o:120:PHE:CD1     | 13:o:235:ILE:HD13    | 2.54                     | 0.43              |
| 1:A:133:LEU:HD23     | 4:D:256[A]:ILE:HG12  | 2.00                     | 0.42              |
| 3:C:135:ARG:HA       | 3:C:135:ARG:HD2      | 1.92                     | 0.42              |
| 4:D:209[A]:LEU:C     | 4:D:209[A]:LEU:HD23  | 2.44                     | 0.42              |
| 23:D:403[B]:CLA:HAA2 | 23:D:403[B]:CLA:HBD  | 2.01                     | 0.42              |
| 14:T:20:ALA:O        | 14:T:24[B]:ARG:HB3   | 2.19                     | 0.42              |
| 1:a:85[B]:SER:HA     | 1:a:109[B]:GLY:HA3   | 2.01                     | 0.42              |
| 1:a:261[A]:GLN:HG3   | 2:b:493[A]:TRP:CH2   | 2.54                     | 0.42              |
| 24:a:408:BCR:H371    | 24:a:408:BCR:H24C    | 1.79                     | 0.42              |
| 23:b:605:CLA:H41     | 23:b:605:CLA:H62     | 1.54                     | 0.42              |
| 23:c:509:CLA:H18     | 36:c:518[B]:DGD:HAT2 | 2.00                     | 0.42              |
| 23:C:504:CLA:H62     | 23:C:504:CLA:H101    | 1.68                     | 0.42              |
| 4:D:205[A]:LEU:HD13  | 31:D:401[A]:PHO:HAB  | 2.00                     | 0.42              |
| 15:U:53:ALA:HB1      | 15:U:54:PRO:HA       | 2.01                     | 0.42              |
| 24:Y:101:BCR:HC7     | 24:Y:101:BCR:H331    | 1.82                     | 0.42              |
| 23:d:403[B]:CLA:HAA2 | 23:d:403[B]:CLA:HBD  | 2.01                     | 0.42              |
| 13:o:42:ARG:O        | 13:o:241:ALA:HA      | 2.20                     | 0.42              |
| 2:B:144:PHE:CE2      | 2:B:148[A]:LEU:HD11  | 2.55                     | 0.42              |
| 23:d:402[B]:CLA:HBB1 | 23:d:402[B]:CLA:CHC  | 2.42                     | 0.42              |
| 20:R:8:VAL:O         | 20:R:11:PRO:HD2      | 2.20                     | 0.42              |
| 23:A:404[B]:CLA:HBD  | 23:A:404[B]:CLA:HAA2 | 2.01                     | 0.42              |
| 23:A:405[A]:CLA:H203 | 23:A:405[A]:CLA:H162 | 1.76                     | 0.42              |
| 3:C:330:SER:HB3      | 13:O:100:GLY:O       | 2.18                     | 0.42              |
| 16:V:57:GLU:CD       | 16:V:57:GLU:H        | 2.27                     | 0.42              |
| 23:c:509:CLA:HBC3    | 23:c:511:CLA:H71     | 2.01                     | 0.42              |
| 23:c:513:CLA:H142    | 23:c:513:CLA:H111    | 1.91                     | 0.42              |
| 26:l:103[B]:GOL:H32  | 14:t:25:GLU:HB2      | 2.00                     | 0.42              |
| 15:u:92:VAL:HG12     | 15:u:97:ARG:HD2      | 2.02                     | 0.42              |
| 18:y:30:ILE:HD12     | 18:y:30:ILE:HA       | 1.91                     | 0.42              |
| 19:Z:7:LEU:HD23      | 19:Z:7:LEU:HA        | 1.87                     | 0.42              |
| 4:D:49:LEU:HD13      | 24:D:405:BCR:C15     | 2.48                     | 0.42              |
| 25:a:409[A]:SQD:H302 | 23:c:509:CLA:H71     | 2.00                     | 0.42              |
| 2:b:160:GLY:HA3      | 2:b:180:PRO:HB3      | 2.00                     | 0.42              |
| 19:Z:48:ILE:HD11     | 34:Z:101:LMG:H202    | 2.02                     | 0.42              |
| 1:A:82[A]:VAL:HB     | 1:A:174[A]:LEU:HB2   | 2.01                     | 0.42              |
| 28:A:413[B]:PL9:H221 | 28:A:413[B]:PL9:H201 | 1.87                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:C:509:CLA:HBC2    | 33:D:408[A]:LHG:H351 | 2.01                     | 0.42              |
| 1:a:153[B]:SER:HB3   | 23:a:404[B]:CLA:H43  | 2.01                     | 0.42              |
| 4:d:14:TRP:CD1       | 35:d:411:HTG:H61     | 2.54                     | 0.42              |
| 17:x:23:LEU:HD23     | 17:x:23:LEU:HA       | 1.86                     | 0.42              |
| 32:A:417:LMT:H6'1    | 41:A:504:HOH:O       | 2.18                     | 0.42              |
| 11:L:14:ARG:HB3      | 14:T:25[A]:GLU:HG2   | 2.01                     | 0.42              |
| 23:b:613:CLA:H111    | 23:b:613:CLA:H72     | 1.84                     | 0.42              |
| 19:Z:4:LEU:HD22      | 19:Z:57:LEU:HD11     | 2.02                     | 0.42              |
| 23:A:404[A]:CLA:HBB1 | 23:A:404[A]:CLA:HMB3 | 2.02                     | 0.42              |
| 2:B:298:LEU:HD12     | 2:B:298:LEU:HA       | 1.89                     | 0.42              |
| 23:B:602:CLA:H203    | 23:B:602:CLA:H162    | 1.75                     | 0.42              |
| 3:C:223:TRP:CG       | 3:C:224:ILE:H        | 2.36                     | 0.42              |
| 13:O:169:ASP:H       | 26:O:303:GOL:H12     | 1.84                     | 0.42              |
| 24:T:102:BCR:H24C    | 24:T:102:BCR:H371    | 1.84                     | 0.42              |
| 23:c:506:CLA:H192    | 23:c:506:CLA:H162    | 1.92                     | 0.42              |
| 23:d:402[B]:CLA:HBA1 | 23:d:402[B]:CLA:C4A  | 2.49                     | 0.42              |
| 15:u:16:LYS:NZ       | 15:u:86:GLU:O        | 2.46                     | 0.42              |
| 1:A:183[A]:MET:HA    | 23:A:404[A]:CLA:HMD1 | 2.01                     | 0.42              |
| 23:A:405[B]:CLA:C4A  | 23:A:405[B]:CLA:HBA1 | 2.49                     | 0.42              |
| 26:D:402:GOL:H11     | 12:M:1:FME:CG        | 2.40                     | 0.42              |
| 33:D:408[A]:LHG:H302 | 33:D:408[A]:LHG:H332 | 1.81                     | 0.42              |
| 16:v:134[B]:LYS:HB3  | 26:v:202[B]:GOL:H32  | 2.02                     | 0.42              |
| 35:B:621:HTG:H4'2    | 35:B:621:HTG:H7'3    | 1.83                     | 0.42              |
| 23:C:506:CLA:H111    | 23:C:506:CLA:H93     | 1.68                     | 0.42              |
| 4:D:214[B]:HIS:HA    | 28:D:406[B]:PL9:O2   | 2.20                     | 0.42              |
| 12:M:20:VAL:CG2      | 12:m:20:VAL:HG11     | 2.50                     | 0.42              |
| 24:T:102:BCR:H19C    | 24:b:618:BCR:H363    | 2.02                     | 0.42              |
| 14:t:8:PHE:CD2       | 32:t:101:LMT:H121    | 2.55                     | 0.42              |
| 1:A:243[A]:GLU:CD    | 1:A:243[A]:GLU:H     | 2.27                     | 0.41              |
| 2:B:58:GLN:C         | 2:B:329:PRO:HB3      | 2.45                     | 0.41              |
| 3:C:391[A]:ARG:NH1   | 41:C:609:HOH:O       | 2.53                     | 0.41              |
| 1:a:92[B]:HIS:HE2    | 3:c:360[B]:ASP:CG    | 2.27                     | 0.41              |
| 23:b:605:CLA:HBB1    | 23:b:605:CLA:CHC     | 2.46                     | 0.41              |
| 3:c:406:SER:HA       | 3:c:420[A]:VAL:HG23  | 2.02                     | 0.41              |
| 24:k:101:BCR:H371    | 24:k:101:BCR:H24C    | 1.65                     | 0.41              |
| 20:R:2:ASP:HB3       | 20:R:5:VAL:HG23      | 2.02                     | 0.41              |
| 2:B:201:HIS:CE1      | 23:B:603:CLA:HMB2    | 2.54                     | 0.41              |
| 2:B:216:HIS:CE1      | 23:B:609:CLA:NA      | 2.88                     | 0.41              |
| 3:C:230:LEU:HD23     | 3:C:230:LEU:HA       | 1.86                     | 0.41              |
| 1:a:105:TRP:CE2      | 1:a:110[A]:GLY:HA3   | 2.54                     | 0.41              |
| 3:c:162:GLY:HA2      | 3:c:248:GLY:HA2      | 2.02                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:c:513:CLA:HMB2    | 23:c:513:CLA:H192    | 2.02                     | 0.41              |
| 24:K:102:BCR:H24C    | 24:K:102:BCR:H371    | 1.63                     | 0.41              |
| 33:a:419[A]:LHG:H241 | 33:a:419[A]:LHG:HC61 | 1.90                     | 0.41              |
| 2:b:299:GLU:HG2      | 2:b:402:TYR:HD2      | 1.86                     | 0.41              |
| 23:b:613:CLA:H203    | 23:b:613:CLA:H161    | 1.88                     | 0.41              |
| 32:t:101:LMT:H112    | 32:t:101:LMT:H81     | 1.61                     | 0.41              |
| 34:C:521:LMG:H331    | 34:C:521:LMG:H362    | 1.84                     | 0.41              |
| 16:V:78:ASN:OD1      | 16:V:96:ARG:NH1      | 2.50                     | 0.41              |
| 24:b:619:BCR:H11C    | 24:b:619:BCR:H341    | 1.91                     | 0.41              |
| 3:c:425[A]:TRP:CD1   | 23:c:505:CLA:HMA3    | 2.54                     | 0.41              |
| 24:c:516:BCR:H24C    | 24:c:516:BCR:H371    | 1.89                     | 0.41              |
| 13:o:43:LEU:HB3      | 13:o:81:ILE:HB       | 2.02                     | 0.41              |
| 24:A:408:BCR:H24C    | 24:A:408:BCR:H371    | 1.71                     | 0.41              |
| 2:B:30:VAL:HG12      | 23:B:605:CLA:HHD     | 2.03                     | 0.41              |
| 2:B:138:MET:HE3      | 23:B:615:CLA:CHD     | 2.51                     | 0.41              |
| 23:B:614:CLA:H71     | 23:B:614:CLA:H112    | 1.52                     | 0.41              |
| 1:a:310:LYS:HD2      | 16:v:1:ALA:HB1       | 2.02                     | 0.41              |
| 23:a:404[B]:CLA:H122 | 23:a:404[B]:CLA:H161 | 1.88                     | 0.41              |
| 2:b:161:LEU:HD12     | 2:b:161:LEU:HA       | 1.84                     | 0.41              |
| 3:c:107:ASP:O        | 3:c:110:PRO:HD2      | 2.20                     | 0.41              |
| 23:d:402[A]:CLA:HHC  | 23:d:402[A]:CLA:CBB  | 2.48                     | 0.41              |
| 24:h:101:BCR:H11C    | 24:h:101:BCR:H341    | 1.97                     | 0.41              |
| 16:v:72:LEU:HD23     | 16:v:72:LEU:HA       | 1.93                     | 0.41              |
| 28:A:413[A]:PL9:H43  | 28:A:413[A]:PL9:H471 | 1.69                     | 0.41              |
| 23:a:407:CLA:H61     | 23:a:407:CLA:H41     | 1.80                     | 0.41              |
| 4:d:103:ARG:HG3      | 5:e:73:LYS:HG3       | 2.02                     | 0.41              |
| 4:d:194:ASN:HA       | 4:d:295[B]:SER:OG    | 2.20                     | 0.41              |
| 4:d:293:LEU:HD12     | 4:d:293:LEU:HA       | 1.86                     | 0.41              |
| 33:d:408[A]:LHG:H131 | 33:d:408[A]:LHG:H102 | 1.91                     | 0.41              |
| 24:h:101:BCR:H24C    | 24:h:101:BCR:H371    | 1.71                     | 0.41              |
| 2:B:314:TYR:CE2      | 2:B:316:GLY:HA3      | 2.55                     | 0.41              |
| 33:E:101[A]:LHG:O2   | 6:F:19:ARG:NH1       | 2.54                     | 0.41              |
| 8:I:2:GLU:O          | 8:I:6:ILE:HG12       | 2.20                     | 0.41              |
| 3:c:238:ILE:O        | 3:c:242:LEU:HG       | 2.20                     | 0.41              |
| 4:d:12:ARG:NE        | 4:d:12:ARG:HA        | 2.36                     | 0.41              |
| 19:z:37:LYS:HE2      | 19:z:41:PHE:HE2      | 1.85                     | 0.41              |
| 2:B:86:ILE:H         | 2:B:86:ILE:HG13      | 1.72                     | 0.41              |
| 2:B:216:HIS:CE1      | 23:B:609:CLA:C1A     | 3.03                     | 0.41              |
| 24:B:617:BCR:H15C    | 24:B:617:BCR:H351    | 1.90                     | 0.41              |
| 32:B:626:LMT:H41     | 32:B:626:LMT:H71     | 1.95                     | 0.41              |
| 3:C:279:LEU:HD22     | 23:C:510:CLA:HED2    | 2.03                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 33:a:419[B]:LHG:H241 | 33:a:419[B]:LHG:HC61 | 1.90                     | 0.41              |
| 2:b:245:VAL:HG22     | 23:b:612:CLA:H202    | 2.03                     | 0.41              |
| 3:c:240:ILE:HD13     | 3:c:240:ILE:HA       | 1.83                     | 0.41              |
| 4:d:244[B]:TYR:OH    | 4:d:264[B]:LYS:HE3   | 2.21                     | 0.41              |
| 20:R:24:LEU:N        | 20:R:25:PRO:HD2      | 2.35                     | 0.41              |
| 19:z:26:ALA:HB3      | 19:z:40:ILE:HD11     | 2.03                     | 0.41              |
| 28:A:413[A]:PL9:H451 | 17:X:28:LEU:HD11     | 2.02                     | 0.41              |
| 2:B:451:PHE:CE2      | 2:B:455:HIS:CE1      | 3.09                     | 0.41              |
| 2:B:491[A]:VAL:HG12  | 4:D:136[A]:VAL:HG13  | 2.03                     | 0.41              |
| 3:C:27:ASP:OD1       | 3:C:30:SER:OG        | 2.38                     | 0.41              |
| 36:C:518[A]:DGD:HAE2 | 36:C:518[A]:DGD:HA81 | 1.91                     | 0.41              |
| 36:C:519:DGD:HB81    | 36:C:519:DGD:HBE2    | 1.79                     | 0.41              |
| 33:D:407[B]:LHG:HC62 | 11:L:15[B]:THR:HG23  | 2.03                     | 0.41              |
| 24:H:101:BCR:H331    | 24:H:101:BCR:C8      | 2.51                     | 0.41              |
| 13:O:24:ASP:HA       | 13:O:203:LYS:HE2     | 2.03                     | 0.41              |
| 13:O:40:ILE:HD12     | 13:O:95:PHE:CD1      | 2.56                     | 0.41              |
| 13:O:130:GLN:H       | 13:O:130:GLN:CD      | 2.27                     | 0.41              |
| 18:Y:20:ALA:O        | 18:Y:24:MET:HG2      | 2.20                     | 0.41              |
| 1:a:93[A]:PHE:CD2    | 1:a:95:PRO:HD3       | 2.56                     | 0.41              |
| 1:a:162[A]:PRO:HB3   | 1:a:168[A]:PHE:HA    | 2.03                     | 0.41              |
| 28:a:413[B]:PL9:H503 | 17:x:24:THR:OG1      | 2.21                     | 0.41              |
| 3:c:257:PHE:O        | 3:c:261:ARG:HG3      | 2.21                     | 0.41              |
| 3:c:426:LEU:HD23     | 3:c:426:LEU:HA       | 1.95                     | 0.41              |
| 23:d:404:CLA:H61     | 23:d:404:CLA:H41     | 1.69                     | 0.41              |
| 34:Z:101:LMG:H141    | 34:Z:101:LMG:H111    | 1.84                     | 0.41              |
| 28:A:413[A]:PL9:HC8  | 28:A:413[A]:PL9:H121 | 1.79                     | 0.41              |
| 9:J:2:SER:HB2        | 9:J:3:GLU:H          | 1.74                     | 0.41              |
| 13:O:147:ASN:OD1     | 13:O:194:LYS:HE3     | 2.21                     | 0.41              |
| 1:a:230:THR:HG21     | 11:l:8:GLN:NE2       | 2.36                     | 0.41              |
| 23:a:405[B]:CLA:C4A  | 23:a:405[B]:CLA:HBA1 | 2.51                     | 0.41              |
| 23:a:407:CLA:H203    | 23:c:507:CLA:H101    | 2.03                     | 0.41              |
| 2:b:98:LEU:HB2       | 35:b:622:HTG:C7'     | 2.46                     | 0.41              |
| 2:b:298:LEU:HD12     | 2:b:298:LEU:HA       | 1.87                     | 0.41              |
| 23:b:606:CLA:H151    | 23:b:616:CLA:H112    | 2.02                     | 0.41              |
| 23:c:513:CLA:HBB1    | 23:c:513:CLA:HHC     | 2.03                     | 0.41              |
| 4:d:186[B]:GLN:HB2   | 23:d:403[B]:CLA:HBC1 | 2.03                     | 0.41              |
| 19:z:26:ALA:HB1      | 19:z:36:SER:HB3      | 2.02                     | 0.41              |
| 1:A:72:LEU:HD23      | 1:A:72:LEU:HA        | 1.93                     | 0.40              |
| 23:a:404[B]:CLA:CBD  | 23:d:402[B]:CLA:HAC2 | 2.51                     | 0.40              |
| 33:a:419[A]:LHG:H142 | 33:a:419[A]:LHG:H172 | 1.83                     | 0.40              |
| 2:b:149[B]:LEU:HD11  | 23:b:604:CLA:H122    | 2.02                     | 0.40              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 3:c:330:SER:HB3      | 13:o:100:GLY:O       | 2.21                     | 0.40              |
| 5:e:68:ASP:O         | 5:e:72:ALA:HB2       | 2.21                     | 0.40              |
| 25:f:102:SQD:H462    | 25:f:102:SQD:O7      | 2.21                     | 0.40              |
| 8:i:2:GLU:O          | 8:i:6:ILE:HG12       | 2.22                     | 0.40              |
| 2:B:67:ALA:HA        | 2:B:71:VAL:O         | 2.21                     | 0.40              |
| 23:C:507:CLA:HBA1    | 23:C:507:CLA:H3A     | 1.72                     | 0.40              |
| 4:D:323[B]:GLU:O     | 26:D:413:GOL:O2      | 2.39                     | 0.40              |
| 18:Y:39:LEU:HD23     | 18:Y:39:LEU:HA       | 1.90                     | 0.40              |
| 2:b:358:ARG:HB2      | 26:b:628:GOL:H31     | 2.02                     | 0.40              |
| 33:d:408[A]:LHG:H242 | 33:d:408[A]:LHG:H272 | 1.92                     | 0.40              |
| 34:B:620:LMG:H112    | 34:B:620:LMG:H141    | 1.84                     | 0.40              |
| 5:E:68:ASP:O         | 5:E:72:ALA:HB2       | 2.22                     | 0.40              |
| 2:b:58:GLN:C         | 2:b:329:PRO:HB3      | 2.46                     | 0.40              |
| 2:b:149[B]:LEU:HD21  | 23:b:604:CLA:H171    | 2.03                     | 0.40              |
| 23:c:507:CLA:HBA1    | 23:c:507:CLA:H3A     | 1.84                     | 0.40              |
| 11:l:20:GLY:O        | 11:l:24:ILE:HG12     | 2.21                     | 0.40              |
| 1:a:261[A]:GLN:HG3   | 2:b:493[A]:TRP:CZ3   | 2.55                     | 0.40              |
| 36:c:518[A]:DGD:HBF2 | 36:c:518[A]:DGD:HBE1 | 1.91                     | 0.40              |
| 25:l:101:SQD:H381    | 32:m:103:LMT:H121    | 2.03                     | 0.40              |
| 19:Z:57:LEU:HA       | 19:Z:57:LEU:HD23     | 1.87                     | 0.40              |
| 23:A:407:CLA:H171    | 23:C:507:CLA:H121    | 2.01                     | 0.40              |
| 3:C:334[B]:PRO:HA    | 13:O:153:THR:OG1     | 2.21                     | 0.40              |
| 4:D:161:PRO:HB3      | 4:D:170:ALA:HB2      | 2.04                     | 0.40              |
| 2:b:243:ALA:HA       | 2:b:246:PHE:CE2      | 2.57                     | 0.40              |
| 23:b:612:CLA:H122    | 23:b:612:CLA:H162    | 1.91                     | 0.40              |
| 23:c:506:CLA:HBD     | 23:c:506:CLA:HAA1    | 2.03                     | 0.40              |
| 23:c:506:CLA:HMD3    | 23:c:508:CLA:HAB     | 2.04                     | 0.40              |
| 4:d:126:MET:HE3      | 4:d:143[A]:ALA:O     | 2.21                     | 0.40              |
| 24:d:405:BCR:H351    | 24:d:405:BCR:H15C    | 1.74                     | 0.40              |
| 24:t:102:BCR:H24C    | 24:t:102:BCR:H371    | 1.89                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 553/344 (161%) | 542 (98%) | 9 (2%)  | 2 (0%)   | 30          | 39  |
| 1   | a     | 552/344 (160%) | 541 (98%) | 9 (2%)  | 2 (0%)   | 30          | 39  |
| 2   | B     | 522/505 (103%) | 515 (99%) | 7 (1%)  | 0        | 100         | 100 |
| 2   | b     | 521/505 (103%) | 510 (98%) | 11 (2%) | 0        | 100         | 100 |
| 3   | C     | 546/455 (120%) | 536 (98%) | 9 (2%)  | 1 (0%)   | 44          | 55  |
| 3   | c     | 553/455 (122%) | 539 (98%) | 13 (2%) | 1 (0%)   | 44          | 55  |
| 4   | D     | 453/342 (132%) | 435 (96%) | 18 (4%) | 0        | 100         | 100 |
| 4   | d     | 454/342 (133%) | 439 (97%) | 15 (3%) | 0        | 100         | 100 |
| 5   | E     | 79/84 (94%)    | 78 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 5   | e     | 79/84 (94%)    | 79 (100%) | 0       | 0        | 100         | 100 |
| 6   | F     | 32/44 (73%)    | 32 (100%) | 0       | 0        | 100         | 100 |
| 6   | f     | 30/44 (68%)    | 30 (100%) | 0       | 0        | 100         | 100 |
| 7   | H     | 62/65 (95%)    | 60 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 7   | h     | 63/65 (97%)    | 59 (94%)  | 3 (5%)  | 1 (2%)   | 8           | 7   |
| 8   | I     | 36/38 (95%)    | 34 (94%)  | 1 (3%)  | 1 (3%)   | 4           | 3   |
| 8   | i     | 36/38 (95%)    | 32 (89%)  | 4 (11%) | 0        | 100         | 100 |
| 9   | J     | 36/39 (92%)    | 35 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 9   | j     | 37/39 (95%)    | 37 (100%) | 0       | 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     | 32/36 (89%)    | 32 (100%) | 0       | 0        | 100         | 100 |
| 12  | m     | 34/36 (94%)    | 34 (100%) | 0       | 0        | 100         | 100 |
| 13  | O     | 251/244 (103%) | 242 (96%) | 7 (3%)  | 2 (1%)   | 16          | 20  |
| 13  | o     | 249/244 (102%) | 243 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 14  | T     | 33/32 (103%)   | 33 (100%) | 0       | 0        | 100         | 100 |
| 14  | t     | 32/32 (100%)   | 32 (100%) | 0       | 0        | 100         | 100 |
| 15  | U     | 97/104 (93%)   | 92 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 15  | u     | 98/104 (94%)   | 93 (95%)  | 5 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 16  | V     | 140/137 (102%)   | 136 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 16  | v     | 140/137 (102%)   | 134 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 17  | X     | 37/40 (92%)      | 36 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 17  | x     | 36/40 (90%)      | 36 (100%)  | 0        | 0        | 100         | 100 |
| 18  | Y     | 27/30 (90%)      | 26 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 18  | y     | 27/30 (90%)      | 27 (100%)  | 0        | 0        | 100         | 100 |
| 19  | Z     | 60/62 (97%)      | 58 (97%)   | 1 (2%)   | 1 (2%)   | 7           | 7   |
| 19  | z     | 60/62 (97%)      | 59 (98%)   | 0        | 1 (2%)   | 7           | 7   |
| 20  | R     | 32/34 (94%)      | 31 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| All | All   | 6171/5384 (115%) | 6019 (98%) | 140 (2%) | 12 (0%)  | 44          | 55  |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 3   | C     | 416    | SER  |
| 8   | I     | 36     | ASP  |
| 13  | O     | 26     | ALA  |
| 3   | c     | 416    | SER  |
| 19  | Z     | 31     | GLN  |
| 19  | z     | 30     | PRO  |
| 13  | O     | 138    | THR  |
| 7   | h     | 63     | LYS  |
| 1   | a     | 259[A] | ILE  |
| 1   | a     | 259[B] | ILE  |
| 1   | A     | 259[A] | ILE  |
| 1   | A     | 259[B] | 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     | 444/279 (159%) | 440 (99%) | 4 (1%)   | 75          | 87 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | a     | 443/279 (159%) | 441 (100%) | 2 (0%)   | 86          | 93  |
| 2   | B     | 421/403 (104%) | 415 (99%)  | 6 (1%)   | 62          | 77  |
| 2   | b     | 420/403 (104%) | 408 (97%)  | 12 (3%)  | 37          | 54  |
| 3   | C     | 430/356 (121%) | 422 (98%)  | 8 (2%)   | 52          | 69  |
| 3   | c     | 436/356 (122%) | 426 (98%)  | 10 (2%)  | 45          | 63  |
| 4   | D     | 368/277 (133%) | 365 (99%)  | 3 (1%)   | 79          | 89  |
| 4   | d     | 369/277 (133%) | 362 (98%)  | 7 (2%)   | 52          | 69  |
| 5   | E     | 72/73 (99%)    | 71 (99%)   | 1 (1%)   | 62          | 77  |
| 5   | e     | 72/73 (99%)    | 71 (99%)   | 1 (1%)   | 62          | 77  |
| 6   | F     | 28/38 (74%)    | 28 (100%)  | 0        | 100         | 100 |
| 6   | f     | 26/38 (68%)    | 26 (100%)  | 0        | 100         | 100 |
| 7   | H     | 54/54 (100%)   | 52 (96%)   | 2 (4%)   | 29          | 43  |
| 7   | h     | 55/54 (102%)   | 53 (96%)   | 2 (4%)   | 30          | 44  |
| 8   | I     | 34/34 (100%)   | 32 (94%)   | 2 (6%)   | 16          | 23  |
| 8   | i     | 34/34 (100%)   | 33 (97%)   | 1 (3%)   | 37          | 54  |
| 9   | J     | 26/27 (96%)    | 24 (92%)   | 2 (8%)   | 10          | 14  |
| 9   | j     | 26/27 (96%)    | 25 (96%)   | 1 (4%)   | 28          | 42  |
| 10  | K     | 30/30 (100%)   | 26 (87%)   | 4 (13%)  | 3           | 3   |
| 10  | k     | 30/30 (100%)   | 27 (90%)   | 3 (10%)  | 6           | 8   |
| 11  | L     | 36/35 (103%)   | 36 (100%)  | 0        | 100         | 100 |
| 11  | l     | 36/35 (103%)   | 35 (97%)   | 1 (3%)   | 38          | 55  |
| 12  | M     | 30/32 (94%)    | 27 (90%)   | 3 (10%)  | 6           | 8   |
| 12  | m     | 32/32 (100%)   | 30 (94%)   | 2 (6%)   | 15          | 21  |
| 13  | O     | 216/207 (104%) | 211 (98%)  | 5 (2%)   | 45          | 63  |
| 13  | o     | 213/207 (103%) | 206 (97%)  | 7 (3%)   | 33          | 48  |
| 14  | T     | 32/28 (114%)   | 28 (88%)   | 4 (12%)  | 3           | 4   |
| 14  | t     | 31/28 (111%)   | 31 (100%)  | 0        | 100         | 100 |
| 15  | U     | 86/89 (97%)    | 84 (98%)   | 2 (2%)   | 45          | 63  |
| 15  | u     | 87/89 (98%)    | 85 (98%)   | 2 (2%)   | 45          | 63  |
| 16  | V     | 123/117 (105%) | 122 (99%)  | 1 (1%)   | 79          | 89  |
| 16  | v     | 123/117 (105%) | 119 (97%)  | 4 (3%)   | 33          | 48  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 17  | X     | 32/33 (97%)      | 32 (100%)  | 0        | 100         | 100 |
| 17  | x     | 31/33 (94%)      | 31 (100%)  | 0        | 100         | 100 |
| 18  | Y     | 22/23 (96%)      | 21 (96%)   | 1 (4%)   | 23          | 34  |
| 18  | y     | 22/23 (96%)      | 19 (86%)   | 3 (14%)  | 3           | 3   |
| 19  | Z     | 52/52 (100%)     | 50 (96%)   | 2 (4%)   | 28          | 42  |
| 19  | z     | 52/52 (100%)     | 44 (85%)   | 8 (15%)  | 2           | 2   |
| 20  | R     | 29/29 (100%)     | 27 (93%)   | 2 (7%)   | 13          | 18  |
| All | All   | 5103/4403 (116%) | 4985 (98%) | 118 (2%) | 44          | 63  |

All (118) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 243[A] | GLU  |
| 1   | A     | 243[B] | GLU  |
| 1   | A     | 244[A] | GLU  |
| 1   | A     | 244[B] | GLU  |
| 2   | B     | 161    | LEU  |
| 2   | B     | 294    | SER  |
| 2   | B     | 299    | GLU  |
| 2   | B     | 389    | LYS  |
| 2   | B     | 419    | SER  |
| 2   | B     | 472    | ARG  |
| 3   | C     | 24     | THR  |
| 3   | C     | 29     | GLU  |
| 3   | C     | 30     | SER  |
| 3   | C     | 142    | GLU  |
| 3   | C     | 289    | PHE  |
| 3   | C     | 315[A] | MET  |
| 3   | C     | 315[B] | MET  |
| 3   | C     | 471    | SER  |
| 4   | D     | 259[A] | ILE  |
| 4   | D     | 259[B] | ILE  |
| 4   | D     | 338    | ASN  |
| 5   | E     | 71     | GLU  |
| 7   | H     | 12     | ARG  |
| 7   | H     | 43     | LEU  |
| 8   | I     | 33     | LYS  |
| 8   | I     | 34     | ARG  |
| 9   | J     | 6      | ARG  |
| 9   | J     | 9      | LEU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 10  | K     | 10     | LYS  |
| 10  | K     | 17     | ILE  |
| 10  | K     | 19     | ASP  |
| 10  | K     | 27     | VAL  |
| 12  | M     | 16[A]  | LEU  |
| 12  | M     | 16[B]  | LEU  |
| 12  | M     | 20     | VAL  |
| 13  | O     | 49     | THR  |
| 13  | O     | 55     | GLU  |
| 13  | O     | 87     | VAL  |
| 13  | O     | 98[A]  | GLU  |
| 13  | O     | 98[B]  | GLU  |
| 14  | T     | 25[A]  | GLU  |
| 14  | T     | 25[B]  | GLU  |
| 14  | T     | 30[A]  | THR  |
| 14  | T     | 30[B]  | THR  |
| 15  | U     | 10     | VAL  |
| 15  | U     | 70     | ARG  |
| 16  | V     | 15     | GLU  |
| 18  | Y     | 30     | ILE  |
| 1   | a     | 13     | LEU  |
| 1   | a     | 35     | VAL  |
| 2   | b     | 63     | LEU  |
| 2   | b     | 128    | THR  |
| 2   | b     | 161    | LEU  |
| 2   | b     | 223    | GLN  |
| 2   | b     | 245    | VAL  |
| 2   | b     | 298    | LEU  |
| 2   | b     | 315    | ILE  |
| 2   | b     | 362    | PHE  |
| 2   | b     | 486[A] | LEU  |
| 2   | b     | 486[B] | LEU  |
| 2   | b     | 491[A] | VAL  |
| 2   | b     | 491[B] | VAL  |
| 3   | c     | 19     | ASN  |
| 3   | c     | 142    | GLU  |
| 3   | c     | 152    | LYS  |
| 3   | c     | 158    | THR  |
| 3   | c     | 240    | ILE  |
| 3   | c     | 255    | THR  |
| 3   | c     | 289    | PHE  |
| 3   | c     | 315[A] | MET  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 3   | c     | 315[B] | MET  |
| 3   | c     | 416    | SER  |
| 4   | d     | 26     | ARG  |
| 4   | d     | 230[A] | SER  |
| 4   | d     | 230[B] | SER  |
| 4   | d     | 259[A] | ILE  |
| 4   | d     | 259[B] | ILE  |
| 4   | d     | 272[A] | LEU  |
| 4   | d     | 272[B] | LEU  |
| 5   | e     | 71     | GLU  |
| 7   | h     | 61     | SER  |
| 7   | h     | 65     | LEU  |
| 8   | i     | 33     | LYS  |
| 9   | j     | 9      | LEU  |
| 10  | k     | 10     | LYS  |
| 10  | k     | 17     | ILE  |
| 10  | k     | 24     | VAL  |
| 11  | l     | 2      | GLU  |
| 12  | m     | 16[A]  | LEU  |
| 12  | m     | 16[B]  | LEU  |
| 13  | o     | 25     | THR  |
| 13  | o     | 36     | GLN  |
| 13  | o     | 37     | THR  |
| 13  | o     | 58     | ASN  |
| 13  | o     | 69     | LYS  |
| 13  | o     | 118    | LEU  |
| 13  | o     | 194    | LYS  |
| 15  | u     | 10[A]  | VAL  |
| 15  | u     | 10[B]  | VAL  |
| 16  | v     | 15     | GLU  |
| 16  | v     | 24     | LYS  |
| 16  | v     | 85     | GLU  |
| 16  | v     | 109    | GLU  |
| 18  | y     | 18     | VAL  |
| 18  | y     | 19     | ILE  |
| 18  | y     | 45     | ASN  |
| 19  | Z     | 3      | ILE  |
| 19  | Z     | 31     | GLN  |
| 20  | R     | 4      | ARG  |
| 20  | R     | 29     | LYS  |
| 19  | z     | 2      | THR  |
| 19  | z     | 3      | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | z     | 4   | LEU  |
| 19  | z     | 7   | LEU  |
| 19  | z     | 20  | VAL  |
| 19  | z     | 32  | ASP  |
| 19  | z     | 34  | ASP  |
| 19  | z     | 42  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 44  | ASN  |
| 3   | C     | 322 | GLN  |
| 3   | C     | 415 | ASN  |
| 1   | a     | 75  | ASN  |
| 2   | b     | 331 | ASN  |
| 3   | c     | 19  | ASN  |
| 3   | c     | 155 | ASN  |
| 3   | c     | 201 | ASN  |
| 10  | k     | 40  | GLN  |
| 11  | l     | 8   | GLN  |
| 13  | o     | 58  | ASN  |
| 16  | v     | 86  | GLN  |

### 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 |
| 8   | FME  | i     | 1   | 8    | 8,9,10       | 0.68 | 0        | 8,9,11      | 1.19 | 1 (12%)  |
| 8   | FME  | I     | 1   | 8    | 8,9,10       | 0.66 | 0        | 8,9,11      | 1.21 | 1 (12%)  |
| 14  | FME  | t     | 1   | 14   | 8,9,10       | 0.79 | 0        | 8,9,11      | 1.26 | 1 (12%)  |
| 12  | FME  | m     | 1   | 12   | 8,9,10       | 0.55 | 0        | 8,9,11      | 1.38 | 1 (12%)  |
| 12  | FME  | M     | 1   | 12   | 8,9,10       | 0.57 | 0        | 8,9,11      | 1.29 | 1 (12%)  |
| 14  | FME  | T     | 1   | 14   | 8,9,10       | 0.60 | 0        | 8,9,11      | 1.76 | 3 (37%)  |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 8   | FME  | i     | 1   | 8    | -       | 2/7/9/11 | -     |
| 8   | FME  | I     | 1   | 8    | -       | 1/7/9/11 | -     |
| 14  | FME  | t     | 1   | 14   | -       | 0/7/9/11 | -     |
| 12  | FME  | m     | 1   | 12   | -       | 2/7/9/11 | -     |
| 12  | FME  | M     | 1   | 12   | -       | 1/7/9/11 | -     |
| 14  | FME  | T     | 1   | 14   | -       | 0/7/9/11 | -     |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | T     | 1   | FME  | CB-CA-N | -2.74 | 105.53      | 110.52   |
| 14  | t     | 1   | FME  | O-C-CA  | -2.41 | 118.58      | 124.77   |
| 12  | m     | 1   | FME  | O1-CN-N | -2.40 | 119.12      | 125.32   |
| 14  | T     | 1   | FME  | CA-N-CN | 2.35  | 126.44      | 122.82   |
| 8   | I     | 1   | FME  | O-C-CA  | -2.23 | 119.03      | 124.77   |
| 12  | M     | 1   | FME  | O-C-CA  | -2.16 | 119.21      | 124.77   |
| 8   | i     | 1   | FME  | O-C-CA  | -2.09 | 119.40      | 124.77   |
| 14  | T     | 1   | FME  | C-CA-N  | 2.07  | 113.50      | 109.50   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms     |
|-----|-------|-----|------|-----------|
| 8   | I     | 1   | FME  | O-C-CA-CB |
| 12  | M     | 1   | FME  | O-C-CA-CB |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 12  | m     | 1   | FME  | O-C-CA-CB   |
| 12  | m     | 1   | FME  | O1-CN-N-CA  |
| 8   | i     | 1   | FME  | CA-CB-CG-SD |
| 8   | i     | 1   | FME  | C-CA-CB-CG  |

There are no ring outliers.

2 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | m     | 1   | FME  | 2       | 0            |
| 12  | M     | 1   | FME  | 3       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 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 | $\# Z  > 2$ |
| 28  | PL9  | a     | 413[A] | -    | 55,55,55     | 0.68 | 2 (3%)      | 68,69,69    | 2.03 | 23 (33%)    |
| 23  | CLA  | B     | 611    | -    | 63,73,73     | 2.64 | 17 (26%)    | 74,113,113  | 2.96 | 27 (36%)    |
| 23  | CLA  | A     | 406[A] | 41   | 63,73,73     | 1.98 | 16 (25%)    | 74,113,113  | 2.67 | 30 (40%)    |
| 23  | CLA  | C     | 505    | 41   | 63,73,73     | 2.05 | 17 (26%)    | 74,113,113  | 2.73 | 30 (40%)    |
| 23  | CLA  | d     | 403[A] | -    | 63,73,73     | 1.99 | 16 (25%)    | 74,113,113  | 2.65 | 29 (39%)    |
| 26  | GOL  | l     | 103[A] | -    | 5,5,5        | 0.98 | 0           | 5,5,5       | 1.05 | 1 (20%)     |
| 23  | CLA  | B     | 614    | -    | 63,73,73     | 2.00 | 15 (23%)    | 74,113,113  | 2.88 | 30 (40%)    |
| 24  | BCR  | c     | 516    | -    | 41,41,41     | 1.03 | 1 (2%)      | 56,56,56    | 1.39 | 9 (16%)     |
| 25  | SQD  | b     | 620    | -    | 52,54,54     | 1.00 | 2 (3%)      | 62,65,65    | 1.68 | 10 (16%)    |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | BCR  | B     | 617    | -    | 41,41,41     | 1.06 | 1 (2%)   | 56,56,56    | 1.46 | 8 (14%)  |
| 26  | GOL  | c     | 526[B] | -    | 5,5,5        | 1.01 | 0        | 5,5,5       | 1.06 | 0        |
| 26  | GOL  | o     | 303    | -    | 5,5,5        | 1.22 | 0        | 5,5,5       | 1.04 | 0        |
| 28  | PL9  | D     | 406[A] | -    | 55,55,55     | 0.65 | 1 (1%)   | 68,69,69    | 1.61 | 17 (25%) |
| 32  | LMT  | a     | 416    | -    | 36,36,36     | 0.98 | 2 (5%)   | 47,47,47    | 1.06 | 2 (4%)   |
| 23  | CLA  | b     | 614    | -    | 63,73,73     | 2.02 | 16 (25%) | 74,113,113  | 2.81 | 28 (37%) |
| 35  | HTG  | o     | 301    | -    | 19,19,19     | 1.04 | 2 (10%)  | 23,24,24    | 1.50 | 4 (17%)  |
| 32  | LMT  | t     | 101    | -    | 26,26,36     | 0.91 | 2 (7%)   | 31,31,47    | 1.31 | 3 (9%)   |
| 35  | HTG  | b     | 623    | -    | 19,19,19     | 0.96 | 1 (5%)   | 23,24,24    | 1.72 | 3 (13%)  |
| 23  | CLA  | D     | 404    | -    | 63,73,73     | 2.12 | 16 (25%) | 74,113,113  | 2.74 | 31 (41%) |
| 23  | CLA  | c     | 514    | -    | 63,73,73     | 2.14 | 17 (26%) | 74,113,113  | 2.69 | 28 (37%) |
| 23  | CLA  | D     | 403[B] | -    | 63,73,73     | 2.08 | 16 (25%) | 74,113,113  | 2.79 | 28 (37%) |
| 23  | CLA  | b     | 615    | -    | 63,73,73     | 2.04 | 14 (22%) | 74,113,113  | 2.67 | 28 (37%) |
| 38  | HEM  | F     | 102    | 6,5  | 42,50,50     | 1.27 | 5 (11%)  | 46,82,82    | 1.99 | 14 (30%) |
| 36  | DGD  | c     | 517[B] | -    | 63,63,67     | 0.87 | 2 (3%)   | 77,77,81    | 1.08 | 5 (6%)   |
| 23  | CLA  | B     | 616    | -    | 63,73,73     | 2.14 | 17 (26%) | 74,113,113  | 2.80 | 26 (35%) |
| 33  | LHG  | E     | 101[B] | -    | 41,41,48     | 1.06 | 2 (4%)   | 44,47,54    | 1.12 | 4 (9%)   |
| 25  | SQD  | a     | 411    | -    | 52,54,54     | 1.02 | 2 (3%)   | 62,65,65    | 1.21 | 8 (12%)  |
| 25  | SQD  | a     | 409[B] | -    | 52,54,54     | 0.91 | 2 (3%)   | 62,65,65    | 1.58 | 11 (17%) |
| 24  | BCR  | y     | 101    | -    | 41,41,41     | 1.04 | 1 (2%)   | 56,56,56    | 1.71 | 12 (21%) |
| 31  | PHO  | a     | 415[B] | -    | 50,69,69     | 1.99 | 8 (16%)  | 48,99,99    | 2.00 | 11 (22%) |
| 23  | CLA  | b     | 603    | -    | 63,73,73     | 2.09 | 16 (25%) | 74,113,113  | 2.75 | 30 (40%) |
| 23  | CLA  | B     | 604    | -    | 63,73,73     | 2.03 | 18 (28%) | 74,113,113  | 2.55 | 30 (40%) |
| 23  | CLA  | B     | 607    | 41   | 63,73,73     | 2.03 | 17 (26%) | 74,113,113  | 2.82 | 29 (39%) |
| 23  | CLA  | D     | 403[A] | -    | 63,73,73     | 2.08 | 16 (25%) | 74,113,113  | 2.77 | 32 (43%) |
| 23  | CLA  | B     | 613    | -    | 63,73,73     | 1.97 | 15 (23%) | 74,113,113  | 2.75 | 28 (37%) |
| 34  | LMG  | z     | 101    | -    | 39,39,55     | 1.11 | 2 (5%)   | 47,47,63    | 1.07 | 2 (4%)   |
| 23  | CLA  | C     | 514    | -    | 63,73,73     | 2.09 | 16 (25%) | 74,113,113  | 2.67 | 27 (36%) |
| 23  | CLA  | b     | 607    | 41   | 63,73,73     | 2.03 | 17 (26%) | 74,113,113  | 2.65 | 29 (39%) |
| 26  | GOL  | D     | 402    | -    | 5,5,5        | 1.42 | 2 (40%)  | 5,5,5       | 0.88 | 0        |
| 35  | HTG  | D     | 411    | -    | 16,16,19     | 0.95 | 1 (6%)   | 20,21,24    | 1.31 | 1 (5%)   |
| 33  | LHG  | E     | 101[A] | -    | 41,41,48     | 1.08 | 2 (4%)   | 44,47,54    | 1.12 | 3 (6%)   |
| 36  | DGD  | C     | 517[B] | -    | 63,63,67     | 0.83 | 2 (3%)   | 77,77,81    | 1.11 | 5 (6%)   |
| 25  | SQD  | a     | 409[A] | -    | 52,54,54     | 0.89 | 2 (3%)   | 62,65,65    | 1.80 | 11 (17%) |
| 35  | HTG  | d     | 411    | -    | 16,16,19     | 0.87 | 1 (6%)   | 20,21,24    | 1.41 | 1 (5%)   |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | BCR  | k     | 101    | -    | 41,41,41     | 1.08 | 1 (2%)   | 56,56,56    | 1.53 | 11 (19%) |
| 23  | CLA  | B     | 609    | -    | 63,73,73     | 2.06 | 15 (23%) | 74,113,113  | 2.62 | 28 (37%) |
| 23  | CLA  | c     | 510    | -    | 63,73,73     | 2.04 | 15 (23%) | 74,113,113  | 2.79 | 29 (39%) |
| 25  | SQD  | A     | 409[B] | -    | 52,54,54     | 0.87 | 2 (3%)   | 62,65,65    | 1.69 | 11 (17%) |
| 26  | GOL  | C     | 523[A] | -    | 5,5,5        | 1.16 | 0        | 5,5,5       | 0.94 | 0        |
| 23  | CLA  | C     | 512    | 3    | 63,73,73     | 2.11 | 18 (28%) | 74,113,113  | 2.58 | 27 (36%) |
| 23  | CLA  | c     | 505    | 41   | 63,73,73     | 2.14 | 16 (25%) | 74,113,113  | 2.68 | 30 (40%) |
| 23  | CLA  | B     | 602    | -    | 63,73,73     | 2.08 | 16 (25%) | 74,113,113  | 2.74 | 28 (37%) |
| 36  | DGD  | C     | 517[A] | -    | 63,63,67     | 0.84 | 2 (3%)   | 77,77,81    | 1.20 | 6 (7%)   |
| 23  | CLA  | b     | 601    | 41   | 63,73,73     | 2.16 | 15 (23%) | 74,113,113  | 2.70 | 28 (37%) |
| 26  | GOL  | A     | 410    | -    | 5,5,5        | 1.14 | 0        | 5,5,5       | 0.86 | 0        |
| 32  | LMT  | B     | 629    | -    | 25,25,36     | 0.89 | 1 (4%)   | 30,30,47    | 1.21 | 3 (10%)  |
| 25  | SQD  | A     | 409[A] | -    | 52,54,54     | 0.86 | 2 (3%)   | 62,65,65    | 1.85 | 10 (16%) |
| 24  | BCR  | b     | 618    | -    | 41,41,41     | 1.02 | 1 (2%)   | 56,56,56    | 1.26 | 6 (10%)  |
| 28  | PL9  | D     | 406[B] | -    | 55,55,55     | 0.67 | 2 (3%)   | 68,69,69    | 1.65 | 17 (25%) |
| 33  | LHG  | b     | 629[A] | -    | 48,48,48     | 0.84 | 3 (6%)   | 51,54,54    | 1.05 | 4 (7%)   |
| 24  | BCR  | H     | 101    | -    | 41,41,41     | 1.05 | 1 (2%)   | 56,56,56    | 1.44 | 8 (14%)  |
| 24  | BCR  | K     | 102    | -    | 41,41,41     | 1.09 | 1 (2%)   | 56,56,56    | 1.48 | 11 (19%) |
| 24  | BCR  | b     | 617    | -    | 41,41,41     | 1.05 | 1 (2%)   | 56,56,56    | 1.44 | 9 (16%)  |
| 25  | SQD  | f     | 102    | -    | 41,43,54     | 1.15 | 2 (4%)   | 51,54,65    | 1.59 | 10 (19%) |
| 23  | CLA  | C     | 506    | -    | 63,73,73     | 2.02 | 16 (25%) | 74,113,113  | 2.74 | 29 (39%) |
| 35  | HTG  | B     | 623    | -    | 19,19,19     | 0.97 | 2 (10%)  | 23,24,24    | 1.28 | 3 (13%)  |
| 23  | CLA  | c     | 504    | -    | 63,73,73     | 2.04 | 17 (26%) | 74,113,113  | 2.71 | 27 (36%) |
| 24  | BCR  | D     | 405    | -    | 41,41,41     | 1.12 | 1 (2%)   | 56,56,56    | 1.81 | 15 (26%) |
| 23  | CLA  | c     | 507    | -    | 63,73,73     | 2.07 | 16 (25%) | 74,113,113  | 2.67 | 29 (39%) |
| 35  | HTG  | V     | 202    | -    | 11,11,19     | 0.31 | 0        | 15,15,24    | 1.25 | 1 (6%)   |
| 23  | CLA  | A     | 407    | -    | 63,73,73     | 2.02 | 17 (26%) | 74,113,113  | 2.78 | 32 (43%) |
| 23  | CLA  | a     | 407    | -    | 63,73,73     | 2.02 | 15 (23%) | 74,113,113  | 2.83 | 29 (39%) |
| 23  | CLA  | B     | 615    | -    | 63,73,73     | 2.08 | 16 (25%) | 74,113,113  | 2.80 | 30 (40%) |
| 35  | HTG  | c     | 522    | -    | 19,19,19     | 0.86 | 1 (5%)   | 23,24,24    | 1.40 | 1 (4%)   |
| 23  | CLA  | b     | 602    | -    | 63,73,73     | 2.07 | 16 (25%) | 74,113,113  | 2.87 | 34 (45%) |
| 23  | CLA  | B     | 603    | -    | 63,73,73     | 2.05 | 15 (23%) | 74,113,113  | 2.85 | 29 (39%) |
| 26  | GOL  | a     | 418    | -    | 5,5,5        | 1.33 | 1 (20%)  | 5,5,5       | 1.03 | 0        |
| 26  | GOL  | B     | 622    | -    | 5,5,5        | 0.88 | 0        | 5,5,5       | 1.24 | 1 (20%)  |
| 23  | CLA  | A     | 404[A] | -    | 63,73,73     | 2.06 | 15 (23%) | 74,113,113  | 2.77 | 30 (40%) |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | CLA  | d     | 402[B] | 41     | 63,73,73     | 2.12 | 15 (23%) | 74,113,113  | 2.69 | 28 (37%) |
| 23  | CLA  | B     | 612    | -      | 63,73,73     | 2.09 | 17 (26%) | 74,113,113  | 2.72 | 29 (39%) |
| 23  | CLA  | b     | 605    | -      | 63,73,73     | 1.98 | 17 (26%) | 74,113,113  | 2.80 | 27 (36%) |
| 26  | GOL  | o     | 304    | -      | 5,5,5        | 1.07 | 1 (20%)  | 5,5,5       | 1.16 | 0        |
| 26  | GOL  | b     | 624    | -      | 5,5,5        | 1.25 | 1 (20%)  | 5,5,5       | 0.88 | 0        |
| 34  | LMG  | C     | 520    | -      | 51,51,55     | 0.95 | 2 (3%)   | 59,59,63    | 1.13 | 4 (6%)   |
| 26  | GOL  | C     | 523[B] | -      | 5,5,5        | 1.29 | 0        | 5,5,5       | 0.83 | 0        |
| 32  | LMT  | A     | 419    | -      | 36,36,36     | 1.02 | 2 (5%)   | 47,47,47    | 1.20 | 4 (8%)   |
| 23  | CLA  | b     | 612    | -      | 63,73,73     | 2.06 | 16 (25%) | 74,113,113  | 2.67 | 28 (37%) |
| 24  | BCR  | T     | 102    | -      | 41,41,41     | 1.06 | 1 (2%)   | 56,56,56    | 1.61 | 14 (25%) |
| 26  | GOL  | v     | 202[B] | -      | 5,5,5        | 1.16 | 0        | 5,5,5       | 0.86 | 0        |
| 27  | OEX  | A     | 412[A] | 1,3,41 | 0,15,15      | -    | -        | -           | -    | -        |
| 23  | CLA  | C     | 503    | -      | 63,73,73     | 2.13 | 16 (25%) | 74,113,113  | 2.55 | 27 (36%) |
| 24  | BCR  | d     | 405    | -      | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.99 | 17 (30%) |
| 35  | HTG  | B     | 621    | -      | 19,19,19     | 0.78 | 1 (5%)   | 23,24,24    | 1.21 | 1 (4%)   |
| 23  | CLA  | c     | 509    | -      | 63,73,73     | 2.22 | 16 (25%) | 74,113,113  | 2.58 | 25 (33%) |
| 23  | CLA  | d     | 402[A] | 41     | 63,73,73     | 2.02 | 14 (22%) | 74,113,113  | 2.71 | 28 (37%) |
| 32  | LMT  | b     | 627    | -      | 25,25,36     | 0.88 | 0        | 30,30,47    | 1.07 | 2 (6%)   |
| 30  | BCT  | A     | 415[B] | 21     | 3,3,3        | 0.54 | 0        | 2,3,3       | 0.83 | 0        |
| 24  | BCR  | A     | 408    | -      | 41,41,41     | 1.04 | 1 (2%)   | 56,56,56    | 1.41 | 8 (14%)  |
| 23  | CLA  | b     | 609    | -      | 63,73,73     | 2.08 | 15 (23%) | 74,113,113  | 2.69 | 29 (39%) |
| 33  | LHG  | A     | 418[B] | -      | 48,48,48     | 0.89 | 2 (4%)   | 51,54,54    | 1.16 | 5 (9%)   |
| 24  | BCR  | c     | 515    | -      | 41,41,41     | 1.03 | 1 (2%)   | 56,56,56    | 1.62 | 11 (19%) |
| 26  | GOL  | v     | 202[A] | -      | 5,5,5        | 1.26 | 0        | 5,5,5       | 0.88 | 0        |
| 23  | CLA  | B     | 610    | 41     | 63,73,73     | 2.05 | 16 (25%) | 74,113,113  | 2.77 | 28 (37%) |
| 33  | LHG  | b     | 629[B] | -      | 48,48,48     | 0.90 | 2 (4%)   | 51,54,54    | 1.05 | 3 (5%)   |
| 34  | LMG  | c     | 521    | -      | 51,51,55     | 1.02 | 2 (3%)   | 59,59,63    | 1.36 | 7 (11%)  |
| 25  | SQD  | A     | 411    | -      | 52,54,54     | 1.00 | 2 (3%)   | 62,65,65    | 1.21 | 7 (11%)  |
| 23  | CLA  | a     | 404[B] | -      | 63,73,73     | 2.12 | 16 (25%) | 74,113,113  | 2.72 | 29 (39%) |
| 26  | GOL  | V     | 203[B] | -      | 5,5,5        | 1.13 | 0        | 5,5,5       | 0.99 | 0        |
| 23  | CLA  | B     | 606    | -      | 63,73,73     | 1.99 | 16 (25%) | 74,113,113  | 2.91 | 29 (39%) |
| 33  | LHG  | d     | 407[B] | -      | 48,48,48     | 0.88 | 2 (4%)   | 51,54,54    | 1.14 | 5 (9%)   |
| 24  | BCR  | a     | 408    | -      | 41,41,41     | 1.05 | 1 (2%)   | 56,56,56    | 1.42 | 9 (16%)  |
| 25  | SQD  | X     | 101    | -      | 41,43,54     | 1.17 | 3 (7%)   | 51,54,65    | 2.13 | 13 (25%) |
| 34  | LMG  | d     | 412    | 39     | 51,51,55     | 0.90 | 2 (3%)   | 59,59,63    | 1.12 | 5 (8%)   |
| 30  | BCT  | A     | 415[A] | 21     | 3,3,3        | 0.55 | 0        | 2,3,3       | 1.29 | 0        |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | GOL  | B     | 625    | -      | 5,5,5        | 1.02 | 0        | 5,5,5       | 1.18 | 1 (20%)  |
| 23  | CLA  | c     | 511    | -      | 63,73,73     | 2.12 | 16 (25%) | 74,113,113  | 2.77 | 31 (41%) |
| 32  | LMT  | B     | 626    | -      | 36,36,36     | 1.18 | 4 (11%)  | 47,47,47    | 1.40 | 5 (10%)  |
| 24  | BCR  | B     | 618    | -      | 41,41,41     | 1.00 | 2 (4%)   | 56,56,56    | 1.35 | 7 (12%)  |
| 33  | LHG  | A     | 418[A] | -      | 48,48,48     | 0.87 | 2 (4%)   | 51,54,54    | 1.29 | 6 (11%)  |
| 36  | DGD  | H     | 102    | -      | 63,63,67     | 0.86 | 4 (6%)   | 77,77,81    | 1.07 | 7 (9%)   |
| 27  | OEX  | a     | 412[B] | 1,3,41 | 0,15,15      | -    | -        | -           | -    | -        |
| 23  | CLA  | a     | 404[A] | -      | 63,73,73     | 2.05 | 16 (25%) | 74,113,113  | 2.79 | 32 (43%) |
| 35  | HTG  | C     | 522    | -      | 19,19,19     | 0.79 | 1 (5%)   | 23,24,24    | 1.22 | 2 (8%)   |
| 23  | CLA  | b     | 608    | -      | 63,73,73     | 2.11 | 15 (23%) | 74,113,113  | 2.69 | 29 (39%) |
| 26  | GOL  | V     | 203[A] | -      | 5,5,5        | 1.41 | 1 (20%)  | 5,5,5       | 0.86 | 0        |
| 40  | HEC  | v     | 201    | 16     | 32,50,50     | 1.96 | 4 (12%)  | 30,82,82    | 2.51 | 9 (30%)  |
| 33  | LHG  | d     | 407[A] | -      | 48,48,48     | 0.87 | 2 (4%)   | 51,54,54    | 1.06 | 4 (7%)   |
| 23  | CLA  | C     | 504    | -      | 63,73,73     | 2.01 | 16 (25%) | 74,113,113  | 2.73 | 26 (35%) |
| 33  | LHG  | d     | 414[B] | -      | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.09 | 4 (7%)   |
| 40  | HEC  | V     | 201    | 16     | 32,50,50     | 1.93 | 3 (9%)   | 30,82,82    | 2.61 | 9 (30%)  |
| 32  | LMT  | M     | 101    | -      | 36,36,36     | 1.09 | 2 (5%)   | 47,47,47    | 1.27 | 6 (12%)  |
| 23  | CLA  | A     | 404[B] | -      | 63,73,73     | 2.13 | 15 (23%) | 74,113,113  | 2.72 | 31 (41%) |
| 23  | CLA  | B     | 601    | 41     | 63,73,73     | 2.11 | 17 (26%) | 74,113,113  | 2.70 | 26 (35%) |
| 35  | HTG  | b     | 625    | -      | 19,19,19     | 0.98 | 2 (10%)  | 23,24,24    | 1.49 | 3 (13%)  |
| 27  | OEX  | a     | 412[A] | 1,3,41 | 0,15,15      | -    | -        | -           | -    | -        |
| 32  | LMT  | A     | 417    | -      | 36,36,36     | 0.91 | 0        | 47,47,47    | 1.07 | 2 (4%)   |
| 24  | BCR  | B     | 619    | -      | 41,41,41     | 1.08 | 2 (4%)   | 56,56,56    | 1.47 | 11 (19%) |
| 33  | LHG  | a     | 419[B] | -      | 41,41,48     | 1.04 | 2 (4%)   | 44,47,54    | 0.95 | 2 (4%)   |
| 23  | CLA  | C     | 502    | -      | 63,73,73     | 2.00 | 16 (25%) | 74,113,113  | 2.77 | 30 (40%) |
| 36  | DGD  | h     | 102    | -      | 63,63,67     | 0.86 | 4 (6%)   | 77,77,81    | 1.14 | 6 (7%)   |
| 23  | CLA  | c     | 503    | -      | 63,73,73     | 2.13 | 16 (25%) | 74,113,113  | 2.53 | 24 (32%) |
| 23  | CLA  | c     | 506    | -      | 63,73,73     | 2.07 | 17 (26%) | 74,113,113  | 2.64 | 26 (35%) |
| 33  | LHG  | d     | 414[A] | -      | 48,48,48     | 0.89 | 3 (6%)   | 51,54,54    | 1.13 | 4 (7%)   |
| 23  | CLA  | b     | 606    | -      | 63,73,73     | 2.04 | 15 (23%) | 74,113,113  | 2.70 | 27 (36%) |
| 27  | OEX  | A     | 412[B] | 1,3,41 | 0,15,15      | -    | -        | -           | -    | -        |
| 23  | CLA  | c     | 513    | -      | 63,73,73     | 2.08 | 15 (23%) | 74,113,113  | 2.69 | 28 (37%) |
| 23  | CLA  | C     | 507    | -      | 63,73,73     | 2.02 | 17 (26%) | 74,113,113  | 2.74 | 29 (39%) |
| 23  | CLA  | c     | 512    | 3      | 63,73,73     | 2.17 | 16 (25%) | 74,113,113  | 2.71 | 29 (39%) |
| 32  | LMT  | b     | 621    | -      | 25,25,36     | 0.95 | 1 (4%)   | 30,30,47    | 1.20 | 3 (10%)  |



| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | DGD  | C     | 519    | -    | 63,63,67     | 0.86 | 3 (4%)   | 77,77,81    | 1.00 | 3 (3%)   |
| 36  | DGD  | c     | 518[A] | -    | 63,63,67     | 0.85 | 3 (4%)   | 77,77,81    | 0.98 | 4 (5%)   |
| 33  | LHG  | a     | 419[A] | -    | 41,41,48     | 1.06 | 2 (4%)   | 44,47,54    | 0.93 | 2 (4%)   |
| 28  | PL9  | A     | 413[B] | -    | 55,55,55     | 0.66 | 2 (3%)   | 68,69,69    | 1.97 | 25 (36%) |
| 31  | PHO  | a     | 406[B] | -    | 50,69,69     | 1.90 | 7 (14%)  | 48,99,99    | 1.97 | 11 (22%) |
| 31  | PHO  | D     | 401[B] | -    | 50,69,69     | 1.88 | 8 (16%)  | 48,99,99    | 1.98 | 9 (18%)  |
| 36  | DGD  | C     | 518[B] | -    | 63,63,67     | 0.86 | 2 (3%)   | 77,77,81    | 1.04 | 5 (6%)   |
| 32  | LMT  | B     | 627    | -    | 36,36,36     | 1.00 | 3 (8%)   | 47,47,47    | 1.17 | 4 (8%)   |
| 34  | LMG  | c     | 501    | -    | 51,51,55     | 0.92 | 2 (3%)   | 59,59,63    | 1.21 | 4 (6%)   |
| 23  | CLA  | c     | 508    | 41   | 63,73,73     | 2.06 | 15 (23%) | 74,113,113  | 2.76 | 27 (36%) |
| 26  | GOL  | D     | 413    | -    | 5,5,5        | 1.59 | 2 (40%)  | 5,5,5       | 0.95 | 0        |
| 34  | LMG  | Z     | 101    | -    | 37,37,55     | 1.02 | 3 (8%)   | 45,45,63    | 1.46 | 5 (11%)  |
| 33  | LHG  | d     | 408[B] | -    | 48,48,48     | 0.91 | 2 (4%)   | 51,54,54    | 1.12 | 5 (9%)   |
| 33  | LHG  | D     | 407[A] | -    | 48,48,48     | 0.88 | 3 (6%)   | 51,54,54    | 1.02 | 3 (5%)   |
| 26  | GOL  | c     | 527    | -    | 5,5,5        | 1.21 | 1 (20%)  | 5,5,5       | 1.05 | 0        |
| 23  | CLA  | a     | 405[B] | 41   | 63,73,73     | 2.07 | 15 (23%) | 74,113,113  | 2.71 | 29 (39%) |
| 26  | GOL  | d     | 413    | -    | 5,5,5        | 1.01 | 0        | 5,5,5       | 1.15 | 0        |
| 24  | BCR  | b     | 619    | -    | 41,41,41     | 1.11 | 2 (4%)   | 56,56,56    | 1.34 | 8 (14%)  |
| 34  | LMG  | m     | 101    | -    | 51,51,55     | 0.90 | 2 (3%)   | 59,59,63    | 1.29 | 6 (10%)  |
| 23  | CLA  | b     | 610    | 41   | 63,73,73     | 2.10 | 16 (25%) | 74,113,113  | 2.84 | 29 (39%) |
| 28  | PL9  | A     | 413[A] | -    | 55,55,55     | 0.71 | 3 (5%)   | 68,69,69    | 2.05 | 25 (36%) |
| 31  | PHO  | a     | 406[A] | -    | 50,69,69     | 1.89 | 8 (16%)  | 48,99,99    | 2.00 | 9 (18%)  |
| 34  | LMG  | C     | 521    | -    | 51,51,55     | 1.08 | 3 (5%)   | 59,59,63    | 1.42 | 8 (13%)  |
| 31  | PHO  | D     | 401[A] | -    | 50,69,69     | 1.82 | 8 (16%)  | 48,99,99    | 1.79 | 10 (20%) |
| 36  | DGD  | C     | 518[A] | -    | 63,63,67     | 0.91 | 3 (4%)   | 77,77,81    | 1.04 | 5 (6%)   |
| 23  | CLA  | c     | 502    | -    | 63,73,73     | 2.07 | 17 (26%) | 74,113,113  | 2.75 | 28 (37%) |
| 28  | PL9  | d     | 406[B] | -    | 55,55,55     | 0.66 | 1 (1%)   | 68,69,69    | 1.69 | 17 (25%) |
| 33  | LHG  | d     | 408[A] | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.02 | 3 (5%)   |
| 26  | GOL  | a     | 417    | -    | 5,5,5        | 1.39 | 1 (20%)  | 5,5,5       | 1.13 | 1 (20%)  |
| 34  | LMG  | B     | 620    | -    | 51,51,55     | 0.93 | 2 (3%)   | 59,59,63    | 1.29 | 4 (6%)   |
| 24  | BCR  | h     | 101    | -    | 41,41,41     | 1.04 | 1 (2%)   | 56,56,56    | 1.45 | 13 (23%) |
| 23  | CLA  | a     | 405[A] | 41   | 63,73,73     | 2.01 | 16 (25%) | 74,113,113  | 2.67 | 28 (37%) |
| 33  | LHG  | L     | 101[B] | -    | 48,48,48     | 0.93 | 3 (6%)   | 51,54,54    | 1.09 | 4 (7%)   |
| 32  | LMT  | T     | 101    | -    | 36,36,36     | 1.05 | 3 (8%)   | 47,47,47    | 1.08 | 2 (4%)   |
| 25  | SQD  | l     | 101    | -    | 52,54,54     | 1.03 | 3 (5%)   | 62,65,65    | 1.77 | 12 (19%) |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | GOL  | b     | 628    | -    | 5,5,5        | 0.57 | 0        | 5,5,5       | 1.48 | 1 (20%)  |
| 23  | CLA  | b     | 611    | -    | 63,73,73     | 2.04 | 16 (25%) | 74,113,113  | 2.73 | 30 (40%) |
| 30  | BCT  | d     | 401[B] | 21   | 3,3,3        | 0.51 | 0        | 2,3,3       | 1.18 | 0        |
| 24  | BCR  | C     | 516    | -    | 41,41,41     | 1.05 | 1 (2%)   | 56,56,56    | 1.36 | 10 (17%) |
| 31  | PHO  | A     | 416[B] | -    | 50,69,69     | 1.97 | 8 (16%)  | 48,99,99    | 2.02 | 12 (25%) |
| 23  | CLA  | A     | 405[B] | 41   | 63,73,73     | 2.07 | 16 (25%) | 74,113,113  | 2.62 | 31 (41%) |
| 23  | CLA  | b     | 616    | -    | 63,73,73     | 2.02 | 15 (23%) | 74,113,113  | 2.79 | 30 (40%) |
| 33  | LHG  | D     | 408[B] | -    | 48,48,48     | 0.91 | 2 (4%)   | 51,54,54    | 1.10 | 3 (5%)   |
| 23  | CLA  | C     | 511    | -    | 63,73,73     | 2.10 | 16 (25%) | 74,113,113  | 2.76 | 28 (37%) |
| 28  | PL9  | d     | 406[A] | -    | 55,55,55     | 0.72 | 1 (1%)   | 68,69,69    | 1.61 | 17 (25%) |
| 34  | LMG  | c     | 520    | -    | 51,51,55     | 0.90 | 2 (3%)   | 59,59,63    | 1.21 | 6 (10%)  |
| 26  | GOL  | c     | 526[A] | -    | 5,5,5        | 1.04 | 0        | 5,5,5       | 1.05 | 0        |
| 33  | LHG  | L     | 101[A] | -    | 48,48,48     | 0.89 | 3 (6%)   | 51,54,54    | 1.16 | 4 (7%)   |
| 26  | GOL  | a     | 410    | -    | 5,5,5        | 0.97 | 0        | 5,5,5       | 1.04 | 0        |
| 34  | LMG  | D     | 412    | 39   | 51,51,55     | 0.81 | 3 (5%)   | 59,59,63    | 1.06 | 3 (5%)   |
| 36  | DGD  | c     | 518[B] | -    | 63,63,67     | 0.87 | 2 (3%)   | 77,77,81    | 1.01 | 6 (7%)   |
| 31  | PHO  | A     | 416[A] | -    | 50,69,69     | 2.00 | 8 (16%)  | 48,99,99    | 1.97 | 10 (20%) |
| 30  | BCT  | d     | 401[A] | 21   | 3,3,3        | 0.49 | 0        | 2,3,3       | 1.49 | 0        |
| 23  | CLA  | b     | 613    | -    | 63,73,73     | 2.07 | 16 (25%) | 74,113,113  | 2.73 | 30 (40%) |
| 23  | CLA  | A     | 405[A] | 41   | 63,73,73     | 2.02 | 15 (23%) | 74,113,113  | 2.70 | 31 (41%) |
| 36  | DGD  | c     | 517[A] | -    | 63,63,67     | 0.86 | 2 (3%)   | 77,77,81    | 1.10 | 8 (10%)  |
| 33  | LHG  | D     | 408[A] | -    | 48,48,48     | 0.94 | 2 (4%)   | 51,54,54    | 1.04 | 4 (7%)   |
| 26  | GOL  | O     | 303    | -    | 5,5,5        | 1.17 | 1 (20%)  | 5,5,5       | 1.18 | 1 (20%)  |
| 23  | CLA  | C     | 508    | 41   | 63,73,73     | 2.02 | 17 (26%) | 74,113,113  | 2.60 | 25 (33%) |
| 24  | BCR  | t     | 102    | -    | 41,41,41     | 1.08 | 1 (2%)   | 56,56,56    | 1.63 | 12 (21%) |
| 23  | CLA  | B     | 608    | -    | 63,73,73     | 1.99 | 15 (23%) | 74,113,113  | 2.72 | 34 (45%) |
| 24  | BCR  | Y     | 101    | -    | 41,41,41     | 1.00 | 1 (2%)   | 56,56,56    | 1.77 | 15 (26%) |
| 31  | PHO  | a     | 415[A] | -    | 50,69,69     | 1.95 | 8 (16%)  | 48,99,99    | 2.11 | 12 (25%) |
| 23  | CLA  | B     | 605    | -    | 63,73,73     | 2.06 | 16 (25%) | 74,113,113  | 2.92 | 31 (41%) |
| 33  | LHG  | D     | 407[B] | -    | 48,48,48     | 0.88 | 2 (4%)   | 51,54,54    | 1.07 | 4 (7%)   |
| 34  | LMG  | C     | 501    | -    | 51,51,55     | 0.92 | 2 (3%)   | 59,59,63    | 1.53 | 8 (13%)  |
| 32  | LMT  | m     | 103    | -    | 36,36,36     | 1.03 | 3 (8%)   | 47,47,47    | 1.09 | 3 (6%)   |
| 28  | PL9  | a     | 413[B] | -    | 55,55,55     | 0.66 | 2 (3%)   | 68,69,69    | 1.95 | 20 (29%) |
| 26  | GOL  | O     | 302    | -    | 5,5,5        | 0.98 | 0        | 5,5,5       | 0.97 | 0        |
| 35  | HTG  | b     | 622    | -    | 19,19,19     | 1.12 | 2 (10%)  | 23,24,24    | 1.89 | 7 (30%)  |
| 23  | CLA  | C     | 509    | -    | 63,73,73     | 2.17 | 17 (26%) | 74,113,113  | 2.65 | 26 (35%) |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | CLA  | A     | 406[B] | 41   | 63,73,73     | 2.10 | 17 (26%) | 74,113,113  | 2.67 | 28 (37%) |
| 23  | CLA  | C     | 513    | -    | 63,73,73     | 2.08 | 15 (23%) | 74,113,113  | 2.74 | 30 (40%) |
| 32  | LMT  | e     | 101    | -    | 36,36,36     | 1.00 | 1 (2%)   | 47,47,47    | 0.99 | 1 (2%)   |
| 36  | DGD  | c     | 519    | -    | 63,63,67     | 0.86 | 4 (6%)   | 77,77,81    | 1.09 | 5 (6%)   |
| 23  | CLA  | C     | 510    | -    | 63,73,73     | 2.13 | 16 (25%) | 74,113,113  | 2.72 | 27 (36%) |
| 38  | HEM  | f     | 101    | 6,5  | 42,50,50     | 1.29 | 5 (11%)  | 46,82,82    | 1.80 | 11 (23%) |
| 23  | CLA  | d     | 404    | -    | 63,73,73     | 2.08 | 17 (26%) | 74,113,113  | 2.72 | 30 (40%) |
| 23  | CLA  | d     | 403[B] | -    | 63,73,73     | 2.08 | 14 (22%) | 74,113,113  | 2.64 | 26 (35%) |
| 32  | LMT  | F     | 101    | -    | 36,36,36     | 1.03 | 1 (2%)   | 47,47,47    | 1.01 | 1 (2%)   |
| 24  | BCR  | C     | 515    | -    | 41,41,41     | 1.08 | 1 (2%)   | 56,56,56    | 1.43 | 7 (12%)  |
| 26  | GOL  | l     | 103[B] | -    | 5,5,5        | 0.89 | 0        | 5,5,5       | 1.15 | 0        |
| 23  | CLA  | b     | 604    | -    | 63,73,73     | 2.09 | 16 (25%) | 74,113,113  | 2.67 | 28 (37%) |

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   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 28  | PL9  | a     | 413[A] | -    | -         | 14/53/73/73   | 0/1/1/1 |
| 23  | CLA  | B     | 611    | -    | 1/1/15/20 | 3/37/115/115  | -       |
| 23  | CLA  | A     | 406[A] | 41   | -         | 5/37/115/115  | -       |
| 23  | CLA  | C     | 505    | 41   | 1/1/15/20 | 7/37/115/115  | -       |
| 23  | CLA  | d     | 403[A] | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 26  | GOL  | l     | 103[A] | -    | -         | 2/4/4/4       | -       |
| 23  | CLA  | B     | 614    | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 24  | BCR  | c     | 516    | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 25  | SQD  | b     | 620    | -    | -         | 18/49/69/69   | 0/1/1/1 |
| 24  | BCR  | B     | 617    | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 26  | GOL  | c     | 526[B] | -    | -         | 0/4/4/4       | -       |
| 26  | GOL  | o     | 303    | -    | -         | 2/4/4/4       | -       |
| 28  | PL9  | D     | 406[A] | -    | -         | 6/53/73/73    | 0/1/1/1 |
| 32  | LMT  | a     | 416    | -    | -         | 10/21/61/61   | 0/2/2/2 |
| 23  | CLA  | b     | 614    | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 35  | HTG  | o     | 301    | -    | -         | 4/10/30/30    | 0/1/1/1 |
| 32  | LMT  | t     | 101    | -    | -         | 10/17/38/61   | 0/1/1/2 |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 35  | HTG  | b     | 623    | -    | -         | 4/10/30/30    | 0/1/1/1 |
| 23  | CLA  | D     | 404    | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 23  | CLA  | D     | 403[B] | -    | 1/1/15/20 | 0/37/115/115  | -       |
| 23  | CLA  | b     | 615    | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 23  | CLA  | c     | 514    | -    | -         | 9/37/115/115  | -       |
| 38  | HEM  | F     | 102    | 6,5  | -         | 3/12/54/54    | -       |
| 36  | DGD  | c     | 517[B] | -    | -         | 19/51/91/95   | 0/2/2/2 |
| 23  | CLA  | B     | 616    | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 33  | LHG  | E     | 101[B] | -    | -         | 19/46/46/53   | -       |
| 25  | SQD  | a     | 411    | -    | -         | 16/49/69/69   | 0/1/1/1 |
| 25  | SQD  | a     | 409[B] | -    | -         | 9/49/69/69    | 0/1/1/1 |
| 24  | BCR  | y     | 101    | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 31  | PHO  | a     | 415[B] | -    | -         | 4/37/103/103  | 0/5/6/6 |
| 23  | CLA  | b     | 603    | -    | 1/1/15/20 | 2/37/115/115  | -       |
| 23  | CLA  | B     | 604    | -    | 1/1/15/20 | 1/37/115/115  | -       |
| 23  | CLA  | B     | 607    | 41   | 1/1/15/20 | 3/37/115/115  | -       |
| 23  | CLA  | D     | 403[A] | -    | 1/1/15/20 | 0/37/115/115  | -       |
| 23  | CLA  | B     | 613    | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 34  | LMG  | z     | 101    | -    | -         | 9/34/54/70    | 0/1/1/1 |
| 23  | CLA  | C     | 514    | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 23  | CLA  | b     | 607    | 41   | 1/1/15/20 | 5/37/115/115  | -       |
| 26  | GOL  | D     | 402    | -    | -         | 2/4/4/4       | -       |
| 35  | HTG  | D     | 411    | -    | -         | 3/7/27/30     | 0/1/1/1 |
| 33  | LHG  | E     | 101[A] | -    | -         | 21/46/46/53   | -       |
| 36  | DGD  | C     | 517[B] | -    | -         | 15/51/91/95   | 0/2/2/2 |
| 25  | SQD  | a     | 409[A] | -    | -         | 9/49/69/69    | 0/1/1/1 |
| 35  | HTG  | d     | 411    | -    | -         | 1/7/27/30     | 0/1/1/1 |
| 24  | BCR  | k     | 101    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 23  | CLA  | B     | 609    | -    | 1/1/15/20 | 0/37/115/115  | -       |
| 23  | CLA  | c     | 510    | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 25  | SQD  | A     | 409[B] | -    | -         | 10/49/69/69   | 0/1/1/1 |
| 26  | GOL  | C     | 523[A] | -    | -         | 0/4/4/4       | -       |
| 23  | CLA  | C     | 512    | 3    | 1/1/15/20 | 5/37/115/115  | -       |
| 23  | CLA  | c     | 505    | 41   | 1/1/15/20 | 5/37/115/115  | -       |
| 23  | CLA  | B     | 602    | -    | 1/1/15/20 | 8/37/115/115  | -       |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 36  | DGD  | C     | 517[A] | -    | -         | 15/51/91/95   | 0/2/2/2 |
| 23  | CLA  | b     | 601    | 41   | 1/1/15/20 | 18/37/115/115 | -       |
| 26  | GOL  | A     | 410    | -    | -         | 2/4/4/4       | -       |
| 32  | LMT  | B     | 629    | -    | -         | 11/17/37/61   | 0/1/1/2 |
| 25  | SQD  | A     | 409[A] | -    | -         | 12/49/69/69   | 0/1/1/1 |
| 24  | BCR  | b     | 618    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 28  | PL9  | D     | 406[B] | -    | -         | 7/53/73/73    | 0/1/1/1 |
| 33  | LHG  | b     | 629[A] | -    | -         | 15/53/53/53   | -       |
| 24  | BCR  | H     | 101    | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 24  | BCR  | K     | 102    | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 24  | BCR  | b     | 617    | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 25  | SQD  | f     | 102    | -    | -         | 11/38/58/69   | 0/1/1/1 |
| 23  | CLA  | C     | 506    | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 35  | HTG  | B     | 623    | -    | -         | 4/10/30/30    | 0/1/1/1 |
| 23  | CLA  | c     | 504    | -    | 1/1/15/20 | 0/37/115/115  | -       |
| 24  | BCR  | D     | 405    | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 23  | CLA  | c     | 507    | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 35  | HTG  | V     | 202    | -    | -         | 0/2/19/30     | 0/1/1/1 |
| 23  | CLA  | A     | 407    | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 23  | CLA  | a     | 407    | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 23  | CLA  | B     | 615    | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 35  | HTG  | c     | 522    | -    | -         | 2/10/30/30    | 0/1/1/1 |
| 23  | CLA  | b     | 602    | -    | 1/1/15/20 | 3/37/115/115  | -       |
| 23  | CLA  | B     | 603    | -    | 1/1/15/20 | 3/37/115/115  | -       |
| 26  | GOL  | a     | 418    | -    | -         | 2/4/4/4       | -       |
| 26  | GOL  | B     | 622    | -    | -         | 4/4/4/4       | -       |
| 23  | CLA  | A     | 404[A] | -    | 1/1/15/20 | 3/37/115/115  | -       |
| 23  | CLA  | d     | 402[B] | 41   | 1/1/15/20 | 2/37/115/115  | -       |
| 23  | CLA  | B     | 612    | -    | 1/1/15/20 | 5/37/115/115  | -       |
| 23  | CLA  | b     | 605    | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 26  | GOL  | o     | 304    | -    | -         | 4/4/4/4       | -       |
| 26  | GOL  | b     | 624    | -    | -         | 2/4/4/4       | -       |
| 34  | LMG  | C     | 520    | -    | -         | 12/46/66/70   | 0/1/1/1 |
| 26  | GOL  | C     | 523[B] | -    | -         | 0/4/4/4       | -       |
| 32  | LMT  | A     | 419    | -    | -         | 15/21/61/61   | 0/2/2/2 |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 23  | CLA  | b     | 612    | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 24  | BCR  | T     | 102    | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 26  | GOL  | v     | 202[B] | -    | -         | 2/4/4/4       | -       |
| 23  | CLA  | C     | 503    | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 24  | BCR  | d     | 405    | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 35  | HTG  | B     | 621    | -    | -         | 2/10/30/30    | 0/1/1/1 |
| 23  | CLA  | c     | 509    | -    | 1/1/15/20 | 2/37/115/115  | -       |
| 23  | CLA  | d     | 402[A] | 41   | 1/1/15/20 | 4/37/115/115  | -       |
| 32  | LMT  | b     | 627    | -    | -         | 11/17/37/61   | 0/1/1/2 |
| 24  | BCR  | A     | 408    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 23  | CLA  | b     | 609    | -    | 1/1/15/20 | 0/37/115/115  | -       |
| 33  | LHG  | A     | 418[B] | -    | -         | 16/53/53/53   | -       |
| 24  | BCR  | c     | 515    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 26  | GOL  | v     | 202[A] | -    | -         | 2/4/4/4       | -       |
| 23  | CLA  | B     | 610    | 41   | 1/1/15/20 | 7/37/115/115  | -       |
| 33  | LHG  | b     | 629[B] | -    | -         | 18/53/53/53   | -       |
| 34  | LMG  | c     | 521    | -    | -         | 10/46/66/70   | 0/1/1/1 |
| 25  | SQD  | A     | 411    | -    | -         | 14/49/69/69   | 0/1/1/1 |
| 23  | CLA  | a     | 404[B] | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 26  | GOL  | V     | 203[B] | -    | -         | 2/4/4/4       | -       |
| 23  | CLA  | B     | 606    | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 33  | LHG  | d     | 407[B] | -    | -         | 16/53/53/53   | -       |
| 24  | BCR  | a     | 408    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 25  | SQD  | X     | 101    | -    | -         | 13/38/58/69   | 0/1/1/1 |
| 34  | LMG  | d     | 412    | 39   | -         | 11/46/66/70   | 0/1/1/1 |
| 26  | GOL  | B     | 625    | -    | -         | 3/4/4/4       | -       |
| 23  | CLA  | c     | 511    | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 32  | LMT  | B     | 626    | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 24  | BCR  | B     | 618    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 33  | LHG  | A     | 418[A] | -    | -         | 14/53/53/53   | -       |
| 36  | DGD  | H     | 102    | -    | -         | 10/51/91/95   | 0/2/2/2 |
| 23  | CLA  | a     | 404[A] | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 35  | HTG  | C     | 522    | -    | -         | 0/10/30/30    | 0/1/1/1 |
| 23  | CLA  | b     | 608    | -    | -         | 4/37/115/115  | -       |
| 26  | GOL  | V     | 203[A] | -    | -         | 2/4/4/4       | -       |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 40  | HEC  | v     | 201    | 16   | -         | 2/10/54/54    | -       |
| 33  | LHG  | d     | 407[A] | -    | -         | 12/53/53/53   | -       |
| 23  | CLA  | C     | 504    | -    | -         | 4/37/115/115  | -       |
| 33  | LHG  | d     | 414[B] | -    | -         | 8/53/53/53    | -       |
| 40  | HEC  | V     | 201    | 16   | -         | 2/10/54/54    | -       |
| 32  | LMT  | M     | 101    | -    | -         | 4/21/61/61    | 0/2/2/2 |
| 23  | CLA  | A     | 404[B] | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 23  | CLA  | B     | 601    | 41   | 1/1/15/20 | 11/37/115/115 | -       |
| 35  | HTG  | b     | 625    | -    | -         | 3/10/30/30    | 0/1/1/1 |
| 32  | LMT  | A     | 417    | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 24  | BCR  | B     | 619    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 33  | LHG  | a     | 419[B] | -    | -         | 16/46/46/53   | -       |
| 23  | CLA  | C     | 502    | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 36  | DGD  | h     | 102    | -    | -         | 16/51/91/95   | 0/2/2/2 |
| 23  | CLA  | c     | 503    | -    | 1/1/15/20 | 3/37/115/115  | -       |
| 23  | CLA  | c     | 506    | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 33  | LHG  | d     | 414[A] | -    | -         | 15/53/53/53   | -       |
| 23  | CLA  | b     | 606    | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 23  | CLA  | c     | 513    | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 23  | CLA  | C     | 507    | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 23  | CLA  | c     | 512    | 3    | 1/1/15/20 | 6/37/115/115  | -       |
| 32  | LMT  | b     | 621    | -    | -         | 8/17/37/61    | 0/1/1/2 |
| 36  | DGD  | C     | 519    | -    | -         | 20/51/91/95   | 0/2/2/2 |
| 36  | DGD  | c     | 518[A] | -    | -         | 16/51/91/95   | 0/2/2/2 |
| 33  | LHG  | a     | 419[A] | -    | -         | 16/46/46/53   | -       |
| 28  | PL9  | A     | 413[B] | -    | -         | 13/53/73/73   | 0/1/1/1 |
| 31  | PHO  | a     | 406[B] | -    | -         | 3/37/103/103  | 0/5/6/6 |
| 31  | PHO  | D     | 401[B] | -    | -         | 2/37/103/103  | 0/5/6/6 |
| 36  | DGD  | C     | 518[B] | -    | -         | 12/51/91/95   | 0/2/2/2 |
| 32  | LMT  | B     | 627    | -    | -         | 10/21/61/61   | 0/2/2/2 |
| 34  | LMG  | c     | 501    | -    | -         | 12/46/66/70   | 0/1/1/1 |
| 23  | CLA  | c     | 508    | 41   | 1/1/15/20 | 7/37/115/115  | -       |
| 26  | GOL  | D     | 413    | -    | -         | 4/4/4/4       | -       |
| 34  | LMG  | Z     | 101    | -    | -         | 11/31/51/70   | 0/1/1/1 |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 33  | LHG  | d     | 408[B] | -    | -         | 14/53/53/53   | -       |
| 33  | LHG  | D     | 407[A] | -    | -         | 17/53/53/53   | -       |
| 26  | GOL  | c     | 527    | -    | -         | 2/4/4/4       | -       |
| 23  | CLA  | a     | 405[B] | 41   | -         | 3/37/115/115  | -       |
| 26  | GOL  | d     | 413    | -    | -         | 2/4/4/4       | -       |
| 24  | BCR  | b     | 619    | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 34  | LMG  | m     | 101    | -    | -         | 11/46/66/70   | 0/1/1/1 |
| 23  | CLA  | b     | 610    | 41   | 1/1/15/20 | 9/37/115/115  | -       |
| 28  | PL9  | A     | 413[A] | -    | -         | 14/53/73/73   | 0/1/1/1 |
| 31  | PHO  | a     | 406[A] | -    | -         | 6/37/103/103  | 0/5/6/6 |
| 34  | LMG  | C     | 521    | -    | -         | 13/46/66/70   | 0/1/1/1 |
| 31  | PHO  | D     | 401[A] | -    | -         | 0/37/103/103  | 0/5/6/6 |
| 36  | DGD  | C     | 518[A] | -    | -         | 12/51/91/95   | 0/2/2/2 |
| 23  | CLA  | c     | 502    | -    | 1/1/15/20 | 2/37/115/115  | -       |
| 28  | PL9  | d     | 406[B] | -    | -         | 8/53/73/73    | 0/1/1/1 |
| 33  | LHG  | d     | 408[A] | -    | -         | 12/53/53/53   | -       |
| 26  | GOL  | a     | 417    | -    | -         | 2/4/4/4       | -       |
| 34  | LMG  | B     | 620    | -    | -         | 17/46/66/70   | 0/1/1/1 |
| 24  | BCR  | h     | 101    | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 23  | CLA  | a     | 405[A] | 41   | -         | 4/37/115/115  | -       |
| 33  | LHG  | L     | 101[B] | -    | -         | 18/53/53/53   | -       |
| 32  | LMT  | T     | 101    | -    | -         | 7/21/61/61    | 0/2/2/2 |
| 25  | SQD  | l     | 101    | -    | -         | 14/49/69/69   | 0/1/1/1 |
| 26  | GOL  | b     | 628    | -    | -         | 0/4/4/4       | -       |
| 23  | CLA  | b     | 611    | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 31  | PHO  | A     | 416[B] | -    | -         | 0/37/103/103  | 0/5/6/6 |
| 24  | BCR  | C     | 516    | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 23  | CLA  | A     | 405[B] | 41   | 1/1/15/20 | 3/37/115/115  | -       |
| 23  | CLA  | b     | 616    | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 33  | LHG  | D     | 408[B] | -    | -         | 12/53/53/53   | -       |
| 23  | CLA  | C     | 511    | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 28  | PL9  | d     | 406[A] | -    | -         | 6/53/73/73    | 0/1/1/1 |
| 34  | LMG  | c     | 520    | -    | -         | 12/46/66/70   | 0/1/1/1 |
| 26  | GOL  | c     | 526[A] | -    | -         | 0/4/4/4       | -       |
| 33  | LHG  | L     | 101[A] | -    | -         | 20/53/53/53   | -       |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|--------|------|-----------|--------------|---------|
| 26  | GOL  | a     | 410    | -    | -         | 4/4/4/4      | -       |
| 34  | LMG  | D     | 412    | 39   | -         | 9/46/66/70   | 0/1/1/1 |
| 36  | DGD  | c     | 518[B] | -    | -         | 13/51/91/95  | 0/2/2/2 |
| 31  | PHO  | A     | 416[A] | -    | -         | 1/37/103/103 | 0/5/6/6 |
| 23  | CLA  | b     | 613    | -    | 1/1/15/20 | 2/37/115/115 | -       |
| 23  | CLA  | A     | 405[A] | 41   | 1/1/15/20 | 1/37/115/115 | -       |
| 36  | DGD  | c     | 517[A] | -    | -         | 17/51/91/95  | 0/2/2/2 |
| 33  | LHG  | D     | 408[A] | -    | -         | 13/53/53/53  | -       |
| 26  | GOL  | O     | 303    | -    | -         | 2/4/4/4      | -       |
| 23  | CLA  | C     | 508    | 41   | 1/1/15/20 | 8/37/115/115 | -       |
| 24  | BCR  | t     | 102    | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 23  | CLA  | B     | 608    | -    | -         | 3/37/115/115 | -       |
| 24  | BCR  | Y     | 101    | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 31  | PHO  | a     | 415[A] | -    | -         | 1/37/103/103 | 0/5/6/6 |
| 23  | CLA  | B     | 605    | -    | 1/1/15/20 | 6/37/115/115 | -       |
| 33  | LHG  | D     | 407[B] | -    | -         | 19/53/53/53  | -       |
| 34  | LMG  | C     | 501    | -    | -         | 11/46/66/70  | 0/1/1/1 |
| 32  | LMT  | m     | 103    | -    | -         | 8/21/61/61   | 0/2/2/2 |
| 28  | PL9  | a     | 413[B] | -    | -         | 15/53/73/73  | 0/1/1/1 |
| 26  | GOL  | O     | 302    | -    | -         | 2/4/4/4      | -       |
| 35  | HTG  | b     | 622    | -    | -         | 5/10/30/30   | 0/1/1/1 |
| 23  | CLA  | C     | 509    | -    | 1/1/15/20 | 3/37/115/115 | -       |
| 23  | CLA  | A     | 406[B] | 41   | -         | 4/37/115/115 | -       |
| 23  | CLA  | C     | 513    | -    | 1/1/15/20 | 6/37/115/115 | -       |
| 32  | LMT  | e     | 101    | -    | -         | 15/21/61/61  | 0/2/2/2 |
| 36  | DGD  | c     | 519    | -    | -         | 9/51/91/95   | 0/2/2/2 |
| 23  | CLA  | C     | 510    | -    | 1/1/15/20 | 7/37/115/115 | -       |
| 38  | HEM  | f     | 101    | 6,5  | -         | 6/12/54/54   | -       |
| 23  | CLA  | d     | 404    | -    | 1/1/15/20 | 8/37/115/115 | -       |
| 23  | CLA  | d     | 403[B] | -    | 1/1/15/20 | 4/37/115/115 | -       |
| 32  | LMT  | F     | 101    | -    | -         | 8/21/61/61   | 0/2/2/2 |
| 24  | BCR  | C     | 515    | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 26  | GOL  | l     | 103[B] | -    | -         | 2/4/4/4      | -       |
| 23  | CLA  | b     | 604    | -    | 1/1/15/20 | 9/37/115/115 | -       |

All (1541) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 611    | CLA  | C3B-C2B | 10.62 | 1.54        | 1.40     |
| 23  | B     | 612    | CLA  | C3B-C2B | 7.60  | 1.50        | 1.40     |
| 23  | B     | 616    | CLA  | C3B-C2B | 7.30  | 1.50        | 1.40     |
| 23  | b     | 608    | CLA  | C3B-C2B | 7.13  | 1.50        | 1.40     |
| 23  | C     | 509    | CLA  | C3B-C2B | 7.00  | 1.49        | 1.40     |
| 23  | C     | 512    | CLA  | C3B-C2B | 6.96  | 1.49        | 1.40     |
| 23  | D     | 403[B] | CLA  | C3B-C2B | 6.79  | 1.49        | 1.40     |
| 23  | c     | 511    | CLA  | C3B-C2B | 6.74  | 1.49        | 1.40     |
| 23  | B     | 611    | CLA  | C1D-ND  | 6.73  | 1.46        | 1.37     |
| 23  | b     | 603    | CLA  | C3B-C2B | 6.71  | 1.49        | 1.40     |
| 23  | B     | 603    | CLA  | C3B-C2B | 6.70  | 1.49        | 1.40     |
| 31  | a     | 415[B] | PHO  | C3B-C2B | 6.68  | 1.49        | 1.40     |
| 23  | C     | 505    | CLA  | C3B-C2B | 6.66  | 1.49        | 1.40     |
| 23  | C     | 510    | CLA  | C3B-C2B | 6.61  | 1.49        | 1.40     |
| 23  | b     | 612    | CLA  | C3B-C2B | 6.60  | 1.49        | 1.40     |
| 23  | d     | 403[B] | CLA  | C3B-C2B | 6.58  | 1.49        | 1.40     |
| 31  | a     | 406[B] | PHO  | C3B-C2B | 6.57  | 1.49        | 1.40     |
| 23  | A     | 407    | CLA  | C3B-C2B | 6.57  | 1.49        | 1.40     |
| 23  | c     | 503    | CLA  | C3B-C2B | 6.57  | 1.49        | 1.40     |
| 23  | D     | 403[A] | CLA  | C3B-C2B | 6.56  | 1.49        | 1.40     |
| 31  | a     | 406[A] | PHO  | C3B-C2B | 6.55  | 1.49        | 1.40     |
| 23  | c     | 512    | CLA  | C3B-C2B | 6.54  | 1.49        | 1.40     |
| 23  | b     | 613    | CLA  | C3B-C2B | 6.54  | 1.49        | 1.40     |
| 23  | c     | 505    | CLA  | C3B-C2B | 6.53  | 1.49        | 1.40     |
| 23  | B     | 602    | CLA  | C3B-C2B | 6.49  | 1.49        | 1.40     |
| 23  | b     | 607    | CLA  | C3B-C2B | 6.49  | 1.49        | 1.40     |
| 23  | b     | 611    | CLA  | C3B-C2B | 6.48  | 1.49        | 1.40     |
| 23  | c     | 510    | CLA  | C3B-C2B | 6.47  | 1.49        | 1.40     |
| 23  | C     | 503    | CLA  | C3B-C2B | 6.46  | 1.49        | 1.40     |
| 23  | c     | 509    | CLA  | C3B-C2B | 6.36  | 1.49        | 1.40     |
| 31  | A     | 416[B] | PHO  | C3B-C2B | 6.31  | 1.48        | 1.40     |
| 31  | D     | 401[B] | PHO  | C3B-C2B | 6.28  | 1.48        | 1.40     |
| 31  | D     | 401[A] | PHO  | C3B-C2B | 6.28  | 1.48        | 1.40     |
| 23  | C     | 511    | CLA  | C3B-C2B | 6.27  | 1.48        | 1.40     |
| 23  | b     | 601    | CLA  | C3B-C2B | 6.25  | 1.48        | 1.40     |
| 23  | B     | 611    | CLA  | CMB-C2B | 6.21  | 1.64        | 1.51     |
| 23  | B     | 613    | CLA  | C3B-C2B | 6.21  | 1.48        | 1.40     |
| 23  | C     | 514    | CLA  | C3B-C2B | 6.17  | 1.48        | 1.40     |
| 23  | A     | 404[A] | CLA  | C3B-C2B | 6.11  | 1.48        | 1.40     |
| 23  | A     | 405[B] | CLA  | C3B-C2B | 6.10  | 1.48        | 1.40     |
| 31  | A     | 416[A] | PHO  | C3B-C2B | 6.09  | 1.48        | 1.40     |
| 23  | C     | 507    | CLA  | C3B-C2B | 6.08  | 1.48        | 1.40     |
| 23  | b     | 604    | CLA  | C3B-C2B | 6.07  | 1.48        | 1.40     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 23  | B     | 614    | CLA  | C3B-C2B | 6.04 | 1.48        | 1.40     |
| 31  | a     | 415[A] | PHO  | C3B-C2B | 6.02 | 1.48        | 1.40     |
| 23  | a     | 404[B] | CLA  | C3B-C2B | 6.01 | 1.48        | 1.40     |
| 23  | A     | 404[B] | CLA  | C3B-C2B | 6.01 | 1.48        | 1.40     |
| 23  | a     | 404[A] | CLA  | C3B-C2B | 6.01 | 1.48        | 1.40     |
| 23  | B     | 611    | CLA  | CHC-C1C | 6.00 | 1.49        | 1.34     |
| 23  | B     | 608    | CLA  | C3B-C2B | 5.96 | 1.48        | 1.40     |
| 23  | c     | 514    | CLA  | C3B-C2B | 5.95 | 1.48        | 1.40     |
| 23  | C     | 513    | CLA  | CHC-C1C | 5.94 | 1.49        | 1.34     |
| 23  | B     | 601    | CLA  | C3B-C2B | 5.90 | 1.48        | 1.40     |
| 23  | b     | 609    | CLA  | C3B-C2B | 5.87 | 1.48        | 1.40     |
| 23  | c     | 513    | CLA  | CHC-C1C | 5.87 | 1.49        | 1.34     |
| 23  | C     | 513    | CLA  | C3B-C2B | 5.86 | 1.48        | 1.40     |
| 23  | B     | 611    | CLA  | C3C-C2C | 5.86 | 1.49        | 1.36     |
| 23  | b     | 610    | CLA  | CHC-C1C | 5.86 | 1.49        | 1.34     |
| 23  | a     | 407    | CLA  | CHC-C1C | 5.82 | 1.48        | 1.34     |
| 23  | d     | 403[A] | CLA  | C3B-C2B | 5.82 | 1.48        | 1.40     |
| 23  | B     | 606    | CLA  | C3B-C2B | 5.79 | 1.48        | 1.40     |
| 23  | b     | 602    | CLA  | CHC-C1C | 5.79 | 1.48        | 1.34     |
| 23  | c     | 507    | CLA  | C3B-C2B | 5.78 | 1.48        | 1.40     |
| 23  | c     | 509    | CLA  | CHC-C1C | 5.78 | 1.48        | 1.34     |
| 23  | b     | 616    | CLA  | C3B-C2B | 5.76 | 1.48        | 1.40     |
| 23  | B     | 601    | CLA  | CHC-C1C | 5.75 | 1.48        | 1.34     |
| 23  | a     | 405[B] | CLA  | C3B-C2B | 5.75 | 1.48        | 1.40     |
| 23  | B     | 602    | CLA  | CHC-C1C | 5.74 | 1.48        | 1.34     |
| 23  | A     | 406[B] | CLA  | CHC-C1C | 5.73 | 1.48        | 1.34     |
| 23  | A     | 404[B] | CLA  | CHC-C1C | 5.73 | 1.48        | 1.34     |
| 23  | b     | 613    | CLA  | CHC-C1C | 5.73 | 1.48        | 1.34     |
| 23  | c     | 502    | CLA  | CHC-C1C | 5.73 | 1.48        | 1.34     |
| 23  | d     | 402[B] | CLA  | C3B-C2B | 5.73 | 1.48        | 1.40     |
| 23  | b     | 609    | CLA  | CHC-C1C | 5.71 | 1.48        | 1.34     |
| 23  | B     | 607    | CLA  | C3B-C2B | 5.70 | 1.48        | 1.40     |
| 23  | a     | 404[B] | CLA  | CHC-C1C | 5.69 | 1.48        | 1.34     |
| 23  | b     | 614    | CLA  | C3B-C2B | 5.69 | 1.48        | 1.40     |
| 23  | A     | 406[A] | CLA  | CHC-C1C | 5.69 | 1.48        | 1.34     |
| 23  | B     | 607    | CLA  | CHC-C1C | 5.68 | 1.48        | 1.34     |
| 23  | a     | 405[B] | CLA  | CHC-C1C | 5.67 | 1.48        | 1.34     |
| 23  | C     | 502    | CLA  | C3B-C2B | 5.66 | 1.48        | 1.40     |
| 23  | b     | 610    | CLA  | C3B-C2B | 5.65 | 1.48        | 1.40     |
| 31  | a     | 415[A] | PHO  | OBD-CAD | 5.65 | 1.29        | 1.22     |
| 23  | c     | 509    | CLA  | O2D-CGD | 5.65 | 1.47        | 1.33     |
| 23  | c     | 504    | CLA  | CHC-C1C | 5.64 | 1.48        | 1.34     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 31  | A     | 416[A] | PHO  | OBD-CAD | 5.63 | 1.29        | 1.22     |
| 23  | C     | 508    | CLA  | C3B-C2B | 5.63 | 1.48        | 1.40     |
| 31  | a     | 415[B] | PHO  | C3D-C2D | 5.62 | 1.49        | 1.39     |
| 31  | a     | 415[A] | PHO  | C3D-C2D | 5.62 | 1.49        | 1.39     |
| 23  | D     | 404    | CLA  | CHC-C1C | 5.62 | 1.48        | 1.34     |
| 23  | c     | 509    | CLA  | C3C-C2C | 5.61 | 1.48        | 1.36     |
| 31  | a     | 406[A] | PHO  | C3D-C2D | 5.61 | 1.49        | 1.39     |
| 23  | C     | 504    | CLA  | C3C-C2C | 5.61 | 1.48        | 1.36     |
| 23  | C     | 504    | CLA  | CHC-C1C | 5.60 | 1.48        | 1.34     |
| 23  | a     | 407    | CLA  | C3B-C2B | 5.60 | 1.48        | 1.40     |
| 23  | b     | 606    | CLA  | C3B-C2B | 5.60 | 1.48        | 1.40     |
| 23  | B     | 605    | CLA  | CHC-C1C | 5.58 | 1.48        | 1.34     |
| 23  | B     | 604    | CLA  | C3B-C2B | 5.58 | 1.47        | 1.40     |
| 23  | d     | 404    | CLA  | CHC-C1C | 5.58 | 1.48        | 1.34     |
| 23  | b     | 603    | CLA  | CHC-C1C | 5.57 | 1.48        | 1.34     |
| 23  | C     | 502    | CLA  | CHC-C1C | 5.57 | 1.48        | 1.34     |
| 23  | b     | 615    | CLA  | CHC-C1C | 5.57 | 1.48        | 1.34     |
| 23  | D     | 404    | CLA  | C3C-C2C | 5.56 | 1.48        | 1.36     |
| 23  | c     | 508    | CLA  | CHC-C1C | 5.56 | 1.48        | 1.34     |
| 23  | B     | 610    | CLA  | C3C-C2C | 5.56 | 1.48        | 1.36     |
| 31  | a     | 406[B] | PHO  | C3D-C2D | 5.55 | 1.49        | 1.39     |
| 23  | c     | 506    | CLA  | CHC-C1C | 5.55 | 1.48        | 1.34     |
| 23  | a     | 405[A] | CLA  | C3B-C2B | 5.55 | 1.47        | 1.40     |
| 23  | b     | 615    | CLA  | C3B-C2B | 5.54 | 1.47        | 1.40     |
| 23  | c     | 513    | CLA  | C3C-C2C | 5.54 | 1.48        | 1.36     |
| 23  | C     | 511    | CLA  | C1D-ND  | 5.53 | 1.45        | 1.37     |
| 23  | d     | 402[B] | CLA  | C3C-C2C | 5.53 | 1.48        | 1.36     |
| 23  | B     | 609    | CLA  | CHC-C1C | 5.52 | 1.48        | 1.34     |
| 23  | C     | 505    | CLA  | CHC-C1C | 5.52 | 1.48        | 1.34     |
| 23  | d     | 404    | CLA  | C3C-C2C | 5.51 | 1.48        | 1.36     |
| 23  | d     | 404    | CLA  | C3B-C2B | 5.51 | 1.47        | 1.40     |
| 23  | B     | 610    | CLA  | CHC-C1C | 5.50 | 1.48        | 1.34     |
| 40  | v     | 201    | HEC  | C3D-C2D | 5.50 | 1.54        | 1.37     |
| 23  | B     | 616    | CLA  | CHC-C1C | 5.49 | 1.48        | 1.34     |
| 23  | b     | 614    | CLA  | CHC-C1C | 5.49 | 1.48        | 1.34     |
| 23  | C     | 506    | CLA  | CHC-C1C | 5.49 | 1.48        | 1.34     |
| 23  | b     | 607    | CLA  | CHC-C1C | 5.49 | 1.48        | 1.34     |
| 23  | B     | 612    | CLA  | CHC-C1C | 5.48 | 1.48        | 1.34     |
| 23  | B     | 613    | CLA  | CHC-C1C | 5.48 | 1.48        | 1.34     |
| 23  | d     | 402[A] | CLA  | C3C-C2C | 5.48 | 1.48        | 1.36     |
| 31  | A     | 416[A] | PHO  | C3D-C2D | 5.48 | 1.49        | 1.39     |
| 23  | B     | 609    | CLA  | C3B-C2B | 5.46 | 1.47        | 1.40     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 31  | a     | 415[B] | PHO  | OBD-CAD | 5.46  | 1.29        | 1.22     |
| 23  | B     | 606    | CLA  | CHC-C1C | 5.46  | 1.48        | 1.34     |
| 40  | v     | 201    | HEC  | C2B-C3B | -5.45 | 1.34        | 1.40     |
| 23  | C     | 508    | CLA  | CHC-C1C | 5.45  | 1.48        | 1.34     |
| 23  | C     | 503    | CLA  | CHC-C1C | 5.44  | 1.48        | 1.34     |
| 23  | c     | 503    | CLA  | C3C-C2C | 5.44  | 1.48        | 1.36     |
| 23  | c     | 511    | CLA  | CHC-C1C | 5.44  | 1.48        | 1.34     |
| 23  | d     | 402[B] | CLA  | CHC-C1C | 5.44  | 1.48        | 1.34     |
| 23  | a     | 404[A] | CLA  | CHC-C1C | 5.43  | 1.47        | 1.34     |
| 31  | A     | 416[B] | PHO  | C3D-C2D | 5.43  | 1.48        | 1.39     |
| 23  | B     | 615    | CLA  | CHC-C1C | 5.43  | 1.47        | 1.34     |
| 23  | b     | 604    | CLA  | CHC-C1C | 5.43  | 1.47        | 1.34     |
| 23  | c     | 514    | CLA  | CHC-C1C | 5.41  | 1.47        | 1.34     |
| 40  | V     | 201    | HEC  | C2B-C3B | -5.41 | 1.34        | 1.40     |
| 23  | c     | 512    | CLA  | CHC-C1C | 5.41  | 1.47        | 1.34     |
| 23  | A     | 406[B] | CLA  | C3C-C2C | 5.41  | 1.48        | 1.36     |
| 23  | A     | 405[A] | CLA  | CHC-C1C | 5.41  | 1.47        | 1.34     |
| 23  | a     | 405[A] | CLA  | CHC-C1C | 5.41  | 1.47        | 1.34     |
| 23  | a     | 404[B] | CLA  | C3C-C2C | 5.40  | 1.48        | 1.36     |
| 23  | b     | 616    | CLA  | CHC-C1C | 5.39  | 1.47        | 1.34     |
| 23  | A     | 404[B] | CLA  | C3C-C2C | 5.38  | 1.48        | 1.36     |
| 23  | B     | 615    | CLA  | C3B-C2B | 5.38  | 1.47        | 1.40     |
| 23  | C     | 513    | CLA  | C3C-C2C | 5.37  | 1.48        | 1.36     |
| 23  | c     | 512    | CLA  | C1D-ND  | 5.37  | 1.44        | 1.37     |
| 23  | b     | 610    | CLA  | C3C-C2C | 5.37  | 1.48        | 1.36     |
| 23  | c     | 513    | CLA  | C3B-C2B | 5.36  | 1.47        | 1.40     |
| 23  | c     | 504    | CLA  | C3C-C2C | 5.36  | 1.48        | 1.36     |
| 23  | b     | 609    | CLA  | O2D-CGD | 5.36  | 1.46        | 1.33     |
| 23  | D     | 403[A] | CLA  | CHC-C1C | 5.35  | 1.47        | 1.34     |
| 23  | b     | 601    | CLA  | CHC-C1C | 5.35  | 1.47        | 1.34     |
| 23  | c     | 506    | CLA  | C3C-C2C | 5.35  | 1.48        | 1.36     |
| 23  | C     | 504    | CLA  | C3B-C2B | 5.35  | 1.47        | 1.40     |
| 23  | B     | 604    | CLA  | C3C-C2C | 5.34  | 1.48        | 1.36     |
| 31  | A     | 416[B] | PHO  | OBD-CAD | 5.34  | 1.29        | 1.22     |
| 23  | A     | 404[A] | CLA  | C3C-C2C | 5.33  | 1.48        | 1.36     |
| 23  | C     | 512    | CLA  | CHC-C1C | 5.33  | 1.47        | 1.34     |
| 23  | b     | 606    | CLA  | CHC-C1C | 5.31  | 1.47        | 1.34     |
| 23  | d     | 403[B] | CLA  | C3C-C2C | 5.31  | 1.48        | 1.36     |
| 23  | b     | 605    | CLA  | C3B-C2B | 5.30  | 1.47        | 1.40     |
| 23  | C     | 514    | CLA  | CHC-C1C | 5.30  | 1.47        | 1.34     |
| 23  | D     | 403[B] | CLA  | C3C-C2C | 5.30  | 1.48        | 1.36     |
| 23  | A     | 404[A] | CLA  | CHC-C1C | 5.30  | 1.47        | 1.34     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | b     | 614    | CLA  | C3C-C2C | 5.30  | 1.48        | 1.36     |
| 23  | c     | 505    | CLA  | C1D-ND  | 5.30  | 1.44        | 1.37     |
| 24  | k     | 101    | BCR  | C23-C22 | -5.30 | 1.34        | 1.46     |
| 23  | c     | 514    | CLA  | C3C-C2C | 5.30  | 1.48        | 1.36     |
| 23  | A     | 405[B] | CLA  | CHC-C1C | 5.30  | 1.47        | 1.34     |
| 24  | C     | 515    | BCR  | C23-C22 | -5.29 | 1.34        | 1.46     |
| 23  | c     | 503    | CLA  | CHC-C1C | 5.29  | 1.47        | 1.34     |
| 23  | c     | 512    | CLA  | C3C-C2C | 5.28  | 1.48        | 1.36     |
| 23  | b     | 601    | CLA  | C3C-C2C | 5.28  | 1.48        | 1.36     |
| 23  | c     | 509    | CLA  | C1D-ND  | 5.27  | 1.44        | 1.37     |
| 23  | d     | 402[A] | CLA  | CHC-C1C | 5.27  | 1.47        | 1.34     |
| 23  | a     | 407    | CLA  | C3C-C2C | 5.27  | 1.48        | 1.36     |
| 23  | B     | 601    | CLA  | C3C-C2C | 5.27  | 1.48        | 1.36     |
| 23  | b     | 605    | CLA  | C3C-C2C | 5.27  | 1.48        | 1.36     |
| 23  | A     | 406[B] | CLA  | C3B-C2B | 5.26  | 1.47        | 1.40     |
| 24  | K     | 102    | BCR  | C23-C22 | -5.26 | 1.34        | 1.46     |
| 23  | b     | 608    | CLA  | CHC-C1C | 5.26  | 1.47        | 1.34     |
| 23  | b     | 612    | CLA  | C3C-C2C | 5.26  | 1.48        | 1.36     |
| 23  | C     | 506    | CLA  | C3B-C2B | 5.25  | 1.47        | 1.40     |
| 23  | B     | 605    | CLA  | C3C-C2C | 5.25  | 1.48        | 1.36     |
| 23  | C     | 509    | CLA  | C3C-C2C | 5.25  | 1.48        | 1.36     |
| 23  | C     | 511    | CLA  | C3C-C2C | 5.25  | 1.48        | 1.36     |
| 23  | b     | 606    | CLA  | C3C-C2C | 5.24  | 1.48        | 1.36     |
| 23  | d     | 402[B] | CLA  | C1D-ND  | 5.24  | 1.44        | 1.37     |
| 23  | c     | 506    | CLA  | C3B-C2B | 5.23  | 1.47        | 1.40     |
| 23  | c     | 502    | CLA  | C3B-C2B | 5.22  | 1.47        | 1.40     |
| 23  | a     | 405[A] | CLA  | C3C-C2C | 5.21  | 1.48        | 1.36     |
| 23  | D     | 403[A] | CLA  | C3C-C2C | 5.21  | 1.48        | 1.36     |
| 23  | c     | 510    | CLA  | O2D-CGD | 5.21  | 1.46        | 1.33     |
| 23  | C     | 509    | CLA  | CHC-C1C | 5.20  | 1.47        | 1.34     |
| 23  | a     | 405[B] | CLA  | C3C-C2C | 5.19  | 1.48        | 1.36     |
| 23  | D     | 404    | CLA  | C1D-ND  | 5.19  | 1.44        | 1.37     |
| 31  | a     | 406[A] | PHO  | O2D-CGD | 5.19  | 1.46        | 1.33     |
| 23  | b     | 613    | CLA  | O2D-CGD | 5.18  | 1.46        | 1.33     |
| 23  | b     | 607    | CLA  | C3C-C2C | 5.18  | 1.47        | 1.36     |
| 23  | C     | 511    | CLA  | CHC-C1C | 5.18  | 1.47        | 1.34     |
| 23  | c     | 505    | CLA  | C3C-C2C | 5.17  | 1.47        | 1.36     |
| 23  | C     | 512    | CLA  | O2D-CGD | 5.17  | 1.45        | 1.33     |
| 23  | b     | 601    | CLA  | C1D-ND  | 5.17  | 1.44        | 1.37     |
| 23  | C     | 510    | CLA  | C3C-C2C | 5.16  | 1.47        | 1.36     |
| 23  | c     | 503    | CLA  | C1D-ND  | 5.15  | 1.44        | 1.37     |
| 23  | B     | 601    | CLA  | O2A-CGA | 5.14  | 1.48        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 511    | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 23  | c     | 514    | CLA  | C1D-ND  | 5.11  | 1.44        | 1.37     |
| 23  | b     | 615    | CLA  | C3C-C2C | 5.10  | 1.47        | 1.36     |
| 23  | A     | 404[B] | CLA  | C1D-ND  | 5.10  | 1.44        | 1.37     |
| 23  | B     | 606    | CLA  | C3C-C2C | 5.10  | 1.47        | 1.36     |
| 23  | B     | 603    | CLA  | C3C-C2C | 5.09  | 1.47        | 1.36     |
| 23  | b     | 602    | CLA  | C3B-C2B | 5.09  | 1.47        | 1.40     |
| 23  | A     | 405[A] | CLA  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 23  | B     | 609    | CLA  | C3C-C2C | 5.09  | 1.47        | 1.36     |
| 23  | D     | 404    | CLA  | C3B-C2B | 5.08  | 1.47        | 1.40     |
| 23  | C     | 502    | CLA  | C3C-C2C | 5.08  | 1.47        | 1.36     |
| 23  | d     | 403[A] | CLA  | CHC-C1C | 5.08  | 1.47        | 1.34     |
| 23  | c     | 505    | CLA  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 23  | B     | 605    | CLA  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 23  | C     | 503    | CLA  | C1D-ND  | 5.06  | 1.44        | 1.37     |
| 23  | b     | 602    | CLA  | C3C-C2C | 5.06  | 1.47        | 1.36     |
| 23  | c     | 507    | CLA  | CHC-C1C | 5.05  | 1.47        | 1.34     |
| 23  | B     | 612    | CLA  | C3C-C2C | 5.05  | 1.47        | 1.36     |
| 23  | B     | 610    | CLA  | C3B-C2B | 5.05  | 1.47        | 1.40     |
| 40  | V     | 201    | HEC  | C3D-C2D | 5.05  | 1.52        | 1.37     |
| 23  | A     | 405[A] | CLA  | C3B-C2B | 5.04  | 1.47        | 1.40     |
| 23  | c     | 510    | CLA  | C3C-C2C | 5.04  | 1.47        | 1.36     |
| 23  | A     | 406[A] | CLA  | C3C-C2C | 5.04  | 1.47        | 1.36     |
| 24  | d     | 405    | BCR  | C23-C22 | -5.04 | 1.35        | 1.46     |
| 23  | C     | 506    | CLA  | C3C-C2C | 5.04  | 1.47        | 1.36     |
| 23  | c     | 511    | CLA  | C1D-ND  | 5.03  | 1.44        | 1.37     |
| 23  | c     | 505    | CLA  | CHC-C1C | 5.03  | 1.47        | 1.34     |
| 23  | c     | 502    | CLA  | C3C-C2C | 5.03  | 1.47        | 1.36     |
| 23  | C     | 509    | CLA  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 23  | b     | 615    | CLA  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 23  | B     | 605    | CLA  | C3B-C2B | 5.02  | 1.47        | 1.40     |
| 23  | b     | 611    | CLA  | CHC-C1C | 5.02  | 1.46        | 1.34     |
| 23  | d     | 402[A] | CLA  | C1D-ND  | 5.01  | 1.44        | 1.37     |
| 23  | C     | 514    | CLA  | C1D-ND  | 5.01  | 1.44        | 1.37     |
| 23  | C     | 508    | CLA  | C3C-C2C | 5.01  | 1.47        | 1.36     |
| 23  | c     | 507    | CLA  | C3C-C2C | 5.01  | 1.47        | 1.36     |
| 23  | C     | 507    | CLA  | CHC-C1C | 5.01  | 1.46        | 1.34     |
| 23  | B     | 614    | CLA  | CHC-C1C | 5.01  | 1.46        | 1.34     |
| 23  | A     | 406[B] | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 24  | T     | 102    | BCR  | C23-C22 | -5.00 | 1.35        | 1.46     |
| 23  | d     | 403[A] | CLA  | C3C-C2C | 5.00  | 1.47        | 1.36     |
| 23  | b     | 602    | CLA  | O2D-CGD | 4.99  | 1.45        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 505    | CLA  | C3C-C2C | 4.99  | 1.47        | 1.36     |
| 23  | D     | 403[B] | CLA  | CHC-C1C | 4.99  | 1.46        | 1.34     |
| 31  | A     | 416[B] | PHO  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 31  | a     | 415[B] | PHO  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 23  | B     | 604    | CLA  | CHC-C1C | 4.98  | 1.46        | 1.34     |
| 23  | C     | 514    | CLA  | C3C-C2C | 4.97  | 1.47        | 1.36     |
| 23  | c     | 508    | CLA  | C3C-C2C | 4.97  | 1.47        | 1.36     |
| 23  | B     | 602    | CLA  | C3C-C2C | 4.97  | 1.47        | 1.36     |
| 23  | B     | 614    | CLA  | C3C-C2C | 4.96  | 1.47        | 1.36     |
| 23  | b     | 603    | CLA  | C3C-C2C | 4.96  | 1.47        | 1.36     |
| 23  | B     | 615    | CLA  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 23  | b     | 605    | CLA  | CHC-C1C | 4.96  | 1.46        | 1.34     |
| 23  | B     | 604    | CLA  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 23  | c     | 502    | CLA  | C1D-ND  | 4.95  | 1.44        | 1.37     |
| 23  | c     | 511    | CLA  | C3C-C2C | 4.95  | 1.47        | 1.36     |
| 23  | b     | 603    | CLA  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 31  | D     | 401[B] | PHO  | OBD-CAD | 4.95  | 1.28        | 1.22     |
| 23  | b     | 612    | CLA  | CHC-C1C | 4.95  | 1.46        | 1.34     |
| 31  | D     | 401[B] | PHO  | C3D-C2D | 4.94  | 1.48        | 1.39     |
| 23  | d     | 402[B] | CLA  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 23  | b     | 601    | CLA  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 23  | C     | 510    | CLA  | CHC-C1C | 4.93  | 1.46        | 1.34     |
| 23  | a     | 404[A] | CLA  | C3C-C2C | 4.93  | 1.47        | 1.36     |
| 23  | C     | 503    | CLA  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 24  | t     | 102    | BCR  | C23-C22 | -4.92 | 1.35        | 1.46     |
| 23  | A     | 405[B] | CLA  | C3C-C2C | 4.92  | 1.47        | 1.36     |
| 23  | D     | 404    | CLA  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 23  | B     | 615    | CLA  | C3C-C2C | 4.92  | 1.47        | 1.36     |
| 23  | B     | 601    | CLA  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 23  | c     | 508    | CLA  | C3B-C2B | 4.91  | 1.47        | 1.40     |
| 23  | d     | 403[B] | CLA  | CHC-C1C | 4.91  | 1.46        | 1.34     |
| 31  | D     | 401[A] | PHO  | C3D-C2D | 4.91  | 1.48        | 1.39     |
| 23  | b     | 609    | CLA  | C3C-C2C | 4.90  | 1.47        | 1.36     |
| 23  | d     | 402[A] | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 31  | A     | 416[A] | PHO  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 23  | b     | 611    | CLA  | C3C-C2C | 4.90  | 1.47        | 1.36     |
| 23  | b     | 604    | CLA  | C1D-ND  | 4.90  | 1.44        | 1.37     |
| 23  | a     | 405[B] | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 23  | a     | 404[B] | CLA  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 23  | b     | 601    | CLA  | O2A-CGA | 4.89  | 1.47        | 1.33     |
| 23  | A     | 407    | CLA  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 23  | B     | 616    | CLA  | C3C-C2C | 4.89  | 1.47        | 1.36     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 514    | CLA  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 23  | C     | 510    | CLA  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 23  | C     | 509    | CLA  | C1D-ND  | 4.88  | 1.44        | 1.37     |
| 23  | b     | 616    | CLA  | O2D-CGD | 4.88  | 1.45        | 1.33     |
| 31  | a     | 406[B] | PHO  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 25  | X     | 101    | SQD  | O47-C7  | 4.87  | 1.48        | 1.34     |
| 23  | A     | 405[A] | CLA  | C3C-C2C | 4.87  | 1.47        | 1.36     |
| 23  | B     | 608    | CLA  | CHC-C1C | 4.86  | 1.46        | 1.34     |
| 23  | B     | 607    | CLA  | C3C-C2C | 4.86  | 1.47        | 1.36     |
| 31  | D     | 401[A] | PHO  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 31  | D     | 401[B] | PHO  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 23  | C     | 507    | CLA  | C3C-C2C | 4.85  | 1.47        | 1.36     |
| 23  | c     | 507    | CLA  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 23  | D     | 403[A] | CLA  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 23  | c     | 504    | CLA  | C3B-C2B | 4.83  | 1.46        | 1.40     |
| 23  | b     | 608    | CLA  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 31  | a     | 406[B] | PHO  | OBD-CAD | 4.82  | 1.28        | 1.22     |
| 23  | C     | 505    | CLA  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 23  | a     | 405[B] | CLA  | C1D-ND  | 4.82  | 1.44        | 1.37     |
| 23  | A     | 404[B] | CLA  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 23  | d     | 404    | CLA  | C1D-ND  | 4.80  | 1.44        | 1.37     |
| 24  | D     | 405    | BCR  | C23-C22 | -4.80 | 1.35        | 1.46     |
| 23  | c     | 503    | CLA  | O2D-CGD | 4.80  | 1.45        | 1.33     |
| 23  | c     | 510    | CLA  | CHC-C1C | 4.80  | 1.46        | 1.34     |
| 23  | b     | 613    | CLA  | C3C-C2C | 4.80  | 1.47        | 1.36     |
| 23  | b     | 616    | CLA  | C3C-C2C | 4.79  | 1.47        | 1.36     |
| 31  | a     | 415[A] | PHO  | O2D-CGD | 4.79  | 1.45        | 1.33     |
| 23  | D     | 403[B] | CLA  | O2D-CGD | 4.79  | 1.45        | 1.33     |
| 23  | a     | 404[B] | CLA  | C1D-ND  | 4.78  | 1.44        | 1.37     |
| 34  | c     | 521    | LMG  | O7-C10  | 4.78  | 1.47        | 1.34     |
| 23  | b     | 611    | CLA  | O2D-CGD | 4.77  | 1.45        | 1.33     |
| 23  | c     | 508    | CLA  | O2D-CGD | 4.77  | 1.45        | 1.33     |
| 23  | A     | 405[B] | CLA  | O2D-CGD | 4.77  | 1.45        | 1.33     |
| 23  | b     | 610    | CLA  | O2D-CGD | 4.77  | 1.45        | 1.33     |
| 23  | b     | 606    | CLA  | C1D-ND  | 4.77  | 1.44        | 1.37     |
| 23  | B     | 608    | CLA  | C3C-C2C | 4.76  | 1.47        | 1.36     |
| 23  | b     | 604    | CLA  | C3C-C2C | 4.76  | 1.47        | 1.36     |
| 23  | B     | 610    | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 23  | B     | 603    | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 23  | a     | 404[A] | CLA  | C1D-ND  | 4.74  | 1.44        | 1.37     |
| 23  | b     | 610    | CLA  | C1D-ND  | 4.74  | 1.44        | 1.37     |
| 24  | C     | 516    | BCR  | C23-C22 | -4.74 | 1.35        | 1.46     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | A     | 404[A] | CLA  | C1D-ND  | 4.74  | 1.44        | 1.37     |
| 24  | c     | 515    | BCR  | C23-C22 | -4.74 | 1.35        | 1.46     |
| 25  | a     | 411    | SQD  | O48-C23 | 4.73  | 1.47        | 1.33     |
| 23  | d     | 403[B] | CLA  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 23  | A     | 404[A] | CLA  | O2D-CGD | 4.72  | 1.44        | 1.33     |
| 23  | A     | 407    | CLA  | C3C-C2C | 4.72  | 1.47        | 1.36     |
| 23  | A     | 406[B] | CLA  | C1D-ND  | 4.72  | 1.44        | 1.37     |
| 23  | c     | 504    | CLA  | CHD-C1D | 4.71  | 1.47        | 1.38     |
| 23  | C     | 506    | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |
| 23  | C     | 514    | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |
| 23  | c     | 504    | CLA  | C1D-ND  | 4.70  | 1.44        | 1.37     |
| 23  | d     | 402[A] | CLA  | C3B-C2B | 4.69  | 1.46        | 1.40     |
| 23  | B     | 611    | CLA  | O2D-CGD | 4.69  | 1.44        | 1.33     |
| 23  | C     | 513    | CLA  | O2D-CGD | 4.69  | 1.44        | 1.33     |
| 23  | B     | 603    | CLA  | CHC-C1C | 4.69  | 1.46        | 1.34     |
| 23  | b     | 608    | CLA  | C3C-C2C | 4.68  | 1.46        | 1.36     |
| 23  | C     | 512    | CLA  | C3C-C2C | 4.68  | 1.46        | 1.36     |
| 23  | A     | 406[A] | CLA  | O2D-CGD | 4.68  | 1.44        | 1.33     |
| 23  | C     | 507    | CLA  | O2D-CGD | 4.68  | 1.44        | 1.33     |
| 23  | B     | 615    | CLA  | C1D-ND  | 4.67  | 1.44        | 1.37     |
| 23  | d     | 404    | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 23  | B     | 614    | CLA  | C1D-ND  | 4.67  | 1.44        | 1.37     |
| 24  | b     | 619    | BCR  | C23-C22 | -4.67 | 1.36        | 1.46     |
| 34  | C     | 521    | LMG  | O7-C10  | 4.66  | 1.47        | 1.34     |
| 24  | B     | 619    | BCR  | C23-C22 | -4.66 | 1.36        | 1.46     |
| 25  | f     | 102    | SQD  | O47-C7  | 4.65  | 1.47        | 1.34     |
| 23  | A     | 407    | CLA  | CHC-C1C | 4.64  | 1.46        | 1.34     |
| 23  | B     | 606    | CLA  | O2D-CGD | 4.64  | 1.44        | 1.33     |
| 24  | y     | 101    | BCR  | C23-C22 | -4.64 | 1.36        | 1.46     |
| 23  | b     | 602    | CLA  | CHD-C1D | 4.63  | 1.47        | 1.38     |
| 25  | l     | 101    | SQD  | O47-C7  | 4.62  | 1.47        | 1.34     |
| 23  | B     | 616    | CLA  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 23  | b     | 605    | CLA  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 31  | A     | 416[A] | PHO  | CHA-CBD | -4.61 | 1.47        | 1.52     |
| 23  | B     | 605    | CLA  | C1D-ND  | 4.61  | 1.43        | 1.37     |
| 23  | b     | 613    | CLA  | C1D-ND  | 4.61  | 1.43        | 1.37     |
| 23  | c     | 513    | CLA  | C1D-ND  | 4.61  | 1.43        | 1.37     |
| 23  | B     | 602    | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 23  | c     | 507    | CLA  | C1D-ND  | 4.61  | 1.43        | 1.37     |
| 23  | a     | 405[A] | CLA  | O2D-CGD | 4.60  | 1.44        | 1.33     |
| 23  | b     | 616    | CLA  | C1D-ND  | 4.60  | 1.43        | 1.37     |
| 23  | B     | 609    | CLA  | O2D-CGD | 4.60  | 1.44        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 503    | CLA  | C3C-C2C | 4.59  | 1.46        | 1.36     |
| 23  | A     | 406[A] | CLA  | C3B-C2B | 4.59  | 1.46        | 1.40     |
| 24  | A     | 408    | BCR  | C23-C22 | -4.59 | 1.36        | 1.46     |
| 23  | a     | 407    | CLA  | O2D-CGD | 4.59  | 1.44        | 1.33     |
| 23  | a     | 407    | CLA  | O2A-CGA | 4.59  | 1.46        | 1.33     |
| 23  | C     | 511    | CLA  | O2D-CGD | 4.59  | 1.44        | 1.33     |
| 33  | E     | 101[A] | LHG  | O8-C23  | 4.58  | 1.46        | 1.33     |
| 23  | c     | 508    | CLA  | O2A-CGA | 4.58  | 1.46        | 1.33     |
| 23  | c     | 506    | CLA  | O2D-CGD | 4.58  | 1.44        | 1.33     |
| 23  | C     | 513    | CLA  | C1D-ND  | 4.57  | 1.43        | 1.37     |
| 23  | b     | 615    | CLA  | C1D-ND  | 4.57  | 1.43        | 1.37     |
| 23  | b     | 606    | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |
| 34  | C     | 521    | LMG  | O8-C28  | 4.56  | 1.46        | 1.33     |
| 24  | c     | 516    | BCR  | C23-C22 | -4.56 | 1.36        | 1.46     |
| 23  | C     | 504    | CLA  | O2D-CGD | 4.55  | 1.44        | 1.33     |
| 34  | z     | 101    | LMG  | O8-C28  | 4.55  | 1.46        | 1.33     |
| 23  | d     | 403[A] | CLA  | O2D-CGD | 4.54  | 1.44        | 1.33     |
| 23  | c     | 514    | CLA  | CHD-C1D | 4.54  | 1.47        | 1.38     |
| 23  | B     | 609    | CLA  | CHD-C1D | 4.53  | 1.47        | 1.38     |
| 23  | B     | 616    | CLA  | C1D-ND  | 4.52  | 1.43        | 1.37     |
| 23  | b     | 607    | CLA  | O2D-CGD | 4.52  | 1.44        | 1.33     |
| 24  | b     | 618    | BCR  | C23-C22 | -4.51 | 1.36        | 1.46     |
| 33  | a     | 419[A] | LHG  | O8-C23  | 4.51  | 1.46        | 1.33     |
| 23  | B     | 613    | CLA  | C3C-C2C | 4.51  | 1.46        | 1.36     |
| 23  | A     | 406[B] | CLA  | CHD-C1D | 4.50  | 1.47        | 1.38     |
| 24  | b     | 617    | BCR  | C23-C22 | -4.50 | 1.36        | 1.46     |
| 23  | C     | 503    | CLA  | C3D-C2D | 4.50  | 1.51        | 1.39     |
| 23  | B     | 613    | CLA  | O2D-CGD | 4.49  | 1.44        | 1.33     |
| 23  | B     | 603    | CLA  | C1D-ND  | 4.49  | 1.43        | 1.37     |
| 23  | d     | 402[B] | CLA  | O2A-CGA | 4.49  | 1.46        | 1.33     |
| 33  | E     | 101[B] | LHG  | O8-C23  | 4.48  | 1.46        | 1.33     |
| 23  | b     | 612    | CLA  | O2D-CGD | 4.47  | 1.44        | 1.33     |
| 23  | A     | 405[B] | CLA  | C1D-ND  | 4.46  | 1.43        | 1.37     |
| 23  | B     | 608    | CLA  | C1D-ND  | 4.46  | 1.43        | 1.37     |
| 23  | c     | 513    | CLA  | O2D-CGD | 4.46  | 1.44        | 1.33     |
| 24  | H     | 101    | BCR  | C23-C22 | -4.46 | 1.36        | 1.46     |
| 23  | b     | 604    | CLA  | O2D-CGD | 4.46  | 1.44        | 1.33     |
| 23  | B     | 610    | CLA  | C1D-ND  | 4.45  | 1.43        | 1.37     |
| 24  | Y     | 101    | BCR  | C23-C22 | -4.45 | 1.36        | 1.46     |
| 25  | A     | 411    | SQD  | O48-C23 | 4.45  | 1.46        | 1.33     |
| 23  | C     | 510    | CLA  | CHD-C1D | 4.45  | 1.47        | 1.38     |
| 23  | B     | 615    | CLA  | CHD-C1D | 4.45  | 1.47        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 512    | CLA  | CHD-C1D | 4.44  | 1.47        | 1.38     |
| 23  | C     | 506    | CLA  | CHD-C1D | 4.43  | 1.47        | 1.38     |
| 23  | B     | 609    | CLA  | O2A-CGA | 4.43  | 1.46        | 1.33     |
| 23  | c     | 512    | CLA  | O2D-CGD | 4.43  | 1.44        | 1.33     |
| 23  | b     | 601    | CLA  | CHD-C1D | 4.43  | 1.47        | 1.38     |
| 23  | c     | 514    | CLA  | O2A-CGA | 4.43  | 1.46        | 1.33     |
| 23  | B     | 608    | CLA  | O2D-CGD | 4.42  | 1.44        | 1.33     |
| 25  | b     | 620    | SQD  | O48-C23 | 4.42  | 1.46        | 1.33     |
| 23  | c     | 508    | CLA  | C1D-ND  | 4.42  | 1.43        | 1.37     |
| 23  | B     | 604    | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 23  | b     | 604    | CLA  | CHD-C1D | 4.41  | 1.47        | 1.38     |
| 23  | D     | 403[B] | CLA  | O2A-CGA | 4.41  | 1.46        | 1.33     |
| 23  | B     | 616    | CLA  | C3D-C2D | 4.41  | 1.51        | 1.39     |
| 31  | D     | 401[A] | PHO  | OBD-CAD | 4.41  | 1.28        | 1.22     |
| 24  | a     | 408    | BCR  | C23-C22 | -4.39 | 1.36        | 1.46     |
| 24  | h     | 101    | BCR  | C23-C22 | -4.39 | 1.36        | 1.46     |
| 23  | b     | 614    | CLA  | O2D-CGD | 4.38  | 1.44        | 1.33     |
| 23  | C     | 502    | CLA  | C1D-ND  | 4.38  | 1.43        | 1.37     |
| 23  | b     | 602    | CLA  | C1D-ND  | 4.37  | 1.43        | 1.37     |
| 25  | b     | 620    | SQD  | O47-C7  | 4.37  | 1.46        | 1.34     |
| 40  | V     | 201    | HEC  | C3C-C2C | -4.36 | 1.35        | 1.40     |
| 23  | C     | 503    | CLA  | CHD-C1D | 4.36  | 1.46        | 1.38     |
| 23  | c     | 513    | CLA  | O2A-CGA | 4.36  | 1.46        | 1.33     |
| 23  | d     | 402[A] | CLA  | C3D-C2D | 4.36  | 1.50        | 1.39     |
| 33  | a     | 419[B] | LHG  | O8-C23  | 4.36  | 1.46        | 1.33     |
| 24  | B     | 617    | BCR  | C23-C22 | -4.35 | 1.36        | 1.46     |
| 23  | b     | 602    | CLA  | CHD-C4C | 4.35  | 1.49        | 1.39     |
| 23  | C     | 510    | CLA  | C3D-C2D | 4.34  | 1.50        | 1.39     |
| 23  | a     | 404[A] | CLA  | O2D-CGD | 4.34  | 1.43        | 1.33     |
| 23  | C     | 514    | CLA  | O2A-CGA | 4.33  | 1.46        | 1.33     |
| 23  | d     | 403[B] | CLA  | O2A-CGA | 4.33  | 1.46        | 1.33     |
| 23  | c     | 502    | CLA  | O2D-CGD | 4.32  | 1.43        | 1.33     |
| 23  | C     | 502    | CLA  | O2D-CGD | 4.32  | 1.43        | 1.33     |
| 23  | b     | 605    | CLA  | C1D-ND  | 4.32  | 1.43        | 1.37     |
| 23  | d     | 404    | CLA  | O2A-CGA | 4.32  | 1.45        | 1.33     |
| 34  | m     | 101    | LMG  | O8-C28  | 4.31  | 1.45        | 1.33     |
| 23  | C     | 507    | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 23  | A     | 407    | CLA  | O2A-CGA | 4.31  | 1.45        | 1.33     |
| 23  | B     | 612    | CLA  | O2D-CGD | 4.30  | 1.43        | 1.33     |
| 23  | b     | 612    | CLA  | C1D-ND  | 4.30  | 1.43        | 1.37     |
| 23  | B     | 611    | CLA  | OBD-CAD | 4.29  | 1.29        | 1.22     |
| 34  | B     | 620    | LMG  | O8-C28  | 4.29  | 1.45        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | b     | 614    | CLA  | C1D-ND  | 4.29  | 1.43        | 1.37     |
| 23  | c     | 505    | CLA  | C3D-C2D | 4.29  | 1.50        | 1.39     |
| 23  | c     | 507    | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 33  | a     | 419[A] | LHG  | O7-C7   | 4.28  | 1.46        | 1.34     |
| 23  | B     | 601    | CLA  | C1D-ND  | 4.28  | 1.43        | 1.37     |
| 40  | v     | 201    | HEC  | C3C-C2C | -4.28 | 1.35        | 1.40     |
| 23  | c     | 507    | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 34  | C     | 520    | LMG  | O8-C28  | 4.28  | 1.45        | 1.33     |
| 23  | d     | 402[B] | CLA  | C3D-C2D | 4.28  | 1.50        | 1.39     |
| 23  | a     | 405[B] | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 25  | f     | 102    | SQD  | O48-C23 | 4.27  | 1.45        | 1.33     |
| 23  | b     | 601    | CLA  | C3D-C2D | 4.27  | 1.50        | 1.39     |
| 23  | d     | 403[B] | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 23  | c     | 513    | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 34  | c     | 521    | LMG  | O8-C28  | 4.25  | 1.45        | 1.33     |
| 23  | C     | 508    | CLA  | O2D-CGD | 4.25  | 1.43        | 1.33     |
| 23  | B     | 603    | CLA  | C3D-C2D | 4.25  | 1.50        | 1.39     |
| 23  | A     | 404[B] | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 23  | A     | 405[B] | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 23  | C     | 510    | CLA  | C1D-ND  | 4.24  | 1.43        | 1.37     |
| 23  | B     | 606    | CLA  | C1D-ND  | 4.24  | 1.43        | 1.37     |
| 23  | C     | 508    | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 23  | c     | 505    | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 23  | D     | 404    | CLA  | CHD-C1D | 4.23  | 1.46        | 1.38     |
| 23  | b     | 608    | CLA  | C3D-C2D | 4.23  | 1.50        | 1.39     |
| 23  | c     | 512    | CLA  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 23  | c     | 503    | CLA  | C3D-C2D | 4.23  | 1.50        | 1.39     |
| 23  | C     | 509    | CLA  | C3D-C2D | 4.22  | 1.50        | 1.39     |
| 23  | A     | 404[B] | CLA  | CHD-C4C | 4.22  | 1.48        | 1.39     |
| 23  | b     | 603    | CLA  | C1D-ND  | 4.22  | 1.43        | 1.37     |
| 33  | E     | 101[A] | LHG  | O7-C7   | 4.22  | 1.46        | 1.34     |
| 23  | B     | 614    | CLA  | O2D-CGD | 4.21  | 1.43        | 1.33     |
| 23  | C     | 512    | CLA  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 23  | b     | 611    | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 33  | d     | 408[A] | LHG  | O8-C23  | 4.20  | 1.45        | 1.33     |
| 25  | A     | 411    | SQD  | O47-C7  | 4.20  | 1.46        | 1.34     |
| 23  | A     | 405[A] | CLA  | C1D-ND  | 4.20  | 1.43        | 1.37     |
| 33  | a     | 419[B] | LHG  | O7-C7   | 4.19  | 1.46        | 1.34     |
| 23  | b     | 609    | CLA  | OBD-CAD | 4.19  | 1.29        | 1.22     |
| 23  | c     | 507    | CLA  | C3D-C2D | 4.19  | 1.50        | 1.39     |
| 36  | c     | 517[B] | DGD  | O2G-C1B | 4.19  | 1.46        | 1.34     |
| 23  | D     | 403[A] | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 23  | C     | 508    | CLA  | CHD-C1D | 4.19 | 1.46        | 1.38     |
| 33  | d     | 408[B] | LHG  | O8-C23  | 4.18 | 1.45        | 1.33     |
| 23  | c     | 510    | CLA  | C1D-ND  | 4.18 | 1.43        | 1.37     |
| 23  | C     | 510    | CLA  | OBD-CAD | 4.18 | 1.29        | 1.22     |
| 33  | E     | 101[B] | LHG  | O7-C7   | 4.18 | 1.46        | 1.34     |
| 34  | Z     | 101    | LMG  | O7-C10  | 4.18 | 1.46        | 1.34     |
| 23  | B     | 610    | CLA  | C3D-C2D | 4.17 | 1.50        | 1.39     |
| 23  | b     | 614    | CLA  | CHD-C1D | 4.17 | 1.46        | 1.38     |
| 23  | c     | 509    | CLA  | O2A-CGA | 4.17 | 1.45        | 1.33     |
| 23  | A     | 407    | CLA  | CHD-C1D | 4.17 | 1.46        | 1.38     |
| 23  | c     | 509    | CLA  | C3D-C2D | 4.17 | 1.50        | 1.39     |
| 23  | c     | 506    | CLA  | CHD-C1D | 4.17 | 1.46        | 1.38     |
| 23  | a     | 404[B] | CLA  | CHD-C4C | 4.16 | 1.48        | 1.39     |
| 23  | c     | 502    | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 23  | B     | 609    | CLA  | C3D-C2D | 4.16 | 1.50        | 1.39     |
| 33  | L     | 101[B] | LHG  | O8-C23  | 4.16 | 1.45        | 1.33     |
| 23  | C     | 512    | CLA  | CHD-C4C | 4.16 | 1.48        | 1.39     |
| 23  | c     | 508    | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 23  | A     | 405[B] | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 23  | D     | 403[A] | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 23  | A     | 405[A] | CLA  | C3D-C2D | 4.15 | 1.50        | 1.39     |
| 23  | b     | 611    | CLA  | C1D-ND  | 4.15 | 1.43        | 1.37     |
| 23  | c     | 514    | CLA  | CHD-C4C | 4.15 | 1.48        | 1.39     |
| 23  | b     | 613    | CLA  | C3D-C2D | 4.14 | 1.50        | 1.39     |
| 23  | b     | 608    | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 23  | c     | 503    | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 23  | d     | 402[B] | CLA  | CHD-C1D | 4.14 | 1.46        | 1.38     |
| 25  | l     | 101    | SQD  | O48-C23 | 4.14 | 1.45        | 1.33     |
| 36  | C     | 517[B] | DGD  | O2G-C1B | 4.14 | 1.46        | 1.34     |
| 23  | A     | 405[B] | CLA  | C3D-C2D | 4.13 | 1.50        | 1.39     |
| 23  | a     | 405[A] | CLA  | C1D-ND  | 4.13 | 1.43        | 1.37     |
| 36  | C     | 517[A] | DGD  | O2G-C1B | 4.13 | 1.46        | 1.34     |
| 23  | d     | 404    | CLA  | CHD-C1D | 4.13 | 1.46        | 1.38     |
| 31  | a     | 406[A] | PHO  | OBD-CAD | 4.13 | 1.27        | 1.22     |
| 23  | a     | 405[B] | CLA  | C3D-C2D | 4.13 | 1.50        | 1.39     |
| 23  | C     | 506    | CLA  | C1D-ND  | 4.13 | 1.43        | 1.37     |
| 23  | d     | 402[A] | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 23  | a     | 404[A] | CLA  | CHD-C4C | 4.12 | 1.48        | 1.39     |
| 23  | c     | 502    | CLA  | CHD-C4C | 4.12 | 1.48        | 1.39     |
| 23  | C     | 514    | CLA  | CHD-C1D | 4.12 | 1.46        | 1.38     |
| 23  | B     | 607    | CLA  | CHD-C1D | 4.11 | 1.46        | 1.38     |
| 23  | C     | 514    | CLA  | CHD-C4C | 4.11 | 1.48        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 36  | c     | 519    | DGD  | O1G-C1A | 4.11 | 1.45        | 1.33     |
| 23  | b     | 608    | CLA  | OBD-CAD | 4.11 | 1.29        | 1.22     |
| 23  | C     | 502    | CLA  | CHD-C1D | 4.10 | 1.46        | 1.38     |
| 36  | c     | 518[B] | DGD  | O1G-C1A | 4.10 | 1.45        | 1.33     |
| 25  | a     | 409[B] | SQD  | O48-C23 | 4.10 | 1.45        | 1.33     |
| 23  | c     | 503    | CLA  | CHD-C1D | 4.10 | 1.46        | 1.38     |
| 23  | c     | 512    | CLA  | CHD-C4C | 4.09 | 1.48        | 1.39     |
| 23  | b     | 606    | CLA  | CHD-C4C | 4.09 | 1.48        | 1.39     |
| 34  | C     | 501    | LMG  | O7-C10  | 4.09 | 1.45        | 1.34     |
| 23  | b     | 616    | CLA  | O2A-CGA | 4.09 | 1.45        | 1.33     |
| 23  | b     | 610    | CLA  | CHD-C4C | 4.09 | 1.48        | 1.39     |
| 34  | z     | 101    | LMG  | O7-C10  | 4.08 | 1.45        | 1.34     |
| 23  | a     | 404[B] | CLA  | O2A-CGA | 4.08 | 1.45        | 1.33     |
| 23  | b     | 603    | CLA  | CHD-C1D | 4.08 | 1.46        | 1.38     |
| 23  | a     | 404[A] | CLA  | CHD-C1D | 4.08 | 1.46        | 1.38     |
| 23  | A     | 405[A] | CLA  | O2A-CGA | 4.08 | 1.45        | 1.33     |
| 23  | b     | 609    | CLA  | CHD-C1D | 4.08 | 1.46        | 1.38     |
| 23  | b     | 615    | CLA  | O2A-CGA | 4.07 | 1.45        | 1.33     |
| 23  | c     | 508    | CLA  | CHD-C4C | 4.07 | 1.48        | 1.39     |
| 23  | A     | 406[A] | CLA  | CHD-C1D | 4.07 | 1.46        | 1.38     |
| 23  | c     | 511    | CLA  | CHD-C4C | 4.07 | 1.48        | 1.39     |
| 23  | c     | 513    | CLA  | CHD-C4C | 4.07 | 1.48        | 1.39     |
| 34  | C     | 520    | LMG  | O7-C10  | 4.07 | 1.45        | 1.34     |
| 33  | D     | 408[B] | LHG  | O7-C7   | 4.07 | 1.45        | 1.34     |
| 23  | c     | 506    | CLA  | OBD-CAD | 4.07 | 1.29        | 1.22     |
| 23  | C     | 514    | CLA  | C3D-C2D | 4.07 | 1.50        | 1.39     |
| 23  | d     | 403[B] | CLA  | C1D-ND  | 4.06 | 1.43        | 1.37     |
| 23  | A     | 406[B] | CLA  | CHD-C4C | 4.06 | 1.48        | 1.39     |
| 23  | B     | 610    | CLA  | OBD-CAD | 4.06 | 1.29        | 1.22     |
| 23  | c     | 509    | CLA  | CHD-C1D | 4.06 | 1.46        | 1.38     |
| 34  | c     | 501    | LMG  | O8-C28  | 4.06 | 1.45        | 1.33     |
| 23  | b     | 610    | CLA  | CHD-C1D | 4.05 | 1.46        | 1.38     |
| 23  | c     | 507    | CLA  | CHD-C4C | 4.05 | 1.48        | 1.39     |
| 25  | a     | 409[A] | SQD  | O47-C7  | 4.05 | 1.45        | 1.34     |
| 23  | C     | 509    | CLA  | O2A-CGA | 4.05 | 1.45        | 1.33     |
| 23  | C     | 513    | CLA  | O2A-CGA | 4.05 | 1.45        | 1.33     |
| 23  | B     | 602    | CLA  | C1D-ND  | 4.05 | 1.43        | 1.37     |
| 23  | B     | 608    | CLA  | CHD-C1D | 4.05 | 1.46        | 1.38     |
| 23  | b     | 606    | CLA  | CHD-C1D | 4.05 | 1.46        | 1.38     |
| 23  | B     | 607    | CLA  | O2D-CGD | 4.04 | 1.43        | 1.33     |
| 23  | b     | 608    | CLA  | CHD-C1D | 4.04 | 1.46        | 1.38     |
| 34  | c     | 520    | LMG  | O7-C10  | 4.04 | 1.45        | 1.34     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 615    | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 33  | d     | 414[B] | LHG  | O8-C23  | 4.04  | 1.45        | 1.33     |
| 23  | c     | 506    | CLA  | C1D-ND  | 4.04  | 1.43        | 1.37     |
| 23  | B     | 615    | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 23  | B     | 612    | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 23  | C     | 513    | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 36  | C     | 519    | DGD  | O1G-C1A | 4.04  | 1.45        | 1.33     |
| 23  | B     | 609    | CLA  | C1D-ND  | 4.03  | 1.43        | 1.37     |
| 31  | A     | 416[A] | PHO  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 25  | X     | 101    | SQD  | O48-C23 | 4.02  | 1.45        | 1.33     |
| 23  | b     | 607    | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 31  | a     | 415[B] | PHO  | C3C-C2C | 4.02  | 1.49        | 1.37     |
| 23  | B     | 614    | CLA  | CHD-C4C | 4.02  | 1.48        | 1.39     |
| 23  | C     | 513    | CLA  | C3D-C2D | 4.02  | 1.50        | 1.39     |
| 23  | D     | 403[B] | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 23  | c     | 514    | CLA  | C3D-C2D | 4.02  | 1.50        | 1.39     |
| 23  | b     | 615    | CLA  | C3D-C2D | 4.01  | 1.49        | 1.39     |
| 23  | d     | 403[B] | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 23  | a     | 405[A] | CLA  | C3D-C2D | 4.01  | 1.49        | 1.39     |
| 23  | C     | 512    | CLA  | CHD-C1D | 4.01  | 1.46        | 1.38     |
| 36  | c     | 518[A] | DGD  | O1G-C1A | 4.01  | 1.45        | 1.33     |
| 23  | C     | 507    | CLA  | C1D-ND  | 4.01  | 1.43        | 1.37     |
| 34  | c     | 520    | LMG  | O8-C28  | 4.01  | 1.45        | 1.33     |
| 23  | A     | 405[B] | CLA  | CHD-C4C | 4.00  | 1.48        | 1.39     |
| 23  | b     | 605    | CLA  | CHD-C1D | 4.00  | 1.46        | 1.38     |
| 23  | C     | 512    | CLA  | C3D-C2D | 4.00  | 1.49        | 1.39     |
| 23  | d     | 404    | CLA  | C3D-C2D | 4.00  | 1.49        | 1.39     |
| 23  | b     | 601    | CLA  | CHD-C4C | 4.00  | 1.48        | 1.39     |
| 23  | a     | 404[B] | CLA  | CHD-C1D | 4.00  | 1.46        | 1.38     |
| 31  | A     | 416[B] | PHO  | CHA-CBD | -4.00 | 1.47        | 1.52     |
| 23  | A     | 406[A] | CLA  | C3D-C2D | 4.00  | 1.49        | 1.39     |
| 23  | b     | 616    | CLA  | CHD-C1D | 3.99  | 1.46        | 1.38     |
| 31  | D     | 401[B] | PHO  | O2A-CGA | 3.99  | 1.45        | 1.33     |
| 23  | C     | 507    | CLA  | O2A-CGA | 3.99  | 1.45        | 1.33     |
| 23  | D     | 404    | CLA  | C3D-C2D | 3.98  | 1.49        | 1.39     |
| 25  | A     | 409[B] | SQD  | O48-C23 | 3.98  | 1.45        | 1.33     |
| 23  | B     | 602    | CLA  | C3D-C2D | 3.98  | 1.49        | 1.39     |
| 34  | d     | 412    | LMG  | O7-C10  | 3.98  | 1.45        | 1.34     |
| 25  | a     | 409[A] | SQD  | O48-C23 | 3.98  | 1.44        | 1.33     |
| 23  | c     | 504    | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 25  | a     | 409[B] | SQD  | O47-C7  | 3.97  | 1.45        | 1.34     |
| 24  | B     | 618    | BCR  | C23-C22 | -3.97 | 1.37        | 1.46     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 34  | B     | 620    | LMG  | O7-C10  | 3.97 | 1.45        | 1.34     |
| 23  | B     | 601    | CLA  | CHD-C1D | 3.97 | 1.46        | 1.38     |
| 23  | C     | 503    | CLA  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 23  | c     | 509    | CLA  | OBD-CAD | 3.97 | 1.29        | 1.22     |
| 23  | a     | 405[B] | CLA  | CHD-C1D | 3.97 | 1.46        | 1.38     |
| 23  | a     | 405[A] | CLA  | O2A-CGA | 3.97 | 1.44        | 1.33     |
| 23  | A     | 406[B] | CLA  | O2A-CGA | 3.96 | 1.44        | 1.33     |
| 23  | B     | 605    | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 23  | d     | 403[A] | CLA  | O2A-CGA | 3.96 | 1.44        | 1.33     |
| 23  | b     | 612    | CLA  | OBD-CAD | 3.96 | 1.29        | 1.22     |
| 23  | C     | 507    | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 34  | c     | 501    | LMG  | O7-C10  | 3.95 | 1.45        | 1.34     |
| 23  | c     | 506    | CLA  | O2A-CGA | 3.95 | 1.44        | 1.33     |
| 23  | B     | 603    | CLA  | O2A-CGA | 3.95 | 1.44        | 1.33     |
| 23  | A     | 406[A] | CLA  | OBD-CAD | 3.95 | 1.29        | 1.22     |
| 23  | b     | 614    | CLA  | C3D-C2D | 3.95 | 1.49        | 1.39     |
| 23  | b     | 608    | CLA  | C1D-ND  | 3.95 | 1.43        | 1.37     |
| 34  | C     | 501    | LMG  | O8-C28  | 3.95 | 1.44        | 1.33     |
| 23  | b     | 605    | CLA  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 23  | B     | 614    | CLA  | O2A-CGA | 3.94 | 1.44        | 1.33     |
| 23  | A     | 405[A] | CLA  | CHD-C1D | 3.94 | 1.46        | 1.38     |
| 23  | B     | 608    | CLA  | C3D-C2D | 3.94 | 1.49        | 1.39     |
| 23  | c     | 511    | CLA  | C3D-C2D | 3.94 | 1.49        | 1.39     |
| 23  | B     | 611    | CLA  | CHD-C1D | 3.94 | 1.46        | 1.38     |
| 33  | b     | 629[B] | LHG  | O8-C23  | 3.93 | 1.44        | 1.33     |
| 36  | c     | 517[B] | DGD  | O1G-C1A | 3.93 | 1.44        | 1.33     |
| 31  | a     | 415[B] | PHO  | O2A-CGA | 3.93 | 1.44        | 1.33     |
| 33  | b     | 629[B] | LHG  | O7-C7   | 3.93 | 1.45        | 1.34     |
| 23  | A     | 406[B] | CLA  | C3D-C2D | 3.93 | 1.49        | 1.39     |
| 23  | c     | 510    | CLA  | CHD-C1D | 3.93 | 1.46        | 1.38     |
| 23  | C     | 504    | CLA  | C1D-ND  | 3.93 | 1.43        | 1.37     |
| 23  | C     | 503    | CLA  | O2A-CGA | 3.93 | 1.44        | 1.33     |
| 33  | L     | 101[A] | LHG  | O8-C23  | 3.92 | 1.44        | 1.33     |
| 23  | c     | 511    | CLA  | CHD-C1D | 3.92 | 1.46        | 1.38     |
| 23  | D     | 403[A] | CLA  | C1D-ND  | 3.92 | 1.43        | 1.37     |
| 23  | C     | 506    | CLA  | CHD-C4C | 3.91 | 1.48        | 1.39     |
| 33  | D     | 408[A] | LHG  | O8-C23  | 3.91 | 1.44        | 1.33     |
| 36  | C     | 518[B] | DGD  | O1G-C1A | 3.91 | 1.44        | 1.33     |
| 23  | C     | 512    | CLA  | C1D-ND  | 3.91 | 1.43        | 1.37     |
| 33  | L     | 101[B] | LHG  | O7-C7   | 3.91 | 1.45        | 1.34     |
| 31  | A     | 416[B] | PHO  | C3C-C2C | 3.91 | 1.49        | 1.37     |
| 36  | C     | 518[B] | DGD  | O2G-C1B | 3.90 | 1.45        | 1.34     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 23  | C     | 511    | CLA  | CHD-C4C | 3.90 | 1.48        | 1.39     |
| 33  | d     | 407[A] | LHG  | O7-C7   | 3.90 | 1.45        | 1.34     |
| 31  | A     | 416[B] | PHO  | O2A-CGA | 3.90 | 1.44        | 1.33     |
| 23  | b     | 603    | CLA  | C3D-C2D | 3.90 | 1.49        | 1.39     |
| 36  | h     | 102    | DGD  | O2G-C1B | 3.90 | 1.45        | 1.34     |
| 23  | d     | 403[A] | CLA  | CHD-C1D | 3.89 | 1.46        | 1.38     |
| 33  | D     | 408[A] | LHG  | O7-C7   | 3.89 | 1.45        | 1.34     |
| 36  | c     | 518[B] | DGD  | O2G-C1B | 3.89 | 1.45        | 1.34     |
| 23  | C     | 504    | CLA  | CHD-C1D | 3.89 | 1.46        | 1.38     |
| 23  | C     | 510    | CLA  | O2A-CGA | 3.89 | 1.44        | 1.33     |
| 31  | a     | 415[A] | PHO  | C3C-C2C | 3.89 | 1.49        | 1.37     |
| 23  | A     | 406[B] | CLA  | OBD-CAD | 3.88 | 1.29        | 1.22     |
| 23  | B     | 602    | CLA  | CHD-C1D | 3.88 | 1.46        | 1.38     |
| 23  | d     | 402[B] | CLA  | CHD-C4C | 3.88 | 1.48        | 1.39     |
| 23  | c     | 503    | CLA  | CHD-C4C | 3.88 | 1.48        | 1.39     |
| 23  | B     | 611    | CLA  | C3D-C2D | 3.87 | 1.49        | 1.39     |
| 23  | c     | 510    | CLA  | CHD-C4C | 3.87 | 1.48        | 1.39     |
| 23  | C     | 510    | CLA  | CHD-C4C | 3.87 | 1.48        | 1.39     |
| 23  | C     | 505    | CLA  | C3D-C2D | 3.87 | 1.49        | 1.39     |
| 23  | b     | 607    | CLA  | C3D-C2D | 3.87 | 1.49        | 1.39     |
| 23  | b     | 616    | CLA  | C3D-C2D | 3.87 | 1.49        | 1.39     |
| 23  | B     | 605    | CLA  | CHD-C1D | 3.87 | 1.46        | 1.38     |
| 23  | B     | 609    | CLA  | CHD-C4C | 3.87 | 1.48        | 1.39     |
| 23  | b     | 606    | CLA  | O2A-CGA | 3.86 | 1.44        | 1.33     |
| 23  | a     | 405[B] | CLA  | CHD-C4C | 3.86 | 1.48        | 1.39     |
| 23  | A     | 404[A] | CLA  | C3D-C2D | 3.86 | 1.49        | 1.39     |
| 23  | B     | 611    | CLA  | O2A-CGA | 3.86 | 1.44        | 1.33     |
| 23  | C     | 511    | CLA  | C3D-C2D | 3.86 | 1.49        | 1.39     |
| 23  | D     | 404    | CLA  | OBD-CAD | 3.86 | 1.29        | 1.22     |
| 23  | B     | 613    | CLA  | CHD-C1D | 3.85 | 1.45        | 1.38     |
| 25  | a     | 411    | SQD  | O47-C7  | 3.85 | 1.45        | 1.34     |
| 23  | D     | 403[B] | CLA  | C3D-C2D | 3.85 | 1.49        | 1.39     |
| 23  | b     | 609    | CLA  | O2A-CGA | 3.85 | 1.44        | 1.33     |
| 31  | D     | 401[B] | PHO  | C3C-C2C | 3.85 | 1.49        | 1.37     |
| 23  | b     | 604    | CLA  | C3D-C2D | 3.85 | 1.49        | 1.39     |
| 31  | a     | 415[A] | PHO  | O2A-CGA | 3.85 | 1.44        | 1.33     |
| 34  | d     | 412    | LMG  | O8-C28  | 3.85 | 1.44        | 1.33     |
| 23  | b     | 611    | CLA  | CHD-C1D | 3.85 | 1.45        | 1.38     |
| 23  | A     | 404[B] | CLA  | O2A-CGA | 3.85 | 1.44        | 1.33     |
| 36  | C     | 518[A] | DGD  | O2G-C1B | 3.85 | 1.45        | 1.34     |
| 23  | D     | 403[B] | CLA  | CHD-C4C | 3.84 | 1.48        | 1.39     |
| 23  | d     | 402[A] | CLA  | OBD-CAD | 3.84 | 1.29        | 1.22     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 23  | c     | 512    | CLA  | C3D-C2D | 3.84 | 1.49        | 1.39     |
| 33  | d     | 407[B] | LHG  | O7-C7   | 3.84 | 1.45        | 1.34     |
| 23  | A     | 404[B] | CLA  | OBD-CAD | 3.84 | 1.29        | 1.22     |
| 23  | c     | 502    | CLA  | O2A-CGA | 3.84 | 1.44        | 1.33     |
| 23  | c     | 504    | CLA  | O2A-CGA | 3.83 | 1.44        | 1.33     |
| 23  | b     | 609    | CLA  | CHD-C4C | 3.83 | 1.47        | 1.39     |
| 23  | c     | 505    | CLA  | O2A-CGA | 3.83 | 1.44        | 1.33     |
| 23  | b     | 608    | CLA  | CHD-C4C | 3.83 | 1.47        | 1.39     |
| 23  | c     | 510    | CLA  | C3D-C2D | 3.83 | 1.49        | 1.39     |
| 23  | C     | 504    | CLA  | CHD-C4C | 3.83 | 1.47        | 1.39     |
| 23  | b     | 606    | CLA  | OBD-CAD | 3.83 | 1.29        | 1.22     |
| 23  | B     | 606    | CLA  | CHD-C1D | 3.83 | 1.45        | 1.38     |
| 23  | b     | 610    | CLA  | OBD-CAD | 3.83 | 1.29        | 1.22     |
| 23  | c     | 502    | CLA  | C3D-C2D | 3.83 | 1.49        | 1.39     |
| 23  | d     | 402[B] | CLA  | OBD-CAD | 3.83 | 1.29        | 1.22     |
| 23  | B     | 616    | CLA  | O2A-CGA | 3.82 | 1.44        | 1.33     |
| 23  | b     | 612    | CLA  | O2A-CGA | 3.82 | 1.44        | 1.33     |
| 23  | c     | 510    | CLA  | O2A-CGA | 3.82 | 1.44        | 1.33     |
| 23  | B     | 616    | CLA  | CHD-C1D | 3.82 | 1.45        | 1.38     |
| 23  | C     | 509    | CLA  | OBD-CAD | 3.81 | 1.29        | 1.22     |
| 33  | A     | 418[B] | LHG  | O8-C23  | 3.81 | 1.44        | 1.33     |
| 23  | A     | 405[A] | CLA  | CHD-C4C | 3.81 | 1.47        | 1.39     |
| 36  | c     | 517[A] | DGD  | O2G-C1B | 3.81 | 1.45        | 1.34     |
| 23  | D     | 404    | CLA  | CHD-C4C | 3.81 | 1.47        | 1.39     |
| 23  | a     | 405[A] | CLA  | CHD-C4C | 3.81 | 1.47        | 1.39     |
| 23  | b     | 611    | CLA  | C3D-C2D | 3.81 | 1.49        | 1.39     |
| 23  | b     | 611    | CLA  | CHD-C4C | 3.81 | 1.47        | 1.39     |
| 23  | b     | 602    | CLA  | C3D-C2D | 3.80 | 1.49        | 1.39     |
| 33  | D     | 408[B] | LHG  | O8-C23  | 3.80 | 1.44        | 1.33     |
| 23  | C     | 509    | CLA  | CHD-C1D | 3.80 | 1.45        | 1.38     |
| 36  | C     | 517[B] | DGD  | O1G-C1A | 3.80 | 1.44        | 1.33     |
| 23  | A     | 407    | CLA  | C3D-C2D | 3.80 | 1.49        | 1.39     |
| 36  | C     | 518[A] | DGD  | O1G-C1A | 3.80 | 1.44        | 1.33     |
| 33  | d     | 414[B] | LHG  | O7-C7   | 3.79 | 1.45        | 1.34     |
| 23  | c     | 509    | CLA  | CHD-C4C | 3.79 | 1.47        | 1.39     |
| 23  | b     | 605    | CLA  | C3D-C2D | 3.79 | 1.49        | 1.39     |
| 23  | b     | 609    | CLA  | C3D-C2D | 3.79 | 1.49        | 1.39     |
| 23  | C     | 505    | CLA  | O2A-CGA | 3.79 | 1.44        | 1.33     |
| 36  | c     | 517[A] | DGD  | O1G-C1A | 3.79 | 1.44        | 1.33     |
| 33  | d     | 408[B] | LHG  | O7-C7   | 3.78 | 1.45        | 1.34     |
| 31  | A     | 416[A] | PHO  | C3C-C2C | 3.78 | 1.48        | 1.37     |
| 23  | c     | 508    | CLA  | C3D-C2D | 3.78 | 1.49        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 23  | B     | 601    | CLA  | C3D-C2D | 3.78 | 1.49        | 1.39     |
| 31  | D     | 401[A] | PHO  | C3C-C2C | 3.78 | 1.48        | 1.37     |
| 23  | c     | 513    | CLA  | C3D-C2D | 3.78 | 1.49        | 1.39     |
| 23  | B     | 613    | CLA  | C3D-C2D | 3.78 | 1.49        | 1.39     |
| 23  | B     | 605    | CLA  | O2A-CGA | 3.77 | 1.44        | 1.33     |
| 31  | D     | 401[A] | PHO  | O2A-CGA | 3.77 | 1.44        | 1.33     |
| 23  | B     | 610    | CLA  | CHD-C1D | 3.77 | 1.45        | 1.38     |
| 23  | A     | 404[B] | CLA  | C3D-C2D | 3.77 | 1.49        | 1.39     |
| 23  | b     | 610    | CLA  | C3D-C2D | 3.77 | 1.49        | 1.39     |
| 23  | B     | 602    | CLA  | O2A-CGA | 3.77 | 1.44        | 1.33     |
| 23  | C     | 502    | CLA  | O2A-CGA | 3.77 | 1.44        | 1.33     |
| 23  | A     | 406[A] | CLA  | C1D-ND  | 3.77 | 1.42        | 1.37     |
| 23  | c     | 505    | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 23  | b     | 612    | CLA  | CHD-C1D | 3.77 | 1.45        | 1.38     |
| 23  | c     | 506    | CLA  | CHD-C4C | 3.76 | 1.47        | 1.39     |
| 25  | A     | 409[A] | SQD  | O48-C23 | 3.76 | 1.44        | 1.33     |
| 23  | B     | 615    | CLA  | C3D-C2D | 3.76 | 1.49        | 1.39     |
| 23  | C     | 508    | CLA  | C3D-C2D | 3.76 | 1.49        | 1.39     |
| 23  | c     | 504    | CLA  | O2D-CGD | 3.75 | 1.42        | 1.33     |
| 23  | b     | 604    | CLA  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 34  | m     | 101    | LMG  | O7-C10  | 3.75 | 1.44        | 1.34     |
| 23  | C     | 505    | CLA  | C1D-ND  | 3.74 | 1.42        | 1.37     |
| 23  | B     | 606    | CLA  | O2A-CGA | 3.74 | 1.44        | 1.33     |
| 23  | a     | 404[A] | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 23  | A     | 406[A] | CLA  | O2A-CGA | 3.74 | 1.44        | 1.33     |
| 33  | D     | 407[B] | LHG  | O7-C7   | 3.73 | 1.44        | 1.34     |
| 23  | C     | 508    | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 23  | A     | 406[A] | CLA  | CHD-C4C | 3.73 | 1.47        | 1.39     |
| 23  | b     | 601    | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 23  | b     | 602    | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 36  | h     | 102    | DGD  | O1G-C1A | 3.73 | 1.44        | 1.33     |
| 23  | b     | 606    | CLA  | C3D-C2D | 3.73 | 1.49        | 1.39     |
| 23  | A     | 407    | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 23  | b     | 615    | CLA  | OBD-CAD | 3.72 | 1.28        | 1.22     |
| 23  | a     | 404[A] | CLA  | C3D-C2D | 3.72 | 1.49        | 1.39     |
| 23  | b     | 615    | CLA  | CHD-C1D | 3.72 | 1.45        | 1.38     |
| 36  | H     | 102    | DGD  | O1G-C1A | 3.72 | 1.44        | 1.33     |
| 33  | D     | 407[B] | LHG  | O8-C23  | 3.72 | 1.44        | 1.33     |
| 23  | C     | 514    | CLA  | OBD-CAD | 3.71 | 1.28        | 1.22     |
| 23  | C     | 505    | CLA  | CHD-C1D | 3.71 | 1.45        | 1.38     |
| 33  | A     | 418[B] | LHG  | O7-C7   | 3.71 | 1.44        | 1.34     |
| 23  | B     | 607    | CLA  | CHD-C4C | 3.71 | 1.47        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 33  | d     | 407[B] | LHG  | O8-C23  | 3.70  | 1.44        | 1.33     |
| 23  | b     | 604    | CLA  | O2A-CGA | 3.70  | 1.44        | 1.33     |
| 23  | C     | 511    | CLA  | CHD-C1D | 3.70  | 1.45        | 1.38     |
| 23  | C     | 513    | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 23  | c     | 513    | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 23  | b     | 615    | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 23  | b     | 612    | CLA  | C3D-C2D | 3.70  | 1.49        | 1.39     |
| 23  | c     | 508    | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 31  | a     | 406[B] | PHO  | O2A-CGA | 3.69  | 1.44        | 1.33     |
| 23  | b     | 605    | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 23  | B     | 611    | CLA  | C1C-C2C | 3.69  | 1.52        | 1.44     |
| 23  | A     | 404[A] | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 23  | B     | 604    | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 23  | D     | 403[B] | CLA  | C1D-ND  | 3.69  | 1.42        | 1.37     |
| 23  | b     | 602    | CLA  | O2A-CGA | 3.69  | 1.44        | 1.33     |
| 23  | d     | 404    | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 23  | C     | 503    | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 33  | L     | 101[A] | LHG  | O7-C7   | 3.69  | 1.44        | 1.34     |
| 23  | B     | 604    | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 25  | A     | 409[A] | SQD  | O47-C7  | 3.68  | 1.44        | 1.34     |
| 36  | c     | 519    | DGD  | O2G-C1B | 3.68  | 1.44        | 1.34     |
| 23  | b     | 613    | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 23  | b     | 609    | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 33  | d     | 408[A] | LHG  | O7-C7   | 3.68  | 1.44        | 1.34     |
| 23  | a     | 404[B] | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 23  | a     | 404[B] | CLA  | C3D-C2D | 3.67  | 1.49        | 1.39     |
| 23  | C     | 509    | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 23  | c     | 511    | CLA  | O2A-CGA | 3.67  | 1.44        | 1.33     |
| 23  | b     | 604    | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 23  | B     | 603    | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 23  | D     | 403[A] | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 23  | A     | 404[A] | CLA  | CHD-C1D | 3.67  | 1.45        | 1.38     |
| 23  | B     | 612    | CLA  | O2A-CGA | 3.67  | 1.44        | 1.33     |
| 33  | D     | 407[A] | LHG  | O7-C7   | 3.67  | 1.44        | 1.34     |
| 23  | c     | 506    | CLA  | C3D-C2D | 3.66  | 1.49        | 1.39     |
| 23  | C     | 511    | CLA  | O2A-CGA | 3.66  | 1.44        | 1.33     |
| 23  | c     | 505    | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 23  | C     | 502    | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 38  | f     | 101    | HEM  | C4D-ND  | -3.66 | 1.33        | 1.40     |
| 23  | B     | 612    | CLA  | C3D-C2D | 3.66  | 1.49        | 1.39     |
| 36  | C     | 517[A] | DGD  | O1G-C1A | 3.66  | 1.44        | 1.33     |
| 23  | B     | 606    | CLA  | CHD-C4C | 3.65  | 1.47        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 33  | d     | 414[A] | LHG  | O8-C23  | 3.65 | 1.44        | 1.33     |
| 23  | B     | 612    | CLA  | C1D-ND  | 3.65 | 1.42        | 1.37     |
| 23  | B     | 608    | CLA  | O2A-CGA | 3.64 | 1.44        | 1.33     |
| 31  | a     | 406[B] | PHO  | C3C-C2C | 3.64 | 1.48        | 1.37     |
| 23  | B     | 611    | CLA  | CHD-C4C | 3.64 | 1.47        | 1.39     |
| 23  | a     | 405[B] | CLA  | OBD-CAD | 3.64 | 1.28        | 1.22     |
| 23  | C     | 506    | CLA  | C3D-C2D | 3.64 | 1.48        | 1.39     |
| 23  | b     | 614    | CLA  | O2A-CGA | 3.64 | 1.44        | 1.33     |
| 23  | B     | 605    | CLA  | C3D-C2D | 3.64 | 1.48        | 1.39     |
| 23  | b     | 614    | CLA  | CHD-C4C | 3.64 | 1.47        | 1.39     |
| 23  | B     | 609    | CLA  | OBD-CAD | 3.64 | 1.28        | 1.22     |
| 23  | b     | 603    | CLA  | CHD-C4C | 3.63 | 1.47        | 1.39     |
| 23  | d     | 403[B] | CLA  | C3D-C2D | 3.63 | 1.48        | 1.39     |
| 23  | B     | 607    | CLA  | CHB-C4A | 3.62 | 1.36        | 1.33     |
| 23  | d     | 403[A] | CLA  | CHD-C4C | 3.62 | 1.47        | 1.39     |
| 23  | C     | 507    | CLA  | C3D-C2D | 3.62 | 1.48        | 1.39     |
| 23  | d     | 402[A] | CLA  | CHD-C1D | 3.62 | 1.45        | 1.38     |
| 23  | B     | 606    | CLA  | C3D-C2D | 3.62 | 1.48        | 1.39     |
| 23  | C     | 508    | CLA  | CHD-C4C | 3.61 | 1.47        | 1.39     |
| 23  | B     | 603    | CLA  | CHD-C4C | 3.61 | 1.47        | 1.39     |
| 23  | B     | 613    | CLA  | OBD-CAD | 3.61 | 1.28        | 1.22     |
| 23  | B     | 604    | CLA  | C1D-ND  | 3.61 | 1.42        | 1.37     |
| 23  | d     | 403[A] | CLA  | OBD-CAD | 3.61 | 1.28        | 1.22     |
| 33  | b     | 629[A] | LHG  | O7-C7   | 3.61 | 1.44        | 1.34     |
| 33  | D     | 407[A] | LHG  | O8-C23  | 3.61 | 1.43        | 1.33     |
| 23  | a     | 407    | CLA  | CHD-C4C | 3.61 | 1.47        | 1.39     |
| 23  | A     | 405[B] | CLA  | OBD-CAD | 3.60 | 1.28        | 1.22     |
| 33  | A     | 418[A] | LHG  | O7-C7   | 3.60 | 1.44        | 1.34     |
| 23  | b     | 613    | CLA  | CHD-C1D | 3.60 | 1.45        | 1.38     |
| 23  | D     | 403[A] | CLA  | C3D-C2D | 3.60 | 1.48        | 1.39     |
| 23  | a     | 407    | CLA  | CHD-C1D | 3.59 | 1.45        | 1.38     |
| 23  | b     | 613    | CLA  | O2A-CGA | 3.58 | 1.43        | 1.33     |
| 33  | d     | 407[A] | LHG  | O8-C23  | 3.58 | 1.43        | 1.33     |
| 23  | c     | 512    | CLA  | OBD-CAD | 3.58 | 1.28        | 1.22     |
| 23  | a     | 405[A] | CLA  | CHD-C1D | 3.58 | 1.45        | 1.38     |
| 23  | d     | 403[A] | CLA  | C3D-C2D | 3.58 | 1.48        | 1.39     |
| 36  | H     | 102    | DGD  | O2G-C1B | 3.58 | 1.44        | 1.34     |
| 25  | A     | 409[B] | SQD  | O47-C7  | 3.57 | 1.44        | 1.34     |
| 23  | b     | 607    | CLA  | C1D-ND  | 3.57 | 1.42        | 1.37     |
| 23  | c     | 507    | CLA  | OBD-CAD | 3.56 | 1.28        | 1.22     |
| 23  | B     | 601    | CLA  | CHD-C4C | 3.56 | 1.47        | 1.39     |
| 23  | C     | 506    | CLA  | O2A-CGA | 3.56 | 1.43        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 505    | CLA  | CHD-C4C | 3.55  | 1.47        | 1.39     |
| 23  | d     | 402[A] | CLA  | CHD-C4C | 3.55  | 1.47        | 1.39     |
| 36  | c     | 518[A] | DGD  | O2G-C1B | 3.54  | 1.44        | 1.34     |
| 23  | B     | 615    | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 31  | a     | 406[A] | PHO  | C3C-C2C | 3.52  | 1.48        | 1.37     |
| 23  | b     | 603    | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 23  | B     | 607    | CLA  | O2A-CGA | 3.52  | 1.43        | 1.33     |
| 23  | C     | 504    | CLA  | O2A-CGA | 3.52  | 1.43        | 1.33     |
| 33  | d     | 414[A] | LHG  | O7-C7   | 3.51  | 1.44        | 1.34     |
| 23  | d     | 404    | CLA  | CHD-C4C | 3.51  | 1.47        | 1.39     |
| 23  | B     | 602    | CLA  | CHD-C4C | 3.51  | 1.47        | 1.39     |
| 23  | B     | 607    | CLA  | C3D-C2D | 3.50  | 1.48        | 1.39     |
| 35  | b     | 622    | HTG  | C1'-S1  | -3.50 | 1.76        | 1.81     |
| 33  | A     | 418[A] | LHG  | O8-C23  | 3.50  | 1.43        | 1.33     |
| 23  | a     | 405[A] | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 23  | B     | 608    | CLA  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 23  | C     | 502    | CLA  | C3D-C2D | 3.49  | 1.48        | 1.39     |
| 23  | B     | 601    | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 23  | B     | 607    | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 23  | a     | 407    | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 34  | D     | 412    | LMG  | O8-C28  | 3.48  | 1.43        | 1.33     |
| 36  | C     | 519    | DGD  | O2G-C1B | 3.47  | 1.44        | 1.34     |
| 23  | c     | 502    | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 23  | C     | 507    | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 23  | B     | 614    | CLA  | CHD-C1D | 3.46  | 1.45        | 1.38     |
| 23  | b     | 605    | CLA  | O2A-CGA | 3.46  | 1.43        | 1.33     |
| 23  | b     | 603    | CLA  | O2A-CGA | 3.45  | 1.43        | 1.33     |
| 23  | c     | 510    | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 23  | b     | 616    | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 23  | C     | 513    | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 23  | C     | 504    | CLA  | C3D-C2D | 3.44  | 1.48        | 1.39     |
| 23  | B     | 610    | CLA  | O2A-CGA | 3.44  | 1.43        | 1.33     |
| 23  | B     | 603    | CLA  | CHD-C1D | 3.43  | 1.45        | 1.38     |
| 23  | b     | 612    | CLA  | CHD-C4C | 3.42  | 1.47        | 1.39     |
| 35  | B     | 623    | HTG  | C1'-S1  | -3.42 | 1.76        | 1.81     |
| 23  | C     | 504    | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 33  | b     | 629[A] | LHG  | O8-C23  | 3.40  | 1.43        | 1.33     |
| 23  | B     | 610    | CLA  | CHD-C4C | 3.39  | 1.46        | 1.39     |
| 23  | B     | 614    | CLA  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 23  | B     | 613    | CLA  | CHD-C4C | 3.38  | 1.46        | 1.39     |
| 23  | b     | 616    | CLA  | CHD-C4C | 3.38  | 1.46        | 1.39     |
| 23  | B     | 602    | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | d     | 403[B] | CLA  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 23  | b     | 607    | CLA  | CHD-C4C | 3.37  | 1.46        | 1.39     |
| 35  | o     | 301    | HTG  | C1'-S1  | -3.37 | 1.76        | 1.81     |
| 23  | D     | 403[B] | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 23  | A     | 405[A] | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 31  | a     | 406[A] | PHO  | O2A-CGA | 3.36  | 1.43        | 1.33     |
| 23  | B     | 613    | CLA  | O2A-CGA | 3.34  | 1.43        | 1.33     |
| 23  | B     | 616    | CLA  | CHD-C4C | 3.33  | 1.46        | 1.39     |
| 34  | D     | 412    | LMG  | O7-C10  | 3.33  | 1.43        | 1.34     |
| 23  | A     | 404[A] | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 38  | F     | 102    | HEM  | C1B-NB  | -3.33 | 1.34        | 1.40     |
| 23  | a     | 407    | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 23  | D     | 404    | CLA  | O2A-CGA | 3.33  | 1.43        | 1.33     |
| 23  | d     | 403[A] | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 23  | c     | 503    | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 23  | A     | 407    | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 23  | B     | 616    | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 23  | B     | 608    | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 23  | B     | 604    | CLA  | C3D-C2D | 3.30  | 1.48        | 1.39     |
| 23  | B     | 612    | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 23  | B     | 607    | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 23  | C     | 511    | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 23  | A     | 404[A] | CLA  | O2A-CGA | 3.28  | 1.42        | 1.33     |
| 35  | b     | 623    | HTG  | C1'-S1  | -3.27 | 1.76        | 1.81     |
| 23  | A     | 407    | CLA  | CHD-C4C | 3.27  | 1.46        | 1.39     |
| 23  | B     | 602    | CLA  | C1C-C2C | 3.25  | 1.51        | 1.44     |
| 23  | D     | 403[A] | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 23  | c     | 514    | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 23  | c     | 504    | CLA  | OBD-CAD | 3.23  | 1.28        | 1.22     |
| 23  | b     | 610    | CLA  | O2A-CGA | 3.21  | 1.42        | 1.33     |
| 23  | B     | 613    | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 23  | a     | 404[A] | CLA  | O2A-CGA | 3.19  | 1.42        | 1.33     |
| 23  | D     | 404    | CLA  | C1C-C2C | 3.19  | 1.51        | 1.44     |
| 23  | C     | 506    | CLA  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 23  | B     | 612    | CLA  | CHD-C4C | 3.17  | 1.46        | 1.39     |
| 23  | c     | 512    | CLA  | C1B-CHB | 3.15  | 1.49        | 1.41     |
| 23  | C     | 512    | CLA  | C4D-CHA | 3.15  | 1.49        | 1.38     |
| 23  | B     | 615    | CLA  | C1C-C2C | 3.15  | 1.50        | 1.44     |
| 23  | c     | 504    | CLA  | C3D-C2D | 3.14  | 1.47        | 1.39     |
| 23  | c     | 511    | CLA  | OBD-CAD | 3.14  | 1.27        | 1.22     |
| 23  | B     | 613    | CLA  | C1C-C2C | 3.13  | 1.50        | 1.44     |
| 23  | B     | 604    | CLA  | O2A-CGA | 3.13  | 1.42        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 38  | F     | 102    | HEM  | C4D-ND  | -3.10 | 1.34        | 1.40     |
| 31  | a     | 406[B] | PHO  | CHA-CBD | -3.06 | 1.49        | 1.52     |
| 23  | B     | 605    | CLA  | CHB-C4A | 3.06  | 1.35        | 1.33     |
| 38  | f     | 101    | HEM  | C1B-NB  | -3.06 | 1.34        | 1.40     |
| 23  | b     | 613    | CLA  | C4D-CHA | 3.05  | 1.48        | 1.38     |
| 23  | b     | 614    | CLA  | OBD-CAD | 3.04  | 1.27        | 1.22     |
| 23  | b     | 604    | CLA  | C4D-CHA | 3.03  | 1.48        | 1.38     |
| 23  | B     | 616    | CLA  | C4D-CHA | 3.02  | 1.48        | 1.38     |
| 23  | C     | 513    | CLA  | C4B-CHC | 3.02  | 1.49        | 1.41     |
| 23  | C     | 505    | CLA  | OBD-CAD | 3.00  | 1.27        | 1.22     |
| 28  | A     | 413[A] | PL9  | C6-C5   | 2.99  | 1.49        | 1.35     |
| 31  | D     | 401[A] | PHO  | CBD-CGD | -2.99 | 1.48        | 1.52     |
| 31  | D     | 401[B] | PHO  | CHA-CBD | -2.97 | 1.49        | 1.52     |
| 23  | b     | 610    | CLA  | C4B-CHC | 2.97  | 1.49        | 1.41     |
| 35  | D     | 411    | HTG  | C1'-S1  | -2.96 | 1.77        | 1.81     |
| 23  | b     | 612    | CLA  | CHB-C4A | 2.95  | 1.35        | 1.33     |
| 23  | C     | 508    | CLA  | C4D-CHA | 2.95  | 1.48        | 1.38     |
| 23  | C     | 505    | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 23  | B     | 611    | CLA  | C4B-CHC | 2.94  | 1.49        | 1.41     |
| 28  | a     | 413[B] | PL9  | C6-C5   | 2.93  | 1.49        | 1.35     |
| 23  | B     | 601    | CLA  | C1C-C2C | 2.93  | 1.50        | 1.44     |
| 23  | b     | 612    | CLA  | C1B-CHB | 2.93  | 1.49        | 1.41     |
| 28  | a     | 413[A] | PL9  | C6-C5   | 2.92  | 1.49        | 1.35     |
| 23  | c     | 509    | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 35  | b     | 625    | HTG  | C1'-S1  | -2.92 | 1.77        | 1.81     |
| 23  | a     | 407    | CLA  | C1C-C2C | 2.91  | 1.50        | 1.44     |
| 23  | B     | 616    | CLA  | C1C-C2C | 2.91  | 1.50        | 1.44     |
| 23  | B     | 607    | CLA  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 23  | c     | 506    | CLA  | C4C-C3C | 2.90  | 1.50        | 1.45     |
| 23  | b     | 607    | CLA  | O2A-CGA | 2.90  | 1.41        | 1.33     |
| 23  | B     | 605    | CLA  | C1C-C2C | 2.90  | 1.50        | 1.44     |
| 23  | c     | 511    | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 23  | A     | 404[A] | CLA  | C4C-C3C | 2.88  | 1.49        | 1.45     |
| 23  | a     | 407    | CLA  | C1D-ND  | 2.88  | 1.41        | 1.37     |
| 28  | A     | 413[B] | PL9  | C6-C5   | 2.87  | 1.49        | 1.35     |
| 23  | b     | 603    | CLA  | C4D-CHA | 2.87  | 1.48        | 1.38     |
| 23  | B     | 606    | CLA  | C1B-CHB | 2.87  | 1.49        | 1.41     |
| 23  | B     | 604    | CLA  | C4D-CHA | 2.87  | 1.48        | 1.38     |
| 23  | B     | 614    | CLA  | OBD-CAD | 2.86  | 1.27        | 1.22     |
| 23  | b     | 602    | CLA  | C4B-CHC | 2.86  | 1.48        | 1.41     |
| 31  | a     | 415[B] | PHO  | CHA-CBD | -2.85 | 1.49        | 1.52     |
| 23  | C     | 506    | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 35  | c     | 522    | HTG  | C1'-S1  | -2.85 | 1.77        | 1.81     |
| 23  | B     | 608    | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 23  | c     | 510    | CLA  | C4C-C3C | 2.84  | 1.49        | 1.45     |
| 23  | B     | 605    | CLA  | C4B-CHC | 2.84  | 1.48        | 1.41     |
| 23  | B     | 616    | CLA  | C1B-CHB | 2.84  | 1.48        | 1.41     |
| 23  | d     | 403[A] | CLA  | C4C-C3C | 2.84  | 1.49        | 1.45     |
| 23  | B     | 612    | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 23  | C     | 502    | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 23  | b     | 605    | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 31  | a     | 415[B] | PHO  | C3A-C2A | -2.82 | 1.52        | 1.54     |
| 23  | C     | 513    | CLA  | C1C-C2C | 2.82  | 1.50        | 1.44     |
| 23  | b     | 611    | CLA  | OBD-CAD | 2.81  | 1.27        | 1.22     |
| 35  | d     | 411    | HTG  | C1'-S1  | -2.81 | 1.77        | 1.81     |
| 23  | c     | 508    | CLA  | C1C-C2C | 2.80  | 1.50        | 1.44     |
| 23  | c     | 504    | CLA  | C1C-C2C | 2.80  | 1.50        | 1.44     |
| 23  | c     | 508    | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 23  | D     | 404    | CLA  | C4C-C3C | 2.80  | 1.49        | 1.45     |
| 23  | c     | 510    | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 23  | b     | 610    | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 23  | b     | 609    | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 23  | b     | 602    | CLA  | C1C-C2C | 2.80  | 1.50        | 1.44     |
| 23  | B     | 606    | CLA  | OBD-CAD | 2.79  | 1.27        | 1.22     |
| 23  | a     | 405[A] | CLA  | C1C-C2C | 2.79  | 1.50        | 1.44     |
| 23  | c     | 505    | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 23  | C     | 512    | CLA  | OBD-CAD | 2.79  | 1.27        | 1.22     |
| 23  | c     | 504    | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 23  | A     | 405[A] | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 31  | a     | 406[A] | PHO  | CBD-CGD | -2.79 | 1.49        | 1.52     |
| 23  | D     | 404    | CLA  | C4B-CHC | 2.79  | 1.48        | 1.41     |
| 23  | C     | 502    | CLA  | C1C-C2C | 2.79  | 1.50        | 1.44     |
| 23  | b     | 607    | CLA  | OBD-CAD | 2.78  | 1.27        | 1.22     |
| 23  | B     | 614    | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 23  | B     | 612    | CLA  | C4C-C3C | 2.78  | 1.49        | 1.45     |
| 23  | a     | 405[A] | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 23  | d     | 403[B] | CLA  | C4C-C3C | 2.77  | 1.49        | 1.45     |
| 23  | C     | 511    | CLA  | C4C-C3C | 2.77  | 1.49        | 1.45     |
| 23  | b     | 610    | CLA  | C4C-C3C | 2.76  | 1.49        | 1.45     |
| 34  | Z     | 101    | LMG  | O8-C28  | 2.76  | 1.46        | 1.33     |
| 23  | D     | 404    | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 23  | d     | 403[B] | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 35  | b     | 625    | HTG  | C1-S1   | -2.76 | 1.76        | 1.80     |
| 31  | a     | 406[A] | PHO  | CHA-CBD | -2.76 | 1.49        | 1.52     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 506    | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 23  | b     | 615    | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 23  | B     | 601    | CLA  | C4B-CHC | 2.73  | 1.48        | 1.41     |
| 36  | C     | 519    | DGD  | O2G-C2G | -2.73 | 1.40        | 1.46     |
| 23  | B     | 613    | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 23  | B     | 603    | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 38  | f     | 101    | HEM  | C1D-ND  | -2.72 | 1.33        | 1.38     |
| 32  | M     | 101    | LMT  | O2'-C2' | -2.72 | 1.36        | 1.43     |
| 31  | a     | 415[A] | PHO  | CHA-CBD | -2.72 | 1.49        | 1.52     |
| 23  | C     | 502    | CLA  | OBD-CAD | 2.72  | 1.27        | 1.22     |
| 23  | B     | 613    | CLA  | C4C-C3C | 2.71  | 1.49        | 1.45     |
| 23  | b     | 608    | CLA  | C1C-C2C | 2.71  | 1.50        | 1.44     |
| 23  | B     | 607    | CLA  | C1B-CHB | 2.71  | 1.48        | 1.41     |
| 23  | D     | 403[A] | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 23  | c     | 506    | CLA  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 23  | C     | 507    | CLA  | C4C-C3C | 2.71  | 1.49        | 1.45     |
| 23  | C     | 506    | CLA  | C4C-C3C | 2.71  | 1.49        | 1.45     |
| 23  | c     | 511    | CLA  | C1B-CHB | 2.70  | 1.48        | 1.41     |
| 23  | c     | 512    | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 23  | C     | 506    | CLA  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 23  | C     | 504    | CLA  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 23  | d     | 403[A] | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 23  | b     | 614    | CLA  | C1C-C2C | 2.69  | 1.50        | 1.44     |
| 23  | B     | 611    | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 23  | B     | 615    | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 23  | b     | 611    | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 23  | C     | 511    | CLA  | CHB-C4A | 2.68  | 1.35        | 1.33     |
| 23  | B     | 615    | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 23  | B     | 612    | CLA  | C1C-C2C | 2.68  | 1.50        | 1.44     |
| 23  | B     | 612    | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 23  | c     | 513    | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 23  | b     | 614    | CLA  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 23  | b     | 609    | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 23  | D     | 403[A] | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 23  | b     | 603    | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 23  | c     | 504    | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 28  | d     | 406[B] | PL9  | C6-C5   | 2.67  | 1.48        | 1.35     |
| 23  | A     | 406[A] | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 31  | a     | 415[A] | PHO  | C3A-C2A | -2.67 | 1.52        | 1.54     |
| 23  | C     | 508    | CLA  | OBD-CAD | 2.67  | 1.27        | 1.22     |
| 23  | a     | 404[A] | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 23  | c     | 504    | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 610    | CLA  | C1C-C2C | 2.67  | 1.49        | 1.44     |
| 23  | c     | 505    | CLA  | C1C-C2C | 2.67  | 1.49        | 1.44     |
| 23  | b     | 614    | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 23  | b     | 613    | CLA  | C1C-C2C | 2.66  | 1.49        | 1.44     |
| 28  | D     | 406[A] | PL9  | C6-C5   | 2.66  | 1.48        | 1.35     |
| 23  | c     | 502    | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 23  | B     | 614    | CLA  | C3D-C4D | -2.66 | 1.38        | 1.44     |
| 23  | C     | 509    | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 23  | C     | 510    | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 23  | A     | 406[B] | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 23  | B     | 602    | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 23  | B     | 608    | CLA  | C3D-C4D | -2.65 | 1.38        | 1.44     |
| 23  | A     | 407    | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 23  | b     | 613    | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 23  | d     | 403[A] | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 23  | A     | 404[B] | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 23  | a     | 404[A] | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 23  | C     | 509    | CLA  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 23  | B     | 602    | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 23  | C     | 510    | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 23  | B     | 611    | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 23  | C     | 504    | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 23  | C     | 514    | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 28  | D     | 406[B] | PL9  | C6-C5   | 2.64  | 1.48        | 1.35     |
| 23  | a     | 407    | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 23  | A     | 404[A] | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 23  | B     | 615    | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 23  | b     | 606    | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 23  | B     | 610    | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 23  | c     | 506    | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 23  | B     | 610    | CLA  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 23  | b     | 601    | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 23  | c     | 508    | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 23  | C     | 509    | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 23  | b     | 607    | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 23  | d     | 402[B] | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 23  | A     | 405[A] | CLA  | C1C-C2C | 2.62  | 1.49        | 1.44     |
| 23  | d     | 404    | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 32  | B     | 626    | LMT  | C3'-C2' | 2.62  | 1.59        | 1.52     |
| 23  | C     | 507    | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 23  | c     | 514    | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 23  | d     | 402[A] | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 504    | CLA  | C3D-C4D | -2.61 | 1.38        | 1.44     |
| 23  | B     | 609    | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 23  | B     | 610    | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 23  | b     | 604    | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 23  | C     | 505    | CLA  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 23  | B     | 614    | CLA  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 23  | c     | 514    | CLA  | C1C-C2C | 2.60  | 1.49        | 1.44     |
| 23  | b     | 616    | CLA  | C1C-C2C | 2.60  | 1.49        | 1.44     |
| 23  | B     | 606    | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 23  | b     | 614    | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 23  | c     | 513    | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 35  | C     | 522    | HTG  | C1'-S1  | -2.59 | 1.77        | 1.81     |
| 23  | b     | 611    | CLA  | C1C-C2C | 2.59  | 1.49        | 1.44     |
| 23  | C     | 503    | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 23  | b     | 603    | CLA  | C1C-C2C | 2.59  | 1.49        | 1.44     |
| 23  | C     | 513    | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 23  | B     | 609    | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 23  | c     | 502    | CLA  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 26  | D     | 413    | GOL  | C3-C2   | 2.59  | 1.61        | 1.51     |
| 23  | A     | 406[B] | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 23  | c     | 511    | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 34  | C     | 521    | LMG  | O1-C1   | 2.58  | 1.44        | 1.40     |
| 23  | C     | 503    | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 23  | A     | 405[B] | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 23  | C     | 512    | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 23  | b     | 609    | CLA  | C3D-C4D | -2.58 | 1.38        | 1.44     |
| 23  | D     | 403[B] | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 23  | B     | 604    | CLA  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 23  | B     | 604    | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 23  | B     | 611    | CLA  | CHB-C4A | 2.57  | 1.35        | 1.33     |
| 23  | b     | 604    | CLA  | C1C-C2C | 2.57  | 1.49        | 1.44     |
| 23  | a     | 405[B] | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 23  | b     | 612    | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 23  | C     | 511    | CLA  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 23  | c     | 505    | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 32  | t     | 101    | LMT  | O3'-C3' | -2.56 | 1.36        | 1.43     |
| 23  | a     | 404[B] | CLA  | C4C-C3C | 2.55  | 1.49        | 1.45     |
| 23  | B     | 603    | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 23  | c     | 502    | CLA  | C3D-C4D | -2.54 | 1.38        | 1.44     |
| 23  | C     | 504    | CLA  | C1B-CHB | 2.54  | 1.48        | 1.41     |
| 23  | d     | 404    | CLA  | C1C-C2C | 2.54  | 1.49        | 1.44     |
| 23  | a     | 404[B] | CLA  | C4D-CHA | 2.54  | 1.47        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 601    | CLA  | C4D-CHA | 2.54  | 1.47        | 1.38     |
| 23  | c     | 510    | CLA  | C1B-CHB | 2.54  | 1.48        | 1.41     |
| 23  | c     | 509    | CLA  | C4C-C3C | 2.54  | 1.49        | 1.45     |
| 23  | B     | 602    | CLA  | C3D-C4D | -2.54 | 1.38        | 1.44     |
| 23  | B     | 603    | CLA  | C1B-CHB | 2.53  | 1.48        | 1.41     |
| 23  | C     | 503    | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 23  | a     | 407    | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 36  | H     | 102    | DGD  | O5D-C1E | 2.53  | 1.44        | 1.40     |
| 23  | b     | 611    | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 23  | b     | 607    | CLA  | C1C-C2C | 2.53  | 1.49        | 1.44     |
| 23  | b     | 610    | CLA  | C1C-C2C | 2.53  | 1.49        | 1.44     |
| 23  | B     | 608    | CLA  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 23  | c     | 508    | CLA  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 23  | B     | 605    | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 23  | b     | 613    | CLA  | OBD-CAD | 2.52  | 1.26        | 1.22     |
| 23  | c     | 507    | CLA  | C1B-CHB | 2.51  | 1.48        | 1.41     |
| 31  | A     | 416[A] | PHO  | C3A-C2A | -2.51 | 1.52        | 1.54     |
| 23  | D     | 403[B] | CLA  | C1B-CHB | 2.51  | 1.48        | 1.41     |
| 23  | C     | 514    | CLA  | C1C-C2C | 2.51  | 1.49        | 1.44     |
| 23  | D     | 403[B] | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 32  | A     | 419    | LMT  | O3'-C3' | -2.50 | 1.36        | 1.43     |
| 23  | c     | 513    | CLA  | C1B-CHB | 2.50  | 1.48        | 1.41     |
| 23  | b     | 616    | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 23  | b     | 616    | CLA  | C3D-C4D | -2.50 | 1.38        | 1.44     |
| 23  | c     | 507    | CLA  | C4C-C3C | 2.50  | 1.49        | 1.45     |
| 23  | b     | 615    | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 23  | c     | 502    | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 23  | c     | 507    | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 31  | D     | 401[B] | PHO  | CBD-CGD | -2.49 | 1.49        | 1.52     |
| 23  | A     | 404[A] | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 23  | B     | 602    | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 23  | c     | 509    | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 23  | c     | 502    | CLA  | C1B-CHB | 2.48  | 1.47        | 1.41     |
| 23  | b     | 604    | CLA  | C4C-C3C | 2.48  | 1.49        | 1.45     |
| 23  | A     | 404[B] | CLA  | C4C-C3C | 2.48  | 1.49        | 1.45     |
| 23  | a     | 407    | CLA  | CHB-C4A | 2.48  | 1.35        | 1.33     |
| 25  | X     | 101    | SQD  | O6-C1   | 2.48  | 1.44        | 1.40     |
| 23  | B     | 605    | CLA  | C3D-C4D | -2.48 | 1.38        | 1.44     |
| 23  | C     | 506    | CLA  | C1B-CHB | 2.48  | 1.47        | 1.41     |
| 23  | B     | 607    | CLA  | C3D-C4D | -2.48 | 1.38        | 1.44     |
| 28  | d     | 406[A] | PL9  | C6-C5   | 2.48  | 1.47        | 1.35     |
| 23  | C     | 505    | CLA  | CHB-C4A | 2.48  | 1.35        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | D     | 403[B] | CLA  | C3D-C4D | -2.48 | 1.38        | 1.44     |
| 23  | C     | 510    | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 23  | b     | 602    | CLA  | C4D-CHA | 2.48  | 1.46        | 1.38     |
| 23  | C     | 509    | CLA  | C1C-C2C | 2.47  | 1.49        | 1.44     |
| 23  | C     | 502    | CLA  | C3D-C4D | -2.47 | 1.38        | 1.44     |
| 23  | C     | 508    | CLA  | C3D-C4D | -2.47 | 1.38        | 1.44     |
| 23  | b     | 616    | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 23  | C     | 511    | CLA  | C4D-CHA | 2.47  | 1.46        | 1.38     |
| 26  | a     | 418    | GOL  | C1-C2   | 2.47  | 1.61        | 1.51     |
| 23  | A     | 405[A] | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 23  | c     | 514    | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 23  | C     | 508    | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 23  | d     | 403[A] | CLA  | C3D-C4D | -2.46 | 1.38        | 1.44     |
| 23  | B     | 603    | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 23  | b     | 609    | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 23  | a     | 405[B] | CLA  | C1C-C2C | 2.46  | 1.49        | 1.44     |
| 23  | B     | 604    | CLA  | CHB-C4A | 2.46  | 1.35        | 1.33     |
| 23  | C     | 508    | CLA  | C1B-CHB | 2.46  | 1.47        | 1.41     |
| 23  | a     | 407    | CLA  | C4D-CHA | 2.45  | 1.46        | 1.38     |
| 23  | B     | 613    | CLA  | C1B-CHB | 2.45  | 1.47        | 1.41     |
| 23  | b     | 607    | CLA  | C1B-CHB | 2.45  | 1.47        | 1.41     |
| 23  | d     | 403[A] | CLA  | C1C-C2C | 2.45  | 1.49        | 1.44     |
| 23  | C     | 502    | CLA  | C4B-CHC | 2.45  | 1.47        | 1.41     |
| 23  | b     | 610    | CLA  | C4D-CHA | 2.45  | 1.46        | 1.38     |
| 23  | C     | 508    | CLA  | C1C-C2C | 2.44  | 1.49        | 1.44     |
| 23  | C     | 511    | CLA  | C3D-C4D | -2.44 | 1.38        | 1.44     |
| 23  | A     | 406[B] | CLA  | C1C-C2C | 2.44  | 1.49        | 1.44     |
| 23  | D     | 403[A] | CLA  | C3D-C4D | -2.44 | 1.38        | 1.44     |
| 32  | b     | 621    | LMT  | C3'-C2' | 2.44  | 1.58        | 1.52     |
| 23  | d     | 403[B] | CLA  | C4D-CHA | 2.44  | 1.46        | 1.38     |
| 23  | d     | 402[B] | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 23  | B     | 602    | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 23  | a     | 404[B] | CLA  | C1B-CHB | 2.43  | 1.47        | 1.41     |
| 23  | C     | 514    | CLA  | C1B-CHB | 2.43  | 1.47        | 1.41     |
| 23  | B     | 605    | CLA  | OBD-CAD | 2.43  | 1.26        | 1.22     |
| 23  | c     | 506    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 23  | C     | 506    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 23  | C     | 507    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 23  | b     | 612    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 23  | C     | 509    | CLA  | CHB-C4A | 2.42  | 1.35        | 1.33     |
| 23  | C     | 504    | CLA  | C3D-C4D | -2.42 | 1.38        | 1.44     |
| 23  | C     | 504    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 502    | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 23  | C     | 507    | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 23  | b     | 608    | CLA  | C1B-CHB | 2.41  | 1.47        | 1.41     |
| 23  | c     | 514    | CLA  | C1B-CHB | 2.41  | 1.47        | 1.41     |
| 23  | b     | 613    | CLA  | C4B-CHC | 2.41  | 1.47        | 1.41     |
| 23  | B     | 606    | CLA  | C1C-C2C | 2.41  | 1.49        | 1.44     |
| 23  | d     | 403[B] | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 23  | b     | 609    | CLA  | C1C-C2C | 2.41  | 1.49        | 1.44     |
| 23  | B     | 608    | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 23  | B     | 609    | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 23  | B     | 611    | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 23  | C     | 508    | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 23  | B     | 614    | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 23  | c     | 514    | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 23  | C     | 512    | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 23  | c     | 502    | CLA  | C1C-C2C | 2.40  | 1.49        | 1.44     |
| 23  | b     | 607    | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 23  | A     | 405[B] | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 23  | B     | 606    | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 23  | A     | 404[B] | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 23  | C     | 510    | CLA  | C1C-C2C | 2.40  | 1.49        | 1.44     |
| 23  | c     | 509    | CLA  | C1C-C2C | 2.40  | 1.49        | 1.44     |
| 23  | a     | 404[A] | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 23  | b     | 603    | CLA  | C1B-CHB | 2.39  | 1.47        | 1.41     |
| 23  | b     | 611    | CLA  | C4D-CHA | 2.39  | 1.46        | 1.38     |
| 23  | A     | 405[B] | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 23  | a     | 404[B] | CLA  | C1C-C2C | 2.39  | 1.49        | 1.44     |
| 23  | a     | 405[A] | CLA  | C3D-C4D | -2.38 | 1.38        | 1.44     |
| 23  | a     | 404[A] | CLA  | C1C-C2C | 2.38  | 1.49        | 1.44     |
| 24  | d     | 405    | BCR  | C30-C25 | -2.38 | 1.50        | 1.53     |
| 23  | A     | 405[A] | CLA  | C1B-CHB | 2.37  | 1.47        | 1.41     |
| 38  | F     | 102    | HEM  | C3B-C4B | 2.37  | 1.49        | 1.44     |
| 23  | C     | 505    | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 23  | D     | 403[A] | CLA  | C1C-C2C | 2.37  | 1.49        | 1.44     |
| 23  | c     | 503    | CLA  | C4D-CHA | 2.37  | 1.46        | 1.38     |
| 23  | B     | 612    | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 23  | B     | 607    | CLA  | C1C-C2C | 2.37  | 1.49        | 1.44     |
| 23  | A     | 406[A] | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 23  | b     | 614    | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 23  | B     | 605    | CLA  | C1B-CHB | 2.36  | 1.47        | 1.41     |
| 23  | C     | 512    | CLA  | C3D-C4D | -2.36 | 1.38        | 1.44     |
| 23  | a     | 405[B] | CLA  | C3D-C4D | -2.36 | 1.38        | 1.44     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 511    | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 35  | b     | 622    | HTG  | O5-C1   | 2.35  | 1.46        | 1.42     |
| 23  | B     | 612    | CLA  | C4B-CHC | 2.35  | 1.47        | 1.41     |
| 23  | b     | 601    | CLA  | C1B-CHB | 2.35  | 1.47        | 1.41     |
| 23  | B     | 609    | CLA  | C1B-CHB | 2.35  | 1.47        | 1.41     |
| 23  | c     | 503    | CLA  | C1B-CHB | 2.35  | 1.47        | 1.41     |
| 23  | A     | 407    | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 35  | B     | 621    | HTG  | C1'-S1  | -2.34 | 1.78        | 1.81     |
| 23  | D     | 404    | CLA  | C4D-CHA | 2.34  | 1.46        | 1.38     |
| 23  | b     | 601    | CLA  | C1C-C2C | 2.34  | 1.49        | 1.44     |
| 23  | b     | 603    | CLA  | C3D-C4D | -2.34 | 1.38        | 1.44     |
| 23  | b     | 615    | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 23  | B     | 604    | CLA  | C3D-C4D | -2.34 | 1.38        | 1.44     |
| 23  | B     | 610    | CLA  | C3D-C4D | -2.34 | 1.38        | 1.44     |
| 23  | A     | 406[A] | CLA  | C1B-CHB | 2.34  | 1.47        | 1.41     |
| 23  | D     | 403[B] | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 23  | b     | 611    | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 23  | B     | 606    | CLA  | C3D-C4D | -2.33 | 1.38        | 1.44     |
| 23  | B     | 607    | CLA  | C4B-CHC | 2.33  | 1.47        | 1.41     |
| 23  | b     | 606    | CLA  | C3D-C4D | -2.33 | 1.38        | 1.44     |
| 23  | B     | 604    | CLA  | C1C-C2C | 2.33  | 1.49        | 1.44     |
| 32  | T     | 101    | LMT  | O3'-C3' | -2.33 | 1.37        | 1.43     |
| 23  | A     | 404[A] | CLA  | C1C-C2C | 2.33  | 1.49        | 1.44     |
| 31  | D     | 401[A] | PHO  | CHA-CBD | -2.33 | 1.49        | 1.52     |
| 23  | c     | 514    | CLA  | C3D-C4D | -2.33 | 1.39        | 1.44     |
| 32  | B     | 626    | LMT  | O3'-C3' | -2.33 | 1.37        | 1.43     |
| 23  | b     | 604    | CLA  | C1B-CHB | 2.33  | 1.47        | 1.41     |
| 26  | b     | 624    | GOL  | C3-C2   | 2.32  | 1.60        | 1.51     |
| 23  | b     | 612    | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 24  | B     | 619    | BCR  | C30-C25 | -2.32 | 1.50        | 1.53     |
| 31  | A     | 416[B] | PHO  | C3A-C2A | -2.32 | 1.52        | 1.54     |
| 23  | C     | 507    | CLA  | C1B-CHB | 2.32  | 1.47        | 1.41     |
| 23  | d     | 404    | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 23  | A     | 405[B] | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 23  | B     | 612    | CLA  | CHB-C4A | 2.31  | 1.35        | 1.33     |
| 23  | c     | 511    | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 23  | c     | 512    | CLA  | CHB-C4A | 2.31  | 1.35        | 1.33     |
| 23  | b     | 608    | CLA  | C4D-CHA | 2.31  | 1.46        | 1.38     |
| 23  | c     | 510    | CLA  | C1C-C2C | 2.31  | 1.49        | 1.44     |
| 23  | c     | 509    | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 23  | C     | 505    | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 23  | A     | 406[A] | CLA  | C1C-C2C | 2.30  | 1.49        | 1.44     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | a     | 404[A] | CLA  | C4B-CHC | 2.30  | 1.47        | 1.41     |
| 32  | e     | 101    | LMT  | O3'-C3' | -2.30 | 1.37        | 1.43     |
| 23  | a     | 405[A] | CLA  | C1B-CHB | 2.29  | 1.47        | 1.41     |
| 32  | B     | 629    | LMT  | O3'-C3' | -2.29 | 1.37        | 1.43     |
| 23  | D     | 403[B] | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 38  | f     | 101    | HEM  | CHB-C1B | 2.29  | 1.40        | 1.34     |
| 23  | b     | 606    | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 23  | b     | 605    | CLA  | C1D-C2D | 2.29  | 1.49        | 1.45     |
| 32  | m     | 103    | LMT  | C3'-C2' | 2.29  | 1.58        | 1.52     |
| 23  | A     | 407    | CLA  | C1C-C2C | 2.28  | 1.49        | 1.44     |
| 23  | c     | 504    | CLA  | C4C-C3C | 2.28  | 1.48        | 1.45     |
| 26  | a     | 417    | GOL  | C3-C2   | 2.28  | 1.60        | 1.51     |
| 36  | c     | 519    | DGD  | O2G-C2G | -2.28 | 1.41        | 1.46     |
| 23  | C     | 512    | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 23  | b     | 602    | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 23  | B     | 604    | CLA  | C1A-CHA | 2.27  | 1.52        | 1.43     |
| 35  | o     | 301    | HTG  | O5-C1   | 2.27  | 1.46        | 1.42     |
| 36  | C     | 518[A] | DGD  | O5D-C1E | 2.27  | 1.44        | 1.40     |
| 23  | c     | 505    | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 23  | A     | 407    | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 23  | b     | 601    | CLA  | C4B-CHC | 2.27  | 1.47        | 1.41     |
| 23  | A     | 405[A] | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 23  | C     | 514    | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 36  | h     | 102    | DGD  | O5D-C1E | 2.26  | 1.44        | 1.40     |
| 35  | B     | 623    | HTG  | C1-S1   | -2.26 | 1.76        | 1.80     |
| 23  | A     | 405[B] | CLA  | C1C-C2C | 2.26  | 1.49        | 1.44     |
| 23  | B     | 615    | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 23  | C     | 510    | CLA  | CHB-C4A | 2.26  | 1.35        | 1.33     |
| 23  | B     | 606    | CLA  | MG-NA   | 2.25  | 2.11        | 2.06     |
| 23  | D     | 403[A] | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 23  | b     | 607    | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 23  | a     | 405[B] | CLA  | C4B-CHC | 2.25  | 1.47        | 1.41     |
| 23  | A     | 407    | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 38  | F     | 102    | HEM  | CHB-C1B | 2.25  | 1.40        | 1.34     |
| 23  | c     | 513    | CLA  | C1C-C2C | 2.25  | 1.49        | 1.44     |
| 23  | b     | 611    | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 23  | b     | 610    | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 26  | o     | 304    | GOL  | C1-C2   | 2.24  | 1.60        | 1.51     |
| 23  | B     | 609    | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 23  | b     | 607    | CLA  | C3D-C4D | -2.24 | 1.39        | 1.44     |
| 23  | d     | 402[A] | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 23  | d     | 404    | CLA  | C1B-CHB | 2.24  | 1.47        | 1.41     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | A     | 406[B] | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 23  | d     | 404    | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 23  | c     | 506    | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 23  | C     | 503    | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 23  | b     | 616    | CLA  | C1B-CHB | 2.23  | 1.47        | 1.41     |
| 23  | c     | 507    | CLA  | C4B-CHC | 2.23  | 1.47        | 1.41     |
| 23  | c     | 513    | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 36  | c     | 519    | DGD  | O5D-C1E | 2.23  | 1.43        | 1.40     |
| 28  | a     | 413[A] | PL9  | C2-C3   | 2.22  | 1.40        | 1.34     |
| 23  | b     | 605    | CLA  | C1C-C2C | 2.22  | 1.49        | 1.44     |
| 23  | B     | 610    | CLA  | C4B-CHC | 2.22  | 1.47        | 1.41     |
| 23  | b     | 608    | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 23  | C     | 504    | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 23  | D     | 403[A] | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 26  | D     | 413    | GOL  | O2-C2   | -2.21 | 1.36        | 1.43     |
| 23  | C     | 502    | CLA  | C1B-CHB | 2.21  | 1.47        | 1.41     |
| 23  | D     | 404    | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 23  | c     | 512    | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 36  | c     | 518[A] | DGD  | O2G-C2G | -2.21 | 1.41        | 1.46     |
| 32  | T     | 101    | LMT  | O2'-C2' | -2.20 | 1.37        | 1.43     |
| 32  | a     | 416    | LMT  | O3'-C3' | -2.20 | 1.37        | 1.43     |
| 23  | A     | 406[B] | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 32  | F     | 101    | LMT  | O3'-C3' | -2.20 | 1.37        | 1.43     |
| 23  | c     | 504    | CLA  | MG-NA   | 2.20  | 2.11        | 2.06     |
| 23  | a     | 404[B] | CLA  | C4B-CHC | 2.19  | 1.47        | 1.41     |
| 23  | c     | 510    | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 23  | a     | 405[B] | CLA  | C1B-CHB | 2.19  | 1.47        | 1.41     |
| 38  | F     | 102    | HEM  | FE-NB   | 2.19  | 2.10        | 1.98     |
| 23  | B     | 603    | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 23  | B     | 604    | CLA  | C4B-CHC | 2.19  | 1.47        | 1.41     |
| 23  | d     | 404    | CLA  | C1D-C2D | 2.18  | 1.49        | 1.45     |
| 23  | b     | 604    | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 23  | B     | 601    | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 32  | B     | 627    | LMT  | O2'-C2' | -2.18 | 1.37        | 1.43     |
| 26  | D     | 402    | GOL  | C3-C2   | 2.18  | 1.60        | 1.51     |
| 23  | C     | 512    | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 23  | B     | 614    | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 23  | d     | 402[B] | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 23  | C     | 510    | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 25  | l     | 101    | SQD  | O6-C1   | 2.17  | 1.43        | 1.40     |
| 23  | b     | 607    | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 23  | d     | 402[B] | CLA  | C1B-CHB | 2.17  | 1.47        | 1.41     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 509    | CLA  | C4B-CHC | 2.17  | 1.47        | 1.41     |
| 23  | C     | 505    | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 23  | A     | 407    | CLA  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 23  | c     | 503    | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 23  | A     | 405[B] | CLA  | C4C-C3C | 2.16  | 1.48        | 1.45     |
| 23  | c     | 508    | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 23  | B     | 601    | CLA  | C1B-CHB | 2.16  | 1.47        | 1.41     |
| 23  | d     | 404    | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 23  | C     | 514    | CLA  | C4B-CHC | 2.15  | 1.47        | 1.41     |
| 23  | d     | 403[A] | CLA  | C4B-CHC | 2.15  | 1.47        | 1.41     |
| 23  | c     | 511    | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 32  | m     | 103    | LMT  | O2B-C2B | -2.15 | 1.37        | 1.43     |
| 23  | B     | 613    | CLA  | C4B-CHC | 2.15  | 1.47        | 1.41     |
| 23  | b     | 606    | CLA  | C1B-CHB | 2.14  | 1.46        | 1.41     |
| 23  | b     | 605    | CLA  | C1C-NC  | -2.14 | 1.34        | 1.37     |
| 23  | C     | 513    | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 23  | c     | 503    | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 26  | O     | 303    | GOL  | O2-C2   | -2.14 | 1.37        | 1.43     |
| 23  | b     | 615    | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 23  | d     | 402[B] | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 23  | b     | 603    | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 23  | c     | 506    | CLA  | CHB-C4A | 2.13  | 1.35        | 1.33     |
| 23  | C     | 506    | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 23  | C     | 503    | CLA  | C4D-CHA | 2.13  | 1.45        | 1.38     |
| 23  | C     | 514    | CLA  | C1C-NC  | -2.13 | 1.34        | 1.37     |
| 23  | a     | 405[A] | CLA  | C4C-C3C | 2.13  | 1.48        | 1.45     |
| 23  | C     | 513    | CLA  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 23  | C     | 507    | CLA  | C4B-CHC | 2.13  | 1.46        | 1.41     |
| 23  | A     | 406[A] | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 23  | A     | 406[B] | CLA  | C1D-C2D | 2.12  | 1.49        | 1.45     |
| 32  | m     | 103    | LMT  | O3'-C3' | -2.12 | 1.37        | 1.43     |
| 33  | d     | 414[A] | LHG  | O7-C5   | -2.12 | 1.41        | 1.46     |
| 23  | A     | 406[B] | CLA  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 28  | D     | 406[B] | PL9  | C2-C3   | 2.12  | 1.39        | 1.34     |
| 23  | B     | 601    | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 28  | A     | 413[A] | PL9  | C2-C1   | -2.12 | 1.39        | 1.44     |
| 23  | c     | 505    | CLA  | C4B-CHC | 2.11  | 1.46        | 1.41     |
| 23  | C     | 509    | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 32  | A     | 419    | LMT  | O2'-C2' | -2.11 | 1.37        | 1.43     |
| 23  | A     | 404[B] | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 32  | a     | 416    | LMT  | O2'-C2' | -2.11 | 1.37        | 1.43     |
| 23  | a     | 404[A] | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | a     | 404[B] | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 23  | c     | 511    | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 23  | B     | 615    | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 23  | c     | 509    | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 34  | D     | 412    | LMG  | O7-C8   | -2.11 | 1.41        | 1.46     |
| 23  | C     | 507    | CLA  | C1D-C2D | 2.10  | 1.49        | 1.45     |
| 23  | B     | 616    | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 32  | B     | 627    | LMT  | O2B-C2B | -2.10 | 1.37        | 1.43     |
| 23  | c     | 503    | CLA  | C4B-CHC | 2.10  | 1.46        | 1.41     |
| 23  | b     | 602    | CLA  | C1D-C2D | 2.10  | 1.49        | 1.45     |
| 28  | A     | 413[B] | PL9  | C2-C3   | 2.10  | 1.39        | 1.34     |
| 32  | B     | 626    | LMT  | O5'-C5' | -2.10 | 1.39        | 1.44     |
| 28  | a     | 413[B] | PL9  | C2-C3   | 2.10  | 1.39        | 1.34     |
| 23  | c     | 514    | CLA  | C1D-C2D | 2.09  | 1.49        | 1.45     |
| 32  | B     | 627    | LMT  | O3'-C3' | -2.09 | 1.37        | 1.43     |
| 24  | b     | 619    | BCR  | C1-C6   | -2.09 | 1.51        | 1.53     |
| 26  | D     | 402    | GOL  | O2-C2   | -2.09 | 1.37        | 1.43     |
| 32  | t     | 101    | LMT  | O2'-C2' | -2.09 | 1.37        | 1.43     |
| 33  | D     | 407[A] | LHG  | O7-C5   | -2.08 | 1.41        | 1.46     |
| 23  | C     | 505    | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 23  | C     | 503    | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 23  | b     | 605    | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 23  | c     | 512    | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 23  | b     | 606    | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 23  | c     | 507    | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 23  | b     | 612    | CLA  | C4B-CHC | 2.07  | 1.46        | 1.41     |
| 23  | A     | 407    | CLA  | C4B-CHC | 2.07  | 1.46        | 1.41     |
| 23  | C     | 512    | CLA  | CHB-C4A | 2.07  | 1.34        | 1.33     |
| 23  | A     | 406[A] | CLA  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 23  | c     | 507    | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 23  | a     | 405[A] | CLA  | C4B-CHC | 2.07  | 1.46        | 1.41     |
| 32  | M     | 101    | LMT  | O3'-C3' | -2.06 | 1.37        | 1.43     |
| 23  | B     | 607    | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 23  | b     | 605    | CLA  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 23  | c     | 505    | CLA  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 23  | b     | 605    | CLA  | C4B-CHC | 2.06  | 1.46        | 1.41     |
| 23  | B     | 608    | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 32  | B     | 626    | LMT  | O4'-C4B | -2.05 | 1.37        | 1.43     |
| 23  | b     | 601    | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 28  | A     | 413[A] | PL9  | C2-C3   | 2.05  | 1.39        | 1.34     |
| 23  | A     | 404[A] | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 33  | b     | 629[A] | LHG  | O7-C5   | -2.04 | 1.41        | 1.46     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 26  | V     | 203[A] | GOL  | C1-C2   | 2.04  | 1.59        | 1.51     |
| 23  | b     | 613    | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 23  | b     | 608    | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 33  | L     | 101[B] | LHG  | O7-C5   | -2.04 | 1.41        | 1.46     |
| 23  | d     | 402[A] | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 23  | d     | 402[A] | CLA  | C4B-CHC | 2.04  | 1.46        | 1.41     |
| 23  | b     | 614    | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 23  | c     | 503    | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 38  | f     | 101    | HEM  | CHA-C4D | 2.03  | 1.39        | 1.34     |
| 32  | T     | 101    | LMT  | O3B-C3B | -2.02 | 1.37        | 1.43     |
| 24  | B     | 618    | BCR  | C19-C18 | 2.02  | 1.50        | 1.46     |
| 33  | L     | 101[A] | LHG  | O7-C5   | -2.02 | 1.41        | 1.46     |
| 26  | c     | 527    | GOL  | C3-C2   | 2.02  | 1.59        | 1.51     |
| 36  | h     | 102    | DGD  | O2G-C2G | -2.02 | 1.41        | 1.46     |
| 40  | v     | 201    | HEC  | C3C-C4C | 2.02  | 1.46        | 1.43     |
| 23  | c     | 502    | CLA  | C1D-C2D | 2.02  | 1.49        | 1.45     |
| 23  | B     | 601    | CLA  | C1C-NC  | -2.02 | 1.34        | 1.37     |
| 23  | c     | 512    | CLA  | C1D-C2D | 2.01  | 1.49        | 1.45     |
| 23  | b     | 602    | CLA  | C1B-CHB | 2.01  | 1.46        | 1.41     |
| 23  | A     | 404[B] | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 36  | H     | 102    | DGD  | O2G-C2G | -2.01 | 1.41        | 1.46     |
| 34  | Z     | 101    | LMG  | O1-C1   | 2.01  | 1.43        | 1.40     |
| 23  | C     | 512    | CLA  | MG-NA   | 2.01  | 2.11        | 2.06     |
| 23  | B     | 616    | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 23  | B     | 616    | CLA  | C4B-CHC | 2.01  | 1.46        | 1.41     |
| 23  | C     | 508    | CLA  | CHB-C4A | 2.00  | 1.34        | 1.33     |
| 23  | B     | 616    | CLA  | C4C-C3C | 2.00  | 1.48        | 1.45     |
| 23  | b     | 613    | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |

All (3139) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|--------|-------------|----------|
| 23  | a     | 407    | CLA  | C1D-ND-C4D | -11.00 | 98.60       | 106.31   |
| 23  | B     | 611    | CLA  | C1D-ND-C4D | -10.88 | 98.68       | 106.31   |
| 23  | a     | 404[B] | CLA  | C1D-ND-C4D | -10.33 | 99.07       | 106.31   |
| 23  | B     | 615    | CLA  | C1D-ND-C4D | -10.23 | 99.13       | 106.31   |
| 23  | b     | 610    | CLA  | C1D-ND-C4D | -10.02 | 99.28       | 106.31   |
| 23  | d     | 404    | CLA  | C1D-ND-C4D | -10.01 | 99.29       | 106.31   |
| 23  | c     | 502    | CLA  | C1D-ND-C4D | -10.01 | 99.29       | 106.31   |
| 23  | b     | 605    | CLA  | C1D-ND-C4D | -9.91  | 99.36       | 106.31   |
| 23  | C     | 504    | CLA  | C1D-ND-C4D | -9.90  | 99.36       | 106.31   |
| 23  | B     | 601    | CLA  | C1D-ND-C4D | -9.89  | 99.37       | 106.31   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 606    | CLA  | C1D-ND-C4D  | -9.86 | 99.40       | 106.31   |
| 23  | b     | 602    | CLA  | C1D-ND-C4D  | -9.84 | 99.41       | 106.31   |
| 23  | a     | 405[B] | CLA  | C1D-ND-C4D  | -9.82 | 99.42       | 106.31   |
| 23  | B     | 607    | CLA  | C1D-ND-C4D  | -9.81 | 99.43       | 106.31   |
| 23  | D     | 404    | CLA  | C1D-ND-C4D  | -9.79 | 99.44       | 106.31   |
| 23  | c     | 512    | CLA  | C1D-ND-C4D  | -9.75 | 99.47       | 106.31   |
| 23  | A     | 406[B] | CLA  | C1D-ND-C4D  | -9.74 | 99.48       | 106.31   |
| 23  | C     | 514    | CLA  | C1D-ND-C4D  | -9.73 | 99.48       | 106.31   |
| 23  | B     | 613    | CLA  | C1D-ND-C4D  | -9.73 | 99.48       | 106.31   |
| 23  | C     | 502    | CLA  | C1D-ND-C4D  | -9.73 | 99.49       | 106.31   |
| 23  | b     | 607    | CLA  | C1D-ND-C4D  | -9.70 | 99.51       | 106.31   |
| 23  | B     | 614    | CLA  | C1D-ND-C4D  | -9.59 | 99.58       | 106.31   |
| 23  | A     | 404[B] | CLA  | C1D-ND-C4D  | -9.55 | 99.61       | 106.31   |
| 23  | c     | 506    | CLA  | C1D-ND-C4D  | -9.53 | 99.63       | 106.31   |
| 23  | C     | 505    | CLA  | C1D-ND-C4D  | -9.52 | 99.63       | 106.31   |
| 23  | c     | 504    | CLA  | C1D-ND-C4D  | -9.48 | 99.66       | 106.31   |
| 23  | B     | 605    | CLA  | C1D-ND-C4D  | -9.48 | 99.66       | 106.31   |
| 23  | A     | 407    | CLA  | C1D-ND-C4D  | -9.46 | 99.68       | 106.31   |
| 23  | C     | 511    | CLA  | C1D-ND-C4D  | -9.46 | 99.68       | 106.31   |
| 23  | C     | 513    | CLA  | C1D-ND-C4D  | -9.46 | 99.68       | 106.31   |
| 31  | a     | 406[A] | PHO  | O2D-CGD-CBD | 9.43  | 121.31      | 110.95   |
| 23  | c     | 513    | CLA  | C1D-ND-C4D  | -9.43 | 99.70       | 106.31   |
| 23  | c     | 514    | CLA  | C1D-ND-C4D  | -9.42 | 99.70       | 106.31   |
| 23  | B     | 612    | CLA  | C1D-ND-C4D  | -9.35 | 99.75       | 106.31   |
| 23  | b     | 614    | CLA  | C1D-ND-C4D  | -9.33 | 99.76       | 106.31   |
| 23  | c     | 508    | CLA  | C1D-ND-C4D  | -9.31 | 99.78       | 106.31   |
| 31  | a     | 406[B] | PHO  | O2D-CGD-CBD | 9.31  | 121.18      | 110.95   |
| 23  | c     | 507    | CLA  | C1D-ND-C4D  | -9.29 | 99.80       | 106.31   |
| 23  | C     | 506    | CLA  | C1D-ND-C4D  | -9.28 | 99.80       | 106.31   |
| 23  | c     | 511    | CLA  | C1D-ND-C4D  | -9.28 | 99.80       | 106.31   |
| 23  | b     | 601    | CLA  | C1D-ND-C4D  | -9.27 | 99.80       | 106.31   |
| 23  | a     | 405[A] | CLA  | C1D-ND-C4D  | -9.26 | 99.82       | 106.31   |
| 23  | D     | 403[A] | CLA  | C1D-ND-C4D  | -9.24 | 99.83       | 106.31   |
| 23  | b     | 615    | CLA  | C1D-ND-C4D  | -9.24 | 99.83       | 106.31   |
| 23  | c     | 510    | CLA  | C1D-ND-C4D  | -9.24 | 99.83       | 106.31   |
| 31  | D     | 401[B] | PHO  | O2D-CGD-CBD | 9.21  | 121.06      | 110.95   |
| 23  | d     | 403[A] | CLA  | C1D-ND-C4D  | -9.17 | 99.88       | 106.31   |
| 23  | A     | 405[B] | CLA  | C1D-ND-C4D  | -9.16 | 99.88       | 106.31   |
| 23  | A     | 406[A] | CLA  | C1D-ND-C4D  | -9.16 | 99.89       | 106.31   |
| 23  | d     | 402[A] | CLA  | C1D-ND-C4D  | -9.12 | 99.91       | 106.31   |
| 23  | D     | 403[B] | CLA  | C1D-ND-C4D  | -9.10 | 99.93       | 106.31   |
| 23  | d     | 402[B] | CLA  | C1D-ND-C4D  | -9.10 | 99.93       | 106.31   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 510    | CLA  | C1D-ND-C4D  | -9.10 | 99.93       | 106.31   |
| 31  | a     | 415[A] | PHO  | O2D-CGD-CBD | 9.07  | 120.91      | 110.95   |
| 23  | b     | 606    | CLA  | C1D-ND-C4D  | -9.03 | 99.98       | 106.31   |
| 23  | C     | 509    | CLA  | C1D-ND-C4D  | -8.99 | 100.00      | 106.31   |
| 23  | A     | 405[A] | CLA  | C1D-ND-C4D  | -8.99 | 100.01      | 106.31   |
| 23  | b     | 609    | CLA  | C1D-ND-C4D  | -8.91 | 100.06      | 106.31   |
| 23  | a     | 404[A] | CLA  | C1D-ND-C4D  | -8.91 | 100.06      | 106.31   |
| 23  | B     | 603    | CLA  | C1D-ND-C4D  | -8.91 | 100.06      | 106.31   |
| 23  | b     | 611    | CLA  | C1D-ND-C4D  | -8.90 | 100.07      | 106.31   |
| 23  | b     | 603    | CLA  | C1D-ND-C4D  | -8.85 | 100.10      | 106.31   |
| 23  | C     | 507    | CLA  | C1D-ND-C4D  | -8.76 | 100.17      | 106.31   |
| 23  | B     | 608    | CLA  | C1D-ND-C4D  | -8.73 | 100.18      | 106.31   |
| 23  | b     | 608    | CLA  | C1D-ND-C4D  | -8.72 | 100.19      | 106.31   |
| 23  | b     | 612    | CLA  | C1D-ND-C4D  | -8.72 | 100.19      | 106.31   |
| 23  | B     | 616    | CLA  | C1D-ND-C4D  | -8.71 | 100.20      | 106.31   |
| 23  | C     | 503    | CLA  | C1D-ND-C4D  | -8.70 | 100.20      | 106.31   |
| 23  | d     | 403[B] | CLA  | C1D-ND-C4D  | -8.65 | 100.25      | 106.31   |
| 31  | A     | 416[A] | PHO  | O2D-CGD-CBD | 8.64  | 120.44      | 110.95   |
| 23  | c     | 509    | CLA  | C1D-ND-C4D  | -8.59 | 100.29      | 106.31   |
| 23  | B     | 610    | CLA  | C1D-ND-C4D  | -8.58 | 100.29      | 106.31   |
| 23  | A     | 404[A] | CLA  | C1D-ND-C4D  | -8.57 | 100.30      | 106.31   |
| 23  | B     | 609    | CLA  | C1D-ND-C4D  | -8.55 | 100.31      | 106.31   |
| 40  | v     | 201    | HEC  | CBB-CAB-C3B | -8.55 | 107.48      | 127.49   |
| 23  | c     | 505    | CLA  | C1D-ND-C4D  | -8.53 | 100.33      | 106.31   |
| 23  | c     | 503    | CLA  | C1D-ND-C4D  | -8.49 | 100.36      | 106.31   |
| 23  | B     | 602    | CLA  | C1D-ND-C4D  | -8.47 | 100.37      | 106.31   |
| 31  | a     | 415[B] | PHO  | O2D-CGD-CBD | 8.42  | 120.20      | 110.95   |
| 40  | V     | 201    | HEC  | CBB-CAB-C3B | -8.39 | 107.85      | 127.49   |
| 31  | A     | 416[B] | PHO  | O2D-CGD-CBD | 8.38  | 120.15      | 110.95   |
| 23  | b     | 616    | CLA  | C1D-ND-C4D  | -8.32 | 100.48      | 106.31   |
| 23  | b     | 602    | CLA  | C4A-NA-C1A  | -8.32 | 102.89      | 106.68   |
| 23  | b     | 613    | CLA  | C1D-ND-C4D  | -8.25 | 100.52      | 106.31   |
| 23  | C     | 512    | CLA  | C1D-ND-C4D  | -8.18 | 100.57      | 106.31   |
| 23  | b     | 604    | CLA  | C1D-ND-C4D  | -8.08 | 100.64      | 106.31   |
| 23  | D     | 403[B] | CLA  | C4A-NA-C1A  | -7.96 | 103.05      | 106.68   |
| 23  | C     | 508    | CLA  | C1D-ND-C4D  | -7.63 | 100.96      | 106.31   |
| 23  | B     | 604    | CLA  | C1D-ND-C4D  | -7.58 | 100.99      | 106.31   |
| 23  | B     | 611    | CLA  | CHD-C4C-C3C | -7.53 | 113.80      | 124.77   |
| 23  | B     | 605    | CLA  | CHD-C4C-C3C | -7.52 | 113.81      | 124.77   |
| 23  | B     | 605    | CLA  | CMD-C2D-C1D | 7.50  | 137.93      | 124.73   |
| 25  | X     | 101    | SQD  | O6-C1-C2    | 7.49  | 119.65      | 108.27   |
| 23  | c     | 502    | CLA  | CMD-C2D-C1D | 7.46  | 137.86      | 124.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 606    | CLA  | CMD-C2D-C1D | 7.43  | 137.81      | 124.73   |
| 23  | b     | 616    | CLA  | O2D-CGD-CBD | 7.34  | 124.06      | 111.23   |
| 23  | c     | 504    | CLA  | CMD-C2D-C1D | 7.30  | 137.58      | 124.73   |
| 23  | B     | 615    | CLA  | C4A-NA-C1A  | -7.27 | 103.36      | 106.68   |
| 23  | B     | 606    | CLA  | C4A-NA-C1A  | -7.23 | 103.38      | 106.68   |
| 31  | D     | 401[A] | PHO  | O2D-CGD-CBD | 7.23  | 118.89      | 110.95   |
| 23  | C     | 505    | CLA  | C2D-C1D-ND  | 7.20  | 117.25      | 110.13   |
| 23  | B     | 616    | CLA  | CHD-C4C-C3C | -7.17 | 114.32      | 124.77   |
| 23  | B     | 610    | CLA  | O2D-CGD-CBD | 7.13  | 123.69      | 111.23   |
| 23  | C     | 507    | CLA  | CMD-C2D-C1D | 7.13  | 137.28      | 124.73   |
| 23  | C     | 511    | CLA  | CMD-C2D-C1D | 7.07  | 137.17      | 124.73   |
| 23  | D     | 403[A] | CLA  | C4A-NA-C1A  | -7.05 | 103.46      | 106.68   |
| 23  | c     | 508    | CLA  | CMD-C2D-C1D | 7.04  | 137.12      | 124.73   |
| 23  | a     | 407    | CLA  | C2D-C1D-ND  | 7.02  | 117.08      | 110.13   |
| 23  | B     | 607    | CLA  | C2D-C1D-ND  | 7.01  | 117.06      | 110.13   |
| 23  | b     | 603    | CLA  | C4A-NA-C1A  | -7.00 | 103.49      | 106.68   |
| 23  | B     | 609    | CLA  | C4A-NA-C1A  | -6.98 | 103.50      | 106.68   |
| 23  | B     | 603    | CLA  | O2D-CGD-CBD | 6.96  | 123.39      | 111.23   |
| 23  | B     | 613    | CLA  | C2D-C1D-ND  | 6.95  | 117.01      | 110.13   |
| 23  | B     | 614    | CLA  | CMD-C2D-C1D | 6.95  | 136.96      | 124.73   |
| 23  | B     | 616    | CLA  | C2D-C1D-ND  | 6.94  | 117.00      | 110.13   |
| 23  | b     | 614    | CLA  | C2D-C1D-ND  | 6.94  | 116.99      | 110.13   |
| 23  | c     | 504    | CLA  | C4A-NA-C1A  | -6.92 | 103.52      | 106.68   |
| 23  | C     | 504    | CLA  | C4A-NA-C1A  | -6.91 | 103.53      | 106.68   |
| 23  | B     | 611    | CLA  | CMD-C2D-C1D | 6.90  | 136.88      | 124.73   |
| 23  | b     | 615    | CLA  | C4A-NA-C1A  | -6.90 | 103.53      | 106.68   |
| 23  | b     | 601    | CLA  | O2D-CGD-CBD | 6.88  | 123.26      | 111.23   |
| 23  | B     | 614    | CLA  | C2D-C1D-ND  | 6.88  | 116.93      | 110.13   |
| 23  | B     | 606    | CLA  | C2D-C1D-ND  | 6.86  | 116.91      | 110.13   |
| 23  | b     | 606    | CLA  | C4A-NA-C1A  | -6.83 | 103.56      | 106.68   |
| 23  | b     | 613    | CLA  | CHD-C4C-C3C | -6.83 | 114.82      | 124.77   |
| 23  | C     | 513    | CLA  | CHD-C4C-C3C | -6.82 | 114.83      | 124.77   |
| 23  | B     | 616    | CLA  | O2D-CGD-CBD | 6.82  | 123.15      | 111.23   |
| 23  | b     | 613    | CLA  | C2D-C1D-ND  | 6.80  | 116.86      | 110.13   |
| 23  | A     | 407    | CLA  | C2D-C1D-ND  | 6.78  | 116.83      | 110.13   |
| 23  | B     | 611    | CLA  | C2D-C1D-ND  | 6.75  | 116.80      | 110.13   |
| 23  | C     | 504    | CLA  | C2D-C1D-ND  | 6.74  | 116.80      | 110.13   |
| 23  | c     | 510    | CLA  | C1-C2-C3    | -6.74 | 115.16      | 126.20   |
| 23  | b     | 610    | CLA  | CHD-C4C-C3C | -6.73 | 114.95      | 124.77   |
| 23  | B     | 615    | CLA  | C2D-C1D-ND  | 6.73  | 116.79      | 110.13   |
| 23  | d     | 404    | CLA  | CMD-C2D-C1D | 6.70  | 136.53      | 124.73   |
| 23  | A     | 404[A] | CLA  | CMD-C2D-C1D | 6.70  | 136.53      | 124.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 508    | CLA  | O2D-CGD-CBD | 6.68  | 122.92      | 111.23   |
| 23  | d     | 403[B] | CLA  | CMD-C2D-C1D | 6.65  | 136.44      | 124.73   |
| 23  | d     | 404    | CLA  | C2D-C1D-ND  | 6.65  | 116.71      | 110.13   |
| 23  | b     | 616    | CLA  | CHD-C4C-C3C | -6.65 | 115.08      | 124.77   |
| 23  | C     | 504    | CLA  | CHD-C4C-C3C | -6.64 | 115.09      | 124.77   |
| 23  | A     | 404[B] | CLA  | CMD-C2D-C1D | 6.64  | 136.42      | 124.73   |
| 25  | A     | 409[A] | SQD  | O6-C1-C2    | 6.64  | 118.36      | 108.27   |
| 23  | d     | 402[A] | CLA  | CHD-C4C-C3C | -6.62 | 115.12      | 124.77   |
| 25  | X     | 101    | SQD  | O47-C7-C8   | 6.60  | 125.76      | 111.48   |
| 23  | B     | 603    | CLA  | C4A-NA-C1A  | -6.60 | 103.67      | 106.68   |
| 23  | b     | 607    | CLA  | C2D-C1D-ND  | 6.59  | 116.65      | 110.13   |
| 23  | B     | 606    | CLA  | O2D-CGD-CBD | 6.58  | 122.73      | 111.23   |
| 23  | B     | 602    | CLA  | CHD-C4C-C3C | -6.55 | 115.22      | 124.77   |
| 23  | B     | 605    | CLA  | C2D-C1D-ND  | 6.54  | 116.60      | 110.13   |
| 23  | a     | 407    | CLA  | CHD-C4C-C3C | -6.53 | 115.25      | 124.77   |
| 23  | B     | 614    | CLA  | CHD-C4C-C3C | -6.50 | 115.30      | 124.77   |
| 23  | d     | 402[A] | CLA  | C2D-C1D-ND  | 6.50  | 116.56      | 110.13   |
| 23  | A     | 407    | CLA  | CHD-C4C-C3C | -6.50 | 115.30      | 124.77   |
| 23  | A     | 406[B] | CLA  | CMD-C2D-C1D | 6.50  | 136.17      | 124.73   |
| 23  | b     | 612    | CLA  | CHD-C4C-C3C | -6.49 | 115.31      | 124.77   |
| 23  | B     | 615    | CLA  | CHD-C4C-C3C | -6.49 | 115.32      | 124.77   |
| 23  | b     | 605    | CLA  | CMD-C2D-C1D | 6.48  | 136.15      | 124.73   |
| 23  | c     | 514    | CLA  | CMD-C2D-C1D | 6.48  | 136.14      | 124.73   |
| 23  | B     | 610    | CLA  | C2D-C1D-ND  | 6.48  | 116.54      | 110.13   |
| 23  | b     | 609    | CLA  | C4A-NA-C1A  | -6.47 | 103.73      | 106.68   |
| 35  | b     | 623    | HTG  | C1'-S1-C1   | 6.45  | 114.38      | 100.45   |
| 23  | b     | 605    | CLA  | CHD-C4C-C3C | -6.45 | 115.37      | 124.77   |
| 23  | B     | 602    | CLA  | O2D-CGD-CBD | 6.44  | 122.50      | 111.23   |
| 23  | b     | 616    | CLA  | CMD-C2D-C1D | 6.43  | 136.05      | 124.73   |
| 23  | B     | 612    | CLA  | O2D-CGD-CBD | 6.42  | 122.46      | 111.23   |
| 23  | a     | 405[A] | CLA  | C2D-C1D-ND  | 6.42  | 116.48      | 110.13   |
| 23  | B     | 601    | CLA  | C2D-C1D-ND  | 6.41  | 116.47      | 110.13   |
| 23  | a     | 405[A] | CLA  | CHD-C4C-C3C | -6.41 | 115.43      | 124.77   |
| 23  | b     | 605    | CLA  | C2D-C1D-ND  | 6.39  | 116.45      | 110.13   |
| 23  | C     | 508    | CLA  | CMD-C2D-C1D | 6.39  | 135.98      | 124.73   |
| 23  | B     | 601    | CLA  | CHD-C4C-C3C | -6.39 | 115.46      | 124.77   |
| 23  | a     | 405[B] | CLA  | CMD-C2D-C1D | 6.38  | 135.97      | 124.73   |
| 23  | b     | 611    | CLA  | CHD-C4C-C3C | -6.38 | 115.47      | 124.77   |
| 23  | b     | 616    | CLA  | C4A-NA-C1A  | -6.38 | 103.77      | 106.68   |
| 23  | b     | 601    | CLA  | C4A-NA-C1A  | -6.38 | 103.77      | 106.68   |
| 23  | c     | 510    | CLA  | C2D-C1D-ND  | 6.37  | 116.43      | 110.13   |
| 23  | b     | 610    | CLA  | C2D-C1D-ND  | 6.36  | 116.42      | 110.13   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 404[B] | CLA  | CMD-C2D-C1D | 6.36  | 135.92      | 124.73   |
| 23  | b     | 606    | CLA  | CMD-C2D-C1D | 6.36  | 135.92      | 124.73   |
| 25  | l     | 101    | SQD  | O6-C1-C2    | 6.35  | 117.92      | 108.27   |
| 23  | b     | 609    | CLA  | CHD-C4C-C3C | -6.33 | 115.54      | 124.77   |
| 23  | C     | 514    | CLA  | C2D-C1D-ND  | 6.31  | 116.37      | 110.13   |
| 23  | D     | 403[A] | CLA  | C2D-C1D-ND  | 6.30  | 116.37      | 110.13   |
| 23  | C     | 509    | CLA  | C2D-C1D-ND  | 6.30  | 116.36      | 110.13   |
| 23  | c     | 508    | CLA  | O2D-CGD-CBD | 6.30  | 122.25      | 111.23   |
| 24  | Y     | 101    | BCR  | C33-C5-C6   | -6.30 | 117.61      | 124.48   |
| 23  | B     | 603    | CLA  | C2D-C1D-ND  | 6.29  | 116.35      | 110.13   |
| 23  | B     | 613    | CLA  | CHD-C4C-C3C | -6.29 | 115.61      | 124.77   |
| 23  | A     | 404[A] | CLA  | C4A-NA-C1A  | -6.29 | 103.81      | 106.68   |
| 23  | a     | 405[B] | CLA  | CHD-C4C-C3C | -6.26 | 115.65      | 124.77   |
| 23  | b     | 614    | CLA  | CMD-C2D-C1D | 6.25  | 135.74      | 124.73   |
| 23  | b     | 611    | CLA  | C2D-C1D-ND  | 6.25  | 116.31      | 110.13   |
| 23  | b     | 615    | CLA  | C2D-C1D-ND  | 6.25  | 116.31      | 110.13   |
| 23  | b     | 603    | CLA  | CHD-C4C-C3C | -6.24 | 115.67      | 124.77   |
| 23  | c     | 508    | CLA  | C2D-C1D-ND  | 6.24  | 116.30      | 110.13   |
| 23  | a     | 405[B] | CLA  | C2D-C1D-ND  | 6.24  | 116.30      | 110.13   |
| 23  | B     | 601    | CLA  | O2D-CGD-CBD | 6.23  | 122.12      | 111.23   |
| 23  | B     | 609    | CLA  | CHD-C4C-C3C | -6.22 | 115.71      | 124.77   |
| 23  | C     | 502    | CLA  | O2D-CGD-CBD | 6.21  | 122.09      | 111.23   |
| 23  | b     | 602    | CLA  | O2D-CGD-CBD | 6.21  | 122.08      | 111.23   |
| 23  | C     | 506    | CLA  | O2D-CGD-CBD | 6.21  | 122.08      | 111.23   |
| 23  | C     | 513    | CLA  | C2D-C1D-ND  | 6.19  | 116.25      | 110.13   |
| 23  | c     | 512    | CLA  | CHD-C4C-C3C | -6.19 | 115.75      | 124.77   |
| 23  | c     | 514    | CLA  | C4A-NA-C1A  | -6.19 | 103.86      | 106.68   |
| 23  | c     | 508    | CLA  | CHD-C4C-C3C | -6.18 | 115.76      | 124.77   |
| 23  | a     | 404[B] | CLA  | C2D-C1D-ND  | 6.18  | 116.24      | 110.13   |
| 23  | C     | 513    | CLA  | C4A-NA-C1A  | -6.17 | 103.86      | 106.68   |
| 23  | C     | 506    | CLA  | C4A-NA-C1A  | -6.16 | 103.87      | 106.68   |
| 23  | A     | 405[B] | CLA  | C2D-C1D-ND  | 6.16  | 116.22      | 110.13   |
| 23  | C     | 509    | CLA  | CHD-C4C-C3C | -6.15 | 115.80      | 124.77   |
| 23  | b     | 601    | CLA  | CMD-C2D-C1D | 6.14  | 135.55      | 124.73   |
| 23  | b     | 606    | CLA  | CHD-C4C-C3C | -6.14 | 115.82      | 124.77   |
| 23  | B     | 612    | CLA  | C2D-C1D-ND  | 6.14  | 116.20      | 110.13   |
| 23  | C     | 510    | CLA  | C2D-C1D-ND  | 6.14  | 116.20      | 110.13   |
| 23  | A     | 405[A] | CLA  | C2D-C1D-ND  | 6.12  | 116.18      | 110.13   |
| 23  | b     | 611    | CLA  | CMD-C2D-C1D | 6.12  | 135.50      | 124.73   |
| 23  | B     | 606    | CLA  | CHD-C4C-C3C | -6.11 | 115.86      | 124.77   |
| 23  | C     | 502    | CLA  | C2D-C1D-ND  | 6.10  | 116.17      | 110.13   |
| 23  | D     | 403[A] | CLA  | CMD-C2D-C1D | 6.10  | 135.47      | 124.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | d     | 402[B] | CLA  | CHD-C4C-C3C | -6.10 | 115.88      | 124.77   |
| 23  | D     | 403[B] | CLA  | C2D-C1D-ND  | 6.10  | 116.16      | 110.13   |
| 23  | b     | 604    | CLA  | C1-C2-C3    | -6.10 | 116.21      | 126.20   |
| 23  | b     | 601    | CLA  | CHD-C4C-C3C | -6.09 | 115.89      | 124.77   |
| 23  | B     | 608    | CLA  | C2D-C1D-ND  | 6.08  | 116.15      | 110.13   |
| 23  | b     | 615    | CLA  | CHD-C4C-C3C | -6.08 | 115.91      | 124.77   |
| 23  | c     | 504    | CLA  | CHD-C4C-C3C | -6.08 | 115.92      | 124.77   |
| 23  | B     | 610    | CLA  | CMD-C2D-C1D | 6.07  | 135.42      | 124.73   |
| 23  | a     | 404[A] | CLA  | CMD-C2D-C1D | 6.07  | 135.41      | 124.73   |
| 23  | B     | 605    | CLA  | O2D-CGD-CBD | 6.07  | 121.84      | 111.23   |
| 23  | c     | 507    | CLA  | C2D-C1D-ND  | 6.07  | 116.13      | 110.13   |
| 23  | D     | 404    | CLA  | CMD-C2D-C1D | 6.06  | 135.40      | 124.73   |
| 23  | b     | 608    | CLA  | CHD-C4C-C3C | -6.06 | 115.94      | 124.77   |
| 23  | c     | 509    | CLA  | C2D-C1D-ND  | 6.06  | 116.12      | 110.13   |
| 23  | c     | 502    | CLA  | C2D-C1D-ND  | 6.05  | 116.12      | 110.13   |
| 23  | d     | 403[B] | CLA  | C2C-C1C-NC  | 6.05  | 116.34      | 109.98   |
| 23  | C     | 502    | CLA  | CHD-C4C-C3C | -6.05 | 115.95      | 124.77   |
| 23  | A     | 406[A] | CLA  | C2D-C1D-ND  | 6.05  | 116.11      | 110.13   |
| 23  | b     | 611    | CLA  | O2D-CGD-CBD | 6.04  | 121.79      | 111.23   |
| 23  | c     | 511    | CLA  | C4A-NA-C1A  | -6.04 | 103.92      | 106.68   |
| 23  | d     | 402[B] | CLA  | C2D-C1D-ND  | 6.03  | 116.10      | 110.13   |
| 23  | b     | 607    | CLA  | CHD-C4C-C3C | -6.03 | 115.98      | 124.77   |
| 23  | a     | 404[A] | CLA  | C4A-NA-C1A  | -6.03 | 103.93      | 106.68   |
| 24  | D     | 405    | BCR  | C7-C8-C9    | -6.03 | 117.32      | 126.23   |
| 23  | C     | 514    | CLA  | CHD-C4C-C3C | -6.03 | 115.98      | 124.77   |
| 23  | c     | 511    | CLA  | CHD-C4C-C3C | -6.03 | 115.99      | 124.77   |
| 23  | a     | 405[A] | CLA  | C4A-NA-C1A  | -6.02 | 103.93      | 106.68   |
| 23  | c     | 513    | CLA  | CHD-C4C-C3C | -6.02 | 116.00      | 124.77   |
| 23  | c     | 512    | CLA  | CMD-C2D-C1D | 6.02  | 135.32      | 124.73   |
| 23  | B     | 607    | CLA  | CHD-C4C-C3C | -6.01 | 116.01      | 124.77   |
| 23  | B     | 601    | CLA  | CMD-C2D-C1D | 6.01  | 135.30      | 124.73   |
| 23  | C     | 510    | CLA  | CHD-C4C-C3C | -6.00 | 116.02      | 124.77   |
| 23  | b     | 616    | CLA  | C2D-C1D-ND  | 5.99  | 116.06      | 110.13   |
| 23  | b     | 604    | CLA  | O2D-CGD-CBD | 5.99  | 121.70      | 111.23   |
| 23  | c     | 512    | CLA  | C2D-C1D-ND  | 5.99  | 116.05      | 110.13   |
| 23  | D     | 404    | CLA  | CHD-C4C-C3C | -5.97 | 116.07      | 124.77   |
| 23  | b     | 601    | CLA  | C2D-C1D-ND  | 5.97  | 116.03      | 110.13   |
| 23  | c     | 503    | CLA  | CHD-C4C-C3C | -5.95 | 116.09      | 124.77   |
| 23  | b     | 605    | CLA  | O2D-CGD-CBD | 5.95  | 121.63      | 111.23   |
| 25  | A     | 409[B] | SQD  | O6-C1-C2    | 5.95  | 117.30      | 108.27   |
| 23  | D     | 404    | CLA  | C4A-NA-C1A  | -5.95 | 103.97      | 106.68   |
| 23  | b     | 614    | CLA  | O2D-CGD-CBD | 5.94  | 121.62      | 111.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 506    | CLA  | O2D-CGD-CBD | 5.94  | 121.62      | 111.23   |
| 23  | c     | 507    | CLA  | CMD-C2D-C1D | 5.94  | 135.18      | 124.73   |
| 23  | C     | 503    | CLA  | CHD-C4C-C3C | -5.93 | 116.13      | 124.77   |
| 23  | d     | 402[A] | CLA  | CMD-C2D-C1D | 5.93  | 135.16      | 124.73   |
| 23  | C     | 506    | CLA  | CHD-C4C-C3C | -5.92 | 116.14      | 124.77   |
| 23  | d     | 402[B] | CLA  | CMD-C2D-C1D | 5.92  | 135.16      | 124.73   |
| 23  | b     | 610    | CLA  | CMD-C2D-C1D | 5.92  | 135.15      | 124.73   |
| 23  | b     | 614    | CLA  | CHD-C4C-C3C | -5.91 | 116.15      | 124.77   |
| 23  | c     | 510    | CLA  | CHD-C4C-C3C | -5.91 | 116.16      | 124.77   |
| 23  | c     | 505    | CLA  | CMD-C2D-C1D | 5.91  | 135.13      | 124.73   |
| 23  | c     | 511    | CLA  | C2D-C1D-ND  | 5.90  | 115.97      | 110.13   |
| 23  | c     | 513    | CLA  | C2D-C1D-ND  | 5.90  | 115.97      | 110.13   |
| 23  | C     | 512    | CLA  | CHD-C4C-C3C | -5.90 | 116.17      | 124.77   |
| 23  | B     | 611    | CLA  | O2D-CGD-CBD | 5.89  | 121.53      | 111.23   |
| 23  | A     | 406[A] | CLA  | CMD-C2D-C1D | 5.89  | 135.10      | 124.73   |
| 23  | c     | 510    | CLA  | CMD-C2D-C1D | 5.89  | 135.09      | 124.73   |
| 23  | C     | 511    | CLA  | CHD-C4C-C3C | -5.88 | 116.20      | 124.77   |
| 23  | C     | 502    | CLA  | C4A-NA-C1A  | -5.88 | 104.00      | 106.68   |
| 23  | B     | 610    | CLA  | CHD-C4C-C3C | -5.88 | 116.20      | 124.77   |
| 23  | D     | 404    | CLA  | C2D-C1D-ND  | 5.88  | 115.94      | 110.13   |
| 25  | a     | 409[A] | SQD  | O6-C1-C2    | 5.87  | 117.19      | 108.27   |
| 23  | b     | 602    | CLA  | CMD-C2D-C1D | 5.87  | 135.06      | 124.73   |
| 23  | D     | 403[B] | CLA  | CMD-C2D-C1D | 5.86  | 135.05      | 124.73   |
| 40  | V     | 201    | HEC  | CBD-CAD-C3D | -5.86 | 102.69      | 112.54   |
| 23  | b     | 609    | CLA  | C2D-C1D-ND  | 5.86  | 115.92      | 110.13   |
| 23  | B     | 604    | CLA  | C2C-C1C-NC  | 5.85  | 116.12      | 109.98   |
| 23  | A     | 406[A] | CLA  | CHD-C4C-C3C | -5.85 | 116.25      | 124.77   |
| 23  | A     | 406[B] | CLA  | C2D-C1D-ND  | 5.84  | 115.91      | 110.13   |
| 23  | c     | 506    | CLA  | CHD-C4C-C3C | -5.84 | 116.26      | 124.77   |
| 23  | c     | 513    | CLA  | CMD-C2D-C1D | 5.84  | 135.00      | 124.73   |
| 23  | B     | 614    | CLA  | C3D-C2D-C1D | -5.82 | 97.88       | 105.83   |
| 23  | B     | 608    | CLA  | CMD-C2D-C1D | 5.82  | 134.98      | 124.73   |
| 23  | C     | 504    | CLA  | CMD-C2D-C1D | 5.82  | 134.97      | 124.73   |
| 23  | C     | 505    | CLA  | CHD-C4C-C3C | -5.82 | 116.29      | 124.77   |
| 23  | c     | 503    | CLA  | C2D-C1D-ND  | 5.81  | 115.88      | 110.13   |
| 23  | B     | 609    | CLA  | CMD-C2D-C1D | 5.81  | 134.97      | 124.73   |
| 23  | C     | 502    | CLA  | CMD-C2D-C1D | 5.81  | 134.96      | 124.73   |
| 23  | B     | 602    | CLA  | C2D-C1D-ND  | 5.81  | 115.88      | 110.13   |
| 23  | a     | 404[B] | CLA  | CHD-C4C-C3C | -5.81 | 116.30      | 124.77   |
| 23  | d     | 403[A] | CLA  | C2D-C1D-ND  | 5.80  | 115.87      | 110.13   |
| 23  | C     | 512    | CLA  | O2D-CGD-CBD | 5.80  | 121.37      | 111.23   |
| 23  | C     | 508    | CLA  | CHD-C4C-C3C | -5.79 | 116.33      | 124.77   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31  | a     | 415[A] | PHO  | C1-C2-C3    | -5.78 | 116.72      | 126.20   |
| 23  | c     | 503    | CLA  | C2C-C1C-NC  | 5.78  | 116.05      | 109.98   |
| 23  | d     | 403[A] | CLA  | C2C-C1C-NC  | 5.78  | 116.05      | 109.98   |
| 23  | c     | 505    | CLA  | C4A-NA-C1A  | -5.77 | 104.05      | 106.68   |
| 23  | b     | 602    | CLA  | C2D-C1D-ND  | 5.77  | 115.84      | 110.13   |
| 23  | A     | 405[A] | CLA  | CHD-C4C-C3C | -5.77 | 116.36      | 124.77   |
| 23  | b     | 604    | CLA  | CMD-C2D-C1D | 5.77  | 134.89      | 124.73   |
| 23  | A     | 406[A] | CLA  | C4A-NA-C1A  | -5.77 | 104.05      | 106.68   |
| 23  | C     | 505    | CLA  | CMD-C2D-C1D | 5.76  | 134.87      | 124.73   |
| 23  | b     | 613    | CLA  | CMD-C2D-C1D | 5.76  | 134.87      | 124.73   |
| 23  | C     | 512    | CLA  | C2D-C1D-ND  | 5.76  | 115.82      | 110.13   |
| 25  | b     | 620    | SQD  | O6-C1-C2    | 5.76  | 117.01      | 108.27   |
| 23  | C     | 514    | CLA  | CMD-C2D-C1D | 5.76  | 134.86      | 124.73   |
| 23  | c     | 513    | CLA  | O2D-CGD-CBD | 5.75  | 121.29      | 111.23   |
| 23  | C     | 510    | CLA  | CMD-C2D-C1D | 5.75  | 134.86      | 124.73   |
| 23  | b     | 615    | CLA  | CMD-C2D-C1D | 5.75  | 134.85      | 124.73   |
| 23  | c     | 514    | CLA  | C2D-C1D-ND  | 5.75  | 115.81      | 110.13   |
| 23  | c     | 502    | CLA  | CHD-C4C-C3C | -5.74 | 116.41      | 124.77   |
| 23  | C     | 509    | CLA  | C2C-C1C-NC  | 5.73  | 116.00      | 109.98   |
| 23  | C     | 506    | CLA  | C2D-C1D-ND  | 5.72  | 115.79      | 110.13   |
| 23  | c     | 506    | CLA  | C2D-C1D-ND  | 5.72  | 115.78      | 110.13   |
| 23  | B     | 603    | CLA  | CHD-C4C-C3C | -5.72 | 116.44      | 124.77   |
| 23  | A     | 404[B] | CLA  | C4A-NA-C1A  | -5.72 | 104.07      | 106.68   |
| 23  | A     | 406[B] | CLA  | C4A-NA-C1A  | -5.71 | 104.07      | 106.68   |
| 23  | a     | 407    | CLA  | O2D-CGD-CBD | 5.71  | 121.21      | 111.23   |
| 23  | c     | 509    | CLA  | CHD-C4C-C3C | -5.71 | 116.45      | 124.77   |
| 25  | l     | 101    | SQD  | O47-C7-C8   | 5.69  | 123.80      | 111.48   |
| 23  | B     | 607    | CLA  | CMD-C2D-C1D | 5.69  | 134.75      | 124.73   |
| 23  | C     | 503    | CLA  | C2D-C1D-ND  | 5.69  | 115.76      | 110.13   |
| 23  | b     | 603    | CLA  | CMD-C2D-C1D | 5.69  | 134.75      | 124.73   |
| 25  | A     | 409[A] | SQD  | C1-O5-C5    | -5.69 | 102.61      | 113.72   |
| 23  | A     | 407    | CLA  | CMD-C2D-C1D | 5.69  | 134.74      | 124.73   |
| 23  | A     | 404[B] | CLA  | C2D-C1D-ND  | 5.68  | 115.75      | 110.13   |
| 23  | B     | 614    | CLA  | C4A-NA-C1A  | -5.68 | 104.09      | 106.68   |
| 23  | A     | 404[A] | CLA  | C2D-C1D-ND  | 5.67  | 115.73      | 110.13   |
| 23  | A     | 405[B] | CLA  | CMD-C2D-C1D | 5.66  | 134.69      | 124.73   |
| 23  | b     | 606    | CLA  | C2D-C1D-ND  | 5.65  | 115.72      | 110.13   |
| 35  | c     | 522    | HTG  | C1'-S1-C1   | 5.65  | 112.66      | 100.45   |
| 23  | d     | 404    | CLA  | CHD-C4C-C3C | -5.65 | 116.53      | 124.77   |
| 23  | b     | 608    | CLA  | O2D-CGD-CBD | 5.65  | 121.10      | 111.23   |
| 23  | B     | 607    | CLA  | O2D-CGD-CBD | 5.64  | 121.10      | 111.23   |
| 23  | B     | 614    | CLA  | O2D-CGD-CBD | 5.64  | 121.09      | 111.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 603    | CLA  | C2D-C1D-ND  | 5.64  | 115.71      | 110.13   |
| 23  | D     | 403[B] | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 23  | A     | 405[B] | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 23  | C     | 506    | CLA  | CMD-C2D-C1D | 5.63  | 134.65      | 124.73   |
| 23  | b     | 614    | CLA  | C3D-C2D-C1D | -5.63 | 98.15       | 105.83   |
| 23  | c     | 504    | CLA  | C2D-C1D-ND  | 5.62  | 115.69      | 110.13   |
| 23  | B     | 611    | CLA  | C3D-C2D-C1D | -5.62 | 98.16       | 105.83   |
| 23  | C     | 508    | CLA  | C2D-C1D-ND  | 5.62  | 115.69      | 110.13   |
| 23  | c     | 506    | CLA  | CMD-C2D-C1D | 5.59  | 134.58      | 124.73   |
| 23  | b     | 610    | CLA  | O2D-CGD-CBD | 5.59  | 121.01      | 111.23   |
| 23  | b     | 613    | CLA  | C3D-C2D-C1D | -5.59 | 98.20       | 105.83   |
| 23  | C     | 512    | CLA  | CMD-C2D-C1D | 5.59  | 134.57      | 124.73   |
| 23  | b     | 602    | CLA  | CHD-C4C-C3C | -5.59 | 116.62      | 124.77   |
| 23  | b     | 607    | CLA  | CMD-C2D-C1D | 5.58  | 134.56      | 124.73   |
| 23  | c     | 513    | CLA  | C4A-NA-C1A  | -5.57 | 104.14      | 106.68   |
| 23  | c     | 505    | CLA  | O2D-CGD-CBD | 5.57  | 120.97      | 111.23   |
| 23  | C     | 505    | CLA  | C2C-C1C-NC  | 5.57  | 115.83      | 109.98   |
| 23  | C     | 511    | CLA  | C2D-C1D-ND  | 5.57  | 115.64      | 110.13   |
| 23  | c     | 505    | CLA  | C2D-C1D-ND  | 5.57  | 115.64      | 110.13   |
| 23  | B     | 612    | CLA  | CMD-C2D-C1D | 5.57  | 134.53      | 124.73   |
| 23  | c     | 502    | CLA  | O2D-CGD-CBD | 5.57  | 120.96      | 111.23   |
| 23  | C     | 511    | CLA  | C2C-C1C-NC  | 5.56  | 115.82      | 109.98   |
| 23  | A     | 406[B] | CLA  | CHD-C4C-C3C | -5.56 | 116.67      | 124.77   |
| 23  | B     | 612    | CLA  | CHD-C4C-C3C | -5.56 | 116.67      | 124.77   |
| 23  | b     | 612    | CLA  | CMD-C2D-C1D | 5.55  | 134.50      | 124.73   |
| 23  | B     | 602    | CLA  | C4A-NA-C1A  | -5.55 | 104.15      | 106.68   |
| 23  | c     | 511    | CLA  | CMD-C2D-C1D | 5.54  | 134.49      | 124.73   |
| 23  | D     | 403[A] | CLA  | CHD-C4C-C3C | -5.54 | 116.70      | 124.77   |
| 23  | A     | 407    | CLA  | C2C-C1C-NC  | 5.53  | 115.80      | 109.98   |
| 23  | b     | 609    | CLA  | CMD-C2D-C1D | 5.53  | 134.47      | 124.73   |
| 23  | a     | 404[A] | CLA  | C2C-C1C-NC  | 5.53  | 115.79      | 109.98   |
| 23  | C     | 513    | CLA  | O2D-CGD-CBD | 5.52  | 120.88      | 111.23   |
| 23  | B     | 608    | CLA  | CHD-C4C-C3C | -5.52 | 116.73      | 124.77   |
| 23  | B     | 609    | CLA  | C2D-C1D-ND  | 5.52  | 115.59      | 110.13   |
| 23  | a     | 405[B] | CLA  | O2D-CGD-CBD | 5.52  | 120.88      | 111.23   |
| 23  | b     | 608    | CLA  | C2D-C1D-ND  | 5.51  | 115.58      | 110.13   |
| 23  | B     | 605    | CLA  | C3D-C2D-C1D | -5.51 | 98.31       | 105.83   |
| 23  | a     | 404[A] | CLA  | CHD-C4C-C3C | -5.51 | 116.74      | 124.77   |
| 23  | C     | 507    | CLA  | C2D-C1D-ND  | 5.50  | 115.57      | 110.13   |
| 23  | C     | 505    | CLA  | C3D-C2D-C1D | -5.50 | 98.32       | 105.83   |
| 23  | d     | 403[A] | CLA  | CHD-C4C-C3C | -5.49 | 116.76      | 124.77   |
| 23  | B     | 608    | CLA  | O2D-CGD-CBD | 5.49  | 120.82      | 111.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 507    | CLA  | C2C-C1C-NC  | 5.48  | 115.74      | 109.98   |
| 23  | a     | 405[A] | CLA  | CMD-C2D-C1D | 5.48  | 134.38      | 124.73   |
| 23  | B     | 605    | CLA  | C4A-NA-C1A  | -5.48 | 104.18      | 106.68   |
| 23  | B     | 616    | CLA  | C3D-C2D-C1D | -5.48 | 98.36       | 105.83   |
| 23  | C     | 513    | CLA  | CMD-C2D-C1D | 5.47  | 134.36      | 124.73   |
| 23  | B     | 601    | CLA  | C4A-NA-C1A  | -5.45 | 104.19      | 106.68   |
| 23  | D     | 403[B] | CLA  | C2C-C1C-NC  | 5.44  | 115.69      | 109.98   |
| 23  | d     | 403[A] | CLA  | CMD-C2D-C1D | 5.43  | 134.30      | 124.73   |
| 23  | B     | 613    | CLA  | C1-C2-C3    | -5.43 | 117.30      | 126.20   |
| 23  | a     | 404[A] | CLA  | C2D-C1D-ND  | 5.43  | 115.50      | 110.13   |
| 23  | A     | 404[B] | CLA  | CHD-C4C-C3C | -5.42 | 116.87      | 124.77   |
| 23  | c     | 507    | CLA  | CHD-C4C-C3C | -5.42 | 116.87      | 124.77   |
| 23  | c     | 514    | CLA  | CHD-C4C-C3C | -5.42 | 116.88      | 124.77   |
| 31  | a     | 415[B] | PHO  | C1-C2-C3    | -5.41 | 117.33      | 126.20   |
| 23  | C     | 511    | CLA  | O2D-CGD-CBD | 5.41  | 120.68      | 111.23   |
| 23  | B     | 604    | CLA  | O2D-CGD-CBD | 5.39  | 120.66      | 111.23   |
| 23  | B     | 616    | CLA  | C2C-C1C-NC  | 5.39  | 115.65      | 109.98   |
| 23  | c     | 505    | CLA  | CHD-C4C-C3C | -5.39 | 116.92      | 124.77   |
| 23  | b     | 612    | CLA  | C2D-C1D-ND  | 5.37  | 115.44      | 110.13   |
| 23  | C     | 507    | CLA  | CHD-C4C-C3C | -5.36 | 116.95      | 124.77   |
| 23  | b     | 604    | CLA  | CHD-C4C-C3C | -5.36 | 116.96      | 124.77   |
| 24  | t     | 102    | BCR  | C33-C5-C6   | -5.36 | 118.64      | 124.48   |
| 23  | B     | 606    | CLA  | C3D-C2D-C1D | -5.35 | 98.53       | 105.83   |
| 23  | c     | 506    | CLA  | C4A-NA-C1A  | -5.35 | 104.24      | 106.68   |
| 23  | B     | 604    | CLA  | CMD-C2D-C1D | 5.34  | 134.14      | 124.73   |
| 23  | c     | 512    | CLA  | O2D-CGD-CBD | 5.34  | 120.56      | 111.23   |
| 23  | B     | 607    | CLA  | C3D-C2D-C1D | -5.34 | 98.55       | 105.83   |
| 23  | b     | 604    | CLA  | C2D-C1D-ND  | 5.33  | 115.41      | 110.13   |
| 23  | C     | 503    | CLA  | CMD-C2D-C1D | 5.32  | 134.10      | 124.73   |
| 23  | B     | 608    | CLA  | C2C-C1C-NC  | 5.32  | 115.57      | 109.98   |
| 23  | d     | 403[B] | CLA  | C4A-NA-C1A  | -5.31 | 104.26      | 106.68   |
| 23  | B     | 610    | CLA  | C3D-C2D-C1D | -5.31 | 98.59       | 105.83   |
| 23  | B     | 604    | CLA  | CHD-C4C-C3C | -5.31 | 117.04      | 124.77   |
| 23  | B     | 616    | CLA  | C3C-C4C-NC  | 5.30  | 117.22      | 110.43   |
| 24  | H     | 101    | BCR  | C38-C26-C25 | -5.30 | 118.70      | 124.48   |
| 23  | c     | 510    | CLA  | C2C-C1C-NC  | 5.30  | 115.55      | 109.98   |
| 25  | A     | 409[A] | SQD  | C1-C2-C3    | -5.30 | 98.86       | 110.01   |
| 23  | d     | 404    | CLA  | O2D-CGD-CBD | 5.30  | 120.49      | 111.23   |
| 35  | D     | 411    | HTG  | C1'-S1-C1   | 5.30  | 111.89      | 100.45   |
| 23  | c     | 509    | CLA  | O2D-CGD-CBD | 5.29  | 120.48      | 111.23   |
| 23  | B     | 602    | CLA  | CMD-C2D-C1D | 5.28  | 134.03      | 124.73   |
| 23  | d     | 403[B] | CLA  | C2D-C1D-ND  | 5.28  | 115.35      | 110.13   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 603    | CLA  | C2C-C1C-NC  | 5.27  | 115.52      | 109.98   |
| 23  | c     | 507    | CLA  | C2C-C1C-NC  | 5.27  | 115.52      | 109.98   |
| 23  | C     | 509    | CLA  | O2D-CGD-CBD | 5.27  | 120.44      | 111.23   |
| 23  | B     | 611    | CLA  | CMB-C2B-C1B | 5.25  | 136.14      | 128.46   |
| 23  | A     | 405[A] | CLA  | C4A-NA-C1A  | -5.24 | 104.29      | 106.68   |
| 23  | d     | 404    | CLA  | C3D-C2D-C1D | -5.24 | 98.68       | 105.83   |
| 23  | b     | 604    | CLA  | C2C-C1C-NC  | 5.24  | 115.48      | 109.98   |
| 23  | D     | 403[A] | CLA  | C2C-C1C-NC  | 5.23  | 115.48      | 109.98   |
| 23  | b     | 607    | CLA  | C2C-C1C-NC  | 5.22  | 115.47      | 109.98   |
| 23  | b     | 608    | CLA  | C4A-NA-C1A  | -5.22 | 104.30      | 106.68   |
| 23  | c     | 511    | CLA  | C1-C2-C3    | -5.22 | 117.64      | 126.20   |
| 23  | B     | 607    | CLA  | C4A-NA-C1A  | -5.22 | 104.30      | 106.68   |
| 23  | A     | 404[A] | CLA  | C2C-C1C-NC  | 5.20  | 115.44      | 109.98   |
| 23  | b     | 616    | CLA  | C3D-C2D-C1D | -5.19 | 98.74       | 105.83   |
| 23  | B     | 608    | CLA  | C3D-C2D-C1D | -5.19 | 98.75       | 105.83   |
| 25  | b     | 620    | SQD  | O47-C7-C8   | 5.19  | 122.70      | 111.48   |
| 23  | b     | 613    | CLA  | C2C-C1C-NC  | 5.18  | 115.42      | 109.98   |
| 23  | c     | 503    | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 23  | b     | 611    | CLA  | C3D-C2D-C1D | -5.16 | 98.78       | 105.83   |
| 23  | b     | 614    | CLA  | C4A-NA-C1A  | -5.16 | 104.33      | 106.68   |
| 23  | B     | 604    | CLA  | C1-C2-C3    | -5.15 | 117.77      | 126.20   |
| 23  | b     | 611    | CLA  | C4A-NA-C1A  | -5.14 | 104.33      | 106.68   |
| 23  | C     | 508    | CLA  | C2C-C1C-NC  | 5.14  | 115.39      | 109.98   |
| 23  | A     | 404[A] | CLA  | CHD-C4C-C3C | -5.13 | 117.30      | 124.77   |
| 23  | c     | 508    | CLA  | C4A-NA-C1A  | -5.12 | 104.34      | 106.68   |
| 23  | B     | 612    | CLA  | CAC-C3C-C4C | 5.11  | 131.44      | 124.79   |
| 23  | A     | 405[A] | CLA  | O2D-CGD-CBD | 5.11  | 120.17      | 111.23   |
| 24  | d     | 405    | BCR  | C15-C14-C13 | -5.11 | 120.11      | 127.28   |
| 23  | B     | 615    | CLA  | CMD-C2D-C1D | 5.11  | 133.72      | 124.73   |
| 23  | c     | 502    | CLA  | CHD-C1D-ND  | -5.10 | 117.62      | 124.80   |
| 23  | C     | 505    | CLA  | O2D-CGD-CBD | 5.10  | 120.15      | 111.23   |
| 23  | C     | 510    | CLA  | C2C-C1C-NC  | 5.10  | 115.34      | 109.98   |
| 23  | b     | 606    | CLA  | O2D-CGD-CBD | 5.10  | 120.14      | 111.23   |
| 23  | A     | 407    | CLA  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 23  | a     | 405[B] | CLA  | C4A-NA-C1A  | -5.09 | 104.36      | 106.68   |
| 23  | d     | 402[A] | CLA  | C3D-C2D-C1D | -5.08 | 98.90       | 105.83   |
| 23  | d     | 403[B] | CLA  | CHD-C4C-C3C | -5.08 | 117.37      | 124.77   |
| 23  | B     | 614    | CLA  | C2C-C1C-NC  | 5.08  | 115.31      | 109.98   |
| 23  | c     | 510    | CLA  | O2D-CGD-CBD | 5.07  | 120.10      | 111.23   |
| 25  | a     | 409[A] | SQD  | O47-C7-C8   | 5.07  | 122.45      | 111.48   |
| 23  | C     | 509    | CLA  | CMD-C2D-C1D | 5.07  | 133.66      | 124.73   |
| 23  | C     | 506    | CLA  | C2C-C1C-NC  | 5.07  | 115.30      | 109.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | D     | 403[A] | CLA  | C3D-C2D-C1D | -5.06 | 98.92       | 105.83   |
| 23  | b     | 612    | CLA  | O2D-CGD-CBD | 5.06  | 120.07      | 111.23   |
| 23  | A     | 405[B] | CLA  | C2C-C1C-NC  | 5.06  | 115.29      | 109.98   |
| 23  | C     | 504    | CLA  | C3D-C2D-C1D | -5.04 | 98.95       | 105.83   |
| 23  | a     | 407    | CLA  | C4A-NA-C1A  | -5.04 | 104.38      | 106.68   |
| 34  | C     | 501    | LMG  | C7-O1-C1    | -5.03 | 103.01      | 113.80   |
| 23  | c     | 509    | CLA  | C4A-NA-C1A  | -5.03 | 104.39      | 106.68   |
| 35  | d     | 411    | HTG  | C1'-S1-C1   | 5.03  | 111.31      | 100.45   |
| 38  | f     | 101    | HEM  | CHC-C4B-NB  | 5.02  | 129.84      | 124.44   |
| 23  | B     | 615    | CLA  | C3D-C2D-C1D | -5.02 | 98.99       | 105.83   |
| 23  | B     | 610    | CLA  | O2A-CGA-CBA | 5.01  | 127.11      | 111.83   |
| 23  | C     | 507    | CLA  | O2D-CGD-CBD | 5.00  | 119.98      | 111.23   |
| 31  | A     | 416[B] | PHO  | C1-C2-C3    | -5.00 | 118.01      | 126.20   |
| 23  | b     | 605    | CLA  | O2D-CGD-O1D | -4.99 | 114.14      | 123.85   |
| 23  | D     | 404    | CLA  | O2D-CGD-CBD | 4.98  | 119.94      | 111.23   |
| 23  | C     | 508    | CLA  | C3D-C2D-C1D | -4.98 | 99.03       | 105.83   |
| 23  | c     | 511    | CLA  | O2D-CGD-CBD | 4.98  | 119.94      | 111.23   |
| 23  | B     | 613    | CLA  | CMD-C2D-C1D | 4.98  | 133.50      | 124.73   |
| 23  | b     | 607    | CLA  | C3D-C2D-C1D | -4.98 | 99.03       | 105.83   |
| 23  | a     | 407    | CLA  | C3D-C4D-ND  | 4.98  | 118.08      | 109.99   |
| 23  | c     | 504    | CLA  | O2D-CGD-CBD | 4.97  | 119.91      | 111.23   |
| 23  | c     | 508    | CLA  | CHD-C1D-ND  | -4.96 | 117.81      | 124.80   |
| 23  | a     | 405[A] | CLA  | C3D-C2D-C1D | -4.96 | 99.06       | 105.83   |
| 23  | d     | 402[B] | CLA  | O2D-CGD-CBD | 4.96  | 119.90      | 111.23   |
| 23  | A     | 406[B] | CLA  | C3D-C4D-ND  | 4.96  | 118.05      | 109.99   |
| 23  | c     | 505    | CLA  | C2C-C1C-NC  | 4.96  | 115.19      | 109.98   |
| 23  | b     | 603    | CLA  | C2C-C1C-NC  | 4.96  | 115.19      | 109.98   |
| 25  | a     | 409[A] | SQD  | C1-O5-C5    | -4.95 | 104.05      | 113.72   |
| 23  | c     | 509    | CLA  | C3D-C2D-C1D | -4.94 | 99.08       | 105.83   |
| 23  | A     | 405[A] | CLA  | C2C-C1C-NC  | 4.93  | 115.17      | 109.98   |
| 23  | c     | 509    | CLA  | C2C-C1C-NC  | 4.93  | 115.16      | 109.98   |
| 23  | B     | 616    | CLA  | C4A-NA-C1A  | -4.93 | 104.43      | 106.68   |
| 23  | b     | 610    | CLA  | C4A-NA-C1A  | -4.92 | 104.44      | 106.68   |
| 23  | B     | 613    | CLA  | C2C-C1C-NC  | 4.91  | 115.14      | 109.98   |
| 23  | B     | 612    | CLA  | O2D-CGD-O1D | -4.91 | 114.29      | 123.85   |
| 23  | b     | 602    | CLA  | C3D-C4D-ND  | 4.91  | 117.96      | 109.99   |
| 23  | c     | 509    | CLA  | CMD-C2D-C1D | 4.91  | 133.37      | 124.73   |
| 23  | b     | 608    | CLA  | CMD-C2D-C1D | 4.91  | 133.37      | 124.73   |
| 23  | c     | 506    | CLA  | C2C-C1C-NC  | 4.90  | 115.13      | 109.98   |
| 23  | D     | 403[B] | CLA  | C1-C2-C3    | -4.90 | 118.17      | 126.20   |
| 23  | b     | 602    | CLA  | O2D-CGD-O1D | -4.90 | 114.31      | 123.85   |
| 23  | d     | 402[A] | CLA  | C2C-C1C-NC  | 4.90  | 115.13      | 109.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 611    | CLA  | C2C-C1C-NC  | 4.90  | 115.13      | 109.98   |
| 23  | a     | 404[B] | CLA  | C3D-C4D-ND  | 4.90  | 117.95      | 109.99   |
| 23  | C     | 507    | CLA  | C4A-NA-C1A  | -4.90 | 104.44      | 106.68   |
| 23  | b     | 603    | CLA  | O2D-CGD-CBD | 4.89  | 119.78      | 111.23   |
| 23  | C     | 504    | CLA  | O2D-CGD-CBD | 4.89  | 119.78      | 111.23   |
| 23  | d     | 402[B] | CLA  | C2C-C1C-NC  | 4.89  | 115.12      | 109.98   |
| 35  | b     | 622    | HTG  | C1-O5-C5    | 4.89  | 121.33      | 112.56   |
| 25  | a     | 409[B] | SQD  | O47-C7-C8   | 4.89  | 122.05      | 111.48   |
| 23  | c     | 508    | CLA  | C2C-C1C-NC  | 4.89  | 115.11      | 109.98   |
| 23  | C     | 510    | CLA  | C1-C2-C3    | -4.88 | 118.20      | 126.20   |
| 23  | b     | 612    | CLA  | C1-C2-C3    | -4.88 | 118.20      | 126.20   |
| 23  | B     | 603    | CLA  | C3D-C2D-C1D | -4.88 | 99.17       | 105.83   |
| 23  | B     | 604    | CLA  | C2D-C1D-ND  | 4.87  | 114.95      | 110.13   |
| 23  | b     | 612    | CLA  | C2C-C1C-NC  | 4.86  | 115.09      | 109.98   |
| 23  | c     | 502    | CLA  | C4A-NA-C1A  | -4.86 | 104.46      | 106.68   |
| 23  | c     | 502    | CLA  | C3D-C2D-C1D | -4.86 | 99.20       | 105.83   |
| 23  | c     | 508    | CLA  | C3D-C2D-C1D | -4.86 | 99.20       | 105.83   |
| 23  | b     | 602    | CLA  | CHD-C1D-ND  | -4.86 | 117.97      | 124.80   |
| 23  | d     | 402[B] | CLA  | C3D-C2D-C1D | -4.85 | 99.21       | 105.83   |
| 23  | C     | 510    | CLA  | C4A-NA-C1A  | -4.84 | 104.47      | 106.68   |
| 23  | A     | 405[B] | CLA  | C3D-C2D-C1D | -4.84 | 99.23       | 105.83   |
| 23  | C     | 509    | CLA  | C3D-C2D-C1D | -4.84 | 99.23       | 105.83   |
| 23  | C     | 514    | CLA  | C2C-C1C-NC  | 4.84  | 115.06      | 109.98   |
| 28  | a     | 413[A] | PL9  | C7-C8-C9    | -4.84 | 118.50      | 126.83   |
| 23  | C     | 506    | CLA  | C1-C2-C3    | -4.84 | 118.28      | 126.20   |
| 23  | b     | 605    | CLA  | C3D-C2D-C1D | -4.83 | 99.24       | 105.83   |
| 23  | B     | 606    | CLA  | CHD-C1D-ND  | -4.82 | 118.01      | 124.80   |
| 23  | B     | 607    | CLA  | C2C-C1C-NC  | 4.81  | 115.03      | 109.98   |
| 23  | C     | 512    | CLA  | C4A-NA-C1A  | -4.80 | 104.49      | 106.68   |
| 28  | A     | 413[A] | PL9  | C7-C8-C9    | -4.80 | 118.56      | 126.83   |
| 23  | D     | 403[B] | CLA  | O2D-CGD-CBD | 4.80  | 119.62      | 111.23   |
| 23  | C     | 514    | CLA  | C3D-C2D-C1D | -4.79 | 99.29       | 105.83   |
| 25  | f     | 102    | SQD  | O47-C7-C8   | 4.79  | 121.85      | 111.48   |
| 23  | c     | 512    | CLA  | C2C-C1C-NC  | 4.79  | 115.01      | 109.98   |
| 23  | c     | 507    | CLA  | C4A-NA-C1A  | -4.79 | 104.49      | 106.68   |
| 23  | c     | 503    | CLA  | C1C-C2C-C3C | -4.78 | 101.95      | 106.98   |
| 23  | A     | 405[A] | CLA  | C3D-C2D-C1D | -4.78 | 99.31       | 105.83   |
| 23  | a     | 405[B] | CLA  | C3D-C2D-C1D | -4.78 | 99.31       | 105.83   |
| 23  | b     | 606    | CLA  | C2C-C1C-NC  | 4.78  | 115.00      | 109.98   |
| 23  | b     | 615    | CLA  | C3D-C2D-C1D | -4.78 | 99.31       | 105.83   |
| 25  | a     | 409[B] | SQD  | O6-C1-C2    | 4.78  | 115.53      | 108.27   |
| 23  | A     | 405[A] | CLA  | CMD-C2D-C1D | 4.77  | 133.12      | 124.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | b     | 617    | BCR  | C33-C5-C6   | -4.77 | 119.28      | 124.48   |
| 23  | d     | 403[A] | CLA  | C4A-NA-C1A  | -4.76 | 104.51      | 106.68   |
| 23  | D     | 404    | CLA  | C3D-C4D-ND  | 4.76  | 117.72      | 109.99   |
| 23  | b     | 609    | CLA  | C1-C2-C3    | -4.76 | 118.40      | 126.20   |
| 23  | a     | 407    | CLA  | CMD-C2D-C1D | 4.76  | 133.10      | 124.73   |
| 23  | c     | 514    | CLA  | C2C-C1C-NC  | 4.75  | 114.98      | 109.98   |
| 23  | c     | 504    | CLA  | C3D-C2D-C1D | -4.75 | 99.34       | 105.83   |
| 23  | b     | 613    | CLA  | C3C-C4C-NC  | 4.74  | 116.51      | 110.43   |
| 23  | c     | 510    | CLA  | C3D-C2D-C1D | -4.74 | 99.36       | 105.83   |
| 23  | b     | 607    | CLA  | C3D-C4D-ND  | 4.74  | 117.70      | 109.99   |
| 38  | F     | 102    | HEM  | CAD-CBD-CGD | 4.74  | 126.24      | 113.67   |
| 25  | f     | 102    | SQD  | C1-O5-C5    | 4.74  | 122.98      | 113.72   |
| 23  | a     | 405[B] | CLA  | C3D-C4D-ND  | 4.73  | 117.68      | 109.99   |
| 23  | c     | 502    | CLA  | C3D-C4D-ND  | 4.73  | 117.68      | 109.99   |
| 23  | b     | 608    | CLA  | C2C-C1C-NC  | 4.73  | 114.95      | 109.98   |
| 28  | A     | 413[B] | PL9  | C7-C8-C9    | -4.73 | 118.68      | 126.83   |
| 23  | d     | 402[A] | CLA  | O2D-CGD-CBD | 4.73  | 119.49      | 111.23   |
| 23  | B     | 615    | CLA  | C2C-C1C-NC  | 4.72  | 114.94      | 109.98   |
| 23  | C     | 511    | CLA  | C1-C2-C3    | -4.72 | 118.46      | 126.20   |
| 23  | D     | 403[B] | CLA  | C3D-C2D-C1D | -4.72 | 99.39       | 105.83   |
| 34  | B     | 620    | LMG  | O7-C10-C11  | 4.72  | 121.69      | 111.48   |
| 23  | d     | 402[B] | CLA  | C4A-NA-C1A  | -4.72 | 104.53      | 106.68   |
| 23  | b     | 605    | CLA  | C3D-C4D-ND  | 4.72  | 117.65      | 109.99   |
| 23  | B     | 601    | CLA  | C3D-C2D-C1D | -4.71 | 99.40       | 105.83   |
| 23  | d     | 404    | CLA  | CHD-C1D-ND  | -4.69 | 118.20      | 124.80   |
| 23  | c     | 505    | CLA  | C3D-C2D-C1D | -4.69 | 99.43       | 105.83   |
| 23  | c     | 507    | CLA  | O2D-CGD-CBD | 4.69  | 119.43      | 111.23   |
| 28  | A     | 413[B] | PL9  | C32-C33-C34 | -4.69 | 116.90      | 127.62   |
| 23  | B     | 608    | CLA  | C4A-NA-C1A  | -4.68 | 104.54      | 106.68   |
| 23  | B     | 607    | CLA  | O2D-CGD-O1D | -4.68 | 114.73      | 123.85   |
| 23  | C     | 505    | CLA  | C4A-NA-C1A  | -4.68 | 104.54      | 106.68   |
| 23  | B     | 612    | CLA  | C2C-C1C-NC  | 4.68  | 114.90      | 109.98   |
| 23  | c     | 503    | CLA  | C3D-C2D-C1D | -4.68 | 99.45       | 105.83   |
| 35  | B     | 621    | HTG  | C1'-S1-C1   | 4.68  | 110.55      | 100.45   |
| 38  | F     | 102    | HEM  | CBA-CAA-C2A | -4.68 | 104.68      | 112.54   |
| 23  | b     | 605    | CLA  | C2C-C1C-NC  | 4.67  | 114.89      | 109.98   |
| 23  | c     | 507    | CLA  | C3D-C4D-ND  | 4.67  | 117.58      | 109.99   |
| 23  | C     | 510    | CLA  | O2D-CGD-CBD | 4.67  | 119.39      | 111.23   |
| 23  | c     | 508    | CLA  | C1C-C2C-C3C | -4.67 | 102.07      | 106.98   |
| 23  | b     | 610    | CLA  | O2A-CGA-CBA | 4.66  | 126.06      | 111.83   |
| 23  | A     | 406[A] | CLA  | C3D-C4D-ND  | 4.66  | 117.56      | 109.99   |
| 23  | c     | 514    | CLA  | C3D-C2D-C1D | -4.66 | 99.47       | 105.83   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 613    | CLA  | C3D-C2D-C1D | -4.66 | 99.47       | 105.83   |
| 23  | b     | 610    | CLA  | C3D-C2D-C1D | -4.66 | 99.47       | 105.83   |
| 23  | C     | 503    | CLA  | O2D-CGD-CBD | 4.66  | 119.37      | 111.23   |
| 23  | B     | 611    | CLA  | C1D-CHD-C4C | -4.66 | 116.12      | 126.02   |
| 23  | c     | 506    | CLA  | C3D-C4D-ND  | 4.66  | 117.56      | 109.99   |
| 23  | b     | 605    | CLA  | CHD-C1D-ND  | -4.65 | 118.26      | 124.80   |
| 23  | B     | 602    | CLA  | C3C-C4C-NC  | 4.65  | 116.38      | 110.43   |
| 23  | C     | 502    | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 23  | B     | 602    | CLA  | C2C-C1C-NC  | 4.64  | 114.86      | 109.98   |
| 23  | C     | 513    | CLA  | C3D-C2D-C1D | -4.63 | 99.51       | 105.83   |
| 23  | C     | 512    | CLA  | C2C-C1C-NC  | 4.63  | 114.84      | 109.98   |
| 23  | d     | 403[A] | CLA  | C3D-C4D-ND  | 4.62  | 117.50      | 109.99   |
| 23  | C     | 509    | CLA  | C3C-C4C-NC  | 4.62  | 116.35      | 110.43   |
| 23  | C     | 507    | CLA  | C3D-C2D-C1D | -4.62 | 99.53       | 105.83   |
| 23  | B     | 615    | CLA  | C3D-C4D-ND  | 4.62  | 117.49      | 109.99   |
| 23  | B     | 604    | CLA  | C3C-C4C-NC  | 4.61  | 116.33      | 110.43   |
| 23  | B     | 601    | CLA  | C3D-C4D-ND  | 4.61  | 117.48      | 109.99   |
| 23  | A     | 406[A] | CLA  | O2D-CGD-CBD | 4.61  | 119.28      | 111.23   |
| 23  | c     | 514    | CLA  | C3D-C4D-ND  | 4.60  | 117.47      | 109.99   |
| 23  | b     | 610    | CLA  | C3D-C4D-ND  | 4.59  | 117.45      | 109.99   |
| 23  | b     | 601    | CLA  | C3D-C2D-C1D | -4.59 | 99.56       | 105.83   |
| 23  | B     | 605    | CLA  | C3C-C4C-NC  | 4.59  | 116.31      | 110.43   |
| 23  | A     | 404[A] | CLA  | C3D-C2D-C1D | -4.59 | 99.56       | 105.83   |
| 23  | A     | 405[A] | CLA  | C1C-C2C-C3C | -4.59 | 102.15      | 106.98   |
| 23  | A     | 404[B] | CLA  | C2C-C1C-NC  | 4.59  | 114.80      | 109.98   |
| 23  | C     | 507    | CLA  | C1C-C2C-C3C | -4.59 | 102.16      | 106.98   |
| 23  | C     | 503    | CLA  | C2C-C1C-NC  | 4.58  | 114.80      | 109.98   |
| 24  | K     | 102    | BCR  | C7-C8-C9    | -4.58 | 119.45      | 126.23   |
| 23  | a     | 404[B] | CLA  | C4A-NA-C1A  | -4.58 | 104.59      | 106.68   |
| 23  | B     | 613    | CLA  | C3C-C4C-NC  | 4.57  | 116.29      | 110.43   |
| 23  | d     | 404    | CLA  | C3D-C4D-ND  | 4.57  | 117.42      | 109.99   |
| 34  | C     | 501    | LMG  | O1-C1-C2    | 4.57  | 115.22      | 108.27   |
| 23  | b     | 613    | CLA  | C4A-NA-C1A  | -4.57 | 104.59      | 106.68   |
| 23  | C     | 511    | CLA  | C3D-C2D-C1D | -4.57 | 99.60       | 105.83   |
| 23  | b     | 616    | CLA  | C1D-CHD-C4C | -4.57 | 116.31      | 126.02   |
| 23  | b     | 601    | CLA  | C3D-C4D-ND  | 4.57  | 117.41      | 109.99   |
| 24  | d     | 405    | BCR  | C29-C30-C25 | 4.57  | 117.07      | 110.44   |
| 23  | C     | 508    | CLA  | C4A-NA-C1A  | -4.57 | 104.60      | 106.68   |
| 23  | b     | 606    | CLA  | C3D-C2D-C1D | -4.56 | 99.60       | 105.83   |
| 23  | B     | 611    | CLA  | CMC-C2C-C1C | 4.56  | 132.16      | 125.03   |
| 23  | a     | 404[B] | CLA  | C2C-C1C-NC  | 4.56  | 114.77      | 109.98   |
| 23  | D     | 404    | CLA  | C3D-C2D-C1D | -4.56 | 99.61       | 105.83   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 503    | CLA  | C3D-C4D-ND  | 4.56  | 117.39      | 109.99   |
| 23  | b     | 608    | CLA  | C3D-C4D-ND  | 4.55  | 117.39      | 109.99   |
| 23  | d     | 402[B] | CLA  | C1C-C2C-C3C | -4.55 | 102.19      | 106.98   |
| 23  | A     | 406[B] | CLA  | O2D-CGD-CBD | 4.55  | 119.18      | 111.23   |
| 23  | B     | 609    | CLA  | C3D-C4D-ND  | 4.55  | 117.38      | 109.99   |
| 23  | B     | 603    | CLA  | CMD-C2D-C1D | 4.55  | 132.73      | 124.73   |
| 23  | c     | 502    | CLA  | O2D-CGD-O1D | -4.54 | 115.00      | 123.85   |
| 23  | A     | 404[B] | CLA  | C3D-C4D-ND  | 4.54  | 117.37      | 109.99   |
| 23  | c     | 511    | CLA  | C2C-C1C-NC  | 4.54  | 114.75      | 109.98   |
| 23  | a     | 405[A] | CLA  | O2D-CGD-CBD | 4.54  | 119.17      | 111.23   |
| 23  | B     | 613    | CLA  | C4A-NA-C1A  | -4.54 | 104.61      | 106.68   |
| 23  | A     | 406[B] | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 23  | c     | 514    | CLA  | CHD-C1D-ND  | -4.54 | 118.42      | 124.80   |
| 23  | C     | 511    | CLA  | C3D-C4D-ND  | 4.54  | 117.36      | 109.99   |
| 23  | c     | 507    | CLA  | C3D-C2D-C1D | -4.53 | 99.64       | 105.83   |
| 28  | D     | 406[B] | PL9  | C42-C43-C44 | -4.53 | 117.25      | 127.62   |
| 23  | A     | 404[B] | CLA  | C1D-CHD-C4C | -4.53 | 116.39      | 126.02   |
| 23  | C     | 507    | CLA  | CHD-C1D-ND  | -4.53 | 118.42      | 124.80   |
| 23  | c     | 514    | CLA  | O2D-CGD-CBD | 4.53  | 119.15      | 111.23   |
| 23  | B     | 609    | CLA  | C2C-C1C-NC  | 4.53  | 114.74      | 109.98   |
| 23  | C     | 510    | CLA  | C3D-C4D-ND  | 4.53  | 117.34      | 109.99   |
| 23  | b     | 607    | CLA  | C3C-C4C-NC  | 4.52  | 116.22      | 110.43   |
| 23  | c     | 513    | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 23  | A     | 407    | CLA  | C3C-C4C-NC  | 4.52  | 116.22      | 110.43   |
| 23  | b     | 614    | CLA  | C2C-C1C-NC  | 4.51  | 114.72      | 109.98   |
| 23  | B     | 612    | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 28  | A     | 413[A] | PL9  | C32-C33-C34 | -4.51 | 117.31      | 127.62   |
| 25  | b     | 620    | SQD  | C1-O5-C5    | -4.51 | 104.92      | 113.72   |
| 23  | C     | 514    | CLA  | C3D-C4D-ND  | 4.50  | 117.31      | 109.99   |
| 23  | A     | 405[A] | CLA  | C3D-C4D-ND  | 4.50  | 117.30      | 109.99   |
| 23  | D     | 403[A] | CLA  | C3C-C4C-NC  | 4.49  | 116.18      | 110.43   |
| 23  | C     | 502    | CLA  | O2D-CGD-O1D | -4.49 | 115.11      | 123.85   |
| 23  | c     | 513    | CLA  | C3D-C4D-ND  | 4.49  | 117.28      | 109.99   |
| 23  | b     | 609    | CLA  | C3D-C2D-C1D | -4.48 | 99.71       | 105.83   |
| 23  | B     | 612    | CLA  | C3C-C4C-NC  | 4.48  | 116.17      | 110.43   |
| 23  | B     | 607    | CLA  | C3D-C4D-ND  | 4.48  | 117.27      | 109.99   |
| 23  | C     | 513    | CLA  | C3D-C4D-ND  | 4.48  | 117.26      | 109.99   |
| 23  | b     | 604    | CLA  | C4A-NA-C1A  | -4.47 | 104.64      | 106.68   |
| 23  | C     | 505    | CLA  | C1C-C2C-C3C | -4.47 | 102.28      | 106.98   |
| 23  | a     | 404[B] | CLA  | C3D-C2D-C1D | -4.47 | 99.74       | 105.83   |
| 23  | c     | 512    | CLA  | C3D-C2D-C1D | -4.47 | 99.74       | 105.83   |
| 24  | d     | 405    | BCR  | C7-C8-C9    | -4.47 | 119.63      | 126.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 405[B] | CLA  | CHD-C1D-ND  | -4.47 | 118.52      | 124.80   |
| 32  | t     | 101    | LMT  | C3'-C4'-C5' | -4.46 | 101.04      | 110.93   |
| 23  | D     | 403[B] | CLA  | C3D-C4D-ND  | 4.46  | 117.23      | 109.99   |
| 24  | B     | 618    | BCR  | C29-C30-C25 | 4.46  | 116.91      | 110.44   |
| 23  | b     | 608    | CLA  | C1-C2-C3    | -4.45 | 118.91      | 126.20   |
| 28  | a     | 413[B] | PL9  | C7-C3-C4    | 4.45  | 120.58      | 116.91   |
| 23  | a     | 404[B] | CLA  | C1D-CHD-C4C | -4.45 | 116.56      | 126.02   |
| 23  | C     | 503    | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 23  | B     | 602    | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 23  | b     | 604    | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 23  | b     | 611    | CLA  | C3C-C4C-NC  | 4.44  | 116.12      | 110.43   |
| 23  | c     | 507    | CLA  | C1-C2-C3    | -4.44 | 118.92      | 126.20   |
| 23  | C     | 506    | CLA  | C3D-C4D-ND  | 4.44  | 117.20      | 109.99   |
| 23  | d     | 403[B] | CLA  | C3D-C4D-ND  | 4.43  | 117.19      | 109.99   |
| 23  | A     | 405[B] | CLA  | C3D-C4D-ND  | 4.43  | 117.19      | 109.99   |
| 23  | b     | 603    | CLA  | C3D-C4D-ND  | 4.43  | 117.19      | 109.99   |
| 23  | B     | 611    | CLA  | C3D-C4D-ND  | 4.43  | 117.19      | 109.99   |
| 23  | C     | 512    | CLA  | C3D-C2D-C1D | -4.43 | 99.79       | 105.83   |
| 23  | a     | 405[A] | CLA  | C3D-C4D-ND  | 4.42  | 117.17      | 109.99   |
| 23  | C     | 514    | CLA  | O2D-CGD-CBD | 4.42  | 118.95      | 111.23   |
| 23  | C     | 507    | CLA  | C3D-C4D-ND  | 4.42  | 117.17      | 109.99   |
| 23  | a     | 404[A] | CLA  | C3D-C4D-ND  | 4.42  | 117.17      | 109.99   |
| 23  | C     | 510    | CLA  | C3D-C2D-C1D | -4.41 | 99.81       | 105.83   |
| 23  | a     | 404[A] | CLA  | C1C-C2C-C3C | -4.41 | 102.34      | 106.98   |
| 23  | d     | 402[A] | CLA  | C1C-C2C-C3C | -4.41 | 102.34      | 106.98   |
| 23  | B     | 610    | CLA  | C2C-C1C-NC  | 4.41  | 114.61      | 109.98   |
| 25  | X     | 101    | SQD  | C1-O5-C5    | -4.41 | 105.12      | 113.72   |
| 35  | C     | 522    | HTG  | C1'-S1-C1   | 4.41  | 109.96      | 100.45   |
| 23  | C     | 508    | CLA  | C3C-C4C-NC  | 4.40  | 116.07      | 110.43   |
| 23  | c     | 511    | CLA  | C3D-C2D-C1D | -4.40 | 99.82       | 105.83   |
| 23  | c     | 506    | CLA  | C3C-C4C-NC  | 4.40  | 116.07      | 110.43   |
| 23  | b     | 610    | CLA  | C2C-C1C-NC  | 4.40  | 114.60      | 109.98   |
| 23  | a     | 407    | CLA  | C3D-C2D-C1D | -4.40 | 99.83       | 105.83   |
| 23  | b     | 615    | CLA  | C2C-C1C-NC  | 4.40  | 114.60      | 109.98   |
| 23  | C     | 502    | CLA  | C3D-C4D-ND  | 4.39  | 117.13      | 109.99   |
| 23  | B     | 606    | CLA  | C2C-C1C-NC  | 4.39  | 114.59      | 109.98   |
| 31  | A     | 416[A] | PHO  | C1-C2-C3    | -4.39 | 119.00      | 126.20   |
| 23  | d     | 402[B] | CLA  | C3D-C4D-ND  | 4.39  | 117.12      | 109.99   |
| 23  | c     | 512    | CLA  | C3D-C4D-ND  | 4.39  | 117.12      | 109.99   |
| 23  | A     | 405[B] | CLA  | O2D-CGD-CBD | 4.38  | 118.89      | 111.23   |
| 23  | b     | 605    | CLA  | C4A-NA-C1A  | -4.38 | 104.68      | 106.68   |
| 23  | B     | 616    | CLA  | CMD-C2D-C1D | 4.38  | 132.43      | 124.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 613    | CLA  | C3D-C4D-ND  | 4.37  | 117.09      | 109.99   |
| 23  | A     | 406[A] | CLA  | C3D-C2D-C1D | -4.37 | 99.87       | 105.83   |
| 23  | a     | 407    | CLA  | C3C-C4C-NC  | 4.36  | 116.02      | 110.43   |
| 23  | d     | 403[A] | CLA  | C1C-C2C-C3C | -4.36 | 102.39      | 106.98   |
| 23  | B     | 612    | CLA  | C3D-C4D-ND  | 4.36  | 117.07      | 109.99   |
| 23  | d     | 403[B] | CLA  | C1C-C2C-C3C | -4.36 | 102.40      | 106.98   |
| 23  | B     | 604    | CLA  | C4A-NA-C1A  | -4.36 | 104.69      | 106.68   |
| 33  | E     | 101[A] | LHG  | O7-C7-C8    | 4.35  | 120.90      | 111.48   |
| 23  | b     | 616    | CLA  | O2D-CGD-O1D | -4.35 | 115.38      | 123.85   |
| 23  | C     | 504    | CLA  | C1D-CHD-C4C | -4.35 | 116.77      | 126.02   |
| 23  | B     | 603    | CLA  | C3D-C4D-ND  | 4.35  | 117.06      | 109.99   |
| 23  | A     | 404[B] | CLA  | C3D-C2D-C1D | -4.35 | 99.89       | 105.83   |
| 23  | c     | 505    | CLA  | CHD-C1D-ND  | -4.35 | 118.68      | 124.80   |
| 23  | A     | 407    | CLA  | C3D-C4D-ND  | 4.35  | 117.05      | 109.99   |
| 34  | C     | 501    | LMG  | O7-C10-C11  | 4.34  | 120.88      | 111.48   |
| 23  | B     | 609    | CLA  | C3D-C2D-C1D | -4.34 | 99.90       | 105.83   |
| 23  | b     | 603    | CLA  | C1D-CHD-C4C | -4.34 | 116.79      | 126.02   |
| 23  | C     | 514    | CLA  | CHD-C1D-ND  | -4.34 | 118.69      | 124.80   |
| 23  | b     | 603    | CLA  | C3D-C2D-C1D | -4.34 | 99.91       | 105.83   |
| 28  | a     | 413[B] | PL9  | C7-C3-C2    | -4.33 | 118.28      | 123.39   |
| 23  | C     | 510    | CLA  | CHD-C1D-ND  | -4.33 | 118.70      | 124.80   |
| 23  | C     | 511    | CLA  | C1C-C2C-C3C | -4.33 | 102.42      | 106.98   |
| 23  | c     | 511    | CLA  | C3D-C4D-ND  | 4.33  | 117.02      | 109.99   |
| 23  | b     | 610    | CLA  | C1-C2-C3    | -4.33 | 119.11      | 126.20   |
| 24  | y     | 101    | BCR  | C33-C5-C6   | -4.33 | 119.76      | 124.48   |
| 23  | c     | 504    | CLA  | C1D-CHD-C4C | -4.32 | 116.83      | 126.02   |
| 23  | A     | 407    | CLA  | C4A-NA-C1A  | -4.32 | 104.71      | 106.68   |
| 23  | d     | 404    | CLA  | C4A-NA-C1A  | -4.32 | 104.71      | 106.68   |
| 24  | C     | 516    | BCR  | C7-C8-C9    | -4.32 | 119.84      | 126.23   |
| 23  | B     | 603    | CLA  | O2D-CGD-O1D | -4.32 | 115.44      | 123.85   |
| 33  | E     | 101[B] | LHG  | O7-C7-C8    | 4.32  | 120.82      | 111.48   |
| 23  | B     | 605    | CLA  | CHD-C1D-ND  | -4.32 | 118.73      | 124.80   |
| 24  | B     | 617    | BCR  | C7-C8-C9    | -4.31 | 119.85      | 126.23   |
| 23  | b     | 614    | CLA  | C3D-C4D-ND  | 4.31  | 116.99      | 109.99   |
| 23  | c     | 502    | CLA  | C2C-C1C-NC  | 4.30  | 114.50      | 109.98   |
| 23  | A     | 406[A] | CLA  | C2C-C1C-NC  | 4.30  | 114.50      | 109.98   |
| 23  | C     | 512    | CLA  | C1D-CHD-C4C | -4.30 | 116.89      | 126.02   |
| 23  | b     | 615    | CLA  | C3D-C4D-ND  | 4.29  | 116.97      | 109.99   |
| 23  | a     | 405[A] | CLA  | C2C-C1C-NC  | 4.29  | 114.49      | 109.98   |
| 23  | C     | 504    | CLA  | C3D-C4D-ND  | 4.29  | 116.96      | 109.99   |
| 23  | C     | 504    | CLA  | C3C-C4C-NC  | 4.29  | 115.92      | 110.43   |
| 23  | c     | 513    | CLA  | C1-C2-C3    | -4.29 | 119.17      | 126.20   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 611    | CLA  | CHD-C4C-NC  | 4.29  | 130.88      | 124.23   |
| 23  | C     | 502    | CLA  | C2C-C1C-NC  | 4.28  | 114.48      | 109.98   |
| 23  | c     | 508    | CLA  | CMC-C2C-C1C | 4.28  | 131.73      | 125.03   |
| 24  | d     | 405    | BCR  | C40-C30-C25 | -4.28 | 103.53      | 110.24   |
| 23  | A     | 406[B] | CLA  | C2C-C1C-NC  | 4.28  | 114.48      | 109.98   |
| 23  | B     | 606    | CLA  | C3D-C4D-ND  | 4.27  | 116.94      | 109.99   |
| 25  | a     | 409[A] | SQD  | C1-C2-C3    | -4.27 | 101.02      | 110.01   |
| 23  | b     | 614    | CLA  | CHD-C1D-ND  | -4.27 | 118.79      | 124.80   |
| 23  | b     | 609    | CLA  | C3C-C4C-NC  | 4.27  | 115.90      | 110.43   |
| 23  | D     | 403[B] | CLA  | CHD-C1D-ND  | -4.27 | 118.80      | 124.80   |
| 23  | B     | 615    | CLA  | C1D-CHD-C4C | -4.26 | 116.96      | 126.02   |
| 23  | c     | 504    | CLA  | C3D-C4D-ND  | 4.26  | 116.92      | 109.99   |
| 23  | a     | 404[A] | CLA  | C3D-C2D-C1D | -4.26 | 100.02      | 105.83   |
| 23  | A     | 406[A] | CLA  | CHD-C1D-ND  | -4.26 | 118.81      | 124.80   |
| 23  | b     | 606    | CLA  | C3D-C4D-ND  | 4.26  | 116.91      | 109.99   |
| 34  | Z     | 101    | LMG  | O7-C10-C11  | 4.26  | 120.69      | 111.48   |
| 23  | d     | 402[A] | CLA  | C3D-C4D-ND  | 4.26  | 116.91      | 109.99   |
| 23  | c     | 503    | CLA  | CMD-C2D-C1D | 4.25  | 132.22      | 124.73   |
| 23  | d     | 402[A] | CLA  | C4A-NA-C1A  | -4.25 | 104.74      | 106.68   |
| 23  | a     | 405[A] | CLA  | CHD-C1D-ND  | -4.25 | 118.81      | 124.80   |
| 23  | a     | 407    | CLA  | C2C-C1C-NC  | 4.25  | 114.45      | 109.98   |
| 23  | A     | 407    | CLA  | C1-C2-C3    | -4.25 | 119.23      | 126.20   |
| 23  | C     | 505    | CLA  | C3C-C4C-NC  | 4.25  | 115.88      | 110.43   |
| 34  | c     | 501    | LMG  | O7-C10-C11  | 4.25  | 120.67      | 111.48   |
| 23  | A     | 405[B] | CLA  | C1C-C2C-C3C | -4.24 | 102.52      | 106.98   |
| 23  | b     | 612    | CLA  | C3B-C4B-NB  | 4.24  | 114.70      | 109.21   |
| 23  | c     | 504    | CLA  | C2C-C1C-NC  | 4.24  | 114.44      | 109.98   |
| 23  | A     | 404[A] | CLA  | CHD-C1D-ND  | -4.24 | 118.83      | 124.80   |
| 23  | B     | 602    | CLA  | O2D-CGD-O1D | -4.24 | 115.60      | 123.85   |
| 23  | B     | 610    | CLA  | CAA-C2A-C3A | -4.24 | 101.54      | 113.00   |
| 23  | b     | 614    | CLA  | O2D-CGD-O1D | -4.24 | 115.60      | 123.85   |
| 23  | c     | 505    | CLA  | C3D-C4D-ND  | 4.24  | 116.87      | 109.99   |
| 33  | A     | 418[A] | LHG  | O8-C23-O10  | -4.23 | 113.04      | 123.63   |
| 23  | c     | 507    | CLA  | CHD-C1D-ND  | -4.23 | 118.84      | 124.80   |
| 23  | c     | 503    | CLA  | C3D-C4D-ND  | 4.23  | 116.87      | 109.99   |
| 23  | B     | 615    | CLA  | C3C-C4C-NC  | 4.23  | 115.85      | 110.43   |
| 23  | b     | 606    | CLA  | CHD-C1D-ND  | -4.22 | 118.86      | 124.80   |
| 23  | d     | 402[A] | CLA  | CAA-C2A-C3A | -4.22 | 101.59      | 113.00   |
| 32  | B     | 626    | LMT  | C1'-O5'-C5' | -4.22 | 105.47      | 113.72   |
| 23  | d     | 403[A] | CLA  | C3D-C2D-C1D | -4.22 | 100.07      | 105.83   |
| 28  | a     | 413[A] | PL9  | C32-C33-C34 | -4.22 | 117.96      | 127.62   |
| 23  | C     | 509    | CLA  | C3D-C4D-ND  | 4.22  | 116.84      | 109.99   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 406[B] | CLA  | CHD-C1D-ND  | -4.22 | 118.87      | 124.80   |
| 23  | d     | 403[B] | CLA  | C3D-C2D-C1D | -4.21 | 100.08      | 105.83   |
| 28  | a     | 413[A] | PL9  | C7-C3-C2    | -4.21 | 118.42      | 123.39   |
| 23  | b     | 612    | CLA  | C3C-C4C-NC  | 4.21  | 115.83      | 110.43   |
| 23  | c     | 510    | CLA  | C3D-C4D-ND  | 4.21  | 116.83      | 109.99   |
| 23  | B     | 601    | CLA  | CHD-C1D-ND  | -4.21 | 118.88      | 124.80   |
| 23  | A     | 404[B] | CLA  | C3B-C4B-NB  | 4.21  | 114.65      | 109.21   |
| 23  | b     | 609    | CLA  | C3D-C4D-ND  | 4.21  | 116.83      | 109.99   |
| 23  | B     | 613    | CLA  | O2D-CGD-CBD | 4.21  | 118.59      | 111.23   |
| 23  | c     | 505    | CLA  | C1-O2A-CGA  | 4.21  | 126.84      | 116.65   |
| 23  | C     | 506    | CLA  | C3C-C4C-NC  | 4.21  | 115.82      | 110.43   |
| 40  | v     | 201    | HEC  | CBC-CAC-C3C | -4.21 | 117.65      | 127.49   |
| 23  | D     | 403[A] | CLA  | C3D-C4D-ND  | 4.21  | 116.82      | 109.99   |
| 23  | a     | 404[A] | CLA  | CAA-C2A-C3A | -4.20 | 101.65      | 113.00   |
| 36  | C     | 518[B] | DGD  | O2G-C1B-C2B | 4.20  | 120.56      | 111.48   |
| 23  | c     | 512    | CLA  | C1D-CHD-C4C | -4.19 | 117.11      | 126.02   |
| 23  | b     | 615    | CLA  | C1D-CHD-C4C | -4.19 | 117.11      | 126.02   |
| 23  | a     | 404[A] | CLA  | C1D-CHD-C4C | -4.19 | 117.12      | 126.02   |
| 23  | C     | 503    | CLA  | C4A-NA-C1A  | -4.19 | 104.77      | 106.68   |
| 23  | b     | 612    | CLA  | C4A-NA-C1A  | -4.18 | 104.77      | 106.68   |
| 31  | D     | 401[B] | PHO  | C1A-C2A-C3A | -4.18 | 98.86       | 102.84   |
| 24  | c     | 515    | BCR  | C11-C10-C9  | -4.18 | 121.41      | 127.28   |
| 23  | d     | 403[A] | CLA  | O2D-CGD-CBD | 4.18  | 118.53      | 111.23   |
| 34  | c     | 521    | LMG  | O7-C10-C11  | 4.18  | 120.52      | 111.48   |
| 23  | b     | 616    | CLA  | C3C-C4C-NC  | 4.18  | 115.78      | 110.43   |
| 23  | b     | 610    | CLA  | C3C-C4C-NC  | 4.18  | 115.78      | 110.43   |
| 23  | C     | 514    | CLA  | C1C-C2C-C3C | -4.17 | 102.59      | 106.98   |
| 23  | B     | 615    | CLA  | O2D-CGD-CBD | 4.17  | 118.52      | 111.23   |
| 23  | B     | 607    | CLA  | C1C-C2C-C3C | -4.17 | 102.59      | 106.98   |
| 28  | a     | 413[B] | PL9  | C32-C33-C34 | -4.17 | 118.08      | 127.62   |
| 40  | v     | 201    | HEC  | CMB-C2B-C1B | -4.17 | 122.35      | 128.46   |
| 23  | B     | 605    | CLA  | C2C-C1C-NC  | 4.16  | 114.36      | 109.98   |
| 34  | m     | 101    | LMG  | O7-C10-C11  | 4.16  | 120.49      | 111.48   |
| 23  | A     | 404[A] | CLA  | C3D-C4D-ND  | 4.16  | 116.75      | 109.99   |
| 23  | B     | 608    | CLA  | C3D-C4D-ND  | 4.16  | 116.75      | 109.99   |
| 23  | B     | 608    | CLA  | O2D-CGD-O1D | -4.16 | 115.75      | 123.85   |
| 23  | A     | 405[B] | CLA  | C4A-NA-C1A  | -4.16 | 104.78      | 106.68   |
| 23  | B     | 614    | CLA  | C1D-CHD-C4C | -4.16 | 117.18      | 126.02   |
| 23  | c     | 504    | CLA  | CHD-C1D-ND  | -4.16 | 118.95      | 124.80   |
| 23  | B     | 616    | CLA  | C1D-CHD-C4C | -4.16 | 117.19      | 126.02   |
| 23  | B     | 604    | CLA  | C1C-C2C-C3C | -4.15 | 102.61      | 106.98   |
| 24  | T     | 102    | BCR  | C15-C16-C17 | -4.15 | 115.02      | 123.52   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | D     | 403[A] | CLA  | O2D-CGD-CBD | 4.15  | 118.49      | 111.23   |
| 33  | d     | 408[B] | LHG  | O7-C7-C8    | 4.15  | 120.46      | 111.48   |
| 23  | b     | 611    | CLA  | C3D-C4D-ND  | 4.15  | 116.73      | 109.99   |
| 23  | B     | 605    | CLA  | C3D-C4D-ND  | 4.15  | 116.73      | 109.99   |
| 23  | B     | 614    | CLA  | C1C-C2C-C3C | -4.14 | 102.62      | 106.98   |
| 23  | B     | 605    | CLA  | C1D-CHD-C4C | -4.14 | 117.21      | 126.02   |
| 23  | b     | 604    | CLA  | C3B-C4B-NB  | 4.14  | 114.56      | 109.21   |
| 23  | c     | 508    | CLA  | C3D-C4D-ND  | 4.14  | 116.71      | 109.99   |
| 23  | b     | 606    | CLA  | C1D-CHD-C4C | -4.14 | 117.23      | 126.02   |
| 23  | C     | 508    | CLA  | O2D-CGD-O1D | -4.14 | 115.80      | 123.85   |
| 35  | V     | 202    | HTG  | C1-O5-C5    | 4.14  | 117.73      | 112.19   |
| 23  | C     | 505    | CLA  | C3D-C4D-ND  | 4.13  | 116.70      | 109.99   |
| 23  | c     | 513    | CLA  | C1D-CHD-C4C | -4.13 | 117.24      | 126.02   |
| 23  | b     | 603    | CLA  | C3C-C4C-NC  | 4.13  | 115.72      | 110.43   |
| 23  | c     | 510    | CLA  | C3B-C4B-NB  | 4.13  | 114.55      | 109.21   |
| 34  | C     | 521    | LMG  | O6-C5-C4    | 4.12  | 117.13      | 109.70   |
| 24  | y     | 101    | BCR  | C15-C14-C13 | -4.12 | 121.50      | 127.28   |
| 23  | C     | 506    | CLA  | CHD-C1D-ND  | -4.12 | 119.01      | 124.80   |
| 34  | c     | 521    | LMG  | O6-C5-C4    | 4.12  | 117.12      | 109.70   |
| 23  | c     | 512    | CLA  | O2D-CGD-O1D | -4.12 | 115.84      | 123.85   |
| 23  | c     | 503    | CLA  | C4A-NA-C1A  | -4.11 | 104.80      | 106.68   |
| 23  | b     | 603    | CLA  | CAA-C2A-C3A | -4.11 | 101.89      | 113.00   |
| 23  | B     | 607    | CLA  | C3C-C4C-NC  | 4.11  | 115.70      | 110.43   |
| 23  | a     | 404[B] | CLA  | C3B-C4B-NB  | 4.11  | 114.52      | 109.21   |
| 23  | b     | 613    | CLA  | C1-C2-C3    | -4.11 | 119.46      | 126.20   |
| 23  | D     | 403[A] | CLA  | CHD-C1D-ND  | -4.11 | 119.02      | 124.80   |
| 23  | b     | 613    | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 23  | B     | 614    | CLA  | CHD-C1D-ND  | -4.11 | 119.03      | 124.80   |
| 23  | d     | 403[B] | CLA  | O2D-CGD-CBD | 4.10  | 118.41      | 111.23   |
| 23  | d     | 402[A] | CLA  | C1D-CHD-C4C | -4.10 | 117.30      | 126.02   |
| 25  | A     | 409[B] | SQD  | C1-C2-C3    | -4.10 | 101.39      | 110.01   |
| 23  | C     | 502    | CLA  | C1D-CHD-C4C | -4.10 | 117.31      | 126.02   |
| 23  | b     | 612    | CLA  | C3D-C4D-ND  | 4.10  | 116.65      | 109.99   |
| 23  | D     | 403[B] | CLA  | C1C-C2C-C3C | -4.10 | 102.67      | 106.98   |
| 23  | C     | 506    | CLA  | C3D-C2D-C1D | -4.10 | 100.24      | 105.83   |
| 23  | D     | 404    | CLA  | C4-C3-C5    | 4.09  | 122.33      | 115.23   |
| 23  | B     | 606    | CLA  | O2D-CGD-O1D | -4.09 | 115.88      | 123.85   |
| 23  | A     | 404[B] | CLA  | CHD-C1D-ND  | -4.09 | 119.04      | 124.80   |
| 23  | B     | 601    | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 23  | B     | 609    | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 23  | c     | 504    | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 23  | b     | 608    | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 503    | CLA  | CHD-C1D-ND  | -4.08 | 119.06      | 124.80   |
| 23  | d     | 403[A] | CLA  | C3C-C4C-NC  | 4.08  | 115.66      | 110.43   |
| 23  | C     | 511    | CLA  | C1D-CHD-C4C | -4.08 | 117.34      | 126.02   |
| 23  | c     | 510    | CLA  | C1D-CHD-C4C | -4.08 | 117.34      | 126.02   |
| 33  | D     | 408[B] | LHG  | O7-C7-C8    | 4.08  | 120.31      | 111.48   |
| 23  | A     | 404[B] | CLA  | O2D-CGD-CBD | 4.08  | 118.37      | 111.23   |
| 23  | b     | 601    | CLA  | CHD-C1D-ND  | -4.08 | 119.06      | 124.80   |
| 23  | d     | 402[B] | CLA  | CHD-C1D-ND  | -4.08 | 119.06      | 124.80   |
| 23  | A     | 405[B] | CLA  | CHD-C1D-ND  | -4.08 | 119.06      | 124.80   |
| 23  | b     | 616    | CLA  | O2A-CGA-CBA | 4.08  | 124.27      | 111.83   |
| 23  | c     | 505    | CLA  | C1C-C2C-C3C | -4.08 | 102.69      | 106.98   |
| 35  | b     | 625    | HTG  | C1-O5-C5    | 4.08  | 119.88      | 112.56   |
| 31  | D     | 401[A] | PHO  | C1A-C2A-C3A | -4.08 | 98.96       | 102.84   |
| 23  | d     | 402[B] | CLA  | C1D-CHD-C4C | -4.07 | 117.36      | 126.02   |
| 23  | c     | 509    | CLA  | C3D-C4D-ND  | 4.07  | 116.61      | 109.99   |
| 23  | B     | 609    | CLA  | CHD-C1D-ND  | -4.07 | 119.08      | 124.80   |
| 23  | C     | 509    | CLA  | O2D-CGD-O1D | -4.07 | 115.93      | 123.85   |
| 23  | b     | 611    | CLA  | CHD-C1D-ND  | -4.07 | 119.08      | 124.80   |
| 23  | C     | 505    | CLA  | CHD-C1D-ND  | -4.06 | 119.08      | 124.80   |
| 38  | F     | 102    | HEM  | CHC-C4B-NB  | 4.06  | 128.81      | 124.44   |
| 23  | D     | 403[A] | CLA  | C1-C2-C3    | -4.06 | 119.54      | 126.20   |
| 23  | b     | 608    | CLA  | CMC-C2C-C1C | 4.06  | 131.38      | 125.03   |
| 23  | b     | 601    | CLA  | C1D-CHD-C4C | -4.06 | 117.40      | 126.02   |
| 23  | b     | 604    | CLA  | C3C-C4C-NC  | 4.06  | 115.62      | 110.43   |
| 23  | c     | 512    | CLA  | CHD-C1D-ND  | -4.05 | 119.10      | 124.80   |
| 23  | C     | 512    | CLA  | O2D-CGD-O1D | -4.05 | 115.96      | 123.85   |
| 23  | C     | 507    | CLA  | C1-C2-C3    | -4.05 | 119.56      | 126.20   |
| 23  | C     | 513    | CLA  | C1-C2-C3    | -4.05 | 119.56      | 126.20   |
| 23  | b     | 610    | CLA  | C1D-CHD-C4C | -4.05 | 117.42      | 126.02   |
| 23  | b     | 601    | CLA  | C2C-C1C-NC  | 4.05  | 114.23      | 109.98   |
| 23  | b     | 616    | CLA  | C2C-C1C-NC  | 4.04  | 114.23      | 109.98   |
| 23  | b     | 610    | CLA  | O2A-CGA-O1A | -4.04 | 113.52      | 123.63   |
| 23  | C     | 504    | CLA  | C2C-C1C-NC  | 4.04  | 114.23      | 109.98   |
| 23  | c     | 503    | CLA  | C1D-CHD-C4C | -4.04 | 117.43      | 126.02   |
| 23  | B     | 602    | CLA  | C3D-C4D-ND  | 4.04  | 116.55      | 109.99   |
| 28  | a     | 413[A] | PL9  | C7-C3-C4    | 4.04  | 120.24      | 116.91   |
| 23  | c     | 510    | CLA  | C1C-C2C-C3C | -4.04 | 102.73      | 106.98   |
| 28  | A     | 413[A] | PL9  | C7-C3-C2    | -4.03 | 118.63      | 123.39   |
| 23  | C     | 514    | CLA  | C4A-NA-C1A  | -4.03 | 104.84      | 106.68   |
| 34  | C     | 521    | LMG  | O7-C10-C11  | 4.03  | 120.20      | 111.48   |
| 23  | B     | 614    | CLA  | O2D-CGD-O1D | -4.03 | 116.00      | 123.85   |
| 23  | A     | 404[A] | CLA  | C1C-C2C-C3C | -4.03 | 102.74      | 106.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 506    | CLA  | C3D-C2D-C1D | -4.02 | 100.34      | 105.83   |
| 23  | C     | 513    | CLA  | C3C-C4C-NC  | 4.02  | 115.58      | 110.43   |
| 23  | B     | 615    | CLA  | C1C-C2C-C3C | -4.02 | 102.75      | 106.98   |
| 23  | D     | 404    | CLA  | CHD-C1D-ND  | -4.02 | 119.14      | 124.80   |
| 23  | a     | 404[B] | CLA  | CHD-C1D-ND  | -4.02 | 119.14      | 124.80   |
| 23  | C     | 510    | CLA  | C3C-C4C-NC  | 4.02  | 115.58      | 110.43   |
| 23  | C     | 513    | CLA  | CHD-C1D-ND  | -4.02 | 119.14      | 124.80   |
| 23  | b     | 602    | CLA  | C3D-C2D-C1D | -4.02 | 100.35      | 105.83   |
| 23  | d     | 404    | CLA  | C2C-C1C-NC  | 4.02  | 114.20      | 109.98   |
| 25  | A     | 409[B] | SQD  | C1-O5-C5    | -4.02 | 105.88      | 113.72   |
| 23  | B     | 610    | CLA  | C3C-C4C-NC  | 4.01  | 115.57      | 110.43   |
| 23  | b     | 612    | CLA  | C1D-CHD-C4C | -4.01 | 117.50      | 126.02   |
| 23  | B     | 616    | CLA  | O2D-CGD-O1D | -4.01 | 116.05      | 123.85   |
| 23  | b     | 604    | CLA  | CAC-C3C-C4C | 4.00  | 130.00      | 124.79   |
| 23  | B     | 613    | CLA  | CMC-C2C-C1C | 4.00  | 131.29      | 125.03   |
| 23  | D     | 404    | CLA  | C2C-C1C-NC  | 4.00  | 114.19      | 109.98   |
| 23  | A     | 404[A] | CLA  | C3B-C4B-NB  | 4.00  | 114.38      | 109.21   |
| 23  | B     | 607    | CLA  | CHD-C1D-ND  | -4.00 | 119.18      | 124.80   |
| 23  | A     | 407    | CLA  | C1C-C2C-C3C | -4.00 | 102.78      | 106.98   |
| 36  | C     | 518[A] | DGD  | O2G-C1B-C2B | 3.99  | 120.12      | 111.48   |
| 23  | D     | 403[B] | CLA  | C3C-C4C-NC  | 3.99  | 115.54      | 110.43   |
| 23  | b     | 604    | CLA  | C1D-CHD-C4C | -3.99 | 117.54      | 126.02   |
| 23  | B     | 609    | CLA  | O2D-CGD-CBD | 3.98  | 118.19      | 111.23   |
| 23  | B     | 606    | CLA  | C1C-C2C-C3C | -3.98 | 102.79      | 106.98   |
| 23  | b     | 612    | CLA  | C3D-C2D-C1D | -3.98 | 100.40      | 105.83   |
| 23  | B     | 603    | CLA  | CAC-C3C-C4C | 3.98  | 129.97      | 124.79   |
| 25  | A     | 411    | SQD  | O47-C7-C8   | 3.98  | 120.09      | 111.48   |
| 23  | B     | 610    | CLA  | C3D-C4D-ND  | 3.98  | 116.45      | 109.99   |
| 23  | A     | 407    | CLA  | C3B-C4B-NB  | 3.98  | 114.35      | 109.21   |
| 23  | c     | 507    | CLA  | C3B-C4B-NB  | 3.98  | 114.35      | 109.21   |
| 23  | B     | 603    | CLA  | C1D-CHD-C4C | -3.98 | 117.57      | 126.02   |
| 23  | c     | 507    | CLA  | C1C-C2C-C3C | -3.97 | 102.80      | 106.98   |
| 23  | b     | 607    | CLA  | C1C-C2C-C3C | -3.97 | 102.80      | 106.98   |
| 23  | b     | 615    | CLA  | O2D-CGD-CBD | 3.97  | 118.17      | 111.23   |
| 23  | c     | 511    | CLA  | CHD-C1D-ND  | -3.97 | 119.21      | 124.80   |
| 23  | B     | 605    | CLA  | C1-C2-C3    | -3.97 | 119.70      | 126.20   |
| 23  | C     | 510    | CLA  | C3B-C4B-NB  | 3.96  | 114.33      | 109.21   |
| 23  | a     | 404[A] | CLA  | O2D-CGD-CBD | 3.96  | 118.16      | 111.23   |
| 36  | C     | 517[A] | DGD  | O2G-C1B-C2B | 3.96  | 120.05      | 111.48   |
| 23  | A     | 404[A] | CLA  | CAA-C2A-C3A | -3.96 | 102.30      | 113.00   |
| 23  | c     | 511    | CLA  | C1C-C2C-C3C | -3.96 | 102.82      | 106.98   |
| 23  | C     | 507    | CLA  | O2D-CGD-O1D | -3.96 | 116.15      | 123.85   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 509    | CLA  | C3B-C4B-NB  | 3.95  | 114.32      | 109.21   |
| 23  | B     | 614    | CLA  | CMC-C2C-C1C | 3.95  | 131.21      | 125.03   |
| 23  | B     | 603    | CLA  | C3C-C4C-NC  | 3.95  | 115.49      | 110.43   |
| 28  | d     | 406[B] | PL9  | C42-C43-C44 | -3.95 | 118.58      | 127.62   |
| 24  | b     | 617    | BCR  | C7-C8-C9    | -3.95 | 120.40      | 126.23   |
| 23  | c     | 514    | CLA  | C1D-CHD-C4C | -3.95 | 117.63      | 126.02   |
| 25  | A     | 409[B] | SQD  | O47-C7-C8   | 3.95  | 120.02      | 111.48   |
| 23  | B     | 616    | CLA  | C3D-C4D-ND  | 3.94  | 116.40      | 109.99   |
| 23  | D     | 404    | CLA  | C3C-C4C-NC  | 3.94  | 115.48      | 110.43   |
| 23  | C     | 509    | CLA  | C1C-C2C-C3C | -3.94 | 102.84      | 106.98   |
| 23  | C     | 512    | CLA  | C3D-C4D-ND  | 3.94  | 116.39      | 109.99   |
| 23  | b     | 608    | CLA  | C3D-C2D-C1D | -3.94 | 100.46      | 105.83   |
| 23  | C     | 513    | CLA  | C1D-CHD-C4C | -3.93 | 117.66      | 126.02   |
| 40  | V     | 201    | HEC  | C1D-C2D-C3D | -3.93 | 104.26      | 107.00   |
| 23  | A     | 404[A] | CLA  | O2A-CGA-CBA | 3.93  | 123.81      | 111.83   |
| 23  | C     | 508    | CLA  | C1D-CHD-C4C | -3.92 | 117.68      | 126.02   |
| 23  | A     | 407    | CLA  | O2D-CGD-CBD | 3.92  | 118.09      | 111.23   |
| 23  | a     | 405[A] | CLA  | C3C-C4C-NC  | 3.92  | 115.45      | 110.43   |
| 23  | c     | 508    | CLA  | C3C-C4C-NC  | 3.92  | 115.45      | 110.43   |
| 23  | A     | 406[B] | CLA  | C1C-C2C-C3C | -3.92 | 102.86      | 106.98   |
| 23  | a     | 407    | CLA  | C1C-C2C-C3C | -3.92 | 102.86      | 106.98   |
| 23  | C     | 510    | CLA  | C1C-C2C-C3C | -3.92 | 102.86      | 106.98   |
| 23  | C     | 511    | CLA  | CHD-C1D-ND  | -3.91 | 119.30      | 124.80   |
| 23  | C     | 502    | CLA  | CHD-C1D-ND  | -3.91 | 119.30      | 124.80   |
| 23  | A     | 406[A] | CLA  | C1C-C2C-C3C | -3.91 | 102.87      | 106.98   |
| 23  | C     | 503    | CLA  | C3C-C4C-NC  | 3.91  | 115.44      | 110.43   |
| 23  | B     | 610    | CLA  | C4A-NA-C1A  | -3.90 | 104.90      | 106.68   |
| 25  | a     | 411    | SQD  | O47-C7-C8   | 3.90  | 119.92      | 111.48   |
| 23  | A     | 407    | CLA  | C1D-CHD-C4C | -3.90 | 117.73      | 126.02   |
| 34  | d     | 412    | LMG  | O7-C10-C11  | 3.90  | 119.92      | 111.48   |
| 23  | c     | 510    | CLA  | CAC-C3C-C4C | 3.90  | 129.87      | 124.79   |
| 23  | b     | 609    | CLA  | O2D-CGD-CBD | 3.89  | 118.03      | 111.23   |
| 23  | c     | 512    | CLA  | C1C-C2C-C3C | -3.89 | 102.89      | 106.98   |
| 23  | b     | 614    | CLA  | C3C-C4C-NC  | 3.89  | 115.41      | 110.43   |
| 23  | b     | 604    | CLA  | C3D-C4D-ND  | 3.88  | 116.30      | 109.99   |
| 23  | b     | 604    | CLA  | C1C-C2C-C3C | -3.88 | 102.90      | 106.98   |
| 23  | c     | 504    | CLA  | O2D-CGD-O1D | -3.87 | 116.31      | 123.85   |
| 23  | B     | 608    | CLA  | C1D-CHD-C4C | -3.87 | 117.80      | 126.02   |
| 23  | b     | 606    | CLA  | C1C-C2C-C3C | -3.86 | 102.92      | 106.98   |
| 23  | c     | 512    | CLA  | C3B-C4B-NB  | 3.86  | 114.20      | 109.21   |
| 25  | X     | 101    | SQD  | O8-S-C6     | 3.86  | 113.43      | 105.97   |
| 40  | V     | 201    | HEC  | CMB-C2B-C1B | -3.86 | 122.80      | 128.46   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 609    | CLA  | C2C-C1C-NC  | 3.86  | 114.03      | 109.98   |
| 23  | b     | 602    | CLA  | CAA-C2A-C3A | -3.86 | 102.58      | 113.00   |
| 23  | C     | 512    | CLA  | C3C-C4C-NC  | 3.85  | 115.36      | 110.43   |
| 23  | b     | 615    | CLA  | C3C-C4C-NC  | 3.85  | 115.36      | 110.43   |
| 34  | c     | 520    | LMG  | O7-C10-C11  | 3.85  | 119.81      | 111.48   |
| 23  | b     | 608    | CLA  | CHD-C1D-ND  | -3.85 | 119.39      | 124.80   |
| 23  | d     | 403[B] | CLA  | CHD-C1D-ND  | -3.85 | 119.39      | 124.80   |
| 23  | c     | 513    | CLA  | CHD-C1D-ND  | -3.85 | 119.39      | 124.80   |
| 34  | Z     | 101    | LMG  | C1-C2-C3    | 3.85  | 118.10      | 110.01   |
| 23  | A     | 405[A] | CLA  | CMC-C2C-C1C | 3.84  | 131.04      | 125.03   |
| 23  | C     | 508    | CLA  | CHD-C1D-ND  | -3.84 | 119.39      | 124.80   |
| 28  | D     | 406[A] | PL9  | C42-C43-C44 | -3.84 | 118.83      | 127.62   |
| 23  | c     | 509    | CLA  | C1C-C2C-C3C | -3.84 | 102.94      | 106.98   |
| 23  | B     | 608    | CLA  | C1C-C2C-C3C | -3.84 | 102.94      | 106.98   |
| 23  | B     | 606    | CLA  | C1D-CHD-C4C | -3.83 | 117.87      | 126.02   |
| 23  | b     | 616    | CLA  | C3D-C4D-ND  | 3.83  | 116.22      | 109.99   |
| 40  | v     | 201    | HEC  | CBA-CAA-C2A | -3.83 | 106.23      | 112.55   |
| 23  | B     | 616    | CLA  | C3B-C4B-NB  | 3.83  | 114.16      | 109.21   |
| 23  | d     | 402[A] | CLA  | CHD-C1D-ND  | -3.83 | 119.41      | 124.80   |
| 23  | B     | 614    | CLA  | C3D-C4D-ND  | 3.82  | 116.20      | 109.99   |
| 23  | C     | 514    | CLA  | C3C-C4C-NC  | 3.82  | 115.33      | 110.43   |
| 23  | c     | 510    | CLA  | CHD-C1D-ND  | -3.82 | 119.43      | 124.80   |
| 23  | B     | 613    | CLA  | CHD-C1D-ND  | -3.82 | 119.43      | 124.80   |
| 23  | B     | 611    | CLA  | C3C-C4C-NC  | 3.82  | 115.32      | 110.43   |
| 23  | b     | 605    | CLA  | C1C-C2C-C3C | -3.81 | 102.97      | 106.98   |
| 23  | b     | 607    | CLA  | CHD-C1D-ND  | -3.81 | 119.44      | 124.80   |
| 23  | A     | 404[A] | CLA  | C1D-CHD-C4C | -3.81 | 117.92      | 126.02   |
| 23  | b     | 605    | CLA  | C3C-C4C-NC  | 3.81  | 115.31      | 110.43   |
| 23  | B     | 608    | CLA  | C3B-C4B-NB  | 3.81  | 114.13      | 109.21   |
| 23  | A     | 405[A] | CLA  | CBC-CAC-C3C | -3.81 | 102.10      | 112.42   |
| 23  | b     | 613    | CLA  | CHD-C1D-ND  | -3.81 | 119.44      | 124.80   |
| 23  | c     | 505    | CLA  | C3B-C4B-NB  | 3.81  | 114.13      | 109.21   |
| 23  | C     | 505    | CLA  | C3B-C4B-NB  | 3.80  | 114.13      | 109.21   |
| 23  | B     | 613    | CLA  | C1C-C2C-C3C | -3.80 | 102.98      | 106.98   |
| 24  | K     | 102    | BCR  | C38-C26-C25 | -3.80 | 120.33      | 124.48   |
| 23  | d     | 403[B] | CLA  | C3C-C4C-NC  | 3.80  | 115.30      | 110.43   |
| 23  | B     | 615    | CLA  | CMC-C2C-C1C | 3.80  | 130.97      | 125.03   |
| 23  | A     | 404[A] | CLA  | O2D-CGD-CBD | 3.80  | 117.88      | 111.23   |
| 23  | c     | 509    | CLA  | C3C-C4C-NC  | 3.80  | 115.30      | 110.43   |
| 23  | C     | 509    | CLA  | C1D-CHD-C4C | -3.80 | 117.95      | 126.02   |
| 23  | d     | 402[A] | CLA  | C3C-C4C-NC  | 3.80  | 115.29      | 110.43   |
| 23  | B     | 611    | CLA  | CMB-C2B-C3B | 3.79  | 132.26      | 124.68   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 407    | CLA  | C1D-CHD-C4C | -3.79 | 117.96      | 126.02   |
| 23  | A     | 406[B] | CLA  | C1D-CHD-C4C | -3.79 | 117.97      | 126.02   |
| 23  | c     | 505    | CLA  | C1D-CHD-C4C | -3.79 | 117.97      | 126.02   |
| 23  | a     | 405[B] | CLA  | C1D-CHD-C4C | -3.79 | 117.97      | 126.02   |
| 23  | B     | 615    | CLA  | C4-C3-C5    | 3.79  | 121.80      | 115.23   |
| 23  | c     | 506    | CLA  | O2D-CGD-O1D | -3.79 | 116.48      | 123.85   |
| 33  | d     | 414[A] | LHG  | O8-C23-O10  | -3.78 | 114.17      | 123.63   |
| 23  | A     | 405[A] | CLA  | CHD-C1D-ND  | -3.78 | 119.48      | 124.80   |
| 23  | B     | 611    | CLA  | O2D-CGD-O1D | -3.78 | 116.49      | 123.85   |
| 23  | b     | 603    | CLA  | C1C-C2C-C3C | -3.78 | 103.01      | 106.98   |
| 23  | A     | 407    | CLA  | CHD-C1D-ND  | -3.78 | 119.49      | 124.80   |
| 23  | b     | 614    | CLA  | C1-C2-C3    | -3.78 | 120.01      | 126.20   |
| 23  | B     | 606    | CLA  | C3C-C4C-NC  | 3.78  | 115.27      | 110.43   |
| 24  | d     | 405    | BCR  | C38-C26-C25 | -3.77 | 120.37      | 124.48   |
| 34  | c     | 521    | LMG  | C3-C4-C5    | 3.77  | 117.07      | 110.23   |
| 23  | B     | 616    | CLA  | C1C-C2C-C3C | -3.77 | 103.01      | 106.98   |
| 23  | b     | 610    | CLA  | CHD-C1D-ND  | -3.77 | 119.50      | 124.80   |
| 24  | T     | 102    | BCR  | C11-C10-C9  | -3.76 | 122.00      | 127.28   |
| 23  | c     | 513    | CLA  | C2C-C1C-NC  | 3.76  | 113.94      | 109.98   |
| 23  | C     | 503    | CLA  | C1-C2-C3    | -3.76 | 120.03      | 126.20   |
| 23  | B     | 602    | CLA  | C1D-CHD-C4C | -3.76 | 118.03      | 126.02   |
| 23  | b     | 611    | CLA  | C1-C2-C3    | -3.76 | 120.03      | 126.20   |
| 23  | C     | 502    | CLA  | C3C-C4C-NC  | 3.76  | 115.25      | 110.43   |
| 28  | d     | 406[A] | PL9  | C42-C43-C44 | -3.76 | 119.02      | 127.62   |
| 23  | b     | 608    | CLA  | CMB-C2B-C3B | 3.75  | 132.18      | 124.68   |
| 25  | l     | 101    | SQD  | C1-O5-C5    | -3.75 | 106.40      | 113.72   |
| 23  | D     | 404    | CLA  | C1D-CHD-C4C | -3.75 | 118.06      | 126.02   |
| 23  | B     | 610    | CLA  | CAA-CBA-CGA | -3.75 | 102.57      | 113.21   |
| 23  | B     | 611    | CLA  | CHB-C4A-NA  | 3.75  | 129.81      | 124.40   |
| 28  | A     | 413[A] | PL9  | C22-C23-C24 | -3.74 | 119.05      | 127.62   |
| 23  | c     | 502    | CLA  | C1C-C2C-C3C | -3.74 | 103.04      | 106.98   |
| 23  | C     | 514    | CLA  | C1D-CHD-C4C | -3.74 | 118.07      | 126.02   |
| 23  | C     | 504    | CLA  | CHD-C1D-ND  | -3.74 | 119.54      | 124.80   |
| 23  | b     | 613    | CLA  | O2A-CGA-O1A | -3.74 | 114.27      | 123.63   |
| 23  | b     | 611    | CLA  | C3B-C4B-NB  | 3.74  | 114.05      | 109.21   |
| 23  | b     | 614    | CLA  | C1C-C2C-C3C | -3.74 | 103.05      | 106.98   |
| 28  | A     | 413[A] | PL9  | C7-C3-C4    | 3.74  | 119.99      | 116.91   |
| 33  | d     | 414[B] | LHG  | O7-C7-C8    | 3.74  | 119.56      | 111.48   |
| 23  | b     | 613    | CLA  | O2D-CGD-CBD | 3.74  | 117.76      | 111.23   |
| 23  | a     | 404[A] | CLA  | CHD-C1D-ND  | -3.73 | 119.55      | 124.80   |
| 33  | d     | 414[A] | LHG  | O8-C23-C24  | 3.73  | 123.21      | 111.83   |
| 31  | a     | 406[A] | PHO  | O1D-CGD-CBD | -3.73 | 119.07      | 124.72   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | d     | 403[B] | CLA  | C3B-C4B-NB  | 3.73  | 114.03      | 109.21   |
| 23  | a     | 405[B] | CLA  | C2C-C1C-NC  | 3.72  | 113.89      | 109.98   |
| 23  | c     | 514    | CLA  | C1C-C2C-C3C | -3.72 | 103.07      | 106.98   |
| 23  | B     | 609    | CLA  | C1C-C2C-C3C | -3.72 | 103.07      | 106.98   |
| 33  | b     | 629[B] | LHG  | O7-C7-C8    | 3.72  | 119.52      | 111.48   |
| 23  | b     | 611    | CLA  | C1D-CHD-C4C | -3.72 | 118.12      | 126.02   |
| 23  | a     | 404[B] | CLA  | O2D-CGD-CBD | 3.71  | 117.72      | 111.23   |
| 23  | b     | 612    | CLA  | O2D-CGD-O1D | -3.71 | 116.62      | 123.85   |
| 23  | b     | 603    | CLA  | O2D-CGD-O1D | -3.71 | 116.62      | 123.85   |
| 23  | D     | 403[A] | CLA  | C3B-C4B-NB  | 3.71  | 114.01      | 109.21   |
| 28  | a     | 413[B] | PL9  | C7-C8-C9    | -3.71 | 120.44      | 126.83   |
| 40  | V     | 201    | HEC  | CBC-CAC-C3C | -3.71 | 118.80      | 127.49   |
| 25  | a     | 409[A] | SQD  | C44-O6-C1   | -3.71 | 105.84      | 113.80   |
| 23  | B     | 601    | CLA  | C1D-CHD-C4C | -3.71 | 118.14      | 126.02   |
| 33  | L     | 101[A] | LHG  | O7-C7-C8    | 3.71  | 119.50      | 111.48   |
| 23  | d     | 403[B] | CLA  | C1D-CHD-C4C | -3.71 | 118.14      | 126.02   |
| 23  | b     | 608    | CLA  | C1D-CHD-C4C | -3.71 | 118.14      | 126.02   |
| 23  | b     | 608    | CLA  | C3C-C4C-NC  | 3.70  | 115.17      | 110.43   |
| 23  | a     | 407    | CLA  | CHD-C1D-ND  | -3.70 | 119.59      | 124.80   |
| 23  | B     | 603    | CLA  | C1C-C2C-C3C | -3.70 | 103.09      | 106.98   |
| 23  | c     | 510    | CLA  | C4A-NA-C1A  | -3.70 | 104.99      | 106.68   |
| 23  | A     | 405[B] | CLA  | CAA-C2A-C3A | -3.69 | 103.02      | 113.00   |
| 23  | B     | 604    | CLA  | C1D-CHD-C4C | -3.69 | 118.17      | 126.02   |
| 33  | d     | 407[B] | LHG  | O7-C7-C8    | 3.69  | 119.47      | 111.48   |
| 23  | B     | 615    | CLA  | CHD-C1D-ND  | -3.69 | 119.61      | 124.80   |
| 23  | b     | 602    | CLA  | C2C-C1C-NC  | 3.69  | 113.85      | 109.98   |
| 23  | B     | 610    | CLA  | O2D-CGD-O1D | -3.68 | 116.68      | 123.85   |
| 28  | A     | 413[B] | PL9  | C22-C23-C24 | -3.68 | 119.19      | 127.62   |
| 23  | B     | 611    | CLA  | CHD-C1D-ND  | -3.68 | 119.62      | 124.80   |
| 23  | D     | 403[A] | CLA  | C1C-C2C-C3C | -3.68 | 103.11      | 106.98   |
| 23  | b     | 614    | CLA  | O2A-CGA-O1A | -3.68 | 114.42      | 123.63   |
| 23  | B     | 604    | CLA  | C3D-C4D-ND  | 3.68  | 115.97      | 109.99   |
| 28  | a     | 413[A] | PL9  | C15-C14-C16 | 3.67  | 121.60      | 115.23   |
| 23  | B     | 609    | CLA  | CBC-CAC-C3C | -3.67 | 102.47      | 112.42   |
| 28  | a     | 413[B] | PL9  | C27-C28-C29 | -3.67 | 119.22      | 127.62   |
| 23  | c     | 509    | CLA  | C1D-CHD-C4C | -3.67 | 118.22      | 126.02   |
| 23  | a     | 405[A] | CLA  | C1D-CHD-C4C | -3.67 | 118.23      | 126.02   |
| 23  | c     | 506    | CLA  | CHD-C1D-ND  | -3.67 | 119.64      | 124.80   |
| 23  | C     | 503    | CLA  | C1C-C2C-C3C | -3.67 | 103.12      | 106.98   |
| 23  | B     | 604    | CLA  | C3D-C2D-C1D | -3.66 | 100.83      | 105.83   |
| 23  | a     | 404[A] | CLA  | O2A-CGA-O1A | -3.66 | 114.47      | 123.63   |
| 23  | B     | 602    | CLA  | C1C-C2C-C3C | -3.66 | 103.13      | 106.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 405[A] | CLA  | C1C-C2C-C3C | -3.66 | 103.13      | 106.98   |
| 23  | c     | 511    | CLA  | C3C-C4C-NC  | 3.66  | 115.12      | 110.43   |
| 23  | B     | 602    | CLA  | CMC-C2C-C1C | 3.66  | 130.75      | 125.03   |
| 24  | A     | 408    | BCR  | C24-C23-C22 | -3.66 | 120.82      | 126.23   |
| 23  | C     | 514    | CLA  | C3B-C4B-NB  | 3.66  | 113.94      | 109.21   |
| 23  | b     | 609    | CLA  | CHD-C1D-ND  | -3.66 | 119.66      | 124.80   |
| 36  | c     | 518[B] | DGD  | O2G-C1B-C2B | 3.65  | 119.39      | 111.48   |
| 38  | F     | 102    | HEM  | C1B-NB-C4B  | 3.65  | 109.53      | 105.21   |
| 23  | C     | 511    | CLA  | C4A-NA-C1A  | -3.65 | 105.01      | 106.68   |
| 23  | c     | 506    | CLA  | C4C-C3C-C2C | -3.65 | 101.58      | 106.89   |
| 23  | A     | 405[A] | CLA  | CAA-C2A-C3A | -3.65 | 103.13      | 113.00   |
| 23  | B     | 610    | CLA  | O2A-CGA-O1A | -3.65 | 114.50      | 123.63   |
| 23  | B     | 616    | CLA  | C4C-C3C-C2C | -3.65 | 101.58      | 106.89   |
| 23  | b     | 601    | CLA  | O2D-CGD-O1D | -3.65 | 116.75      | 123.85   |
| 33  | L     | 101[B] | LHG  | O7-C7-C8    | 3.65  | 119.37      | 111.48   |
| 35  | o     | 301    | HTG  | O5-C1-C2    | 3.64  | 115.34      | 110.32   |
| 23  | b     | 611    | CLA  | O2D-CGD-O1D | -3.64 | 116.76      | 123.85   |
| 23  | a     | 404[A] | CLA  | C3C-C4C-NC  | 3.64  | 115.09      | 110.43   |
| 23  | d     | 404    | CLA  | C1C-C2C-C3C | -3.64 | 103.16      | 106.98   |
| 23  | B     | 605    | CLA  | CHD-C4C-NC  | 3.64  | 129.87      | 124.23   |
| 36  | c     | 517[A] | DGD  | O2G-C1B-C2B | 3.64  | 119.34      | 111.48   |
| 23  | C     | 506    | CLA  | C1C-C2C-C3C | -3.63 | 103.16      | 106.98   |
| 23  | B     | 613    | CLA  | C3B-C4B-NB  | 3.63  | 113.91      | 109.21   |
| 23  | B     | 603    | CLA  | CHD-C1D-ND  | -3.63 | 119.69      | 124.80   |
| 23  | d     | 403[A] | CLA  | CHD-C1D-ND  | -3.63 | 119.69      | 124.80   |
| 23  | c     | 510    | CLA  | C3C-C4C-NC  | 3.63  | 115.08      | 110.43   |
| 23  | C     | 511    | CLA  | C3B-C4B-NB  | 3.63  | 113.90      | 109.21   |
| 23  | B     | 612    | CLA  | C4C-C3C-C2C | -3.63 | 101.61      | 106.89   |
| 23  | b     | 607    | CLA  | C4A-NA-C1A  | -3.63 | 105.02      | 106.68   |
| 23  | b     | 604    | CLA  | O2D-CGD-O1D | -3.63 | 116.79      | 123.85   |
| 28  | d     | 406[A] | PL9  | C37-C38-C39 | -3.63 | 119.33      | 127.62   |
| 36  | C     | 517[B] | DGD  | O2G-C1B-C2B | 3.62  | 119.32      | 111.48   |
| 23  | C     | 509    | CLA  | C1-C2-C3    | -3.62 | 120.26      | 126.20   |
| 23  | B     | 608    | CLA  | CHD-C1D-ND  | -3.62 | 119.71      | 124.80   |
| 23  | A     | 405[B] | CLA  | C1D-CHD-C4C | -3.62 | 118.32      | 126.02   |
| 40  | V     | 201    | HEC  | CMC-C2C-C1C | -3.62 | 123.15      | 128.46   |
| 23  | c     | 512    | CLA  | C4A-NA-C1A  | -3.62 | 105.03      | 106.68   |
| 23  | C     | 508    | CLA  | C3D-C4D-ND  | 3.62  | 115.87      | 109.99   |
| 23  | c     | 506    | CLA  | CAC-C3C-C4C | 3.62  | 129.50      | 124.79   |
| 23  | a     | 404[A] | CLA  | C1-C2-C3    | -3.61 | 120.28      | 126.20   |
| 23  | B     | 612    | CLA  | CMB-C2B-C3B | 3.61  | 131.90      | 124.68   |
| 23  | B     | 614    | CLA  | C1-C2-C3    | -3.61 | 120.28      | 126.20   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 506    | CLA  | C1D-CHD-C4C | -3.61 | 118.35      | 126.02   |
| 23  | c     | 514    | CLA  | C3C-C4C-NC  | 3.61  | 115.05      | 110.43   |
| 23  | d     | 403[A] | CLA  | O2A-CGA-CBA | 3.61  | 122.83      | 111.83   |
| 23  | C     | 504    | CLA  | C4C-C3C-C2C | -3.60 | 101.64      | 106.89   |
| 23  | b     | 606    | CLA  | C4-C3-C5    | 3.60  | 121.48      | 115.23   |
| 23  | c     | 511    | CLA  | CMC-C2C-C1C | 3.60  | 130.66      | 125.03   |
| 25  | l     | 101    | SQD  | C3-C4-C5    | 3.60  | 116.76      | 110.23   |
| 23  | a     | 407    | CLA  | CMC-C2C-C1C | 3.60  | 130.65      | 125.03   |
| 23  | D     | 404    | CLA  | O2D-CGD-O1D | -3.59 | 116.85      | 123.85   |
| 23  | A     | 405[A] | CLA  | C1D-CHD-C4C | -3.59 | 118.38      | 126.02   |
| 38  | f     | 101    | HEM  | CHD-C1D-ND  | 3.59  | 128.29      | 124.44   |
| 33  | d     | 414[B] | LHG  | O8-C23-C24  | 3.59  | 122.77      | 111.83   |
| 24  | B     | 617    | BCR  | C16-C17-C18 | -3.58 | 122.25      | 127.28   |
| 23  | c     | 514    | CLA  | C3B-C4B-NB  | 3.58  | 113.84      | 109.21   |
| 23  | C     | 505    | CLA  | C1D-CHD-C4C | -3.58 | 118.41      | 126.02   |
| 28  | a     | 413[A] | PL9  | C30-C29-C31 | 3.58  | 121.44      | 115.23   |
| 23  | A     | 406[A] | CLA  | C3C-C4C-NC  | 3.58  | 115.02      | 110.43   |
| 24  | t     | 102    | BCR  | C11-C10-C9  | -3.58 | 122.26      | 127.28   |
| 23  | C     | 507    | CLA  | C3B-C4B-NB  | 3.58  | 113.83      | 109.21   |
| 23  | B     | 608    | CLA  | C3C-C4C-NC  | 3.58  | 115.01      | 110.43   |
| 23  | b     | 609    | CLA  | CBC-CAC-C3C | -3.58 | 102.73      | 112.42   |
| 23  | A     | 406[A] | CLA  | C1D-CHD-C4C | -3.57 | 118.42      | 126.02   |
| 23  | B     | 614    | CLA  | C3C-C4C-NC  | 3.57  | 115.01      | 110.43   |
| 23  | B     | 612    | CLA  | CHD-C1D-ND  | -3.57 | 119.78      | 124.80   |
| 23  | b     | 612    | CLA  | C1C-C2C-C3C | -3.57 | 103.22      | 106.98   |
| 25  | a     | 411    | SQD  | O48-C23-C24 | 3.57  | 122.72      | 111.83   |
| 23  | c     | 507    | CLA  | O2D-CGD-O1D | -3.57 | 116.90      | 123.85   |
| 23  | c     | 503    | CLA  | C3C-C4C-NC  | 3.57  | 115.00      | 110.43   |
| 23  | b     | 615    | CLA  | CHD-C1D-ND  | -3.57 | 119.78      | 124.80   |
| 36  | c     | 518[A] | DGD  | O2G-C1B-C2B | 3.56  | 119.19      | 111.48   |
| 28  | A     | 413[A] | PL9  | C15-C14-C16 | 3.56  | 121.41      | 115.23   |
| 23  | B     | 604    | CLA  | C3B-C4B-NB  | 3.56  | 113.82      | 109.21   |
| 23  | d     | 404    | CLA  | C3C-C4C-NC  | 3.56  | 114.99      | 110.43   |
| 33  | A     | 418[B] | LHG  | O7-C7-C8    | 3.56  | 119.19      | 111.48   |
| 24  | h     | 101    | BCR  | C38-C26-C25 | -3.56 | 120.60      | 124.48   |
| 24  | t     | 102    | BCR  | C21-C20-C19 | -3.56 | 112.89      | 123.20   |
| 23  | b     | 603    | CLA  | CHD-C1D-ND  | -3.56 | 119.80      | 124.80   |
| 23  | a     | 404[B] | CLA  | CAA-C2A-C3A | -3.56 | 103.39      | 113.00   |
| 23  | B     | 613    | CLA  | CAC-C3C-C4C | 3.56  | 129.42      | 124.79   |
| 31  | D     | 401[B] | PHO  | O1D-CGD-CBD | -3.55 | 119.34      | 124.72   |
| 23  | c     | 507    | CLA  | C1D-CHD-C4C | -3.55 | 118.47      | 126.02   |
| 24  | h     | 101    | BCR  | C7-C8-C9    | -3.55 | 120.98      | 126.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 404[A] | CLA  | C3C-C4C-NC  | 3.55  | 114.98      | 110.43   |
| 25  | A     | 409[A] | SQD  | O47-C7-C8   | 3.55  | 119.16      | 111.48   |
| 23  | b     | 608    | CLA  | O2D-CGD-O1D | -3.55 | 116.94      | 123.85   |
| 23  | C     | 507    | CLA  | CBC-CAC-C3C | -3.55 | 102.81      | 112.42   |
| 28  | A     | 413[B] | PL9  | C17-C18-C19 | -3.55 | 119.51      | 127.62   |
| 24  | Y     | 101    | BCR  | C16-C17-C18 | -3.55 | 122.31      | 127.28   |
| 23  | B     | 610    | CLA  | C1C-C2C-C3C | -3.55 | 103.25      | 106.98   |
| 28  | A     | 413[B] | PL9  | C15-C14-C16 | 3.54  | 121.38      | 115.23   |
| 23  | b     | 613    | CLA  | C1D-CHD-C4C | -3.54 | 118.50      | 126.02   |
| 23  | c     | 502    | CLA  | C1-C2-C3    | -3.54 | 120.40      | 126.20   |
| 28  | a     | 413[A] | PL9  | C27-C28-C29 | -3.54 | 119.53      | 127.62   |
| 34  | C     | 520    | LMG  | O8-C28-C29  | 3.53  | 122.61      | 111.83   |
| 23  | b     | 614    | CLA  | C1D-CHD-C4C | -3.53 | 118.51      | 126.02   |
| 28  | A     | 413[A] | PL9  | C37-C38-C39 | -3.53 | 119.54      | 127.62   |
| 23  | B     | 610    | CLA  | CHD-C1D-ND  | -3.53 | 119.83      | 124.80   |
| 23  | b     | 601    | CLA  | C3C-C4C-NC  | 3.53  | 114.95      | 110.43   |
| 23  | A     | 404[B] | CLA  | CAA-C2A-C3A | -3.53 | 103.46      | 113.00   |
| 24  | C     | 515    | BCR  | C15-C14-C13 | -3.53 | 122.33      | 127.28   |
| 23  | b     | 609    | CLA  | C1D-CHD-C4C | -3.53 | 118.52      | 126.02   |
| 23  | B     | 610    | CLA  | C1D-CHD-C4C | -3.53 | 118.52      | 126.02   |
| 23  | C     | 512    | CLA  | C1C-C2C-C3C | -3.52 | 103.27      | 106.98   |
| 23  | B     | 603    | CLA  | CAA-C2A-C3A | -3.52 | 103.48      | 113.00   |
| 23  | B     | 601    | CLA  | C4C-C3C-C2C | -3.52 | 101.77      | 106.89   |
| 31  | a     | 406[B] | PHO  | C1-C2-C3    | -3.52 | 120.43      | 126.20   |
| 28  | A     | 413[A] | PL9  | C27-C28-C29 | -3.52 | 119.56      | 127.62   |
| 25  | a     | 409[A] | SQD  | O9-S-C6     | 3.52  | 112.01      | 106.76   |
| 23  | d     | 403[A] | CLA  | C1-C2-C3    | -3.52 | 120.43      | 126.20   |
| 23  | c     | 511    | CLA  | C1D-CHD-C4C | -3.51 | 118.55      | 126.02   |
| 25  | a     | 409[B] | SQD  | C1-O5-C5    | -3.51 | 106.86      | 113.72   |
| 23  | b     | 613    | CLA  | C3B-C4B-NB  | 3.51  | 113.75      | 109.21   |
| 23  | B     | 614    | CLA  | CHD-C4C-NC  | 3.51  | 129.67      | 124.23   |
| 23  | B     | 612    | CLA  | CMC-C2C-C1C | 3.51  | 130.52      | 125.03   |
| 23  | B     | 601    | CLA  | C2C-C1C-NC  | 3.50  | 113.66      | 109.98   |
| 31  | A     | 416[B] | PHO  | C1A-C2A-C3A | -3.50 | 99.51       | 102.84   |
| 23  | d     | 403[A] | CLA  | C3B-C4B-NB  | 3.50  | 113.73      | 109.21   |
| 25  | A     | 409[B] | SQD  | C44-O6-C1   | -3.50 | 106.30      | 113.80   |
| 23  | C     | 508    | CLA  | C1C-C2C-C3C | -3.50 | 103.30      | 106.98   |
| 23  | c     | 511    | CLA  | C3B-C4B-NB  | 3.50  | 113.73      | 109.21   |
| 23  | A     | 404[A] | CLA  | O2A-CGA-O1A | -3.50 | 114.89      | 123.63   |
| 23  | b     | 615    | CLA  | C4-C3-C5    | 3.49  | 121.29      | 115.23   |
| 23  | B     | 603    | CLA  | CMC-C2C-C1C | 3.49  | 130.50      | 125.03   |
| 33  | A     | 418[A] | LHG  | O7-C7-C8    | 3.49  | 119.04      | 111.48   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 513    | CLA  | C4-C3-C5    | 3.49  | 121.28      | 115.23   |
| 23  | b     | 613    | CLA  | O2A-CGA-CBA | 3.49  | 122.47      | 111.83   |
| 28  | d     | 406[A] | PL9  | C40-C39-C41 | 3.49  | 121.28      | 115.23   |
| 23  | b     | 606    | CLA  | C3C-C4C-NC  | 3.49  | 114.89      | 110.43   |
| 23  | b     | 607    | CLA  | C3B-C4B-NB  | 3.49  | 113.72      | 109.21   |
| 23  | d     | 402[B] | CLA  | CBC-CAC-C3C | -3.48 | 102.98      | 112.42   |
| 28  | A     | 413[B] | PL9  | C37-C38-C39 | -3.48 | 119.65      | 127.62   |
| 23  | a     | 404[A] | CLA  | O2A-CGA-CBA | 3.48  | 122.45      | 111.83   |
| 23  | B     | 609    | CLA  | C1D-CHD-C4C | -3.48 | 118.62      | 126.02   |
| 23  | d     | 402[B] | CLA  | CAA-C2A-C3A | -3.48 | 103.59      | 113.00   |
| 23  | a     | 404[B] | CLA  | C3C-C4C-NC  | 3.48  | 114.89      | 110.43   |
| 23  | c     | 505    | CLA  | C3C-C4C-NC  | 3.48  | 114.89      | 110.43   |
| 28  | a     | 413[B] | PL9  | C15-C14-C16 | 3.48  | 121.27      | 115.23   |
| 24  | C     | 515    | BCR  | C7-C8-C9    | -3.48 | 121.09      | 126.23   |
| 23  | d     | 403[B] | CLA  | C1-C2-C3    | -3.48 | 120.50      | 126.20   |
| 23  | B     | 611    | CLA  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 23  | b     | 606    | CLA  | O2D-CGD-O1D | -3.47 | 117.09      | 123.85   |
| 28  | A     | 413[B] | PL9  | C27-C28-C29 | -3.47 | 119.68      | 127.62   |
| 23  | B     | 605    | CLA  | C4-C3-C5    | 3.47  | 121.25      | 115.23   |
| 36  | c     | 517[B] | DGD  | O2G-C1B-C2B | 3.47  | 118.98      | 111.48   |
| 23  | B     | 601    | CLA  | O2D-CGD-O1D | -3.47 | 117.10      | 123.85   |
| 28  | D     | 406[B] | PL9  | C25-C24-C26 | 3.47  | 121.24      | 115.23   |
| 31  | A     | 416[A] | PHO  | C1A-C2A-C3A | -3.46 | 99.54       | 102.84   |
| 23  | c     | 504    | CLA  | C1-C2-C3    | -3.46 | 120.53      | 126.20   |
| 34  | C     | 520    | LMG  | O7-C10-C11  | 3.46  | 118.97      | 111.48   |
| 23  | b     | 612    | CLA  | C4-C3-C5    | 3.46  | 121.23      | 115.23   |
| 23  | A     | 405[A] | CLA  | C3C-C4C-NC  | 3.46  | 114.86      | 110.43   |
| 28  | a     | 413[A] | PL9  | C37-C38-C39 | -3.46 | 119.71      | 127.62   |
| 23  | B     | 603    | CLA  | O2A-CGA-CBA | 3.46  | 122.38      | 111.83   |
| 23  | C     | 513    | CLA  | CHD-C4C-NC  | 3.46  | 129.59      | 124.23   |
| 23  | C     | 512    | CLA  | CHD-C1D-ND  | -3.46 | 119.94      | 124.80   |
| 23  | b     | 613    | CLA  | C3D-C4D-ND  | 3.46  | 115.60      | 109.99   |
| 24  | C     | 515    | BCR  | C33-C5-C6   | -3.45 | 120.72      | 124.48   |
| 23  | C     | 509    | CLA  | C4C-C3C-C2C | -3.45 | 101.87      | 106.89   |
| 23  | d     | 402[A] | CLA  | CHD-C4C-NC  | 3.45  | 129.58      | 124.23   |
| 23  | A     | 407    | CLA  | CAA-C2A-C3A | -3.45 | 103.69      | 113.00   |
| 23  | B     | 607    | CLA  | C4-C3-C5    | 3.45  | 121.21      | 115.23   |
| 24  | B     | 617    | BCR  | C33-C5-C6   | -3.44 | 120.73      | 124.48   |
| 23  | B     | 602    | CLA  | CAA-C2A-C3A | -3.44 | 103.70      | 113.00   |
| 23  | b     | 602    | CLA  | CMC-C2C-C1C | 3.44  | 130.41      | 125.03   |
| 23  | b     | 605    | CLA  | C1D-CHD-C4C | -3.44 | 118.71      | 126.02   |
| 23  | b     | 607    | CLA  | C1D-CHD-C4C | -3.44 | 118.71      | 126.02   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 33  | D     | 407[B] | LHG  | O7-C7-C8    | 3.44  | 118.91      | 111.48   |
| 23  | b     | 610    | CLA  | C4C-C3C-C2C | -3.43 | 101.89      | 106.89   |
| 23  | d     | 402[A] | CLA  | C3B-C4B-NB  | 3.43  | 113.65      | 109.21   |
| 23  | a     | 404[A] | CLA  | CMB-C2B-C3B | 3.43  | 131.54      | 124.68   |
| 23  | a     | 405[B] | CLA  | CHD-C4C-NC  | 3.43  | 129.55      | 124.23   |
| 31  | a     | 406[A] | PHO  | C1A-C2A-C3A | -3.43 | 99.58       | 102.84   |
| 33  | A     | 418[A] | LHG  | O8-C23-C24  | 3.42  | 122.28      | 111.83   |
| 24  | K     | 102    | BCR  | C24-C23-C22 | -3.42 | 121.17      | 126.23   |
| 23  | B     | 605    | CLA  | C4C-C3C-C2C | -3.42 | 101.91      | 106.89   |
| 23  | B     | 607    | CLA  | C1D-CHD-C4C | -3.42 | 118.75      | 126.02   |
| 23  | C     | 505    | CLA  | O2D-CGD-O1D | -3.42 | 117.19      | 123.85   |
| 23  | b     | 602    | CLA  | C3C-C4C-NC  | 3.42  | 114.81      | 110.43   |
| 38  | F     | 102    | HEM  | CHB-C1B-NB  | 3.41  | 128.60      | 124.37   |
| 33  | d     | 408[A] | LHG  | O7-C7-C8    | 3.41  | 118.86      | 111.48   |
| 23  | b     | 602    | CLA  | C1C-C2C-C3C | -3.41 | 103.39      | 106.98   |
| 23  | B     | 603    | CLA  | CMB-C2B-C3B | 3.41  | 131.50      | 124.68   |
| 24  | y     | 101    | BCR  | C38-C26-C25 | -3.41 | 120.76      | 124.48   |
| 34  | C     | 521    | LMG  | C3-C4-C5    | 3.41  | 116.42      | 110.23   |
| 23  | A     | 406[A] | CLA  | CAA-C2A-C3A | -3.41 | 103.78      | 113.00   |
| 23  | a     | 405[B] | CLA  | C3C-C4C-NC  | 3.41  | 114.80      | 110.43   |
| 24  | k     | 101    | BCR  | C7-C8-C9    | -3.41 | 121.19      | 126.23   |
| 23  | A     | 405[B] | CLA  | C3C-C4C-NC  | 3.41  | 114.80      | 110.43   |
| 23  | C     | 504    | CLA  | C4-C3-C5    | 3.41  | 121.14      | 115.23   |
| 23  | C     | 510    | CLA  | C1D-CHD-C4C | -3.41 | 118.78      | 126.02   |
| 33  | A     | 418[B] | LHG  | C5-O7-C7    | -3.40 | 109.66      | 117.80   |
| 23  | C     | 508    | CLA  | C4C-C3C-C2C | -3.40 | 101.94      | 106.89   |
| 23  | A     | 404[B] | CLA  | C1C-C2C-C3C | -3.40 | 103.41      | 106.98   |
| 23  | C     | 506    | CLA  | C4-C3-C5    | 3.40  | 121.13      | 115.23   |
| 38  | F     | 102    | HEM  | CBD-CAD-C3D | -3.40 | 103.14      | 112.53   |
| 38  | f     | 101    | HEM  | CHA-C4D-ND  | 3.40  | 128.58      | 124.37   |
| 23  | b     | 611    | CLA  | C1C-C2C-C3C | -3.40 | 103.41      | 106.98   |
| 23  | C     | 513    | CLA  | C2C-C1C-NC  | 3.40  | 113.55      | 109.98   |
| 23  | A     | 404[A] | CLA  | C1-C2-C3    | -3.40 | 120.63      | 126.20   |
| 28  | d     | 406[B] | PL9  | C7-C3-C4    | 3.40  | 119.71      | 116.91   |
| 23  | C     | 503    | CLA  | O2D-CGD-O1D | -3.40 | 117.24      | 123.85   |
| 35  | b     | 622    | HTG  | O2-C2-C1    | 3.39  | 116.33      | 110.30   |
| 28  | D     | 406[B] | PL9  | C27-C28-C29 | -3.39 | 119.86      | 127.62   |
| 23  | B     | 616    | CLA  | CAC-C3C-C4C | 3.39  | 129.20      | 124.79   |
| 23  | d     | 402[B] | CLA  | CHD-C4C-NC  | 3.39  | 129.49      | 124.23   |
| 23  | c     | 512    | CLA  | C3C-C4C-NC  | 3.39  | 114.77      | 110.43   |
| 23  | c     | 507    | CLA  | C3C-C4C-NC  | 3.39  | 114.77      | 110.43   |
| 23  | C     | 506    | CLA  | CAC-C3C-C4C | 3.39  | 129.20      | 124.79   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 510    | CLA  | O2A-CGA-CBA | 3.39  | 122.16      | 111.83   |
| 23  | b     | 616    | CLA  | CHD-C1D-ND  | -3.39 | 120.04      | 124.80   |
| 34  | c     | 521    | LMG  | C9-C8-C7    | -3.38 | 103.89      | 111.78   |
| 23  | a     | 404[B] | CLA  | C1C-C2C-C3C | -3.38 | 103.42      | 106.98   |
| 23  | B     | 605    | CLA  | O2D-CGD-O1D | -3.38 | 117.26      | 123.85   |
| 23  | b     | 614    | CLA  | C3B-C4B-NB  | 3.38  | 113.58      | 109.21   |
| 23  | c     | 512    | CLA  | CHD-C4C-NC  | 3.38  | 129.47      | 124.23   |
| 23  | a     | 404[A] | CLA  | C3B-C4B-NB  | 3.38  | 113.58      | 109.21   |
| 40  | v     | 201    | HEC  | CBD-CAD-C3D | -3.38 | 106.86      | 112.54   |
| 23  | B     | 609    | CLA  | O2D-CGD-O1D | -3.37 | 117.28      | 123.85   |
| 23  | c     | 513    | CLA  | CHD-C4C-NC  | 3.37  | 129.46      | 124.23   |
| 23  | d     | 402[B] | CLA  | C3B-C4B-NB  | 3.37  | 113.57      | 109.21   |
| 23  | b     | 612    | CLA  | O2A-CGA-CBA | 3.37  | 122.12      | 111.83   |
| 23  | C     | 503    | CLA  | CAC-C3C-C4C | 3.37  | 129.18      | 124.79   |
| 23  | C     | 507    | CLA  | C1D-CHD-C4C | -3.37 | 118.85      | 126.02   |
| 25  | A     | 409[A] | SQD  | C44-O6-C1   | -3.37 | 106.57      | 113.80   |
| 23  | b     | 604    | CLA  | CMC-C2C-C1C | 3.37  | 130.30      | 125.03   |
| 23  | c     | 512    | CLA  | CBC-CAC-C3C | -3.37 | 103.28      | 112.42   |
| 23  | c     | 513    | CLA  | O2D-CGD-O1D | -3.37 | 117.29      | 123.85   |
| 23  | D     | 404    | CLA  | C4C-C3C-C2C | -3.37 | 101.99      | 106.89   |
| 23  | A     | 406[A] | CLA  | C3B-C4B-NB  | 3.37  | 113.56      | 109.21   |
| 25  | X     | 101    | SQD  | C1-C2-C3    | -3.36 | 102.93      | 110.01   |
| 23  | c     | 513    | CLA  | C1C-C2C-C3C | -3.36 | 103.44      | 106.98   |
| 23  | b     | 606    | CLA  | C3B-C4B-NB  | 3.36  | 113.55      | 109.21   |
| 23  | B     | 613    | CLA  | O2A-CGA-O1A | -3.36 | 115.23      | 123.63   |
| 23  | c     | 509    | CLA  | O2D-CGD-O1D | -3.36 | 117.31      | 123.85   |
| 28  | a     | 413[A] | PL9  | C17-C18-C19 | -3.36 | 119.94      | 127.62   |
| 23  | c     | 506    | CLA  | C1D-CHD-C4C | -3.36 | 118.89      | 126.02   |
| 23  | D     | 403[A] | CLA  | C4C-C3C-C2C | -3.35 | 102.01      | 106.89   |
| 23  | A     | 404[A] | CLA  | CAC-C3C-C4C | 3.35  | 129.15      | 124.79   |
| 23  | b     | 604    | CLA  | CHD-C1D-ND  | -3.35 | 120.08      | 124.80   |
| 36  | h     | 102    | DGD  | O2G-C1B-C2B | 3.35  | 118.73      | 111.48   |
| 23  | C     | 503    | CLA  | CMC-C2C-C1C | 3.35  | 130.27      | 125.03   |
| 23  | C     | 511    | CLA  | C3C-C4C-NC  | 3.35  | 114.72      | 110.43   |
| 23  | c     | 509    | CLA  | C1-C2-C3    | -3.35 | 120.71      | 126.20   |
| 28  | D     | 406[A] | PL9  | C17-C18-C19 | -3.35 | 119.96      | 127.62   |
| 23  | a     | 405[B] | CLA  | C1C-C2C-C3C | -3.35 | 103.46      | 106.98   |
| 23  | d     | 403[B] | CLA  | O2A-CGA-CBA | 3.34  | 122.03      | 111.83   |
| 33  | b     | 629[A] | LHG  | O7-C7-C8    | 3.34  | 118.72      | 111.48   |
| 23  | b     | 602    | CLA  | C1-C2-C3    | -3.34 | 120.72      | 126.20   |
| 23  | b     | 607    | CLA  | O2D-CGD-CBD | 3.34  | 117.07      | 111.23   |
| 23  | B     | 603    | CLA  | O2A-CGA-O1A | -3.34 | 115.27      | 123.63   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 509    | CLA  | C4A-NA-C1A  | -3.34 | 105.16      | 106.68   |
| 40  | v     | 201    | HEC  | CMC-C2C-C1C | -3.34 | 123.57      | 128.46   |
| 23  | C     | 502    | CLA  | C1C-C2C-C3C | -3.34 | 103.47      | 106.98   |
| 23  | b     | 609    | CLA  | C4C-C3C-C2C | -3.34 | 102.03      | 106.89   |
| 23  | A     | 404[A] | CLA  | CAA-C2A-C1A | -3.33 | 101.05      | 111.97   |
| 23  | d     | 403[B] | CLA  | CHC-C1C-C2C | -3.33 | 117.50      | 126.94   |
| 23  | b     | 611    | CLA  | C4C-C3C-C2C | -3.33 | 102.04      | 106.89   |
| 34  | Z     | 101    | LMG  | O6-C1-C2    | 3.33  | 117.21      | 110.37   |
| 23  | c     | 502    | CLA  | C3C-C4C-NC  | 3.33  | 114.69      | 110.43   |
| 23  | b     | 608    | CLA  | C3B-C4B-NB  | 3.33  | 113.51      | 109.21   |
| 23  | B     | 614    | CLA  | O2A-CGA-O1A | -3.33 | 115.31      | 123.63   |
| 23  | d     | 403[A] | CLA  | C1D-CHD-C4C | -3.33 | 118.95      | 126.02   |
| 32  | A     | 417    | LMT  | O5B-C5B-C4B | 3.32  | 115.69      | 109.70   |
| 23  | B     | 610    | CLA  | C4C-C3C-C2C | -3.32 | 102.05      | 106.89   |
| 23  | B     | 615    | CLA  | CED-O2D-CGD | 3.32  | 123.46      | 115.92   |
| 23  | B     | 605    | CLA  | C1C-C2C-C3C | -3.32 | 103.49      | 106.98   |
| 23  | C     | 507    | CLA  | C3C-C4C-NC  | 3.32  | 114.68      | 110.43   |
| 23  | a     | 404[A] | CLA  | CAA-C2A-C1A | -3.32 | 101.10      | 111.97   |
| 24  | D     | 405    | BCR  | C28-C27-C26 | -3.32 | 108.14      | 114.06   |
| 35  | b     | 625    | HTG  | O5-C5-C4    | 3.32  | 115.67      | 109.70   |
| 23  | b     | 609    | CLA  | CAC-C3C-C4C | 3.32  | 129.10      | 124.79   |
| 23  | C     | 510    | CLA  | CMB-C2B-C3B | 3.32  | 131.31      | 124.68   |
| 23  | c     | 509    | CLA  | C3B-C4B-NB  | 3.31  | 113.49      | 109.21   |
| 23  | A     | 404[B] | CLA  | C3C-C4C-NC  | 3.31  | 114.67      | 110.43   |
| 23  | a     | 407    | CLA  | O2A-CGA-CBA | 3.31  | 121.93      | 111.83   |
| 23  | b     | 603    | CLA  | C3B-C4B-NB  | 3.31  | 113.49      | 109.21   |
| 24  | c     | 515    | BCR  | C15-C14-C13 | -3.31 | 122.64      | 127.28   |
| 24  | D     | 405    | BCR  | C29-C30-C25 | 3.31  | 115.25      | 110.44   |
| 23  | C     | 506    | CLA  | C4C-C3C-C2C | -3.31 | 102.08      | 106.89   |
| 25  | a     | 409[A] | SQD  | C45-O47-C7  | -3.31 | 109.88      | 117.80   |
| 23  | A     | 407    | CLA  | C4C-C3C-C2C | -3.31 | 102.08      | 106.89   |
| 23  | B     | 616    | CLA  | O2A-CGA-CBA | 3.30  | 121.91      | 111.83   |
| 23  | c     | 503    | CLA  | O2D-CGD-O1D | -3.30 | 117.42      | 123.85   |
| 23  | a     | 404[A] | CLA  | O2D-CGD-O1D | -3.30 | 117.43      | 123.85   |
| 23  | C     | 506    | CLA  | O2D-CGD-O1D | -3.30 | 117.43      | 123.85   |
| 23  | C     | 503    | CLA  | C4-C3-C5    | 3.29  | 120.94      | 115.23   |
| 28  | d     | 406[B] | PL9  | C40-C39-C41 | 3.29  | 120.94      | 115.23   |
| 23  | b     | 615    | CLA  | C1C-C2C-C3C | -3.29 | 103.52      | 106.98   |
| 23  | A     | 405[B] | CLA  | C3B-C4B-NB  | 3.29  | 113.46      | 109.21   |
| 34  | m     | 101    | LMG  | O8-C28-C29  | 3.28  | 121.85      | 111.83   |
| 31  | a     | 406[B] | PHO  | O1D-CGD-CBD | -3.28 | 119.74      | 124.72   |
| 23  | B     | 607    | CLA  | CBC-CAC-C3C | -3.28 | 103.52      | 112.42   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | D     | 403[B] | CLA  | C1D-CHD-C4C | -3.28 | 119.05      | 126.02   |
| 23  | b     | 605    | CLA  | CHD-C4C-NC  | 3.28  | 129.32      | 124.23   |
| 23  | C     | 502    | CLA  | CAC-C3C-C4C | 3.28  | 129.06      | 124.79   |
| 34  | C     | 521    | LMG  | O8-C28-C29  | 3.28  | 121.82      | 111.83   |
| 23  | d     | 402[B] | CLA  | C3C-C4C-NC  | 3.28  | 114.63      | 110.43   |
| 24  | D     | 405    | BCR  | C10-C11-C12 | -3.27 | 113.71      | 123.20   |
| 25  | A     | 409[A] | SQD  | O9-S-C6     | 3.27  | 111.64      | 106.76   |
| 23  | A     | 406[A] | CLA  | O2A-CGA-O1A | -3.27 | 115.45      | 123.63   |
| 23  | A     | 404[B] | CLA  | CHC-C1C-C2C | -3.27 | 117.68      | 126.94   |
| 31  | a     | 415[A] | PHO  | C4-C3-C5    | 3.27  | 120.90      | 115.23   |
| 23  | C     | 509    | CLA  | CHD-C1D-ND  | -3.27 | 120.20      | 124.80   |
| 23  | b     | 607    | CLA  | C4C-C3C-C2C | -3.27 | 102.14      | 106.89   |
| 28  | d     | 406[B] | PL9  | C10-C9-C11  | 3.27  | 120.90      | 115.23   |
| 23  | b     | 609    | CLA  | CMC-C2C-C1C | 3.26  | 130.13      | 125.03   |
| 23  | d     | 403[A] | CLA  | C4-C3-C5    | 3.26  | 120.89      | 115.23   |
| 23  | b     | 606    | CLA  | CHD-C4C-NC  | 3.26  | 129.29      | 124.23   |
| 23  | c     | 510    | CLA  | CHC-C1C-C2C | -3.26 | 117.71      | 126.94   |
| 23  | C     | 510    | CLA  | O2A-CGA-CBA | 3.26  | 121.77      | 111.83   |
| 23  | c     | 507    | CLA  | CHC-C1C-C2C | -3.26 | 117.71      | 126.94   |
| 23  | a     | 407    | CLA  | C3B-C4B-NB  | 3.26  | 113.42      | 109.21   |
| 24  | Y     | 101    | BCR  | C15-C14-C13 | -3.26 | 122.71      | 127.28   |
| 23  | b     | 612    | CLA  | C4C-C3C-C2C | -3.26 | 102.15      | 106.89   |
| 28  | a     | 413[B] | PL9  | C17-C18-C19 | -3.25 | 120.17      | 127.62   |
| 23  | C     | 507    | CLA  | CAC-C3C-C4C | 3.25  | 129.02      | 124.79   |
| 25  | X     | 101    | SQD  | O48-C23-C24 | 3.25  | 121.75      | 111.83   |
| 23  | a     | 405[B] | CLA  | CMC-C2C-C1C | 3.25  | 130.11      | 125.03   |
| 34  | c     | 501    | LMG  | C7-O1-C1    | -3.25 | 106.83      | 113.80   |
| 23  | D     | 403[B] | CLA  | C3B-C4B-NB  | 3.25  | 113.41      | 109.21   |
| 24  | k     | 101    | BCR  | C29-C30-C25 | 3.25  | 115.16      | 110.44   |
| 23  | b     | 616    | CLA  | O2A-CGA-O1A | -3.25 | 115.51      | 123.63   |
| 23  | b     | 610    | CLA  | CHD-C4C-NC  | 3.25  | 129.26      | 124.23   |
| 23  | C     | 511    | CLA  | C4-C3-C5    | 3.25  | 120.86      | 115.23   |
| 31  | a     | 406[A] | PHO  | O2A-CGA-O1A | -3.25 | 115.51      | 123.63   |
| 34  | c     | 520    | LMG  | O1-C7-C8    | -3.25 | 102.92      | 110.82   |
| 25  | X     | 101    | SQD  | C44-O6-C1   | -3.24 | 106.84      | 113.80   |
| 23  | B     | 602    | CLA  | C4C-C3C-C2C | -3.24 | 102.17      | 106.89   |
| 23  | b     | 616    | CLA  | C4C-C3C-C2C | -3.24 | 102.17      | 106.89   |
| 23  | B     | 603    | CLA  | C3B-C4B-NB  | 3.24  | 113.40      | 109.21   |
| 38  | f     | 101    | HEM  | CAD-CBD-CGD | 3.24  | 122.26      | 113.67   |
| 23  | c     | 506    | CLA  | C1C-C2C-C3C | -3.24 | 103.57      | 106.98   |
| 23  | C     | 510    | CLA  | C4C-C3C-C2C | -3.23 | 102.19      | 106.89   |
| 23  | c     | 511    | CLA  | C4-C3-C5    | 3.23  | 120.84      | 115.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 504    | CLA  | C1-C2-C3    | -3.23 | 120.90      | 126.20   |
| 23  | C     | 513    | CLA  | CMC-C2C-C1C | 3.23  | 130.08      | 125.03   |
| 23  | A     | 406[B] | CLA  | C3C-C4C-NC  | 3.23  | 114.57      | 110.43   |
| 23  | A     | 406[B] | CLA  | O2A-CGA-O1A | -3.23 | 115.55      | 123.63   |
| 23  | d     | 404    | CLA  | O2D-CGD-O1D | -3.23 | 117.57      | 123.85   |
| 23  | c     | 504    | CLA  | C4C-C3C-C2C | -3.22 | 102.20      | 106.89   |
| 23  | d     | 403[A] | CLA  | O2A-CGA-O1A | -3.22 | 115.57      | 123.63   |
| 23  | C     | 507    | CLA  | CMC-C2C-C1C | 3.22  | 130.07      | 125.03   |
| 23  | b     | 610    | CLA  | C1C-C2C-C3C | -3.22 | 103.59      | 106.98   |
| 23  | b     | 608    | CLA  | CAC-C3C-C4C | 3.22  | 128.98      | 124.79   |
| 23  | C     | 510    | CLA  | CAC-C3C-C4C | 3.22  | 128.98      | 124.79   |
| 23  | a     | 405[A] | CLA  | C3B-C4B-NB  | 3.22  | 113.37      | 109.21   |
| 23  | c     | 503    | CLA  | C3B-C4B-NB  | 3.22  | 113.37      | 109.21   |
| 28  | D     | 406[A] | PL9  | C25-C24-C26 | 3.22  | 120.81      | 115.23   |
| 23  | a     | 405[A] | CLA  | CAA-C2A-C3A | -3.22 | 104.31      | 113.00   |
| 23  | B     | 616    | CLA  | CMC-C2C-C1C | 3.21  | 130.06      | 125.03   |
| 31  | a     | 406[A] | PHO  | O2A-CGA-CBA | 3.21  | 121.63      | 111.83   |
| 23  | b     | 613    | CLA  | C4C-C3C-C2C | -3.21 | 102.21      | 106.89   |
| 32  | B     | 626    | LMT  | O1'-C1'-C2' | 3.21  | 113.14      | 108.27   |
| 23  | d     | 404    | CLA  | C1D-CHD-C4C | -3.21 | 119.20      | 126.02   |
| 23  | c     | 513    | CLA  | C3C-C4C-NC  | 3.21  | 114.54      | 110.43   |
| 23  | c     | 513    | CLA  | C4-C3-C5    | 3.20  | 120.79      | 115.23   |
| 34  | z     | 101    | LMG  | O7-C10-C11  | 3.20  | 118.41      | 111.48   |
| 25  | a     | 409[B] | SQD  | C45-O47-C7  | -3.20 | 110.14      | 117.80   |
| 23  | c     | 508    | CLA  | O2D-CGD-O1D | -3.20 | 117.62      | 123.85   |
| 23  | B     | 602    | CLA  | CHD-C1D-ND  | -3.20 | 120.30      | 124.80   |
| 23  | A     | 407    | CLA  | CMA-C3A-C2A | -3.20 | 101.61      | 113.98   |
| 25  | l     | 101    | SQD  | O7-S-C6     | 3.20  | 111.53      | 106.76   |
| 23  | b     | 612    | CLA  | CHD-C1D-ND  | -3.20 | 120.30      | 124.80   |
| 23  | a     | 404[B] | CLA  | CHC-C1C-C2C | -3.19 | 117.90      | 126.94   |
| 23  | b     | 609    | CLA  | C3B-C4B-NB  | 3.19  | 113.34      | 109.21   |
| 25  | f     | 102    | SQD  | O5-C1-C2    | 3.19  | 116.93      | 110.37   |
| 28  | A     | 413[A] | PL9  | O1-C4-C3    | -3.19 | 117.37      | 120.73   |
| 23  | a     | 407    | CLA  | O2D-CGD-O1D | -3.18 | 117.65      | 123.85   |
| 23  | c     | 512    | CLA  | C4-C3-C5    | 3.18  | 120.75      | 115.23   |
| 23  | c     | 507    | CLA  | CAC-C3C-C4C | 3.18  | 128.93      | 124.79   |
| 23  | A     | 405[A] | CLA  | C3B-C4B-NB  | 3.18  | 113.32      | 109.21   |
| 23  | b     | 601    | CLA  | CHD-C4C-NC  | 3.18  | 129.16      | 124.23   |
| 23  | b     | 605    | CLA  | C4-C3-C5    | 3.18  | 120.74      | 115.23   |
| 33  | d     | 414[B] | LHG  | O8-C23-O10  | -3.18 | 115.69      | 123.63   |
| 23  | B     | 612    | CLA  | C1C-C2C-C3C | -3.17 | 103.64      | 106.98   |
| 23  | c     | 502    | CLA  | C1D-CHD-C4C | -3.17 | 119.27      | 126.02   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 602    | CLA  | C1D-CHD-C4C | -3.17 | 119.28      | 126.02   |
| 23  | C     | 514    | CLA  | CBC-CAC-C3C | -3.17 | 103.82      | 112.42   |
| 40  | V     | 201    | HEC  | CBA-CAA-C2A | -3.17 | 107.33      | 112.55   |
| 24  | k     | 101    | BCR  | C24-C23-C22 | -3.17 | 121.55      | 126.23   |
| 23  | C     | 508    | CLA  | C1-C2-C3    | -3.17 | 121.01      | 126.20   |
| 23  | b     | 616    | CLA  | CHD-C4C-NC  | 3.17  | 129.14      | 124.23   |
| 23  | A     | 407    | CLA  | CBC-CAC-C3C | -3.16 | 103.85      | 112.42   |
| 32  | B     | 627    | LMT  | O1'-C1'-C2' | 3.16  | 113.07      | 108.27   |
| 34  | B     | 620    | LMG  | O8-C28-C29  | 3.16  | 121.47      | 111.83   |
| 23  | C     | 503    | CLA  | C1D-CHD-C4C | -3.16 | 119.31      | 126.02   |
| 23  | C     | 502    | CLA  | C3B-C4B-NB  | 3.16  | 113.29      | 109.21   |
| 33  | D     | 408[A] | LHG  | O8-C23-C24  | 3.16  | 121.46      | 111.83   |
| 23  | B     | 604    | CLA  | C4C-C3C-C2C | -3.16 | 102.30      | 106.89   |
| 23  | C     | 507    | CLA  | CHC-C1C-C2C | -3.16 | 118.00      | 126.94   |
| 24  | y     | 101    | BCR  | C10-C11-C12 | -3.15 | 114.06      | 123.20   |
| 24  | a     | 408    | BCR  | C29-C30-C25 | 3.15  | 115.02      | 110.44   |
| 23  | a     | 405[A] | CLA  | CHD-C4C-NC  | 3.15  | 129.12      | 124.23   |
| 28  | a     | 413[B] | PL9  | C42-C43-C44 | -3.15 | 120.42      | 127.62   |
| 23  | C     | 510    | CLA  | O2A-CGA-O1A | -3.15 | 115.75      | 123.63   |
| 23  | a     | 405[B] | CLA  | O2D-CGD-O1D | -3.15 | 117.72      | 123.85   |
| 23  | B     | 613    | CLA  | C4-C3-C5    | 3.15  | 120.69      | 115.23   |
| 23  | d     | 404    | CLA  | C3B-C4B-NB  | 3.15  | 113.28      | 109.21   |
| 24  | B     | 619    | BCR  | C21-C20-C19 | -3.15 | 114.09      | 123.20   |
| 23  | b     | 612    | CLA  | CMC-C2C-C1C | 3.14  | 129.95      | 125.03   |
| 23  | c     | 505    | CLA  | CAC-C3C-C4C | 3.14  | 128.88      | 124.79   |
| 25  | l     | 101    | SQD  | O48-C23-C24 | 3.14  | 121.42      | 111.83   |
| 28  | d     | 406[A] | PL9  | C22-C23-C24 | -3.14 | 120.44      | 127.62   |
| 23  | D     | 404    | CLA  | CAC-C3C-C4C | 3.14  | 128.87      | 124.79   |
| 23  | c     | 514    | CLA  | CAC-C3C-C4C | 3.14  | 128.87      | 124.79   |
| 23  | d     | 402[B] | CLA  | O2D-CGD-O1D | -3.14 | 117.74      | 123.85   |
| 23  | B     | 613    | CLA  | O2A-CGA-CBA | 3.14  | 121.39      | 111.83   |
| 23  | D     | 403[A] | CLA  | C1D-CHD-C4C | -3.13 | 119.36      | 126.02   |
| 23  | C     | 513    | CLA  | O2A-CGA-CBA | 3.13  | 121.39      | 111.83   |
| 23  | b     | 601    | CLA  | C1C-C2C-C3C | -3.13 | 103.68      | 106.98   |
| 23  | b     | 605    | CLA  | C4C-C3C-C2C | -3.13 | 102.33      | 106.89   |
| 28  | A     | 413[A] | PL9  | C17-C18-C19 | -3.13 | 120.45      | 127.62   |
| 23  | C     | 513    | CLA  | C1C-C2C-C3C | -3.13 | 103.69      | 106.98   |
| 28  | a     | 413[B] | PL9  | C37-C38-C39 | -3.13 | 120.46      | 127.62   |
| 23  | C     | 506    | CLA  | C3B-C4B-NB  | 3.13  | 113.26      | 109.21   |
| 23  | A     | 405[A] | CLA  | CAC-C3C-C4C | 3.13  | 128.86      | 124.79   |
| 24  | a     | 408    | BCR  | C38-C26-C25 | -3.13 | 121.07      | 124.48   |
| 28  | a     | 413[A] | PL9  | C25-C24-C26 | 3.12  | 120.65      | 115.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 611    | CLA  | C4C-C3C-C2C | -3.12 | 102.34      | 106.89   |
| 23  | C     | 511    | CLA  | CHD-C4C-NC  | 3.12  | 129.08      | 124.23   |
| 23  | B     | 612    | CLA  | C11-C12-C13 | -3.12 | 105.58      | 115.97   |
| 23  | B     | 607    | CLA  | C2A-C1A-CHA | -3.12 | 118.45      | 123.87   |
| 24  | y     | 101    | BCR  | C24-C23-C22 | -3.12 | 121.61      | 126.23   |
| 33  | D     | 407[A] | LHG  | O8-C23-O10  | -3.12 | 115.82      | 123.63   |
| 23  | B     | 613    | CLA  | O2D-CGD-O1D | -3.12 | 117.77      | 123.85   |
| 23  | d     | 404    | CLA  | CAA-C2A-C3A | -3.12 | 104.57      | 113.00   |
| 31  | A     | 416[A] | PHO  | C4-C3-C5    | 3.12  | 120.64      | 115.23   |
| 23  | B     | 613    | CLA  | C4C-C3C-C2C | -3.12 | 102.35      | 106.89   |
| 23  | c     | 502    | CLA  | C3B-C4B-NB  | 3.12  | 113.24      | 109.21   |
| 23  | c     | 509    | CLA  | C4C-C3C-C2C | -3.11 | 102.36      | 106.89   |
| 25  | A     | 411    | SQD  | O48-C23-C24 | 3.11  | 121.33      | 111.83   |
| 28  | D     | 406[B] | PL9  | C17-C18-C19 | -3.11 | 120.50      | 127.62   |
| 23  | c     | 509    | CLA  | CHD-C1D-ND  | -3.11 | 120.42      | 124.80   |
| 23  | B     | 606    | CLA  | CBC-CAC-C3C | -3.11 | 103.98      | 112.42   |
| 23  | c     | 506    | CLA  | C1-C2-C3    | -3.11 | 121.10      | 126.20   |
| 28  | a     | 413[A] | PL9  | C42-C43-C44 | -3.11 | 120.50      | 127.62   |
| 24  | c     | 516    | BCR  | C11-C10-C9  | -3.11 | 122.92      | 127.28   |
| 23  | B     | 613    | CLA  | C1D-CHD-C4C | -3.11 | 119.41      | 126.02   |
| 23  | c     | 513    | CLA  | O2A-CGA-CBA | 3.11  | 121.31      | 111.83   |
| 24  | b     | 618    | BCR  | C37-C22-C21 | -3.11 | 117.78      | 122.82   |
| 24  | B     | 617    | BCR  | C15-C14-C13 | -3.10 | 122.93      | 127.28   |
| 23  | b     | 612    | CLA  | CAC-C3C-C4C | 3.10  | 128.83      | 124.79   |
| 23  | C     | 512    | CLA  | C3B-C4B-NB  | 3.10  | 113.22      | 109.21   |
| 23  | c     | 503    | CLA  | CBC-CAC-C3C | -3.10 | 104.02      | 112.42   |
| 33  | D     | 408[A] | LHG  | O7-C7-C8    | 3.10  | 118.19      | 111.48   |
| 23  | b     | 601    | CLA  | C4C-C3C-C2C | -3.10 | 102.38      | 106.89   |
| 36  | h     | 102    | DGD  | O1G-C1A-C2A | 3.10  | 121.29      | 111.83   |
| 23  | b     | 606    | CLA  | CHC-C1C-C2C | -3.10 | 118.17      | 126.94   |
| 24  | D     | 405    | BCR  | C37-C22-C23 | 3.10  | 122.82      | 118.09   |
| 23  | b     | 602    | CLA  | C2A-C1A-CHA | -3.10 | 118.49      | 123.87   |
| 23  | c     | 512    | CLA  | CHC-C1C-C2C | -3.10 | 118.17      | 126.94   |
| 23  | a     | 405[B] | CLA  | C3B-C4B-NB  | 3.10  | 113.21      | 109.21   |
| 24  | y     | 101    | BCR  | C21-C20-C19 | -3.10 | 114.23      | 123.20   |
| 23  | B     | 606    | CLA  | O2A-CGA-CBA | 3.10  | 121.27      | 111.83   |
| 23  | C     | 509    | CLA  | CHC-C1C-C2C | -3.09 | 118.19      | 126.94   |
| 23  | d     | 402[A] | CLA  | CMA-C3A-C2A | -3.09 | 102.03      | 113.98   |
| 23  | b     | 601    | CLA  | C4-C3-C5    | 3.09  | 120.59      | 115.23   |
| 25  | b     | 620    | SQD  | C3-C4-C5    | 3.09  | 115.83      | 110.23   |
| 32  | A     | 419    | LMT  | O5B-C5B-C4B | 3.09  | 115.26      | 109.70   |
| 23  | b     | 614    | CLA  | CMC-C2C-C1C | 3.09  | 129.86      | 125.03   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 511    | CLA  | O2A-CGA-O1A | -3.09 | 115.91      | 123.63   |
| 23  | A     | 406[B] | CLA  | C3B-C4B-NB  | 3.09  | 113.20      | 109.21   |
| 23  | C     | 512    | CLA  | CMB-C2B-C3B | 3.08  | 130.85      | 124.68   |
| 28  | d     | 406[B] | PL9  | C7-C8-C9    | -3.08 | 121.52      | 126.83   |
| 23  | b     | 607    | CLA  | CBC-CAC-C3C | -3.08 | 104.07      | 112.42   |
| 24  | B     | 619    | BCR  | C38-C26-C25 | -3.08 | 121.12      | 124.48   |
| 38  | f     | 101    | HEM  | CBD-CAD-C3D | -3.08 | 104.02      | 112.53   |
| 23  | A     | 404[A] | CLA  | CMB-C2B-C3B | 3.08  | 130.84      | 124.68   |
| 34  | C     | 521    | LMG  | O1-C1-C2    | 3.08  | 112.95      | 108.27   |
| 23  | a     | 404[A] | CLA  | C4-C3-C5    | 3.08  | 120.57      | 115.23   |
| 23  | a     | 404[B] | CLA  | C4C-C3C-C2C | -3.08 | 102.41      | 106.89   |
| 23  | b     | 610    | CLA  | C4-C3-C5    | 3.07  | 120.56      | 115.23   |
| 23  | B     | 612    | CLA  | C1D-CHD-C4C | -3.07 | 119.48      | 126.02   |
| 23  | D     | 403[B] | CLA  | O2A-CGA-CBA | 3.07  | 121.21      | 111.83   |
| 23  | b     | 612    | CLA  | O2A-CGA-O1A | -3.07 | 115.94      | 123.63   |
| 23  | B     | 608    | CLA  | CHC-C1C-C2C | -3.07 | 118.24      | 126.94   |
| 23  | b     | 605    | CLA  | O2A-CGA-O1A | -3.07 | 115.95      | 123.63   |
| 23  | B     | 603    | CLA  | C4C-C3C-C2C | -3.07 | 102.42      | 106.89   |
| 23  | c     | 504    | CLA  | C1C-C2C-C3C | -3.07 | 103.75      | 106.98   |
| 23  | b     | 614    | CLA  | O2A-CGA-CBA | 3.07  | 121.19      | 111.83   |
| 23  | b     | 602    | CLA  | CMA-C3A-C4A | -3.07 | 103.53      | 111.77   |
| 23  | C     | 504    | CLA  | CHD-C4C-NC  | 3.06  | 128.98      | 124.23   |
| 23  | D     | 404    | CLA  | C1C-C2C-C3C | -3.06 | 103.76      | 106.98   |
| 23  | B     | 614    | CLA  | O2A-CGA-CBA | 3.06  | 121.17      | 111.83   |
| 32  | B     | 626    | LMT  | C4B-C3B-C2B | 3.06  | 116.21      | 110.83   |
| 23  | b     | 603    | CLA  | O2A-CGA-CBA | 3.06  | 121.17      | 111.83   |
| 36  | C     | 517[A] | DGD  | C2G-O2G-C1B | -3.06 | 110.47      | 117.80   |
| 23  | b     | 610    | CLA  | CAA-C2A-C3A | -3.06 | 104.73      | 113.00   |
| 23  | d     | 403[B] | CLA  | C4C-C3C-C2C | -3.06 | 102.44      | 106.89   |
| 23  | B     | 601    | CLA  | C1-O2A-CGA  | 3.06  | 124.05      | 116.65   |
| 28  | a     | 413[B] | PL9  | C30-C29-C31 | 3.06  | 120.53      | 115.23   |
| 23  | C     | 507    | CLA  | C4-C3-C5    | 3.06  | 120.53      | 115.23   |
| 38  | F     | 102    | HEM  | CHD-C1D-ND  | 3.05  | 127.72      | 124.44   |
| 33  | D     | 408[A] | LHG  | O8-C23-O10  | -3.05 | 115.99      | 123.63   |
| 24  | d     | 405    | BCR  | C16-C17-C18 | -3.05 | 123.00      | 127.28   |
| 33  | a     | 419[A] | LHG  | O7-C7-C8    | 3.05  | 118.08      | 111.48   |
| 23  | a     | 407    | CLA  | CMA-C3A-C2A | -3.05 | 102.18      | 113.98   |
| 40  | v     | 201    | HEC  | C1D-C2D-C3D | -3.05 | 104.87      | 107.00   |
| 36  | c     | 519    | DGD  | O2G-C1B-C2B | 3.05  | 118.08      | 111.48   |
| 23  | B     | 606    | CLA  | CMC-C2C-C1C | 3.05  | 129.80      | 125.03   |
| 34  | c     | 520    | LMG  | O8-C28-C29  | 3.05  | 121.12      | 111.83   |
| 23  | b     | 613    | CLA  | CMB-C2B-C3B | 3.04  | 130.76      | 124.68   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 514    | CLA  | O2A-CGA-CBA | 3.04  | 121.11      | 111.83   |
| 23  | D     | 403[B] | CLA  | C4C-C3C-C2C | -3.04 | 102.47      | 106.89   |
| 23  | c     | 514    | CLA  | CAA-C2A-C3A | -3.04 | 104.78      | 113.00   |
| 23  | B     | 608    | CLA  | C1-C2-C3    | -3.04 | 121.22      | 126.20   |
| 33  | A     | 418[B] | LHG  | O8-C23-O10  | -3.04 | 116.03      | 123.63   |
| 23  | c     | 508    | CLA  | C4-C3-C5    | 3.04  | 120.50      | 115.23   |
| 31  | A     | 416[A] | PHO  | CMC-C2C-C3C | 3.03  | 130.66      | 124.94   |
| 28  | a     | 413[A] | PL9  | C35-C34-C36 | 3.03  | 120.49      | 115.23   |
| 23  | b     | 615    | CLA  | C4C-C3C-C2C | -3.03 | 102.48      | 106.89   |
| 31  | a     | 415[B] | PHO  | C4-C3-C5    | 3.03  | 120.49      | 115.23   |
| 33  | d     | 414[A] | LHG  | O7-C7-C8    | 3.03  | 118.04      | 111.48   |
| 23  | c     | 506    | CLA  | C3B-C4B-NB  | 3.03  | 113.13      | 109.21   |
| 33  | a     | 419[B] | LHG  | O7-C7-C8    | 3.03  | 118.04      | 111.48   |
| 28  | A     | 413[B] | PL9  | C20-C19-C21 | 3.03  | 120.49      | 115.23   |
| 23  | B     | 611    | CLA  | C3B-C4B-NB  | 3.03  | 113.13      | 109.21   |
| 23  | A     | 405[B] | CLA  | CHC-C1C-C2C | -3.03 | 118.36      | 126.94   |
| 23  | A     | 406[A] | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 25  | a     | 409[B] | SQD  | C1-C2-C3    | -3.03 | 103.64      | 110.01   |
| 24  | B     | 619    | BCR  | C7-C8-C9    | -3.03 | 121.76      | 126.23   |
| 23  | b     | 614    | CLA  | CAC-C3C-C4C | 3.03  | 128.73      | 124.79   |
| 33  | E     | 101[A] | LHG  | O8-C23-C24  | 3.03  | 121.06      | 111.83   |
| 23  | c     | 511    | CLA  | CAC-C3C-C4C | 3.03  | 128.73      | 124.79   |
| 23  | B     | 607    | CLA  | CAA-C2A-C3A | -3.02 | 104.83      | 113.00   |
| 34  | c     | 501    | LMG  | C8-O7-C10   | -3.02 | 110.56      | 117.80   |
| 23  | b     | 603    | CLA  | C2A-C1A-CHA | -3.02 | 118.62      | 123.87   |
| 23  | D     | 404    | CLA  | CMC-C2C-C1C | 3.02  | 129.75      | 125.03   |
| 23  | A     | 406[B] | CLA  | O2D-CGD-O1D | -3.02 | 117.97      | 123.85   |
| 33  | E     | 101[B] | LHG  | O8-C23-C24  | 3.02  | 121.03      | 111.83   |
| 23  | c     | 503    | CLA  | CHD-C4C-NC  | 3.02  | 128.91      | 124.23   |
| 23  | a     | 404[B] | CLA  | O2A-CGA-CBA | 3.01  | 121.02      | 111.83   |
| 28  | a     | 413[B] | PL9  | C25-C24-C26 | 3.01  | 120.46      | 115.23   |
| 28  | a     | 413[B] | PL9  | C22-C23-C24 | -3.01 | 120.73      | 127.62   |
| 23  | C     | 511    | CLA  | CHC-C1C-C2C | -3.01 | 118.42      | 126.94   |
| 23  | c     | 502    | CLA  | CHD-C4C-NC  | 3.01  | 128.90      | 124.23   |
| 25  | A     | 411    | SQD  | O8-S-C6     | 3.01  | 111.78      | 105.97   |
| 23  | C     | 513    | CLA  | C4C-C3C-C2C | -3.01 | 102.51      | 106.89   |
| 34  | z     | 101    | LMG  | O8-C28-C29  | 3.01  | 121.01      | 111.83   |
| 23  | D     | 403[A] | CLA  | O2A-CGA-CBA | 3.01  | 121.00      | 111.83   |
| 23  | c     | 508    | CLA  | O2A-CGA-CBA | 3.01  | 121.00      | 111.83   |
| 23  | C     | 511    | CLA  | O2D-CGD-O1D | -3.01 | 118.00      | 123.85   |
| 23  | a     | 404[A] | CLA  | CHC-C1C-C2C | -3.01 | 118.43      | 126.94   |
| 23  | d     | 403[B] | CLA  | C4-C3-C5    | 3.01  | 120.44      | 115.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25  | A     | 409[B] | SQD  | O48-C23-C24 | 3.01  | 121.00      | 111.83   |
| 25  | f     | 102    | SQD  | O5-C5-C4    | 3.01  | 115.11      | 109.70   |
| 23  | c     | 511    | CLA  | CBC-CAC-C3C | -3.00 | 104.27      | 112.42   |
| 23  | B     | 603    | CLA  | CHC-C1C-C2C | -3.00 | 118.43      | 126.94   |
| 35  | b     | 622    | HTG  | O5-C5-C4    | 3.00  | 115.11      | 109.70   |
| 23  | D     | 403[A] | CLA  | CAA-C2A-C3A | -3.00 | 104.89      | 113.00   |
| 23  | B     | 605    | CLA  | O2A-CGA-O1A | -3.00 | 116.12      | 123.63   |
| 23  | d     | 403[A] | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 23  | b     | 608    | CLA  | CHD-C4C-NC  | 3.00  | 128.88      | 124.23   |
| 23  | c     | 510    | CLA  | CMC-C2C-C1C | 3.00  | 129.72      | 125.03   |
| 33  | D     | 408[B] | LHG  | O8-C23-C24  | 3.00  | 120.98      | 111.83   |
| 23  | B     | 614    | CLA  | C3B-C4B-NB  | 3.00  | 113.09      | 109.21   |
| 32  | M     | 101    | LMT  | C3'-C4'-C5' | -3.00 | 104.28      | 110.93   |
| 34  | Z     | 101    | LMG  | C4-C3-C2    | 3.00  | 116.09      | 110.83   |
| 23  | c     | 509    | CLA  | CAA-C2A-C3A | -3.00 | 104.90      | 113.00   |
| 23  | a     | 405[A] | CLA  | C4C-C3C-C2C | -3.00 | 102.53      | 106.89   |
| 23  | A     | 405[B] | CLA  | O2D-CGD-O1D | -3.00 | 118.02      | 123.85   |
| 23  | b     | 605    | CLA  | CHC-C1C-C2C | -2.99 | 118.46      | 126.94   |
| 23  | B     | 604    | CLA  | CAC-C3C-C4C | 2.99  | 128.69      | 124.79   |
| 23  | B     | 602    | CLA  | C3B-C4B-NB  | 2.99  | 113.08      | 109.21   |
| 23  | B     | 607    | CLA  | O2A-CGA-O1A | -2.99 | 116.14      | 123.63   |
| 36  | C     | 519    | DGD  | O1G-C1A-C2A | 2.99  | 120.96      | 111.83   |
| 23  | A     | 404[B] | CLA  | O2A-CGA-CBA | 2.99  | 120.96      | 111.83   |
| 23  | a     | 407    | CLA  | C2A-C1A-CHA | -2.99 | 118.68      | 123.87   |
| 24  | H     | 101    | BCR  | C16-C17-C18 | -2.99 | 123.08      | 127.28   |
| 23  | c     | 511    | CLA  | CHD-C4C-NC  | 2.99  | 128.87      | 124.23   |
| 23  | B     | 611    | CLA  | C2A-C1A-CHA | -2.99 | 118.68      | 123.87   |
| 23  | D     | 403[B] | CLA  | CAA-C2A-C3A | -2.99 | 104.92      | 113.00   |
| 23  | b     | 612    | CLA  | CHD-C4C-NC  | 2.99  | 128.86      | 124.23   |
| 23  | B     | 606    | CLA  | CHD-C4C-NC  | 2.99  | 128.86      | 124.23   |
| 23  | B     | 601    | CLA  | CHD-C4C-NC  | 2.99  | 128.86      | 124.23   |
| 23  | c     | 510    | CLA  | C4C-C3C-C2C | -2.98 | 102.55      | 106.89   |
| 23  | B     | 614    | CLA  | C2A-C1A-CHA | -2.98 | 118.69      | 123.87   |
| 36  | h     | 102    | DGD  | O1G-C1A-O1A | -2.98 | 116.17      | 123.63   |
| 38  | f     | 101    | HEM  | C1B-NB-C4B  | 2.98  | 108.74      | 105.21   |
| 31  | a     | 415[A] | PHO  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 23  | D     | 404    | CLA  | C1-C2-C3    | -2.98 | 121.31      | 126.20   |
| 31  | a     | 415[A] | PHO  | CBA-CAA-C2A | -2.98 | 105.00      | 113.78   |
| 23  | D     | 403[B] | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 23  | a     | 404[A] | CLA  | CMA-C3A-C4A | -2.98 | 103.77      | 111.77   |
| 24  | B     | 619    | BCR  | C29-C30-C25 | 2.98  | 114.76      | 110.44   |
| 23  | c     | 503    | CLA  | CHC-C1C-C2C | -2.98 | 118.51      | 126.94   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 616    | CLA  | CMB-C2B-C3B | 2.97  | 130.63      | 124.68   |
| 24  | D     | 405    | BCR  | C38-C26-C25 | -2.97 | 121.24      | 124.48   |
| 23  | C     | 512    | CLA  | C4-C3-C5    | 2.97  | 120.39      | 115.23   |
| 28  | a     | 413[A] | PL9  | C10-C9-C11  | 2.97  | 120.39      | 115.23   |
| 25  | f     | 102    | SQD  | C4-C3-C2    | -2.97 | 105.61      | 110.83   |
| 25  | a     | 409[A] | SQD  | O47-C7-O49  | -2.97 | 116.75      | 123.70   |
| 23  | d     | 403[A] | CLA  | C4C-C3C-C2C | -2.97 | 102.56      | 106.89   |
| 23  | c     | 505    | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 23  | b     | 603    | CLA  | CMA-C3A-C2A | -2.97 | 102.49      | 113.98   |
| 23  | A     | 404[A] | CLA  | CMC-C2C-C1C | 2.97  | 129.68      | 125.03   |
| 23  | B     | 606    | CLA  | O2A-CGA-O1A | -2.97 | 116.20      | 123.63   |
| 23  | B     | 615    | CLA  | O2D-CGD-O1D | -2.97 | 118.07      | 123.85   |
| 23  | D     | 403[A] | CLA  | O2D-CGD-O1D | -2.97 | 118.07      | 123.85   |
| 28  | A     | 413[A] | PL9  | C20-C19-C21 | 2.97  | 120.38      | 115.23   |
| 23  | A     | 407    | CLA  | CHC-C1C-C2C | -2.97 | 118.53      | 126.94   |
| 40  | v     | 201    | HEC  | CMB-C2B-C3B | 2.97  | 129.31      | 125.82   |
| 23  | B     | 607    | CLA  | C3B-C4B-NB  | 2.97  | 113.05      | 109.21   |
| 23  | b     | 615    | CLA  | C3B-C4B-NB  | 2.97  | 113.05      | 109.21   |
| 23  | C     | 506    | CLA  | CMC-C2C-C1C | 2.97  | 129.67      | 125.03   |
| 23  | B     | 615    | CLA  | CHD-C4C-NC  | 2.97  | 128.83      | 124.23   |
| 23  | b     | 601    | CLA  | C3B-C4B-NB  | 2.97  | 113.05      | 109.21   |
| 23  | b     | 609    | CLA  | C1C-C2C-C3C | -2.96 | 103.86      | 106.98   |
| 23  | C     | 510    | CLA  | CHC-C1C-C2C | -2.96 | 118.55      | 126.94   |
| 23  | c     | 504    | CLA  | C3B-C4B-NB  | 2.96  | 113.04      | 109.21   |
| 23  | A     | 406[B] | CLA  | O2A-CGA-CBA | 2.96  | 120.87      | 111.83   |
| 34  | D     | 412    | LMG  | O7-C10-C11  | 2.96  | 117.89      | 111.48   |
| 23  | C     | 514    | CLA  | CMC-C2C-C1C | 2.96  | 129.66      | 125.03   |
| 23  | c     | 509    | CLA  | O2A-CGA-CBA | 2.96  | 120.86      | 111.83   |
| 25  | l     | 101    | SQD  | C4-C3-C2    | 2.96  | 116.02      | 110.83   |
| 38  | f     | 101    | HEM  | C4D-ND-C1D  | 2.96  | 108.71      | 105.21   |
| 28  | D     | 406[A] | PL9  | C37-C38-C39 | -2.96 | 120.85      | 127.62   |
| 23  | a     | 407    | CLA  | C4C-C3C-C2C | -2.96 | 102.59      | 106.89   |
| 24  | t     | 102    | BCR  | C1-C6-C7    | 2.96  | 123.67      | 115.65   |
| 23  | b     | 611    | CLA  | CMB-C2B-C3B | 2.96  | 130.59      | 124.68   |
| 23  | c     | 514    | CLA  | C4C-C3C-C2C | -2.96 | 102.59      | 106.89   |
| 24  | c     | 515    | BCR  | C28-C27-C26 | -2.95 | 108.79      | 114.06   |
| 23  | B     | 609    | CLA  | C3B-C4B-NB  | 2.95  | 113.03      | 109.21   |
| 24  | C     | 516    | BCR  | C32-C1-C6   | -2.95 | 105.61      | 110.24   |
| 28  | A     | 413[B] | PL9  | C7-C3-C2    | -2.95 | 119.91      | 123.39   |
| 23  | A     | 404[B] | CLA  | C4C-C3C-C2C | -2.95 | 102.59      | 106.89   |
| 23  | a     | 404[B] | CLA  | CHD-C4C-NC  | 2.95  | 128.81      | 124.23   |
| 33  | A     | 418[A] | LHG  | C5-O7-C7    | -2.95 | 110.73      | 117.80   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | A     | 408    | BCR  | C40-C30-C25 | -2.95 | 105.62      | 110.24   |
| 24  | H     | 101    | BCR  | C24-C23-C22 | -2.95 | 121.87      | 126.23   |
| 23  | C     | 514    | CLA  | C1-C2-C3    | -2.95 | 121.36      | 126.20   |
| 23  | c     | 503    | CLA  | CHD-C1D-ND  | -2.95 | 120.65      | 124.80   |
| 23  | a     | 407    | CLA  | C4-C3-C5    | 2.95  | 120.35      | 115.23   |
| 23  | C     | 512    | CLA  | C4C-C3C-C2C | -2.95 | 102.60      | 106.89   |
| 23  | C     | 502    | CLA  | C4-C3-C5    | 2.95  | 120.34      | 115.23   |
| 23  | C     | 502    | CLA  | CHD-C4C-NC  | 2.95  | 128.80      | 124.23   |
| 23  | D     | 404    | CLA  | C3B-C4B-NB  | 2.95  | 113.02      | 109.21   |
| 23  | B     | 608    | CLA  | CAC-C3C-C4C | 2.95  | 128.62      | 124.79   |
| 23  | a     | 405[B] | CLA  | CAC-C3C-C4C | 2.95  | 128.62      | 124.79   |
| 25  | A     | 409[A] | SQD  | O48-C23-C24 | 2.95  | 120.82      | 111.83   |
| 23  | C     | 504    | CLA  | O2A-CGA-O1A | -2.95 | 116.26      | 123.63   |
| 24  | T     | 102    | BCR  | C2-C1-C6    | 2.95  | 114.72      | 110.44   |
| 23  | d     | 402[B] | CLA  | O2A-CGA-CBA | 2.95  | 120.81      | 111.83   |
| 23  | b     | 603    | CLA  | CBC-CAC-C3C | -2.95 | 104.44      | 112.42   |
| 23  | c     | 502    | CLA  | CHC-C1C-C2C | -2.94 | 118.60      | 126.94   |
| 23  | B     | 607    | CLA  | C1-C2-C3    | -2.94 | 121.38      | 126.20   |
| 23  | C     | 511    | CLA  | CMC-C2C-C1C | 2.94  | 129.63      | 125.03   |
| 23  | B     | 615    | CLA  | C11-C10-C8  | -2.94 | 106.19      | 115.97   |
| 23  | a     | 407    | CLA  | CAA-C2A-C3A | -2.94 | 105.05      | 113.00   |
| 23  | B     | 608    | CLA  | CHB-C4A-NA  | 2.94  | 128.65      | 124.40   |
| 23  | B     | 608    | CLA  | C4C-C3C-C2C | -2.94 | 102.61      | 106.89   |
| 23  | A     | 406[A] | CLA  | O2A-CGA-CBA | 2.94  | 120.80      | 111.83   |
| 35  | o     | 301    | HTG  | C1-O5-C5    | 2.94  | 117.84      | 112.56   |
| 23  | b     | 615    | CLA  | C11-C10-C8  | -2.94 | 106.20      | 115.97   |
| 23  | A     | 404[A] | CLA  | C2A-C1A-CHA | -2.94 | 118.77      | 123.87   |
| 23  | D     | 404    | CLA  | C2A-C1A-CHA | -2.93 | 118.77      | 123.87   |
| 23  | B     | 614    | CLA  | CAC-C3C-C4C | 2.93  | 128.61      | 124.79   |
| 23  | c     | 508    | CLA  | CHD-C4C-NC  | 2.93  | 128.78      | 124.23   |
| 23  | b     | 611    | CLA  | CHC-C1C-C2C | -2.93 | 118.63      | 126.94   |
| 23  | b     | 616    | CLA  | CMC-C2C-C1C | 2.93  | 129.62      | 125.03   |
| 24  | c     | 515    | BCR  | C16-C17-C18 | -2.93 | 123.17      | 127.28   |
| 23  | c     | 509    | CLA  | CHC-C1C-C2C | -2.93 | 118.64      | 126.94   |
| 23  | b     | 616    | CLA  | C1C-C2C-C3C | -2.93 | 103.90      | 106.98   |
| 23  | A     | 405[A] | CLA  | CHD-C4C-NC  | 2.93  | 128.78      | 124.23   |
| 28  | a     | 413[A] | PL9  | C22-C23-C24 | -2.93 | 120.92      | 127.62   |
| 23  | A     | 405[A] | CLA  | CMA-C3A-C4A | -2.93 | 103.90      | 111.77   |
| 23  | A     | 406[B] | CLA  | CHD-C4C-NC  | 2.93  | 128.77      | 124.23   |
| 31  | a     | 406[B] | PHO  | O2A-CGA-CBA | 2.92  | 120.75      | 111.83   |
| 23  | A     | 404[A] | CLA  | C4C-C3C-C2C | -2.92 | 102.64      | 106.89   |
| 23  | b     | 601    | CLA  | C1-O2A-CGA  | 2.92  | 123.73      | 116.65   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 33  | L     | 101[A] | LHG  | O8-C23-C24  | 2.92  | 120.75      | 111.83   |
| 23  | c     | 510    | CLA  | CHD-C4C-NC  | 2.92  | 128.76      | 124.23   |
| 23  | c     | 511    | CLA  | CMB-C2B-C3B | 2.92  | 130.52      | 124.68   |
| 23  | d     | 404    | CLA  | C4-C3-C5    | 2.92  | 120.30      | 115.23   |
| 23  | a     | 405[B] | CLA  | C4C-C3C-C2C | -2.92 | 102.64      | 106.89   |
| 23  | C     | 505    | CLA  | CMC-C2C-C1C | 2.92  | 129.60      | 125.03   |
| 24  | T     | 102    | BCR  | C21-C20-C19 | -2.92 | 114.75      | 123.20   |
| 38  | f     | 101    | HEM  | CHB-C1B-NB  | 2.92  | 127.99      | 124.37   |
| 23  | D     | 404    | CLA  | O2A-CGA-O1A | -2.91 | 116.34      | 123.63   |
| 23  | A     | 404[B] | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.79   |
| 28  | d     | 406[B] | PL9  | C15-C14-C16 | 2.91  | 120.28      | 115.23   |
| 25  | f     | 102    | SQD  | O48-C23-C24 | 2.91  | 120.71      | 111.83   |
| 36  | c     | 518[B] | DGD  | C2G-O2G-C1B | -2.91 | 110.84      | 117.80   |
| 23  | d     | 403[A] | CLA  | CHC-C1C-C2C | -2.91 | 118.71      | 126.94   |
| 23  | A     | 406[A] | CLA  | CHD-C4C-NC  | 2.90  | 128.73      | 124.23   |
| 23  | b     | 605    | CLA  | C3B-C4B-NB  | 2.90  | 112.96      | 109.21   |
| 23  | C     | 502    | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.89   |
| 23  | A     | 406[A] | CLA  | CMC-C2C-C1C | 2.90  | 129.57      | 125.03   |
| 23  | b     | 603    | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.89   |
| 23  | a     | 407    | CLA  | CHD-C4C-NC  | 2.90  | 128.73      | 124.23   |
| 28  | d     | 406[A] | PL9  | C10-C9-C11  | 2.90  | 120.27      | 115.23   |
| 23  | A     | 406[B] | CLA  | C2A-C1A-CHA | -2.90 | 118.83      | 123.87   |
| 23  | d     | 402[B] | CLA  | CHC-C1C-C2C | -2.90 | 118.73      | 126.94   |
| 23  | b     | 615    | CLA  | CHD-C4C-NC  | 2.90  | 128.73      | 124.23   |
| 23  | a     | 404[A] | CLA  | CMC-C2C-C1C | 2.90  | 129.56      | 125.03   |
| 23  | C     | 508    | CLA  | CHC-C1C-C2C | -2.90 | 118.73      | 126.94   |
| 31  | D     | 401[A] | PHO  | C1-C2-C3    | -2.90 | 121.45      | 126.20   |
| 23  | b     | 606    | CLA  | CAA-C2A-C3A | -2.90 | 105.17      | 113.00   |
| 23  | b     | 614    | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.89   |
| 23  | B     | 612    | CLA  | C1-C2-C3    | -2.90 | 121.45      | 126.20   |
| 24  | t     | 102    | BCR  | C7-C6-C5    | -2.90 | 114.88      | 121.56   |
| 23  | b     | 604    | CLA  | C4C-C3C-C2C | -2.89 | 102.68      | 106.89   |
| 23  | B     | 610    | CLA  | C3B-C4B-NB  | 2.89  | 112.95      | 109.21   |
| 23  | B     | 609    | CLA  | C4C-C3C-C2C | -2.89 | 102.68      | 106.89   |
| 23  | B     | 608    | CLA  | CMA-C3A-C4A | -2.89 | 104.00      | 111.77   |
| 23  | b     | 607    | CLA  | CAA-C2A-C3A | -2.89 | 105.18      | 113.00   |
| 23  | B     | 602    | CLA  | CAC-C3C-C4C | 2.89  | 128.55      | 124.79   |
| 31  | A     | 416[A] | PHO  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 32  | B     | 626    | LMT  | C2'-C3'-C4' | 2.89  | 116.24      | 109.68   |
| 23  | C     | 512    | CLA  | CMC-C2C-C1C | 2.89  | 129.55      | 125.03   |
| 23  | b     | 616    | CLA  | C3B-C4B-NB  | 2.89  | 112.94      | 109.21   |
| 31  | D     | 401[B] | PHO  | C1-C2-C3    | -2.89 | 121.47      | 126.20   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 407    | CLA  | O2A-CGA-CBA | 2.89  | 120.63      | 111.83   |
| 36  | c     | 519    | DGD  | O3G-C1D-C2D | -2.88 | 103.90      | 108.27   |
| 31  | A     | 416[B] | PHO  | C4-C3-C5    | 2.88  | 120.23      | 115.23   |
| 23  | B     | 604    | CLA  | CHC-C1C-C2C | -2.88 | 118.78      | 126.94   |
| 24  | d     | 405    | BCR  | C10-C11-C12 | -2.88 | 114.85      | 123.20   |
| 36  | C     | 517[A] | DGD  | O6D-C1D-O3G | -2.88 | 103.24      | 110.04   |
| 23  | a     | 405[B] | CLA  | CAA-C2A-C3A | -2.88 | 105.21      | 113.00   |
| 33  | d     | 407[A] | LHG  | O7-C7-C8    | 2.88  | 117.71      | 111.48   |
| 23  | D     | 403[B] | CLA  | CHC-C1C-C2C | -2.88 | 118.78      | 126.94   |
| 28  | d     | 406[B] | PL9  | C27-C28-C29 | -2.88 | 121.03      | 127.62   |
| 24  | C     | 516    | BCR  | C33-C5-C6   | -2.88 | 121.34      | 124.48   |
| 23  | C     | 512    | CLA  | C1-O2A-CGA  | 2.88  | 123.62      | 116.65   |
| 31  | a     | 415[A] | PHO  | C4A-C3A-C2A | -2.88 | 100.10      | 102.84   |
| 36  | c     | 517[B] | DGD  | O3G-C3G-C2G | -2.88 | 103.82      | 110.82   |
| 23  | B     | 602    | CLA  | C11-C12-C13 | -2.88 | 106.41      | 115.97   |
| 34  | c     | 520    | LMG  | C8-O7-C10   | -2.88 | 110.91      | 117.80   |
| 23  | a     | 404[A] | CLA  | CAC-C3C-C4C | 2.88  | 128.53      | 124.79   |
| 23  | C     | 514    | CLA  | CHD-C4C-NC  | 2.87  | 128.69      | 124.23   |
| 23  | d     | 404    | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 23  | c     | 505    | CLA  | CMC-C2C-C1C | 2.87  | 129.53      | 125.03   |
| 23  | C     | 511    | CLA  | CAC-C3C-C4C | 2.87  | 128.53      | 124.79   |
| 23  | a     | 407    | CLA  | CBC-CAC-C3C | -2.87 | 104.63      | 112.42   |
| 23  | d     | 402[A] | CLA  | CHC-C1C-C2C | -2.87 | 118.81      | 126.94   |
| 25  | a     | 409[B] | SQD  | C44-O6-C1   | -2.87 | 107.64      | 113.80   |
| 23  | c     | 505    | CLA  | CHC-C1C-C2C | -2.87 | 118.82      | 126.94   |
| 23  | d     | 402[A] | CLA  | O2A-CGA-CBA | 2.87  | 120.58      | 111.83   |
| 23  | c     | 513    | CLA  | C3B-C4B-NB  | 2.87  | 112.92      | 109.21   |
| 28  | D     | 406[A] | PL9  | C10-C9-C11  | 2.87  | 120.20      | 115.23   |
| 23  | b     | 607    | CLA  | CHC-C1C-C2C | -2.86 | 118.83      | 126.94   |
| 24  | D     | 405    | BCR  | C31-C1-C6   | -2.86 | 105.75      | 110.24   |
| 23  | b     | 613    | CLA  | CHD-C4C-NC  | 2.86  | 128.67      | 124.23   |
| 23  | B     | 601    | CLA  | C1C-C2C-C3C | -2.86 | 103.97      | 106.98   |
| 23  | B     | 601    | CLA  | CAC-C3C-C4C | 2.86  | 128.51      | 124.79   |
| 23  | d     | 403[B] | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 23  | C     | 502    | CLA  | C1-C2-C3    | -2.86 | 121.51      | 126.20   |
| 23  | c     | 503    | CLA  | C1-C2-C3    | -2.86 | 121.51      | 126.20   |
| 23  | B     | 613    | CLA  | CMB-C2B-C3B | 2.86  | 130.39      | 124.68   |
| 23  | C     | 511    | CLA  | O2A-CGA-CBA | 2.86  | 120.55      | 111.83   |
| 23  | A     | 404[B] | CLA  | C2A-C1A-CHA | -2.86 | 118.91      | 123.87   |
| 28  | D     | 406[A] | PL9  | C53-C6-C1   | 2.86  | 121.13      | 115.28   |
| 23  | C     | 505    | CLA  | C4C-C3C-C2C | -2.86 | 102.73      | 106.89   |
| 23  | c     | 503    | CLA  | CMC-C2C-C1C | 2.86  | 129.50      | 125.03   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31  | a     | 406[B] | PHO  | C1A-C2A-C3A | -2.85 | 100.12      | 102.84   |
| 33  | d     | 407[B] | LHG  | O8-C23-C24  | 2.85  | 120.54      | 111.83   |
| 23  | a     | 405[A] | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 23  | b     | 610    | CLA  | CMC-C2C-C1C | 2.85  | 129.49      | 125.03   |
| 23  | c     | 509    | CLA  | C4-C3-C5    | 2.85  | 120.18      | 115.23   |
| 23  | C     | 506    | CLA  | CHC-C1C-C2C | -2.85 | 118.87      | 126.94   |
| 23  | A     | 405[B] | CLA  | CHD-C4C-NC  | 2.85  | 128.65      | 124.23   |
| 23  | D     | 403[A] | CLA  | C4-C3-C5    | 2.85  | 120.17      | 115.23   |
| 23  | c     | 508    | CLA  | C1D-CHD-C4C | -2.85 | 119.97      | 126.02   |
| 28  | d     | 406[A] | PL9  | C27-C28-C29 | -2.85 | 121.11      | 127.62   |
| 23  | b     | 606    | CLA  | C1-O2A-CGA  | 2.84  | 123.54      | 116.65   |
| 23  | C     | 502    | CLA  | CMC-C2C-C1C | 2.84  | 129.48      | 125.03   |
| 23  | B     | 616    | CLA  | CHC-C1C-C2C | -2.84 | 118.89      | 126.94   |
| 23  | b     | 616    | CLA  | CBC-CAC-C3C | -2.84 | 104.72      | 112.42   |
| 23  | B     | 612    | CLA  | C3B-C4B-NB  | 2.84  | 112.88      | 109.21   |
| 23  | b     | 613    | CLA  | CHC-C1C-C2C | -2.84 | 118.90      | 126.94   |
| 23  | A     | 406[B] | CLA  | CHC-C1C-C2C | -2.84 | 118.90      | 126.94   |
| 23  | c     | 510    | CLA  | C4-C3-C5    | 2.84  | 120.15      | 115.23   |
| 23  | B     | 616    | CLA  | CHD-C1D-ND  | -2.84 | 120.81      | 124.80   |
| 23  | c     | 513    | CLA  | CHC-C1C-C2C | -2.84 | 118.91      | 126.94   |
| 23  | C     | 502    | CLA  | CHC-C1C-C2C | -2.84 | 118.91      | 126.94   |
| 23  | A     | 404[A] | CLA  | CHC-C1C-C2C | -2.83 | 118.92      | 126.94   |
| 23  | B     | 609    | CLA  | CHD-C4C-NC  | 2.83  | 128.62      | 124.23   |
| 23  | b     | 609    | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 31  | D     | 401[A] | PHO  | CMC-C2C-C3C | 2.83  | 130.28      | 124.94   |
| 23  | A     | 404[A] | CLA  | CMA-C3A-C2A | -2.83 | 103.05      | 113.98   |
| 24  | c     | 516    | BCR  | C21-C20-C19 | -2.83 | 115.01      | 123.20   |
| 24  | d     | 405    | BCR  | C37-C22-C23 | 2.83  | 122.41      | 118.09   |
| 25  | X     | 101    | SQD  | O47-C7-O49  | -2.83 | 117.10      | 123.70   |
| 24  | a     | 408    | BCR  | C40-C30-C25 | -2.82 | 105.81      | 110.24   |
| 23  | C     | 512    | CLA  | CAC-C3C-C4C | 2.82  | 128.47      | 124.79   |
| 32  | b     | 627    | LMT  | C3'-C4'-C5' | -2.82 | 104.67      | 110.93   |
| 28  | d     | 406[B] | PL9  | C37-C38-C39 | -2.82 | 121.16      | 127.62   |
| 23  | B     | 603    | CLA  | C2A-C1A-CHA | -2.82 | 118.97      | 123.87   |
| 23  | B     | 607    | CLA  | C4C-C3C-C2C | -2.82 | 102.79      | 106.89   |
| 23  | B     | 605    | CLA  | CMC-C2C-C1C | 2.82  | 129.44      | 125.03   |
| 23  | b     | 603    | CLA  | CHD-C4C-NC  | 2.82  | 128.60      | 124.23   |
| 33  | d     | 407[B] | LHG  | C5-O7-C7    | -2.82 | 111.06      | 117.80   |
| 28  | a     | 413[B] | PL9  | C35-C34-C36 | 2.82  | 120.12      | 115.23   |
| 23  | c     | 506    | CLA  | CHC-C1C-C2C | -2.82 | 118.96      | 126.94   |
| 23  | A     | 404[B] | CLA  | CMB-C2B-C3B | 2.82  | 130.31      | 124.68   |
| 23  | b     | 612    | CLA  | C2A-C1A-CHA | -2.81 | 118.98      | 123.87   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 28  | A     | 413[B] | PL9  | C35-C34-C36 | 2.81  | 120.11      | 115.23   |
| 23  | A     | 405[A] | CLA  | CHC-C1C-C2C | -2.81 | 118.97      | 126.94   |
| 24  | k     | 101    | BCR  | C2-C1-C6    | 2.81  | 114.53      | 110.44   |
| 31  | a     | 415[A] | PHO  | CMB-C2B-C3B | 2.81  | 130.30      | 124.68   |
| 25  | l     | 101    | SQD  | O48-C23-O10 | -2.81 | 116.59      | 123.63   |
| 23  | A     | 406[B] | CLA  | CAA-C2A-C3A | -2.81 | 105.40      | 113.00   |
| 31  | D     | 401[A] | PHO  | O1D-CGD-CBD | -2.81 | 120.46      | 124.72   |
| 31  | D     | 401[B] | PHO  | CMA-C3A-C4A | -2.81 | 108.55      | 114.61   |
| 23  | A     | 406[A] | CLA  | C4C-C3C-C2C | -2.81 | 102.80      | 106.89   |
| 23  | A     | 407    | CLA  | CAC-C3C-C4C | 2.81  | 128.45      | 124.79   |
| 23  | a     | 405[A] | CLA  | CHC-C1C-C2C | -2.81 | 118.98      | 126.94   |
| 23  | C     | 514    | CLA  | O2A-CGA-CBA | 2.81  | 120.40      | 111.83   |
| 23  | c     | 512    | CLA  | O2A-CGA-CBA | 2.81  | 120.40      | 111.83   |
| 23  | b     | 614    | CLA  | CBC-CAC-C3C | -2.81 | 104.81      | 112.42   |
| 24  | T     | 102    | BCR  | C15-C14-C13 | 2.80  | 131.21      | 127.28   |
| 23  | a     | 404[B] | CLA  | C1-C2-C3    | -2.80 | 121.60      | 126.20   |
| 31  | A     | 416[B] | PHO  | CED-O2D-CGD | 2.80  | 122.27      | 115.92   |
| 23  | c     | 502    | CLA  | C4C-C3C-C2C | -2.80 | 102.81      | 106.89   |
| 23  | B     | 608    | CLA  | O2A-CGA-O1A | -2.80 | 116.62      | 123.63   |
| 23  | a     | 404[B] | CLA  | C2A-C1A-CHA | -2.80 | 119.01      | 123.87   |
| 23  | a     | 405[A] | CLA  | O2A-CGA-O1A | -2.80 | 116.62      | 123.63   |
| 23  | c     | 511    | CLA  | CHC-C1C-C2C | -2.80 | 119.01      | 126.94   |
| 33  | A     | 418[B] | LHG  | O8-C23-C24  | 2.80  | 120.36      | 111.83   |
| 23  | B     | 615    | CLA  | C4C-C3C-C2C | -2.80 | 102.82      | 106.89   |
| 23  | C     | 503    | CLA  | C3B-C4B-NB  | 2.80  | 112.83      | 109.21   |
| 23  | b     | 602    | CLA  | CHD-C4C-NC  | 2.80  | 128.57      | 124.23   |
| 23  | A     | 405[B] | CLA  | CBC-CAC-C3C | -2.79 | 104.84      | 112.42   |
| 32  | T     | 101    | LMT  | C1'-O5'-C5' | -2.79 | 108.26      | 113.72   |
| 23  | B     | 609    | CLA  | O2A-CGA-CBA | 2.79  | 120.34      | 111.83   |
| 23  | b     | 607    | CLA  | C4-C3-C5    | 2.79  | 120.07      | 115.23   |
| 24  | c     | 516    | BCR  | C37-C22-C23 | 2.79  | 122.35      | 118.09   |
| 23  | b     | 615    | CLA  | CHC-C1C-C2C | -2.79 | 119.04      | 126.94   |
| 23  | A     | 405[A] | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 24  | B     | 619    | BCR  | C24-C23-C22 | -2.79 | 122.11      | 126.23   |
| 23  | c     | 505    | CLA  | CMB-C2B-C3B | 2.79  | 130.25      | 124.68   |
| 28  | A     | 413[B] | PL9  | C10-C9-C11  | 2.78  | 120.06      | 115.23   |
| 23  | b     | 603    | CLA  | O2A-CGA-O1A | -2.78 | 116.66      | 123.63   |
| 33  | b     | 629[A] | LHG  | O8-C23-C24  | 2.78  | 120.32      | 111.83   |
| 23  | b     | 613    | CLA  | CMC-C2C-C1C | 2.78  | 129.38      | 125.03   |
| 23  | b     | 609    | CLA  | CHD-C4C-NC  | 2.78  | 128.55      | 124.23   |
| 23  | c     | 511    | CLA  | O2A-CGA-O1A | -2.78 | 116.67      | 123.63   |
| 24  | B     | 618    | BCR  | C2-C1-C6    | 2.78  | 114.48      | 110.44   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 604    | CLA  | O2A-CGA-O1A | -2.78 | 116.67      | 123.63   |
| 24  | b     | 617    | BCR  | C24-C23-C22 | -2.78 | 122.12      | 126.23   |
| 23  | C     | 503    | CLA  | CHC-C1C-C2C | -2.78 | 119.07      | 126.94   |
| 24  | B     | 618    | BCR  | C38-C26-C25 | -2.78 | 121.45      | 124.48   |
| 23  | c     | 510    | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 23  | c     | 504    | CLA  | CMC-C2C-C1C | 2.78  | 129.37      | 125.03   |
| 23  | B     | 604    | CLA  | CMC-C2C-C1C | 2.78  | 129.37      | 125.03   |
| 24  | A     | 408    | BCR  | C33-C5-C6   | -2.78 | 121.45      | 124.48   |
| 23  | c     | 507    | CLA  | C4C-C3C-C2C | -2.78 | 102.85      | 106.89   |
| 28  | d     | 406[B] | PL9  | C53-C6-C1   | 2.77  | 120.96      | 115.28   |
| 34  | c     | 521    | LMG  | O8-C28-C29  | 2.77  | 120.29      | 111.83   |
| 23  | B     | 606    | CLA  | C2A-C1A-CHA | -2.77 | 119.05      | 123.87   |
| 33  | D     | 408[B] | LHG  | O8-C23-O10  | -2.77 | 116.69      | 123.63   |
| 23  | b     | 614    | CLA  | CHC-C1C-C2C | -2.77 | 119.09      | 126.94   |
| 23  | B     | 607    | CLA  | CMC-C2C-C1C | 2.77  | 129.37      | 125.03   |
| 23  | C     | 505    | CLA  | CHC-C1C-C2C | -2.77 | 119.09      | 126.94   |
| 23  | B     | 614    | CLA  | CMB-C2B-C3B | 2.77  | 130.22      | 124.68   |
| 23  | b     | 602    | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 23  | d     | 404    | CLA  | O2A-CGA-CBA | 2.77  | 120.28      | 111.83   |
| 23  | C     | 510    | CLA  | CMC-C2C-C1C | 2.77  | 129.36      | 125.03   |
| 32  | T     | 101    | LMT  | C3'-C4'-C5' | -2.77 | 104.80      | 110.93   |
| 23  | c     | 503    | CLA  | O2A-CGA-CBA | 2.77  | 120.27      | 111.83   |
| 28  | D     | 406[B] | PL9  | C20-C19-C21 | 2.76  | 120.03      | 115.23   |
| 23  | B     | 609    | CLA  | CHC-C1C-C2C | -2.76 | 119.11      | 126.94   |
| 23  | C     | 505    | CLA  | O2A-CGA-O1A | -2.76 | 116.71      | 123.63   |
| 23  | C     | 504    | CLA  | C1C-C2C-C3C | -2.76 | 104.07      | 106.98   |
| 33  | a     | 419[A] | LHG  | O8-C23-C24  | 2.76  | 120.25      | 111.83   |
| 40  | V     | 201    | HEC  | CMB-C2B-C3B | 2.76  | 129.07      | 125.82   |
| 33  | a     | 419[B] | LHG  | O8-C23-C24  | 2.76  | 120.25      | 111.83   |
| 23  | b     | 612    | CLA  | CHC-C1C-C2C | -2.76 | 119.12      | 126.94   |
| 23  | C     | 514    | CLA  | O2D-CGD-O1D | -2.76 | 118.48      | 123.85   |
| 24  | B     | 619    | BCR  | C31-C1-C6   | -2.76 | 105.92      | 110.24   |
| 28  | A     | 413[A] | PL9  | C35-C34-C36 | 2.76  | 120.01      | 115.23   |
| 36  | H     | 102    | DGD  | O1G-C1A-C2A | 2.76  | 120.24      | 111.83   |
| 23  | B     | 604    | CLA  | C6-C5-C3    | -2.76 | 106.75      | 113.47   |
| 23  | c     | 505    | CLA  | C4C-C3C-C2C | -2.75 | 102.88      | 106.89   |
| 23  | A     | 405[A] | CLA  | CMA-C3A-C2A | -2.75 | 103.33      | 113.98   |
| 33  | D     | 407[A] | LHG  | O7-C7-C8    | 2.75  | 117.44      | 111.48   |
| 23  | b     | 605    | CLA  | C1-C2-C3    | -2.75 | 121.69      | 126.20   |
| 28  | D     | 406[A] | PL9  | C51-C49-C50 | 2.75  | 120.92      | 114.59   |
| 24  | Y     | 101    | BCR  | C10-C11-C12 | -2.75 | 115.24      | 123.20   |
| 31  | A     | 416[B] | PHO  | C6-C5-C3    | -2.75 | 106.78      | 113.47   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 406[A] | CLA  | C4-C3-C5    | 2.75  | 119.99      | 115.23   |
| 36  | c     | 519    | DGD  | O1G-C1A-C2A | 2.75  | 120.21      | 111.83   |
| 28  | A     | 413[A] | PL9  | C30-C29-C31 | 2.75  | 119.99      | 115.23   |
| 23  | c     | 514    | CLA  | C1-C2-C3    | -2.74 | 121.70      | 126.20   |
| 24  | B     | 617    | BCR  | C37-C22-C23 | 2.74  | 122.28      | 118.09   |
| 33  | D     | 407[A] | LHG  | O8-C23-C24  | 2.74  | 120.20      | 111.83   |
| 28  | A     | 413[B] | PL9  | C42-C43-C44 | -2.74 | 121.34      | 127.62   |
| 24  | k     | 101    | BCR  | C36-C18-C19 | 2.74  | 122.28      | 118.09   |
| 23  | c     | 505    | CLA  | O2A-CGA-O1A | -2.74 | 116.78      | 123.63   |
| 23  | C     | 507    | CLA  | C2A-C1A-CHA | -2.74 | 119.11      | 123.87   |
| 23  | b     | 609    | CLA  | O2A-CGA-CBA | 2.74  | 120.18      | 111.83   |
| 23  | A     | 407    | CLA  | CHD-C4C-NC  | 2.74  | 128.47      | 124.23   |
| 23  | C     | 512    | CLA  | C1-C2-C3    | -2.74 | 121.72      | 126.20   |
| 28  | D     | 406[B] | PL9  | C10-C9-C11  | 2.74  | 119.98      | 115.23   |
| 26  | b     | 628    | GOL  | C3-C2-C1    | -2.73 | 101.77      | 111.80   |
| 33  | d     | 408[B] | LHG  | O8-C23-C24  | 2.73  | 120.17      | 111.83   |
| 31  | D     | 401[B] | PHO  | O2A-CGA-CBA | 2.73  | 120.17      | 111.83   |
| 33  | d     | 407[B] | LHG  | O8-C23-O10  | -2.73 | 116.79      | 123.63   |
| 23  | d     | 404    | CLA  | CHD-C4C-NC  | 2.73  | 128.47      | 124.23   |
| 24  | B     | 618    | BCR  | C7-C8-C9    | -2.73 | 122.19      | 126.23   |
| 24  | b     | 618    | BCR  | C37-C22-C23 | 2.73  | 122.26      | 118.09   |
| 33  | L     | 101[A] | LHG  | O8-C23-O10  | -2.73 | 116.80      | 123.63   |
| 23  | B     | 612    | CLA  | O2A-CGA-CBA | 2.73  | 120.16      | 111.83   |
| 32  | B     | 629    | LMT  | C3'-C4'-C5' | -2.73 | 104.88      | 110.93   |
| 23  | C     | 512    | CLA  | CHD-C4C-NC  | 2.73  | 128.46      | 124.23   |
| 23  | b     | 610    | CLA  | CAA-CBA-CGA | -2.73 | 105.46      | 113.21   |
| 23  | b     | 604    | CLA  | CHC-C1C-C2C | -2.73 | 119.22      | 126.94   |
| 24  | k     | 101    | BCR  | C15-C14-C13 | -2.73 | 123.45      | 127.28   |
| 23  | B     | 611    | CLA  | C1C-C2C-C3C | -2.72 | 104.11      | 106.98   |
| 28  | d     | 406[A] | PL9  | C36-C34-C33 | -2.72 | 115.05      | 121.17   |
| 23  | B     | 615    | CLA  | C3B-C4B-NB  | 2.72  | 112.73      | 109.21   |
| 24  | K     | 102    | BCR  | C2-C1-C6    | 2.72  | 114.40      | 110.44   |
| 23  | A     | 404[B] | CLA  | CHD-C4C-NC  | 2.72  | 128.46      | 124.23   |
| 23  | c     | 504    | CLA  | CAC-C3C-C4C | 2.72  | 128.33      | 124.79   |
| 23  | C     | 514    | CLA  | C2A-C1A-CHA | -2.72 | 119.14      | 123.87   |
| 28  | D     | 406[B] | PL9  | C53-C6-C1   | 2.72  | 120.86      | 115.28   |
| 23  | B     | 616    | CLA  | CHD-C4C-NC  | 2.72  | 128.45      | 124.23   |
| 23  | B     | 605    | CLA  | CED-O2D-CGD | 2.72  | 122.09      | 115.92   |
| 23  | b     | 602    | CLA  | C11-C12-C13 | -2.72 | 106.92      | 115.97   |
| 23  | D     | 404    | CLA  | CHD-C4C-NC  | 2.72  | 128.45      | 124.23   |
| 24  | c     | 516    | BCR  | C32-C1-C6   | -2.72 | 105.98      | 110.24   |
| 23  | a     | 404[A] | CLA  | C2A-C1A-CHA | -2.72 | 119.15      | 123.87   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 28  | A     | 413[B] | PL9  | C30-C29-C31 | 2.72  | 119.94      | 115.23   |
| 23  | C     | 503    | CLA  | C2A-C1A-CHA | -2.72 | 119.15      | 123.87   |
| 23  | c     | 506    | CLA  | O2A-CGA-CBA | 2.71  | 120.11      | 111.83   |
| 23  | b     | 603    | CLA  | CHC-C1C-C2C | -2.71 | 119.25      | 126.94   |
| 23  | b     | 615    | CLA  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 23  | a     | 405[A] | CLA  | O2A-CGA-CBA | 2.71  | 120.10      | 111.83   |
| 23  | b     | 614    | CLA  | CHD-C4C-NC  | 2.71  | 128.43      | 124.23   |
| 28  | d     | 406[B] | PL9  | C12-C13-C14 | -2.71 | 121.42      | 127.62   |
| 24  | C     | 515    | BCR  | C16-C17-C18 | -2.71 | 123.48      | 127.28   |
| 23  | b     | 611    | CLA  | O2A-CGA-O1A | -2.71 | 116.85      | 123.63   |
| 33  | d     | 408[A] | LHG  | O8-C23-C24  | 2.71  | 120.09      | 111.83   |
| 23  | b     | 613    | CLA  | CAC-C3C-C4C | 2.71  | 128.31      | 124.79   |
| 23  | C     | 514    | CLA  | C4C-C3C-C2C | -2.71 | 102.95      | 106.89   |
| 28  | D     | 406[A] | PL9  | C2-C1-C6    | 2.71  | 122.22      | 119.00   |
| 23  | C     | 503    | CLA  | C4C-C3C-C2C | -2.71 | 102.95      | 106.89   |
| 34  | C     | 520    | LMG  | O8-C28-O10  | -2.71 | 116.86      | 123.63   |
| 32  | M     | 101    | LMT  | C1'-O5'-C5' | -2.71 | 108.44      | 113.72   |
| 23  | c     | 514    | CLA  | CHC-C1C-C2C | -2.71 | 119.28      | 126.94   |
| 28  | a     | 413[A] | PL9  | C53-C6-C1   | 2.71  | 120.82      | 115.28   |
| 24  | h     | 101    | BCR  | C33-C5-C6   | -2.71 | 121.53      | 124.48   |
| 33  | b     | 629[B] | LHG  | O8-C23-C24  | 2.70  | 120.08      | 111.83   |
| 23  | B     | 605    | CLA  | C3B-C4B-NB  | 2.70  | 112.70      | 109.21   |
| 23  | c     | 511    | CLA  | O2A-CGA-CBA | 2.70  | 120.08      | 111.83   |
| 23  | C     | 503    | CLA  | CHD-C4C-NC  | 2.70  | 128.42      | 124.23   |
| 23  | b     | 606    | CLA  | C4C-C3C-C2C | -2.70 | 102.96      | 106.89   |
| 23  | B     | 609    | CLA  | C16-C15-C13 | -2.70 | 106.98      | 115.97   |
| 23  | C     | 502    | CLA  | O2A-CGA-O1A | -2.70 | 116.87      | 123.63   |
| 25  | a     | 409[B] | SQD  | O47-C7-O49  | -2.70 | 117.39      | 123.70   |
| 24  | d     | 405    | BCR  | C40-C30-C39 | 2.70  | 116.37      | 108.63   |
| 35  | B     | 623    | HTG  | C3-C4-C5    | 2.70  | 115.13      | 110.23   |
| 23  | C     | 513    | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 25  | X     | 101    | SQD  | O48-C23-O10 | -2.70 | 116.88      | 123.63   |
| 25  | A     | 409[B] | SQD  | O7-S-C6     | 2.70  | 110.78      | 106.76   |
| 35  | b     | 622    | HTG  | O5-C1-C2    | 2.70  | 114.03      | 110.32   |
| 23  | B     | 603    | CLA  | CMA-C3A-C2A | -2.70 | 103.55      | 113.98   |
| 23  | D     | 403[A] | CLA  | CAC-C3C-C4C | 2.70  | 128.30      | 124.79   |
| 23  | b     | 611    | CLA  | CHD-C4C-NC  | 2.70  | 128.41      | 124.23   |
| 24  | y     | 101    | BCR  | C16-C17-C18 | -2.70 | 123.50      | 127.28   |
| 31  | D     | 401[A] | PHO  | O2A-CGA-CBA | 2.69  | 120.05      | 111.83   |
| 28  | a     | 413[B] | PL9  | C10-C9-C11  | 2.69  | 119.91      | 115.23   |
| 23  | B     | 610    | CLA  | CHC-C1C-C2C | -2.69 | 119.31      | 126.94   |
| 28  | A     | 413[A] | PL9  | C2-C1-C6    | 2.69  | 122.20      | 119.00   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 601    | CLA  | O2A-CGA-CBA | 2.69  | 120.04      | 111.83   |
| 23  | d     | 404    | CLA  | CHC-C1C-C2C | -2.69 | 119.32      | 126.94   |
| 23  | b     | 608    | CLA  | CHC-C1C-C2C | -2.69 | 119.32      | 126.94   |
| 23  | C     | 510    | CLA  | CHD-C4C-NC  | 2.69  | 128.40      | 124.23   |
| 23  | c     | 504    | CLA  | CHD-C4C-NC  | 2.69  | 128.40      | 124.23   |
| 36  | C     | 518[A] | DGD  | O1G-C1A-O1A | -2.69 | 116.90      | 123.63   |
| 28  | a     | 413[B] | PL9  | C40-C39-C41 | 2.69  | 119.89      | 115.23   |
| 35  | b     | 622    | HTG  | C1'-S1-C1   | 2.69  | 106.25      | 100.45   |
| 25  | f     | 102    | SQD  | O7-S-C6     | 2.69  | 110.77      | 106.76   |
| 32  | a     | 416    | LMT  | C3'-C4'-C5' | -2.69 | 104.98      | 110.93   |
| 23  | b     | 616    | CLA  | CAC-C3C-C4C | 2.68  | 128.28      | 124.79   |
| 23  | A     | 404[B] | CLA  | C1-C2-C3    | -2.68 | 121.80      | 126.20   |
| 23  | C     | 511    | CLA  | C2A-C1A-CHA | -2.68 | 119.21      | 123.87   |
| 23  | C     | 503    | CLA  | O2A-CGA-CBA | 2.68  | 120.02      | 111.83   |
| 23  | C     | 504    | CLA  | O2D-CGD-O1D | -2.68 | 118.63      | 123.85   |
| 23  | B     | 602    | CLA  | CHD-C4C-NC  | 2.68  | 128.39      | 124.23   |
| 23  | D     | 404    | CLA  | CMA-C3A-C4A | -2.68 | 104.56      | 111.77   |
| 23  | c     | 513    | CLA  | C4C-C3C-C2C | -2.68 | 102.99      | 106.89   |
| 34  | C     | 501    | LMG  | O6-C1-O1    | -2.68 | 103.71      | 110.04   |
| 23  | b     | 604    | CLA  | C4-C3-C5    | 2.68  | 119.88      | 115.23   |
| 23  | B     | 608    | CLA  | CMB-C2B-C3B | 2.68  | 130.04      | 124.68   |
| 23  | d     | 403[B] | CLA  | CAC-C3C-C4C | 2.68  | 128.27      | 124.79   |
| 23  | D     | 403[A] | CLA  | CHC-C1C-C2C | -2.68 | 119.36      | 126.94   |
| 38  | F     | 102    | HEM  | O2A-CGA-CBA | 2.68  | 122.45      | 114.00   |
| 23  | b     | 608    | CLA  | O2A-CGA-CBA | 2.68  | 119.99      | 111.83   |
| 23  | C     | 508    | CLA  | C3B-C4B-NB  | 2.68  | 112.67      | 109.21   |
| 23  | d     | 403[A] | CLA  | C2A-C1A-CHA | -2.67 | 119.23      | 123.87   |
| 23  | b     | 609    | CLA  | O2A-CGA-O1A | -2.67 | 116.95      | 123.63   |
| 36  | C     | 517[B] | DGD  | C3G-C2G-C1G | -2.67 | 105.56      | 111.78   |
| 23  | B     | 614    | CLA  | CHC-C1C-C2C | -2.67 | 119.38      | 126.94   |
| 23  | B     | 603    | CLA  | C4-C3-C5    | 2.67  | 119.86      | 115.23   |
| 23  | D     | 403[A] | CLA  | C2A-C1A-CHA | -2.67 | 119.24      | 123.87   |
| 23  | d     | 402[A] | CLA  | O2D-CGD-O1D | -2.67 | 118.66      | 123.85   |
| 23  | d     | 404    | CLA  | CAC-C3C-C4C | 2.67  | 128.26      | 124.79   |
| 23  | C     | 507    | CLA  | CHD-C4C-NC  | 2.67  | 128.37      | 124.23   |
| 23  | B     | 601    | CLA  | C3B-C4B-NB  | 2.67  | 112.66      | 109.21   |
| 23  | d     | 402[A] | CLA  | C4C-C3C-C2C | -2.67 | 103.01      | 106.89   |
| 23  | B     | 606    | CLA  | C3B-C4B-NB  | 2.66  | 112.66      | 109.21   |
| 23  | b     | 608    | CLA  | O2A-CGA-O1A | -2.66 | 116.96      | 123.63   |
| 25  | b     | 620    | SQD  | O48-C23-C24 | 2.66  | 119.95      | 111.83   |
| 34  | D     | 412    | LMG  | O8-C28-C29  | 2.66  | 119.95      | 111.83   |
| 24  | B     | 617    | BCR  | C37-C22-C21 | -2.66 | 118.50      | 122.82   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | d     | 403[A] | CLA  | CAA-C2A-C3A | -2.66 | 105.81      | 113.00   |
| 36  | c     | 518[B] | DGD  | O1G-C1A-C2A | 2.66  | 119.95      | 111.83   |
| 23  | c     | 507    | CLA  | CHD-C4C-NC  | 2.66  | 128.36      | 124.23   |
| 23  | A     | 404[B] | CLA  | O2A-CGA-O1A | -2.66 | 116.97      | 123.63   |
| 35  | B     | 623    | HTG  | C1'-S1-C1   | 2.66  | 106.19      | 100.45   |
| 23  | d     | 403[A] | CLA  | CAC-C3C-C4C | 2.66  | 128.25      | 124.79   |
| 23  | d     | 404    | CLA  | C2A-C1A-CHA | -2.66 | 119.25      | 123.87   |
| 24  | Y     | 101    | BCR  | C28-C27-C26 | -2.66 | 109.32      | 114.06   |
| 23  | A     | 406[B] | CLA  | CBC-CAC-C3C | -2.66 | 105.22      | 112.42   |
| 23  | C     | 507    | CLA  | CMB-C2B-C3B | 2.65  | 129.99      | 124.68   |
| 23  | b     | 601    | CLA  | CHC-C1C-C2C | -2.65 | 119.43      | 126.94   |
| 23  | C     | 502    | CLA  | O2A-CGA-CBA | 2.65  | 119.92      | 111.83   |
| 24  | D     | 405    | BCR  | C40-C30-C25 | -2.65 | 106.08      | 110.24   |
| 23  | c     | 512    | CLA  | C4C-C3C-C2C | -2.65 | 103.03      | 106.89   |
| 28  | D     | 406[B] | PL9  | C51-C49-C50 | 2.65  | 120.69      | 114.59   |
| 23  | b     | 610    | CLA  | O2D-CGD-O1D | -2.65 | 118.69      | 123.85   |
| 23  | b     | 609    | CLA  | C7-C6-C5    | -2.65 | 106.20      | 113.26   |
| 23  | A     | 406[A] | CLA  | C1-C2-C3    | -2.65 | 121.86      | 126.20   |
| 36  | h     | 102    | DGD  | O3G-C1D-C2D | 2.65  | 112.29      | 108.27   |
| 23  | b     | 603    | CLA  | CMB-C2B-C3B | 2.65  | 129.97      | 124.68   |
| 24  | c     | 515    | BCR  | C37-C22-C21 | -2.65 | 118.53      | 122.82   |
| 28  | a     | 413[A] | PL9  | C47-C48-C49 | -2.64 | 118.83      | 127.64   |
| 28  | a     | 413[B] | PL9  | C20-C19-C21 | 2.64  | 119.81      | 115.23   |
| 23  | A     | 406[B] | CLA  | C4C-C3C-C2C | -2.64 | 103.05      | 106.89   |
| 23  | c     | 512    | CLA  | CMA-C3A-C4A | 2.64  | 118.87      | 111.77   |
| 23  | a     | 404[B] | CLA  | CAA-C2A-C1A | -2.64 | 103.33      | 111.97   |
| 23  | d     | 402[B] | CLA  | C2A-C1A-CHA | -2.64 | 119.29      | 123.87   |
| 31  | a     | 406[B] | PHO  | O2A-CGA-O1A | -2.64 | 117.03      | 123.63   |
| 23  | c     | 505    | CLA  | CBC-CAC-C3C | -2.64 | 105.28      | 112.42   |
| 36  | C     | 518[B] | DGD  | C2G-O2G-C1B | -2.64 | 111.49      | 117.80   |
| 23  | B     | 609    | CLA  | C1-C2-C3    | -2.63 | 121.89      | 126.20   |
| 23  | b     | 607    | CLA  | CMB-C2B-C3B | 2.63  | 129.94      | 124.68   |
| 32  | A     | 419    | LMT  | O5'-C5'-C6' | 2.63  | 112.96      | 106.44   |
| 23  | C     | 509    | CLA  | CMB-C2B-C3B | 2.63  | 129.94      | 124.68   |
| 23  | D     | 403[B] | CLA  | C2A-C1A-CHA | -2.63 | 119.30      | 123.87   |
| 23  | B     | 611    | CLA  | OBD-CAD-C3D | -2.63 | 122.27      | 128.42   |
| 23  | c     | 502    | CLA  | O2A-CGA-CBA | 2.63  | 119.85      | 111.83   |
| 23  | B     | 612    | CLA  | CHC-C1C-C2C | -2.63 | 119.50      | 126.94   |
| 23  | B     | 611    | CLA  | O2A-CGA-O1A | -2.63 | 117.06      | 123.63   |
| 23  | b     | 601    | CLA  | CMB-C2B-C3B | 2.63  | 129.93      | 124.68   |
| 23  | d     | 402[A] | CLA  | O2A-CGA-O1A | -2.63 | 117.06      | 123.63   |
| 23  | D     | 404    | CLA  | CAA-C2A-C3A | -2.63 | 105.91      | 113.00   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 611    | CLA  | CAC-C3C-C4C | 2.62  | 128.21      | 124.79   |
| 23  | A     | 405[B] | CLA  | C4-C3-C5    | 2.62  | 119.78      | 115.23   |
| 23  | c     | 512    | CLA  | C1-C2-C3    | -2.62 | 121.90      | 126.20   |
| 33  | d     | 408[B] | LHG  | C5-O7-C7    | -2.62 | 111.52      | 117.80   |
| 23  | C     | 511    | CLA  | C4C-C3C-C2C | -2.62 | 103.08      | 106.89   |
| 23  | B     | 606    | CLA  | CHC-C1C-C2C | -2.62 | 119.52      | 126.94   |
| 23  | B     | 607    | CLA  | CHD-C4C-NC  | 2.62  | 128.29      | 124.23   |
| 24  | a     | 408    | BCR  | C7-C8-C9    | -2.62 | 122.36      | 126.23   |
| 23  | B     | 614    | CLA  | CBC-CAC-C3C | -2.61 | 105.33      | 112.42   |
| 24  | b     | 617    | BCR  | C16-C15-C14 | -2.61 | 118.18      | 123.52   |
| 23  | D     | 403[A] | CLA  | O2A-CGA-O1A | -2.61 | 117.10      | 123.63   |
| 28  | A     | 413[B] | PL9  | C12-C13-C14 | -2.61 | 121.65      | 127.62   |
| 23  | b     | 603    | CLA  | C4-C3-C5    | 2.61  | 119.76      | 115.23   |
| 23  | B     | 602    | CLA  | C2A-C1A-CHA | -2.61 | 119.34      | 123.87   |
| 36  | c     | 517[B] | DGD  | C2G-O2G-C1B | -2.61 | 111.55      | 117.80   |
| 23  | B     | 608    | CLA  | C1B-CHB-C4A | -2.61 | 125.06      | 130.04   |
| 23  | B     | 616    | CLA  | C1-O2A-CGA  | 2.61  | 122.96      | 116.65   |
| 23  | C     | 514    | CLA  | CHC-C1C-C2C | -2.61 | 119.56      | 126.94   |
| 23  | A     | 406[A] | CLA  | CMB-C2B-C1B | 2.61  | 132.27      | 128.46   |
| 25  | A     | 409[A] | SQD  | O48-C23-O10 | -2.61 | 117.11      | 123.63   |
| 23  | C     | 502    | CLA  | C1-O2A-CGA  | 2.60  | 122.96      | 116.65   |
| 31  | D     | 401[A] | PHO  | O2A-CGA-O1A | -2.60 | 117.12      | 123.63   |
| 23  | c     | 514    | CLA  | CMC-C2C-C1C | 2.60  | 129.10      | 125.03   |
| 23  | B     | 616    | CLA  | CBC-CAC-C3C | -2.60 | 105.36      | 112.42   |
| 23  | A     | 406[A] | CLA  | CHC-C1C-C2C | -2.60 | 119.57      | 126.94   |
| 23  | d     | 402[A] | CLA  | CAA-CBA-CGA | 2.60  | 120.59      | 113.21   |
| 23  | A     | 405[A] | CLA  | C2A-C1A-CHA | -2.60 | 119.35      | 123.87   |
| 23  | b     | 605    | CLA  | C2A-C1A-CHA | -2.60 | 119.35      | 123.87   |
| 23  | b     | 602    | CLA  | CAC-C3C-C4C | 2.60  | 128.17      | 124.79   |
| 23  | B     | 608    | CLA  | CHD-C4C-NC  | 2.60  | 128.26      | 124.23   |
| 24  | b     | 619    | BCR  | C38-C26-C25 | -2.60 | 121.65      | 124.48   |
| 23  | b     | 608    | CLA  | C4C-C3C-C2C | -2.60 | 103.11      | 106.89   |
| 36  | c     | 518[A] | DGD  | O1G-C1A-C2A | 2.59  | 119.74      | 111.83   |
| 23  | A     | 405[A] | CLA  | C4-C3-C5    | 2.59  | 119.73      | 115.23   |
| 24  | T     | 102    | BCR  | C12-C13-C14 | -2.59 | 114.93      | 119.01   |
| 23  | c     | 508    | CLA  | CMB-C2B-C1B | 2.59  | 132.25      | 128.46   |
| 23  | c     | 509    | CLA  | CHD-C4C-NC  | 2.59  | 128.25      | 124.23   |
| 23  | C     | 508    | CLA  | O2A-CGA-CBA | 2.59  | 119.73      | 111.83   |
| 31  | a     | 406[A] | PHO  | CMB-C2B-C3B | 2.59  | 129.86      | 124.68   |
| 23  | c     | 512    | CLA  | C1-O2A-CGA  | 2.59  | 122.92      | 116.65   |
| 28  | a     | 413[A] | PL9  | C40-C39-C41 | 2.59  | 119.72      | 115.23   |
| 23  | b     | 608    | CLA  | C2A-C1A-CHA | -2.59 | 119.37      | 123.87   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 28  | A     | 413[B] | PL9  | C40-C39-C41 | 2.59  | 119.72      | 115.23   |
| 36  | H     | 102    | DGD  | O6E-C5E-C6E | 2.59  | 112.85      | 106.44   |
| 25  | a     | 411    | SQD  | C1-O5-C5    | 2.59  | 118.77      | 113.72   |
| 23  | c     | 514    | CLA  | C2A-C1A-CHA | -2.59 | 119.38      | 123.87   |
| 23  | B     | 607    | CLA  | CHC-C1C-C2C | -2.59 | 119.62      | 126.94   |
| 23  | a     | 405[B] | CLA  | CHC-C1C-C2C | -2.58 | 119.62      | 126.94   |
| 23  | D     | 404    | CLA  | CMA-C3A-C2A | -2.58 | 103.99      | 113.98   |
| 31  | a     | 415[B] | PHO  | CMB-C2B-C3B | 2.58  | 129.84      | 124.68   |
| 23  | A     | 405[A] | CLA  | O2A-CGA-O1A | -2.58 | 117.17      | 123.63   |
| 23  | c     | 503    | CLA  | C4C-C3C-C2C | -2.58 | 103.13      | 106.89   |
| 32  | b     | 621    | LMT  | C1'-O5'-C5' | -2.58 | 108.68      | 113.72   |
| 28  | a     | 413[A] | PL9  | C10-C9-C8   | -2.58 | 117.01      | 123.63   |
| 28  | A     | 413[B] | PL9  | C53-C6-C1   | 2.58  | 120.56      | 115.28   |
| 23  | B     | 610    | CLA  | CHD-C4C-NC  | 2.58  | 128.23      | 124.23   |
| 36  | c     | 518[B] | DGD  | C1D-O6D-C5D | 2.58  | 118.75      | 113.72   |
| 23  | B     | 604    | CLA  | CHD-C1D-ND  | -2.58 | 121.18      | 124.80   |
| 23  | C     | 502    | CLA  | C11-C12-C13 | -2.58 | 107.40      | 115.97   |
| 28  | A     | 413[A] | PL9  | C40-C39-C41 | 2.58  | 119.70      | 115.23   |
| 23  | C     | 504    | CLA  | C3B-C4B-NB  | 2.58  | 112.54      | 109.21   |
| 23  | a     | 405[A] | CLA  | C1-C2-C3    | -2.58 | 121.98      | 126.20   |
| 28  | A     | 413[A] | PL9  | C47-C48-C49 | -2.58 | 119.05      | 127.64   |
| 25  | b     | 620    | SQD  | O8-S-C6     | 2.58  | 110.94      | 105.97   |
| 23  | C     | 510    | CLA  | C16-C15-C13 | -2.57 | 107.41      | 115.97   |
| 23  | B     | 602    | CLA  | CMB-C2B-C3B | 2.57  | 129.82      | 124.68   |
| 28  | d     | 406[B] | PL9  | C35-C34-C36 | 2.57  | 119.69      | 115.23   |
| 23  | A     | 404[B] | CLA  | CAA-C2A-C1A | -2.57 | 103.56      | 111.97   |
| 23  | C     | 512    | CLA  | CHC-C1C-C2C | -2.57 | 119.67      | 126.94   |
| 23  | b     | 616    | CLA  | OBD-CAD-C3D | -2.57 | 122.42      | 128.42   |
| 23  | C     | 505    | CLA  | CBC-CAC-C3C | -2.57 | 105.46      | 112.42   |
| 23  | C     | 504    | CLA  | CHC-C1C-C2C | -2.57 | 119.67      | 126.94   |
| 23  | B     | 612    | CLA  | C4-C3-C5    | 2.57  | 119.68      | 115.23   |
| 23  | a     | 405[B] | CLA  | C2A-C1A-CHA | -2.57 | 119.41      | 123.87   |
| 23  | C     | 513    | CLA  | CHB-C4A-NA  | 2.57  | 128.10      | 124.40   |
| 23  | b     | 607    | CLA  | O2A-CGA-O1A | -2.57 | 117.21      | 123.63   |
| 31  | a     | 415[B] | PHO  | O2D-CGD-O1D | -2.57 | 118.85      | 123.85   |
| 23  | c     | 507    | CLA  | C4-C3-C5    | 2.56  | 119.68      | 115.23   |
| 23  | d     | 404    | CLA  | CMC-C2C-C1C | 2.56  | 129.04      | 125.03   |
| 23  | C     | 513    | CLA  | C2A-C1A-CHA | -2.56 | 119.42      | 123.87   |
| 23  | D     | 404    | CLA  | O2A-CGA-CBA | 2.56  | 119.66      | 111.83   |
| 36  | C     | 518[B] | DGD  | O1G-C1A-O1A | -2.56 | 117.22      | 123.63   |
| 23  | d     | 403[B] | CLA  | C2A-C1A-CHA | -2.56 | 119.42      | 123.87   |
| 23  | A     | 405[B] | CLA  | C4C-C3C-C2C | -2.56 | 103.16      | 106.89   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 36  | C     | 518[B] | DGD  | O1G-C1A-C2A | 2.56  | 119.64      | 111.83   |
| 38  | F     | 102    | HEM  | C3B-C4B-NB  | -2.56 | 107.63      | 109.47   |
| 23  | b     | 613    | CLA  | CED-O2D-CGD | 2.56  | 121.72      | 115.92   |
| 23  | c     | 505    | CLA  | CHD-C4C-NC  | 2.56  | 128.20      | 124.23   |
| 23  | c     | 513    | CLA  | CMA-C3A-C4A | -2.56 | 104.90      | 111.77   |
| 23  | B     | 616    | CLA  | O2A-CGA-O1A | -2.56 | 117.23      | 123.63   |
| 23  | a     | 405[B] | CLA  | C4-C3-C5    | 2.56  | 119.67      | 115.23   |
| 23  | b     | 607    | CLA  | C2A-C1A-CHA | -2.56 | 119.43      | 123.87   |
| 31  | D     | 401[A] | PHO  | CMA-C3A-C4A | -2.56 | 109.11      | 114.61   |
| 23  | C     | 503    | CLA  | CMB-C2B-C3B | 2.55  | 129.79      | 124.68   |
| 28  | a     | 413[B] | PL9  | C47-C48-C49 | -2.55 | 119.12      | 127.64   |
| 23  | A     | 407    | CLA  | CMC-C2C-C1C | 2.55  | 129.03      | 125.03   |
| 24  | H     | 101    | BCR  | C10-C11-C12 | -2.55 | 115.80      | 123.20   |
| 23  | B     | 614    | CLA  | C4C-C3C-C2C | -2.55 | 103.17      | 106.89   |
| 23  | B     | 614    | CLA  | CMA-C3A-C2A | -2.55 | 104.11      | 113.98   |
| 34  | C     | 501    | LMG  | C8-O7-C10   | -2.55 | 111.69      | 117.80   |
| 31  | A     | 416[B] | PHO  | O2D-CGD-O1D | -2.55 | 118.88      | 123.85   |
| 24  | b     | 617    | BCR  | C29-C30-C25 | 2.55  | 114.14      | 110.44   |
| 24  | d     | 405    | BCR  | C39-C30-C25 | -2.55 | 106.25      | 110.24   |
| 23  | d     | 403[B] | CLA  | O2A-CGA-O1A | -2.55 | 117.26      | 123.63   |
| 23  | a     | 407    | CLA  | O2A-CGA-O1A | -2.55 | 117.26      | 123.63   |
| 23  | b     | 608    | CLA  | C11-C12-C13 | -2.55 | 107.50      | 115.97   |
| 28  | D     | 406[A] | PL9  | C42-C41-C39 | -2.55 | 104.75      | 113.19   |
| 36  | c     | 517[A] | DGD  | C2G-O2G-C1B | -2.55 | 111.70      | 117.80   |
| 23  | A     | 407    | CLA  | C4-C3-C5    | 2.54  | 119.64      | 115.23   |
| 25  | A     | 409[B] | SQD  | O9-S-C6     | 2.54  | 110.55      | 106.76   |
| 28  | A     | 413[B] | PL9  | C47-C48-C49 | -2.54 | 119.16      | 127.64   |
| 23  | c     | 511    | CLA  | C4C-C3C-C2C | -2.54 | 103.19      | 106.89   |
| 23  | d     | 402[B] | CLA  | C1-C2-C3    | -2.54 | 122.04      | 126.20   |
| 34  | m     | 101    | LMG  | C8-O7-C10   | -2.54 | 111.72      | 117.80   |
| 28  | A     | 413[A] | PL9  | C10-C9-C8   | -2.54 | 117.11      | 123.63   |
| 25  | a     | 409[B] | SQD  | O48-C23-C24 | 2.54  | 119.57      | 111.83   |
| 23  | B     | 605    | CLA  | C7-C6-C5    | -2.53 | 106.51      | 113.26   |
| 23  | a     | 405[A] | CLA  | CMC-C2C-C1C | 2.53  | 128.99      | 125.03   |
| 23  | B     | 608    | CLA  | CMA-C3A-C2A | -2.53 | 104.19      | 113.98   |
| 23  | c     | 502    | CLA  | O2A-CGA-O1A | -2.53 | 117.30      | 123.63   |
| 23  | A     | 406[A] | CLA  | C2A-C1A-CHA | -2.53 | 119.47      | 123.87   |
| 23  | c     | 505    | CLA  | CAA-C2A-C3A | -2.53 | 106.16      | 113.00   |
| 24  | Y     | 101    | BCR  | C15-C16-C17 | -2.53 | 118.34      | 123.52   |
| 23  | a     | 404[A] | CLA  | CHD-C4C-NC  | 2.53  | 128.15      | 124.23   |
| 23  | C     | 504    | CLA  | O2A-CGA-CBA | 2.53  | 119.55      | 111.83   |
| 23  | C     | 503    | CLA  | CBC-CAC-C3C | -2.53 | 105.57      | 112.42   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31  | A     | 416[B] | PHO  | CMA-C3A-C4A | -2.53 | 109.17      | 114.61   |
| 23  | a     | 404[A] | CLA  | CMA-C3A-C2A | -2.53 | 104.22      | 113.98   |
| 34  | D     | 412    | LMG  | O8-C28-O10  | -2.53 | 117.31      | 123.63   |
| 23  | b     | 609    | CLA  | CHC-C1C-C2C | -2.52 | 119.80      | 126.94   |
| 24  | Y     | 101    | BCR  | C38-C26-C25 | -2.52 | 121.73      | 124.48   |
| 23  | D     | 403[B] | CLA  | CAC-C3C-C4C | 2.52  | 128.07      | 124.79   |
| 23  | C     | 513    | CLA  | CMA-C3A-C4A | -2.52 | 105.00      | 111.77   |
| 23  | d     | 402[A] | CLA  | CBC-CAC-C3C | -2.52 | 105.59      | 112.42   |
| 23  | B     | 608    | CLA  | O2A-CGA-CBA | 2.52  | 119.52      | 111.83   |
| 33  | A     | 418[B] | LHG  | O7-C7-O9    | -2.52 | 117.81      | 123.70   |
| 24  | D     | 405    | BCR  | C3-C4-C5    | -2.52 | 109.56      | 114.06   |
| 23  | b     | 606    | CLA  | O2A-CGA-O1A | -2.52 | 117.33      | 123.63   |
| 24  | a     | 408    | BCR  | C8-C7-C6    | -2.52 | 120.27      | 127.00   |
| 23  | B     | 615    | CLA  | O2A-CGA-CBA | 2.52  | 119.51      | 111.83   |
| 23  | B     | 606    | CLA  | C4-C3-C5    | 2.52  | 119.60      | 115.23   |
| 23  | D     | 403[B] | CLA  | CMB-C2B-C3B | 2.52  | 129.71      | 124.68   |
| 23  | a     | 407    | CLA  | CMB-C2B-C3B | 2.52  | 129.71      | 124.68   |
| 34  | C     | 501    | LMG  | C6-C5-C4    | 2.51  | 119.19      | 113.02   |
| 23  | b     | 605    | CLA  | C1-O2A-CGA  | 2.51  | 122.74      | 116.65   |
| 24  | B     | 619    | BCR  | C39-C30-C25 | -2.51 | 106.30      | 110.24   |
| 23  | A     | 404[A] | CLA  | C1B-CHB-C4A | -2.51 | 125.25      | 130.04   |
| 23  | B     | 606    | CLA  | C4C-C3C-C2C | -2.51 | 103.23      | 106.89   |
| 23  | c     | 504    | CLA  | C2A-C1A-CHA | -2.51 | 119.51      | 123.87   |
| 31  | a     | 406[B] | PHO  | CMB-C2B-C3B | 2.51  | 129.70      | 124.68   |
| 25  | X     | 101    | SQD  | O8-S-O7     | -2.51 | 105.12      | 111.40   |
| 23  | A     | 405[A] | CLA  | CAA-CBA-CGA | 2.51  | 120.34      | 113.21   |
| 28  | D     | 406[B] | PL9  | C40-C39-C41 | 2.51  | 119.58      | 115.23   |
| 35  | b     | 623    | HTG  | O5-C1-C2    | 2.51  | 113.78      | 110.32   |
| 28  | D     | 406[B] | PL9  | C22-C23-C24 | -2.51 | 121.88      | 127.62   |
| 24  | D     | 405    | BCR  | C16-C17-C18 | -2.51 | 123.76      | 127.28   |
| 28  | d     | 406[A] | PL9  | C17-C18-C19 | -2.51 | 121.89      | 127.62   |
| 24  | T     | 102    | BCR  | C16-C17-C18 | -2.51 | 123.76      | 127.28   |
| 23  | C     | 507    | CLA  | CAA-C2A-C3A | -2.51 | 106.23      | 113.00   |
| 23  | A     | 404[A] | CLA  | CAA-CBA-CGA | -2.51 | 106.09      | 113.21   |
| 23  | B     | 607    | CLA  | CMA-C3A-C2A | -2.51 | 104.30      | 113.98   |
| 25  | b     | 620    | SQD  | C1-C2-C3    | -2.51 | 104.74      | 110.01   |
| 23  | c     | 510    | CLA  | C1-O2A-CGA  | 2.50  | 122.71      | 116.65   |
| 23  | b     | 608    | CLA  | CBC-CAC-C3C | -2.50 | 105.64      | 112.42   |
| 23  | C     | 510    | CLA  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |
| 23  | C     | 514    | CLA  | CAA-C2A-C3A | -2.50 | 106.25      | 113.00   |
| 24  | h     | 101    | BCR  | C11-C10-C9  | -2.50 | 123.78      | 127.28   |
| 23  | c     | 510    | CLA  | O2A-CGA-O1A | -2.50 | 117.38      | 123.63   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 28  | d     | 406[B] | PL9  | C22-C23-C24 | -2.50 | 121.91      | 127.62   |
| 33  | A     | 418[A] | LHG  | O7-C7-O9    | -2.50 | 117.87      | 123.70   |
| 23  | B     | 613    | CLA  | CHD-C4C-NC  | 2.50  | 128.10      | 124.23   |
| 34  | d     | 412    | LMG  | O8-C28-O10  | -2.49 | 117.39      | 123.63   |
| 23  | a     | 404[A] | CLA  | C4C-C3C-C2C | -2.49 | 103.26      | 106.89   |
| 31  | A     | 416[B] | PHO  | O2A-CGA-CBA | 2.49  | 119.43      | 111.83   |
| 23  | c     | 513    | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 31  | a     | 415[B] | PHO  | O1D-CGD-CBD | -2.49 | 120.95      | 124.72   |
| 23  | a     | 405[B] | CLA  | O2A-CGA-CBA | 2.49  | 119.42      | 111.83   |
| 23  | c     | 508    | CLA  | C3B-C4B-NB  | 2.49  | 112.43      | 109.21   |
| 23  | C     | 506    | CLA  | O2A-CGA-CBA | 2.49  | 119.42      | 111.83   |
| 23  | A     | 407    | CLA  | C1-O2A-CGA  | 2.49  | 122.67      | 116.65   |
| 23  | B     | 615    | CLA  | C2A-C1A-CHA | -2.49 | 119.55      | 123.87   |
| 24  | c     | 515    | BCR  | C20-C21-C22 | -2.49 | 123.79      | 127.28   |
| 23  | A     | 406[A] | CLA  | CMA-C3A-C2A | -2.48 | 104.38      | 113.98   |
| 23  | B     | 610    | CLA  | O1D-CGD-CBD | -2.48 | 119.62      | 124.52   |
| 34  | d     | 412    | LMG  | C7-O1-C1    | -2.48 | 108.47      | 113.80   |
| 32  | m     | 103    | LMT  | C3B-C4B-C5B | -2.48 | 105.73      | 110.23   |
| 23  | B     | 611    | CLA  | O2A-CGA-CBA | 2.48  | 119.40      | 111.83   |
| 31  | A     | 416[B] | PHO  | O1D-CGD-CBD | -2.48 | 120.96      | 124.72   |
| 24  | c     | 515    | BCR  | C37-C22-C23 | 2.48  | 121.88      | 118.09   |
| 23  | b     | 615    | CLA  | O2A-CGA-CBA | 2.48  | 119.39      | 111.83   |
| 23  | c     | 514    | CLA  | CHD-C4C-NC  | 2.48  | 128.07      | 124.23   |
| 23  | B     | 605    | CLA  | CHC-C1C-C2C | -2.48 | 119.93      | 126.94   |
| 23  | d     | 402[B] | CLA  | C4-C3-C5    | 2.48  | 119.53      | 115.23   |
| 23  | B     | 608    | CLA  | CMC-C2C-C1C | 2.48  | 128.90      | 125.03   |
| 24  | Y     | 101    | BCR  | C37-C22-C23 | 2.48  | 121.87      | 118.09   |
| 31  | a     | 406[B] | PHO  | CMA-C3A-C4A | -2.47 | 109.28      | 114.61   |
| 23  | B     | 608    | CLA  | C2A-C1A-CHA | -2.47 | 119.57      | 123.87   |
| 23  | B     | 605    | CLA  | O2A-CGA-CBA | 2.47  | 119.38      | 111.83   |
| 23  | C     | 507    | CLA  | O2A-CGA-CBA | 2.47  | 119.38      | 111.83   |
| 23  | B     | 603    | CLA  | CHD-C4C-NC  | 2.47  | 128.07      | 124.23   |
| 24  | k     | 101    | BCR  | C20-C21-C22 | -2.47 | 123.81      | 127.28   |
| 32  | m     | 103    | LMT  | C3'-C4'-C5' | -2.47 | 105.45      | 110.93   |
| 23  | a     | 404[B] | CLA  | CMA-C3A-C2A | -2.47 | 104.43      | 113.98   |
| 24  | K     | 102    | BCR  | C29-C30-C25 | 2.47  | 114.03      | 110.44   |
| 24  | k     | 101    | BCR  | C16-C17-C18 | -2.47 | 123.81      | 127.28   |
| 23  | A     | 407    | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 24  | B     | 617    | BCR  | C21-C20-C19 | -2.47 | 116.05      | 123.20   |
| 36  | H     | 102    | DGD  | O1G-C1A-O1A | -2.47 | 117.45      | 123.63   |
| 24  | c     | 515    | BCR  | C33-C5-C6   | -2.47 | 121.79      | 124.48   |
| 23  | b     | 615    | CLA  | O2A-CGA-O1A | -2.47 | 117.46      | 123.63   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 38  | F     | 102    | HEM  | CHA-C4D-ND  | 2.47  | 127.43      | 124.37   |
| 28  | d     | 406[B] | PL9  | C7-C3-C2    | -2.46 | 120.48      | 123.39   |
| 25  | A     | 409[B] | SQD  | O9-S-O7     | -2.46 | 105.81      | 113.82   |
| 28  | d     | 406[B] | PL9  | C20-C19-C21 | 2.46  | 119.50      | 115.23   |
| 38  | F     | 102    | HEM  | CMD-C2D-C1D | 2.46  | 128.88      | 125.03   |
| 23  | B     | 604    | CLA  | O2D-CGD-O1D | -2.46 | 119.06      | 123.85   |
| 28  | d     | 406[A] | PL9  | C12-C13-C14 | -2.46 | 121.99      | 127.62   |
| 32  | A     | 419    | LMT  | O1'-C1'-C2' | 2.46  | 112.01      | 108.27   |
| 24  | K     | 102    | BCR  | C3-C4-C5    | -2.46 | 109.67      | 114.06   |
| 31  | a     | 406[B] | PHO  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 23  | C     | 512    | CLA  | O2A-CGA-CBA | 2.45  | 119.31      | 111.83   |
| 25  | A     | 411    | SQD  | O48-C23-O10 | -2.45 | 117.50      | 123.63   |
| 23  | B     | 604    | CLA  | C6-C7-C8    | -2.45 | 107.82      | 115.97   |
| 23  | b     | 611    | CLA  | O2A-CGA-CBA | 2.45  | 119.30      | 111.83   |
| 23  | d     | 403[A] | CLA  | CMC-C2C-C1C | 2.45  | 128.86      | 125.03   |
| 24  | A     | 408    | BCR  | C38-C26-C25 | -2.45 | 121.81      | 124.48   |
| 24  | c     | 516    | BCR  | C37-C22-C21 | -2.45 | 118.85      | 122.82   |
| 23  | C     | 506    | CLA  | CHD-C4C-NC  | 2.45  | 128.03      | 124.23   |
| 28  | A     | 413[A] | PL9  | C42-C43-C44 | -2.44 | 122.03      | 127.62   |
| 24  | B     | 619    | BCR  | C2-C1-C6    | 2.44  | 113.99      | 110.44   |
| 23  | c     | 508    | CLA  | O2A-CGA-O1A | -2.44 | 117.52      | 123.63   |
| 23  | b     | 615    | CLA  | CBC-CAC-C3C | -2.44 | 105.81      | 112.42   |
| 23  | C     | 514    | CLA  | CMB-C2B-C3B | 2.44  | 129.55      | 124.68   |
| 33  | b     | 629[A] | LHG  | O8-C23-O10  | -2.44 | 117.53      | 123.63   |
| 24  | c     | 516    | BCR  | C16-C17-C18 | -2.44 | 123.86      | 127.28   |
| 23  | C     | 508    | CLA  | C4-C3-C5    | 2.44  | 119.45      | 115.23   |
| 23  | b     | 605    | CLA  | CMC-C2C-C1C | 2.43  | 128.84      | 125.03   |
| 33  | d     | 408[A] | LHG  | O8-C23-O10  | -2.43 | 117.54      | 123.63   |
| 23  | b     | 616    | CLA  | CHC-C1C-C2C | -2.43 | 120.05      | 126.94   |
| 23  | c     | 507    | CLA  | CAA-C2A-C3A | -2.43 | 106.42      | 113.00   |
| 23  | A     | 407    | CLA  | C2A-C1A-CHA | -2.43 | 119.65      | 123.87   |
| 32  | B     | 629    | LMT  | O1'-C1'-C2' | 2.43  | 111.97      | 108.27   |
| 23  | B     | 613    | CLA  | C4-C3-C2    | -2.43 | 117.39      | 123.63   |
| 23  | C     | 510    | CLA  | C2A-C1A-CHA | -2.43 | 119.65      | 123.87   |
| 31  | a     | 415[A] | PHO  | O1D-CGD-CBD | -2.43 | 121.04      | 124.72   |
| 23  | C     | 503    | CLA  | O2A-CGA-O1A | -2.43 | 117.55      | 123.63   |
| 23  | c     | 505    | CLA  | O2A-CGA-CBA | 2.43  | 119.24      | 111.83   |
| 23  | c     | 508    | CLA  | C1-C2-C3    | -2.43 | 122.22      | 126.20   |
| 32  | B     | 629    | LMT  | O5'-C5'-C4' | 2.43  | 114.74      | 109.72   |
| 35  | o     | 301    | HTG  | C1'-S1-C1   | 2.43  | 105.69      | 100.45   |
| 23  | c     | 504    | CLA  | C4-C3-C5    | 2.43  | 119.44      | 115.23   |
| 23  | B     | 604    | CLA  | C11-C12-C13 | -2.43 | 107.90      | 115.97   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 514    | CLA  | O2A-CGA-O1A | -2.42 | 117.56      | 123.63   |
| 23  | C     | 513    | CLA  | O2A-CGA-O1A | -2.42 | 117.56      | 123.63   |
| 23  | B     | 613    | CLA  | CHC-C1C-C2C | -2.42 | 120.08      | 126.94   |
| 24  | Y     | 101    | BCR  | C36-C18-C19 | 2.42  | 121.79      | 118.09   |
| 28  | D     | 406[A] | PL9  | C20-C19-C21 | 2.42  | 119.43      | 115.23   |
| 23  | a     | 404[A] | CLA  | C1B-CHB-C4A | -2.42 | 125.42      | 130.04   |
| 23  | b     | 611    | CLA  | CMC-C2C-C1C | 2.42  | 128.82      | 125.03   |
| 36  | c     | 517[B] | DGD  | O6D-C1D-O3G | -2.42 | 104.33      | 110.04   |
| 33  | D     | 407[B] | LHG  | O8-C23-O10  | -2.42 | 117.58      | 123.63   |
| 23  | b     | 602    | CLA  | C1-O2A-CGA  | 2.42  | 122.50      | 116.65   |
| 23  | d     | 402[B] | CLA  | C4C-C3C-C2C | -2.42 | 103.37      | 106.89   |
| 28  | d     | 406[B] | PL9  | C17-C18-C19 | -2.42 | 122.09      | 127.62   |
| 23  | B     | 606    | CLA  | CAC-C3C-C4C | 2.42  | 127.93      | 124.79   |
| 23  | B     | 601    | CLA  | CMC-C2C-C1C | 2.42  | 128.81      | 125.03   |
| 33  | L     | 101[B] | LHG  | O8-C23-C24  | 2.41  | 119.19      | 111.83   |
| 23  | B     | 612    | CLA  | O2A-CGA-O1A | -2.41 | 117.59      | 123.63   |
| 23  | c     | 502    | CLA  | C4-C3-C5    | 2.41  | 119.42      | 115.23   |
| 23  | B     | 605    | CLA  | CBC-CAC-C3C | -2.41 | 105.88      | 112.42   |
| 23  | c     | 507    | CLA  | C2A-C1A-CHA | -2.41 | 119.68      | 123.87   |
| 23  | B     | 610    | CLA  | CMA-C3A-C2A | -2.41 | 104.66      | 113.98   |
| 23  | b     | 601    | CLA  | O2A-CGA-CBA | 2.41  | 119.19      | 111.83   |
| 33  | d     | 408[B] | LHG  | O7-C7-O9    | -2.41 | 118.07      | 123.70   |
| 24  | D     | 405    | BCR  | C21-C20-C19 | -2.41 | 116.22      | 123.20   |
| 23  | C     | 508    | CLA  | CBC-CAC-C3C | -2.41 | 105.89      | 112.42   |
| 24  | b     | 619    | BCR  | C39-C30-C25 | -2.41 | 106.47      | 110.24   |
| 28  | a     | 413[B] | PL9  | C53-C6-C1   | 2.41  | 120.21      | 115.28   |
| 24  | H     | 101    | BCR  | C16-C15-C14 | -2.41 | 118.59      | 123.52   |
| 35  | o     | 301    | HTG  | O2-C2-C3    | -2.41 | 104.70      | 110.38   |
| 23  | c     | 514    | CLA  | CMB-C2B-C3B | 2.41  | 129.49      | 124.68   |
| 24  | C     | 516    | BCR  | C29-C30-C25 | 2.41  | 113.93      | 110.44   |
| 34  | d     | 412    | LMG  | O8-C28-C29  | 2.41  | 119.17      | 111.83   |
| 23  | C     | 507    | CLA  | O2A-CGA-O1A | -2.41 | 117.61      | 123.63   |
| 23  | b     | 613    | CLA  | C4-C3-C5    | 2.40  | 119.40      | 115.23   |
| 36  | c     | 517[B] | DGD  | C3G-C2G-C1G | -2.40 | 106.18      | 111.78   |
| 23  | A     | 405[B] | CLA  | O2A-CGA-O1A | -2.40 | 117.62      | 123.63   |
| 25  | b     | 620    | SQD  | O7-S-C6     | 2.40  | 110.34      | 106.76   |
| 23  | c     | 512    | CLA  | C2A-C1A-CHA | -2.40 | 119.70      | 123.87   |
| 23  | c     | 509    | CLA  | O2A-CGA-O1A | -2.40 | 117.63      | 123.63   |
| 23  | B     | 609    | CLA  | CMC-C2C-C1C | 2.40  | 128.78      | 125.03   |
| 32  | b     | 627    | LMT  | C1'-O5'-C5' | -2.40 | 109.04      | 113.72   |
| 23  | A     | 406[B] | CLA  | C1-C2-C3    | -2.40 | 122.27      | 126.20   |
| 23  | C     | 506    | CLA  | O2A-CGA-O1A | -2.40 | 117.63      | 123.63   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 31  | a     | 406[A] | PHO  | CMA-C3A-C4A | -2.40 | 109.45      | 114.61   |
| 28  | D     | 406[A] | PL9  | C40-C39-C41 | 2.40  | 119.39      | 115.23   |
| 23  | B     | 611    | CLA  | C4A-NA-C1A  | -2.40 | 105.59      | 106.68   |
| 25  | a     | 409[B] | SQD  | O8-S-C6     | 2.40  | 110.60      | 105.97   |
| 32  | B     | 627    | LMT  | O5'-C5'-C6' | 2.39  | 112.37      | 106.44   |
| 23  | C     | 505    | CLA  | C2A-C1A-CHA | -2.39 | 119.71      | 123.87   |
| 23  | c     | 502    | CLA  | CAC-C3C-C4C | 2.39  | 127.90      | 124.79   |
| 36  | C     | 517[B] | DGD  | O1G-C1A-O1A | -2.39 | 117.64      | 123.63   |
| 36  | c     | 517[A] | DGD  | C3G-C2G-C1G | -2.39 | 106.21      | 111.78   |
| 23  | b     | 604    | CLA  | C6-C5-C3    | -2.39 | 107.64      | 113.47   |
| 24  | A     | 408    | BCR  | C8-C7-C6    | -2.39 | 120.61      | 127.00   |
| 24  | K     | 102    | BCR  | C36-C18-C19 | 2.39  | 121.74      | 118.09   |
| 23  | c     | 512    | CLA  | CMC-C2C-C1C | 2.39  | 128.77      | 125.03   |
| 23  | b     | 601    | CLA  | C2A-C1A-CHA | -2.39 | 119.72      | 123.87   |
| 23  | B     | 612    | CLA  | C2A-C1A-CHA | -2.39 | 119.72      | 123.87   |
| 25  | a     | 409[A] | SQD  | O48-C23-C24 | 2.39  | 119.11      | 111.83   |
| 23  | C     | 505    | CLA  | C1-C2-C3    | -2.39 | 122.29      | 126.20   |
| 23  | a     | 405[B] | CLA  | C1-C2-C3    | -2.39 | 122.29      | 126.20   |
| 31  | a     | 415[B] | PHO  | C1A-C2A-C3A | -2.39 | 100.57      | 102.84   |
| 24  | b     | 618    | BCR  | C2-C1-C6    | 2.38  | 113.90      | 110.44   |
| 24  | C     | 516    | BCR  | C2-C1-C6    | 2.38  | 113.90      | 110.44   |
| 32  | b     | 621    | LMT  | C2'-C3'-C4' | 2.38  | 115.09      | 109.68   |
| 24  | T     | 102    | BCR  | C35-C13-C12 | 2.38  | 121.73      | 118.09   |
| 23  | c     | 511    | CLA  | C2A-C1A-CHA | -2.38 | 119.73      | 123.87   |
| 23  | b     | 607    | CLA  | CAC-C3C-C4C | 2.38  | 127.89      | 124.79   |
| 31  | a     | 415[B] | PHO  | O2A-CGA-CBA | 2.38  | 119.09      | 111.83   |
| 23  | A     | 406[A] | CLA  | CAC-C3C-C4C | 2.38  | 127.89      | 124.79   |
| 24  | Y     | 101    | BCR  | C1-C6-C7    | 2.38  | 122.11      | 115.65   |
| 23  | B     | 615    | CLA  | C6-C7-C8    | -2.38 | 108.06      | 115.97   |
| 23  | c     | 511    | CLA  | C11-C10-C8  | -2.38 | 108.06      | 115.97   |
| 23  | B     | 608    | CLA  | CBC-CAC-C3C | -2.38 | 105.97      | 112.42   |
| 23  | c     | 507    | CLA  | O2A-CGA-O1A | -2.38 | 117.69      | 123.63   |
| 32  | e     | 101    | LMT  | O1'-C1'-C2' | 2.38  | 111.88      | 108.27   |
| 36  | C     | 518[A] | DGD  | C2G-O2G-C1B | -2.38 | 112.11      | 117.80   |
| 24  | b     | 619    | BCR  | C16-C15-C14 | -2.38 | 118.66      | 123.52   |
| 38  | F     | 102    | HEM  | O2D-CGD-CBD | 2.37  | 121.50      | 114.00   |
| 24  | T     | 102    | BCR  | C1-C6-C7    | 2.37  | 122.08      | 115.65   |
| 23  | c     | 510    | CLA  | CMB-C2B-C3B | 2.37  | 129.42      | 124.68   |
| 24  | c     | 516    | BCR  | C33-C5-C6   | -2.37 | 121.90      | 124.48   |
| 23  | D     | 404    | CLA  | CMB-C2B-C1B | 2.37  | 131.93      | 128.46   |
| 23  | C     | 504    | CLA  | CBC-CAC-C3C | -2.37 | 106.00      | 112.42   |
| 33  | d     | 407[A] | LHG  | C6-C5-C4    | -2.37 | 106.27      | 111.78   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 507    | CLA  | C4C-C3C-C2C | -2.37 | 103.45      | 106.89   |
| 24  | B     | 618    | BCR  | C37-C22-C23 | 2.37  | 121.70      | 118.09   |
| 23  | C     | 502    | CLA  | CAA-C2A-C3A | -2.37 | 106.61      | 113.00   |
| 23  | b     | 609    | CLA  | CMA-C3A-C4A | -2.36 | 105.42      | 111.77   |
| 23  | D     | 404    | CLA  | CHC-C1C-C2C | -2.36 | 120.25      | 126.94   |
| 25  | l     | 101    | SQD  | O9-S-C6     | 2.36  | 110.28      | 106.76   |
| 23  | C     | 509    | CLA  | O2A-CGA-O1A | -2.36 | 117.72      | 123.63   |
| 23  | b     | 602    | CLA  | C4-C3-C5    | 2.36  | 119.33      | 115.23   |
| 31  | a     | 415[A] | PHO  | C1A-C2A-C3A | -2.36 | 100.59      | 102.84   |
| 23  | b     | 607    | CLA  | C1-O2A-CGA  | 2.36  | 122.37      | 116.65   |
| 24  | D     | 405    | BCR  | C29-C28-C27 | -2.36 | 106.08      | 111.28   |
| 34  | B     | 620    | LMG  | C12-C11-C10 | -2.36 | 105.04      | 113.69   |
| 24  | h     | 101    | BCR  | C24-C23-C22 | -2.36 | 122.74      | 126.23   |
| 23  | D     | 403[B] | CLA  | CHD-C4C-NC  | 2.36  | 127.89      | 124.23   |
| 31  | a     | 415[A] | PHO  | O2A-CGA-CBA | 2.36  | 119.03      | 111.83   |
| 36  | C     | 517[B] | DGD  | O1G-C1A-C2A | 2.36  | 119.02      | 111.83   |
| 25  | f     | 102    | SQD  | O47-C7-O49  | -2.36 | 118.19      | 123.70   |
| 28  | D     | 406[A] | PL9  | C7-C8-C9    | -2.36 | 122.77      | 126.83   |
| 24  | C     | 515    | BCR  | C38-C26-C25 | -2.36 | 121.91      | 124.48   |
| 24  | b     | 618    | BCR  | C29-C30-C25 | 2.35  | 113.86      | 110.44   |
| 23  | c     | 504    | CLA  | CHC-C1C-C2C | -2.35 | 120.28      | 126.94   |
| 35  | b     | 622    | HTG  | C6-C5-C4    | -2.35 | 107.24      | 113.02   |
| 23  | c     | 513    | CLA  | CMC-C2C-C1C | 2.35  | 128.71      | 125.03   |
| 23  | c     | 504    | CLA  | OBD-CAD-C3D | -2.35 | 122.92      | 128.42   |
| 25  | a     | 411    | SQD  | O48-C23-O10 | -2.35 | 117.75      | 123.63   |
| 24  | h     | 101    | BCR  | C10-C11-C12 | -2.35 | 116.39      | 123.20   |
| 23  | b     | 609    | CLA  | CAA-C2A-C3A | -2.35 | 106.65      | 113.00   |
| 23  | B     | 614    | CLA  | OBD-CAD-C3D | -2.35 | 122.93      | 128.42   |
| 34  | C     | 521    | LMG  | C1-C2-C3    | -2.35 | 105.07      | 110.01   |
| 23  | B     | 601    | CLA  | CHC-C1C-C2C | -2.35 | 120.29      | 126.94   |
| 24  | b     | 619    | BCR  | C15-C14-C13 | -2.35 | 123.98      | 127.28   |
| 23  | B     | 614    | CLA  | CAA-C2A-C3A | -2.35 | 106.65      | 113.00   |
| 23  | B     | 615    | CLA  | CHC-C1C-C2C | -2.35 | 120.29      | 126.94   |
| 23  | b     | 606    | CLA  | CBC-CAC-C3C | -2.35 | 106.06      | 112.42   |
| 23  | b     | 616    | CLA  | C4-C3-C5    | 2.35  | 119.30      | 115.23   |
| 23  | B     | 613    | CLA  | CAA-C2A-C3A | -2.35 | 106.66      | 113.00   |
| 23  | c     | 507    | CLA  | CMC-C2C-C1C | 2.35  | 128.70      | 125.03   |
| 24  | d     | 405    | BCR  | C33-C5-C6   | -2.35 | 121.92      | 124.48   |
| 23  | C     | 505    | CLA  | CAC-C3C-C4C | 2.35  | 127.84      | 124.79   |
| 23  | B     | 603    | CLA  | CBC-CAC-C3C | -2.34 | 106.07      | 112.42   |
| 23  | b     | 614    | CLA  | C2A-C1A-CHA | -2.34 | 119.80      | 123.87   |
| 23  | B     | 611    | CLA  | C2C-C1C-NC  | 2.34  | 112.44      | 109.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 610    | CLA  | CHC-C1C-C2C | -2.34 | 120.31      | 126.94   |
| 23  | b     | 611    | CLA  | C2A-C1A-CHA | -2.34 | 119.81      | 123.87   |
| 23  | b     | 601    | CLA  | CAA-C2A-C3A | -2.34 | 106.68      | 113.00   |
| 36  | C     | 518[A] | DGD  | O2G-C1B-O1B | -2.34 | 118.24      | 123.70   |
| 24  | C     | 515    | BCR  | C29-C30-C25 | 2.34  | 113.83      | 110.44   |
| 24  | B     | 617    | BCR  | C31-C1-C6   | -2.34 | 106.58      | 110.24   |
| 23  | B     | 602    | CLA  | CHC-C1C-C2C | -2.34 | 120.33      | 126.94   |
| 28  | d     | 406[A] | PL9  | C7-C8-C9    | -2.34 | 122.81      | 126.83   |
| 23  | B     | 602    | CLA  | O2A-CGA-CBA | 2.34  | 118.95      | 111.83   |
| 28  | A     | 413[B] | PL9  | C45-C44-C46 | 2.33  | 119.28      | 115.23   |
| 23  | C     | 509    | CLA  | CHD-C4C-NC  | 2.33  | 127.85      | 124.23   |
| 23  | b     | 613    | CLA  | CBC-CAC-C3C | -2.33 | 106.09      | 112.42   |
| 24  | A     | 408    | BCR  | C15-C14-C13 | -2.33 | 124.00      | 127.28   |
| 25  | X     | 101    | SQD  | O5-C1-C2    | -2.33 | 105.58      | 110.37   |
| 23  | C     | 502    | CLA  | C2A-C1A-CHA | -2.33 | 119.82      | 123.87   |
| 24  | a     | 408    | BCR  | C33-C5-C6   | -2.33 | 121.94      | 124.48   |
| 23  | C     | 510    | CLA  | C11-C12-C13 | -2.33 | 108.21      | 115.97   |
| 23  | c     | 513    | CLA  | O2A-CGA-O1A | -2.33 | 117.79      | 123.63   |
| 28  | a     | 413[A] | PL9  | C20-C19-C21 | 2.33  | 119.28      | 115.23   |
| 24  | B     | 618    | BCR  | C37-C22-C21 | -2.33 | 119.04      | 122.82   |
| 32  | M     | 101    | LMT  | C1-O1'-C1'  | 2.33  | 117.66      | 113.68   |
| 34  | c     | 521    | LMG  | O8-C28-O10  | -2.33 | 117.80      | 123.63   |
| 23  | B     | 610    | CLA  | CAC-C3C-C4C | 2.33  | 127.82      | 124.79   |
| 23  | A     | 405[B] | CLA  | CMC-C2C-C1C | 2.33  | 128.67      | 125.03   |
| 23  | D     | 403[B] | CLA  | CMC-C2C-C1C | 2.33  | 128.67      | 125.03   |
| 25  | A     | 409[A] | SQD  | O9-S-O7     | -2.33 | 106.25      | 113.82   |
| 23  | c     | 508    | CLA  | C2A-C1A-CHA | -2.33 | 119.83      | 123.87   |
| 24  | d     | 405    | BCR  | C11-C10-C9  | -2.33 | 124.02      | 127.28   |
| 23  | B     | 608    | CLA  | C11-C12-C13 | -2.33 | 108.23      | 115.97   |
| 23  | C     | 514    | CLA  | O2A-CGA-O1A | -2.33 | 117.81      | 123.63   |
| 32  | A     | 419    | LMT  | O5'-C5'-C4' | 2.33  | 114.53      | 109.72   |
| 25  | A     | 409[A] | SQD  | O8-S-C6     | 2.33  | 110.46      | 105.97   |
| 24  | K     | 102    | BCR  | C39-C30-C25 | -2.33 | 106.60      | 110.24   |
| 23  | D     | 403[A] | CLA  | CMC-C2C-C1C | 2.33  | 128.67      | 125.03   |
| 33  | D     | 407[B] | LHG  | O8-C23-C24  | 2.33  | 118.92      | 111.83   |
| 28  | A     | 413[A] | PL9  | C12-C13-C14 | -2.33 | 122.30      | 127.62   |
| 23  | D     | 403[A] | CLA  | C1B-CHB-C4A | -2.32 | 125.61      | 130.04   |
| 24  | Y     | 101    | BCR  | C7-C6-C5    | -2.32 | 116.20      | 121.56   |
| 35  | B     | 623    | HTG  | O5-C5-C4    | 2.32  | 113.88      | 109.70   |
| 23  | c     | 508    | CLA  | CBC-CAC-C3C | -2.32 | 106.13      | 112.42   |
| 40  | V     | 201    | HEC  | CAD-CBD-CGD | -2.32 | 107.58      | 113.83   |
| 36  | C     | 517[A] | DGD  | O6E-C5E-C4E | 2.32  | 113.88      | 109.70   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 36  | C     | 519    | DGD  | O2G-C1B-C2B | 2.32  | 116.50      | 111.48   |
| 36  | C     | 517[A] | DGD  | C3G-C2G-C1G | -2.32 | 106.38      | 111.78   |
| 23  | B     | 615    | CLA  | CMB-C2B-C1B | 2.32  | 131.85      | 128.46   |
| 23  | B     | 608    | CLA  | CAA-C2A-C3A | -2.32 | 106.74      | 113.00   |
| 23  | C     | 502    | CLA  | OBD-CAD-C3D | -2.32 | 123.00      | 128.42   |
| 24  | A     | 408    | BCR  | C31-C1-C6   | -2.32 | 106.61      | 110.24   |
| 24  | h     | 101    | BCR  | C16-C17-C18 | -2.32 | 124.03      | 127.28   |
| 31  | a     | 415[B] | PHO  | CMC-C2C-C3C | 2.32  | 129.31      | 124.94   |
| 23  | A     | 405[B] | CLA  | C2A-C1A-CHA | -2.31 | 119.85      | 123.87   |
| 36  | c     | 518[B] | DGD  | O1G-C1A-O1A | -2.31 | 117.84      | 123.63   |
| 23  | A     | 405[B] | CLA  | C1-C2-C3    | -2.31 | 122.41      | 126.20   |
| 23  | B     | 604    | CLA  | O2A-CGA-CBA | 2.31  | 118.89      | 111.83   |
| 23  | C     | 505    | CLA  | CHD-C4C-NC  | 2.31  | 127.82      | 124.23   |
| 23  | c     | 505    | CLA  | C2A-C1A-CHA | -2.31 | 119.86      | 123.87   |
| 23  | B     | 605    | CLA  | C2A-C1A-CHA | -2.31 | 119.86      | 123.87   |
| 25  | b     | 620    | SQD  | O5-C1-C2    | -2.31 | 105.62      | 110.37   |
| 23  | a     | 404[B] | CLA  | C4-C3-C5    | 2.31  | 119.24      | 115.23   |
| 23  | b     | 610    | CLA  | C2A-C1A-CHA | -2.31 | 119.86      | 123.87   |
| 23  | b     | 607    | CLA  | O2D-CGD-O1D | -2.31 | 119.36      | 123.85   |
| 23  | d     | 402[B] | CLA  | C1-O2A-CGA  | 2.31  | 122.23      | 116.65   |
| 32  | b     | 621    | LMT  | C1-O1'-C1'  | 2.31  | 117.62      | 113.68   |
| 25  | A     | 409[B] | SQD  | O48-C23-O10 | -2.30 | 117.86      | 123.63   |
| 23  | B     | 610    | CLA  | C1-C2-C3    | -2.30 | 122.42      | 126.20   |
| 23  | C     | 511    | CLA  | CBC-CAC-C3C | -2.30 | 106.17      | 112.42   |
| 32  | B     | 627    | LMT  | O5'-C5'-C4' | 2.30  | 114.49      | 109.72   |
| 31  | D     | 401[A] | PHO  | CMB-C2B-C3B | 2.30  | 129.29      | 124.68   |
| 23  | b     | 607    | CLA  | CHD-C4C-NC  | 2.30  | 127.80      | 124.23   |
| 24  | b     | 617    | BCR  | C21-C20-C19 | -2.30 | 116.53      | 123.20   |
| 28  | A     | 413[A] | PL9  | C45-C44-C46 | 2.30  | 119.22      | 115.23   |
| 24  | d     | 405    | BCR  | C21-C20-C19 | -2.30 | 116.53      | 123.20   |
| 25  | a     | 409[A] | SQD  | O9-S-O7     | -2.30 | 106.34      | 113.82   |
| 25  | A     | 411    | SQD  | C4-C3-C2    | -2.30 | 106.79      | 110.83   |
| 23  | c     | 511    | CLA  | C11-C12-C13 | -2.30 | 108.32      | 115.97   |
| 32  | a     | 416    | LMT  | O5B-C1B-C2B | 2.30  | 115.09      | 110.37   |
| 23  | D     | 403[B] | CLA  | O2A-CGA-O1A | -2.30 | 117.88      | 123.63   |
| 23  | b     | 614    | CLA  | CAA-C2A-C3A | -2.30 | 106.79      | 113.00   |
| 23  | c     | 508    | CLA  | C4C-C3C-C2C | -2.30 | 103.55      | 106.89   |
| 24  | t     | 102    | BCR  | C37-C22-C23 | 2.30  | 121.59      | 118.09   |
| 23  | b     | 601    | CLA  | O1D-CGD-CBD | -2.30 | 119.99      | 124.52   |
| 23  | C     | 504    | CLA  | CAC-C3C-C4C | 2.30  | 127.78      | 124.79   |
| 23  | c     | 510    | CLA  | C4-C3-C2    | -2.29 | 117.73      | 123.63   |
| 25  | a     | 411    | SQD  | O7-S-C6     | 2.29  | 110.18      | 106.76   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 505    | CLA  | O2A-CGA-CBA | 2.29  | 118.83      | 111.83   |
| 23  | b     | 610    | CLA  | C4-C3-C2    | -2.29 | 117.73      | 123.63   |
| 23  | c     | 508    | CLA  | CHC-C1C-C2C | -2.29 | 120.44      | 126.94   |
| 23  | B     | 605    | CLA  | CHA-C1A-NA  | -2.29 | 121.20      | 126.39   |
| 23  | B     | 612    | CLA  | C4A-NA-C1A  | -2.29 | 105.63      | 106.68   |
| 23  | C     | 505    | CLA  | OBD-CAD-C3D | -2.29 | 123.06      | 128.42   |
| 24  | b     | 618    | BCR  | C28-C27-C26 | -2.29 | 109.97      | 114.06   |
| 23  | c     | 502    | CLA  | CMC-C2C-C1C | 2.29  | 128.61      | 125.03   |
| 28  | d     | 406[A] | PL9  | C20-C19-C21 | 2.29  | 119.20      | 115.23   |
| 23  | b     | 610    | CLA  | C3B-C4B-NB  | 2.29  | 112.17      | 109.21   |
| 23  | b     | 604    | CLA  | CHB-C4A-NA  | 2.29  | 127.70      | 124.40   |
| 25  | b     | 620    | SQD  | O47-C7-O49  | -2.29 | 118.36      | 123.70   |
| 33  | E     | 101[A] | LHG  | O7-C7-O9    | -2.28 | 118.37      | 123.70   |
| 33  | d     | 407[B] | LHG  | O7-C7-O9    | -2.28 | 118.37      | 123.70   |
| 23  | B     | 612    | CLA  | CMA-C3A-C2A | -2.28 | 105.17      | 113.98   |
| 23  | C     | 513    | CLA  | CMB-C2B-C3B | 2.28  | 129.24      | 124.68   |
| 23  | b     | 603    | CLA  | CMC-C2C-C1C | 2.28  | 128.59      | 125.03   |
| 23  | C     | 509    | CLA  | CAC-C3C-C4C | 2.28  | 127.75      | 124.79   |
| 25  | a     | 411    | SQD  | C3-C4-C5    | 2.28  | 114.36      | 110.23   |
| 33  | D     | 407[B] | LHG  | C5-O7-C7    | -2.28 | 112.35      | 117.80   |
| 28  | D     | 406[B] | PL9  | C30-C29-C31 | 2.28  | 119.18      | 115.23   |
| 23  | B     | 601    | CLA  | C2A-C1A-CHA | -2.27 | 119.92      | 123.87   |
| 24  | c     | 515    | BCR  | C36-C18-C19 | 2.27  | 121.56      | 118.09   |
| 23  | d     | 404    | CLA  | C1-O2A-CGA  | 2.27  | 122.16      | 116.65   |
| 24  | a     | 408    | BCR  | C37-C22-C21 | -2.27 | 119.13      | 122.82   |
| 28  | D     | 406[B] | PL9  | C47-C48-C49 | -2.27 | 120.06      | 127.64   |
| 28  | A     | 413[B] | PL9  | C25-C24-C26 | 2.27  | 119.17      | 115.23   |
| 23  | c     | 502    | CLA  | CBC-CAC-C3C | -2.27 | 106.26      | 112.42   |
| 23  | B     | 604    | CLA  | C4-C3-C5    | 2.27  | 119.17      | 115.23   |
| 31  | D     | 401[B] | PHO  | CMB-C2B-C3B | 2.27  | 129.22      | 124.68   |
| 23  | a     | 404[A] | CLA  | C7-C6-C5    | -2.27 | 107.20      | 113.26   |
| 23  | d     | 402[A] | CLA  | C2A-C1A-CHA | -2.27 | 119.92      | 123.87   |
| 23  | c     | 506    | CLA  | O2A-CGA-O1A | -2.27 | 117.95      | 123.63   |
| 23  | A     | 407    | CLA  | CMB-C2B-C3B | 2.27  | 129.22      | 124.68   |
| 23  | b     | 613    | CLA  | C16-C15-C13 | -2.27 | 108.42      | 115.97   |
| 24  | k     | 101    | BCR  | C34-C9-C8   | 2.27  | 121.55      | 118.09   |
| 28  | d     | 406[A] | PL9  | C47-C48-C49 | -2.27 | 120.08      | 127.64   |
| 24  | a     | 408    | BCR  | C11-C10-C9  | -2.27 | 124.10      | 127.28   |
| 25  | a     | 411    | SQD  | O5-C5-C4    | 2.27  | 113.78      | 109.70   |
| 23  | B     | 605    | CLA  | OBD-CAD-C3D | -2.26 | 123.12      | 128.42   |
| 23  | d     | 403[B] | CLA  | CAA-C2A-C3A | -2.26 | 106.88      | 113.00   |
| 23  | c     | 505    | CLA  | CED-O2D-CGD | 2.26  | 121.05      | 115.92   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 506    | CLA  | CMC-C2C-C1C | 2.26  | 128.57      | 125.03   |
| 36  | c     | 519    | DGD  | O6D-C5D-C6D | 2.26  | 111.18      | 106.69   |
| 33  | A     | 418[A] | LHG  | O4-P-O5     | 2.26  | 122.96      | 112.44   |
| 23  | c     | 507    | CLA  | C1-O2A-CGA  | 2.26  | 122.12      | 116.65   |
| 23  | b     | 605    | CLA  | CAC-C3C-C4C | 2.26  | 127.73      | 124.79   |
| 23  | C     | 513    | CLA  | CBC-CAC-C3C | -2.26 | 106.30      | 112.42   |
| 23  | b     | 615    | CLA  | C6-C7-C8    | -2.26 | 108.46      | 115.97   |
| 24  | B     | 619    | BCR  | C3-C4-C5    | -2.26 | 110.03      | 114.06   |
| 32  | A     | 417    | LMT  | O1'-C1'-C2' | 2.26  | 111.70      | 108.27   |
| 25  | A     | 409[B] | SQD  | O47-C7-O49  | -2.26 | 118.43      | 123.70   |
| 31  | a     | 415[B] | PHO  | CBA-CAA-C2A | -2.26 | 107.13      | 113.78   |
| 23  | d     | 402[A] | CLA  | CMC-C2C-C1C | 2.26  | 128.56      | 125.03   |
| 23  | D     | 403[A] | CLA  | CED-O2D-CGD | 2.25  | 121.03      | 115.92   |
| 26  | B     | 625    | GOL  | C3-C2-C1    | -2.25 | 103.53      | 111.80   |
| 33  | d     | 407[A] | LHG  | O8-C23-O10  | -2.25 | 117.99      | 123.63   |
| 23  | A     | 404[B] | CLA  | O2D-CGD-O1D | -2.25 | 119.46      | 123.85   |
| 24  | h     | 101    | BCR  | C36-C18-C17 | -2.25 | 119.17      | 122.82   |
| 31  | a     | 415[B] | PHO  | C4A-C3A-C2A | -2.25 | 100.70      | 102.84   |
| 23  | D     | 403[B] | CLA  | CBC-CAC-C3C | -2.25 | 106.31      | 112.42   |
| 23  | d     | 404    | CLA  | CMA-C3A-C2A | -2.25 | 105.28      | 113.98   |
| 23  | b     | 612    | CLA  | OBD-CAD-C3D | -2.25 | 123.16      | 128.42   |
| 31  | a     | 406[A] | PHO  | C1-C2-C3    | -2.25 | 122.51      | 126.20   |
| 34  | C     | 501    | LMG  | O8-C28-C29  | 2.25  | 118.69      | 111.83   |
| 24  | b     | 619    | BCR  | C21-C20-C19 | -2.25 | 116.69      | 123.20   |
| 24  | t     | 102    | BCR  | C29-C30-C25 | 2.25  | 113.70      | 110.44   |
| 28  | D     | 406[A] | PL9  | C12-C13-C14 | -2.25 | 122.48      | 127.62   |
| 23  | a     | 404[B] | CLA  | CAC-C3C-C4C | 2.25  | 127.71      | 124.79   |
| 23  | A     | 405[A] | CLA  | O2A-CGA-CBA | 2.25  | 118.68      | 111.83   |
| 28  | A     | 413[A] | PL9  | C35-C34-C33 | -2.25 | 117.86      | 123.63   |
| 36  | H     | 102    | DGD  | C1E-O6E-C5E | -2.24 | 109.34      | 113.72   |
| 23  | b     | 609    | CLA  | OBD-CAD-C3D | -2.24 | 123.17      | 128.42   |
| 23  | a     | 405[B] | CLA  | CBC-CAC-C3C | -2.24 | 106.33      | 112.42   |
| 25  | X     | 101    | SQD  | C46-C45-C44 | -2.24 | 106.55      | 111.78   |
| 23  | C     | 506    | CLA  | C11-C10-C8  | -2.24 | 108.51      | 115.97   |
| 23  | c     | 511    | CLA  | C4-C3-C2    | -2.24 | 117.87      | 123.63   |
| 23  | c     | 508    | CLA  | O1D-CGD-CBD | -2.24 | 120.09      | 124.52   |
| 24  | C     | 515    | BCR  | C40-C30-C25 | -2.24 | 106.73      | 110.24   |
| 23  | A     | 404[A] | CLA  | CHD-C4C-NC  | 2.24  | 127.71      | 124.23   |
| 23  | d     | 403[A] | CLA  | CMA-C3A-C2A | -2.24 | 105.31      | 113.98   |
| 23  | B     | 609    | CLA  | O2A-CGA-O1A | -2.24 | 118.02      | 123.63   |
| 23  | c     | 504    | CLA  | O2A-CGA-O1A | -2.24 | 118.02      | 123.63   |
| 31  | A     | 416[A] | PHO  | O1D-CGD-CBD | -2.24 | 121.33      | 124.72   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | y     | 101    | BCR  | C28-C27-C26 | -2.24 | 110.06      | 114.06   |
| 23  | b     | 606    | CLA  | CMB-C2B-C3B | 2.24  | 129.16      | 124.68   |
| 23  | b     | 602    | CLA  | CHC-C1C-C2C | -2.24 | 120.60      | 126.94   |
| 23  | C     | 514    | CLA  | C4-C3-C5    | 2.24  | 119.11      | 115.23   |
| 23  | c     | 510    | CLA  | C2A-C1A-CHA | -2.24 | 119.98      | 123.87   |
| 25  | f     | 102    | SQD  | O48-C23-O10 | -2.24 | 118.03      | 123.63   |
| 23  | c     | 514    | CLA  | CBC-CAC-C3C | -2.24 | 106.36      | 112.42   |
| 23  | A     | 406[B] | CLA  | C4-C3-C5    | 2.23  | 119.11      | 115.23   |
| 24  | C     | 516    | BCR  | C11-C10-C9  | -2.23 | 124.15      | 127.28   |
| 23  | c     | 509    | CLA  | C2A-C1A-CHA | -2.23 | 119.99      | 123.87   |
| 23  | b     | 613    | CLA  | CMA-C3A-C4A | -2.23 | 105.78      | 111.77   |
| 23  | C     | 506    | CLA  | CHA-C1A-NA  | -2.23 | 121.34      | 126.39   |
| 23  | C     | 509    | CLA  | O2A-CGA-CBA | 2.23  | 118.64      | 111.83   |
| 24  | b     | 617    | BCR  | C32-C1-C6   | -2.23 | 106.75      | 110.24   |
| 25  | A     | 411    | SQD  | O6-C44-C45  | -2.23 | 105.40      | 110.82   |
| 23  | B     | 607    | CLA  | O2A-CGA-CBA | 2.23  | 118.63      | 111.83   |
| 23  | b     | 603    | CLA  | C1B-CHB-C4A | -2.23 | 125.79      | 130.04   |
| 31  | A     | 416[A] | PHO  | CED-O2D-CGD | 2.23  | 120.97      | 115.92   |
| 23  | b     | 604    | CLA  | O2A-CGA-CBA | 2.23  | 118.63      | 111.83   |
| 36  | c     | 518[A] | DGD  | O1G-C1A-O1A | -2.23 | 118.06      | 123.63   |
| 23  | c     | 502    | CLA  | C1-O2A-CGA  | 2.23  | 122.04      | 116.65   |
| 24  | D     | 405    | BCR  | C30-C25-C24 | 2.23  | 121.69      | 115.65   |
| 23  | d     | 403[B] | CLA  | CMB-C2B-C3B | 2.23  | 129.13      | 124.68   |
| 25  | f     | 102    | SQD  | O6-C1-C2    | 2.23  | 111.65      | 108.27   |
| 23  | c     | 507    | CLA  | CBC-CAC-C3C | -2.23 | 106.39      | 112.42   |
| 23  | b     | 607    | CLA  | C1-C2-C3    | -2.22 | 122.55      | 126.20   |
| 36  | C     | 519    | DGD  | O3G-C3G-C2G | -2.22 | 105.41      | 110.82   |
| 23  | b     | 611    | CLA  | CAA-C2A-C3A | -2.22 | 106.99      | 113.00   |
| 24  | T     | 102    | BCR  | C33-C5-C6   | -2.22 | 122.06      | 124.48   |
| 33  | d     | 414[A] | LHG  | O7-C7-O9    | -2.22 | 118.51      | 123.70   |
| 23  | A     | 405[A] | CLA  | C4C-C3C-C2C | -2.22 | 103.66      | 106.89   |
| 23  | B     | 602    | CLA  | CMA-C3A-C4A | -2.22 | 105.81      | 111.77   |
| 23  | b     | 614    | CLA  | CMB-C2B-C3B | 2.22  | 129.12      | 124.68   |
| 28  | a     | 413[B] | PL9  | C45-C44-C46 | 2.22  | 119.08      | 115.23   |
| 28  | A     | 413[B] | PL9  | C51-C49-C50 | 2.22  | 119.69      | 114.59   |
| 23  | b     | 607    | CLA  | CAA-CBA-CGA | 2.22  | 119.50      | 113.21   |
| 31  | D     | 401[B] | PHO  | O2A-CGA-O1A | -2.22 | 118.08      | 123.63   |
| 23  | A     | 407    | CLA  | O2A-CGA-O1A | -2.21 | 118.09      | 123.63   |
| 33  | d     | 407[A] | LHG  | O8-C23-C24  | 2.21  | 118.59      | 111.83   |
| 23  | D     | 403[A] | CLA  | CMA-C3A-C4A | -2.21 | 105.82      | 111.77   |
| 23  | b     | 604    | CLA  | CMB-C2B-C3B | 2.21  | 129.11      | 124.68   |
| 24  | h     | 101    | BCR  | C16-C15-C14 | -2.21 | 118.99      | 123.52   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 506    | CLA  | CHD-C4C-NC  | 2.21  | 127.66      | 124.23   |
| 34  | m     | 101    | LMG  | O7-C10-O9   | -2.21 | 118.53      | 123.70   |
| 23  | b     | 611    | CLA  | CBC-CAC-C3C | -2.21 | 106.42      | 112.42   |
| 35  | C     | 522    | HTG  | C1-O5-C5    | 2.21  | 116.53      | 112.56   |
| 24  | d     | 405    | BCR  | C36-C18-C17 | -2.21 | 119.23      | 122.82   |
| 24  | h     | 101    | BCR  | C34-C9-C8   | 2.21  | 121.47      | 118.09   |
| 34  | C     | 520    | LMG  | C8-O7-C10   | -2.21 | 112.50      | 117.80   |
| 35  | b     | 623    | HTG  | C1-C2-C3    | 2.21  | 114.87      | 110.55   |
| 23  | a     | 404[B] | CLA  | C1B-CHB-C4A | -2.21 | 125.82      | 130.04   |
| 24  | T     | 102    | BCR  | C7-C8-C9    | -2.21 | 122.96      | 126.23   |
| 24  | b     | 618    | BCR  | C8-C7-C6    | -2.21 | 121.09      | 127.00   |
| 35  | b     | 622    | HTG  | O2-C2-C3    | -2.21 | 105.17      | 110.38   |
| 24  | c     | 516    | BCR  | C38-C26-C25 | -2.21 | 122.07      | 124.48   |
| 24  | b     | 619    | BCR  | C11-C10-C9  | -2.21 | 124.18      | 127.28   |
| 28  | a     | 413[A] | PL9  | C35-C34-C33 | -2.21 | 117.95      | 123.63   |
| 23  | d     | 402[B] | CLA  | CHB-C4A-NA  | 2.21  | 127.59      | 124.40   |
| 31  | D     | 401[A] | PHO  | C4-C3-C5    | 2.21  | 119.06      | 115.23   |
| 25  | l     | 101    | SQD  | C9-C8-C7    | -2.21 | 105.61      | 113.69   |
| 34  | m     | 101    | LMG  | O8-C28-O10  | -2.20 | 118.12      | 123.63   |
| 25  | l     | 101    | SQD  | O5-C1-C2    | -2.20 | 105.84      | 110.37   |
| 23  | d     | 402[B] | CLA  | CMA-C3A-C2A | -2.20 | 105.46      | 113.98   |
| 23  | c     | 505    | CLA  | C4-C3-C5    | 2.20  | 119.05      | 115.23   |
| 23  | C     | 505    | CLA  | CAA-C2A-C3A | -2.20 | 107.05      | 113.00   |
| 23  | c     | 513    | CLA  | CBA-CAA-C2A | -2.20 | 107.24      | 113.79   |
| 24  | B     | 619    | BCR  | C2-C3-C4    | -2.20 | 106.44      | 111.28   |
| 23  | C     | 508    | CLA  | CAC-C3C-C4C | 2.20  | 127.65      | 124.79   |
| 24  | h     | 101    | BCR  | C36-C18-C19 | 2.20  | 121.45      | 118.09   |
| 23  | c     | 503    | CLA  | O2A-CGA-O1A | -2.20 | 118.12      | 123.63   |
| 23  | B     | 601    | CLA  | CHB-C4A-NA  | 2.20  | 127.57      | 124.40   |
| 23  | b     | 616    | CLA  | C11-C12-C13 | -2.20 | 108.66      | 115.97   |
| 23  | b     | 613    | CLA  | O2D-CGD-O1D | -2.20 | 119.57      | 123.85   |
| 23  | d     | 404    | CLA  | CHB-C4A-NA  | 2.20  | 127.57      | 124.40   |
| 24  | c     | 516    | BCR  | C7-C8-C9    | -2.20 | 122.99      | 126.23   |
| 23  | B     | 608    | CLA  | C11-C10-C8  | -2.20 | 108.67      | 115.97   |
| 36  | C     | 518[A] | DGD  | O1G-C1A-C2A | 2.19  | 118.53      | 111.83   |
| 25  | a     | 409[B] | SQD  | C3-C4-C5    | 2.19  | 114.21      | 110.23   |
| 23  | C     | 512    | CLA  | O2A-CGA-O1A | -2.19 | 118.14      | 123.63   |
| 36  | c     | 517[A] | DGD  | O3G-C3G-C2G | -2.19 | 105.48      | 110.82   |
| 23  | D     | 403[B] | CLA  | C4-C3-C5    | 2.19  | 119.03      | 115.23   |
| 24  | t     | 102    | BCR  | C36-C18-C19 | 2.19  | 121.44      | 118.09   |
| 23  | c     | 514    | CLA  | O2D-CGD-O1D | -2.19 | 119.58      | 123.85   |
| 28  | d     | 406[A] | PL9  | C51-C49-C50 | 2.19  | 119.63      | 114.59   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 507    | CLA  | CGD-CBD-CAD | -2.19 | 103.75      | 110.85   |
| 33  | d     | 414[B] | LHG  | O7-C7-O9    | -2.19 | 118.58      | 123.70   |
| 23  | B     | 615    | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |
| 23  | c     | 509    | CLA  | CAC-C3C-C4C | 2.19  | 127.64      | 124.79   |
| 24  | y     | 101    | BCR  | C35-C13-C12 | 2.19  | 121.43      | 118.09   |
| 23  | c     | 512    | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |
| 23  | C     | 509    | CLA  | C2A-C1A-CHA | -2.19 | 120.07      | 123.87   |
| 28  | A     | 413[B] | PL9  | C32-C31-C29 | -2.19 | 105.94      | 113.19   |
| 23  | B     | 610    | CLA  | CMC-C2C-C1C | 2.19  | 128.45      | 125.03   |
| 24  | Y     | 101    | BCR  | C35-C13-C12 | 2.19  | 121.43      | 118.09   |
| 28  | a     | 413[B] | PL9  | C51-C49-C50 | 2.18  | 119.61      | 114.59   |
| 28  | A     | 413[A] | PL9  | C25-C24-C26 | 2.18  | 119.02      | 115.23   |
| 23  | a     | 407    | CLA  | C1B-CHB-C4A | -2.18 | 125.88      | 130.04   |
| 31  | D     | 401[B] | PHO  | O2D-CGD-O1D | -2.18 | 119.60      | 123.85   |
| 26  | B     | 622    | GOL  | C3-C2-C1    | -2.18 | 103.80      | 111.80   |
| 23  | C     | 508    | CLA  | O2A-CGA-O1A | -2.18 | 118.17      | 123.63   |
| 24  | b     | 619    | BCR  | C31-C1-C6   | -2.18 | 106.82      | 110.24   |
| 28  | D     | 406[B] | PL9  | C37-C38-C39 | -2.18 | 122.64      | 127.62   |
| 23  | b     | 615    | CLA  | C2A-C1A-CHA | -2.18 | 120.09      | 123.87   |
| 23  | b     | 615    | CLA  | C1-C2-C3    | -2.18 | 122.63      | 126.20   |
| 23  | A     | 405[B] | CLA  | CAC-C3C-C4C | 2.18  | 127.62      | 124.79   |
| 31  | A     | 416[B] | PHO  | CMC-C2C-C3C | 2.18  | 129.04      | 124.94   |
| 23  | b     | 602    | CLA  | O2A-CGA-CBA | 2.17  | 118.47      | 111.83   |
| 23  | C     | 513    | CLA  | CBA-CAA-C2A | -2.17 | 107.32      | 113.79   |
| 23  | C     | 508    | CLA  | CHD-C4C-NC  | 2.17  | 127.60      | 124.23   |
| 33  | E     | 101[B] | LHG  | O7-C7-O9    | -2.17 | 118.62      | 123.70   |
| 23  | b     | 611    | CLA  | C7-C6-C5    | -2.17 | 107.47      | 113.26   |
| 31  | a     | 406[A] | PHO  | O2D-CGD-O1D | -2.17 | 119.62      | 123.85   |
| 23  | C     | 505    | CLA  | C1-O2A-CGA  | 2.17  | 121.91      | 116.65   |
| 24  | d     | 405    | BCR  | C30-C25-C24 | 2.17  | 121.54      | 115.65   |
| 24  | Y     | 101    | BCR  | C40-C30-C25 | -2.17 | 106.84      | 110.24   |
| 23  | A     | 405[B] | CLA  | CAA-CBA-CGA | 2.17  | 119.36      | 113.21   |
| 23  | b     | 603    | CLA  | CAC-C3C-C4C | 2.17  | 127.61      | 124.79   |
| 23  | B     | 616    | CLA  | CHA-C1A-NA  | -2.17 | 121.48      | 126.39   |
| 23  | a     | 407    | CLA  | CHC-C1C-C2C | -2.17 | 120.81      | 126.94   |
| 24  | y     | 101    | BCR  | C1-C6-C7    | 2.17  | 121.52      | 115.65   |
| 23  | B     | 609    | CLA  | C2A-C1A-CHA | -2.16 | 120.11      | 123.87   |
| 36  | c     | 517[A] | DGD  | O6D-C1D-O3G | -2.16 | 104.93      | 110.04   |
| 31  | a     | 415[A] | PHO  | C4-C3-C2    | -2.16 | 118.07      | 123.63   |
| 28  | d     | 406[A] | PL9  | O2-C1-C6    | -2.16 | 117.04      | 120.48   |
| 23  | B     | 604    | CLA  | CAA-C2A-C3A | -2.16 | 107.16      | 113.00   |
| 23  | b     | 616    | CLA  | C2A-C1A-CHA | -2.16 | 120.11      | 123.87   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 28  | A     | 413[B] | PL9  | C35-C34-C33 | -2.16 | 118.07      | 123.63   |
| 31  | A     | 416[B] | PHO  | CMB-C2B-C3B | 2.16  | 129.00      | 124.68   |
| 23  | D     | 403[A] | CLA  | OBD-CAD-C3D | -2.16 | 123.37      | 128.42   |
| 28  | d     | 406[B] | PL9  | C51-C49-C50 | 2.16  | 119.56      | 114.59   |
| 36  | C     | 518[B] | DGD  | O2G-C1B-O1B | -2.16 | 118.66      | 123.70   |
| 23  | a     | 405[A] | CLA  | CBC-CAC-C3C | -2.16 | 106.57      | 112.42   |
| 23  | C     | 511    | CLA  | CHB-C4A-NA  | 2.16  | 127.51      | 124.40   |
| 23  | B     | 602    | CLA  | C11-C10-C8  | -2.16 | 108.80      | 115.97   |
| 34  | d     | 412    | LMG  | O8-C9-C8    | -2.15 | 102.19      | 108.40   |
| 24  | D     | 405    | BCR  | C2-C1-C6    | 2.15  | 113.57      | 110.44   |
| 28  | d     | 406[B] | PL9  | C45-C44-C46 | 2.15  | 118.97      | 115.23   |
| 23  | c     | 513    | CLA  | CAA-C2A-C3A | -2.15 | 107.18      | 113.00   |
| 23  | A     | 404[B] | CLA  | CBC-CAC-C3C | -2.15 | 106.58      | 112.42   |
| 23  | B     | 604    | CLA  | O1D-CGD-CBD | -2.15 | 120.27      | 124.52   |
| 23  | d     | 404    | CLA  | CBC-CAC-C3C | -2.15 | 106.59      | 112.42   |
| 28  | D     | 406[B] | PL9  | O2-C1-C6    | -2.15 | 117.06      | 120.48   |
| 34  | c     | 501    | LMG  | O6-C5-C4    | 2.15  | 113.58      | 109.70   |
| 23  | a     | 405[B] | CLA  | CMB-C2B-C3B | 2.15  | 128.98      | 124.68   |
| 36  | C     | 517[A] | DGD  | O3G-C3G-C2G | -2.15 | 105.59      | 110.82   |
| 25  | X     | 101    | SQD  | O5-C1-O6    | 2.15  | 115.12      | 110.04   |
| 23  | C     | 504    | CLA  | C2A-C1A-CHA | -2.15 | 120.14      | 123.87   |
| 23  | c     | 502    | CLA  | C2A-C1A-CHA | -2.15 | 120.14      | 123.87   |
| 28  | D     | 406[A] | PL9  | C27-C28-C29 | -2.15 | 122.71      | 127.62   |
| 36  | C     | 517[B] | DGD  | O3G-C3G-C2G | -2.15 | 105.60      | 110.82   |
| 23  | a     | 407    | CLA  | CHB-C4A-NA  | 2.15  | 127.50      | 124.40   |
| 36  | c     | 517[A] | DGD  | O1G-C1A-O1A | -2.15 | 118.26      | 123.63   |
| 23  | d     | 402[A] | CLA  | CMB-C2B-C1B | 2.15  | 131.60      | 128.46   |
| 23  | c     | 511    | CLA  | O1D-CGD-CBD | -2.15 | 120.29      | 124.52   |
| 23  | b     | 604    | CLA  | C4-C3-C2    | -2.15 | 118.12      | 123.63   |
| 23  | B     | 615    | CLA  | C1-O2A-CGA  | 2.14  | 121.84      | 116.65   |
| 23  | C     | 508    | CLA  | CHA-C1A-NA  | -2.14 | 121.53      | 126.39   |
| 36  | H     | 102    | DGD  | O2G-C1B-C2B | 2.14  | 116.12      | 111.48   |
| 23  | b     | 608    | CLA  | CAA-C2A-C3A | -2.14 | 107.21      | 113.00   |
| 24  | b     | 619    | BCR  | C24-C23-C22 | -2.14 | 123.06      | 126.23   |
| 23  | B     | 608    | CLA  | OBD-CAD-C3D | -2.14 | 123.41      | 128.42   |
| 36  | c     | 518[B] | DGD  | O2G-C1B-O1B | -2.14 | 118.70      | 123.70   |
| 23  | d     | 403[A] | CLA  | CHD-C4C-NC  | 2.14  | 127.55      | 124.23   |
| 23  | B     | 612    | CLA  | C7-C6-C5    | -2.14 | 107.56      | 113.26   |
| 33  | L     | 101[B] | LHG  | O8-C23-O10  | -2.14 | 118.28      | 123.63   |
| 23  | b     | 606    | CLA  | O2A-CGA-CBA | 2.14  | 118.36      | 111.83   |
| 23  | b     | 610    | CLA  | O1D-CGD-CBD | -2.14 | 120.30      | 124.52   |
| 23  | B     | 613    | CLA  | C2A-C1A-CHA | -2.14 | 120.16      | 123.87   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 32  | t     | 101    | LMT  | O5'-C5'-C6' | 2.14  | 111.73      | 106.44   |
| 23  | C     | 513    | CLA  | CHC-C1C-C2C | -2.14 | 120.89      | 126.94   |
| 33  | b     | 629[B] | LHG  | C5-O7-C7    | -2.14 | 112.68      | 117.80   |
| 23  | b     | 603    | CLA  | C7-C6-C5    | -2.13 | 107.57      | 113.26   |
| 23  | B     | 614    | CLA  | C4-C3-C5    | 2.13  | 118.93      | 115.23   |
| 28  | D     | 406[B] | PL9  | C45-C44-C46 | 2.13  | 118.93      | 115.23   |
| 33  | L     | 101[A] | LHG  | O4-P-O5     | 2.13  | 122.36      | 112.44   |
| 31  | A     | 416[A] | PHO  | C6-C5-C3    | -2.13 | 108.28      | 113.47   |
| 24  | c     | 515    | BCR  | C21-C20-C19 | -2.13 | 117.03      | 123.20   |
| 38  | F     | 102    | HEM  | C3C-C4C-NC  | -2.13 | 106.92      | 110.94   |
| 23  | b     | 605    | CLA  | O2A-CGA-CBA | 2.13  | 118.33      | 111.83   |
| 24  | B     | 619    | BCR  | C16-C15-C14 | -2.13 | 119.16      | 123.52   |
| 23  | a     | 405[A] | CLA  | C4-C3-C5    | 2.13  | 118.92      | 115.23   |
| 23  | b     | 611    | CLA  | CHB-C4A-NA  | 2.13  | 127.47      | 124.40   |
| 23  | A     | 404[B] | CLA  | CHC-C1C-NC  | 2.13  | 127.52      | 124.31   |
| 32  | M     | 101    | LMT  | O6'-C6'-C5' | -2.13 | 104.09      | 111.33   |
| 23  | B     | 603    | CLA  | C7-C6-C5    | -2.13 | 107.59      | 113.26   |
| 23  | C     | 513    | CLA  | C1B-CHB-C4A | -2.13 | 125.98      | 130.04   |
| 23  | b     | 606    | CLA  | CMC-C2C-C1C | 2.13  | 128.36      | 125.03   |
| 23  | b     | 602    | CLA  | CHB-C4A-NA  | 2.13  | 127.47      | 124.40   |
| 23  | B     | 609    | CLA  | C7-C6-C5    | -2.13 | 107.59      | 113.26   |
| 23  | c     | 506    | CLA  | CMB-C2B-C1B | 2.13  | 131.57      | 128.46   |
| 23  | B     | 609    | CLA  | CHA-C1A-NA  | -2.13 | 121.58      | 126.39   |
| 23  | A     | 404[B] | CLA  | C7-C6-C5    | -2.12 | 107.60      | 113.26   |
| 24  | h     | 101    | BCR  | C2-C1-C6    | 2.12  | 113.52      | 110.44   |
| 23  | A     | 405[B] | CLA  | O2A-CGA-CBA | 2.12  | 118.31      | 111.83   |
| 23  | c     | 507    | CLA  | O2A-CGA-CBA | 2.12  | 118.31      | 111.83   |
| 25  | l     | 101    | SQD  | C44-O6-C1   | -2.12 | 109.25      | 113.80   |
| 28  | a     | 413[A] | PL9  | C45-C44-C46 | 2.12  | 118.91      | 115.23   |
| 23  | C     | 505    | CLA  | CMB-C2B-C3B | 2.12  | 128.92      | 124.68   |
| 24  | H     | 101    | BCR  | C36-C18-C17 | -2.12 | 119.38      | 122.82   |
| 34  | C     | 521    | LMG  | C9-C8-C7    | -2.12 | 106.84      | 111.78   |
| 24  | b     | 617    | BCR  | C8-C7-C6    | -2.12 | 121.33      | 127.00   |
| 23  | B     | 606    | CLA  | CAA-C2A-C3A | -2.12 | 107.27      | 113.00   |
| 23  | A     | 406[B] | CLA  | CAC-C3C-C4C | 2.12  | 127.55      | 124.79   |
| 24  | t     | 102    | BCR  | C20-C21-C22 | -2.12 | 124.31      | 127.28   |
| 36  | H     | 102    | DGD  | C3E-C4E-C5E | -2.12 | 106.39      | 110.23   |
| 23  | A     | 406[A] | CLA  | CHB-C4A-NA  | 2.12  | 127.46      | 124.40   |
| 23  | c     | 511    | CLA  | O2D-CGD-O1D | -2.12 | 119.73      | 123.85   |
| 23  | b     | 609    | CLA  | CMB-C2B-C3B | 2.12  | 128.91      | 124.68   |
| 34  | C     | 521    | LMG  | O6-C1-C2    | -2.12 | 106.02      | 110.37   |
| 32  | M     | 101    | LMT  | C3B-C4B-C5B | -2.12 | 106.40      | 110.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 614    | CLA  | C4-C3-C5    | 2.11  | 118.90      | 115.23   |
| 34  | Z     | 101    | LMG  | C1-O6-C5    | 2.11  | 117.85      | 113.72   |
| 23  | B     | 607    | CLA  | C11-C10-C8  | -2.11 | 108.94      | 115.97   |
| 24  | c     | 515    | BCR  | C7-C8-C9    | -2.11 | 123.11      | 126.23   |
| 23  | B     | 606    | CLA  | C1-O2A-CGA  | 2.11  | 121.76      | 116.65   |
| 23  | D     | 404    | CLA  | C4-C3-C2    | -2.11 | 118.20      | 123.63   |
| 23  | D     | 403[A] | CLA  | CMB-C2B-C3B | 2.11  | 128.90      | 124.68   |
| 23  | A     | 405[A] | CLA  | CHB-C4A-NA  | 2.11  | 127.44      | 124.40   |
| 33  | b     | 629[A] | LHG  | O7-C7-O9    | -2.11 | 118.77      | 123.70   |
| 24  | b     | 617    | BCR  | C35-C13-C12 | 2.11  | 121.31      | 118.09   |
| 23  | b     | 610    | CLA  | CMA-C3A-C2A | -2.11 | 105.83      | 113.98   |
| 33  | E     | 101[B] | LHG  | C5-O7-C7    | -2.11 | 112.75      | 117.80   |
| 23  | B     | 607    | CLA  | OBD-CAD-C3D | -2.11 | 123.49      | 128.42   |
| 36  | H     | 102    | DGD  | C2G-O2G-C1B | -2.11 | 112.75      | 117.80   |
| 23  | C     | 509    | CLA  | C4-C3-C5    | 2.11  | 118.89      | 115.23   |
| 23  | c     | 504    | CLA  | O2A-CGA-CBA | 2.11  | 118.26      | 111.83   |
| 23  | D     | 403[A] | CLA  | CBC-CAC-C3C | -2.11 | 106.71      | 112.42   |
| 23  | A     | 404[A] | CLA  | C7-C6-C5    | -2.11 | 107.65      | 113.26   |
| 23  | a     | 404[B] | CLA  | O2A-CGA-O1A | -2.10 | 118.36      | 123.63   |
| 23  | b     | 615    | CLA  | CHA-C1A-NA  | -2.10 | 121.63      | 126.39   |
| 31  | a     | 406[B] | PHO  | C4-C3-C5    | 2.10  | 118.88      | 115.23   |
| 24  | T     | 102    | BCR  | C7-C6-C5    | -2.10 | 116.71      | 121.56   |
| 23  | c     | 512    | CLA  | CMB-C2B-C3B | 2.10  | 128.88      | 124.68   |
| 23  | b     | 612    | CLA  | CMB-C2B-C3B | 2.10  | 128.88      | 124.68   |
| 23  | c     | 506    | CLA  | C4-C3-C5    | 2.10  | 118.88      | 115.23   |
| 23  | b     | 611    | CLA  | OBD-CAD-C3D | -2.10 | 123.50      | 128.42   |
| 23  | d     | 402[A] | CLA  | CHB-C4A-NA  | 2.10  | 127.43      | 124.40   |
| 24  | y     | 101    | BCR  | C11-C10-C9  | -2.10 | 124.33      | 127.28   |
| 34  | C     | 501    | LMG  | C9-C8-C7    | -2.10 | 106.89      | 111.78   |
| 28  | d     | 406[A] | PL9  | C45-C44-C46 | 2.10  | 118.87      | 115.23   |
| 23  | C     | 502    | CLA  | CBC-CAC-C3C | -2.10 | 106.73      | 112.42   |
| 23  | A     | 405[B] | CLA  | CMA-C3A-C2A | -2.10 | 105.86      | 113.98   |
| 24  | A     | 408    | BCR  | C11-C10-C9  | -2.10 | 124.33      | 127.28   |
| 24  | K     | 102    | BCR  | C33-C5-C6   | -2.10 | 122.19      | 124.48   |
| 24  | B     | 618    | BCR  | C10-C11-C12 | -2.10 | 117.12      | 123.20   |
| 23  | b     | 606    | CLA  | C1-C2-C3    | -2.10 | 122.76      | 126.20   |
| 23  | C     | 509    | CLA  | CAA-C2A-C3A | -2.10 | 107.33      | 113.00   |
| 24  | t     | 102    | BCR  | C2-C1-C6    | 2.10  | 113.48      | 110.44   |
| 23  | d     | 404    | CLA  | CGD-CBD-CAD | -2.10 | 104.06      | 110.85   |
| 36  | c     | 517[A] | DGD  | O1G-C1A-C2A | 2.10  | 118.23      | 111.83   |
| 23  | a     | 405[A] | CLA  | CAC-C3C-C4C | 2.09  | 127.52      | 124.79   |
| 24  | H     | 101    | BCR  | C11-C10-C9  | -2.09 | 124.34      | 127.28   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 511    | CLA  | C4-C3-C2    | -2.09 | 118.25      | 123.63   |
| 23  | b     | 602    | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 23  | b     | 616    | CLA  | C1B-CHB-C4A | -2.09 | 126.05      | 130.04   |
| 23  | b     | 605    | CLA  | OBD-CAD-C3D | -2.09 | 123.53      | 128.42   |
| 23  | B     | 604    | CLA  | CED-O2D-CGD | 2.09  | 120.66      | 115.92   |
| 23  | d     | 403[A] | CLA  | CBC-CAC-C3C | -2.09 | 106.75      | 112.42   |
| 23  | C     | 505    | CLA  | C4-C3-C5    | 2.09  | 118.86      | 115.23   |
| 24  | C     | 516    | BCR  | C21-C20-C19 | -2.09 | 117.15      | 123.20   |
| 32  | B     | 627    | LMT  | O5B-C5B-C4B | 2.09  | 113.46      | 109.70   |
| 23  | c     | 513    | CLA  | CAC-C3C-C4C | 2.09  | 127.50      | 124.79   |
| 28  | d     | 406[A] | PL9  | C2-C1-C6    | 2.08  | 121.48      | 119.00   |
| 24  | d     | 405    | BCR  | C28-C27-C26 | -2.08 | 110.34      | 114.06   |
| 25  | A     | 411    | SQD  | C9-C8-C7    | -2.08 | 106.07      | 113.69   |
| 32  | m     | 103    | LMT  | C1'-O5'-C5' | -2.08 | 109.66      | 113.72   |
| 38  | f     | 101    | HEM  | C3C-C4C-NC  | -2.08 | 107.01      | 110.94   |
| 23  | b     | 601    | CLA  | CAC-C3C-C4C | 2.08  | 127.50      | 124.79   |
| 28  | A     | 413[A] | PL9  | C53-C6-C1   | 2.08  | 119.54      | 115.28   |
| 25  | a     | 409[A] | SQD  | C3-C4-C5    | 2.08  | 114.00      | 110.23   |
| 26  | a     | 417    | GOL  | C3-C2-C1    | -2.08 | 104.18      | 111.80   |
| 36  | h     | 102    | DGD  | C2G-O2G-C1B | -2.08 | 112.83      | 117.80   |
| 23  | b     | 602    | CLA  | C1B-CHB-C4A | -2.08 | 126.08      | 130.04   |
| 23  | D     | 403[A] | CLA  | CMA-C3A-C2A | -2.08 | 105.96      | 113.98   |
| 23  | A     | 406[A] | CLA  | CBC-CAC-C3C | -2.08 | 106.79      | 112.42   |
| 23  | c     | 506    | CLA  | C2A-C1A-CHA | -2.07 | 120.27      | 123.87   |
| 31  | a     | 415[A] | PHO  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 24  | H     | 101    | BCR  | C7-C8-C9    | -2.07 | 123.17      | 126.23   |
| 23  | B     | 609    | CLA  | CMB-C2B-C1B | 2.07  | 131.49      | 128.46   |
| 23  | c     | 502    | CLA  | CMD-C2D-C3D | -2.07 | 122.94      | 127.69   |
| 23  | b     | 601    | CLA  | CBC-CAC-C3C | -2.07 | 106.81      | 112.42   |
| 24  | Y     | 101    | BCR  | C21-C20-C19 | -2.07 | 117.20      | 123.20   |
| 24  | Y     | 101    | BCR  | C36-C18-C17 | -2.07 | 119.46      | 122.82   |
| 23  | B     | 606    | CLA  | C1B-CHB-C4A | -2.07 | 126.09      | 130.04   |
| 23  | d     | 403[B] | CLA  | CMA-C3A-C2A | -2.07 | 105.99      | 113.98   |
| 33  | d     | 408[B] | LHG  | O8-C23-O10  | -2.07 | 118.46      | 123.63   |
| 23  | B     | 601    | CLA  | CAA-C2A-C3A | -2.07 | 107.42      | 113.00   |
| 23  | A     | 405[B] | CLA  | CED-O2D-CGD | 2.06  | 120.60      | 115.92   |
| 34  | m     | 101    | LMG  | C3-C4-C5    | 2.06  | 113.97      | 110.23   |
| 23  | C     | 506    | CLA  | O1D-CGD-CBD | -2.06 | 120.45      | 124.52   |
| 23  | b     | 608    | CLA  | C4-C3-C5    | 2.06  | 118.81      | 115.23   |
| 23  | a     | 405[A] | CLA  | CAA-CBA-CGA | 2.06  | 119.06      | 113.21   |
| 24  | D     | 405    | BCR  | C39-C30-C25 | -2.06 | 107.01      | 110.24   |
| 38  | f     | 101    | HEM  | O2D-CGD-CBD | 2.06  | 120.52      | 114.00   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 611    | CLA  | C1-O2A-CGA  | 2.06  | 121.64      | 116.65   |
| 24  | y     | 101    | BCR  | C40-C30-C25 | -2.06 | 107.01      | 110.24   |
| 23  | b     | 612    | CLA  | CMA-C3A-C2A | -2.06 | 106.02      | 113.98   |
| 23  | c     | 512    | CLA  | CAC-C3C-C4C | 2.06  | 127.47      | 124.79   |
| 24  | K     | 102    | BCR  | C20-C21-C22 | -2.06 | 124.39      | 127.28   |
| 23  | c     | 505    | CLA  | CMA-C3A-C2A | -2.06 | 106.02      | 113.98   |
| 23  | B     | 601    | CLA  | CMB-C2B-C3B | 2.06  | 128.80      | 124.68   |
| 23  | A     | 405[A] | CLA  | C1-C2-C3    | -2.06 | 122.82      | 126.20   |
| 23  | A     | 406[B] | CLA  | CHB-C4A-NA  | 2.06  | 127.37      | 124.40   |
| 24  | k     | 101    | BCR  | C3-C4-C5    | -2.06 | 110.39      | 114.06   |
| 23  | D     | 404    | CLA  | CHB-C4A-NA  | 2.06  | 127.37      | 124.40   |
| 24  | T     | 102    | BCR  | C3-C4-C5    | -2.06 | 110.39      | 114.06   |
| 32  | B     | 626    | LMT  | C1B-C2B-C3B | 2.06  | 114.33      | 110.01   |
| 23  | b     | 604    | CLA  | CHD-C4C-NC  | 2.06  | 127.42      | 124.23   |
| 23  | C     | 504    | CLA  | CMC-C2C-C1C | 2.05  | 128.25      | 125.03   |
| 31  | A     | 416[A] | PHO  | O2A-CGA-CBA | 2.05  | 118.10      | 111.83   |
| 23  | c     | 514    | CLA  | C4-C3-C5    | 2.05  | 118.79      | 115.23   |
| 36  | h     | 102    | DGD  | O2G-C1B-O1B | -2.05 | 118.90      | 123.70   |
| 23  | B     | 615    | CLA  | CHA-C1A-NA  | -2.05 | 121.74      | 126.39   |
| 23  | d     | 402[B] | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 23  | A     | 407    | CLA  | OBD-CAD-C3D | -2.05 | 123.62      | 128.42   |
| 23  | A     | 404[B] | CLA  | C1B-CHB-C4A | -2.05 | 126.13      | 130.04   |
| 23  | c     | 507    | CLA  | CMB-C2B-C3B | 2.05  | 128.78      | 124.68   |
| 23  | a     | 405[B] | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 34  | B     | 620    | LMG  | O6-C5-C4    | 2.05  | 113.39      | 109.70   |
| 38  | F     | 102    | HEM  | C4B-C3B-C2B | -2.05 | 105.39      | 107.28   |
| 28  | D     | 406[A] | PL9  | C47-C48-C49 | -2.05 | 120.81      | 127.64   |
| 24  | C     | 516    | BCR  | C3-C4-C5    | -2.05 | 110.40      | 114.06   |
| 24  | h     | 101    | BCR  | C29-C30-C25 | 2.05  | 113.42      | 110.44   |
| 28  | d     | 406[A] | PL9  | C40-C39-C38 | -2.05 | 118.37      | 123.63   |
| 23  | b     | 602    | CLA  | C3B-C4B-NB  | 2.05  | 111.86      | 109.21   |
| 23  | b     | 602    | CLA  | CMB-C2B-C3B | 2.05  | 128.77      | 124.68   |
| 28  | D     | 406[B] | PL9  | C42-C41-C39 | -2.05 | 106.41      | 113.19   |
| 24  | C     | 516    | BCR  | C39-C30-C25 | -2.05 | 107.03      | 110.24   |
| 23  | B     | 615    | CLA  | CAC-C3C-C4C | 2.05  | 127.45      | 124.79   |
| 25  | a     | 411    | SQD  | O47-C7-O49  | -2.05 | 118.92      | 123.70   |
| 23  | b     | 616    | CLA  | CHA-C1A-NA  | -2.05 | 121.76      | 126.39   |
| 25  | a     | 409[B] | SQD  | O5-C1-C2    | -2.04 | 106.17      | 110.37   |
| 23  | b     | 604    | CLA  | C1B-CHB-C4A | -2.04 | 126.14      | 130.04   |
| 23  | b     | 602    | CLA  | CAA-CBA-CGA | -2.04 | 107.41      | 113.21   |
| 24  | t     | 102    | BCR  | C29-C28-C27 | -2.04 | 106.79      | 111.28   |
| 28  | A     | 413[B] | PL9  | C10-C9-C8   | -2.04 | 118.39      | 123.63   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 405[A] | CLA  | CHA-C1A-NA  | -2.04 | 121.77      | 126.39   |
| 23  | b     | 602    | CLA  | C11-C10-C8  | -2.04 | 109.19      | 115.97   |
| 40  | v     | 201    | HEC  | CAD-CBD-CGD | -2.04 | 108.34      | 113.83   |
| 28  | A     | 413[A] | PL9  | C10-C9-C11  | 2.04  | 118.77      | 115.23   |
| 32  | F     | 101    | LMT  | C1'-O5'-C5' | -2.04 | 109.74      | 113.72   |
| 23  | d     | 404    | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 23  | B     | 610    | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.40   |
| 24  | K     | 102    | BCR  | C10-C11-C12 | -2.04 | 117.30      | 123.20   |
| 34  | c     | 520    | LMG  | O8-C28-O10  | -2.04 | 118.53      | 123.63   |
| 28  | a     | 413[A] | PL9  | C47-C46-C44 | -2.04 | 106.43      | 113.19   |
| 24  | t     | 102    | BCR  | C15-C14-C13 | -2.04 | 124.42      | 127.28   |
| 24  | a     | 408    | BCR  | C37-C22-C23 | 2.04  | 121.20      | 118.09   |
| 23  | A     | 405[B] | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.40   |
| 23  | b     | 613    | CLA  | OBD-CAD-C3D | -2.03 | 123.66      | 128.42   |
| 28  | A     | 413[B] | PL9  | C2-C3-C4    | 2.03  | 121.51      | 118.78   |
| 23  | a     | 405[B] | CLA  | CHB-C4A-NA  | 2.03  | 127.33      | 124.40   |
| 23  | d     | 403[A] | CLA  | CMB-C2B-C3B | 2.03  | 128.74      | 124.68   |
| 23  | B     | 604    | CLA  | CHA-C1A-NA  | -2.03 | 121.79      | 126.39   |
| 26  | l     | 103[A] | GOL  | C3-C2-C1    | -2.03 | 104.36      | 111.80   |
| 32  | M     | 101    | LMT  | O5B-C5B-C6B | 2.03  | 111.47      | 106.44   |
| 23  | C     | 513    | CLA  | O1D-CGD-CBD | -2.03 | 120.52      | 124.52   |
| 24  | d     | 405    | BCR  | C36-C18-C19 | 2.03  | 121.19      | 118.09   |
| 36  | c     | 518[A] | DGD  | O6E-C1E-O5D | -2.03 | 105.26      | 110.04   |
| 28  | a     | 413[A] | PL9  | C51-C49-C50 | 2.02  | 119.25      | 114.59   |
| 28  | D     | 406[B] | PL9  | C7-C3-C4    | 2.02  | 118.58      | 116.91   |
| 23  | C     | 506    | CLA  | CMB-C2B-C1B | 2.02  | 131.42      | 128.46   |
| 35  | b     | 625    | HTG  | C4-C3-C2    | -2.02 | 107.28      | 110.83   |
| 23  | c     | 503    | CLA  | C2A-C1A-CHA | -2.02 | 120.36      | 123.87   |
| 33  | L     | 101[B] | LHG  | C5-O7-C7    | -2.02 | 112.96      | 117.80   |
| 23  | b     | 607    | CLA  | CMA-C3A-C2A | -2.02 | 106.18      | 113.98   |
| 23  | A     | 404[B] | CLA  | CED-O2D-CGD | 2.02  | 120.50      | 115.92   |
| 23  | C     | 512    | CLA  | CBC-CAC-C3C | -2.02 | 106.95      | 112.42   |
| 23  | A     | 407    | CLA  | C11-C12-C13 | -2.02 | 109.26      | 115.97   |
| 23  | C     | 506    | CLA  | C4-C3-C2    | -2.02 | 118.44      | 123.63   |
| 32  | t     | 101    | LMT  | C1-O1'-C1'  | 2.02  | 117.13      | 113.68   |
| 24  | k     | 101    | BCR  | C10-C11-C12 | -2.02 | 117.35      | 123.20   |
| 33  | D     | 408[A] | LHG  | O4-P-O5     | 2.01  | 121.82      | 112.44   |
| 28  | A     | 413[A] | PL9  | C51-C49-C50 | 2.01  | 119.22      | 114.59   |
| 34  | c     | 520    | LMG  | O6-C5-C4    | 2.01  | 113.33      | 109.70   |
| 23  | c     | 504    | CLA  | CMD-C2D-C3D | -2.01 | 123.07      | 127.69   |
| 24  | C     | 516    | BCR  | C37-C22-C23 | 2.01  | 121.16      | 118.09   |
| 23  | A     | 406[B] | CLA  | CMC-C2C-C1C | 2.01  | 128.18      | 125.03   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 601    | CLA  | CMC-C2C-C1C | 2.01  | 128.18      | 125.03   |
| 23  | B     | 605    | CLA  | CAC-C3C-C2C | 2.01  | 131.25      | 127.56   |
| 28  | D     | 406[A] | PL9  | C45-C44-C46 | 2.01  | 118.72      | 115.23   |
| 23  | B     | 612    | CLA  | CHB-C4A-NA  | 2.01  | 127.30      | 124.40   |
| 23  | B     | 602    | CLA  | C1-C2-C3    | -2.01 | 122.90      | 126.20   |
| 24  | T     | 102    | BCR  | C10-C11-C12 | -2.01 | 117.38      | 123.20   |
| 23  | B     | 606    | CLA  | C1-C2-C3    | -2.01 | 122.91      | 126.20   |
| 38  | f     | 101    | HEM  | O2A-CGA-CBA | 2.01  | 120.35      | 114.00   |
| 23  | B     | 605    | CLA  | CAA-C2A-C3A | -2.01 | 107.57      | 113.00   |
| 26  | O     | 303    | GOL  | C3-C2-C1    | -2.01 | 104.43      | 111.80   |
| 28  | A     | 413[B] | PL9  | C7-C3-C4    | 2.01  | 118.56      | 116.91   |
| 36  | c     | 517[A] | DGD  | O2G-C1B-O1B | -2.01 | 119.01      | 123.70   |
| 34  | c     | 521    | LMG  | C13-C12-C11 | -2.00 | 105.77      | 113.13   |
| 23  | b     | 616    | CLA  | O1D-CGD-CBD | -2.00 | 120.57      | 124.52   |
| 23  | a     | 404[B] | CLA  | CHC-C1C-NC  | 2.00  | 127.33      | 124.31   |
| 23  | c     | 510    | CLA  | O2A-C1-C2   | 2.00  | 115.81      | 108.11   |
| 28  | D     | 406[A] | PL9  | C22-C23-C24 | -2.00 | 123.04      | 127.62   |
| 23  | b     | 615    | CLA  | CAC-C3C-C4C | 2.00  | 127.39      | 124.79   |
| 23  | a     | 404[B] | CLA  | CHB-C4A-NA  | 2.00  | 127.29      | 124.40   |
| 36  | c     | 519    | DGD  | O2G-C1B-O1B | -2.00 | 119.03      | 123.70   |
| 31  | a     | 406[B] | PHO  | CMC-C2C-C3C | 2.00  | 128.71      | 124.94   |

All (70) chirality outliers are listed below:

| Mol | Chain | Res    | Type | Atom |
|-----|-------|--------|------|------|
| 23  | A     | 404[A] | CLA  | ND   |
| 23  | A     | 404[B] | CLA  | ND   |
| 23  | A     | 405[A] | CLA  | ND   |
| 23  | A     | 405[B] | CLA  | ND   |
| 23  | A     | 407    | CLA  | ND   |
| 23  | B     | 601    | CLA  | ND   |
| 23  | B     | 602    | CLA  | ND   |
| 23  | B     | 603    | CLA  | ND   |
| 23  | B     | 604    | CLA  | ND   |
| 23  | B     | 605    | CLA  | ND   |
| 23  | B     | 606    | CLA  | ND   |
| 23  | B     | 607    | CLA  | ND   |
| 23  | B     | 609    | CLA  | ND   |
| 23  | B     | 610    | CLA  | ND   |
| 23  | B     | 611    | CLA  | ND   |
| 23  | B     | 612    | CLA  | ND   |
| 23  | B     | 613    | CLA  | ND   |

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| Mol | Chain | Res    | Type | Atom |
|-----|-------|--------|------|------|
| 23  | B     | 614    | CLA  | ND   |
| 23  | B     | 615    | CLA  | ND   |
| 23  | B     | 616    | CLA  | ND   |
| 23  | C     | 502    | CLA  | ND   |
| 23  | C     | 503    | CLA  | ND   |
| 23  | C     | 505    | CLA  | ND   |
| 23  | C     | 506    | CLA  | ND   |
| 23  | C     | 507    | CLA  | ND   |
| 23  | C     | 508    | CLA  | ND   |
| 23  | C     | 509    | CLA  | ND   |
| 23  | C     | 510    | CLA  | ND   |
| 23  | C     | 511    | CLA  | ND   |
| 23  | C     | 512    | CLA  | ND   |
| 23  | C     | 513    | CLA  | ND   |
| 23  | C     | 514    | CLA  | ND   |
| 23  | D     | 403[A] | CLA  | ND   |
| 23  | D     | 403[B] | CLA  | ND   |
| 23  | D     | 404    | CLA  | ND   |
| 23  | a     | 404[A] | CLA  | ND   |
| 23  | a     | 404[B] | CLA  | ND   |
| 23  | a     | 407    | CLA  | ND   |
| 23  | b     | 601    | CLA  | ND   |
| 23  | b     | 602    | CLA  | ND   |
| 23  | b     | 603    | CLA  | ND   |
| 23  | b     | 604    | CLA  | ND   |
| 23  | b     | 605    | CLA  | ND   |
| 23  | b     | 606    | CLA  | ND   |
| 23  | b     | 607    | CLA  | ND   |
| 23  | b     | 609    | CLA  | ND   |
| 23  | b     | 610    | CLA  | ND   |
| 23  | b     | 611    | CLA  | ND   |
| 23  | b     | 612    | CLA  | ND   |
| 23  | b     | 613    | CLA  | ND   |
| 23  | b     | 614    | CLA  | ND   |
| 23  | b     | 615    | CLA  | ND   |
| 23  | b     | 616    | CLA  | ND   |
| 23  | c     | 502    | CLA  | ND   |
| 23  | c     | 503    | CLA  | ND   |
| 23  | c     | 504    | CLA  | ND   |
| 23  | c     | 505    | CLA  | ND   |
| 23  | c     | 506    | CLA  | ND   |
| 23  | c     | 507    | CLA  | ND   |

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| Mol | Chain | Res    | Type | Atom |
|-----|-------|--------|------|------|
| 23  | c     | 508    | CLA  | ND   |
| 23  | c     | 509    | CLA  | ND   |
| 23  | c     | 510    | CLA  | ND   |
| 23  | c     | 511    | CLA  | ND   |
| 23  | c     | 512    | CLA  | ND   |
| 23  | c     | 513    | CLA  | ND   |
| 23  | d     | 402[A] | CLA  | ND   |
| 23  | d     | 402[B] | CLA  | ND   |
| 23  | d     | 403[A] | CLA  | ND   |
| 23  | d     | 403[B] | CLA  | ND   |
| 23  | d     | 404    | CLA  | ND   |

All (1566) torsion outliers are listed below:

| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | B     | 614    | CLA  | CAD-CBD-CGD-O1D |
| 23  | B     | 614    | CLA  | CAD-CBD-CGD-O2D |
| 23  | C     | 505    | CLA  | C2-C3-C5-C6     |
| 23  | C     | 505    | CLA  | C4-C3-C5-C6     |
| 23  | C     | 510    | CLA  | CHA-CBD-CGD-O1D |
| 23  | C     | 510    | CLA  | CHA-CBD-CGD-O2D |
| 23  | b     | 606    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 614    | CLA  | CAD-CBD-CGD-O1D |
| 23  | b     | 614    | CLA  | CAD-CBD-CGD-O2D |
| 23  | c     | 505    | CLA  | C11-C12-C13-C14 |
| 23  | c     | 508    | CLA  | CHA-CBD-CGD-O1D |
| 23  | c     | 508    | CLA  | CHA-CBD-CGD-O2D |
| 23  | c     | 510    | CLA  | C2-C1-O2A-CGA   |
| 23  | c     | 510    | CLA  | C11-C10-C8-C9   |
| 24  | T     | 102    | BCR  | C13-C14-C15-C16 |
| 24  | Y     | 101    | BCR  | C1-C6-C7-C8     |
| 24  | Y     | 101    | BCR  | C5-C6-C7-C8     |
| 24  | d     | 405    | BCR  | C21-C22-C23-C24 |
| 24  | y     | 101    | BCR  | C1-C6-C7-C8     |
| 24  | y     | 101    | BCR  | C5-C6-C7-C8     |
| 25  | A     | 409[B] | SQD  | C8-C7-O47-C45   |
| 25  | A     | 411    | SQD  | O6-C44-C45-O47  |
| 25  | X     | 101    | SQD  | C2-C1-O6-C44    |
| 25  | X     | 101    | SQD  | O49-C7-O47-C45  |
| 25  | X     | 101    | SQD  | C8-C7-O47-C45   |
| 25  | a     | 411    | SQD  | O6-C44-C45-O47  |
| 25  | a     | 411    | SQD  | C5-C6-S-O7      |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 25  | a     | 411    | SQD  | C5-C6-S-O8      |
| 25  | a     | 411    | SQD  | C5-C6-S-O9      |
| 25  | b     | 620    | SQD  | C8-C7-O47-C45   |
| 25  | f     | 102    | SQD  | O6-C44-C45-O47  |
| 25  | f     | 102    | SQD  | O49-C7-O47-C45  |
| 25  | f     | 102    | SQD  | C8-C7-O47-C45   |
| 25  | l     | 101    | SQD  | O49-C7-O47-C45  |
| 26  | A     | 410    | GOL  | O1-C1-C2-C3     |
| 26  | B     | 622    | GOL  | C1-C2-C3-O3     |
| 26  | D     | 402    | GOL  | O1-C1-C2-C3     |
| 26  | D     | 413    | GOL  | C1-C2-C3-O3     |
| 26  | O     | 303    | GOL  | O1-C1-C2-C3     |
| 26  | V     | 203[A] | GOL  | C1-C2-C3-O3     |
| 26  | V     | 203[B] | GOL  | C1-C2-C3-O3     |
| 26  | V     | 203[B] | GOL  | O2-C2-C3-O3     |
| 26  | a     | 410    | GOL  | O1-C1-C2-C3     |
| 26  | b     | 624    | GOL  | C1-C2-C3-O3     |
| 26  | c     | 527    | GOL  | C1-C2-C3-O3     |
| 26  | o     | 304    | GOL  | O1-C1-C2-C3     |
| 26  | o     | 304    | GOL  | C1-C2-C3-O3     |
| 28  | A     | 413[A] | PL9  | C9-C11-C12-C13  |
| 28  | A     | 413[B] | PL9  | C9-C11-C12-C13  |
| 28  | A     | 413[B] | PL9  | C30-C29-C31-C32 |
| 28  | a     | 413[A] | PL9  | C23-C24-C26-C27 |
| 28  | a     | 413[A] | PL9  | C25-C24-C26-C27 |
| 32  | A     | 417    | LMT  | C2'-C1'-O1'-C1  |
| 32  | A     | 417    | LMT  | O5'-C1'-O1'-C1  |
| 32  | A     | 419    | LMT  | C2'-C1'-O1'-C1  |
| 32  | A     | 419    | LMT  | O5'-C1'-O1'-C1  |
| 32  | B     | 627    | LMT  | C2'-C1'-O1'-C1  |
| 32  | B     | 629    | LMT  | O5'-C1'-O1'-C1  |
| 32  | B     | 629    | LMT  | C2-C1-O1'-C1'   |
| 32  | F     | 101    | LMT  | C2'-C1'-O1'-C1  |
| 32  | F     | 101    | LMT  | O5'-C1'-O1'-C1  |
| 32  | b     | 621    | LMT  | C2'-C1'-O1'-C1  |
| 32  | b     | 627    | LMT  | C2'-C1'-O1'-C1  |
| 32  | b     | 627    | LMT  | O5'-C1'-O1'-C1  |
| 32  | t     | 101    | LMT  | O5'-C1'-O1'-C1  |
| 32  | t     | 101    | LMT  | C2-C1-O1'-C1'   |
| 33  | D     | 407[A] | LHG  | O2-C2-C3-O3     |
| 33  | D     | 407[A] | LHG  | C3-O3-P-O4      |
| 33  | D     | 407[A] | LHG  | C3-O3-P-O5      |

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| Mol | Chain | Res    | Type | Atoms         |
|-----|-------|--------|------|---------------|
| 33  | D     | 407[A] | LHG  | C3-O3-P-O6    |
| 33  | D     | 407[A] | LHG  | C4-O6-P-O4    |
| 33  | D     | 407[B] | LHG  | O2-C2-C3-O3   |
| 33  | D     | 407[B] | LHG  | C3-O3-P-O4    |
| 33  | D     | 407[B] | LHG  | C3-O3-P-O5    |
| 33  | D     | 407[B] | LHG  | C3-O3-P-O6    |
| 33  | D     | 407[B] | LHG  | C4-O6-P-O3    |
| 33  | D     | 407[B] | LHG  | C4-O6-P-O4    |
| 33  | D     | 407[B] | LHG  | C4-O6-P-O5    |
| 33  | E     | 101[A] | LHG  | C3-O3-P-O4    |
| 33  | E     | 101[A] | LHG  | C3-O3-P-O5    |
| 33  | E     | 101[A] | LHG  | C3-O3-P-O6    |
| 33  | E     | 101[A] | LHG  | C4-O6-P-O3    |
| 33  | E     | 101[A] | LHG  | O10-C23-O8-C6 |
| 33  | E     | 101[A] | LHG  | C24-C23-O8-C6 |
| 33  | E     | 101[B] | LHG  | C3-O3-P-O4    |
| 33  | E     | 101[B] | LHG  | C3-O3-P-O5    |
| 33  | E     | 101[B] | LHG  | C3-O3-P-O6    |
| 33  | E     | 101[B] | LHG  | C4-O6-P-O3    |
| 33  | E     | 101[B] | LHG  | O10-C23-O8-C6 |
| 33  | E     | 101[B] | LHG  | C24-C23-O8-C6 |
| 33  | L     | 101[A] | LHG  | C4-O6-P-O3    |
| 33  | L     | 101[A] | LHG  | C4-O6-P-O4    |
| 33  | L     | 101[A] | LHG  | C4-O6-P-O5    |
| 33  | L     | 101[B] | LHG  | C4-O6-P-O3    |
| 33  | L     | 101[B] | LHG  | C4-O6-P-O4    |
| 33  | L     | 101[B] | LHG  | C4-O6-P-O5    |
| 33  | a     | 419[A] | LHG  | C3-O3-P-O4    |
| 33  | a     | 419[A] | LHG  | C3-O3-P-O6    |
| 33  | a     | 419[A] | LHG  | C4-O6-P-O3    |
| 33  | a     | 419[A] | LHG  | C4-O6-P-O5    |
| 33  | a     | 419[A] | LHG  | O10-C23-O8-C6 |
| 33  | a     | 419[A] | LHG  | C24-C23-O8-C6 |
| 33  | a     | 419[B] | LHG  | C3-O3-P-O4    |
| 33  | a     | 419[B] | LHG  | C3-O3-P-O6    |
| 33  | a     | 419[B] | LHG  | C4-O6-P-O3    |
| 33  | a     | 419[B] | LHG  | C4-O6-P-O5    |
| 33  | a     | 419[B] | LHG  | O10-C23-O8-C6 |
| 33  | a     | 419[B] | LHG  | C24-C23-O8-C6 |
| 33  | b     | 629[A] | LHG  | C4-O6-P-O3    |
| 33  | b     | 629[A] | LHG  | C4-O6-P-O4    |
| 33  | b     | 629[A] | LHG  | C4-O6-P-O5    |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | b     | 629[B] | LHG  | C4-O6-P-O3      |
| 33  | b     | 629[B] | LHG  | C4-O6-P-O4      |
| 33  | b     | 629[B] | LHG  | C4-O6-P-O5      |
| 33  | d     | 407[A] | LHG  | C3-O3-P-O4      |
| 33  | d     | 407[A] | LHG  | C3-O3-P-O5      |
| 33  | d     | 407[A] | LHG  | C3-O3-P-O6      |
| 33  | d     | 407[A] | LHG  | C4-O6-P-O4      |
| 33  | d     | 407[B] | LHG  | O2-C2-C3-O3     |
| 33  | d     | 407[B] | LHG  | C3-O3-P-O4      |
| 33  | d     | 407[B] | LHG  | C3-O3-P-O6      |
| 33  | d     | 407[B] | LHG  | C4-O6-P-O3      |
| 33  | d     | 407[B] | LHG  | C4-O6-P-O4      |
| 33  | d     | 407[B] | LHG  | C4-O6-P-O5      |
| 33  | d     | 414[A] | LHG  | C3-O3-P-O5      |
| 34  | C     | 521    | LMG  | C11-C10-O7-C8   |
| 34  | c     | 521    | LMG  | O9-C10-O7-C8    |
| 34  | c     | 521    | LMG  | C11-C10-O7-C8   |
| 34  | Z     | 101    | LMG  | O9-C10-O7-C8    |
| 34  | Z     | 101    | LMG  | C11-C10-O7-C8   |
| 34  | z     | 101    | LMG  | O6-C1-O1-C7     |
| 34  | z     | 101    | LMG  | O9-C10-O7-C8    |
| 32  | A     | 419    | LMT  | O5B-C1B-O1B-C4' |
| 32  | B     | 627    | LMT  | C4'-C5'-C6'-O6' |
| 32  | T     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 25  | A     | 409[A] | SQD  | O49-C7-O47-C45  |
| 25  | A     | 409[B] | SQD  | O49-C7-O47-C45  |
| 25  | b     | 620    | SQD  | O49-C7-O47-C45  |
| 34  | C     | 521    | LMG  | O9-C10-O7-C8    |
| 23  | B     | 614    | CLA  | C3-C5-C6-C7     |
| 23  | c     | 513    | CLA  | C3-C5-C6-C7     |
| 23  | d     | 404    | CLA  | C3-C5-C6-C7     |
| 32  | a     | 416    | LMT  | O5B-C5B-C6B-O6B |
| 23  | c     | 514    | CLA  | CBD-CGD-O2D-CED |
| 25  | l     | 101    | SQD  | C8-C7-O47-C45   |
| 34  | z     | 101    | LMG  | C11-C10-O7-C8   |
| 32  | T     | 101    | LMT  | C4B-C5B-C6B-O6B |
| 23  | A     | 407    | CLA  | C4-C3-C5-C6     |
| 23  | B     | 605    | CLA  | C4-C3-C5-C6     |
| 23  | a     | 407    | CLA  | C4-C3-C5-C6     |
| 23  | d     | 404    | CLA  | C4-C3-C5-C6     |
| 28  | A     | 413[A] | PL9  | C15-C14-C16-C17 |
| 23  | a     | 407    | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | d     | 404    | CLA  | C2-C3-C5-C6     |
| 23  | b     | 616    | CLA  | C3-C5-C6-C7     |
| 32  | B     | 626    | LMT  | C4'-C5'-C6'-O6' |
| 32  | m     | 103    | LMT  | C4B-C5B-C6B-O6B |
| 32  | F     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 32  | B     | 626    | LMT  | O5'-C5'-C6'-O6' |
| 32  | b     | 627    | LMT  | O5'-C5'-C6'-O6' |
| 35  | D     | 411    | HTG  | O5-C5-C6-O6     |
| 33  | d     | 407[A] | LHG  | O2-C2-C3-O3     |
| 32  | B     | 627    | LMT  | O5B-C5B-C6B-O6B |
| 34  | C     | 521    | LMG  | O6-C5-C6-O5     |
| 32  | T     | 101    | LMT  | C4'-C5'-C6'-O6' |
| 32  | a     | 416    | LMT  | C4B-C5B-C6B-O6B |
| 32  | e     | 101    | LMT  | C4'-C5'-C6'-O6' |
| 25  | A     | 409[A] | SQD  | C8-C7-O47-C45   |
| 35  | B     | 623    | HTG  | O5-C5-C6-O6     |
| 23  | D     | 404    | CLA  | CBD-CGD-O2D-CED |
| 23  | c     | 513    | CLA  | CBD-CGD-O2D-CED |
| 32  | B     | 626    | LMT  | O5B-C5B-C6B-O6B |
| 32  | m     | 103    | LMT  | O5B-C5B-C6B-O6B |
| 35  | D     | 411    | HTG  | C4-C5-C6-O6     |
| 35  | D     | 411    | HTG  | S1-C1'-C2'-C3'  |
| 35  | b     | 625    | HTG  | S1-C1'-C2'-C3'  |
| 23  | C     | 508    | CLA  | C4-C3-C5-C6     |
| 23  | b     | 614    | CLA  | C4-C3-C5-C6     |
| 23  | c     | 508    | CLA  | C4-C3-C5-C6     |
| 28  | A     | 413[A] | PL9  | C20-C19-C21-C22 |
| 28  | a     | 413[A] | PL9  | C15-C14-C16-C17 |
| 28  | a     | 413[A] | PL9  | C30-C29-C31-C32 |
| 28  | a     | 413[B] | PL9  | C15-C14-C16-C17 |
| 23  | A     | 407    | CLA  | C2-C3-C5-C6     |
| 23  | C     | 508    | CLA  | C2-C3-C5-C6     |
| 23  | b     | 603    | CLA  | C2-C3-C5-C6     |
| 23  | b     | 605    | CLA  | C2-C3-C5-C6     |
| 23  | b     | 614    | CLA  | C2-C3-C5-C6     |
| 23  | c     | 508    | CLA  | C2-C3-C5-C6     |
| 28  | A     | 413[A] | PL9  | C13-C14-C16-C17 |
| 28  | A     | 413[A] | PL9  | C18-C19-C21-C22 |
| 28  | A     | 413[B] | PL9  | C13-C14-C16-C17 |
| 28  | A     | 413[B] | PL9  | C18-C19-C21-C22 |
| 28  | a     | 413[A] | PL9  | C13-C14-C16-C17 |
| 28  | a     | 413[A] | PL9  | C28-C29-C31-C32 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 28  | a     | 413[B] | PL9  | C13-C14-C16-C17 |
| 28  | a     | 413[B] | PL9  | C28-C29-C31-C32 |
| 28  | A     | 413[A] | PL9  | C14-C16-C17-C18 |
| 28  | A     | 413[A] | PL9  | C44-C46-C47-C48 |
| 28  | A     | 413[B] | PL9  | C14-C16-C17-C18 |
| 28  | A     | 413[B] | PL9  | C44-C46-C47-C48 |
| 28  | D     | 406[A] | PL9  | C39-C41-C42-C43 |
| 28  | D     | 406[B] | PL9  | C39-C41-C42-C43 |
| 28  | a     | 413[A] | PL9  | C9-C11-C12-C13  |
| 28  | a     | 413[A] | PL9  | C14-C16-C17-C18 |
| 28  | a     | 413[B] | PL9  | C9-C11-C12-C13  |
| 28  | a     | 413[B] | PL9  | C14-C16-C17-C18 |
| 28  | d     | 406[B] | PL9  | C39-C41-C42-C43 |
| 32  | F     | 101    | LMT  | C4'-C5'-C6'-O6' |
| 34  | c     | 521    | LMG  | C4-C5-C6-O5     |
| 32  | B     | 629    | LMT  | O5'-C5'-C6'-O6' |
| 32  | b     | 621    | LMT  | O5'-C1'-O1'-C1  |
| 23  | c     | 510    | CLA  | CBA-CGA-O2A-C1  |
| 23  | C     | 510    | CLA  | CBD-CGD-O2D-CED |
| 23  | c     | 511    | CLA  | CBD-CGD-O2D-CED |
| 23  | c     | 512    | CLA  | CBD-CGD-O2D-CED |
| 32  | A     | 419    | LMT  | O5B-C5B-C6B-O6B |
| 32  | A     | 419    | LMT  | O5'-C5'-C6'-O6' |
| 32  | B     | 627    | LMT  | O5'-C5'-C6'-O6' |
| 32  | b     | 621    | LMT  | O5'-C5'-C6'-O6' |
| 35  | b     | 625    | HTG  | O5-C5-C6-O6     |
| 32  | T     | 101    | LMT  | O5B-C5B-C6B-O6B |
| 23  | C     | 514    | CLA  | CBD-CGD-O2D-CED |
| 33  | D     | 407[B] | LHG  | C1-C2-C3-O3     |
| 33  | d     | 407[A] | LHG  | C1-C2-C3-O3     |
| 23  | a     | 407    | CLA  | CBA-CGA-O2A-C1  |
| 32  | B     | 627    | LMT  | C4B-C5B-C6B-O6B |
| 32  | B     | 629    | LMT  | C4'-C5'-C6'-O6' |
| 23  | b     | 603    | CLA  | C4-C3-C5-C6     |
| 23  | b     | 605    | CLA  | C4-C3-C5-C6     |
| 28  | A     | 413[B] | PL9  | C15-C14-C16-C17 |
| 28  | A     | 413[B] | PL9  | C20-C19-C21-C22 |
| 28  | a     | 413[B] | PL9  | C30-C29-C31-C32 |
| 23  | B     | 605    | CLA  | C2-C3-C5-C6     |
| 23  | C     | 503    | CLA  | C14-C13-C15-C16 |
| 23  | C     | 507    | CLA  | C14-C13-C15-C16 |
| 23  | b     | 601    | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | b     | 604    | CLA  | C6-C7-C8-C9     |
| 23  | b     | 616    | CLA  | C6-C7-C8-C9     |
| 32  | b     | 627    | LMT  | C4'-C5'-C6'-O6' |
| 34  | c     | 520    | LMG  | C4-C5-C6-O5     |
| 32  | e     | 101    | LMT  | C2'-C1'-O1'-C1  |
| 25  | X     | 101    | SQD  | C23-C24-C25-C26 |
| 32  | e     | 101    | LMT  | O5B-C5B-C6B-O6B |
| 24  | b     | 619    | BCR  | C7-C8-C9-C34    |
| 24  | c     | 516    | BCR  | C7-C8-C9-C34    |
| 24  | b     | 619    | BCR  | C7-C8-C9-C10    |
| 23  | b     | 606    | CLA  | C2A-CAA-CBA-CGA |
| 23  | a     | 407    | CLA  | O1A-CGA-O2A-C1  |
| 32  | e     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 23  | c     | 502    | CLA  | CBD-CGD-O2D-CED |
| 32  | A     | 419    | LMT  | C5'-C4'-O1B-C1B |
| 32  | B     | 626    | LMT  | C5'-C4'-O1B-C1B |
| 23  | C     | 508    | CLA  | C5-C6-C7-C8     |
| 26  | B     | 622    | GOL  | O2-C2-C3-O3     |
| 26  | a     | 410    | GOL  | O1-C1-C2-O2     |
| 23  | A     | 407    | CLA  | C3-C5-C6-C7     |
| 32  | A     | 419    | LMT  | C4B-C5B-C6B-O6B |
| 36  | c     | 518[B] | DGD  | C1B-C2B-C3B-C4B |
| 23  | C     | 511    | CLA  | C11-C12-C13-C15 |
| 28  | A     | 413[A] | PL9  | C30-C29-C31-C32 |
| 28  | a     | 413[B] | PL9  | C25-C24-C26-C27 |
| 34  | c     | 521    | LMG  | O6-C5-C6-O5     |
| 28  | a     | 413[B] | PL9  | C24-C26-C27-C28 |
| 28  | d     | 406[A] | PL9  | C39-C41-C42-C43 |
| 23  | c     | 510    | CLA  | C3-C5-C6-C7     |
| 23  | B     | 601    | CLA  | C10-C11-C12-C13 |
| 32  | a     | 416    | LMT  | O1'-C1-C2-C3    |
| 32  | t     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 36  | c     | 518[A] | DGD  | C1B-C2B-C3B-C4B |
| 23  | A     | 407    | CLA  | C5-C6-C7-C8     |
| 23  | B     | 606    | CLA  | C2A-CAA-CBA-CGA |
| 23  | C     | 509    | CLA  | C10-C11-C12-C13 |
| 23  | b     | 606    | CLA  | C10-C11-C12-C13 |
| 23  | b     | 606    | CLA  | C13-C15-C16-C17 |
| 25  | l     | 101    | SQD  | C7-C8-C9-C10    |
| 33  | E     | 101[A] | LHG  | C23-C24-C25-C26 |
| 23  | C     | 512    | CLA  | C3-C5-C6-C7     |
| 25  | X     | 101    | SQD  | O5-C1-O6-C44    |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 32  | B     | 627    | LMT  | O5'-C1'-O1'-C1  |
| 32  | e     | 101    | LMT  | O5'-C1'-O1'-C1  |
| 23  | B     | 601    | CLA  | C5-C6-C7-C8     |
| 23  | B     | 602    | CLA  | C13-C15-C16-C17 |
| 23  | D     | 404    | CLA  | C10-C11-C12-C13 |
| 23  | b     | 601    | CLA  | C10-C11-C12-C13 |
| 23  | c     | 510    | CLA  | O1A-CGA-O2A-C1  |
| 34  | Z     | 101    | LMG  | C10-C11-C12-C13 |
| 23  | c     | 514    | CLA  | C10-C11-C12-C13 |
| 32  | A     | 419    | LMT  | O1'-C1-C2-C3    |
| 23  | c     | 514    | CLA  | O1D-CGD-O2D-CED |
| 23  | b     | 604    | CLA  | C8-C10-C11-C12  |
| 23  | c     | 513    | CLA  | C15-C16-C17-C18 |
| 23  | B     | 606    | CLA  | C10-C11-C12-C13 |
| 34  | B     | 620    | LMG  | C39-C40-C41-C42 |
| 35  | b     | 622    | HTG  | S1-C1'-C2'-C3'  |
| 23  | B     | 614    | CLA  | C8-C10-C11-C12  |
| 23  | D     | 404    | CLA  | C3-C5-C6-C7     |
| 23  | a     | 404[A] | CLA  | C15-C16-C17-C18 |
| 34  | B     | 620    | LMG  | O9-C10-O7-C8    |
| 33  | D     | 407[A] | LHG  | C1-C2-C3-O3     |
| 33  | d     | 407[B] | LHG  | C1-C2-C3-O3     |
| 25  | l     | 101    | SQD  | C30-C31-C32-C33 |
| 33  | D     | 408[A] | LHG  | C33-C34-C35-C36 |
| 35  | b     | 623    | HTG  | C1'-C2'-C3'-C4' |
| 23  | B     | 614    | CLA  | C10-C11-C12-C13 |
| 23  | C     | 512    | CLA  | C8-C10-C11-C12  |
| 23  | a     | 404[B] | CLA  | C15-C16-C17-C18 |
| 23  | b     | 614    | CLA  | C8-C10-C11-C12  |
| 36  | C     | 519    | DGD  | C6B-C7B-C8B-C9B |
| 36  | c     | 517[B] | DGD  | O6D-C5D-C6D-O5D |
| 23  | b     | 604    | CLA  | C5-C6-C7-C8     |
| 23  | b     | 611    | CLA  | C8-C10-C11-C12  |
| 23  | c     | 508    | CLA  | C5-C6-C7-C8     |
| 33  | D     | 408[B] | LHG  | C33-C34-C35-C36 |
| 36  | h     | 102    | DGD  | C6B-C7B-C8B-C9B |
| 32  | B     | 626    | LMT  | C6-C7-C8-C9     |
| 23  | b     | 611    | CLA  | C15-C16-C17-C18 |
| 36  | C     | 517[B] | DGD  | O6D-C5D-C6D-O5D |
| 32  | A     | 419    | LMT  | C4'-C5'-C6'-O6' |
| 34  | B     | 620    | LMG  | C11-C10-O7-C8   |
| 25  | A     | 411    | SQD  | C2-C1-O6-C44    |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 32  | B     | 629    | LMT  | C2'-C1'-O1'-C1  |
| 32  | t     | 101    | LMT  | C2'-C1'-O1'-C1  |
| 36  | C     | 518[A] | DGD  | C2E-C1E-O5D-C6D |
| 36  | C     | 518[B] | DGD  | C2E-C1E-O5D-C6D |
| 25  | A     | 409[A] | SQD  | C7-C8-C9-C10    |
| 23  | c     | 510    | CLA  | C16-C17-C18-C20 |
| 23  | b     | 614    | CLA  | C10-C11-C12-C13 |
| 24  | Y     | 101    | BCR  | C37-C22-C23-C24 |
| 24  | d     | 405    | BCR  | C37-C22-C23-C24 |
| 35  | B     | 623    | HTG  | S1-C1'-C2'-C3'  |
| 24  | Y     | 101    | BCR  | C21-C22-C23-C24 |
| 23  | b     | 610    | CLA  | C2A-CAA-CBA-CGA |
| 36  | c     | 517[B] | DGD  | C4D-C5D-C6D-O5D |
| 26  | B     | 622    | GOL  | O1-C1-C2-C3     |
| 26  | B     | 625    | GOL  | C1-C2-C3-O3     |
| 26  | D     | 413    | GOL  | O1-C1-C2-C3     |
| 26  | O     | 302    | GOL  | O1-C1-C2-C3     |
| 26  | a     | 410    | GOL  | C1-C2-C3-O3     |
| 26  | a     | 417    | GOL  | O1-C1-C2-C3     |
| 26  | a     | 418    | GOL  | C1-C2-C3-O3     |
| 26  | d     | 413    | GOL  | O1-C1-C2-C3     |
| 26  | o     | 303    | GOL  | C1-C2-C3-O3     |
| 26  | v     | 202[A] | GOL  | O1-C1-C2-C3     |
| 26  | v     | 202[B] | GOL  | O1-C1-C2-C3     |
| 33  | A     | 418[B] | LHG  | O1-C1-C2-C3     |
| 25  | A     | 409[B] | SQD  | C7-C8-C9-C10    |
| 35  | B     | 623    | HTG  | C4-C5-C6-O6     |
| 23  | b     | 602    | CLA  | C16-C17-C18-C20 |
| 23  | b     | 614    | CLA  | C16-C17-C18-C20 |
| 23  | d     | 404    | CLA  | C16-C17-C18-C20 |
| 23  | B     | 616    | CLA  | C3-C5-C6-C7     |
| 23  | b     | 606    | CLA  | C15-C16-C17-C18 |
| 25  | A     | 411    | SQD  | O5-C1-O6-C44    |
| 25  | l     | 101    | SQD  | O5-C1-O6-C44    |
| 32  | A     | 417    | LMT  | O1'-C1-C2-C3    |
| 25  | b     | 620    | SQD  | C18-C19-C20-C21 |
| 23  | c     | 513    | CLA  | O1D-CGD-O2D-CED |
| 25  | A     | 409[A] | SQD  | C12-C13-C14-C15 |
| 23  | B     | 616    | CLA  | C2-C1-O2A-CGA   |
| 23  | B     | 603    | CLA  | C16-C17-C18-C19 |
| 23  | a     | 407    | CLA  | C16-C17-C18-C19 |
| 23  | b     | 602    | CLA  | C16-C17-C18-C19 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | b     | 615    | CLA  | C16-C17-C18-C19 |
| 23  | c     | 509    | CLA  | C16-C17-C18-C19 |
| 23  | c     | 510    | CLA  | C16-C17-C18-C19 |
| 33  | L     | 101[A] | LHG  | C15-C16-C17-C18 |
| 33  | L     | 101[A] | LHG  | C17-C18-C19-C20 |
| 36  | c     | 518[A] | DGD  | C9A-CAA-CBA-CCA |
| 32  | a     | 416    | LMT  | C1-C2-C3-C4     |
| 32  | t     | 101    | LMT  | C4-C5-C6-C7     |
| 33  | L     | 101[B] | LHG  | C13-C14-C15-C16 |
| 33  | b     | 629[B] | LHG  | C27-C28-C29-C30 |
| 34  | D     | 412    | LMG  | C19-C20-C21-C22 |
| 35  | B     | 621    | HTG  | C3'-C4'-C5'-C6' |
| 36  | c     | 517[B] | DGD  | C2B-C3B-C4B-C5B |
| 25  | f     | 102    | SQD  | C32-C33-C34-C35 |
| 34  | B     | 620    | LMG  | C17-C18-C19-C20 |
| 36  | c     | 517[A] | DGD  | O6D-C5D-C6D-O5D |
| 32  | A     | 419    | LMT  | C1-C2-C3-C4     |
| 25  | X     | 101    | SQD  | C30-C31-C32-C33 |
| 33  | b     | 629[B] | LHG  | C16-C17-C18-C19 |
| 36  | c     | 517[A] | DGD  | C9A-CAA-CBA-CCA |
| 36  | c     | 518[B] | DGD  | C9A-CAA-CBA-CCA |
| 36  | c     | 518[B] | DGD  | CBA-CCA-CDA-CEA |
| 26  | A     | 410    | GOL  | O1-C1-C2-O2     |
| 26  | D     | 402    | GOL  | O1-C1-C2-O2     |
| 26  | D     | 413    | GOL  | O2-C2-C3-O3     |
| 26  | O     | 302    | GOL  | O1-C1-C2-O2     |
| 26  | V     | 203[A] | GOL  | O2-C2-C3-O3     |
| 26  | b     | 624    | GOL  | O2-C2-C3-O3     |
| 26  | c     | 527    | GOL  | O2-C2-C3-O3     |
| 26  | o     | 304    | GOL  | O1-C1-C2-O2     |
| 32  | T     | 101    | LMT  | C2-C1-O1'-C1'   |
| 25  | A     | 409[B] | SQD  | C15-C16-C17-C18 |
| 25  | a     | 411    | SQD  | C25-C26-C27-C28 |
| 33  | D     | 408[B] | LHG  | C32-C33-C34-C35 |
| 33  | L     | 101[B] | LHG  | C12-C13-C14-C15 |
| 36  | C     | 518[B] | DGD  | CCB-CDB-CEB-CFB |
| 36  | h     | 102    | DGD  | CAA-CBA-CCA-CDA |
| 36  | h     | 102    | DGD  | C2B-C3B-C4B-C5B |
| 35  | o     | 301    | HTG  | C1'-C2'-C3'-C4' |
| 33  | d     | 414[A] | LHG  | C16-C17-C18-C19 |
| 23  | B     | 603    | CLA  | C16-C17-C18-C20 |
| 23  | b     | 615    | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | D     | 404    | CLA  | O1D-CGD-O2D-CED |
| 32  | b     | 627    | LMT  | C7-C8-C9-C10    |
| 35  | b     | 622    | HTG  | C2'-C3'-C4'-C5' |
| 23  | A     | 405[A] | CLA  | C15-C16-C17-C18 |
| 23  | B     | 615    | CLA  | C5-C6-C7-C8     |
| 23  | C     | 507    | CLA  | C15-C16-C17-C18 |
| 36  | c     | 517[B] | DGD  | C9A-CAA-CBA-CCA |
| 23  | A     | 407    | CLA  | C12-C13-C15-C16 |
| 23  | C     | 505    | CLA  | C12-C13-C15-C16 |
| 36  | c     | 517[A] | DGD  | C5A-C6A-C7A-C8A |
| 23  | B     | 614    | CLA  | C5-C6-C7-C8     |
| 34  | c     | 520    | LMG  | O6-C5-C6-O5     |
| 33  | d     | 407[B] | LHG  | C34-C35-C36-C37 |
| 33  | d     | 408[B] | LHG  | C27-C28-C29-C30 |
| 33  | d     | 414[A] | LHG  | C32-C33-C34-C35 |
| 34  | B     | 620    | LMG  | C34-C35-C36-C37 |
| 34  | c     | 501    | LMG  | C30-C31-C32-C33 |
| 36  | C     | 517[B] | DGD  | C4D-C5D-C6D-O5D |
| 23  | C     | 507    | CLA  | C3A-C2A-CAA-CBA |
| 23  | D     | 404    | CLA  | C4-C3-C5-C6     |
| 32  | M     | 101    | LMT  | C3-C4-C5-C6     |
| 33  | a     | 419[A] | LHG  | C26-C27-C28-C29 |
| 36  | C     | 517[A] | DGD  | C5B-C6B-C7B-C8B |
| 33  | D     | 407[A] | LHG  | C16-C17-C18-C19 |
| 23  | b     | 614    | CLA  | C16-C17-C18-C19 |
| 23  | d     | 403[A] | CLA  | C16-C17-C18-C20 |
| 36  | C     | 517[A] | DGD  | O6D-C5D-C6D-O5D |
| 36  | C     | 517[B] | DGD  | C5B-C6B-C7B-C8B |
| 36  | c     | 518[A] | DGD  | CBA-CCA-CDA-CEA |
| 33  | D     | 408[A] | LHG  | C32-C33-C34-C35 |
| 32  | B     | 629    | LMT  | C3-C4-C5-C6     |
| 32  | T     | 101    | LMT  | C7-C8-C9-C10    |
| 32  | e     | 101    | LMT  | C5-C6-C7-C8     |
| 36  | H     | 102    | DGD  | C5B-C6B-C7B-C8B |
| 36  | c     | 517[A] | DGD  | C2B-C3B-C4B-C5B |
| 36  | c     | 518[A] | DGD  | CAA-CBA-CCA-CDA |
| 36  | h     | 102    | DGD  | C7B-C8B-C9B-CAB |
| 23  | c     | 512    | CLA  | C3-C5-C6-C7     |
| 34  | C     | 501    | LMG  | C10-C11-C12-C13 |
| 34  | c     | 501    | LMG  | C10-C11-C12-C13 |
| 33  | E     | 101[B] | LHG  | C24-C25-C26-C27 |
| 33  | L     | 101[A] | LHG  | C12-C13-C14-C15 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | L     | 101[A] | LHG  | C13-C14-C15-C16 |
| 33  | L     | 101[B] | LHG  | C25-C26-C27-C28 |
| 33  | a     | 419[B] | LHG  | C26-C27-C28-C29 |
| 33  | b     | 629[A] | LHG  | C16-C17-C18-C19 |
| 33  | d     | 414[B] | LHG  | C16-C17-C18-C19 |
| 34  | C     | 501    | LMG  | C17-C18-C19-C20 |
| 34  | C     | 501    | LMG  | C36-C37-C38-C39 |
| 36  | C     | 517[A] | DGD  | C4B-C5B-C6B-C7B |
| 36  | C     | 518[A] | DGD  | CCB-CDB-CEB-CFB |
| 36  | c     | 519    | DGD  | C2B-C3B-C4B-C5B |
| 36  | h     | 102    | DGD  | C9A-CAA-CBA-CCA |
| 34  | c     | 501    | LMG  | C4-C5-C6-O5     |
| 32  | A     | 419    | LMT  | C3'-C4'-O1B-C1B |
| 32  | B     | 626    | LMT  | C3'-C4'-O1B-C1B |
| 25  | A     | 409[A] | SQD  | C15-C16-C17-C18 |
| 25  | b     | 620    | SQD  | C27-C28-C29-C30 |
| 33  | E     | 101[A] | LHG  | C24-C25-C26-C27 |
| 33  | d     | 414[A] | LHG  | C29-C30-C31-C32 |
| 23  | c     | 512    | CLA  | O1D-CGD-O2D-CED |
| 32  | B     | 626    | LMT  | C4B-C5B-C6B-O6B |
| 34  | D     | 412    | LMG  | C35-C36-C37-C38 |
| 23  | a     | 407    | CLA  | C16-C17-C18-C20 |
| 23  | d     | 404    | CLA  | C16-C17-C18-C19 |
| 34  | C     | 520    | LMG  | C16-C17-C18-C19 |
| 32  | A     | 419    | LMT  | C3-C4-C5-C6     |
| 32  | e     | 101    | LMT  | C4-C5-C6-C7     |
| 32  | b     | 621    | LMT  | C3'-C4'-O1B-C1B |
| 34  | C     | 521    | LMG  | C19-C20-C21-C22 |
| 23  | B     | 610    | CLA  | C2A-CAA-CBA-CGA |
| 33  | E     | 101[B] | LHG  | C23-C24-C25-C26 |
| 33  | L     | 101[A] | LHG  | C25-C26-C27-C28 |
| 28  | a     | 413[B] | PL9  | C4-C3-C7-C8     |
| 23  | C     | 507    | CLA  | C4-C3-C5-C6     |
| 25  | b     | 620    | SQD  | C13-C14-C15-C16 |
| 32  | m     | 103    | LMT  | C7-C8-C9-C10    |
| 34  | c     | 501    | LMG  | C34-C35-C36-C37 |
| 36  | c     | 517[B] | DGD  | C5A-C6A-C7A-C8A |
| 23  | D     | 404    | CLA  | C2-C3-C5-C6     |
| 28  | A     | 413[B] | PL9  | C28-C29-C31-C32 |
| 25  | l     | 101    | SQD  | C11-C10-C9-C8   |
| 33  | b     | 629[B] | LHG  | C14-C15-C16-C17 |
| 33  | d     | 414[B] | LHG  | C32-C33-C34-C35 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | c     | 513    | CLA  | CBA-CGA-O2A-C1  |
| 23  | B     | 602    | CLA  | C6-C7-C8-C9     |
| 23  | c     | 514    | CLA  | C6-C7-C8-C9     |
| 25  | a     | 411    | SQD  | C31-C32-C33-C34 |
| 32  | B     | 626    | LMT  | C5-C6-C7-C8     |
| 32  | B     | 627    | LMT  | C2-C3-C4-C5     |
| 32  | b     | 627    | LMT  | C3-C4-C5-C6     |
| 34  | C     | 501    | LMG  | C39-C40-C41-C42 |
| 36  | c     | 518[B] | DGD  | CAA-CBA-CCA-CDA |
| 23  | C     | 511    | CLA  | C10-C11-C12-C13 |
| 33  | D     | 407[B] | LHG  | C16-C17-C18-C19 |
| 34  | m     | 101    | LMG  | C35-C36-C37-C38 |
| 36  | C     | 518[A] | DGD  | O6E-C1E-O5D-C6D |
| 36  | C     | 518[B] | DGD  | O6E-C1E-O5D-C6D |
| 36  | c     | 519    | DGD  | CBB-CCB-CDB-CEB |
| 25  | b     | 620    | SQD  | C31-C32-C33-C34 |
| 33  | b     | 629[A] | LHG  | C14-C15-C16-C17 |
| 36  | C     | 517[B] | DGD  | C4B-C5B-C6B-C7B |
| 36  | c     | 519    | DGD  | CBA-CCA-CDA-CEA |
| 33  | E     | 101[A] | LHG  | O2-C2-C3-O3     |
| 33  | L     | 101[B] | LHG  | C17-C18-C19-C20 |
| 34  | C     | 501    | LMG  | C12-C13-C14-C15 |
| 34  | D     | 412    | LMG  | C30-C31-C32-C33 |
| 34  | m     | 101    | LMG  | C11-C10-O7-C8   |
| 32  | e     | 101    | LMT  | C1-C2-C3-C4     |
| 23  | B     | 615    | CLA  | C10-C11-C12-C13 |
| 25  | X     | 101    | SQD  | C24-C25-C26-C27 |
| 33  | d     | 408[B] | LHG  | C25-C26-C27-C28 |
| 32  | b     | 621    | LMT  | C4'-C5'-C6'-O6' |
| 25  | b     | 620    | SQD  | C14-C15-C16-C17 |
| 33  | L     | 101[B] | LHG  | C15-C16-C17-C18 |
| 34  | C     | 520    | LMG  | C34-C35-C36-C37 |
| 24  | D     | 405    | BCR  | C37-C22-C23-C24 |
| 36  | c     | 517[A] | DGD  | C7A-C8A-C9A-CAA |
| 24  | D     | 405    | BCR  | C21-C22-C23-C24 |
| 34  | C     | 501    | LMG  | C19-C20-C21-C22 |
| 34  | d     | 412    | LMG  | C29-C30-C31-C32 |
| 36  | C     | 517[B] | DGD  | C8A-C9A-CAA-CBA |
| 23  | B     | 610    | CLA  | C16-C17-C18-C19 |
| 23  | B     | 610    | CLA  | C16-C17-C18-C20 |
| 23  | c     | 509    | CLA  | C16-C17-C18-C20 |
| 23  | C     | 504    | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 25  | A     | 411    | SQD  | C17-C18-C19-C20 |
| 32  | B     | 629    | LMT  | C11-C10-C9-C8   |
| 34  | c     | 520    | LMG  | C31-C32-C33-C34 |
| 28  | D     | 406[B] | PL9  | C15-C14-C16-C17 |
| 28  | d     | 406[B] | PL9  | C15-C14-C16-C17 |
| 34  | C     | 521    | LMG  | C18-C19-C20-C21 |
| 23  | A     | 405[B] | CLA  | C15-C16-C17-C18 |
| 33  | d     | 408[A] | LHG  | C29-C30-C31-C32 |
| 25  | X     | 101    | SQD  | C29-C30-C31-C32 |
| 23  | b     | 607    | CLA  | C3-C5-C6-C7     |
| 25  | b     | 620    | SQD  | C24-C23-O48-C46 |
| 33  | A     | 418[A] | LHG  | C12-C13-C14-C15 |
| 34  | c     | 520    | LMG  | C33-C34-C35-C36 |
| 36  | C     | 517[A] | DGD  | C9A-CAA-CBA-CCA |
| 32  | B     | 629    | LMT  | C4-C5-C6-C7     |
| 33  | D     | 408[B] | LHG  | C15-C16-C17-C18 |
| 33  | d     | 408[A] | LHG  | C27-C28-C29-C30 |
| 33  | d     | 408[B] | LHG  | C34-C35-C36-C37 |
| 35  | b     | 622    | HTG  | C1'-C2'-C3'-C4' |
| 33  | A     | 418[B] | LHG  | C12-C13-C14-C15 |
| 33  | d     | 408[A] | LHG  | C25-C26-C27-C28 |
| 36  | H     | 102    | DGD  | CCB-CDB-CEB-CFB |
| 32  | B     | 629    | LMT  | O1'-C1-C2-C3    |
| 25  | A     | 409[A] | SQD  | O6-C44-C45-O47  |
| 25  | A     | 409[B] | SQD  | O6-C44-C45-O47  |
| 25  | X     | 101    | SQD  | O47-C45-C46-O48 |
| 34  | m     | 101    | LMG  | C39-C40-C41-C42 |
| 33  | d     | 414[A] | LHG  | C24-C25-C26-C27 |
| 34  | m     | 101    | LMG  | C38-C39-C40-C41 |
| 23  | C     | 513    | CLA  | C10-C11-C12-C13 |
| 32  | A     | 419    | LMT  | C5-C6-C7-C8     |
| 33  | b     | 629[A] | LHG  | C27-C28-C29-C30 |
| 36  | c     | 517[A] | DGD  | C4D-C5D-C6D-O5D |
| 25  | b     | 620    | SQD  | C26-C27-C28-C29 |
| 33  | D     | 407[A] | LHG  | C12-C13-C14-C15 |
| 33  | d     | 414[B] | LHG  | C25-C26-C27-C28 |
| 32  | M     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 34  | Z     | 101    | LMG  | O6-C5-C6-O5     |
| 23  | d     | 403[A] | CLA  | C16-C17-C18-C19 |
| 23  | A     | 406[B] | CLA  | C13-C15-C16-C17 |
| 32  | B     | 626    | LMT  | C7-C8-C9-C10    |
| 33  | L     | 101[B] | LHG  | C27-C28-C29-C30 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 34  | m     | 101    | LMG  | O9-C10-O7-C8    |
| 33  | D     | 408[A] | LHG  | C15-C16-C17-C18 |
| 34  | C     | 501    | LMG  | C20-C21-C22-C23 |
| 35  | b     | 622    | HTG  | C3'-C4'-C5'-C6' |
| 36  | c     | 517[B] | DGD  | C7A-C8A-C9A-CAA |
| 23  | b     | 614    | CLA  | CBD-CGD-O2D-CED |
| 34  | c     | 520    | LMG  | C34-C35-C36-C37 |
| 32  | b     | 627    | LMT  | C5-C6-C7-C8     |
| 32  | B     | 627    | LMT  | C5-C6-C7-C8     |
| 33  | A     | 418[A] | LHG  | C34-C35-C36-C37 |
| 23  | B     | 608    | CLA  | C16-C17-C18-C20 |
| 26  | B     | 622    | GOL  | O1-C1-C2-O2     |
| 26  | a     | 410    | GOL  | O2-C2-C3-O3     |
| 26  | o     | 303    | GOL  | O2-C2-C3-O3     |
| 26  | o     | 304    | GOL  | O2-C2-C3-O3     |
| 33  | d     | 408[A] | LHG  | C34-C35-C36-C37 |
| 23  | A     | 405[B] | CLA  | C1A-C2A-CAA-CBA |
| 23  | B     | 611    | CLA  | C1A-C2A-CAA-CBA |
| 23  | C     | 502    | CLA  | C1A-C2A-CAA-CBA |
| 23  | C     | 507    | CLA  | C1A-C2A-CAA-CBA |
| 23  | c     | 514    | CLA  | C1A-C2A-CAA-CBA |
| 23  | b     | 605    | CLA  | C5-C6-C7-C8     |
| 36  | c     | 517[B] | DGD  | O6E-C1E-O5D-C6D |
| 36  | C     | 519    | DGD  | C2B-C3B-C4B-C5B |
| 34  | C     | 521    | LMG  | C13-C14-C15-C16 |
| 36  | C     | 517[B] | DGD  | C9A-CAA-CBA-CCA |
| 36  | c     | 518[A] | DGD  | C6A-C7A-C8A-C9A |
| 23  | c     | 507    | CLA  | C15-C16-C17-C18 |
| 23  | C     | 510    | CLA  | O1D-CGD-O2D-CED |
| 33  | D     | 407[B] | LHG  | O6-C4-C5-C6     |
| 33  | d     | 407[A] | LHG  | C34-C35-C36-C37 |
| 34  | c     | 501    | LMG  | C29-C30-C31-C32 |
| 23  | B     | 614    | CLA  | C11-C10-C8-C7   |
| 23  | C     | 506    | CLA  | C11-C12-C13-C15 |
| 23  | C     | 514    | CLA  | C11-C10-C8-C7   |
| 23  | C     | 514    | CLA  | C11-C12-C13-C15 |
| 23  | b     | 601    | CLA  | C6-C7-C8-C10    |
| 23  | b     | 601    | CLA  | C11-C10-C8-C7   |
| 23  | c     | 506    | CLA  | C11-C12-C13-C15 |
| 23  | c     | 511    | CLA  | C12-C13-C15-C16 |
| 23  | c     | 513    | CLA  | C12-C13-C15-C16 |
| 23  | B     | 608    | CLA  | C16-C17-C18-C19 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | d     | 403[B] | CLA  | C16-C17-C18-C20 |
| 23  | A     | 406[A] | CLA  | C13-C15-C16-C17 |
| 23  | B     | 608    | CLA  | C13-C15-C16-C17 |
| 23  | b     | 605    | CLA  | C8-C10-C11-C12  |
| 36  | c     | 518[A] | DGD  | C4A-C5A-C6A-C7A |
| 28  | a     | 413[A] | PL9  | C12-C11-C9-C10  |
| 31  | a     | 406[B] | PHO  | C4-C3-C5-C6     |
| 23  | b     | 605    | CLA  | C3-C5-C6-C7     |
| 23  | C     | 506    | CLA  | C11-C12-C13-C14 |
| 23  | C     | 511    | CLA  | C14-C13-C15-C16 |
| 23  | b     | 610    | CLA  | C11-C12-C13-C14 |
| 23  | c     | 506    | CLA  | C11-C12-C13-C14 |
| 23  | c     | 511    | CLA  | C11-C10-C8-C9   |
| 32  | e     | 101    | LMT  | C9-C10-C11-C12  |
| 32  | B     | 627    | LMT  | C6-C7-C8-C9     |
| 36  | c     | 517[B] | DGD  | O6E-C5E-C6E-O5E |
| 34  | D     | 412    | LMG  | C12-C13-C14-C15 |
| 33  | D     | 408[B] | LHG  | C24-C23-O8-C6   |
| 23  | b     | 601    | CLA  | C8-C10-C11-C12  |
| 25  | f     | 102    | SQD  | C25-C26-C27-C28 |
| 34  | m     | 101    | LMG  | C14-C15-C16-C17 |
| 35  | b     | 623    | HTG  | O5-C5-C6-O6     |
| 25  | A     | 411    | SQD  | O6-C44-C45-C46  |
| 25  | a     | 409[A] | SQD  | O6-C44-C45-C46  |
| 25  | a     | 411    | SQD  | O6-C44-C45-C46  |
| 25  | b     | 620    | SQD  | C44-C45-C46-O48 |
| 25  | f     | 102    | SQD  | O6-C44-C45-C46  |
| 25  | f     | 102    | SQD  | C44-C45-C46-O48 |
| 33  | E     | 101[A] | LHG  | C4-C5-C6-O8     |
| 33  | E     | 101[B] | LHG  | C4-C5-C6-O8     |
| 32  | e     | 101    | LMT  | C4B-C5B-C6B-O6B |
| 33  | D     | 408[A] | LHG  | C13-C14-C15-C16 |
| 34  | C     | 520    | LMG  | C11-C12-C13-C14 |
| 36  | c     | 517[A] | DGD  | CAA-CBA-CCA-CDA |
| 32  | a     | 416    | LMT  | O5'-C5'-C6'-O6' |
| 36  | C     | 517[B] | DGD  | O6E-C5E-C6E-O5E |
| 33  | A     | 418[A] | LHG  | O2-C2-C3-O3     |
| 23  | B     | 601    | CLA  | CBA-CGA-O2A-C1  |
| 36  | c     | 517[A] | DGD  | C2A-C1A-O1G-C1G |
| 36  | c     | 519    | DGD  | C2A-C1A-O1G-C1G |
| 34  | d     | 412    | LMG  | O6-C5-C6-O5     |
| 36  | C     | 517[A] | DGD  | O6E-C5E-C6E-O5E |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | c     | 517[A] | DGD  | O6E-C5E-C6E-O5E |
| 33  | D     | 408[B] | LHG  | C29-C30-C31-C32 |
| 34  | C     | 521    | LMG  | C17-C18-C19-C20 |
| 33  | D     | 408[B] | LHG  | O10-C23-O8-C6   |
| 33  | D     | 407[B] | LHG  | C26-C27-C28-C29 |
| 23  | C     | 514    | CLA  | O1D-CGD-O2D-CED |
| 23  | c     | 507    | CLA  | C10-C11-C12-C13 |
| 23  | c     | 513    | CLA  | C10-C11-C12-C13 |
| 32  | a     | 416    | LMT  | C3-C4-C5-C6     |
| 34  | B     | 620    | LMG  | C37-C38-C39-C40 |
| 34  | C     | 520    | LMG  | C37-C38-C39-C40 |
| 31  | a     | 406[B] | PHO  | C2-C3-C5-C6     |
| 33  | d     | 414[A] | LHG  | C25-C26-C27-C28 |
| 36  | c     | 518[B] | DGD  | C2B-C3B-C4B-C5B |
| 34  | D     | 412    | LMG  | O6-C5-C6-O5     |
| 23  | c     | 513    | CLA  | O1A-CGA-O2A-C1  |
| 25  | b     | 620    | SQD  | O10-C23-O48-C46 |
| 23  | C     | 507    | CLA  | C5-C6-C7-C8     |
| 33  | d     | 414[B] | LHG  | C24-C25-C26-C27 |
| 36  | c     | 517[B] | DGD  | CAA-CBA-CCA-CDA |
| 36  | h     | 102    | DGD  | CAB-CBB-CCB-CDB |
| 25  | A     | 411    | SQD  | C26-C27-C28-C29 |
| 33  | D     | 408[A] | LHG  | C29-C30-C31-C32 |
| 36  | C     | 517[A] | DGD  | C8A-C9A-CAA-CBA |
| 36  | c     | 518[A] | DGD  | C2B-C3B-C4B-C5B |
| 36  | c     | 518[B] | DGD  | C6A-C7A-C8A-C9A |
| 26  | l     | 103[A] | GOL  | O1-C1-C2-C3     |
| 34  | c     | 521    | LMG  | C29-C28-O8-C9   |
| 25  | b     | 620    | SQD  | C46-C45-O47-C7  |
| 25  | l     | 101    | SQD  | C46-C45-O47-C7  |
| 23  | d     | 402[A] | CLA  | C2C-C3C-CAC-CBC |
| 25  | a     | 409[B] | SQD  | C9-C10-C11-C12  |
| 33  | A     | 418[B] | LHG  | C18-C19-C20-C21 |
| 36  | c     | 518[B] | DGD  | C4A-C5A-C6A-C7A |
| 23  | b     | 610    | CLA  | C15-C16-C17-C18 |
| 25  | a     | 409[A] | SQD  | C9-C10-C11-C12  |
| 33  | A     | 418[A] | LHG  | C26-C27-C28-C29 |
| 33  | D     | 407[B] | LHG  | C12-C13-C14-C15 |
| 36  | h     | 102    | DGD  | C9B-CAB-CBB-CCB |
| 23  | d     | 403[B] | CLA  | C16-C17-C18-C19 |
| 32  | b     | 627    | LMT  | O1'-C1-C2-C3    |
| 34  | z     | 101    | LMG  | C20-C21-C22-C23 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | b     | 601    | CLA  | C13-C15-C16-C17 |
| 33  | d     | 408[A] | LHG  | C28-C29-C30-C31 |
| 23  | C     | 511    | CLA  | CBA-CGA-O2A-C1  |
| 23  | d     | 404    | CLA  | CBA-CGA-O2A-C1  |
| 25  | A     | 409[B] | SQD  | C11-C10-C9-C8   |
| 34  | Z     | 101    | LMG  | C11-C12-C13-C14 |
| 23  | c     | 502    | CLA  | O1D-CGD-O2D-CED |
| 23  | c     | 511    | CLA  | O1D-CGD-O2D-CED |
| 32  | t     | 101    | LMT  | C7-C8-C9-C10    |
| 23  | c     | 514    | CLA  | C4-C3-C5-C6     |
| 33  | D     | 407[B] | LHG  | C11-C10-C9-C8   |
| 36  | H     | 102    | DGD  | CAB-CBB-CCB-CDB |
| 36  | C     | 518[A] | DGD  | CDA-CEA-CFA-CGA |
| 25  | a     | 409[A] | SQD  | C12-C13-C14-C15 |
| 34  | z     | 101    | LMG  | C14-C15-C16-C17 |
| 33  | D     | 407[A] | LHG  | C10-C11-C12-C13 |
| 34  | C     | 520    | LMG  | C17-C18-C19-C20 |
| 34  | C     | 521    | LMG  | C20-C21-C22-C23 |
| 36  | H     | 102    | DGD  | C9B-CAB-CBB-CCB |
| 23  | C     | 513    | CLA  | CBA-CGA-O2A-C1  |
| 32  | a     | 416    | LMT  | C9-C10-C11-C12  |
| 25  | A     | 409[B] | SQD  | C12-C13-C14-C15 |
| 34  | z     | 101    | LMG  | C19-C20-C21-C22 |
| 25  | l     | 101    | SQD  | C34-C35-C36-C37 |
| 33  | D     | 408[B] | LHG  | C13-C14-C15-C16 |
| 33  | b     | 629[A] | LHG  | C9-C10-C11-C12  |
| 36  | h     | 102    | DGD  | CDB-CEB-CFB-CGB |
| 34  | m     | 101    | LMG  | C37-C38-C39-C40 |
| 32  | B     | 626    | LMT  | C1-C2-C3-C4     |
| 33  | A     | 418[B] | LHG  | C26-C27-C28-C29 |
| 33  | E     | 101[A] | LHG  | C25-C26-C27-C28 |
| 34  | D     | 412    | LMG  | C36-C37-C38-C39 |
| 25  | A     | 411    | SQD  | C24-C23-O48-C46 |
| 33  | d     | 408[B] | LHG  | C24-C23-O8-C6   |
| 33  | b     | 629[B] | LHG  | C9-C10-C11-C12  |
| 33  | d     | 414[A] | LHG  | C33-C34-C35-C36 |
| 36  | C     | 518[B] | DGD  | CDA-CEA-CFA-CGA |
| 25  | A     | 411    | SQD  | C27-C28-C29-C30 |
| 32  | M     | 101    | LMT  | C2-C3-C4-C5     |
| 34  | C     | 521    | LMG  | C4-C5-C6-O5     |
| 33  | D     | 407[B] | LHG  | C34-C35-C36-C37 |
| 28  | D     | 406[A] | PL9  | C45-C44-C46-C47 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 28  | a     | 413[B] | PL9  | C12-C11-C9-C10  |
| 28  | d     | 406[B] | PL9  | C45-C44-C46-C47 |
| 28  | A     | 413[B] | PL9  | C12-C11-C9-C8   |
| 28  | d     | 406[A] | PL9  | C13-C14-C16-C17 |
| 23  | C     | 503    | CLA  | C13-C15-C16-C17 |
| 34  | B     | 620    | LMG  | C15-C16-C17-C18 |
| 25  | A     | 409[A] | SQD  | C11-C10-C9-C8   |
| 26  | D     | 413    | GOL  | O1-C1-C2-O2     |
| 26  | O     | 303    | GOL  | O1-C1-C2-O2     |
| 26  | v     | 202[A] | GOL  | O1-C1-C2-O2     |
| 32  | A     | 419    | LMT  | C2-C1-O1'-C1'   |
| 32  | F     | 101    | LMT  | C2-C1-O1'-C1'   |
| 32  | e     | 101    | LMT  | C2-C1-O1'-C1'   |
| 32  | m     | 103    | LMT  | C2-C1-O1'-C1'   |
| 23  | B     | 614    | CLA  | C14-C13-C15-C16 |
| 23  | C     | 505    | CLA  | C14-C13-C15-C16 |
| 23  | C     | 507    | CLA  | C6-C7-C8-C9     |
| 23  | C     | 510    | CLA  | C6-C7-C8-C9     |
| 23  | C     | 514    | CLA  | C11-C10-C8-C9   |
| 23  | b     | 601    | CLA  | C6-C7-C8-C9     |
| 35  | o     | 301    | HTG  | C2'-C3'-C4'-C5' |
| 23  | B     | 610    | CLA  | C13-C15-C16-C17 |
| 23  | b     | 604    | CLA  | C13-C15-C16-C17 |
| 36  | c     | 519    | DGD  | O1A-C1A-O1G-C1G |
| 33  | d     | 408[A] | LHG  | C33-C34-C35-C36 |
| 23  | A     | 404[A] | CLA  | C13-C15-C16-C17 |
| 32  | a     | 416    | LMT  | C2-C3-C4-C5     |
| 33  | D     | 408[A] | LHG  | C17-C18-C19-C20 |
| 25  | X     | 101    | SQD  | C34-C35-C36-C37 |
| 32  | F     | 101    | LMT  | C4-C5-C6-C7     |
| 32  | F     | 101    | LMT  | C6-C7-C8-C9     |
| 36  | C     | 517[A] | DGD  | C4D-C5D-C6D-O5D |
| 36  | C     | 519    | DGD  | CDB-CEB-CFB-CGB |
| 23  | A     | 406[B] | CLA  | C12-C13-C15-C16 |
| 23  | C     | 507    | CLA  | C6-C7-C8-C10    |
| 23  | C     | 511    | CLA  | C12-C13-C15-C16 |
| 23  | a     | 407    | CLA  | C11-C10-C8-C7   |
| 23  | b     | 604    | CLA  | C6-C7-C8-C10    |
| 23  | b     | 615    | CLA  | C12-C13-C15-C16 |
| 23  | c     | 505    | CLA  | C11-C12-C13-C15 |
| 23  | c     | 506    | CLA  | C12-C13-C15-C16 |
| 23  | c     | 510    | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | c     | 510    | CLA  | C11-C10-C8-C7   |
| 23  | c     | 511    | CLA  | C11-C10-C8-C7   |
| 23  | d     | 403[B] | CLA  | C11-C12-C13-C15 |
| 23  | A     | 404[B] | CLA  | C13-C15-C16-C17 |
| 23  | B     | 612    | CLA  | C10-C11-C12-C13 |
| 23  | c     | 513    | CLA  | C13-C15-C16-C17 |
| 23  | B     | 601    | CLA  | O1A-CGA-O2A-C1  |
| 36  | c     | 517[A] | DGD  | O1A-C1A-O1G-C1G |
| 33  | E     | 101[A] | LHG  | C13-C14-C15-C16 |
| 36  | c     | 517[B] | DGD  | C2A-C1A-O1G-C1G |
| 23  | B     | 615    | CLA  | C16-C17-C18-C20 |
| 23  | c     | 507    | CLA  | C3A-C2A-CAA-CBA |
| 28  | A     | 413[A] | PL9  | C12-C11-C9-C8   |
| 28  | D     | 406[A] | PL9  | C13-C14-C16-C17 |
| 25  | a     | 409[B] | SQD  | C12-C13-C14-C15 |
| 23  | a     | 404[B] | CLA  | C2C-C3C-CAC-CBC |
| 23  | d     | 404    | CLA  | O1A-CGA-O2A-C1  |
| 23  | c     | 510    | CLA  | C8-C10-C11-C12  |
| 23  | B     | 603    | CLA  | C13-C15-C16-C17 |
| 33  | A     | 418[B] | LHG  | C32-C33-C34-C35 |
| 23  | B     | 601    | CLA  | C15-C16-C17-C18 |
| 33  | d     | 407[B] | LHG  | C25-C26-C27-C28 |
| 33  | A     | 418[B] | LHG  | C1-C2-C3-O3     |
| 33  | D     | 407[B] | LHG  | C13-C14-C15-C16 |
| 34  | c     | 501    | LMG  | C35-C36-C37-C38 |
| 25  | A     | 409[A] | SQD  | O6-C44-C45-C46  |
| 25  | A     | 409[B] | SQD  | O6-C44-C45-C46  |
| 28  | A     | 413[B] | PL9  | C39-C41-C42-C43 |
| 33  | a     | 419[A] | LHG  | C4-C5-C6-O8     |
| 33  | a     | 419[B] | LHG  | C4-C5-C6-O8     |
| 34  | c     | 501    | LMG  | C7-C8-C9-O8     |
| 32  | b     | 627    | LMT  | C6-C7-C8-C9     |
| 23  | b     | 606    | CLA  | C16-C17-C18-C19 |
| 36  | c     | 518[A] | DGD  | CBB-CCB-CDB-CEB |
| 23  | C     | 511    | CLA  | C4-C3-C5-C6     |
| 23  | c     | 506    | CLA  | C4-C3-C5-C6     |
| 28  | A     | 413[A] | PL9  | C45-C44-C46-C47 |
| 33  | a     | 419[A] | LHG  | C23-C24-C25-C26 |
| 34  | c     | 520    | LMG  | C10-C11-C12-C13 |
| 28  | D     | 406[A] | PL9  | C43-C44-C46-C47 |
| 34  | c     | 521    | LMG  | O10-C28-O8-C9   |
| 23  | B     | 615    | CLA  | C16-C17-C18-C19 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | H     | 101    | BCR  | C23-C24-C25-C30 |
| 24  | b     | 617    | BCR  | C1-C6-C7-C8     |
| 33  | A     | 418[B] | LHG  | O2-C2-C3-O3     |
| 23  | b     | 608    | CLA  | C13-C15-C16-C17 |
| 23  | d     | 402[B] | CLA  | C15-C16-C17-C18 |
| 32  | B     | 627    | LMT  | C3-C4-C5-C6     |
| 36  | C     | 517[A] | DGD  | CCA-CDA-CEA-CFA |
| 33  | a     | 419[A] | LHG  | C10-C11-C12-C13 |
| 23  | C     | 503    | CLA  | C15-C16-C17-C18 |
| 36  | C     | 517[B] | DGD  | C7A-C8A-C9A-CAA |
| 35  | c     | 522    | HTG  | C4'-C5'-C6'-C7' |
| 23  | b     | 616    | CLA  | C5-C6-C7-C8     |
| 25  | a     | 409[A] | SQD  | O6-C44-C45-O47  |
| 25  | a     | 409[B] | SQD  | O6-C44-C45-O47  |
| 25  | b     | 620    | SQD  | O47-C45-C46-O48 |
| 33  | d     | 408[B] | LHG  | C9-C10-C11-C12  |
| 36  | C     | 518[B] | DGD  | C7A-C8A-C9A-CAA |
| 33  | L     | 101[A] | LHG  | C27-C28-C29-C30 |
| 33  | L     | 101[B] | LHG  | C26-C27-C28-C29 |
| 36  | H     | 102    | DGD  | C7A-C8A-C9A-CAA |
| 23  | c     | 506    | CLA  | C2-C3-C5-C6     |
| 28  | D     | 406[B] | PL9  | C13-C14-C16-C17 |
| 25  | b     | 620    | SQD  | C11-C10-C9-C8   |
| 36  | C     | 517[A] | DGD  | C7A-C8A-C9A-CAA |
| 36  | C     | 517[A] | DGD  | C3B-C4B-C5B-C6B |
| 33  | a     | 419[B] | LHG  | C23-C24-C25-C26 |
| 34  | c     | 520    | LMG  | C28-C29-C30-C31 |
| 23  | c     | 512    | CLA  | CBA-CGA-O2A-C1  |
| 25  | a     | 409[B] | SQD  | C34-C35-C36-C37 |
| 23  | B     | 610    | CLA  | C14-C13-C15-C16 |
| 23  | d     | 403[B] | CLA  | C11-C12-C13-C14 |
| 34  | C     | 521    | LMG  | C38-C39-C40-C41 |
| 33  | L     | 101[B] | LHG  | C10-C11-C12-C13 |
| 33  | d     | 414[B] | LHG  | C33-C34-C35-C36 |
| 36  | c     | 517[A] | DGD  | O6E-C1E-O5D-C6D |
| 34  | d     | 412    | LMG  | C10-C11-C12-C13 |
| 23  | C     | 511    | CLA  | O1A-CGA-O2A-C1  |
| 34  | Z     | 101    | LMG  | C19-C20-C21-C22 |
| 36  | c     | 517[B] | DGD  | C7B-C8B-C9B-CAB |
| 32  | a     | 416    | LMT  | C4'-C5'-C6'-O6' |
| 36  | c     | 518[B] | DGD  | C9B-CAB-CBB-CCB |
| 28  | A     | 413[A] | PL9  | C39-C41-C42-C43 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 28  | a     | 413[A] | PL9  | C24-C26-C27-C28 |
| 36  | C     | 517[A] | DGD  | C1B-C2B-C3B-C4B |
| 26  | B     | 625    | GOL  | O1-C1-C2-O2     |
| 26  | a     | 418    | GOL  | O2-C2-C3-O3     |
| 23  | b     | 601    | CLA  | CBA-CGA-O2A-C1  |
| 23  | C     | 506    | CLA  | C2-C3-C5-C6     |
| 23  | C     | 511    | CLA  | C2-C3-C5-C6     |
| 28  | d     | 406[B] | PL9  | C13-C14-C16-C17 |
| 23  | A     | 406[A] | CLA  | C16-C17-C18-C20 |
| 33  | b     | 629[B] | LHG  | C10-C11-C12-C13 |
| 36  | C     | 519    | DGD  | CAB-CBB-CCB-CDB |
| 36  | C     | 519    | DGD  | C8A-C9A-CAA-CBA |
| 33  | A     | 418[A] | LHG  | C1-C2-C3-O3     |
| 32  | e     | 101    | LMT  | C3-C4-C5-C6     |
| 23  | b     | 616    | CLA  | CBA-CGA-O2A-C1  |
| 23  | c     | 508    | CLA  | C8-C10-C11-C12  |
| 33  | b     | 629[B] | LHG  | O6-C4-C5-C6     |
| 34  | C     | 501    | LMG  | C18-C19-C20-C21 |
| 36  | C     | 519    | DGD  | C6A-C7A-C8A-C9A |
| 23  | B     | 610    | CLA  | C12-C13-C15-C16 |
| 23  | B     | 614    | CLA  | C12-C13-C15-C16 |
| 23  | C     | 506    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 607    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 614    | CLA  | C12-C13-C15-C16 |
| 23  | c     | 507    | CLA  | C11-C10-C8-C7   |
| 33  | D     | 408[A] | LHG  | C27-C28-C29-C30 |
| 33  | b     | 629[A] | LHG  | C34-C35-C36-C37 |
| 33  | E     | 101[B] | LHG  | C13-C14-C15-C16 |
| 33  | d     | 408[B] | LHG  | C28-C29-C30-C31 |
| 23  | B     | 605    | CLA  | C5-C6-C7-C8     |
| 23  | c     | 510    | CLA  | C13-C15-C16-C17 |
| 32  | B     | 626    | LMT  | C9-C10-C11-C12  |
| 33  | E     | 101[B] | LHG  | C25-C26-C27-C28 |
| 23  | C     | 513    | CLA  | O1A-CGA-O2A-C1  |
| 23  | c     | 512    | CLA  | O1A-CGA-O2A-C1  |
| 33  | d     | 408[B] | LHG  | O10-C23-O8-C6   |
| 36  | C     | 518[A] | DGD  | C2G-C3G-O3G-C1D |
| 36  | C     | 518[B] | DGD  | C5D-C6D-O5D-C1E |
| 36  | c     | 518[A] | DGD  | C5D-C6D-O5D-C1E |
| 36  | c     | 518[B] | DGD  | C5D-C6D-O5D-C1E |
| 32  | b     | 621    | LMT  | C11-C10-C9-C8   |
| 23  | B     | 601    | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | C     | 502    | CLA  | C2A-CAA-CBA-CGA |
| 33  | L     | 101[A] | LHG  | C11-C10-C9-C8   |
| 36  | C     | 519    | DGD  | CAA-CBA-CCA-CDA |
| 23  | b     | 606    | CLA  | C16-C17-C18-C20 |
| 28  | d     | 406[A] | PL9  | C45-C44-C46-C47 |
| 25  | A     | 411    | SQD  | O10-C23-O48-C46 |
| 28  | a     | 413[A] | PL9  | C12-C11-C9-C8   |
| 38  | f     | 101    | HEM  | C2B-C3B-CAB-CBB |
| 26  | l     | 103[B] | GOL  | O1-C1-C2-C3     |
| 34  | B     | 620    | LMG  | C14-C15-C16-C17 |
| 33  | D     | 408[B] | LHG  | C17-C18-C19-C20 |
| 36  | c     | 517[B] | DGD  | O1A-C1A-O1G-C1G |
| 25  | A     | 409[A] | SQD  | C18-C19-C20-C21 |
| 36  | C     | 518[A] | DGD  | C5B-C6B-C7B-C8B |
| 23  | c     | 510    | CLA  | C10-C11-C12-C13 |
| 25  | b     | 620    | SQD  | C28-C29-C30-C31 |
| 33  | b     | 629[A] | LHG  | C13-C14-C15-C16 |
| 36  | C     | 518[A] | DGD  | C8B-C9B-CAB-CBB |
| 33  | D     | 407[A] | LHG  | C11-C10-C9-C8   |
| 36  | C     | 519    | DGD  | C4A-C5A-C6A-C7A |
| 36  | c     | 517[A] | DGD  | CCB-CDB-CEB-CFB |
| 34  | d     | 412    | LMG  | C35-C36-C37-C38 |
| 33  | E     | 101[A] | LHG  | O6-C4-C5-O7     |
| 33  | L     | 101[A] | LHG  | O6-C4-C5-O7     |
| 33  | b     | 629[B] | LHG  | O6-C4-C5-O7     |
| 25  | a     | 409[A] | SQD  | C27-C28-C29-C30 |
| 36  | c     | 518[A] | DGD  | O6E-C1E-O5D-C6D |
| 34  | c     | 501    | LMG  | C21-C22-C23-C24 |
| 25  | l     | 101    | SQD  | C44-C45-C46-O48 |
| 33  | L     | 101[A] | LHG  | C24-C25-C26-C27 |
| 33  | a     | 419[B] | LHG  | C10-C11-C12-C13 |
| 23  | b     | 601    | CLA  | O1A-CGA-O2A-C1  |
| 23  | B     | 613    | CLA  | C15-C16-C17-C18 |
| 33  | d     | 407[A] | LHG  | C13-C14-C15-C16 |
| 23  | C     | 506    | CLA  | C4-C3-C5-C6     |
| 23  | C     | 507    | CLA  | C2-C3-C5-C6     |
| 28  | a     | 413[B] | PL9  | C23-C24-C26-C27 |
| 33  | D     | 408[A] | LHG  | C10-C11-C12-C13 |
| 36  | C     | 518[A] | DGD  | C7A-C8A-C9A-CAA |
| 25  | a     | 409[A] | SQD  | C34-C35-C36-C37 |
| 36  | C     | 517[B] | DGD  | C6A-C7A-C8A-C9A |
| 35  | B     | 623    | HTG  | C4'-C5'-C6'-C7' |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | C     | 511    | CLA  | C8-C10-C11-C12  |
| 23  | b     | 615    | CLA  | C5-C6-C7-C8     |
| 23  | C     | 504    | CLA  | O1D-CGD-O2D-CED |
| 25  | f     | 102    | SQD  | O47-C45-C46-O48 |
| 25  | l     | 101    | SQD  | O47-C45-C46-O48 |
| 33  | a     | 419[A] | LHG  | O7-C5-C6-O8     |
| 34  | c     | 501    | LMG  | O7-C8-C9-O8     |
| 23  | B     | 610    | CLA  | C11-C12-C13-C14 |
| 23  | b     | 615    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 513    | CLA  | C6-C7-C8-C9     |
| 33  | b     | 629[B] | LHG  | C13-C14-C15-C16 |
| 34  | d     | 412    | LMG  | C11-C12-C13-C14 |
| 33  | D     | 408[B] | LHG  | C10-C11-C12-C13 |
| 23  | b     | 616    | CLA  | O1A-CGA-O2A-C1  |
| 23  | C     | 508    | CLA  | C13-C15-C16-C17 |
| 31  | A     | 416[A] | PHO  | C2C-C3C-CAC-CBC |
| 36  | C     | 517[B] | DGD  | CCA-CDA-CEA-CFA |
| 33  | a     | 419[A] | LHG  | C7-C8-C9-C10    |
| 23  | b     | 601    | CLA  | C2-C1-O2A-CGA   |
| 36  | C     | 517[B] | DGD  | C2E-C1E-O5D-C6D |
| 36  | c     | 517[A] | DGD  | C2E-C1E-O5D-C6D |
| 36  | c     | 518[A] | DGD  | C2E-C1E-O5D-C6D |
| 23  | C     | 503    | CLA  | C16-C17-C18-C19 |
| 23  | c     | 507    | CLA  | C13-C15-C16-C17 |
| 33  | D     | 408[B] | LHG  | C27-C28-C29-C30 |
| 34  | d     | 412    | LMG  | C18-C19-C20-C21 |
| 25  | X     | 101    | SQD  | C32-C33-C34-C35 |
| 33  | A     | 418[A] | LHG  | C32-C33-C34-C35 |
| 33  | A     | 418[B] | LHG  | C34-C35-C36-C37 |
| 36  | C     | 519    | DGD  | CDA-CEA-CFA-CGA |
| 23  | A     | 406[B] | CLA  | C16-C17-C18-C20 |
| 33  | b     | 629[B] | LHG  | C28-C29-C30-C31 |
| 33  | d     | 408[A] | LHG  | C9-C10-C11-C12  |
| 25  | A     | 409[A] | SQD  | C34-C35-C36-C37 |
| 34  | C     | 520    | LMG  | C31-C32-C33-C34 |
| 23  | B     | 611    | CLA  | C8-C10-C11-C12  |
| 25  | a     | 411    | SQD  | C16-C17-C18-C19 |
| 33  | d     | 407[A] | LHG  | C11-C10-C9-C8   |
| 36  | h     | 102    | DGD  | CDA-CEA-CFA-CGA |
| 26  | a     | 417    | GOL  | O1-C1-C2-O2     |
| 33  | A     | 418[B] | LHG  | O1-C1-C2-O2     |
| 23  | B     | 607    | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | B     | 604    | CLA  | C1A-C2A-CAA-CBA |
| 23  | d     | 402[A] | CLA  | C1A-C2A-CAA-CBA |
| 36  | C     | 518[B] | DGD  | C1A-C2A-C3A-C4A |
| 25  | a     | 409[A] | SQD  | C35-C36-C37-C38 |
| 24  | K     | 102    | BCR  | C7-C8-C9-C10    |
| 24  | c     | 516    | BCR  | C7-C8-C9-C10    |
| 34  | Z     | 101    | LMG  | C29-C28-O8-C9   |
| 33  | L     | 101[A] | LHG  | O6-C4-C5-C6     |
| 33  | d     | 414[A] | LHG  | C18-C19-C20-C21 |
| 23  | C     | 502    | CLA  | CBD-CGD-O2D-CED |
| 23  | A     | 406[A] | CLA  | C12-C13-C15-C16 |
| 23  | C     | 507    | CLA  | C12-C13-C15-C16 |
| 23  | C     | 508    | CLA  | C11-C12-C13-C15 |
| 23  | D     | 404    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 601    | CLA  | C11-C12-C13-C15 |
| 23  | b     | 616    | CLA  | C6-C7-C8-C10    |
| 23  | d     | 403[A] | CLA  | C11-C12-C13-C15 |
| 32  | m     | 103    | LMT  | O5'-C5'-C6'-O6' |
| 33  | d     | 407[B] | LHG  | C13-C14-C15-C16 |
| 32  | b     | 627    | LMT  | C1-C2-C3-C4     |
| 33  | d     | 407[A] | LHG  | C16-C17-C18-C19 |
| 36  | C     | 519    | DGD  | C7B-C8B-C9B-CAB |
| 36  | c     | 518[B] | DGD  | C5A-C6A-C7A-C8A |
| 23  | b     | 604    | CLA  | C15-C16-C17-C18 |
| 33  | L     | 101[B] | LHG  | C11-C12-C13-C14 |
| 34  | C     | 521    | LMG  | C35-C36-C37-C38 |
| 34  | c     | 520    | LMG  | C30-C31-C32-C33 |
| 33  | d     | 408[B] | LHG  | C11-C10-C9-C8   |
| 33  | D     | 407[B] | LHG  | O6-C4-C5-O7     |
| 23  | D     | 404    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 507    | CLA  | C11-C10-C8-C9   |
| 36  | C     | 517[A] | DGD  | C6A-C7A-C8A-C9A |
| 35  | b     | 625    | HTG  | C4-C5-C6-O6     |
| 23  | B     | 602    | CLA  | C15-C16-C17-C18 |
| 34  | B     | 620    | LMG  | C18-C19-C20-C21 |
| 33  | L     | 101[A] | LHG  | C26-C27-C28-C29 |
| 36  | c     | 518[A] | DGD  | C7B-C8B-C9B-CAB |
| 25  | l     | 101    | SQD  | C33-C34-C35-C36 |
| 33  | E     | 101[A] | LHG  | O7-C5-C6-O8     |
| 33  | a     | 419[B] | LHG  | O7-C5-C6-O8     |
| 34  | z     | 101    | LMG  | C13-C14-C15-C16 |
| 36  | c     | 517[B] | DGD  | C2E-C1E-O5D-C6D |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | L     | 101[B] | LHG  | C24-C25-C26-C27 |
| 25  | a     | 409[B] | SQD  | O6-C44-C45-C46  |
| 28  | a     | 413[A] | PL9  | C43-C44-C46-C47 |
| 28  | d     | 406[B] | PL9  | C43-C44-C46-C47 |
| 34  | z     | 101    | LMG  | C10-C11-C12-C13 |
| 25  | a     | 409[B] | SQD  | C35-C36-C37-C38 |
| 23  | B     | 601    | CLA  | CAD-CBD-CGD-O2D |
| 23  | B     | 607    | CLA  | CAD-CBD-CGD-O2D |
| 23  | C     | 503    | CLA  | CAD-CBD-CGD-O2D |
| 23  | b     | 601    | CLA  | CAD-CBD-CGD-O2D |
| 23  | c     | 503    | CLA  | CAD-CBD-CGD-O2D |
| 23  | B     | 613    | CLA  | C13-C15-C16-C17 |
| 25  | A     | 409[A] | SQD  | C13-C14-C15-C16 |
| 23  | b     | 604    | CLA  | C10-C11-C12-C13 |
| 33  | E     | 101[B] | LHG  | C11-C10-C9-C8   |
| 33  | D     | 407[A] | LHG  | C34-C35-C36-C37 |
| 36  | C     | 517[B] | DGD  | C3B-C4B-C5B-C6B |
| 36  | C     | 518[A] | DGD  | C8A-C9A-CAA-CBA |
| 36  | h     | 102    | DGD  | C3B-C4B-C5B-C6B |
| 33  | A     | 418[B] | LHG  | C29-C30-C31-C32 |
| 34  | c     | 501    | LMG  | C14-C15-C16-C17 |
| 23  | B     | 601    | CLA  | CAD-CBD-CGD-O1D |
| 23  | B     | 607    | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 503    | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 505    | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 508    | CLA  | CHA-CBD-CGD-O1D |
| 23  | C     | 508    | CLA  | CHA-CBD-CGD-O2D |
| 23  | b     | 601    | CLA  | CAD-CBD-CGD-O1D |
| 23  | c     | 503    | CLA  | CAD-CBD-CGD-O1D |
| 23  | c     | 510    | CLA  | CHA-CBD-CGD-O1D |
| 23  | c     | 510    | CLA  | CHA-CBD-CGD-O2D |
| 23  | c     | 513    | CLA  | CHA-CBD-CGD-O1D |
| 23  | c     | 513    | CLA  | CHA-CBD-CGD-O2D |
| 33  | D     | 407[A] | LHG  | C4-O6-P-O3      |
| 33  | D     | 407[A] | LHG  | C4-O6-P-O5      |
| 33  | E     | 101[A] | LHG  | C4-O6-P-O5      |
| 33  | E     | 101[B] | LHG  | C4-O6-P-O5      |
| 33  | a     | 419[A] | LHG  | C4-O6-P-O4      |
| 33  | a     | 419[B] | LHG  | C4-O6-P-O4      |
| 33  | d     | 407[B] | LHG  | C11-C10-C9-C8   |
| 36  | c     | 518[A] | DGD  | C5A-C6A-C7A-C8A |
| 32  | B     | 629    | LMT  | C2-C3-C4-C5     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 34  | c     | 520    | LMG  | C32-C33-C34-C35 |
| 23  | D     | 404    | CLA  | C8-C10-C11-C12  |
| 33  | d     | 414[B] | LHG  | C29-C30-C31-C32 |
| 23  | b     | 601    | CLA  | CAA-CBA-CGA-O2A |
| 34  | B     | 620    | LMG  | O8-C28-C29-C30  |
| 28  | A     | 413[A] | PL9  | C28-C29-C31-C32 |
| 28  | a     | 413[B] | PL9  | C12-C11-C9-C8   |
| 28  | d     | 406[B] | PL9  | C28-C29-C31-C32 |
| 24  | K     | 102    | BCR  | C7-C8-C9-C34    |
| 33  | D     | 408[A] | LHG  | C2-C3-O3-P      |
| 33  | d     | 408[A] | LHG  | C2-C3-O3-P      |
| 33  | d     | 408[B] | LHG  | C2-C3-O3-P      |
| 36  | c     | 519    | DGD  | CDA-CEA-CFA-CGA |
| 33  | d     | 408[A] | LHG  | C32-C33-C34-C35 |
| 34  | C     | 501    | LMG  | C11-C12-C13-C14 |
| 36  | H     | 102    | DGD  | C8A-C9A-CAA-CBA |
| 25  | A     | 411    | SQD  | C30-C31-C32-C33 |
| 33  | D     | 407[A] | LHG  | C26-C27-C28-C29 |
| 33  | d     | 407[B] | LHG  | C9-C10-C11-C12  |
| 36  | C     | 518[B] | DGD  | C5B-C6B-C7B-C8B |
| 28  | A     | 413[B] | PL9  | C4-C3-C7-C8     |
| 28  | a     | 413[A] | PL9  | C4-C3-C7-C8     |
| 34  | C     | 520    | LMG  | C30-C31-C32-C33 |
| 33  | A     | 418[A] | LHG  | O1-C1-C2-C3     |
| 32  | T     | 101    | LMT  | C3-C4-C5-C6     |
| 23  | a     | 404[B] | CLA  | C4C-C3C-CAC-CBC |
| 23  | b     | 612    | CLA  | C10-C11-C12-C13 |
| 33  | d     | 414[A] | LHG  | C34-C35-C36-C37 |
| 23  | c     | 511    | CLA  | C4-C3-C5-C6     |
| 34  | C     | 520    | LMG  | C29-C30-C31-C32 |
| 23  | C     | 511    | CLA  | C13-C15-C16-C17 |
| 23  | b     | 602    | CLA  | C10-C11-C12-C13 |
| 32  | m     | 103    | LMT  | C11-C10-C9-C8   |
| 36  | C     | 519    | DGD  | C7A-C8A-C9A-CAA |
| 36  | c     | 517[B] | DGD  | CBA-CCA-CDA-CEA |
| 32  | A     | 417    | LMT  | O5B-C5B-C6B-O6B |
| 33  | d     | 414[A] | LHG  | C11-C12-C13-C14 |
| 33  | E     | 101[A] | LHG  | O6-C4-C5-C6     |
| 33  | L     | 101[B] | LHG  | O6-C4-C5-C6     |
| 36  | C     | 518[A] | DGD  | C7B-C8B-C9B-CAB |
| 23  | A     | 406[B] | CLA  | C14-C13-C15-C16 |
| 23  | C     | 514    | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | D     | 404    | CLA  | C11-C10-C8-C9   |
| 23  | a     | 407    | CLA  | C11-C10-C8-C9   |
| 23  | c     | 506    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 510    | CLA  | C6-C7-C8-C9     |
| 23  | d     | 403[A] | CLA  | C11-C12-C13-C14 |
| 23  | D     | 404    | CLA  | C11-C10-C8-C7   |
| 23  | b     | 615    | CLA  | C11-C12-C13-C15 |
| 34  | m     | 101    | LMG  | C30-C31-C32-C33 |
| 23  | c     | 511    | CLA  | O1A-CGA-O2A-C1  |
| 33  | L     | 101[B] | LHG  | O6-C4-C5-O7     |
| 36  | C     | 517[B] | DGD  | O6E-C1E-O5D-C6D |
| 36  | c     | 519    | DGD  | O6D-C5D-C6D-O5D |
| 23  | C     | 503    | CLA  | C16-C17-C18-C20 |
| 28  | D     | 406[A] | PL9  | C15-C14-C16-C17 |
| 36  | H     | 102    | DGD  | O2G-C1B-C2B-C3B |
| 28  | d     | 406[B] | PL9  | C18-C19-C21-C22 |
| 25  | a     | 411    | SQD  | C18-C19-C20-C21 |
| 33  | D     | 407[A] | LHG  | C13-C14-C15-C16 |
| 33  | d     | 414[B] | LHG  | C17-C18-C19-C20 |
| 36  | c     | 517[B] | DGD  | CCB-CDB-CEB-CFB |
| 33  | D     | 408[B] | LHG  | C2-C3-O3-P      |
| 33  | E     | 101[B] | LHG  | O7-C5-C6-O8     |
| 23  | c     | 510    | CLA  | C15-C16-C17-C18 |
| 34  | Z     | 101    | LMG  | C21-C22-C23-C24 |
| 33  | D     | 407[B] | LHG  | C10-C11-C12-C13 |
| 33  | b     | 629[A] | LHG  | C28-C29-C30-C31 |
| 33  | d     | 408[A] | LHG  | C10-C11-C12-C13 |
| 36  | H     | 102    | DGD  | CCA-CDA-CEA-CFA |
| 23  | C     | 510    | CLA  | C2-C1-O2A-CGA   |
| 23  | B     | 614    | CLA  | C4-C3-C5-C6     |
| 23  | b     | 601    | CLA  | C4-C3-C5-C6     |
| 25  | A     | 411    | SQD  | C15-C16-C17-C18 |
| 23  | d     | 402[A] | CLA  | C15-C16-C17-C18 |
| 25  | X     | 101    | SQD  | C44-C45-C46-O48 |
| 23  | B     | 601    | CLA  | CAA-CBA-CGA-O2A |
| 32  | m     | 103    | LMT  | C4-C5-C6-C7     |
| 36  | c     | 517[B] | DGD  | C5D-C6D-O5D-C1E |
| 36  | c     | 518[A] | DGD  | C2G-C3G-O3G-C1D |
| 32  | t     | 101    | LMT  | C2-C3-C4-C5     |
| 36  | C     | 519    | DGD  | C9A-CAA-CBA-CCA |
| 28  | a     | 413[A] | PL9  | C45-C44-C46-C47 |
| 23  | b     | 601    | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 28  | a     | 413[B] | PL9  | C43-C44-C46-C47 |
| 25  | A     | 409[A] | SQD  | C16-C17-C18-C19 |
| 34  | D     | 412    | LMG  | C18-C19-C20-C21 |
| 23  | A     | 406[A] | CLA  | C14-C13-C15-C16 |
| 23  | C     | 508    | CLA  | C11-C12-C13-C14 |
| 23  | C     | 511    | CLA  | C11-C12-C13-C14 |
| 33  | D     | 407[A] | LHG  | C28-C29-C30-C31 |
| 23  | c     | 511    | CLA  | CBA-CGA-O2A-C1  |
| 40  | V     | 201    | HEC  | CAD-CBD-CGD-O2D |
| 36  | C     | 519    | DGD  | O6D-C5D-C6D-O5D |
| 23  | b     | 608    | CLA  | C16-C17-C18-C20 |
| 33  | L     | 101[A] | LHG  | C23-C24-C25-C26 |
| 28  | a     | 413[B] | PL9  | C45-C44-C46-C47 |
| 23  | c     | 511    | CLA  | C2-C3-C5-C6     |
| 28  | d     | 406[A] | PL9  | C43-C44-C46-C47 |
| 33  | D     | 408[A] | LHG  | O10-C23-O8-C6   |
| 33  | d     | 408[B] | LHG  | C33-C34-C35-C36 |
| 25  | a     | 411    | SQD  | C15-C16-C17-C18 |
| 23  | d     | 402[A] | CLA  | C4C-C3C-CAC-CBC |
| 23  | B     | 602    | CLA  | C11-C12-C13-C15 |
| 23  | B     | 606    | CLA  | C11-C10-C8-C7   |
| 23  | B     | 613    | CLA  | C11-C10-C8-C7   |
| 23  | B     | 616    | CLA  | C12-C13-C15-C16 |
| 23  | C     | 504    | CLA  | C6-C7-C8-C10    |
| 23  | D     | 404    | CLA  | C15-C16-C17-C18 |
| 23  | b     | 607    | CLA  | C8-C10-C11-C12  |
| 23  | b     | 610    | CLA  | C3-C5-C6-C7     |
| 33  | D     | 408[A] | LHG  | C24-C23-O8-C6   |
| 32  | b     | 621    | LMT  | C7-C8-C9-C10    |
| 33  | D     | 407[B] | LHG  | C28-C29-C30-C31 |
| 25  | a     | 411    | SQD  | C26-C27-C28-C29 |
| 25  | a     | 409[A] | SQD  | C11-C12-C13-C14 |
| 23  | b     | 611    | CLA  | C3-C5-C6-C7     |
| 32  | t     | 101    | LMT  | O1'-C1-C2-C3    |
| 33  | d     | 408[B] | LHG  | C29-C30-C31-C32 |
| 35  | d     | 411    | HTG  | S1-C1'-C2'-C3'  |
| 40  | V     | 201    | HEC  | CAD-CBD-CGD-O1D |
| 23  | d     | 402[B] | CLA  | C2C-C3C-CAC-CBC |
| 25  | b     | 620    | SQD  | C33-C34-C35-C36 |
| 23  | b     | 616    | CLA  | C4-C3-C5-C6     |
| 28  | D     | 406[B] | PL9  | C45-C44-C46-C47 |
| 28  | D     | 406[B] | PL9  | C28-C29-C31-C32 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | d     | 414[A] | LHG  | C1-C2-C3-O3     |
| 34  | c     | 501    | LMG  | C38-C39-C40-C41 |
| 23  | B     | 602    | CLA  | C2A-CAA-CBA-CGA |
| 32  | F     | 101    | LMT  | C2-C3-C4-C5     |
| 23  | C     | 513    | CLA  | C3-C5-C6-C7     |
| 23  | b     | 601    | CLA  | C3-C5-C6-C7     |
| 33  | b     | 629[B] | LHG  | C17-C18-C19-C20 |
| 23  | A     | 407    | CLA  | C11-C12-C13-C14 |
| 23  | B     | 602    | CLA  | C11-C12-C13-C14 |
| 23  | B     | 606    | CLA  | C11-C10-C8-C9   |
| 23  | B     | 613    | CLA  | C11-C12-C13-C14 |
| 23  | C     | 505    | CLA  | C11-C12-C13-C14 |
| 23  | C     | 506    | CLA  | C14-C13-C15-C16 |
| 23  | a     | 405[A] | CLA  | C14-C13-C15-C16 |
| 23  | c     | 505    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 507    | CLA  | C6-C7-C8-C9     |
| 23  | c     | 503    | CLA  | C16-C17-C18-C19 |
| 25  | l     | 101    | SQD  | C24-C25-C26-C27 |
| 32  | A     | 417    | LMT  | C9-C10-C11-C12  |
| 33  | E     | 101[B] | LHG  | C12-C13-C14-C15 |
| 33  | a     | 419[B] | LHG  | C24-C25-C26-C27 |
| 36  | c     | 517[A] | DGD  | C4B-C5B-C6B-C7B |
| 36  | c     | 517[B] | DGD  | C6B-C7B-C8B-C9B |
| 34  | c     | 501    | LMG  | O8-C28-C29-C30  |
| 23  | b     | 616    | CLA  | C2-C3-C5-C6     |
| 23  | c     | 514    | CLA  | C2-C3-C5-C6     |
| 33  | E     | 101[A] | LHG  | C12-C13-C14-C15 |
| 25  | a     | 409[A] | SQD  | C10-C11-C12-C13 |
| 23  | a     | 407    | CLA  | C15-C16-C17-C18 |
| 33  | d     | 407[A] | LHG  | C9-C10-C11-C12  |
| 23  | a     | 405[A] | CLA  | C1A-C2A-CAA-CBA |
| 25  | a     | 409[B] | SQD  | C27-C28-C29-C30 |
| 38  | f     | 101    | HEM  | CAD-CBD-CGD-O1D |
| 24  | B     | 617    | BCR  | C1-C6-C7-C8     |
| 24  | D     | 405    | BCR  | C23-C24-C25-C30 |
| 24  | H     | 101    | BCR  | C23-C24-C25-C26 |
| 24  | b     | 617    | BCR  | C5-C6-C7-C8     |
| 24  | d     | 405    | BCR  | C23-C24-C25-C30 |
| 24  | h     | 101    | BCR  | C23-C24-C25-C30 |
| 36  | C     | 517[B] | DGD  | C1B-C2B-C3B-C4B |
| 23  | b     | 610    | CLA  | C13-C15-C16-C17 |
| 33  | D     | 407[A] | LHG  | C17-C18-C19-C20 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | d     | 408[B] | LHG  | C32-C33-C34-C35 |
| 23  | A     | 406[A] | CLA  | C16-C17-C18-C19 |
| 35  | b     | 622    | HTG  | O5-C5-C6-O6     |
| 38  | F     | 102    | HEM  | CAD-CBD-CGD-O1D |
| 33  | A     | 418[A] | LHG  | C29-C30-C31-C32 |
| 23  | B     | 601    | CLA  | C11-C12-C13-C15 |
| 23  | C     | 503    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 606    | CLA  | C11-C10-C8-C7   |
| 33  | b     | 629[A] | LHG  | C10-C11-C12-C13 |
| 32  | e     | 101    | LMT  | C2-C3-C4-C5     |
| 28  | A     | 413[A] | PL9  | C4-C3-C7-C8     |
| 23  | B     | 615    | CLA  | C8-C10-C11-C12  |
| 32  | b     | 621    | LMT  | C3-C4-C5-C6     |
| 36  | c     | 517[A] | DGD  | CBA-CCA-CDA-CEA |
| 25  | f     | 102    | SQD  | C26-C27-C28-C29 |
| 28  | D     | 406[A] | PL9  | C35-C34-C36-C37 |
| 28  | d     | 406[B] | PL9  | C20-C19-C21-C22 |
| 28  | D     | 406[B] | PL9  | C43-C44-C46-C47 |
| 34  | C     | 521    | LMG  | C11-C12-C13-C14 |
| 34  | d     | 412    | LMG  | C16-C17-C18-C19 |
| 36  | C     | 519    | DGD  | C3B-C4B-C5B-C6B |
| 33  | L     | 101[A] | LHG  | C10-C11-C12-C13 |
| 32  | e     | 101    | LMT  | O1'-C1-C2-C3    |
| 23  | B     | 612    | CLA  | O1A-CGA-O2A-C1  |
| 23  | C     | 512    | CLA  | C11-C12-C13-C14 |
| 23  | b     | 606    | CLA  | C11-C10-C8-C9   |
| 33  | A     | 418[B] | LHG  | C11-C12-C13-C14 |
| 23  | B     | 606    | CLA  | C8-C10-C11-C12  |
| 25  | l     | 101    | SQD  | C29-C30-C31-C32 |
| 33  | a     | 419[A] | LHG  | C24-C25-C26-C27 |
| 34  | B     | 620    | LMG  | C20-C21-C22-C23 |
| 23  | b     | 604    | CLA  | C4-C3-C5-C6     |
| 28  | A     | 413[A] | PL9  | C25-C24-C26-C27 |
| 28  | D     | 406[B] | PL9  | C35-C34-C36-C37 |
| 23  | D     | 404    | CLA  | O1A-CGA-O2A-C1  |
| 23  | B     | 612    | CLA  | CBA-CGA-O2A-C1  |
| 34  | m     | 101    | LMG  | C2-C1-O1-C7     |
| 36  | c     | 518[B] | DGD  | C2E-C1E-O5D-C6D |
| 33  | d     | 407[B] | LHG  | O10-C23-O8-C6   |
| 36  | C     | 518[B] | DGD  | C8A-C9A-CAA-CBA |
| 36  | C     | 518[B] | DGD  | C8B-C9B-CAB-CBB |
| 25  | a     | 409[B] | SQD  | C11-C12-C13-C14 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | H     | 102    | DGD  | O1G-C1G-C2G-C3G |
| 36  | h     | 102    | DGD  | O1G-C1G-C2G-C3G |
| 36  | h     | 102    | DGD  | CBA-CCA-CDA-CEA |
| 23  | a     | 404[B] | CLA  | C2A-CAA-CBA-CGA |
| 38  | f     | 101    | HEM  | CAA-CBA-CGA-O2A |
| 26  | l     | 103[B] | GOL  | O1-C1-C2-O2     |
| 26  | v     | 202[B] | GOL  | O1-C1-C2-O2     |
| 32  | b     | 627    | LMT  | C2-C1-O1'-C1'   |
| 33  | A     | 418[A] | LHG  | O1-C1-C2-O2     |
| 33  | d     | 414[A] | LHG  | C27-C28-C29-C30 |
| 33  | E     | 101[B] | LHG  | O6-C4-C5-O7     |
| 35  | B     | 621    | HTG  | C4'-C5'-C6'-C7' |
| 33  | d     | 414[A] | LHG  | C17-C18-C19-C20 |
| 23  | B     | 614    | CLA  | C2-C3-C5-C6     |
| 32  | t     | 101    | LMT  | C4'-C5'-C6'-O6' |
| 33  | A     | 418[B] | LHG  | C17-C18-C19-C20 |
| 33  | d     | 407[A] | LHG  | C25-C26-C27-C28 |
| 38  | f     | 101    | HEM  | CAD-CBD-CGD-O2D |
| 25  | A     | 411    | SQD  | C19-C20-C21-C22 |
| 38  | F     | 102    | HEM  | CAD-CBD-CGD-O2D |
| 34  | c     | 521    | LMG  | C31-C32-C33-C34 |
| 31  | a     | 406[A] | PHO  | CHA-CBD-CGD-O1D |
| 23  | C     | 509    | CLA  | C13-C15-C16-C17 |
| 23  | C     | 503    | CLA  | C3-C5-C6-C7     |
| 34  | C     | 501    | LMG  | C13-C14-C15-C16 |
| 33  | d     | 407[B] | LHG  | C24-C23-O8-C6   |
| 23  | c     | 505    | CLA  | C4-C3-C5-C6     |
| 25  | b     | 620    | SQD  | C30-C31-C32-C33 |
| 36  | H     | 102    | DGD  | O1G-C1G-C2G-O2G |
| 36  | C     | 518[B] | DGD  | C7B-C8B-C9B-CAB |
| 36  | c     | 518[B] | DGD  | O6E-C1E-O5D-C6D |
| 23  | c     | 505    | CLA  | C12-C13-C15-C16 |
| 35  | b     | 623    | HTG  | C4'-C5'-C6'-C7' |
| 34  | z     | 101    | LMG  | O7-C10-C11-C12  |
| 33  | d     | 414[A] | LHG  | C9-C10-C11-C12  |
| 34  | C     | 520    | LMG  | C36-C37-C38-C39 |
| 36  | h     | 102    | DGD  | CCA-CDA-CEA-CFA |
| 32  | B     | 629    | LMT  | C1-C2-C3-C4     |
| 33  | A     | 418[A] | LHG  | C17-C18-C19-C20 |
| 23  | B     | 614    | CLA  | C6-C7-C8-C9     |
| 23  | a     | 405[A] | CLA  | C11-C12-C13-C14 |
| 23  | a     | 405[B] | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | b     | 601    | CLA  | C11-C12-C13-C14 |
| 23  | b     | 606    | CLA  | C14-C13-C15-C16 |
| 23  | d     | 404    | CLA  | C11-C12-C13-C14 |
| 36  | C     | 517[B] | DGD  | C5D-C6D-O5D-C1E |
| 36  | c     | 517[A] | DGD  | CDB-CEB-CFB-CGB |
| 40  | v     | 201    | HEC  | CAD-CBD-CGD-O2D |
| 23  | A     | 404[B] | CLA  | C2-C1-O2A-CGA   |
| 23  | b     | 613    | CLA  | C2-C1-O2A-CGA   |
| 23  | b     | 614    | CLA  | C2-C1-O2A-CGA   |
| 23  | B     | 616    | CLA  | C16-C17-C18-C20 |
| 33  | d     | 407[B] | LHG  | C16-C17-C18-C19 |
| 33  | a     | 419[B] | LHG  | C7-C8-C9-C10    |
| 23  | b     | 615    | CLA  | C3A-C2A-CAA-CBA |
| 38  | F     | 102    | HEM  | C2B-C3B-CAB-CBB |
| 36  | c     | 519    | DGD  | C1A-C2A-C3A-C4A |
| 23  | B     | 605    | CLA  | CBD-CGD-O2D-CED |
| 33  | d     | 414[B] | LHG  | C23-C24-C25-C26 |
| 31  | a     | 406[A] | PHO  | O2A-C1-C2-C3    |
| 25  | a     | 411    | SQD  | C27-C28-C29-C30 |
| 34  | d     | 412    | LMG  | C13-C14-C15-C16 |
| 33  | b     | 629[A] | LHG  | C25-C26-C27-C28 |
| 32  | e     | 101    | LMT  | C2B-C1B-O1B-C4' |
| 38  | f     | 101    | HEM  | CAA-CBA-CGA-O1A |
| 32  | t     | 101    | LMT  | C11-C10-C9-C8   |
| 33  | L     | 101[B] | LHG  | C11-C10-C9-C8   |
| 31  | a     | 415[B] | PHO  | C4C-C3C-CAC-CBC |
| 23  | c     | 512    | CLA  | C8-C10-C11-C12  |
| 33  | E     | 101[B] | LHG  | C17-C18-C19-C20 |
| 23  | D     | 404    | CLA  | CBA-CGA-O2A-C1  |
| 34  | B     | 620    | LMG  | O1-C7-C8-C9     |
| 38  | f     | 101    | HEM  | C4B-C3B-CAB-CBB |
| 23  | B     | 602    | CLA  | C8-C10-C11-C12  |
| 34  | c     | 520    | LMG  | C14-C15-C16-C17 |
| 40  | v     | 201    | HEC  | CAD-CBD-CGD-O1D |
| 33  | D     | 407[B] | LHG  | C32-C33-C34-C35 |
| 34  | C     | 501    | LMG  | C31-C32-C33-C34 |
| 23  | B     | 616    | CLA  | C16-C17-C18-C19 |
| 23  | b     | 608    | CLA  | C16-C17-C18-C19 |
| 33  | L     | 101[A] | LHG  | C11-C12-C13-C14 |
| 32  | a     | 416    | LMT  | C7-C8-C9-C10    |
| 25  | A     | 411    | SQD  | C7-C8-C9-C10    |
| 36  | h     | 102    | DGD  | O1G-C1G-C2G-O2G |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | B     | 605    | CLA  | C6-C7-C8-C9     |
| 23  | B     | 611    | CLA  | C11-C12-C13-C14 |
| 23  | B     | 614    | CLA  | C11-C10-C8-C9   |
| 23  | b     | 607    | CLA  | C14-C13-C15-C16 |
| 23  | C     | 507    | CLA  | C16-C17-C18-C20 |
| 23  | a     | 404[A] | CLA  | C2C-C3C-CAC-CBC |
| 23  | C     | 511    | CLA  | CAA-CBA-CGA-O2A |
| 33  | A     | 418[A] | LHG  | O8-C23-C24-C25  |
| 23  | A     | 404[A] | CLA  | C2C-C3C-CAC-CBC |
| 36  | c     | 519    | DGD  | C7B-C8B-C9B-CAB |
| 25  | a     | 411    | SQD  | C28-C29-C30-C31 |
| 31  | D     | 401[B] | PHO  | C2C-C3C-CAC-CBC |
| 31  | a     | 406[A] | PHO  | C2C-C3C-CAC-CBC |
| 31  | a     | 406[B] | PHO  | C2C-C3C-CAC-CBC |
| 31  | a     | 415[A] | PHO  | C2C-C3C-CAC-CBC |
| 31  | a     | 415[B] | PHO  | C2C-C3C-CAC-CBC |
| 34  | m     | 101    | LMG  | C32-C33-C34-C35 |
| 33  | A     | 418[B] | LHG  | O8-C23-C24-C25  |
| 36  | c     | 518[A] | DGD  | C1A-C2A-C3A-C4A |
| 23  | C     | 509    | CLA  | C12-C13-C15-C16 |
| 23  | C     | 512    | CLA  | C11-C12-C13-C15 |
| 23  | a     | 405[A] | CLA  | C11-C12-C13-C15 |
| 23  | c     | 514    | CLA  | C12-C13-C15-C16 |
| 36  | C     | 519    | DGD  | CCB-CDB-CEB-CFB |
| 24  | B     | 617    | BCR  | C5-C6-C7-C8     |
| 24  | D     | 405    | BCR  | C23-C24-C25-C26 |
| 24  | d     | 405    | BCR  | C23-C24-C25-C26 |
| 24  | h     | 101    | BCR  | C23-C24-C25-C26 |
| 33  | a     | 419[A] | LHG  | O8-C23-C24-C25  |
| 23  | A     | 407    | CLA  | C2-C1-O2A-CGA   |
| 23  | b     | 608    | CLA  | C2-C1-O2A-CGA   |
| 23  | b     | 610    | CLA  | C16-C17-C18-C19 |
| 23  | b     | 605    | CLA  | C13-C15-C16-C17 |
| 34  | Z     | 101    | LMG  | O7-C10-C11-C12  |
| 32  | M     | 101    | LMT  | O5'-C1'-O1'-C1  |
| 36  | C     | 519    | DGD  | C2A-C3A-C4A-C5A |
| 31  | a     | 415[B] | PHO  | C8-C10-C11-C12  |
| 23  | b     | 612    | CLA  | C13-C15-C16-C17 |
| 33  | E     | 101[B] | LHG  | O7-C7-C8-C9     |
| 31  | a     | 406[A] | PHO  | C2-C3-C5-C6     |
| 35  | c     | 522    | HTG  | C2'-C1'-S1-C1   |
| 35  | o     | 301    | HTG  | C2'-C1'-S1-C1   |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 34  | Z     | 101    | LMG  | O10-C28-O8-C9   |
| 25  | l     | 101    | SQD  | C9-C10-C11-C12  |
| 33  | L     | 101[A] | LHG  | O7-C7-C8-C9     |
| 33  | b     | 629[A] | LHG  | O7-C7-C8-C9     |
| 25  | b     | 620    | SQD  | C25-C26-C27-C28 |
| 35  | b     | 623    | HTG  | S1-C1'-C2'-C3'  |
| 35  | o     | 301    | HTG  | C4'-C5'-C6'-C7' |
| 23  | B     | 605    | CLA  | O1D-CGD-O2D-CED |
| 34  | d     | 412    | LMG  | C28-C29-C30-C31 |
| 34  | B     | 620    | LMG  | C32-C33-C34-C35 |
| 36  | C     | 519    | DGD  | CBA-CCA-CDA-CEA |
| 31  | a     | 406[A] | PHO  | C4-C3-C5-C6     |
| 36  | C     | 519    | DGD  | C8B-C9B-CAB-CBB |
| 33  | a     | 419[B] | LHG  | O8-C23-C24-C25  |
| 26  | B     | 625    | GOL  | O2-C2-C3-O3     |
| 33  | d     | 414[A] | LHG  | C30-C31-C32-C33 |
| 36  | c     | 517[B] | DGD  | C8B-C9B-CAB-CBB |
| 23  | B     | 601    | CLA  | C11-C12-C13-C14 |
| 23  | B     | 613    | CLA  | CAA-CBA-CGA-O2A |
| 25  | A     | 409[B] | SQD  | C16-C17-C18-C19 |
| 34  | C     | 520    | LMG  | O1-C7-C8-C9     |
| 23  | C     | 512    | CLA  | C1A-C2A-CAA-CBA |
| 23  | a     | 405[B] | CLA  | C1A-C2A-CAA-CBA |
| 23  | c     | 507    | CLA  | C1A-C2A-CAA-CBA |
| 34  | B     | 620    | LMG  | O6-C1-O1-C7     |
| 34  | c     | 521    | LMG  | O1-C7-C8-O7     |
| 24  | H     | 101    | BCR  | C9-C10-C11-C12  |
| 33  | d     | 407[B] | LHG  | C30-C31-C32-C33 |
| 25  | a     | 411    | SQD  | O48-C23-C24-C25 |
| 33  | L     | 101[B] | LHG  | O7-C7-C8-C9     |
| 36  | c     | 518[B] | DGD  | CBB-CCB-CDB-CEB |
| 23  | c     | 508    | CLA  | C2A-CAA-CBA-CGA |
| 36  | c     | 517[B] | DGD  | CDB-CEB-CFB-CGB |
| 23  | b     | 615    | CLA  | C13-C15-C16-C17 |
| 33  | A     | 418[B] | LHG  | C9-C10-C11-C12  |
| 23  | B     | 613    | CLA  | C2-C1-O2A-CGA   |
| 23  | a     | 404[A] | CLA  | C2-C1-O2A-CGA   |
| 23  | b     | 610    | CLA  | C2-C1-O2A-CGA   |
| 23  | c     | 513    | CLA  | C2-C1-O2A-CGA   |
| 23  | B     | 612    | CLA  | CAA-CBA-CGA-O2A |
| 23  | C     | 513    | CLA  | CAA-CBA-CGA-O2A |
| 36  | C     | 519    | DGD  | O1G-C1A-C2A-C3A |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | B     | 602    | CLA  | C6-C7-C8-C10    |
| 23  | B     | 615    | CLA  | C12-C13-C15-C16 |
| 23  | a     | 405[B] | CLA  | C11-C12-C13-C15 |
| 23  | b     | 607    | CLA  | C6-C7-C8-C10    |
| 23  | a     | 404[A] | CLA  | C4C-C3C-CAC-CBC |
| 23  | b     | 610    | CLA  | C16-C17-C18-C20 |
| 31  | D     | 401[B] | PHO  | O2A-C1-C2-C3    |
| 32  | A     | 419    | LMT  | C7-C8-C9-C10    |
| 34  | B     | 620    | LMG  | C36-C37-C38-C39 |
| 36  | C     | 517[A] | DGD  | C3A-C4A-C5A-C6A |
| 33  | b     | 629[B] | LHG  | C34-C35-C36-C37 |
| 33  | b     | 629[B] | LHG  | O7-C7-C8-C9     |
| 34  | C     | 520    | LMG  | O7-C10-C11-C12  |
| 23  | b     | 611    | CLA  | C13-C15-C16-C17 |
| 23  | A     | 404[B] | CLA  | C2A-CAA-CBA-CGA |
| 33  | A     | 418[A] | LHG  | C18-C19-C20-C21 |
| 33  | d     | 408[A] | LHG  | C30-C31-C32-C33 |
| 23  | b     | 610    | CLA  | C5-C6-C7-C8     |
| 34  | c     | 520    | LMG  | C29-C30-C31-C32 |
| 34  | Z     | 101    | LMG  | O9-C10-C11-C12  |
| 33  | A     | 418[B] | LHG  | C16-C17-C18-C19 |
| 28  | d     | 406[A] | PL9  | C34-C36-C37-C38 |
| 28  | a     | 413[B] | PL9  | C35-C34-C36-C37 |
| 33  | d     | 408[B] | LHG  | C10-C11-C12-C13 |
| 33  | E     | 101[A] | LHG  | O7-C7-C8-C9     |
| 34  | c     | 520    | LMG  | O7-C10-C11-C12  |
| 25  | a     | 409[B] | SQD  | C10-C11-C12-C13 |
| 33  | E     | 101[B] | LHG  | O9-C7-C8-C9     |
| 33  | b     | 629[A] | LHG  | O9-C7-C8-C9     |
| 23  | A     | 404[A] | CLA  | C4C-C3C-CAC-CBC |
| 32  | m     | 103    | LMT  | C9-C10-C11-C12  |
| 33  | d     | 408[A] | LHG  | O10-C23-O8-C6   |
| 33  | b     | 629[B] | LHG  | C12-C13-C14-C15 |
| 23  | B     | 615    | CLA  | C14-C13-C15-C16 |
| 23  | B     | 616    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 514    | CLA  | C14-C13-C15-C16 |
| 33  | a     | 419[B] | LHG  | O10-C23-C24-C25 |
| 24  | C     | 516    | BCR  | C9-C10-C11-C12  |
| 33  | L     | 101[A] | LHG  | O9-C7-C8-C9     |
| 23  | b     | 612    | CLA  | C8-C10-C11-C12  |
| 25  | A     | 409[B] | SQD  | C18-C19-C20-C21 |
| 26  | d     | 413    | GOL  | O1-C1-C2-O2     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | l     | 103[A] | GOL  | O1-C1-C2-O2     |
| 33  | b     | 629[B] | LHG  | O1-C1-C2-O2     |
| 33  | A     | 418[A] | LHG  | C30-C31-C32-C33 |
| 23  | b     | 612    | CLA  | O1A-CGA-O2A-C1  |
| 23  | b     | 613    | CLA  | CAA-CBA-CGA-O2A |
| 23  | c     | 511    | CLA  | CAA-CBA-CGA-O2A |
| 24  | y     | 101    | BCR  | C21-C22-C23-C24 |
| 23  | C     | 511    | CLA  | CAA-CBA-CGA-O1A |
| 33  | A     | 418[A] | LHG  | O10-C23-C24-C25 |
| 33  | A     | 418[B] | LHG  | O10-C23-C24-C25 |
| 33  | a     | 419[A] | LHG  | O10-C23-C24-C25 |
| 34  | C     | 520    | LMG  | O9-C10-C11-C12  |
| 33  | D     | 408[A] | LHG  | C28-C29-C30-C31 |
| 25  | a     | 411    | SQD  | C45-C44-O6-C1   |
| 34  | C     | 521    | LMG  | C8-C7-O1-C1     |
| 34  | m     | 101    | LMG  | C8-C7-O1-C1     |
| 36  | C     | 517[A] | DGD  | C5D-C6D-O5D-C1E |
| 36  | C     | 518[A] | DGD  | C5D-C6D-O5D-C1E |
| 36  | c     | 517[A] | DGD  | C5D-C6D-O5D-C1E |
| 33  | E     | 101[A] | LHG  | C11-C10-C9-C8   |
| 34  | d     | 412    | LMG  | C38-C39-C40-C41 |
| 36  | C     | 519    | DGD  | O1A-C1A-C2A-C3A |
| 36  | C     | 518[A] | DGD  | O2G-C1B-C2B-C3B |
| 25  | f     | 102    | SQD  | C34-C35-C36-C37 |
| 36  | C     | 517[A] | DGD  | CBA-CCA-CDA-CEA |
| 33  | b     | 629[B] | LHG  | O9-C7-C8-C9     |
| 28  | d     | 406[A] | PL9  | C11-C12-C13-C14 |
| 23  | A     | 405[B] | CLA  | C2C-C3C-CAC-CBC |
| 36  | c     | 518[A] | DGD  | CDA-CEA-CFA-CGA |
| 34  | B     | 620    | LMG  | O6-C5-C6-O5     |
| 23  | C     | 513    | CLA  | CAA-CBA-CGA-O1A |
| 33  | L     | 101[B] | LHG  | O9-C7-C8-C9     |
| 23  | A     | 404[B] | CLA  | CAD-CBD-CGD-O2D |
| 23  | B     | 616    | CLA  | CAD-CBD-CGD-O2D |
| 23  | C     | 502    | CLA  | CAD-CBD-CGD-O2D |
| 23  | C     | 505    | CLA  | CAD-CBD-CGD-O2D |
| 23  | C     | 507    | CLA  | CAD-CBD-CGD-O2D |
| 23  | b     | 616    | CLA  | CAD-CBD-CGD-O2D |
| 31  | a     | 406[A] | PHO  | CAD-CBD-CGD-O2D |
| 31  | a     | 415[B] | PHO  | CAD-CBD-CGD-O2D |
| 33  | L     | 101[A] | LHG  | C32-C33-C34-C35 |
| 34  | D     | 412    | LMG  | O7-C10-C11-C12  |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 25  | a     | 411    | SQD  | O10-C23-C24-C25 |
| 23  | b     | 604    | CLA  | O1A-CGA-O2A-C1  |
| 25  | f     | 102    | SQD  | C11-C10-C9-C8   |
| 23  | C     | 507    | CLA  | C2-C1-O2A-CGA   |
| 33  | E     | 101[A] | LHG  | O8-C23-C24-C25  |
| 28  | A     | 413[B] | PL9  | C46-C47-C48-C49 |
| 32  | A     | 417    | LMT  | C2B-C1B-O1B-C4' |
| 33  | b     | 629[A] | LHG  | C17-C18-C19-C20 |
| 23  | B     | 606    | CLA  | C15-C16-C17-C18 |
| 23  | C     | 510    | CLA  | C13-C15-C16-C17 |
| 33  | D     | 408[A] | LHG  | O8-C23-C24-C25  |
| 33  | d     | 408[B] | LHG  | O8-C23-C24-C25  |
| 36  | C     | 518[B] | DGD  | O2G-C1B-C2B-C3B |
| 23  | B     | 612    | CLA  | CAA-CBA-CGA-O1A |
| 23  | B     | 613    | CLA  | CAA-CBA-CGA-O1A |
| 33  | E     | 101[A] | LHG  | O9-C7-C8-C9     |
| 34  | D     | 412    | LMG  | O9-C10-C11-C12  |
| 34  | d     | 412    | LMG  | C19-C20-C21-C22 |
| 36  | h     | 102    | DGD  | C6A-C7A-C8A-C9A |
| 25  | A     | 411    | SQD  | O48-C23-C24-C25 |
| 33  | D     | 408[B] | LHG  | O8-C23-C24-C25  |
| 34  | c     | 521    | LMG  | O7-C10-C11-C12  |
| 36  | h     | 102    | DGD  | O2G-C1B-C2B-C3B |
| 23  | C     | 504    | CLA  | C5-C6-C7-C8     |
| 34  | c     | 521    | LMG  | O9-C10-C11-C12  |
| 25  | X     | 101    | SQD  | C28-C29-C30-C31 |
| 34  | B     | 620    | LMG  | C29-C30-C31-C32 |

There are no ring outliers.

181 monomers are involved in 372 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 28  | a     | 413[A] | PL9  | 4       | 0            |
| 23  | A     | 406[A] | CLA  | 1       | 0            |
| 23  | C     | 505    | CLA  | 1       | 0            |
| 23  | d     | 403[A] | CLA  | 1       | 0            |
| 26  | l     | 103[A] | GOL  | 1       | 0            |
| 23  | B     | 614    | CLA  | 2       | 0            |
| 24  | c     | 516    | BCR  | 1       | 0            |
| 25  | b     | 620    | SQD  | 2       | 0            |
| 24  | B     | 617    | BCR  | 1       | 0            |
| 28  | D     | 406[A] | PL9  | 1       | 0            |

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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 32  | a     | 416    | LMT  | 1       | 0            |
| 23  | b     | 614    | CLA  | 1       | 0            |
| 35  | o     | 301    | HTG  | 1       | 0            |
| 32  | t     | 101    | LMT  | 3       | 0            |
| 23  | D     | 404    | CLA  | 1       | 0            |
| 23  | c     | 514    | CLA  | 2       | 0            |
| 23  | D     | 403[B] | CLA  | 5       | 0            |
| 23  | b     | 615    | CLA  | 1       | 0            |
| 38  | F     | 102    | HEM  | 1       | 0            |
| 36  | c     | 517[B] | DGD  | 2       | 0            |
| 23  | B     | 616    | CLA  | 3       | 0            |
| 33  | E     | 101[B] | LHG  | 2       | 0            |
| 25  | a     | 411    | SQD  | 1       | 0            |
| 25  | a     | 409[B] | SQD  | 4       | 0            |
| 24  | y     | 101    | BCR  | 1       | 0            |
| 31  | a     | 415[B] | PHO  | 1       | 0            |
| 23  | B     | 604    | CLA  | 1       | 0            |
| 23  | D     | 403[A] | CLA  | 3       | 0            |
| 23  | B     | 613    | CLA  | 4       | 0            |
| 34  | z     | 101    | LMG  | 2       | 0            |
| 23  | C     | 514    | CLA  | 1       | 0            |
| 23  | b     | 607    | CLA  | 2       | 0            |
| 26  | D     | 402    | GOL  | 4       | 0            |
| 33  | E     | 101[A] | LHG  | 4       | 0            |
| 36  | C     | 517[B] | DGD  | 1       | 0            |
| 25  | a     | 409[A] | SQD  | 5       | 0            |
| 35  | d     | 411    | HTG  | 1       | 0            |
| 24  | k     | 101    | BCR  | 1       | 0            |
| 23  | B     | 609    | CLA  | 3       | 0            |
| 23  | c     | 510    | CLA  | 3       | 0            |
| 25  | A     | 409[B] | SQD  | 1       | 0            |
| 23  | C     | 512    | CLA  | 2       | 0            |
| 23  | c     | 505    | CLA  | 2       | 0            |
| 23  | B     | 602    | CLA  | 1       | 0            |
| 36  | C     | 517[A] | DGD  | 1       | 0            |
| 23  | b     | 601    | CLA  | 1       | 0            |
| 32  | B     | 629    | LMT  | 1       | 0            |
| 25  | A     | 409[A] | SQD  | 1       | 0            |
| 24  | b     | 618    | BCR  | 3       | 0            |
| 28  | D     | 406[B] | PL9  | 1       | 0            |
| 24  | H     | 101    | BCR  | 1       | 0            |
| 24  | K     | 102    | BCR  | 1       | 0            |

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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 24  | b     | 617    | BCR  | 1       | 0            |
| 25  | f     | 102    | SQD  | 1       | 0            |
| 23  | C     | 506    | CLA  | 4       | 0            |
| 35  | B     | 623    | HTG  | 1       | 0            |
| 23  | c     | 504    | CLA  | 4       | 0            |
| 24  | D     | 405    | BCR  | 1       | 0            |
| 23  | c     | 507    | CLA  | 4       | 0            |
| 23  | A     | 407    | CLA  | 3       | 0            |
| 23  | a     | 407    | CLA  | 4       | 0            |
| 23  | B     | 615    | CLA  | 5       | 0            |
| 35  | c     | 522    | HTG  | 1       | 0            |
| 23  | B     | 603    | CLA  | 1       | 0            |
| 26  | a     | 418    | GOL  | 3       | 0            |
| 26  | B     | 622    | GOL  | 2       | 0            |
| 23  | A     | 404[A] | CLA  | 2       | 0            |
| 23  | d     | 402[B] | CLA  | 4       | 0            |
| 23  | B     | 612    | CLA  | 3       | 0            |
| 23  | b     | 605    | CLA  | 4       | 0            |
| 32  | A     | 419    | LMT  | 1       | 0            |
| 23  | b     | 612    | CLA  | 3       | 0            |
| 24  | T     | 102    | BCR  | 5       | 0            |
| 26  | v     | 202[B] | GOL  | 2       | 0            |
| 23  | C     | 503    | CLA  | 2       | 0            |
| 24  | d     | 405    | BCR  | 2       | 0            |
| 35  | B     | 621    | HTG  | 1       | 0            |
| 23  | c     | 509    | CLA  | 9       | 0            |
| 23  | d     | 402[A] | CLA  | 3       | 0            |
| 24  | A     | 408    | BCR  | 1       | 0            |
| 23  | b     | 609    | CLA  | 4       | 0            |
| 24  | c     | 515    | BCR  | 2       | 0            |
| 26  | v     | 202[A] | GOL  | 1       | 0            |
| 23  | B     | 610    | CLA  | 2       | 0            |
| 34  | c     | 521    | LMG  | 1       | 0            |
| 25  | A     | 411    | SQD  | 1       | 0            |
| 23  | a     | 404[B] | CLA  | 10      | 0            |
| 23  | B     | 606    | CLA  | 2       | 0            |
| 33  | d     | 407[B] | LHG  | 2       | 0            |
| 24  | a     | 408    | BCR  | 1       | 0            |
| 25  | X     | 101    | SQD  | 1       | 0            |
| 34  | d     | 412    | LMG  | 3       | 0            |
| 23  | c     | 511    | CLA  | 2       | 0            |
| 32  | B     | 626    | LMT  | 1       | 0            |

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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 24  | B     | 618    | BCR  | 2       | 0            |
| 33  | A     | 418[A] | LHG  | 2       | 0            |
| 36  | H     | 102    | DGD  | 1       | 0            |
| 23  | a     | 404[A] | CLA  | 2       | 0            |
| 23  | b     | 608    | CLA  | 1       | 0            |
| 33  | d     | 407[A] | LHG  | 2       | 0            |
| 23  | C     | 504    | CLA  | 4       | 0            |
| 32  | M     | 101    | LMT  | 2       | 0            |
| 23  | A     | 404[B] | CLA  | 6       | 0            |
| 23  | B     | 601    | CLA  | 1       | 0            |
| 35  | b     | 625    | HTG  | 1       | 0            |
| 32  | A     | 417    | LMT  | 1       | 0            |
| 24  | B     | 619    | BCR  | 2       | 0            |
| 33  | a     | 419[B] | LHG  | 3       | 0            |
| 23  | C     | 502    | CLA  | 4       | 0            |
| 36  | h     | 102    | DGD  | 2       | 0            |
| 23  | c     | 503    | CLA  | 2       | 0            |
| 23  | c     | 506    | CLA  | 8       | 0            |
| 23  | b     | 606    | CLA  | 2       | 0            |
| 23  | c     | 513    | CLA  | 7       | 0            |
| 23  | C     | 507    | CLA  | 6       | 0            |
| 23  | c     | 512    | CLA  | 6       | 0            |
| 32  | b     | 621    | LMT  | 1       | 0            |
| 36  | C     | 519    | DGD  | 2       | 0            |
| 36  | c     | 518[A] | DGD  | 3       | 0            |
| 33  | a     | 419[A] | LHG  | 5       | 0            |
| 28  | A     | 413[B] | PL9  | 10      | 0            |
| 31  | a     | 406[B] | PHO  | 2       | 0            |
| 31  | D     | 401[B] | PHO  | 2       | 0            |
| 36  | C     | 518[B] | DGD  | 2       | 0            |
| 32  | B     | 627    | LMT  | 1       | 0            |
| 34  | c     | 501    | LMG  | 1       | 0            |
| 23  | c     | 508    | CLA  | 2       | 0            |
| 26  | D     | 413    | GOL  | 3       | 0            |
| 34  | Z     | 101    | LMG  | 3       | 0            |
| 33  | d     | 408[B] | LHG  | 7       | 0            |
| 33  | D     | 407[A] | LHG  | 2       | 0            |
| 23  | a     | 405[B] | CLA  | 4       | 0            |
| 24  | b     | 619    | BCR  | 4       | 0            |
| 23  | b     | 610    | CLA  | 1       | 0            |
| 28  | A     | 413[A] | PL9  | 11      | 0            |
| 34  | C     | 521    | LMG  | 3       | 0            |

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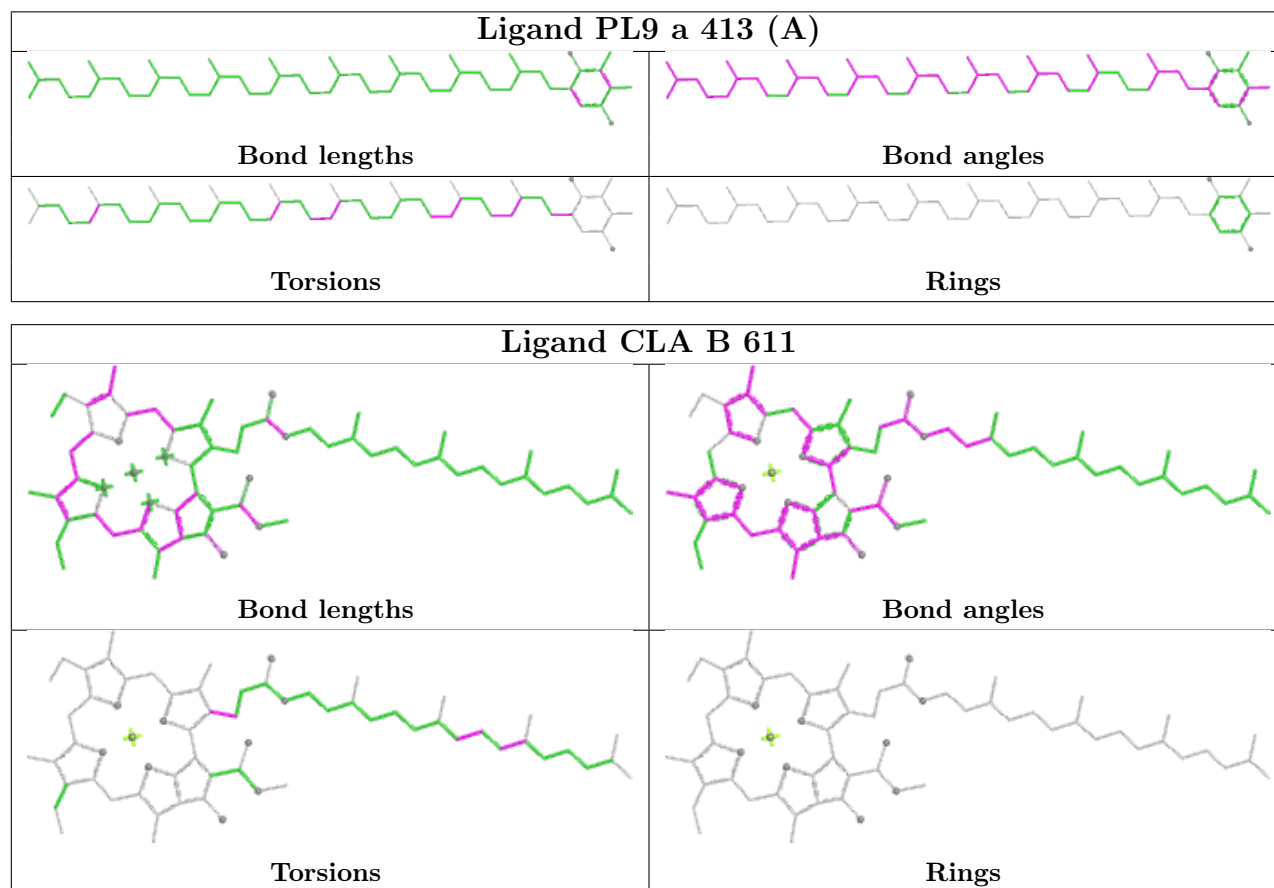
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 31  | D     | 401[A] | PHO  | 1       | 0            |
| 36  | C     | 518[A] | DGD  | 1       | 0            |
| 23  | c     | 502    | CLA  | 2       | 0            |
| 33  | d     | 408[A] | LHG  | 11      | 0            |
| 26  | a     | 417    | GOL  | 2       | 0            |
| 34  | B     | 620    | LMG  | 2       | 0            |
| 24  | h     | 101    | BCR  | 5       | 0            |
| 23  | a     | 405[A] | CLA  | 2       | 0            |
| 33  | L     | 101[B] | LHG  | 1       | 0            |
| 25  | l     | 101    | SQD  | 2       | 0            |
| 26  | b     | 628    | GOL  | 2       | 0            |
| 31  | A     | 416[B] | PHO  | 1       | 0            |
| 23  | A     | 405[B] | CLA  | 5       | 0            |
| 23  | b     | 616    | CLA  | 3       | 0            |
| 33  | D     | 408[B] | LHG  | 3       | 0            |
| 23  | C     | 511    | CLA  | 2       | 0            |
| 34  | c     | 520    | LMG  | 1       | 0            |
| 36  | c     | 518[B] | DGD  | 2       | 0            |
| 31  | A     | 416[A] | PHO  | 1       | 0            |
| 23  | b     | 613    | CLA  | 4       | 0            |
| 23  | A     | 405[A] | CLA  | 1       | 0            |
| 36  | c     | 517[A] | DGD  | 1       | 0            |
| 33  | D     | 408[A] | LHG  | 4       | 0            |
| 26  | O     | 303    | GOL  | 2       | 0            |
| 23  | C     | 508    | CLA  | 2       | 0            |
| 24  | t     | 102    | BCR  | 7       | 0            |
| 24  | Y     | 101    | BCR  | 2       | 0            |
| 31  | a     | 415[A] | PHO  | 1       | 0            |
| 23  | B     | 605    | CLA  | 3       | 0            |
| 33  | D     | 407[B] | LHG  | 2       | 0            |
| 32  | m     | 103    | LMT  | 2       | 0            |
| 28  | a     | 413[B] | PL9  | 4       | 0            |
| 26  | O     | 302    | GOL  | 1       | 0            |
| 35  | b     | 622    | HTG  | 2       | 0            |
| 23  | C     | 509    | CLA  | 4       | 0            |
| 23  | A     | 406[B] | CLA  | 2       | 0            |
| 23  | C     | 513    | CLA  | 2       | 0            |
| 32  | e     | 101    | LMT  | 1       | 0            |
| 36  | c     | 519    | DGD  | 2       | 0            |
| 23  | C     | 510    | CLA  | 2       | 0            |
| 23  | d     | 404    | CLA  | 2       | 0            |
| 23  | d     | 403[B] | CLA  | 5       | 0            |

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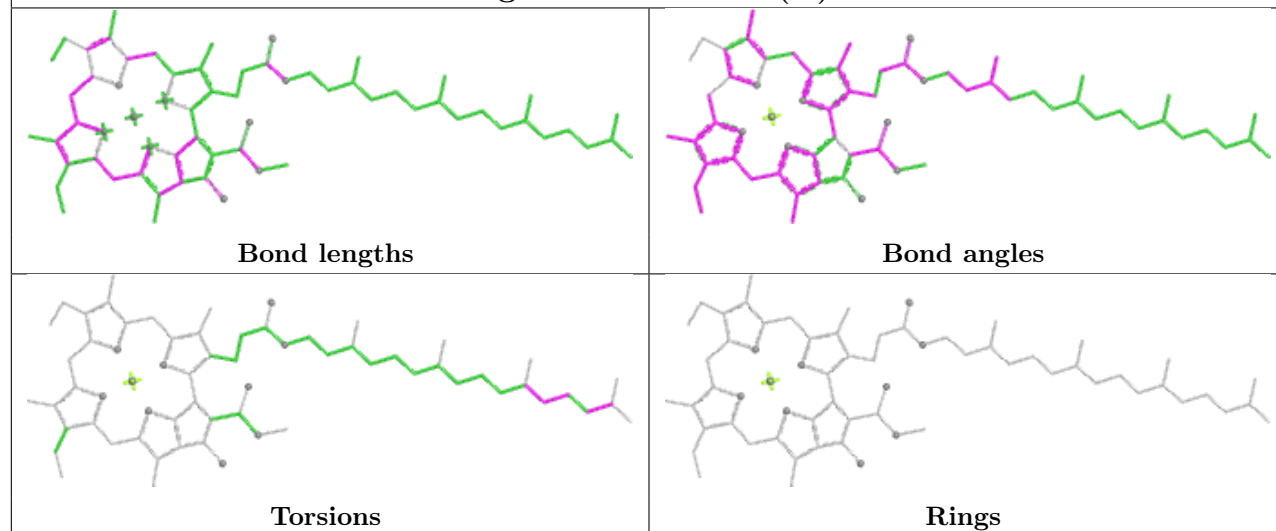
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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 24  | C     | 515    | BCR  | 1       | 0            |
| 26  | l     | 103[B] | GOL  | 1       | 0            |
| 23  | b     | 604    | CLA  | 5       | 0            |

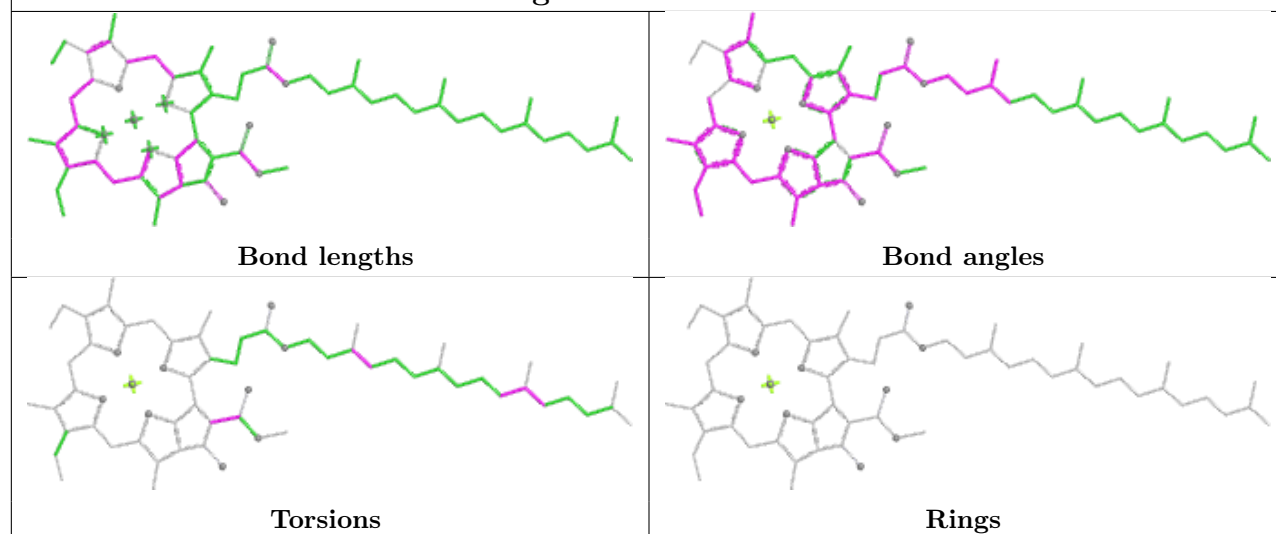
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



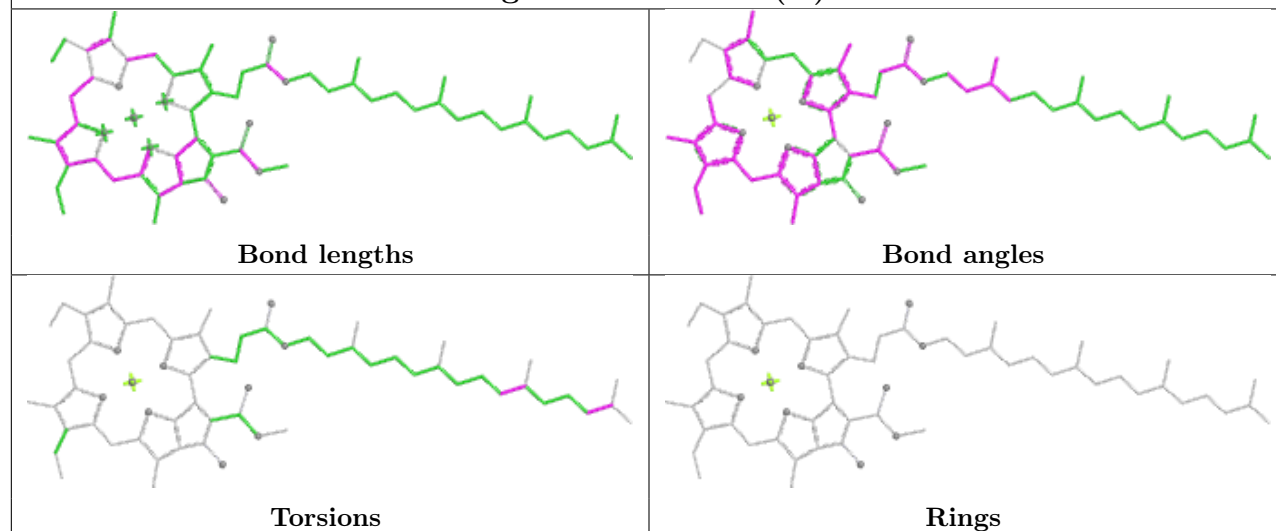
## Ligand CLA A 406 (A)



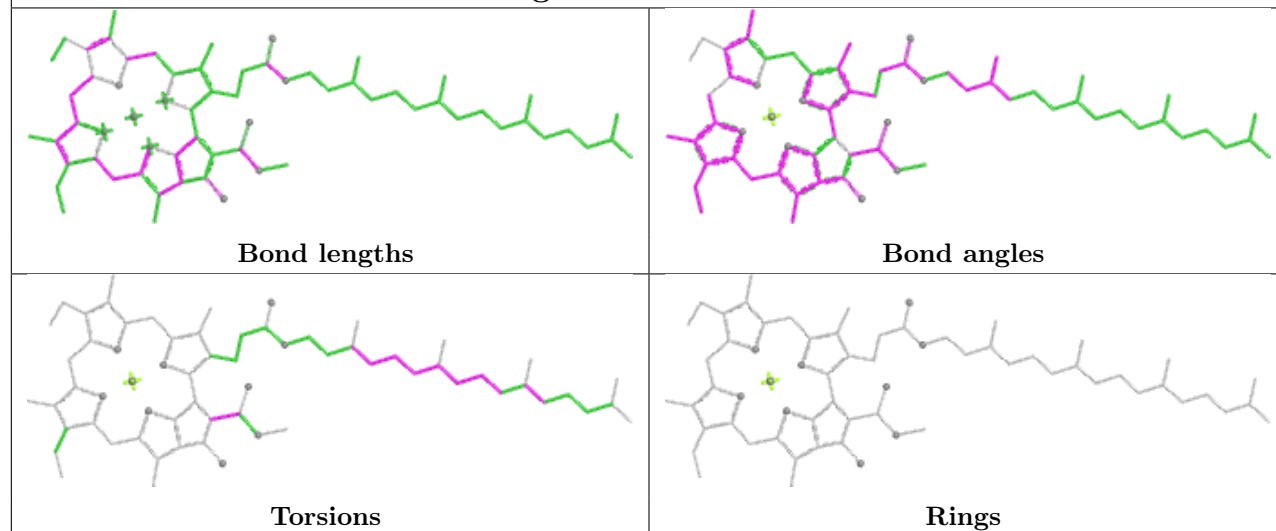
## Ligand CLA C 505



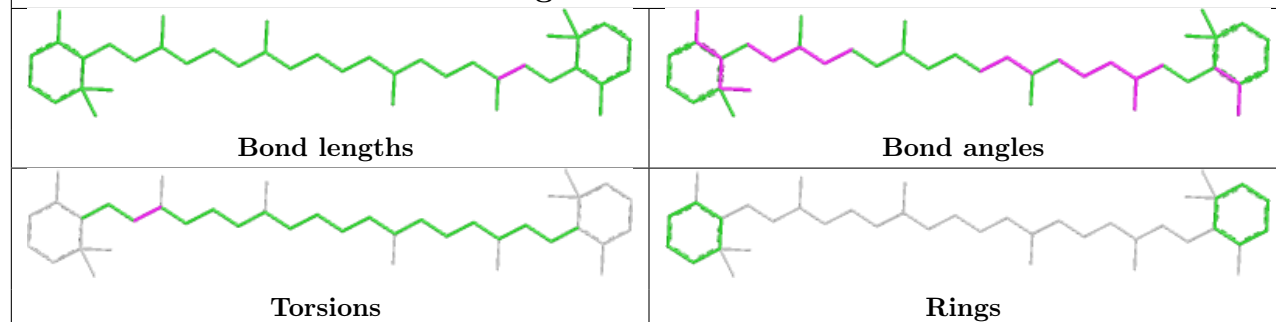
## Ligand CLA d 403 (A)



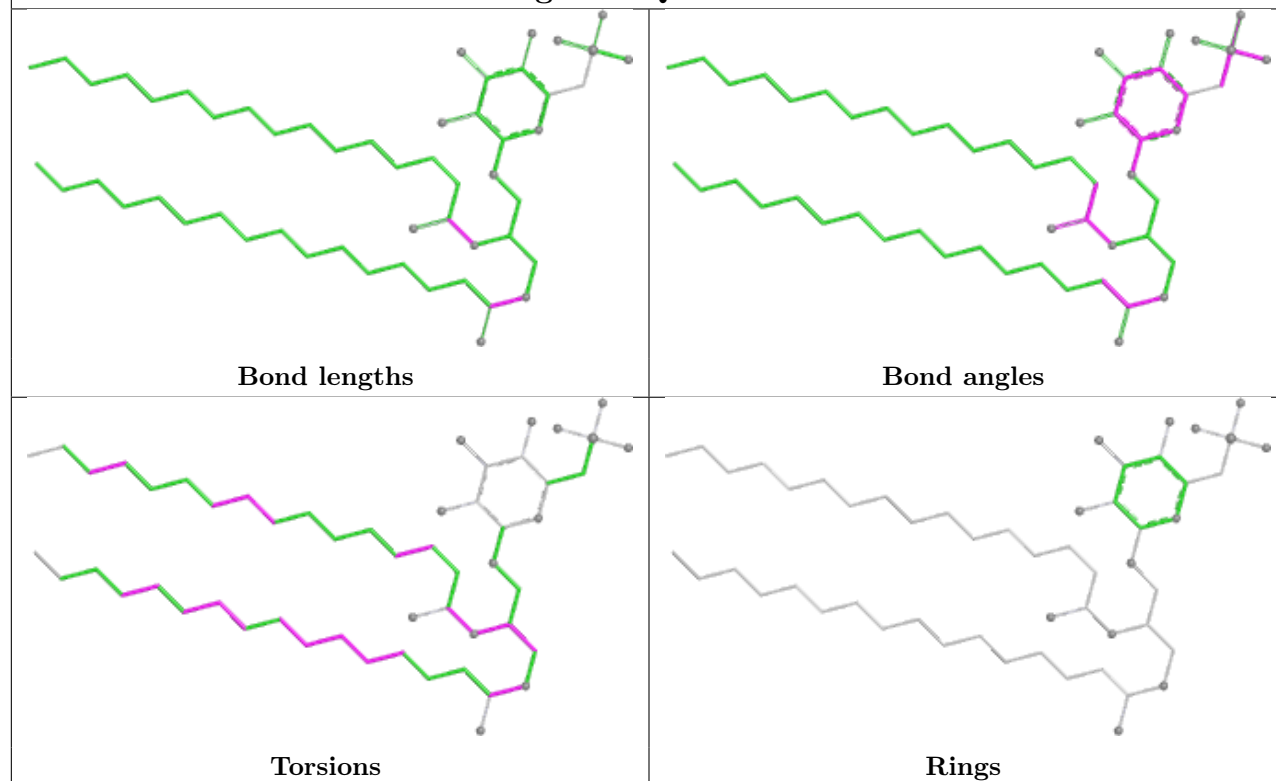
## Ligand CLA B 614

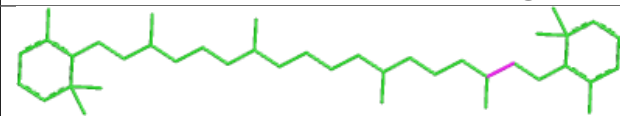
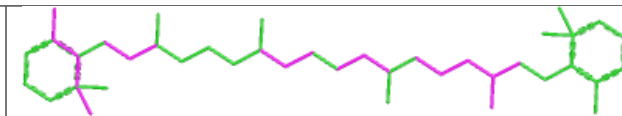
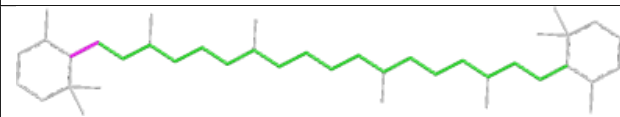
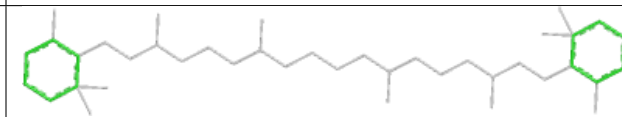


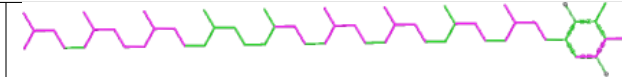
## Ligand BCR c 516

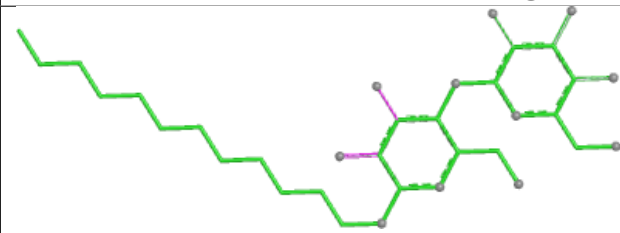
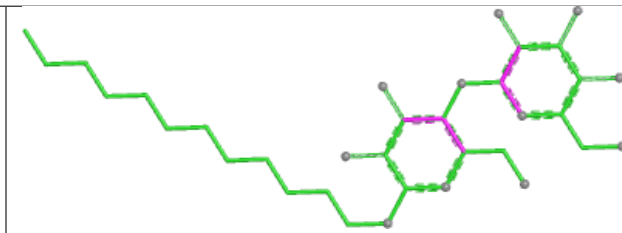
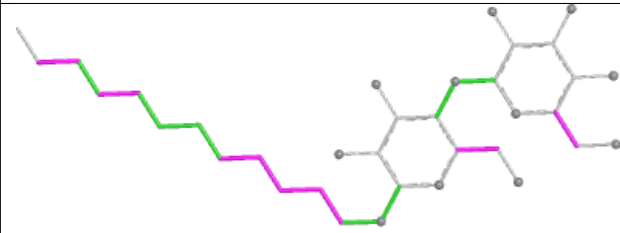
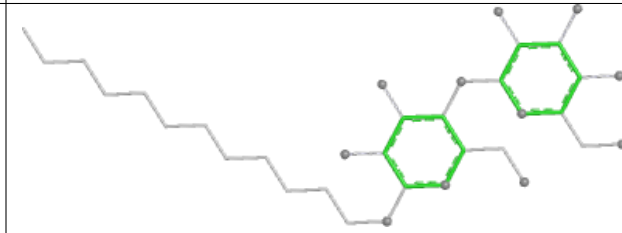


## Ligand SQD b 620

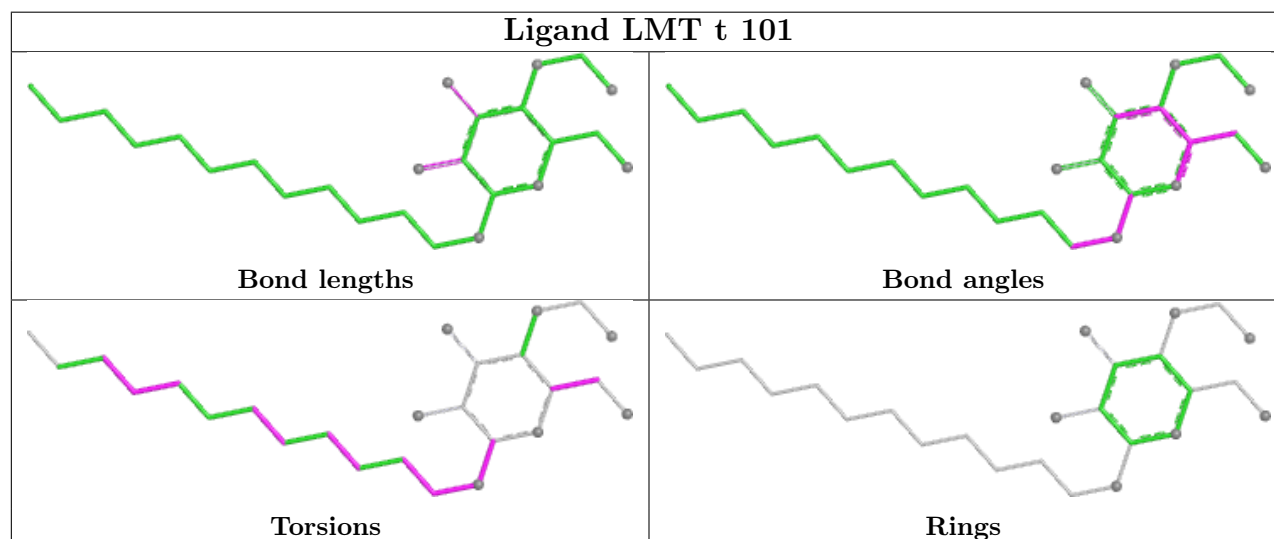
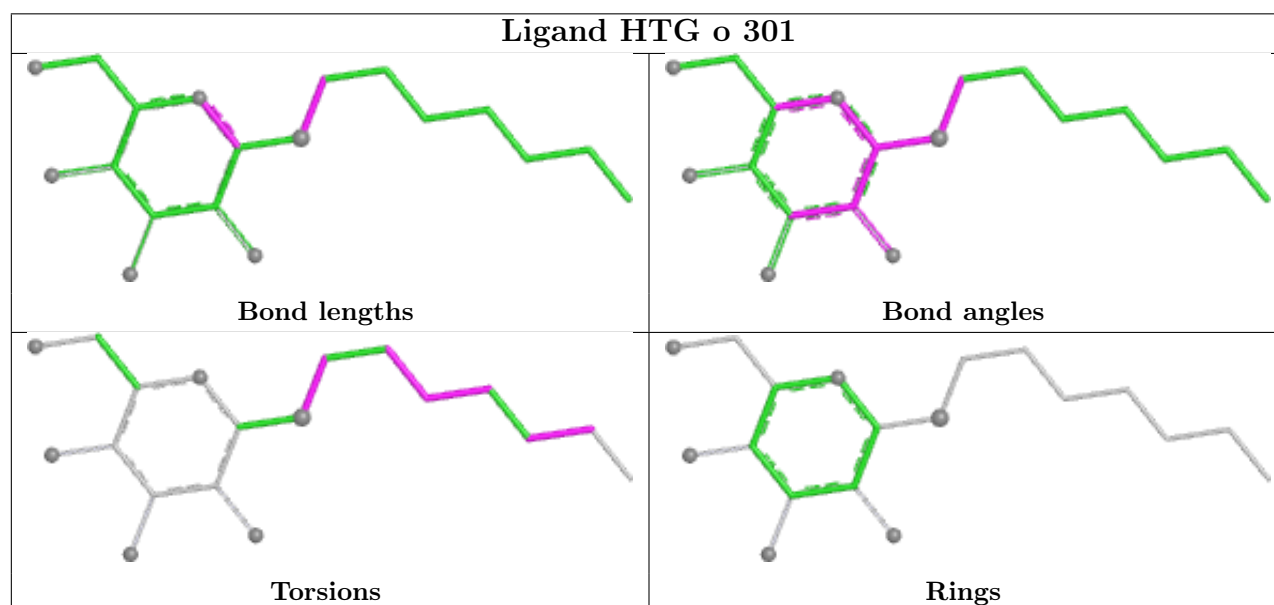
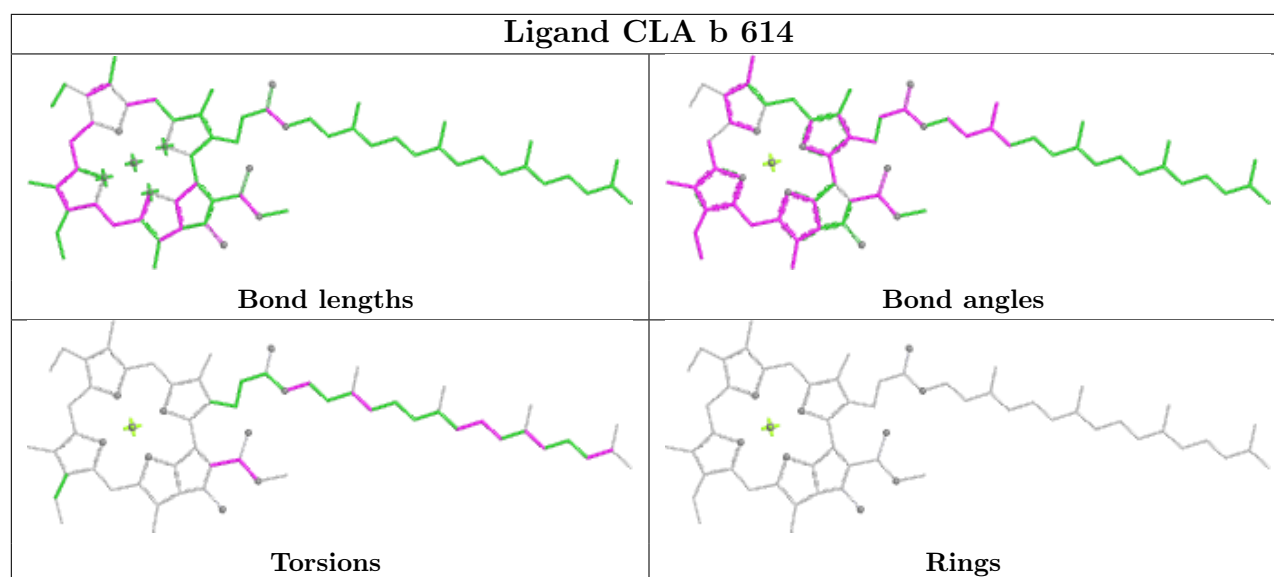


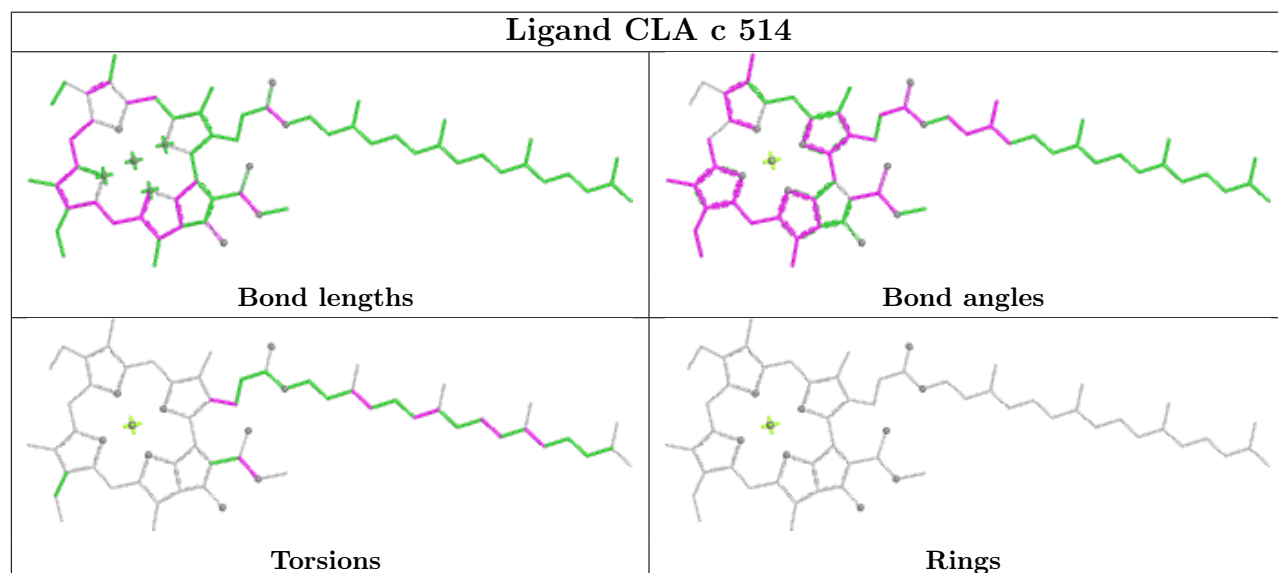
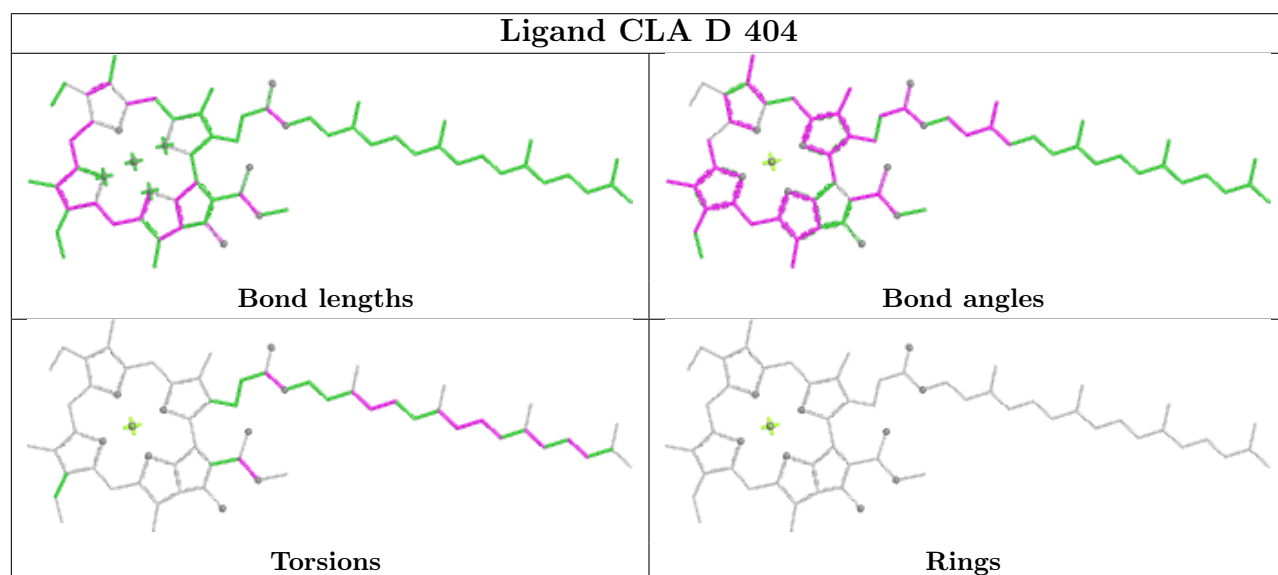
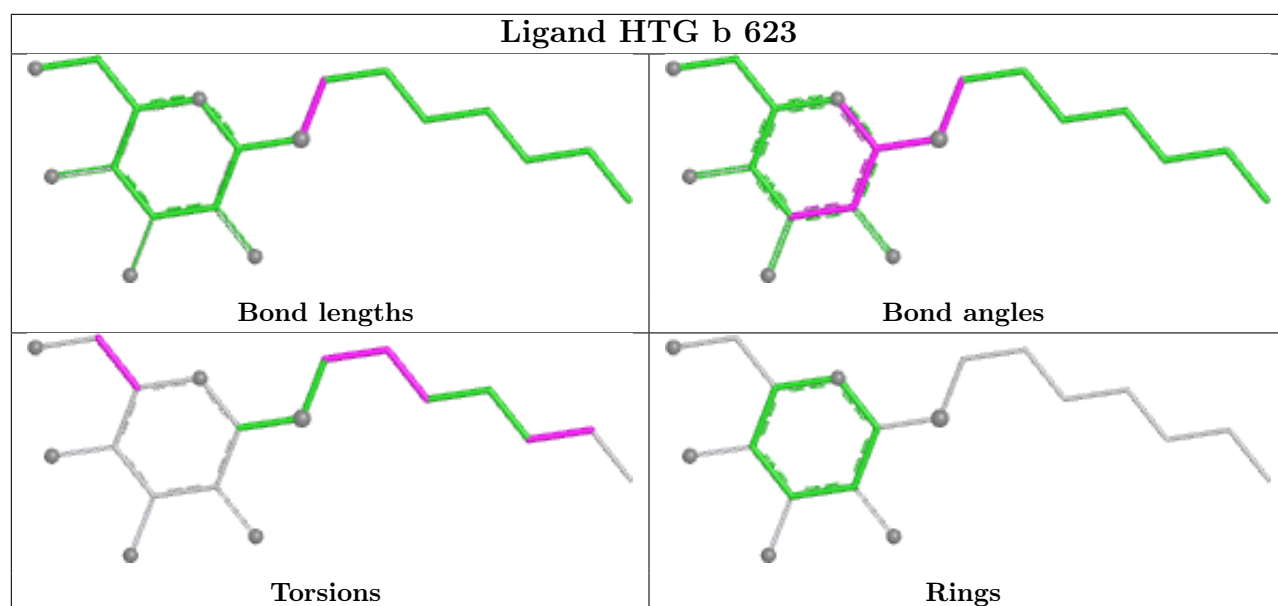
| Ligand BCR B 617                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand PL9 D 406 (A)                                                              |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

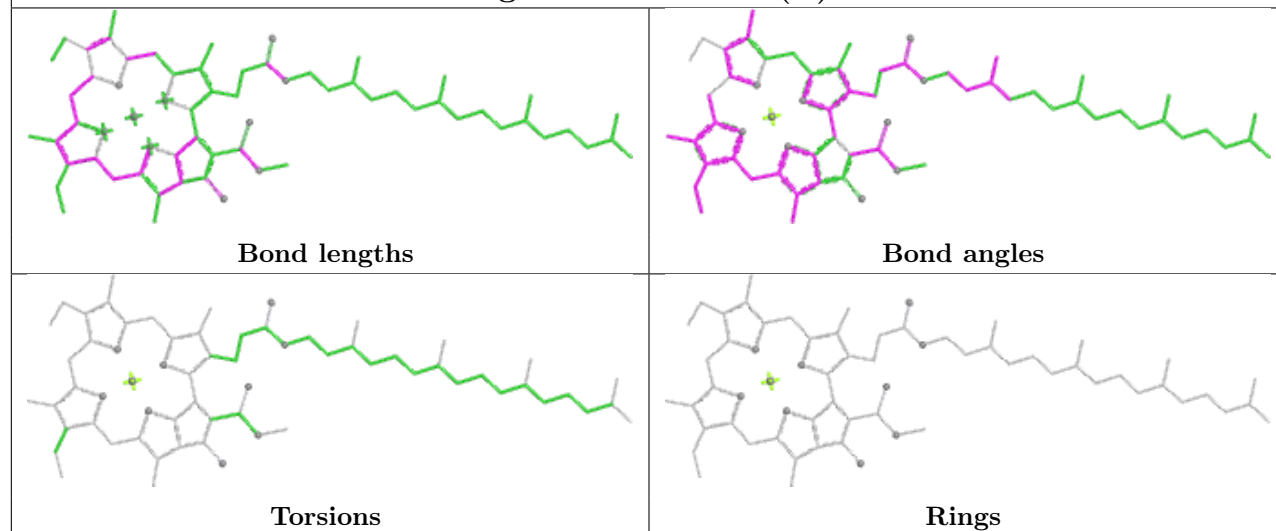
| Ligand LMT a 416                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



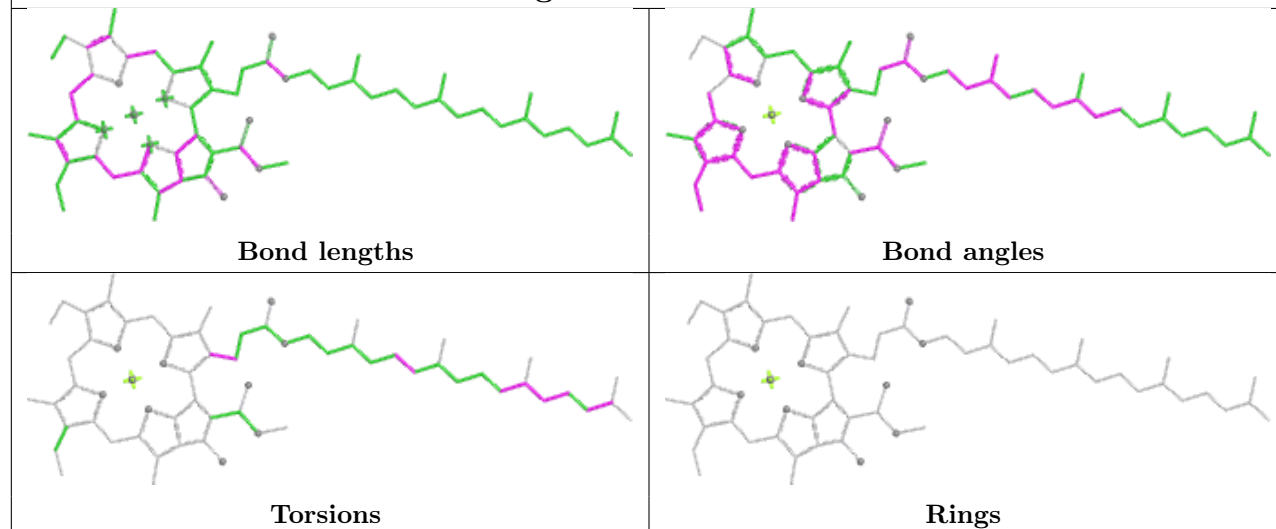


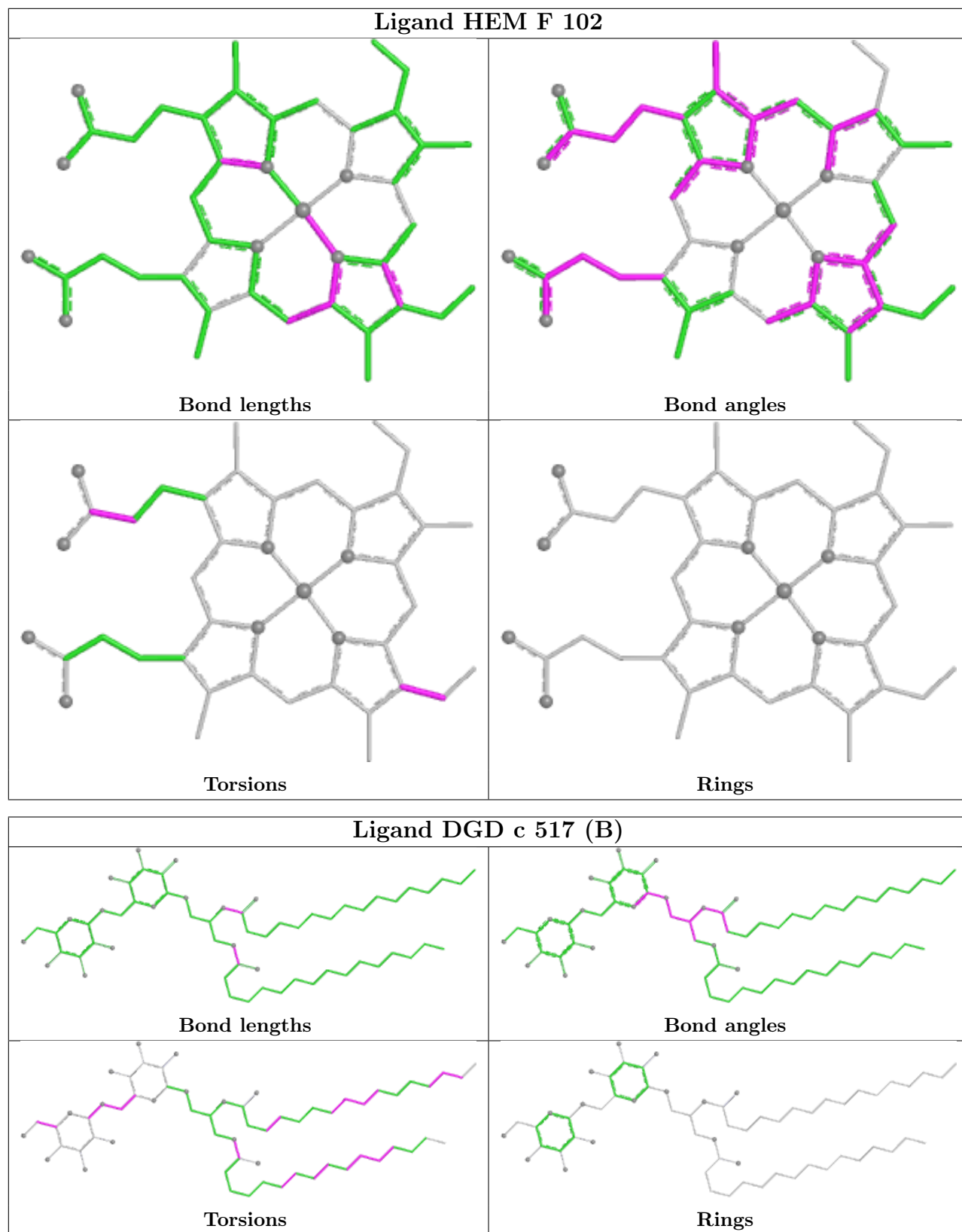


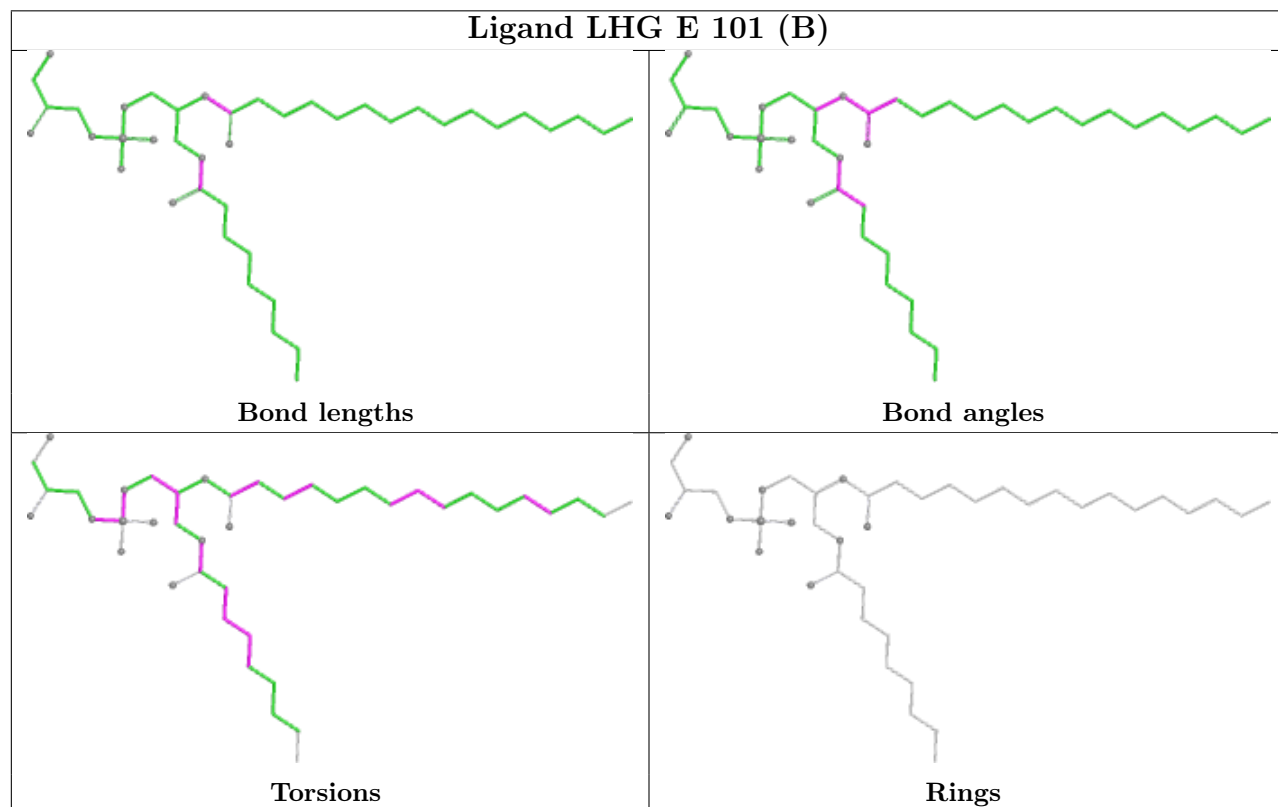
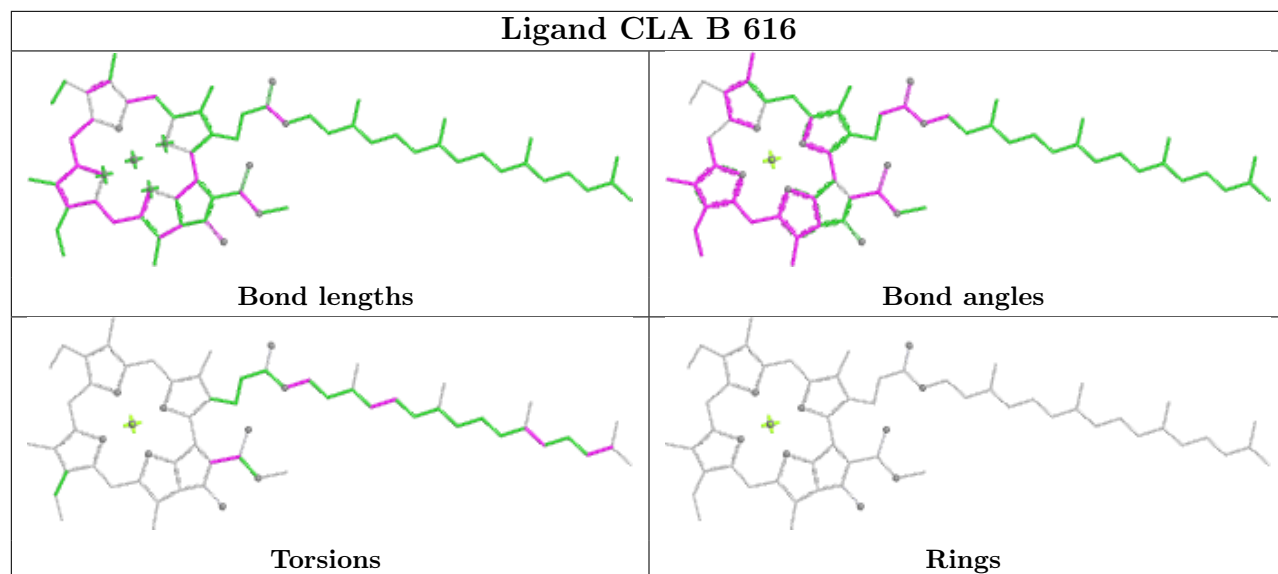
## Ligand CLA D 403 (B)

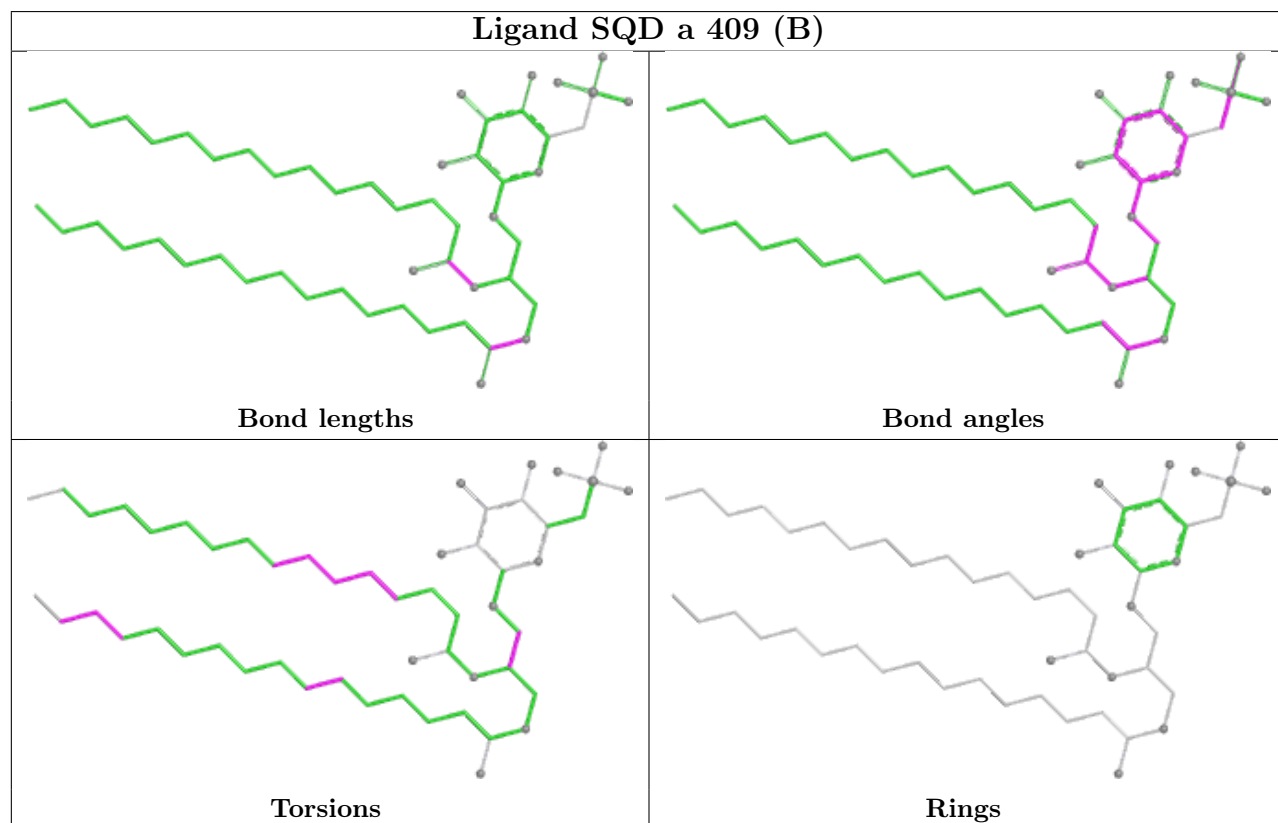
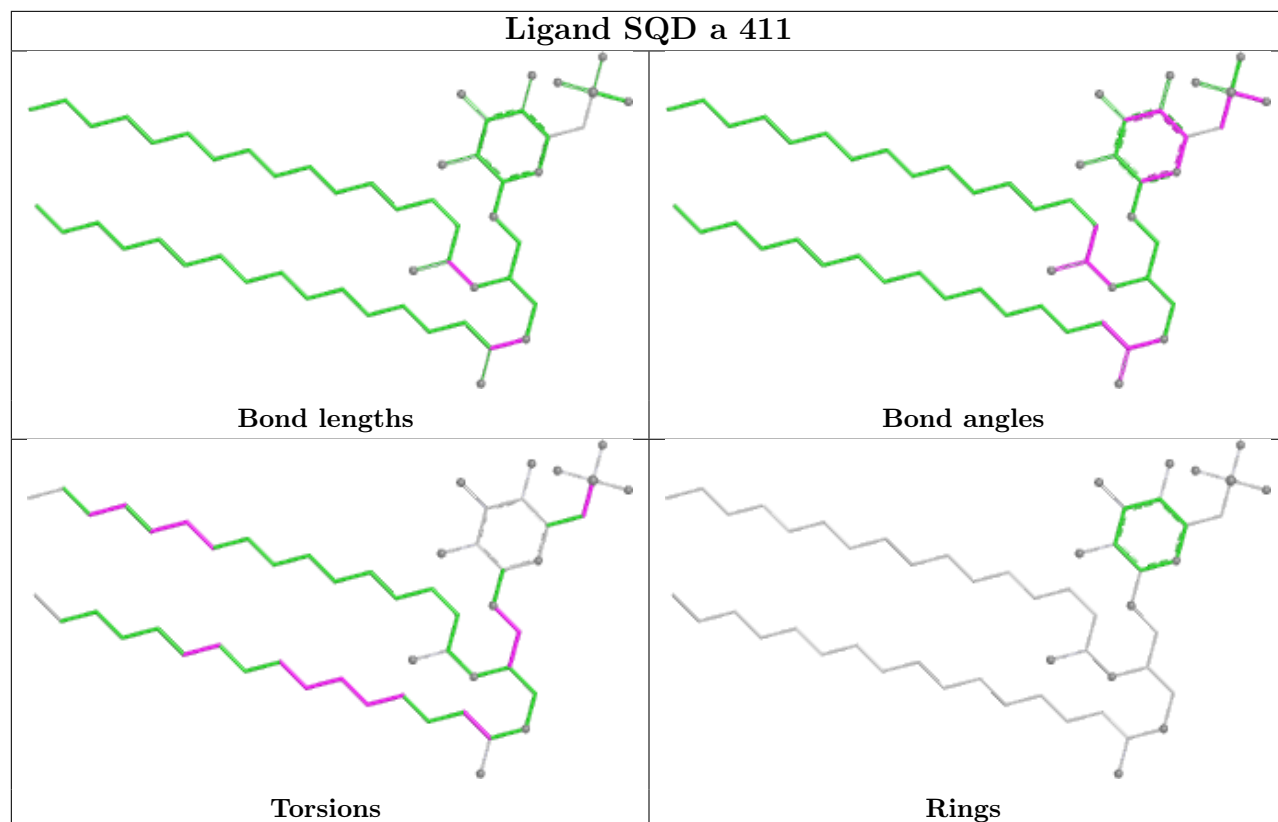


## Ligand CLA b 615

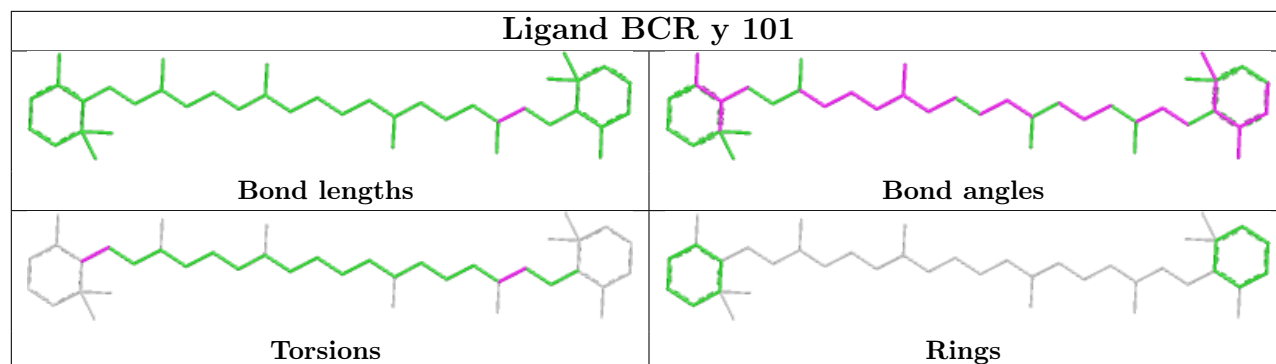




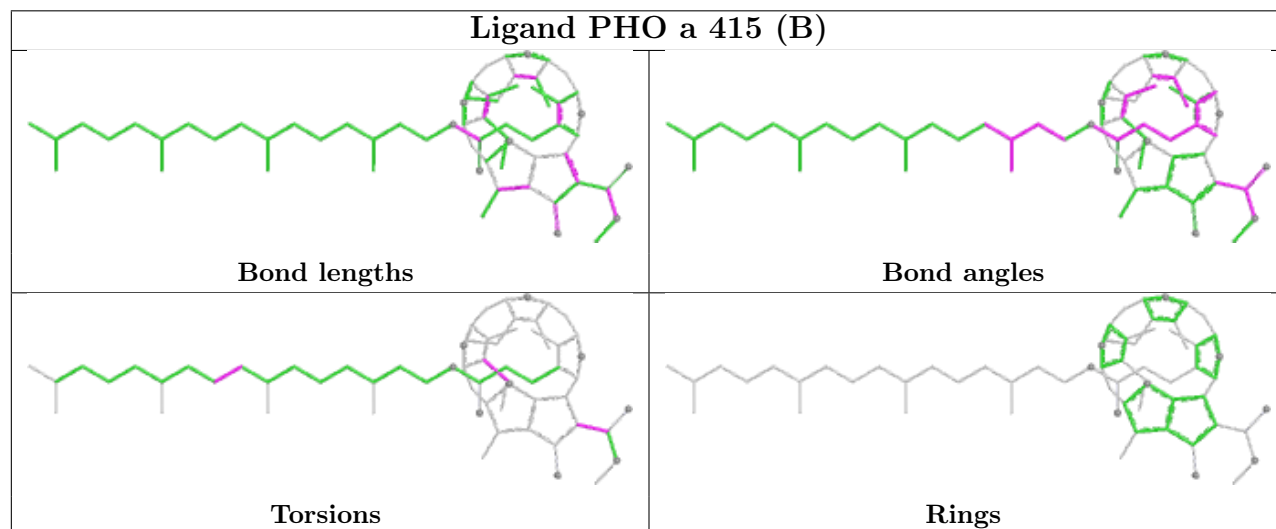




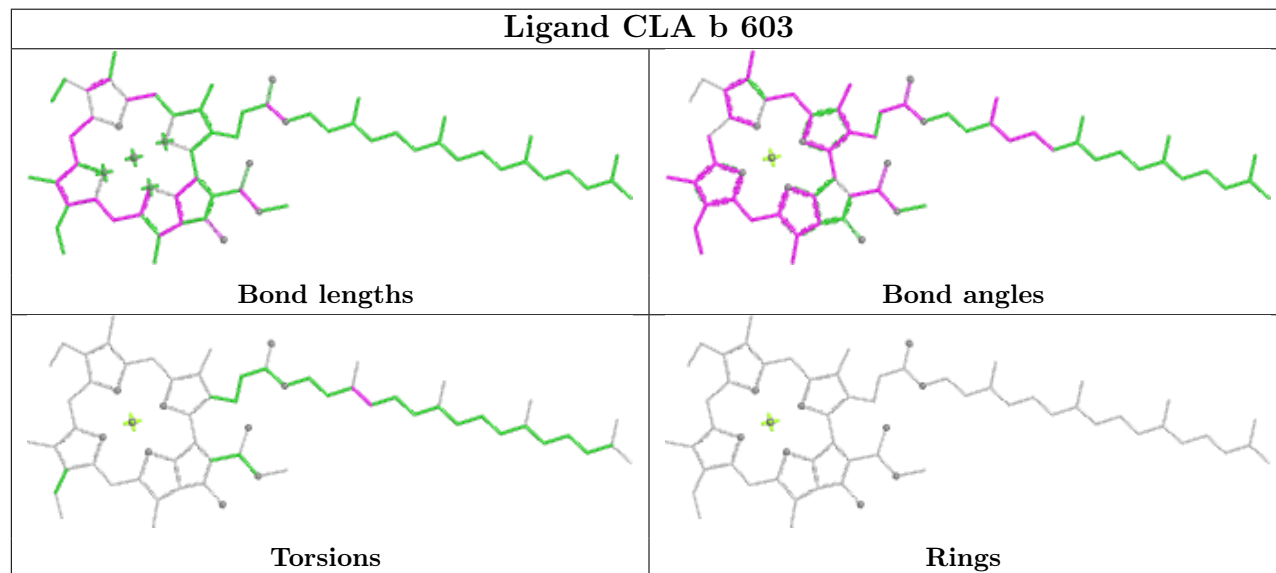
## Ligand BCR y 101



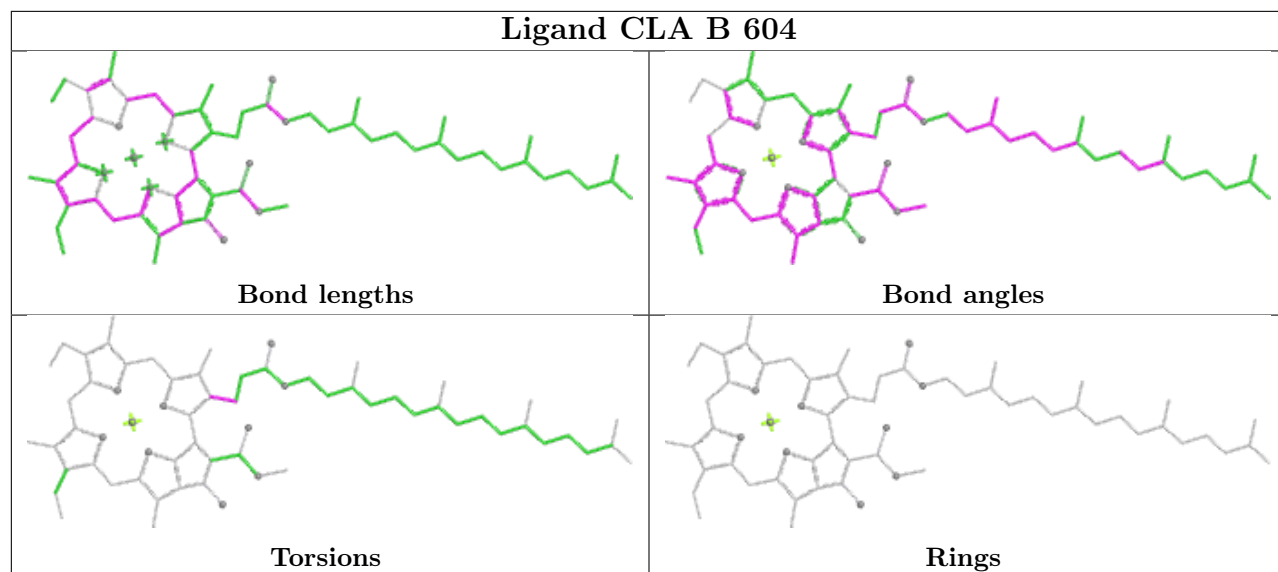
## Ligand PHO a 415 (B)



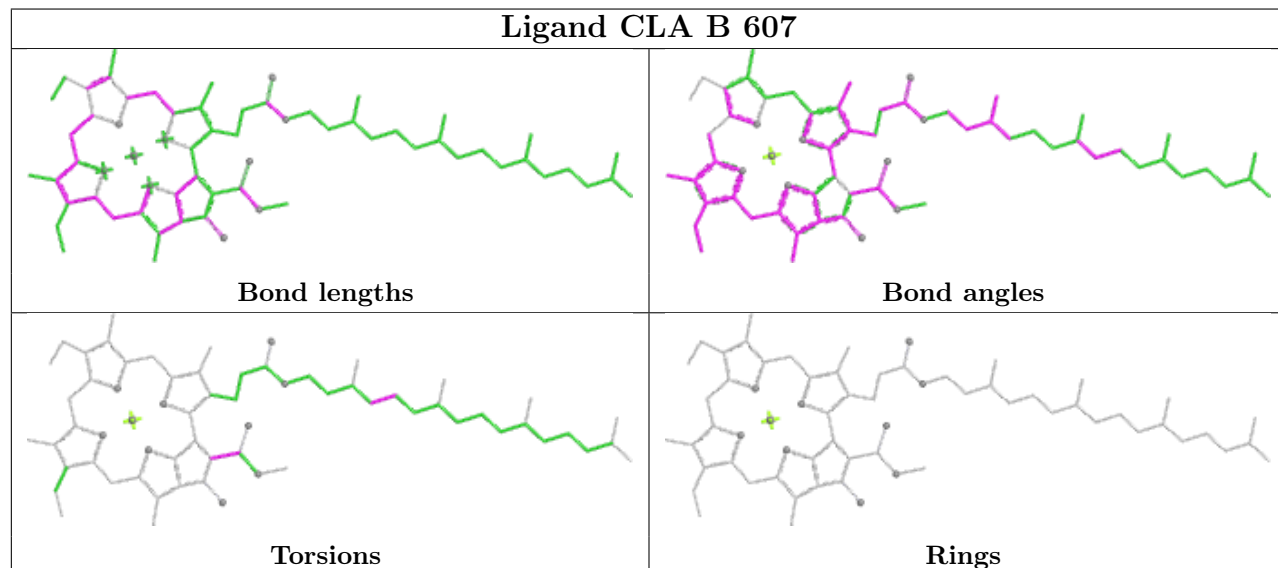
## Ligand CLA b 603



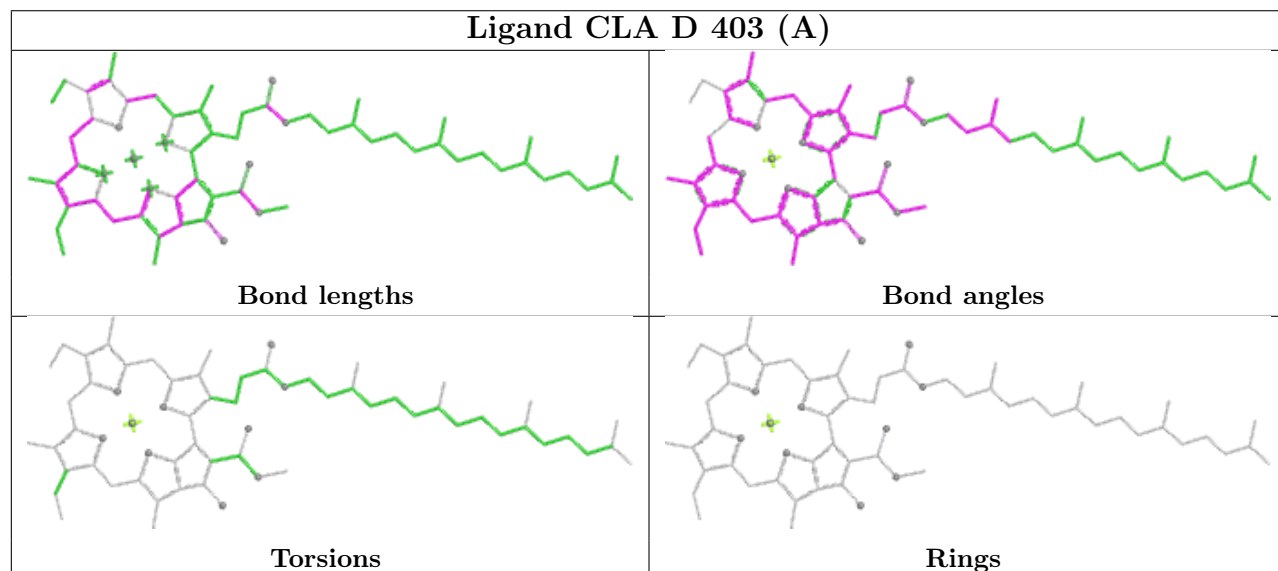
## Ligand CLA B 604



## Ligand CLA B 607

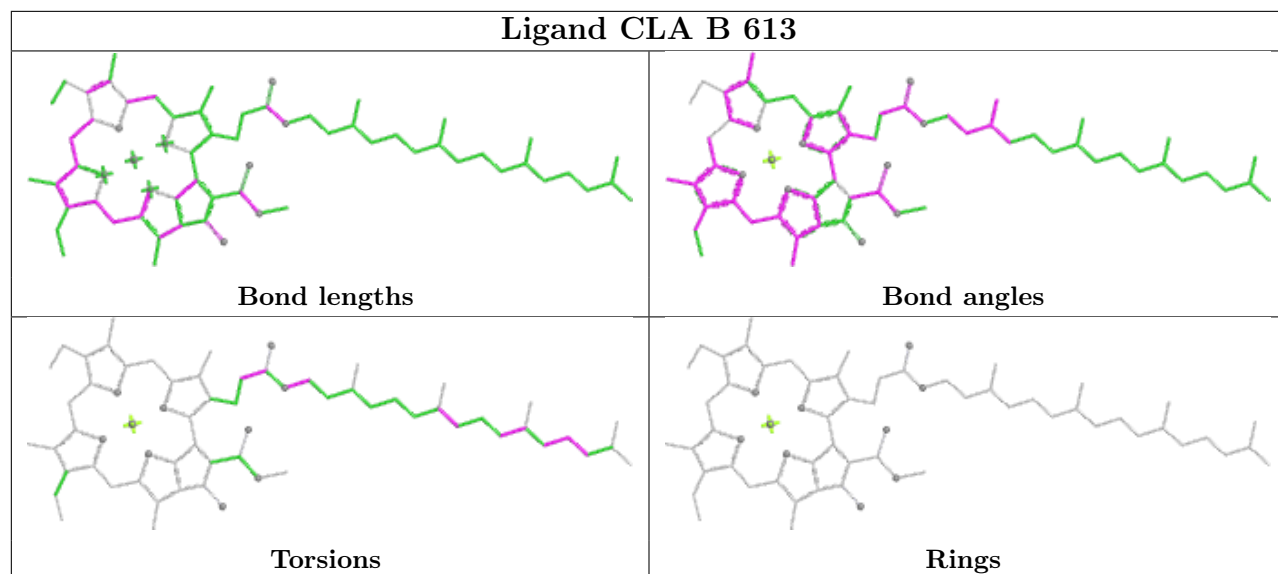


## Ligand CLA D 403 (A)

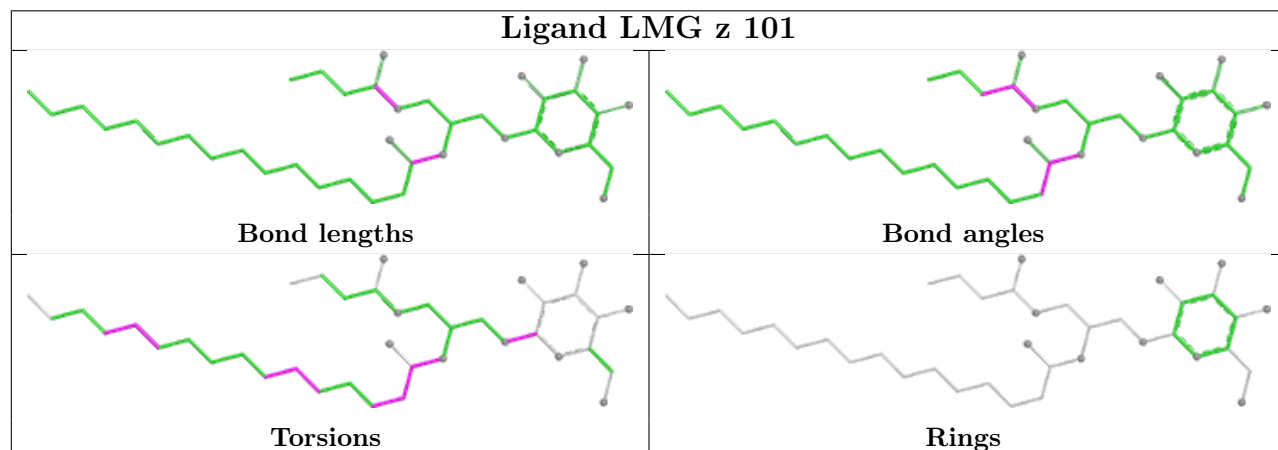




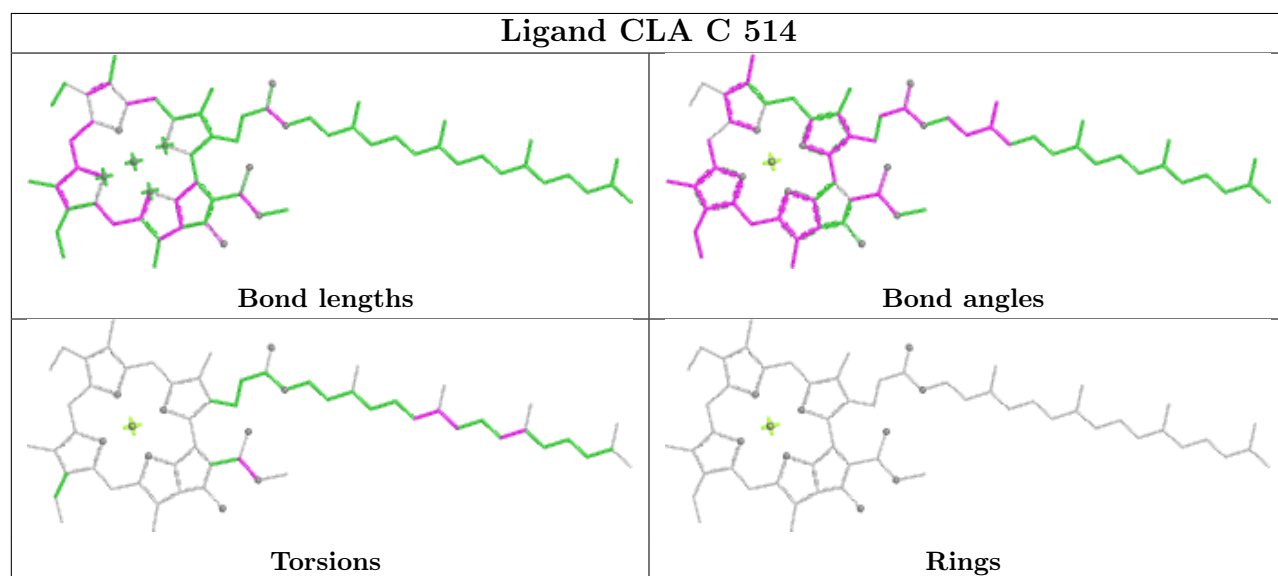
## Ligand CLA B 613



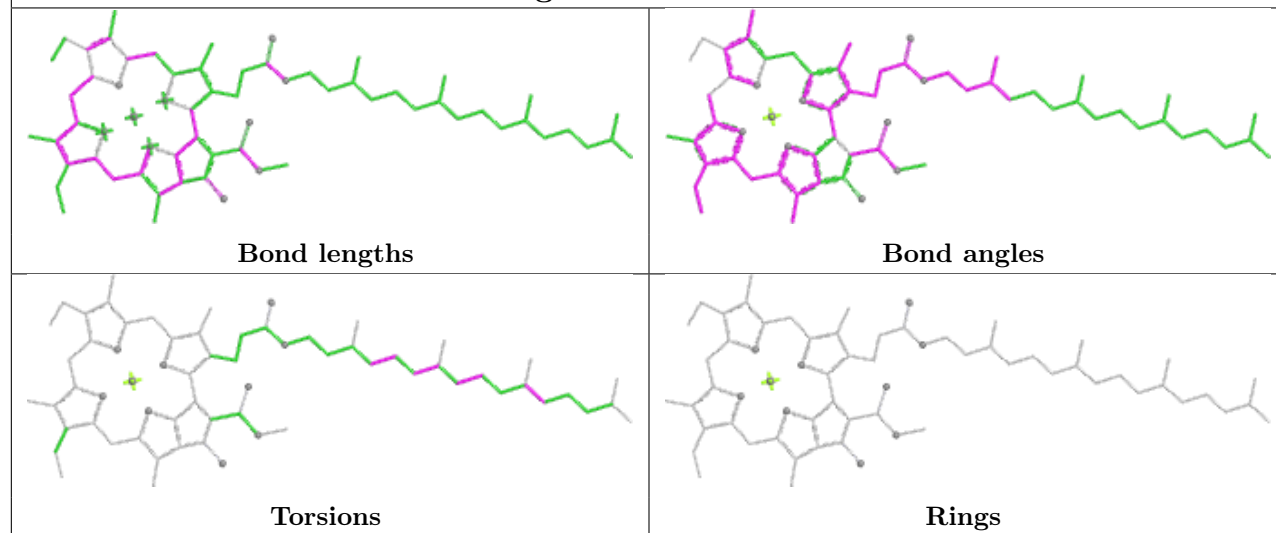
## Ligand LMG z 101



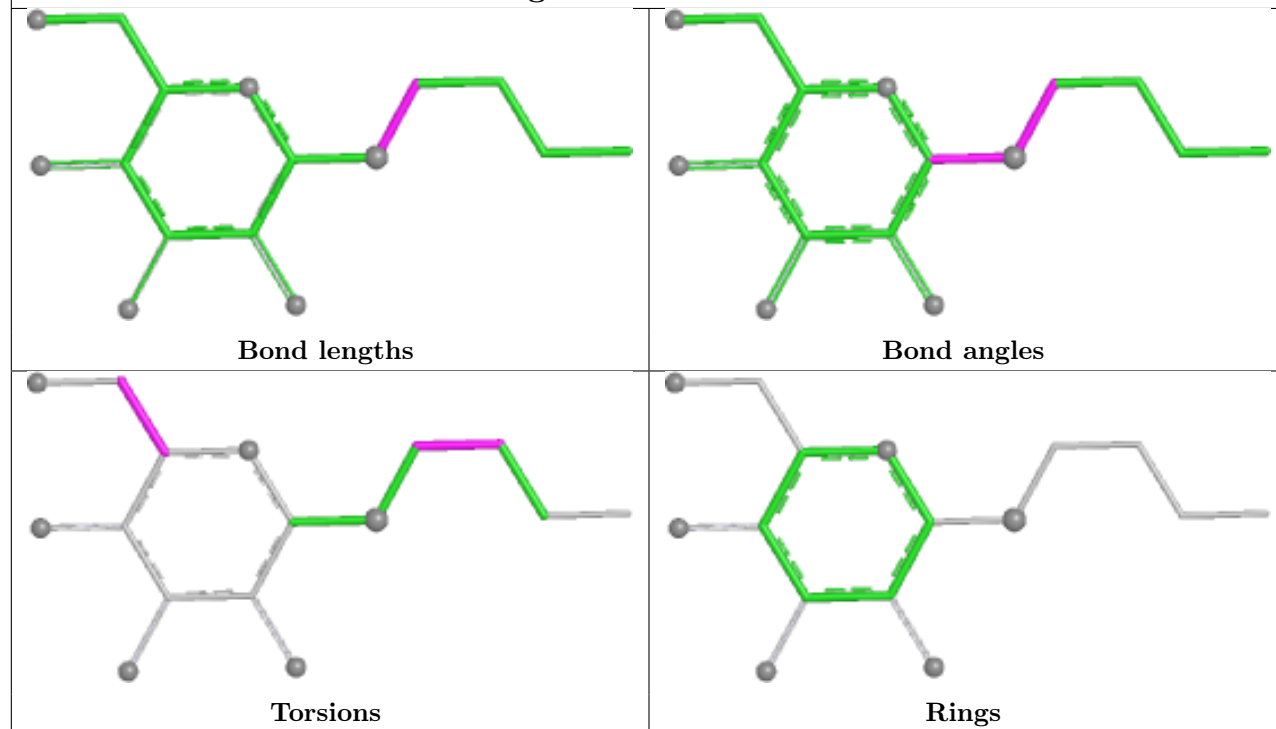
## Ligand CLA C 514

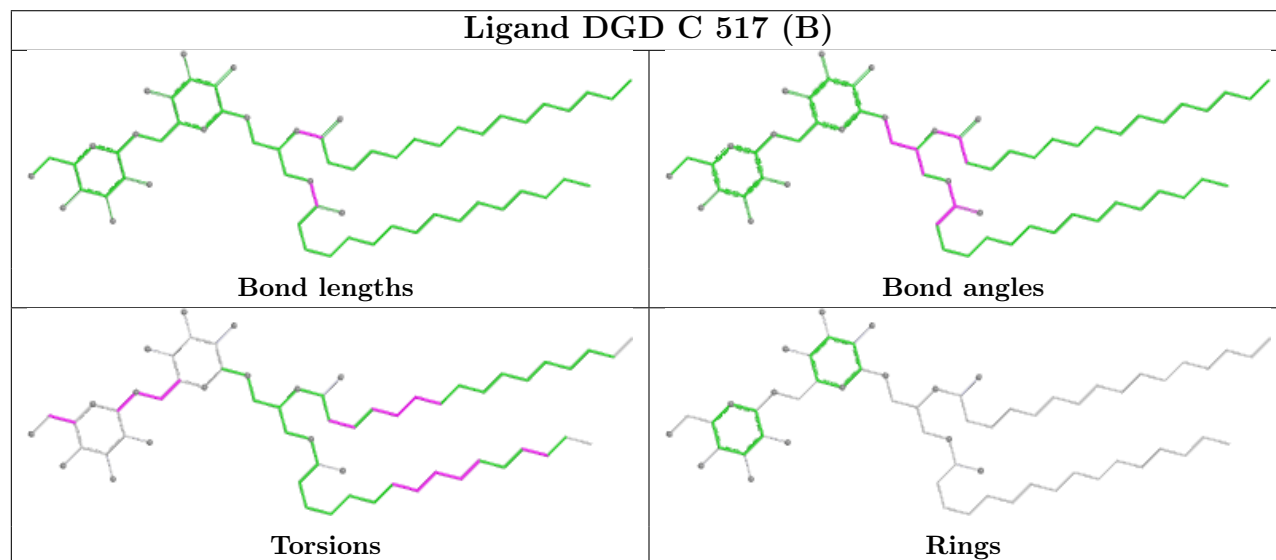
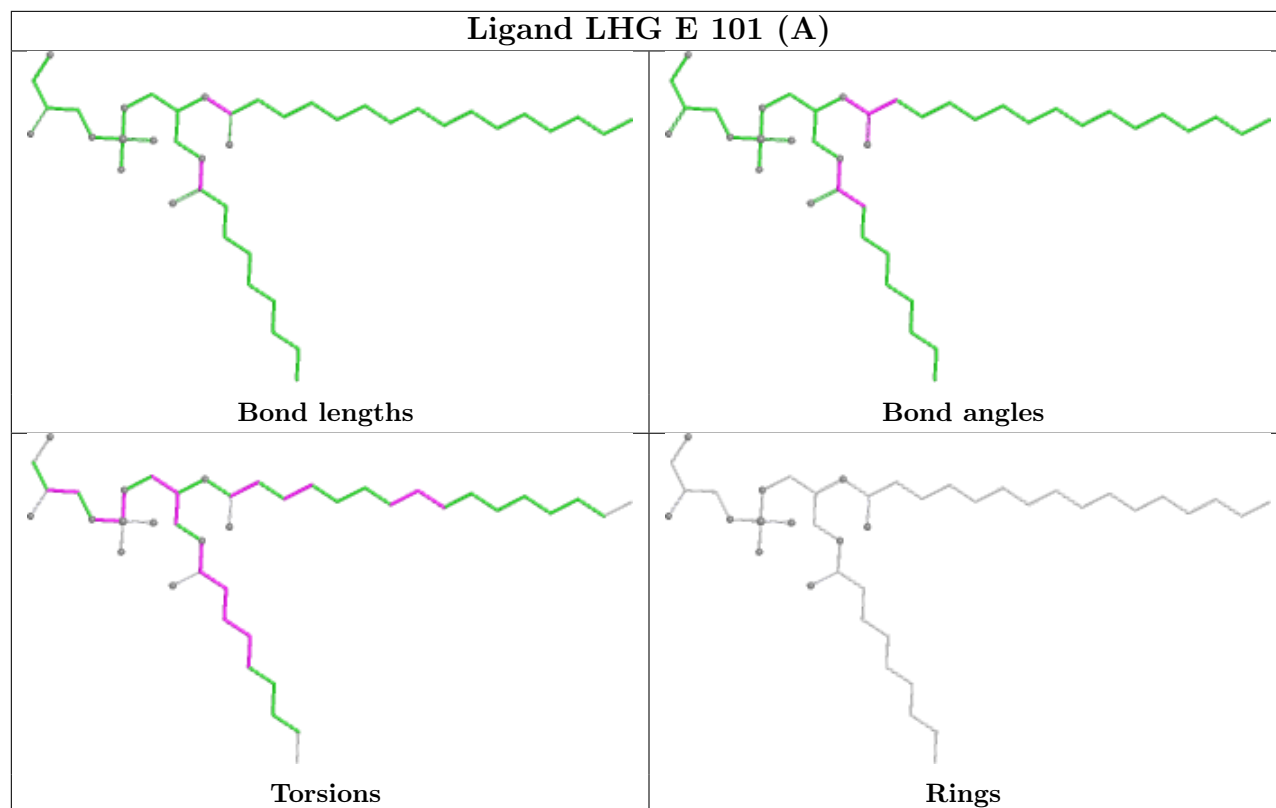


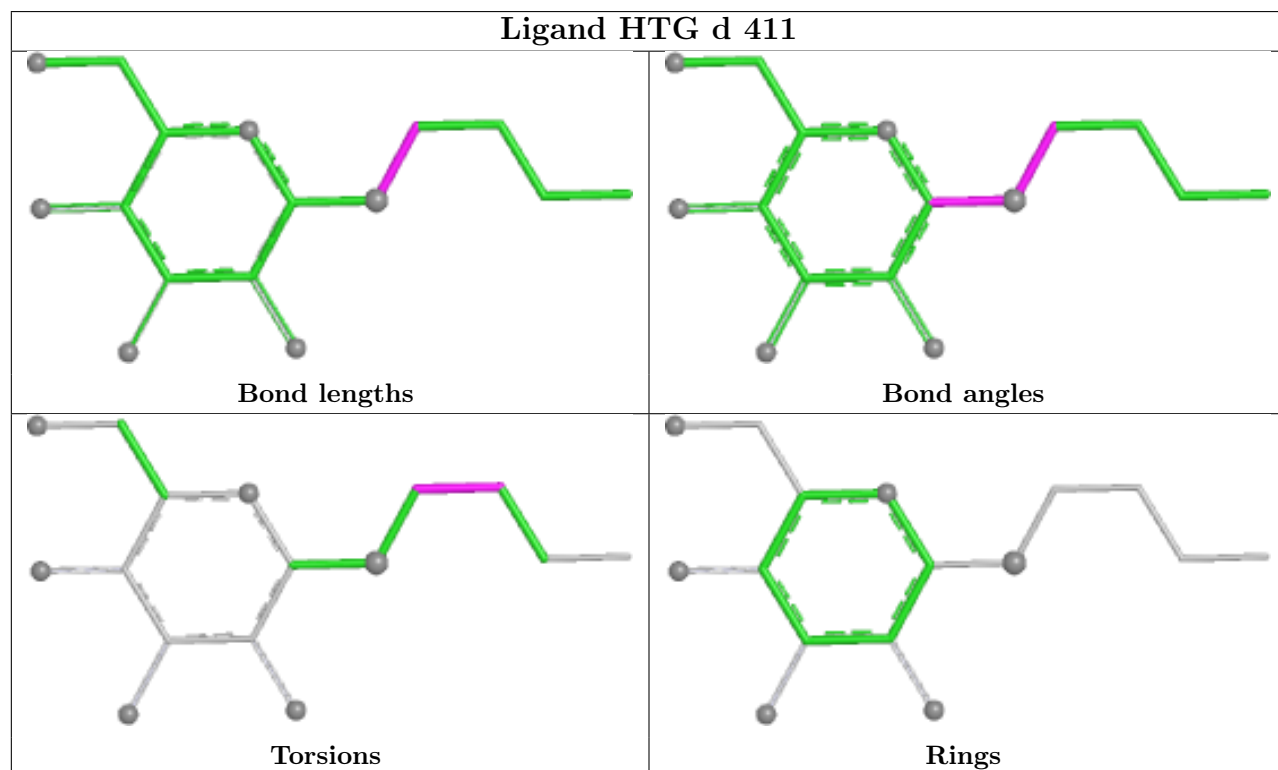
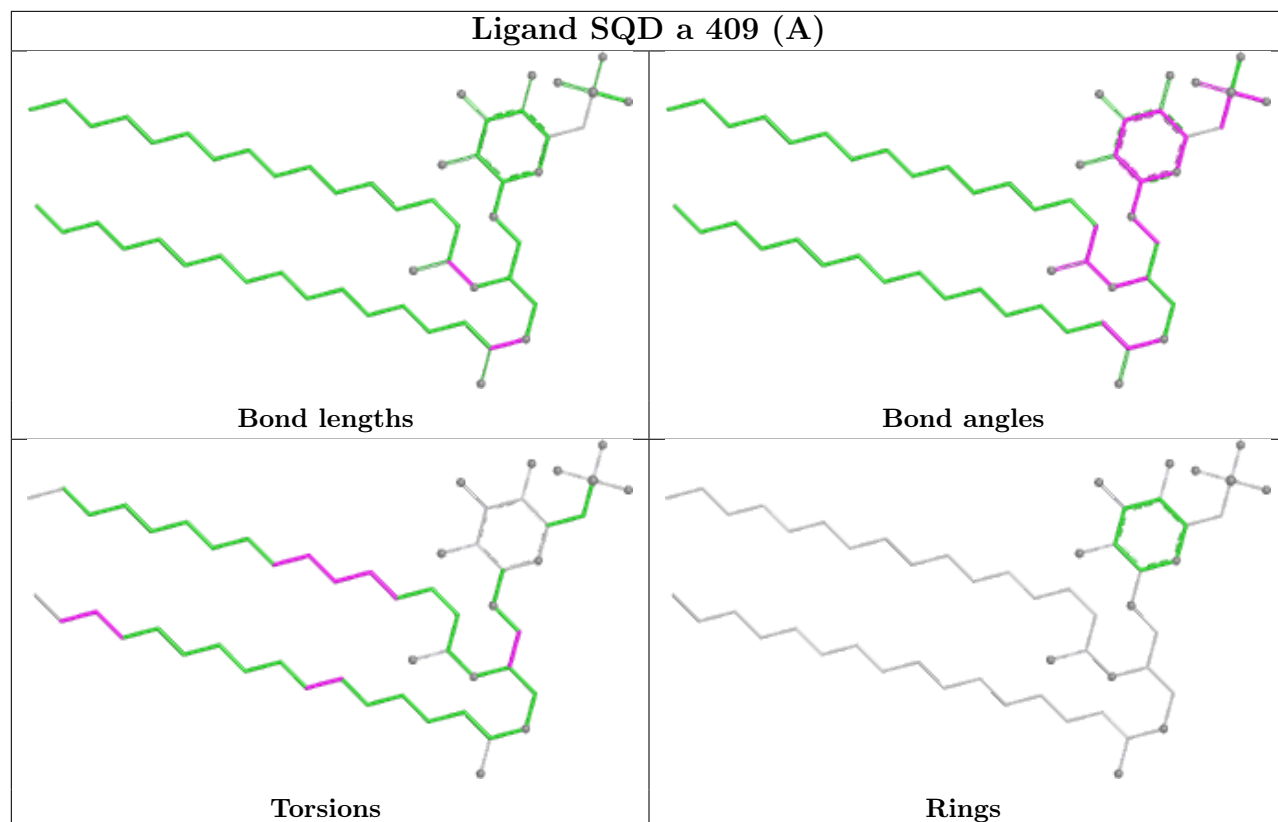
## Ligand CLA b 607



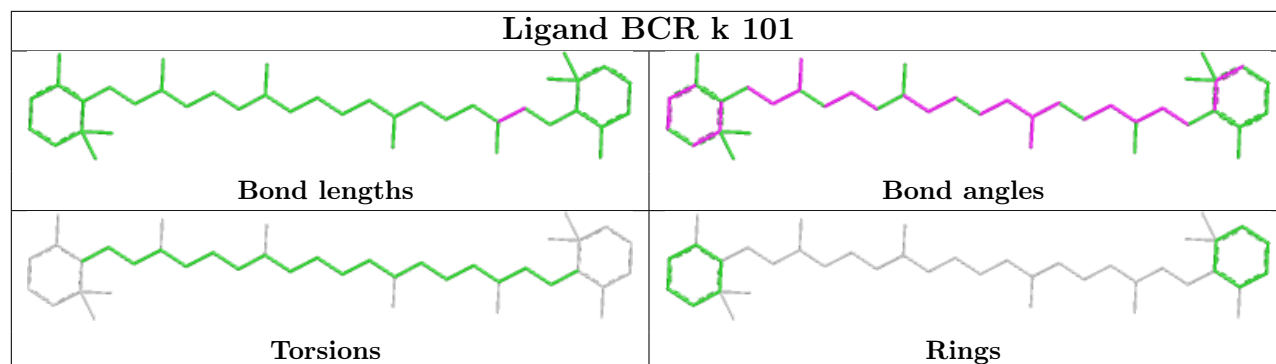
## Ligand HTG D 411



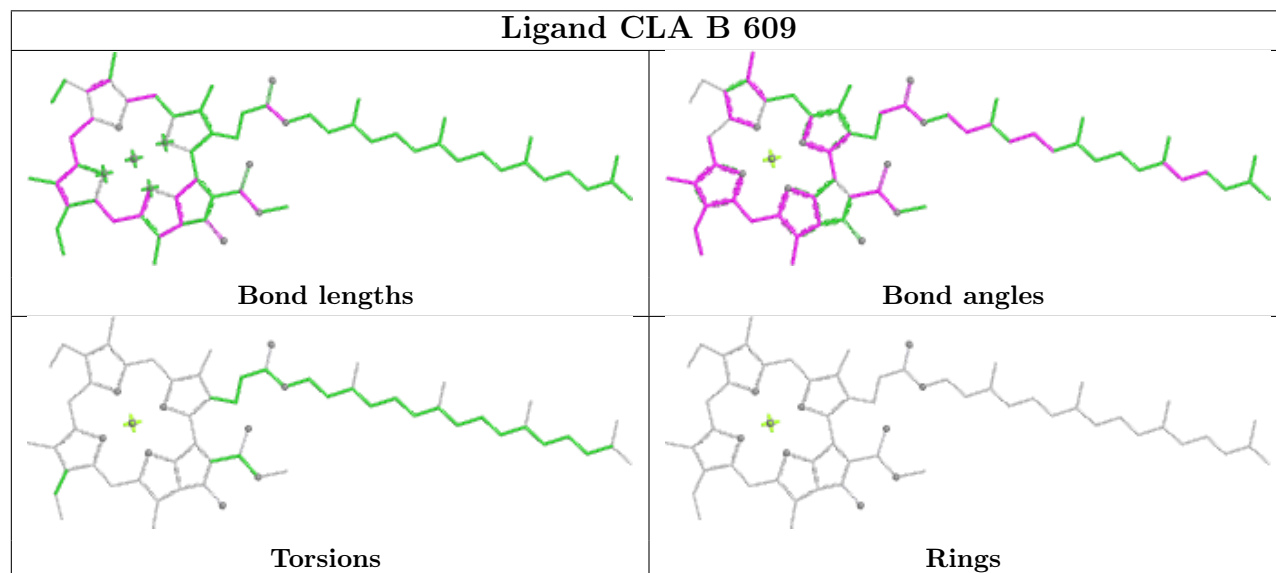




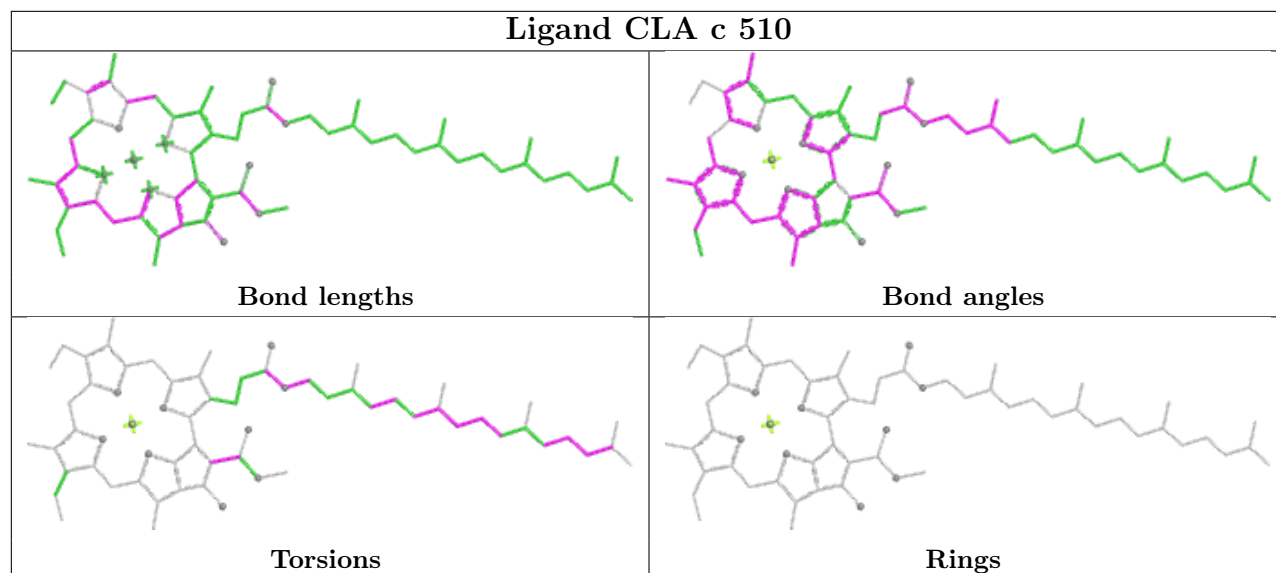
## Ligand BCR k 101



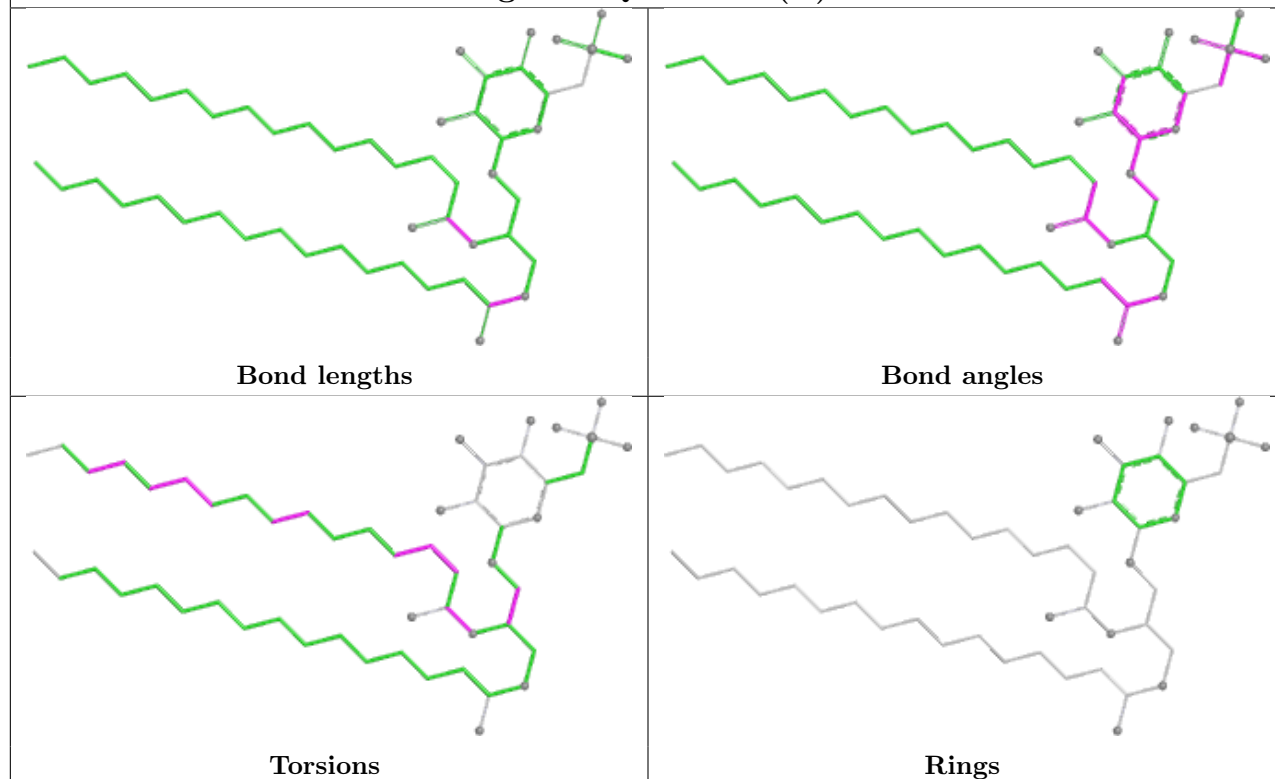
## Ligand CLA B 609



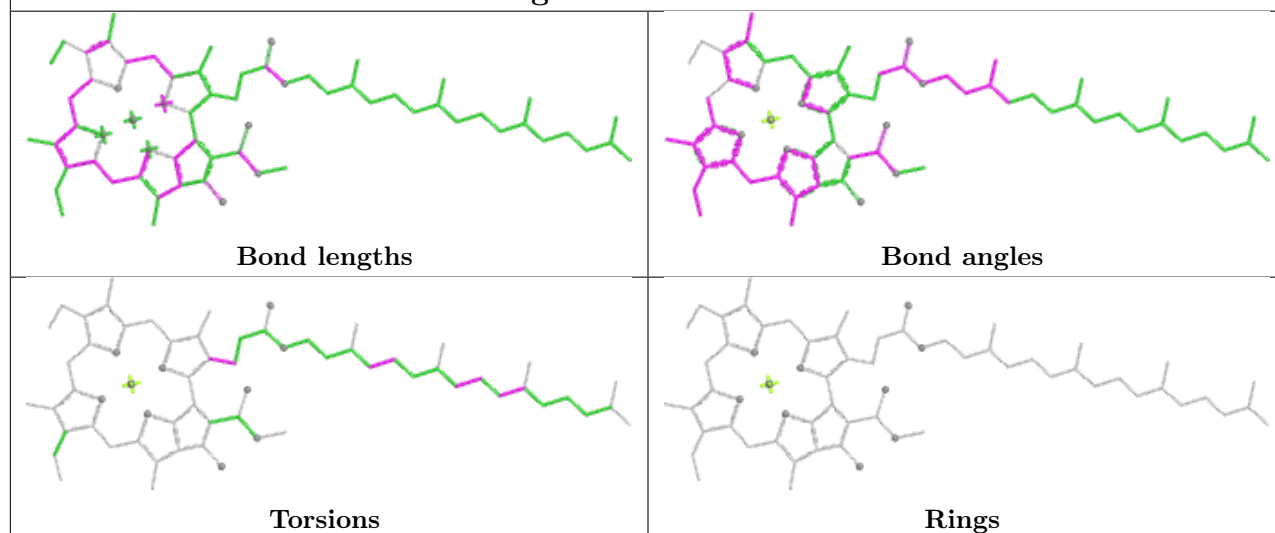
## Ligand CLA c 510



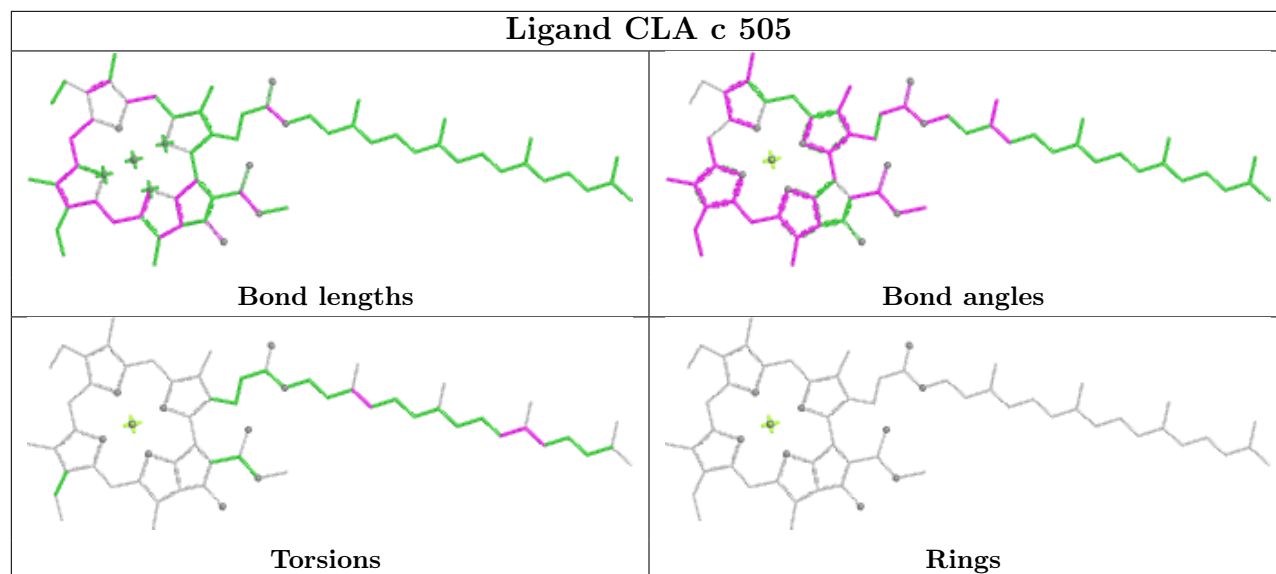
## Ligand SQD A 409 (B)



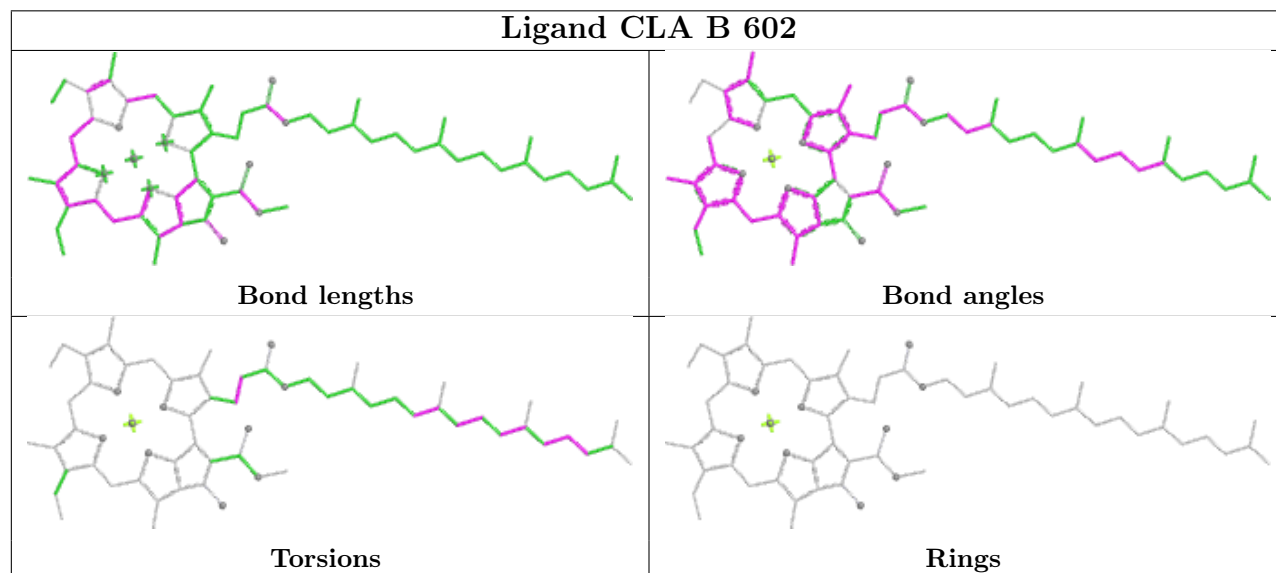
## Ligand CLA C 512



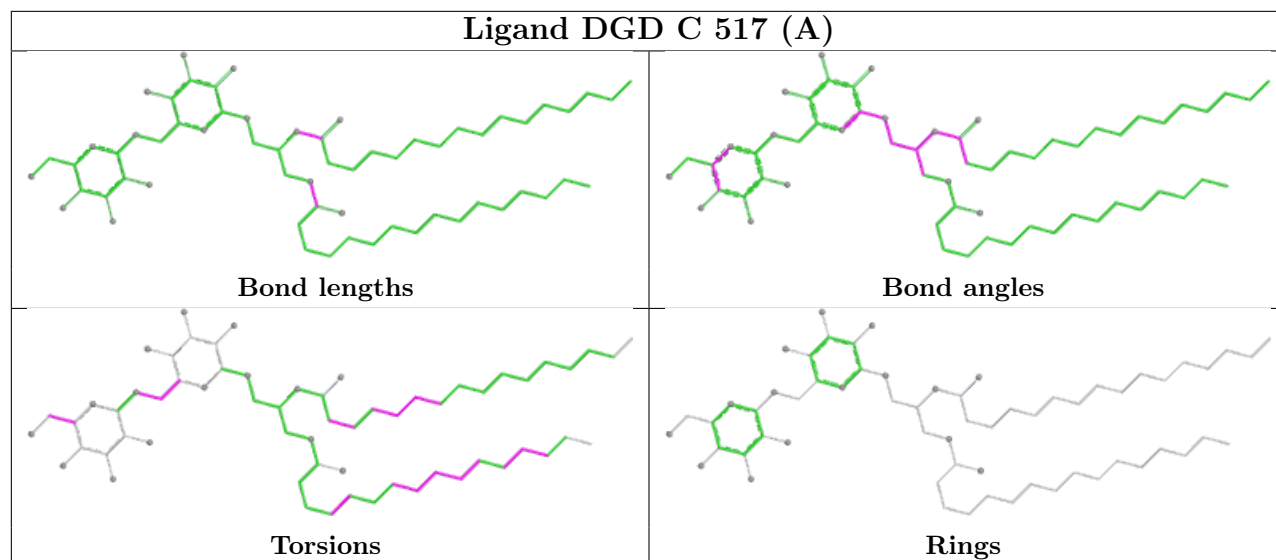
## Ligand CLA c 505



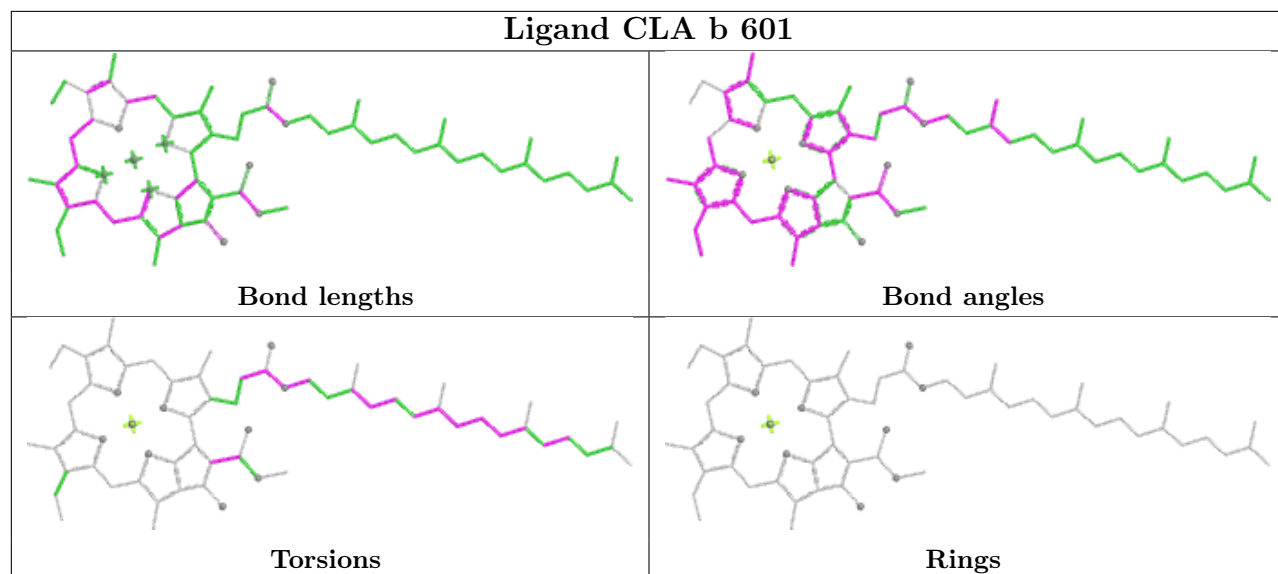
## Ligand CLA B 602



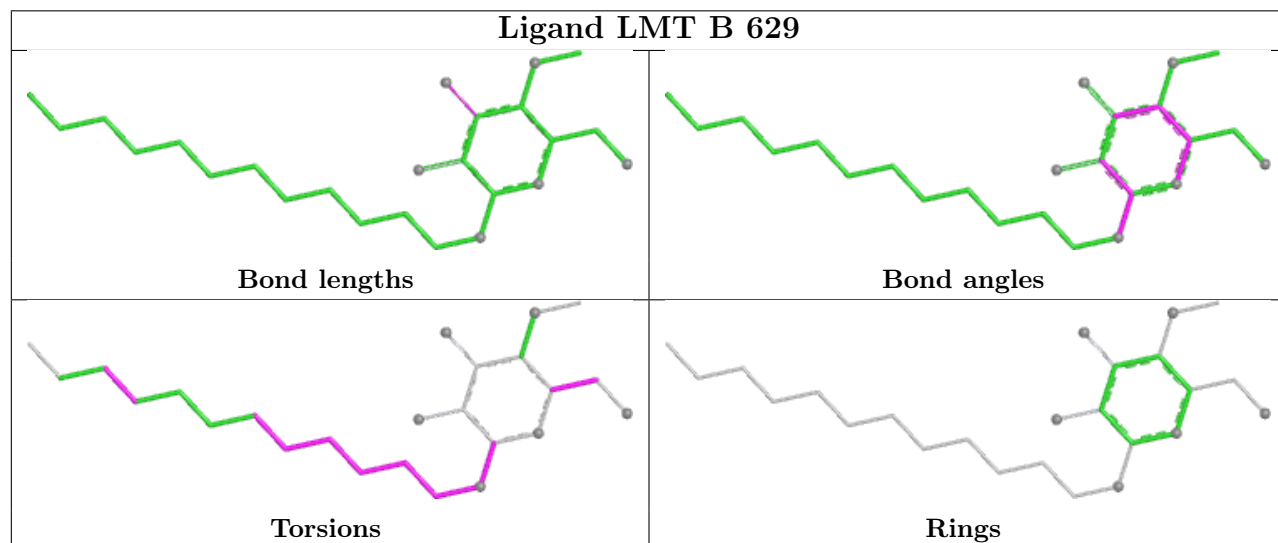
## Ligand DGD C 517 (A)



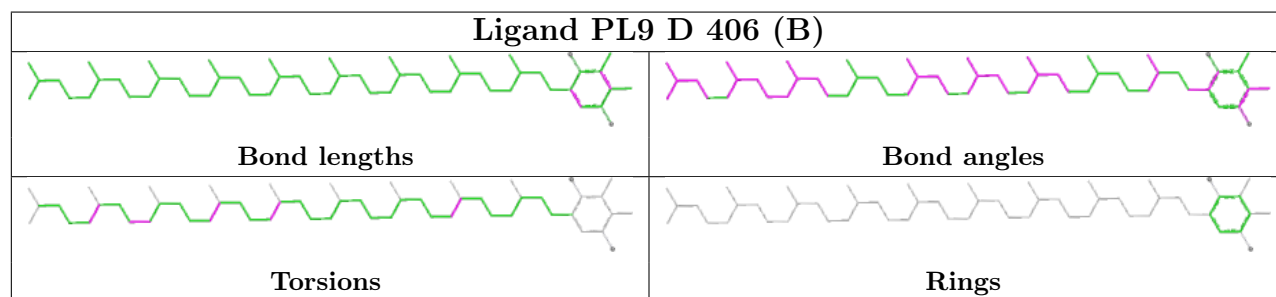
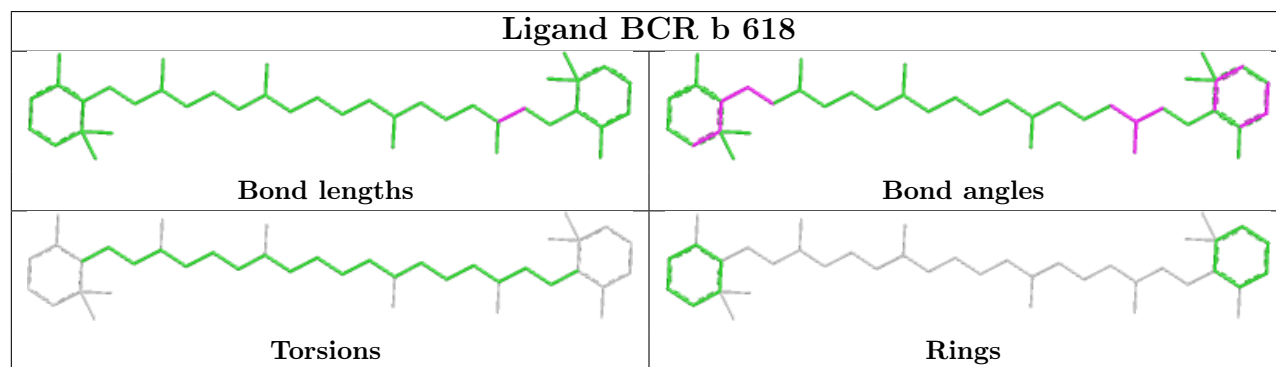
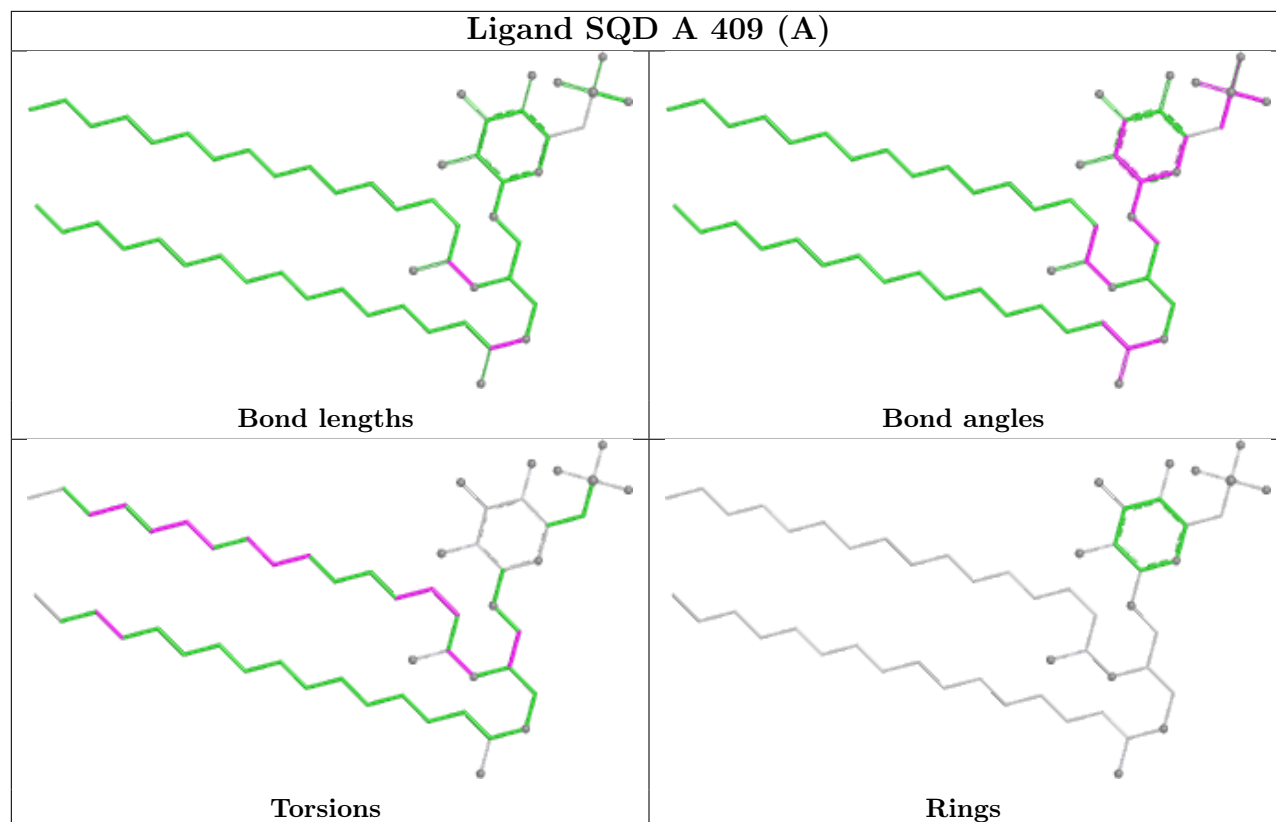
## Ligand CLA b 601



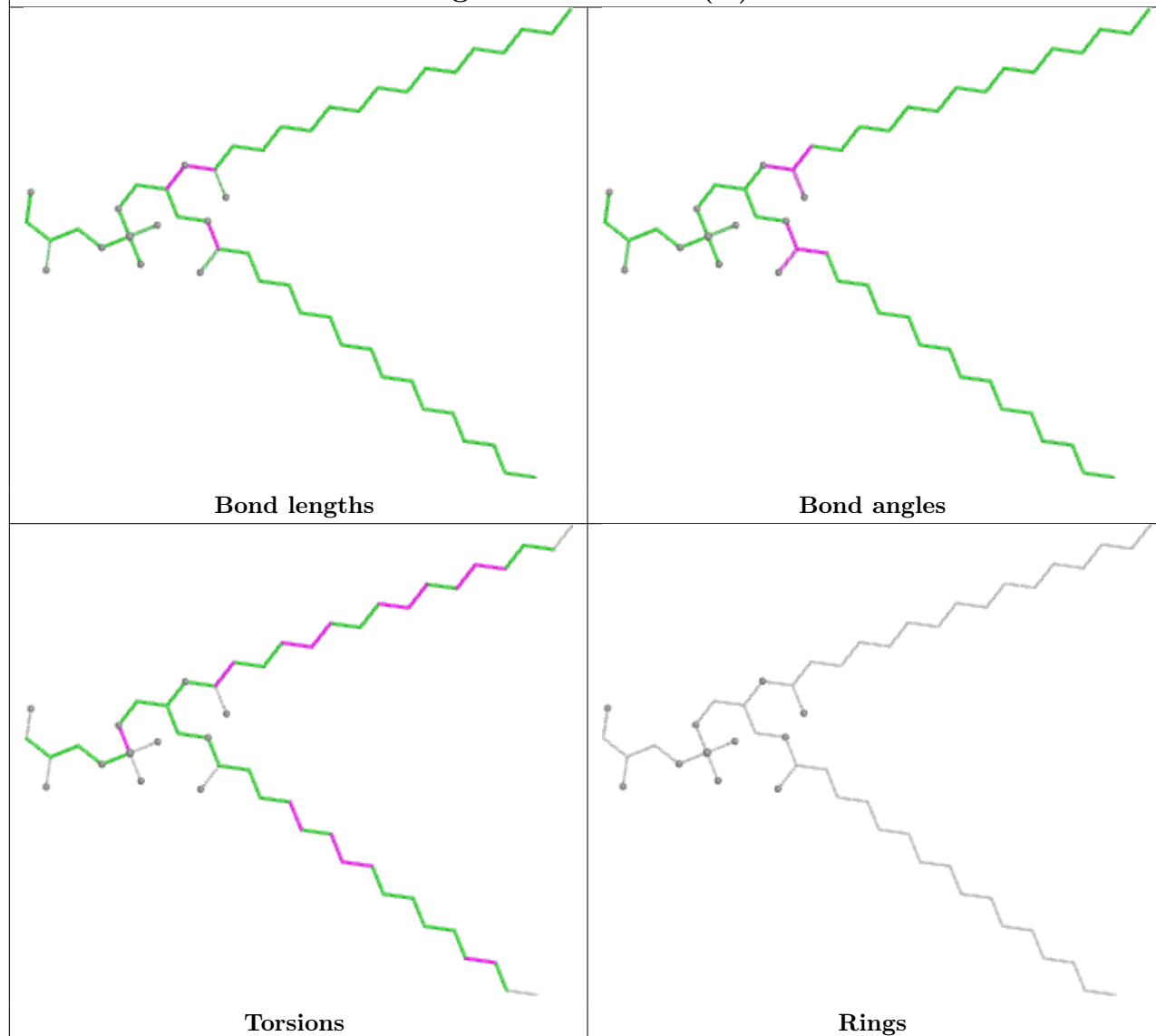
## Ligand LMT B 629



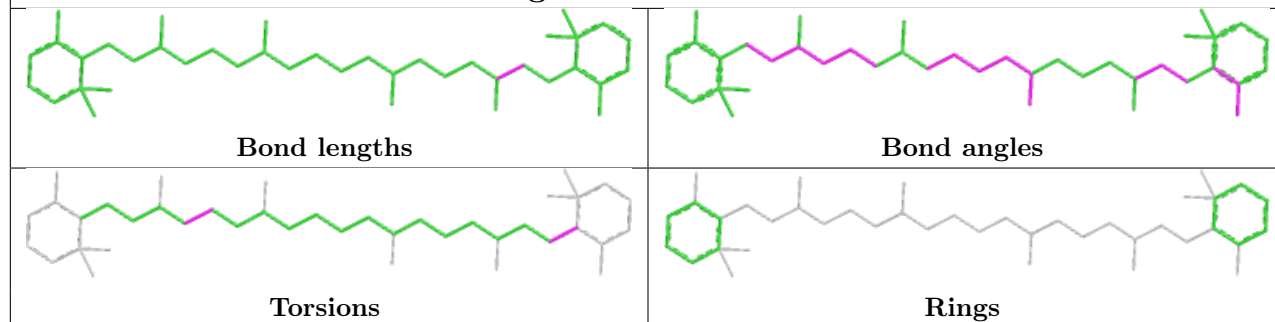


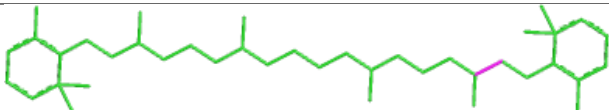
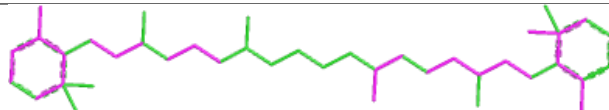
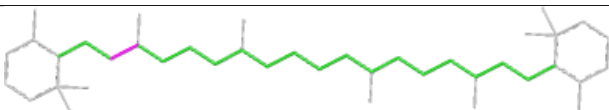
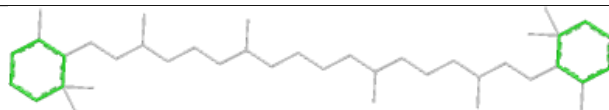


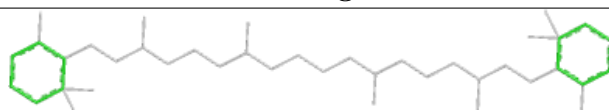
## Ligand LHG b 629 (A)

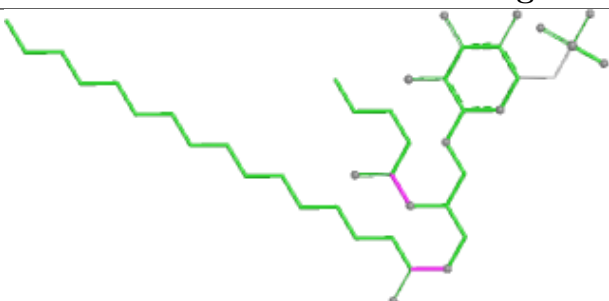
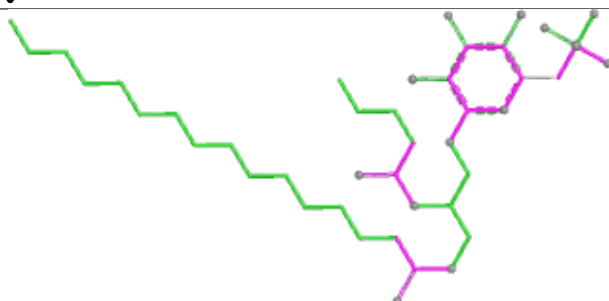
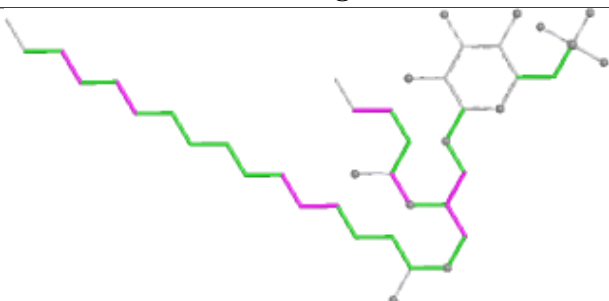
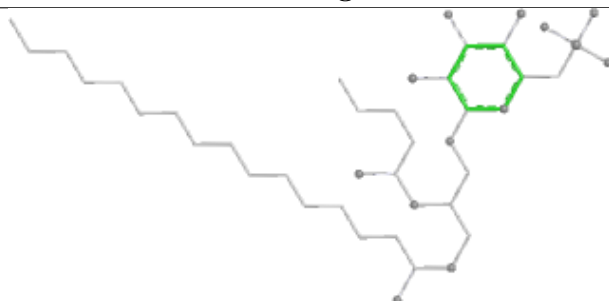


## Ligand BCR H 101

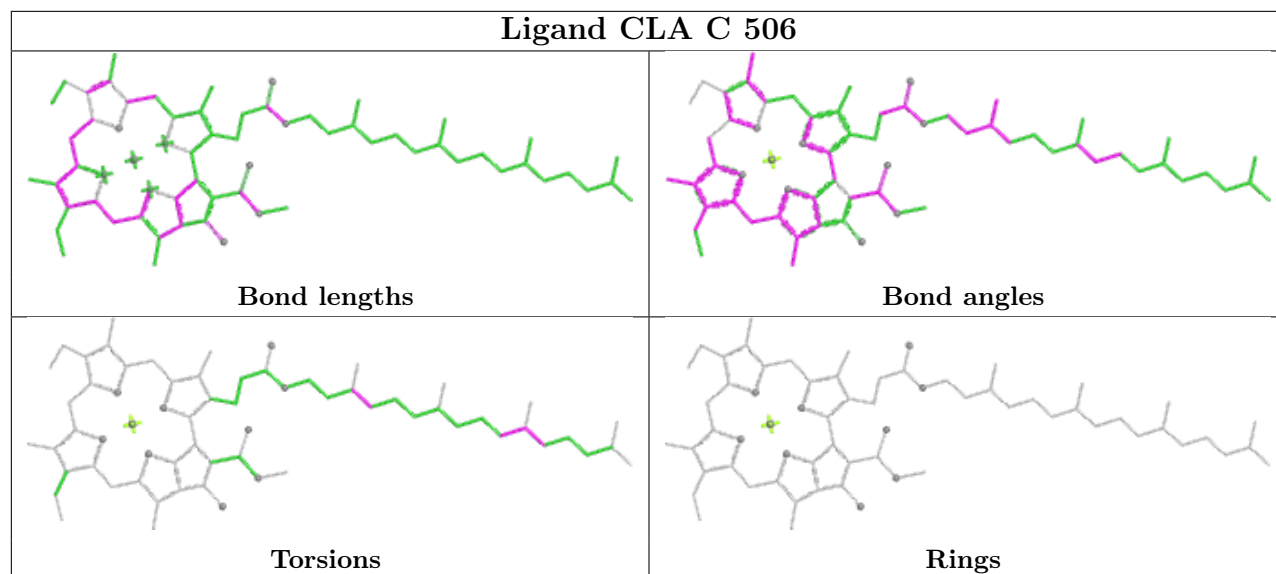


| Ligand BCR K 102                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

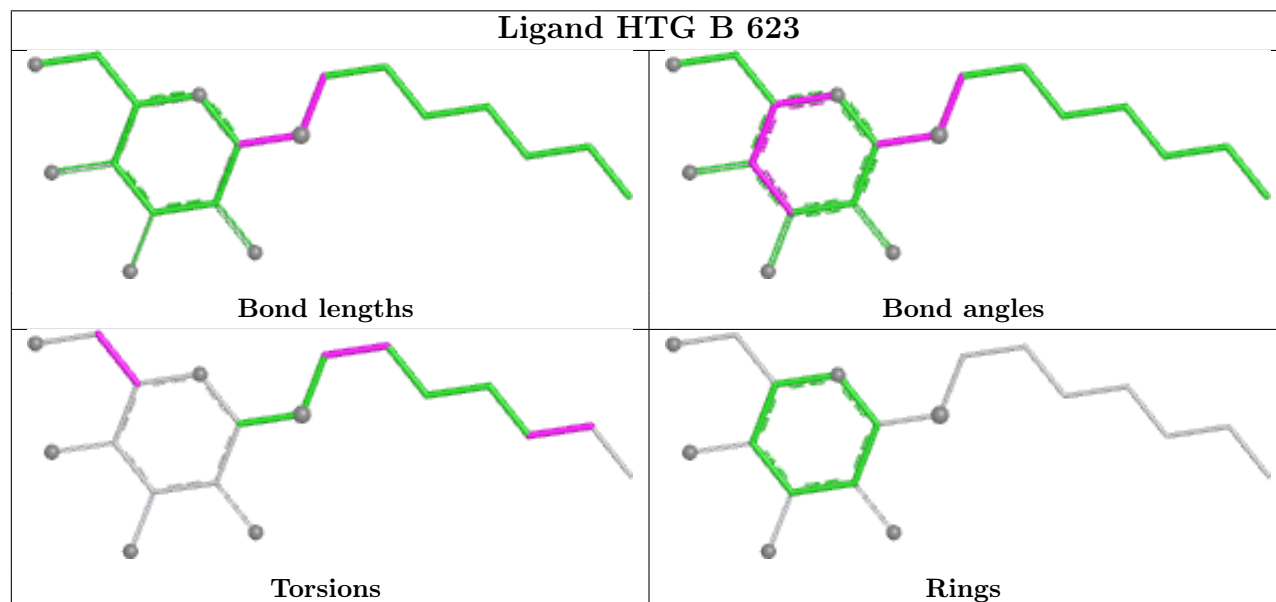
| Ligand BCR b 617                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|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

| Ligand SQD f 102                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

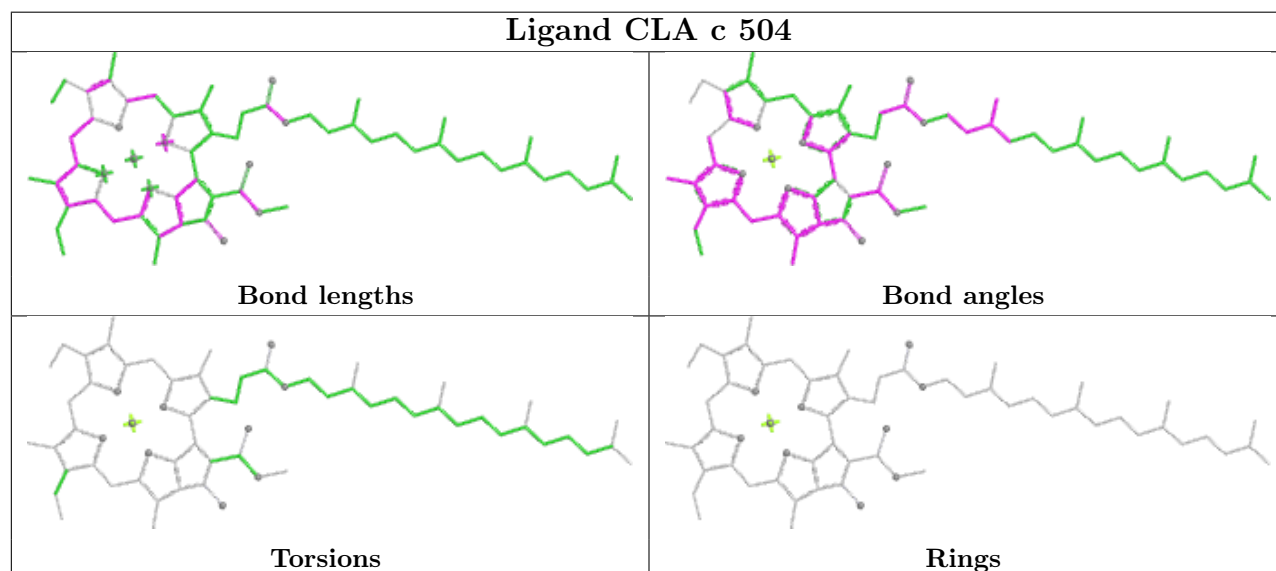
## Ligand CLA C 506

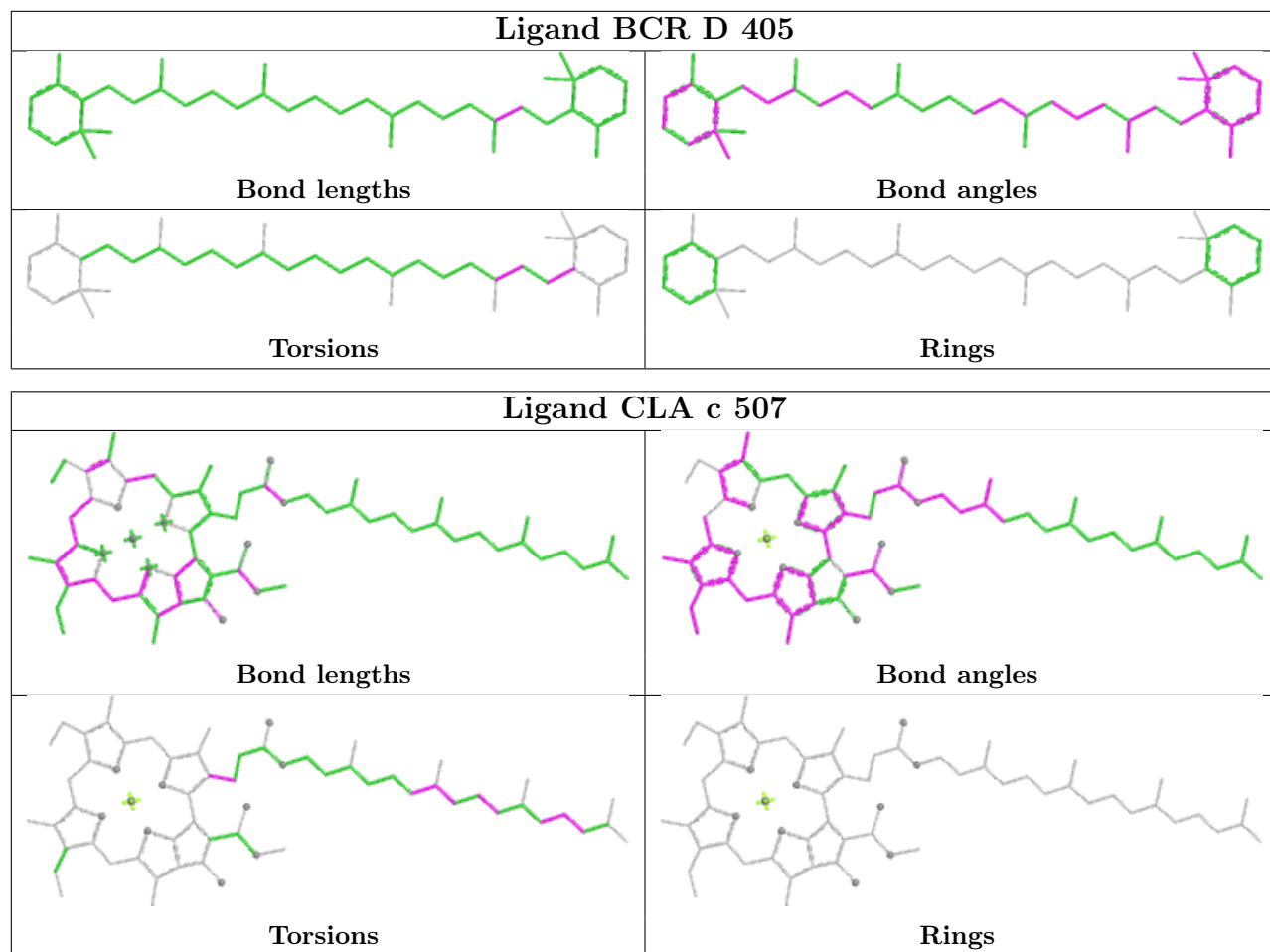


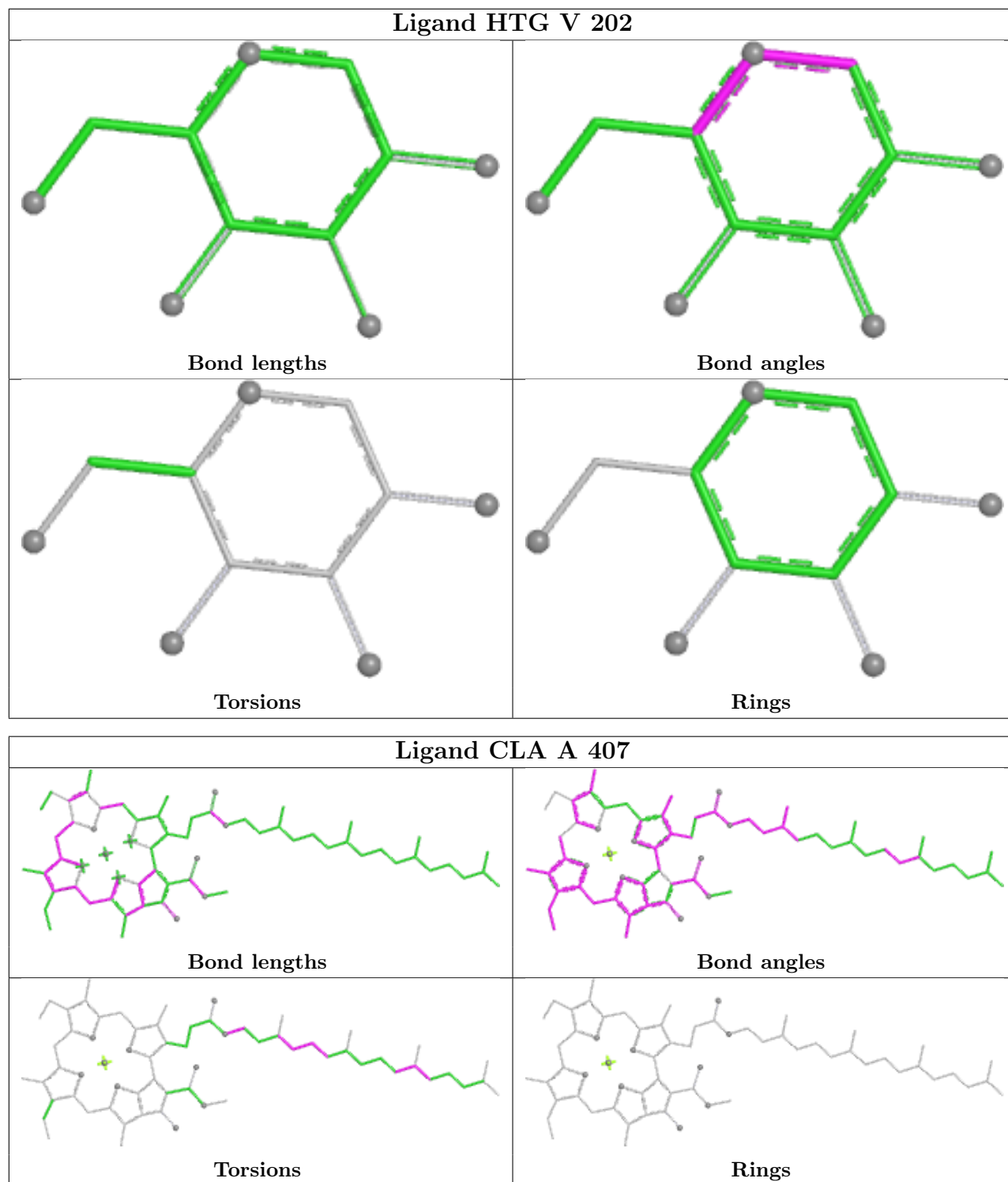
## Ligand HTG B 623



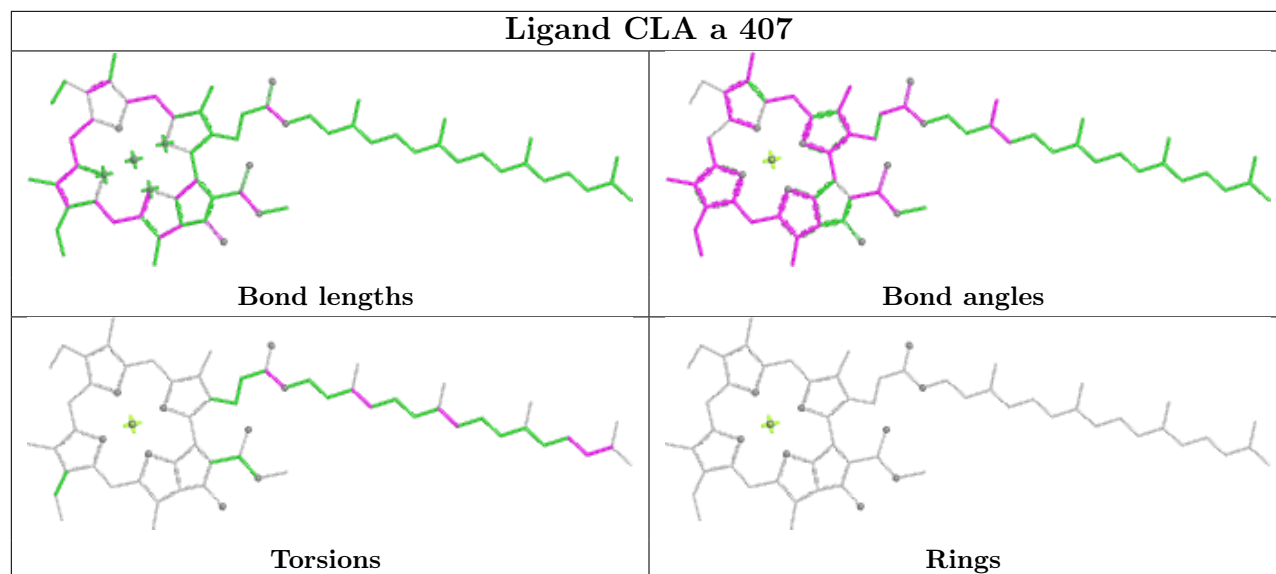
## Ligand CLA c 504



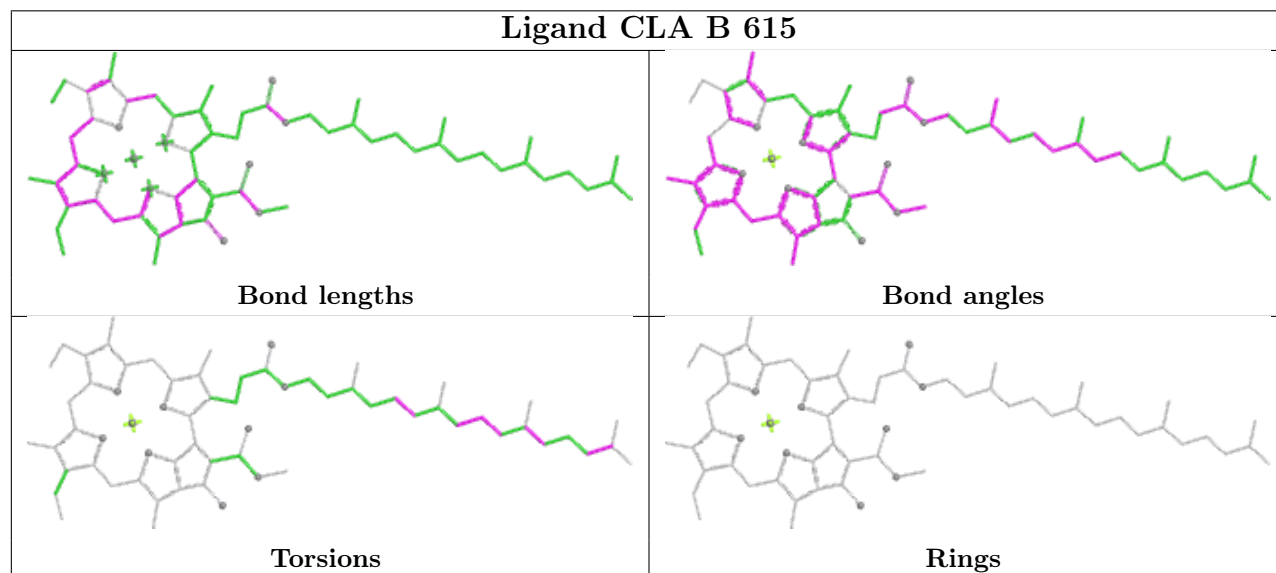




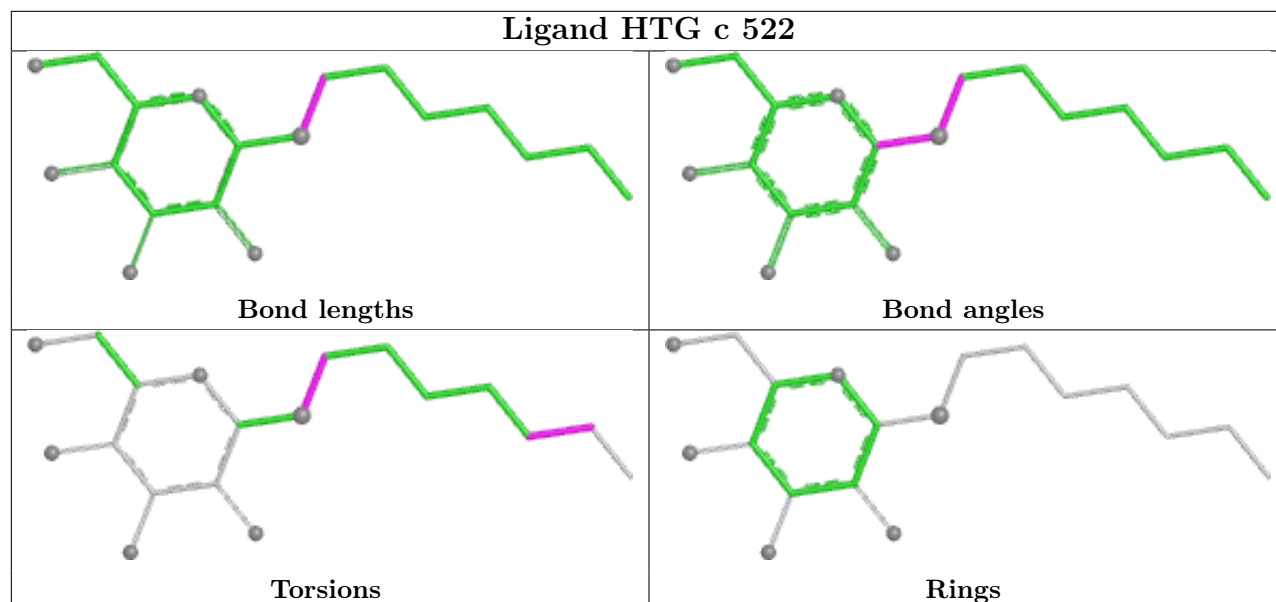
## Ligand CLA a 407



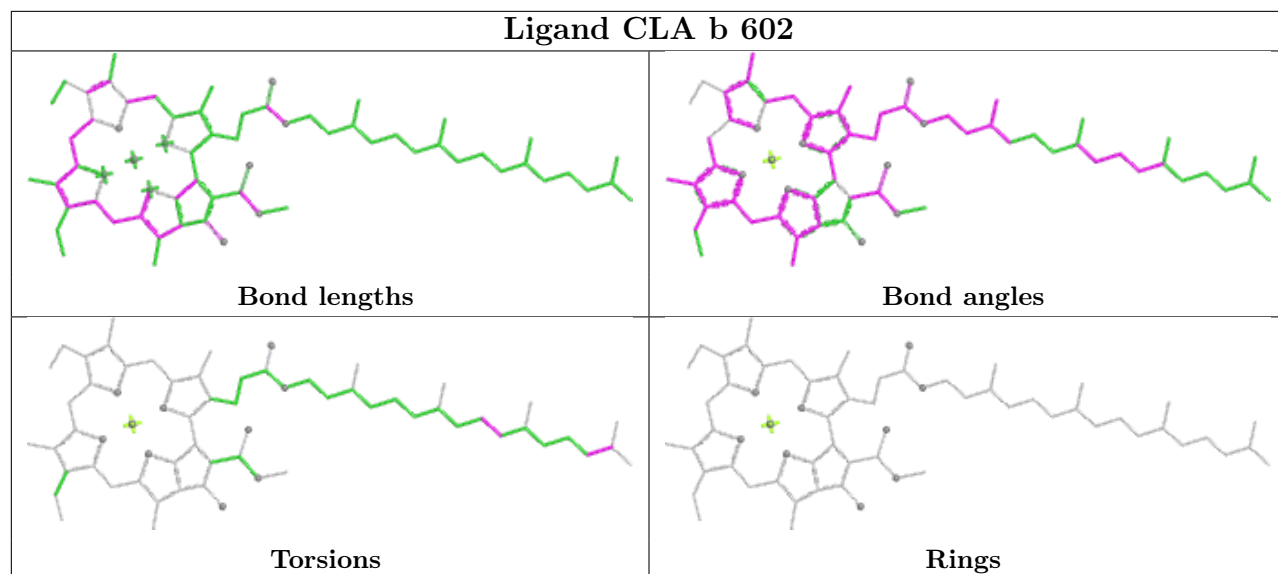
## Ligand CLA B 615



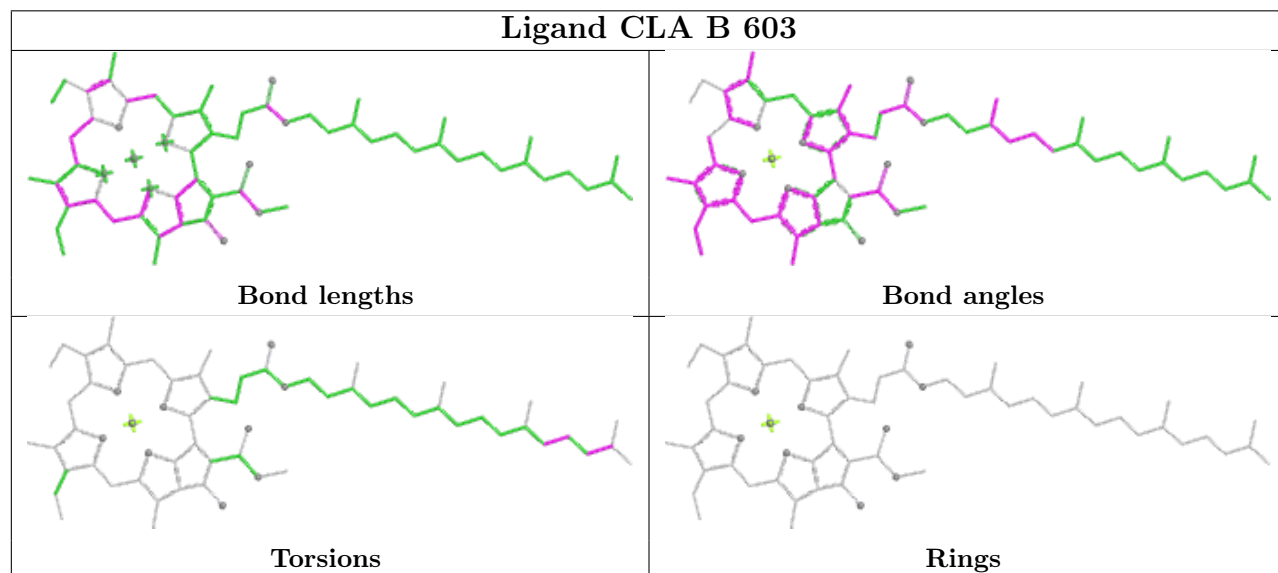
## Ligand HTG c 522



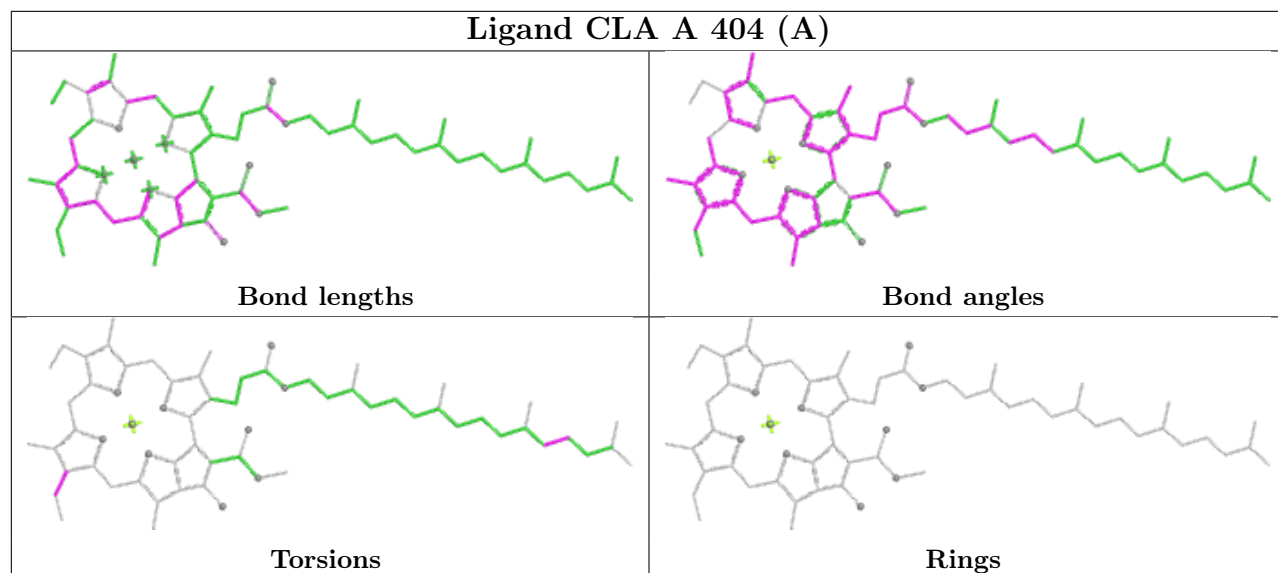
## Ligand CLA b 602



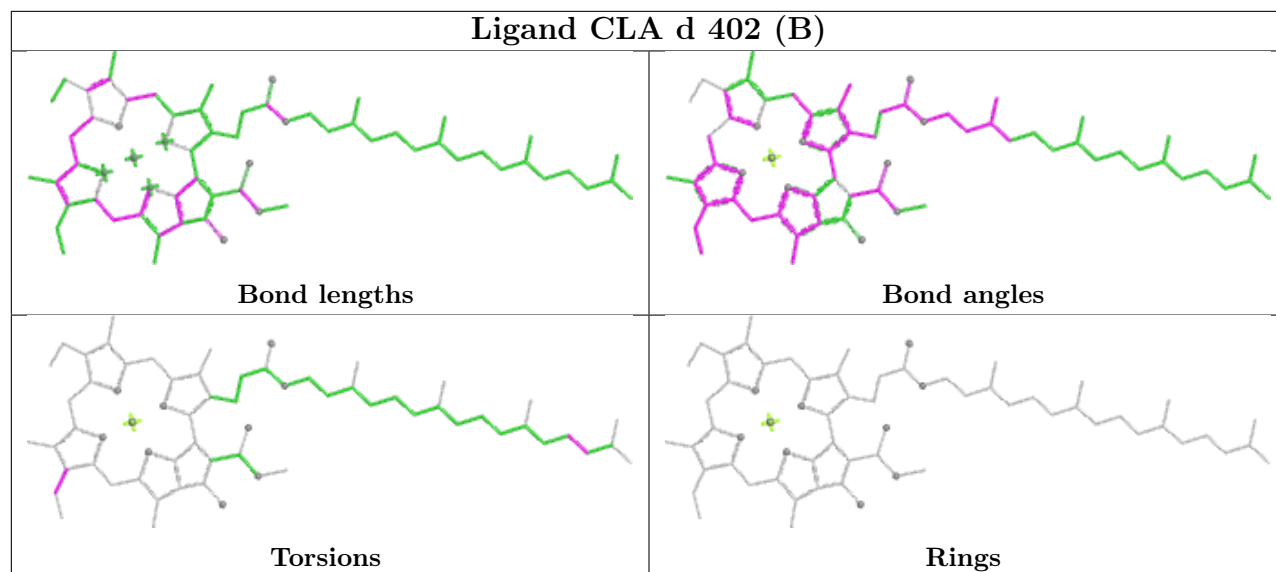
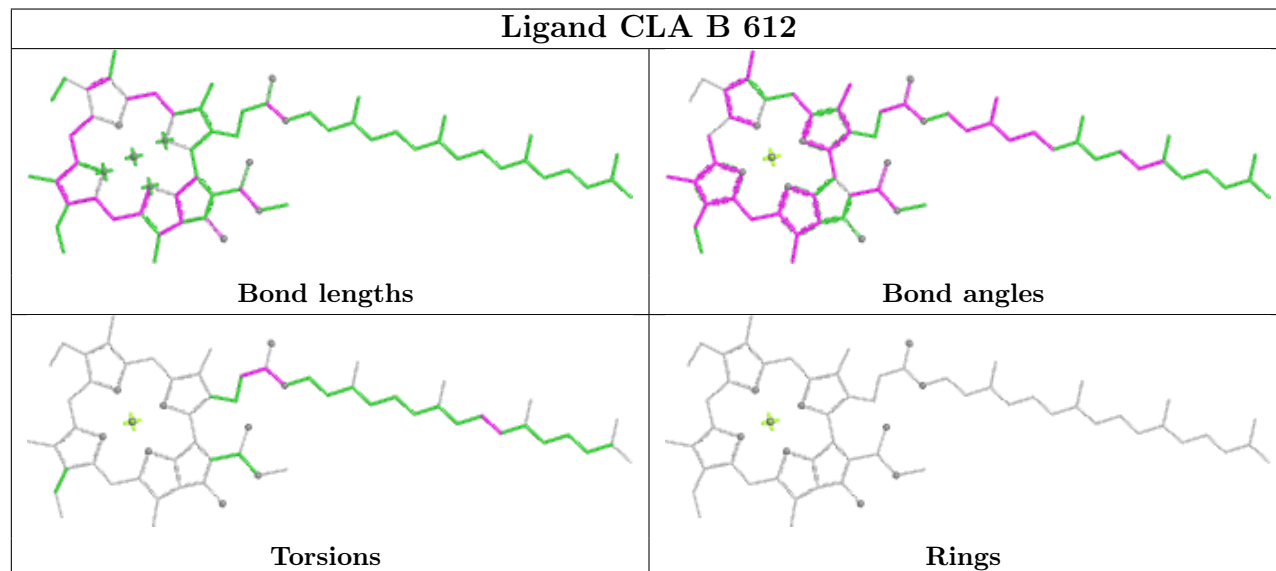
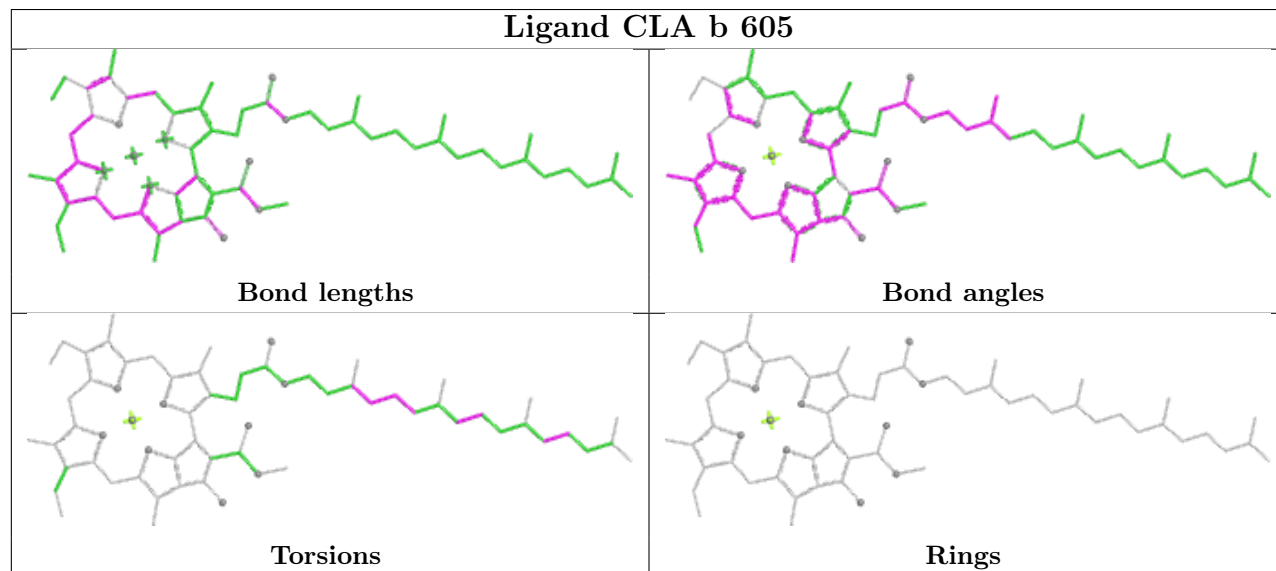
## Ligand CLA B 603

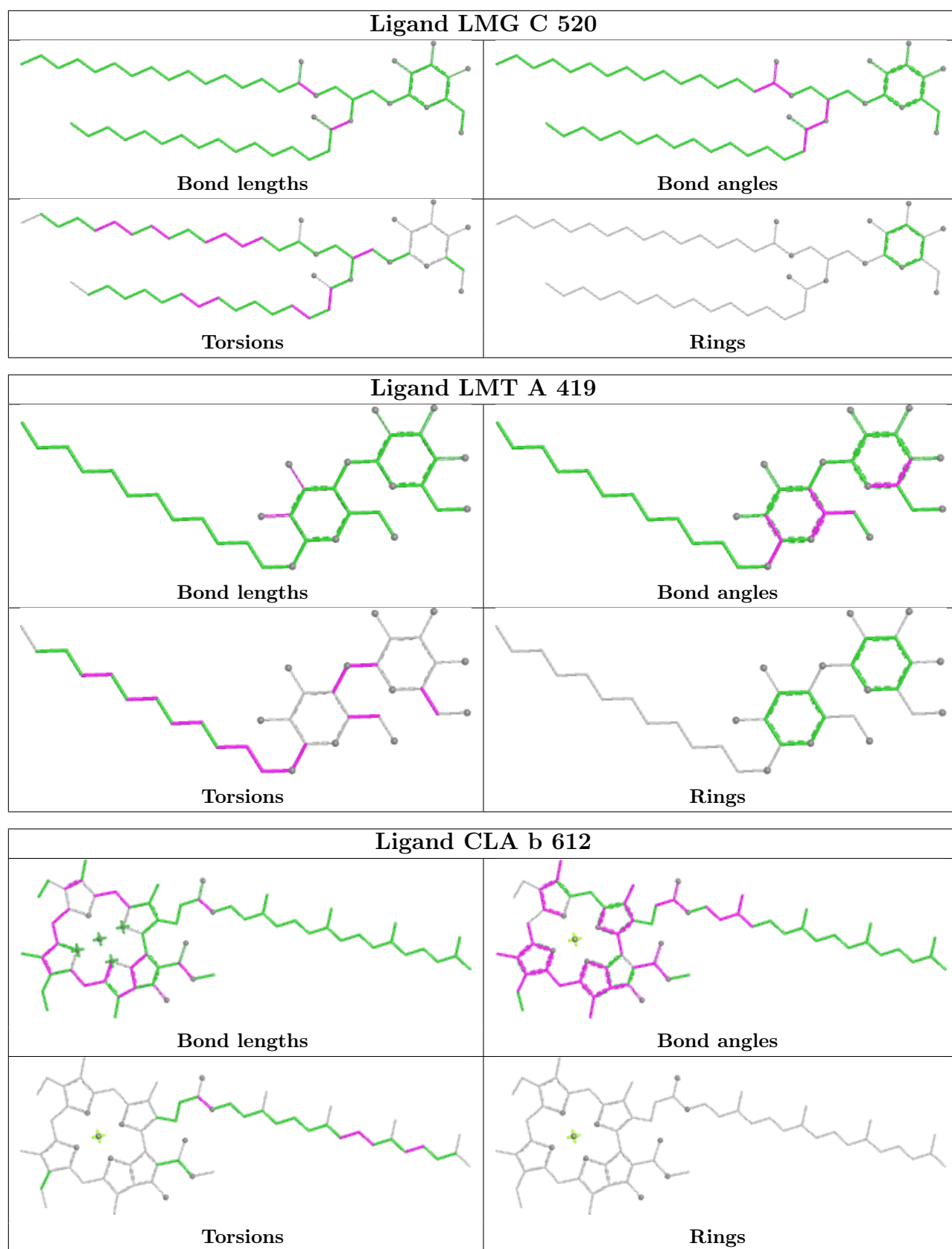


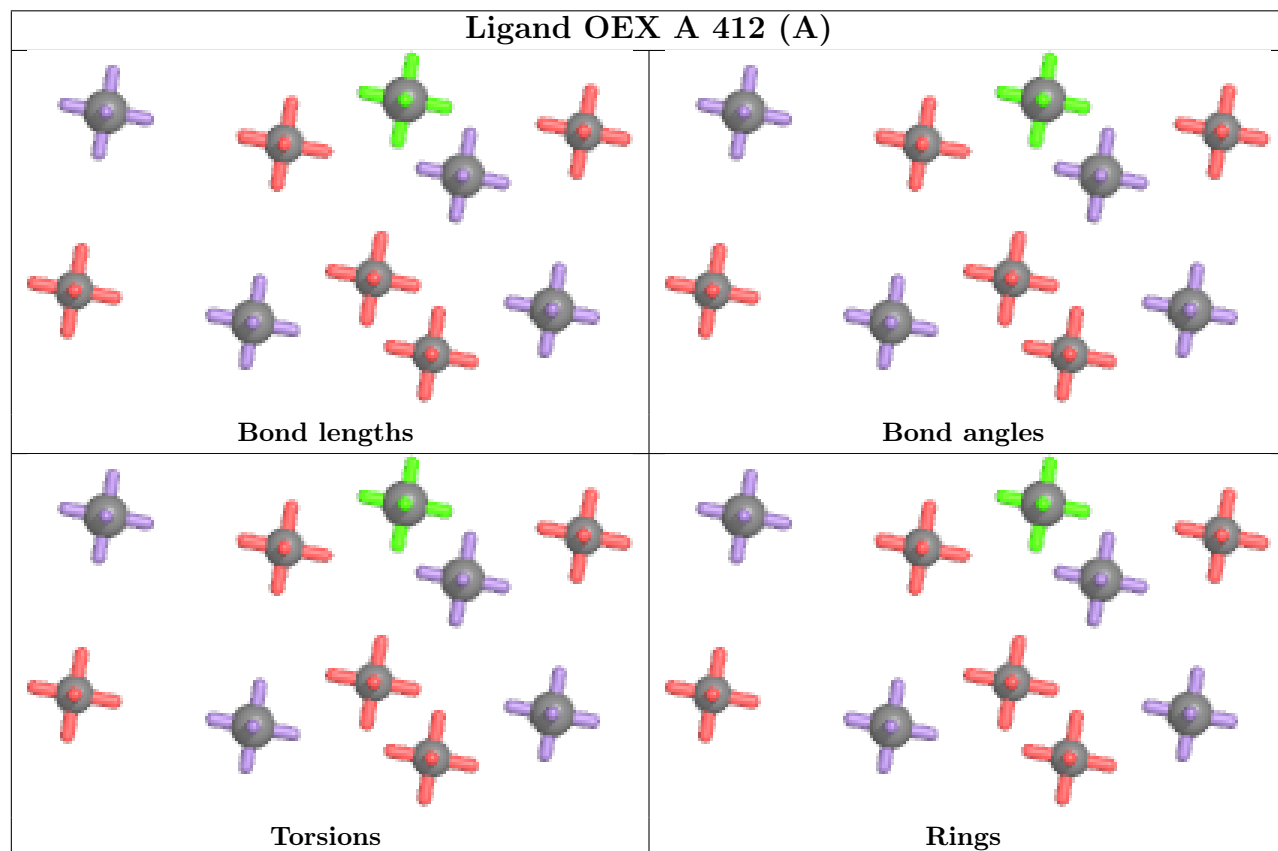
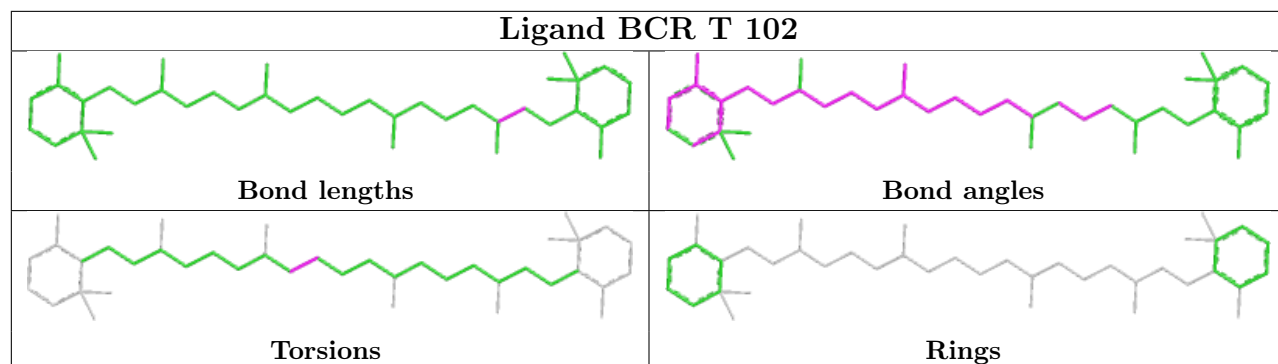
## Ligand CLA A 404 (A)

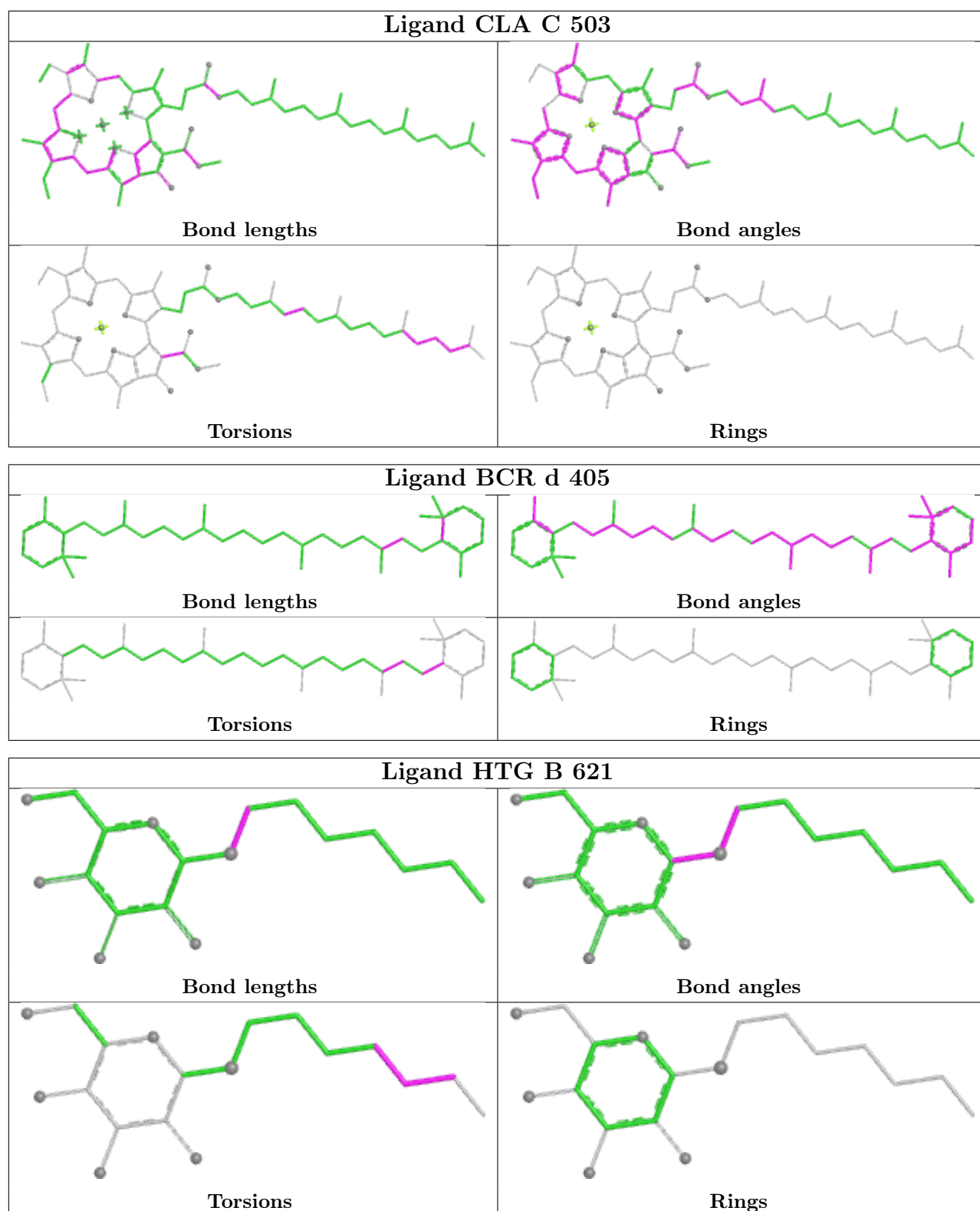


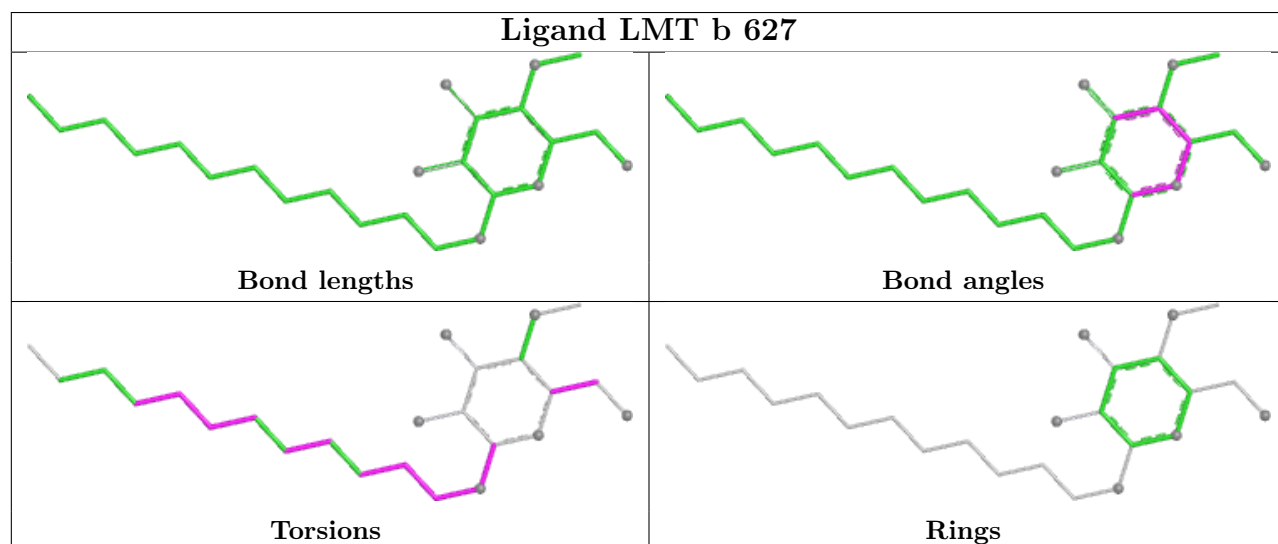
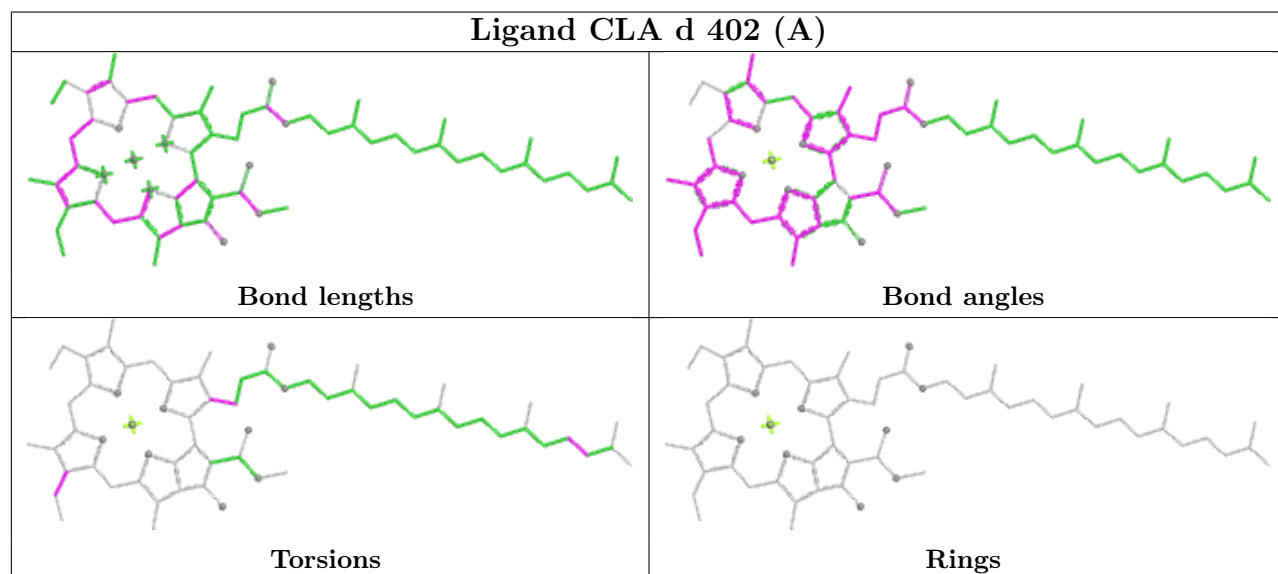
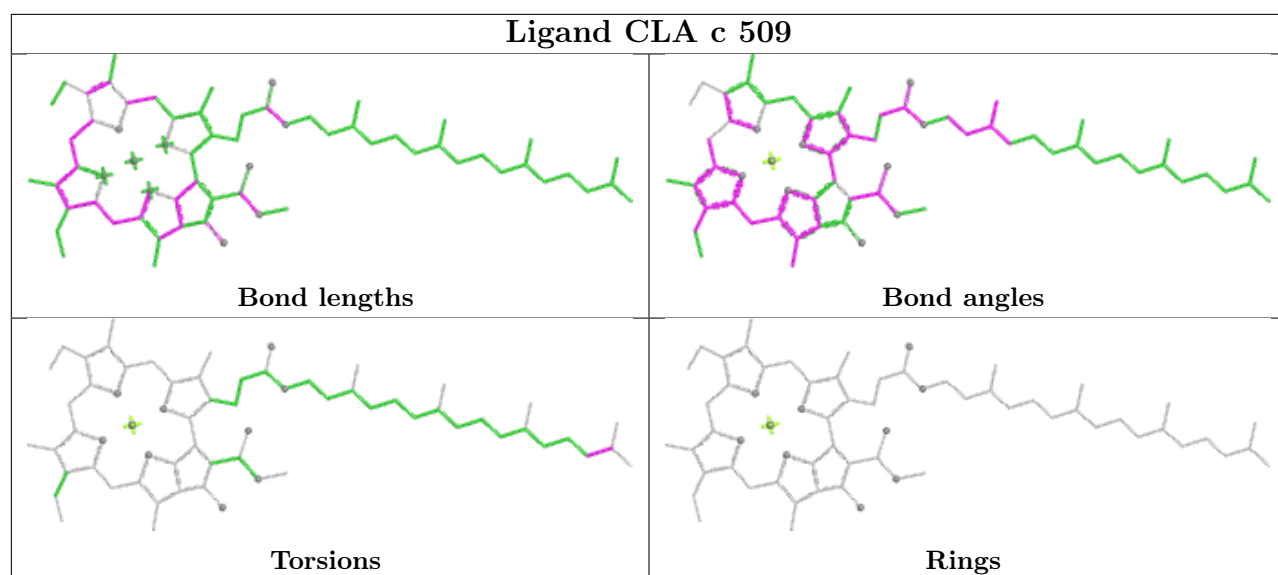


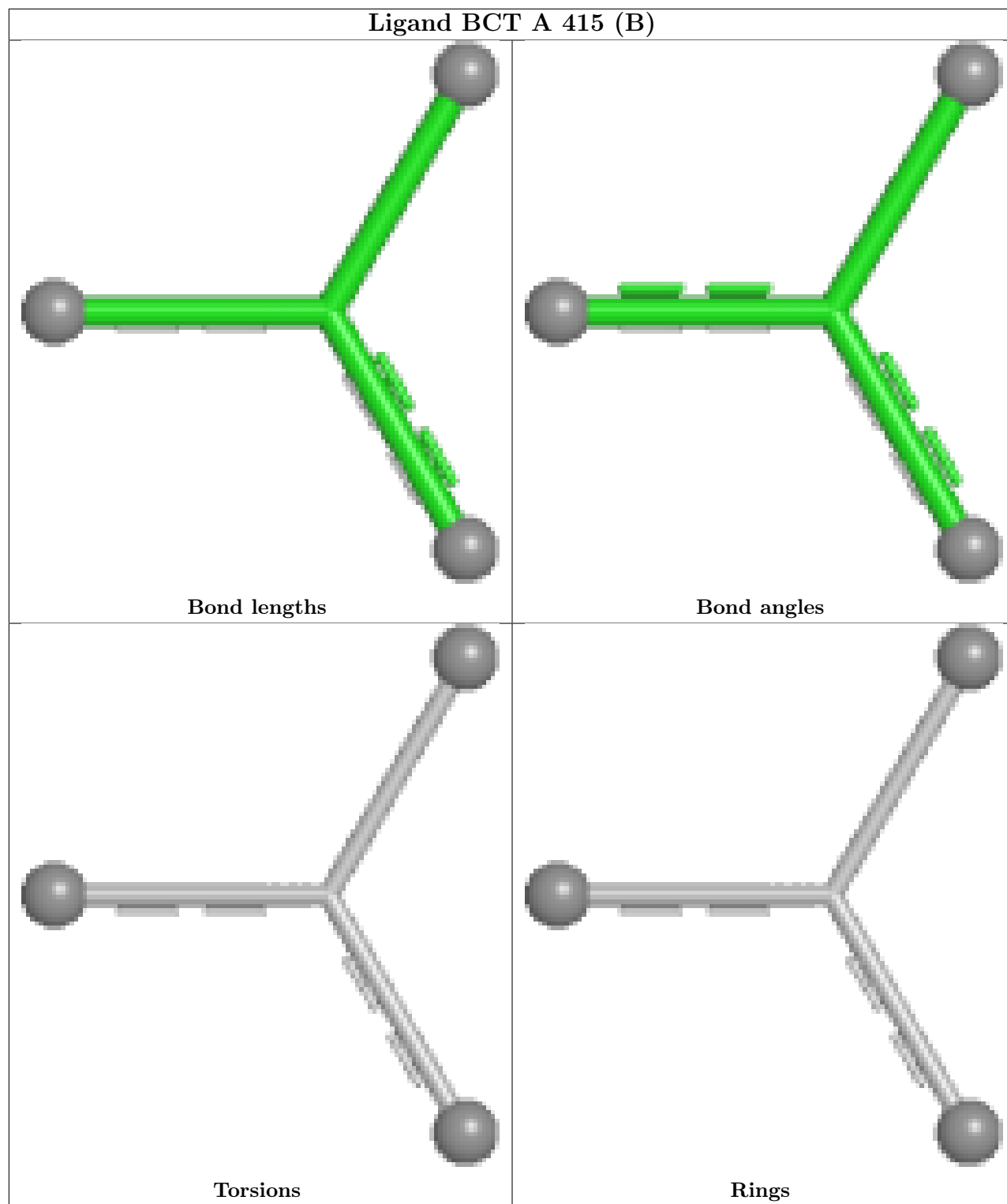
**Ligand CLA d 402 (B)****Ligand CLA B 612****Ligand CLA b 605**

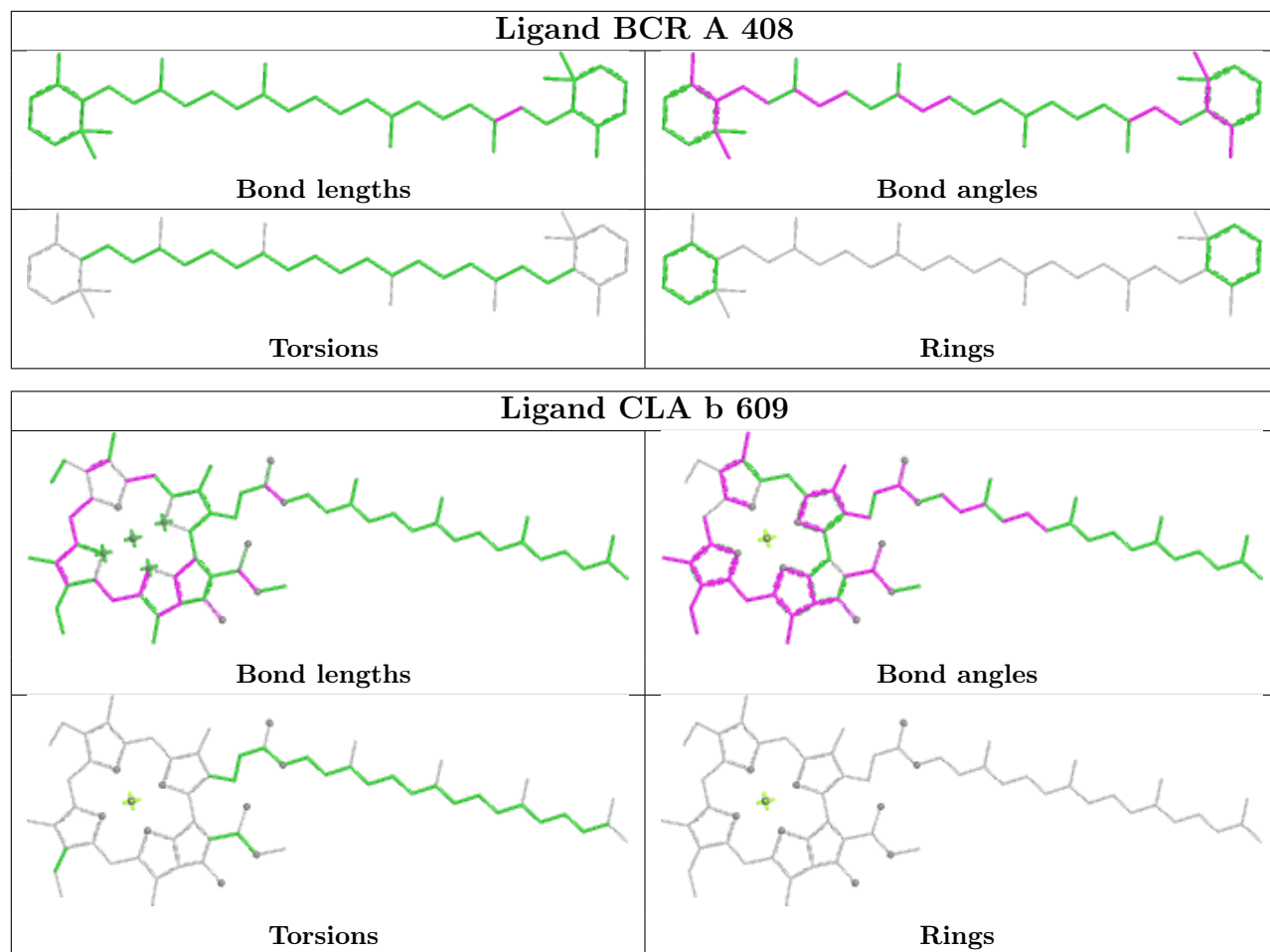




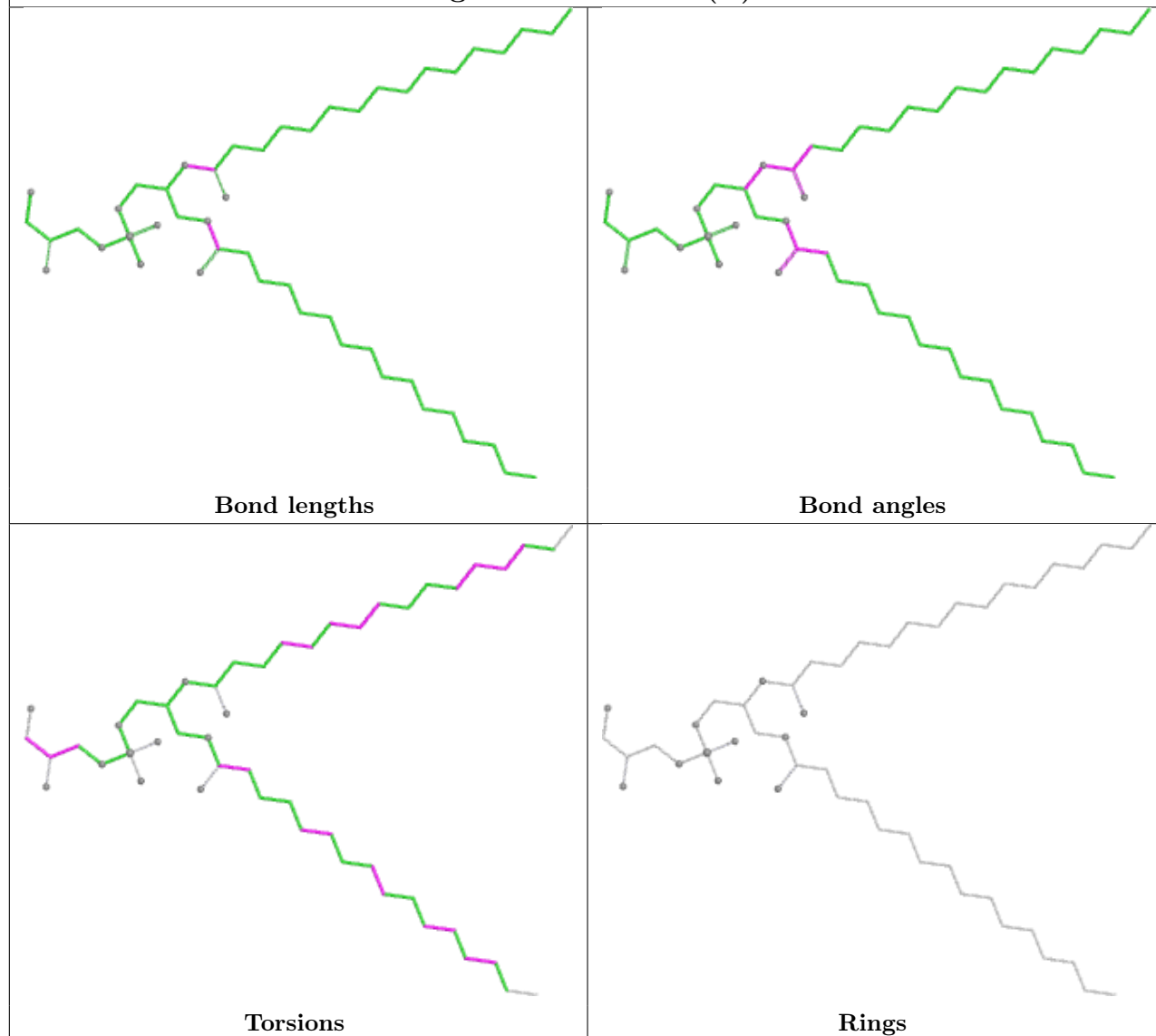




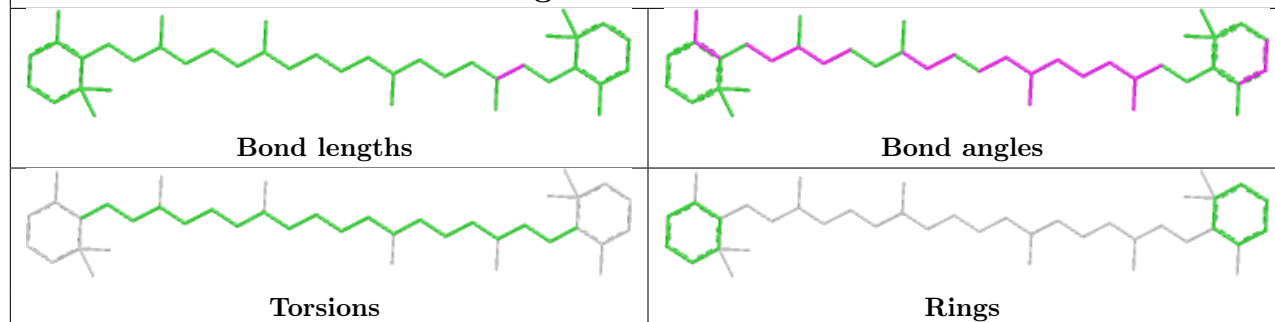




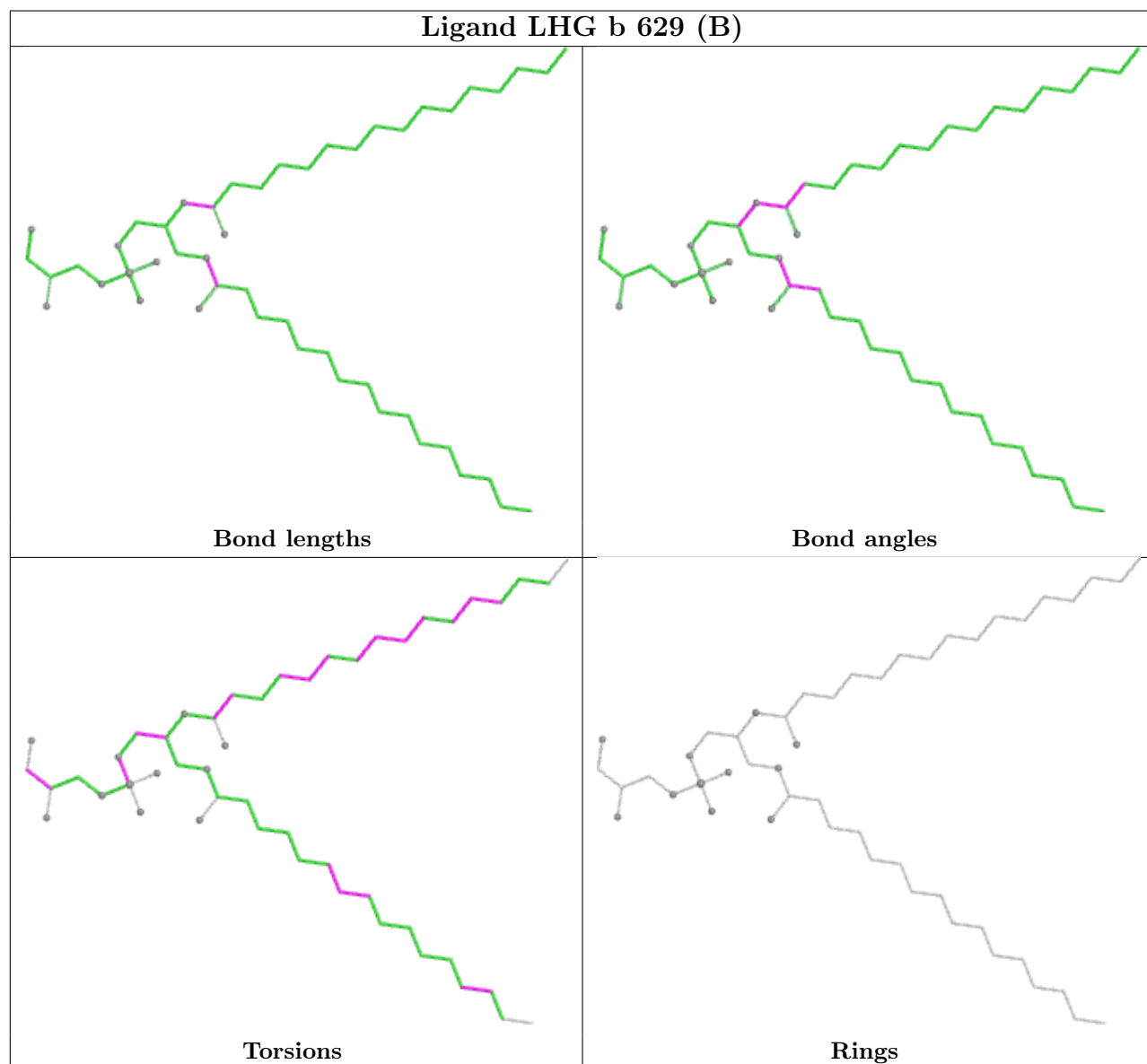
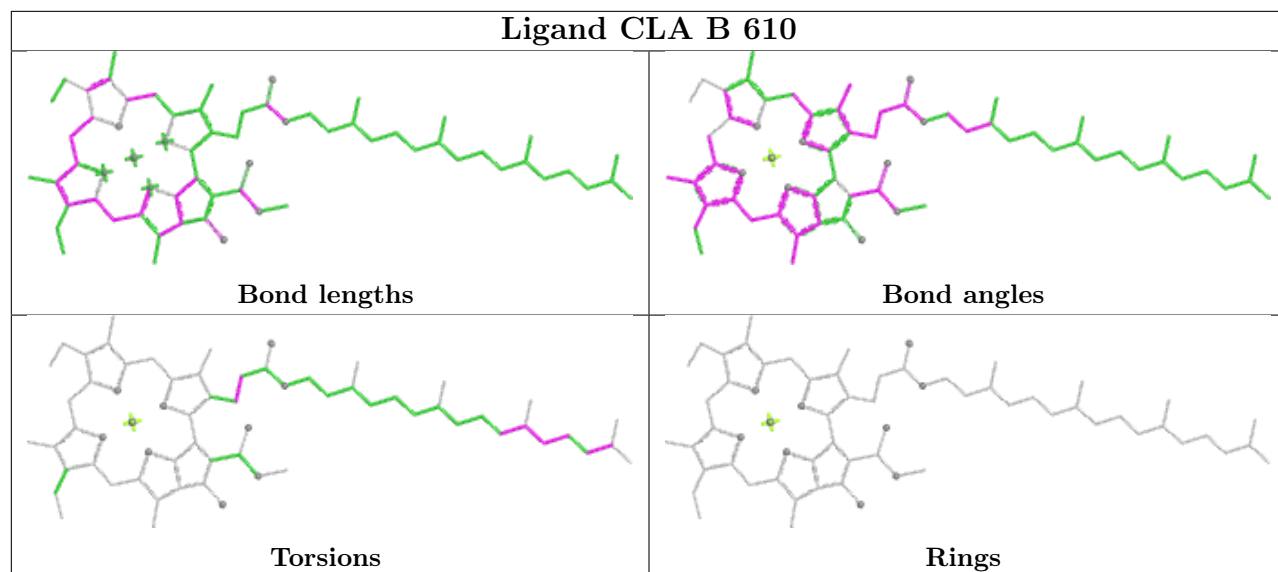
## Ligand LHG A 418 (B)

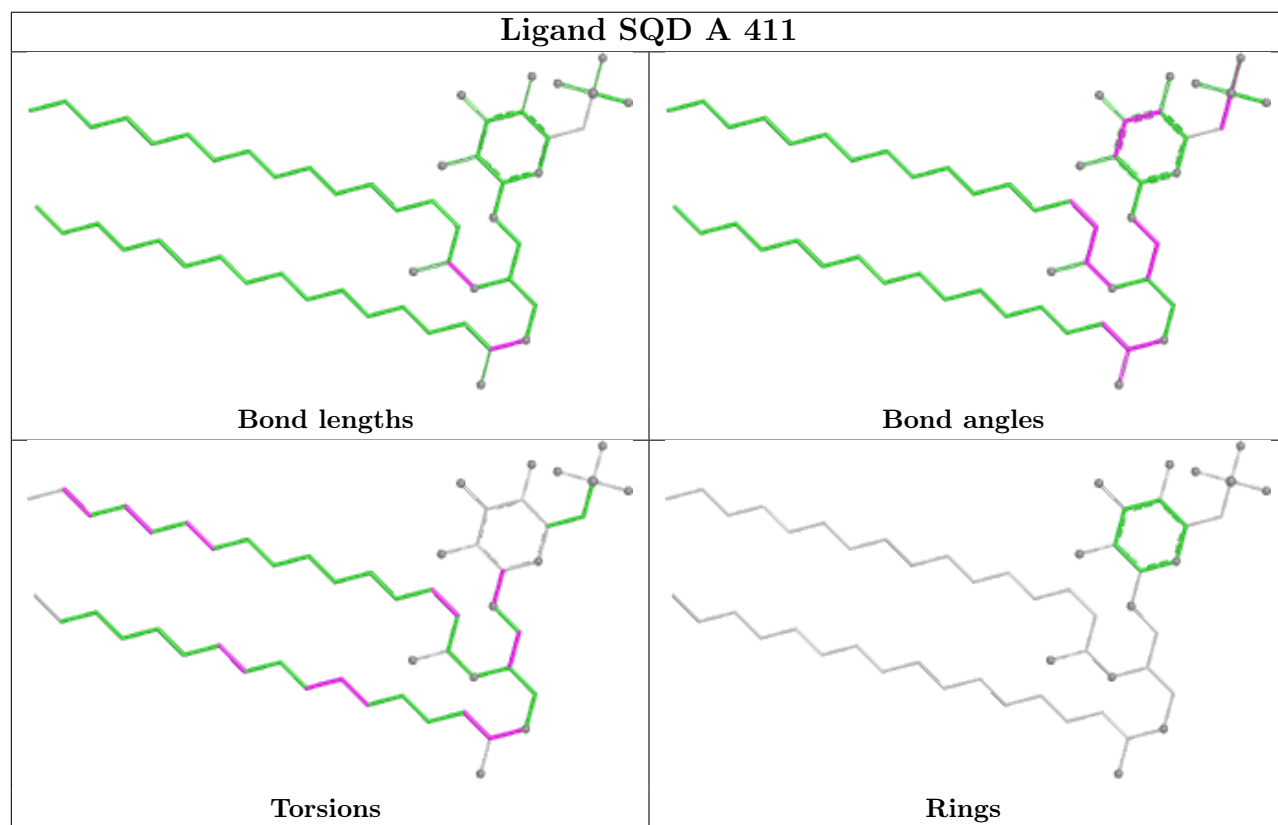
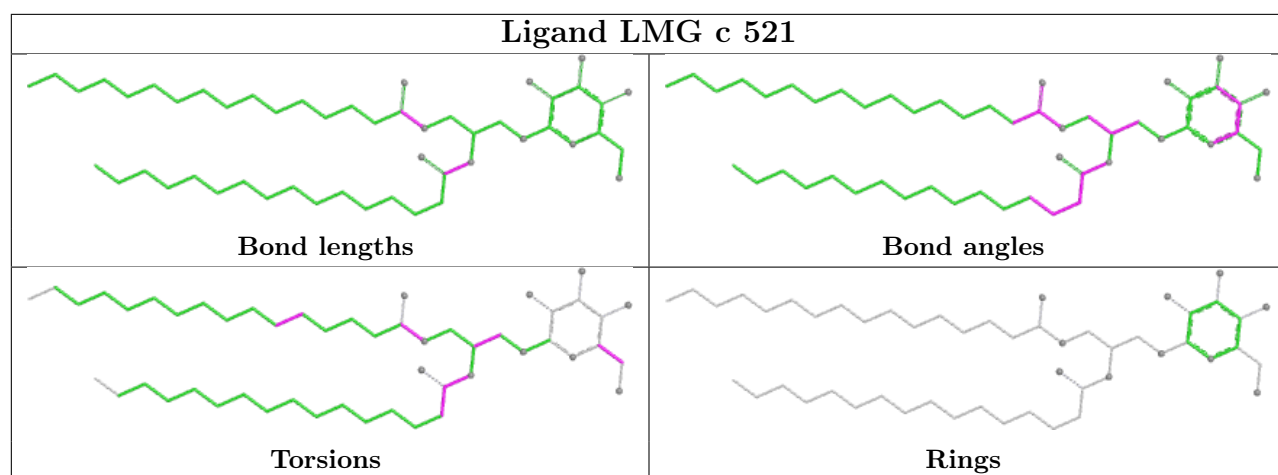


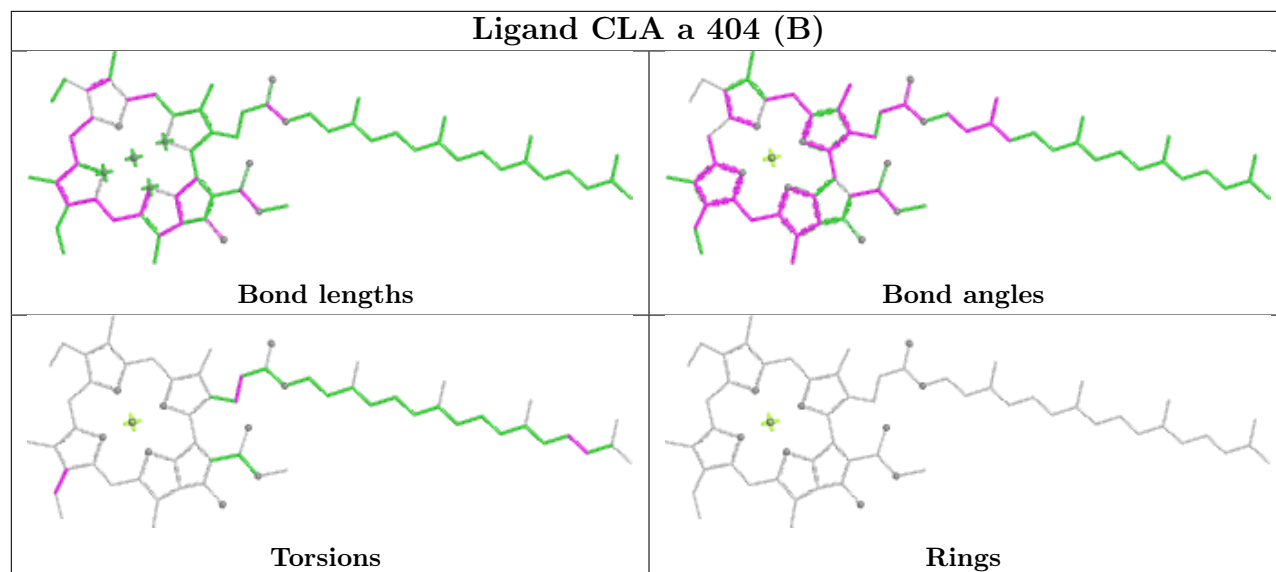
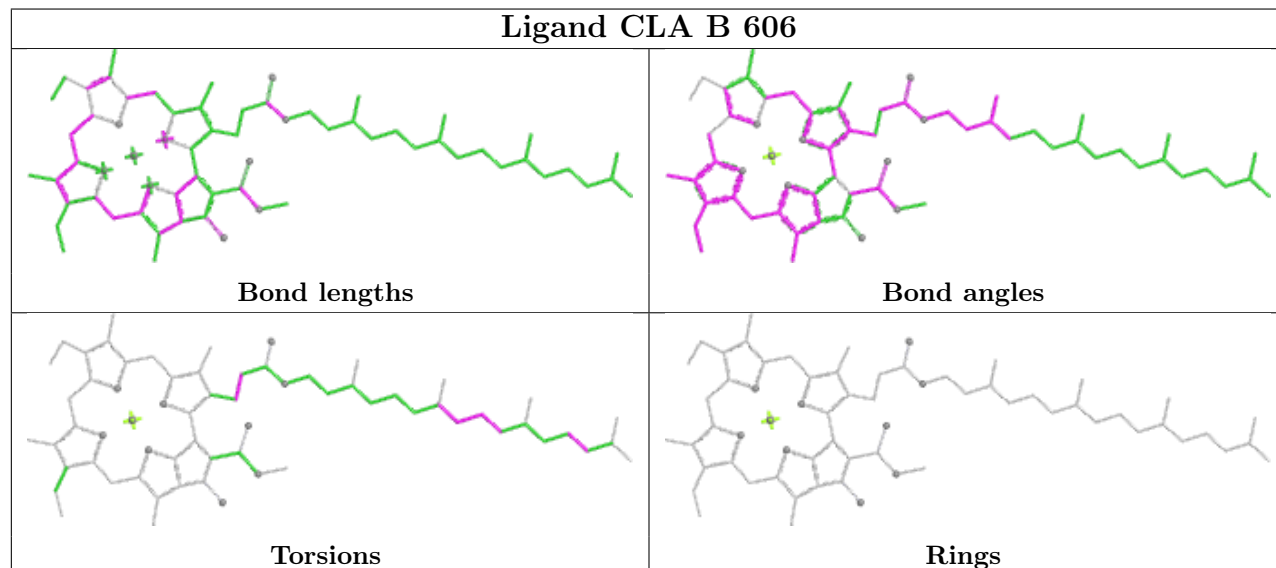
## Ligand BCR c 515



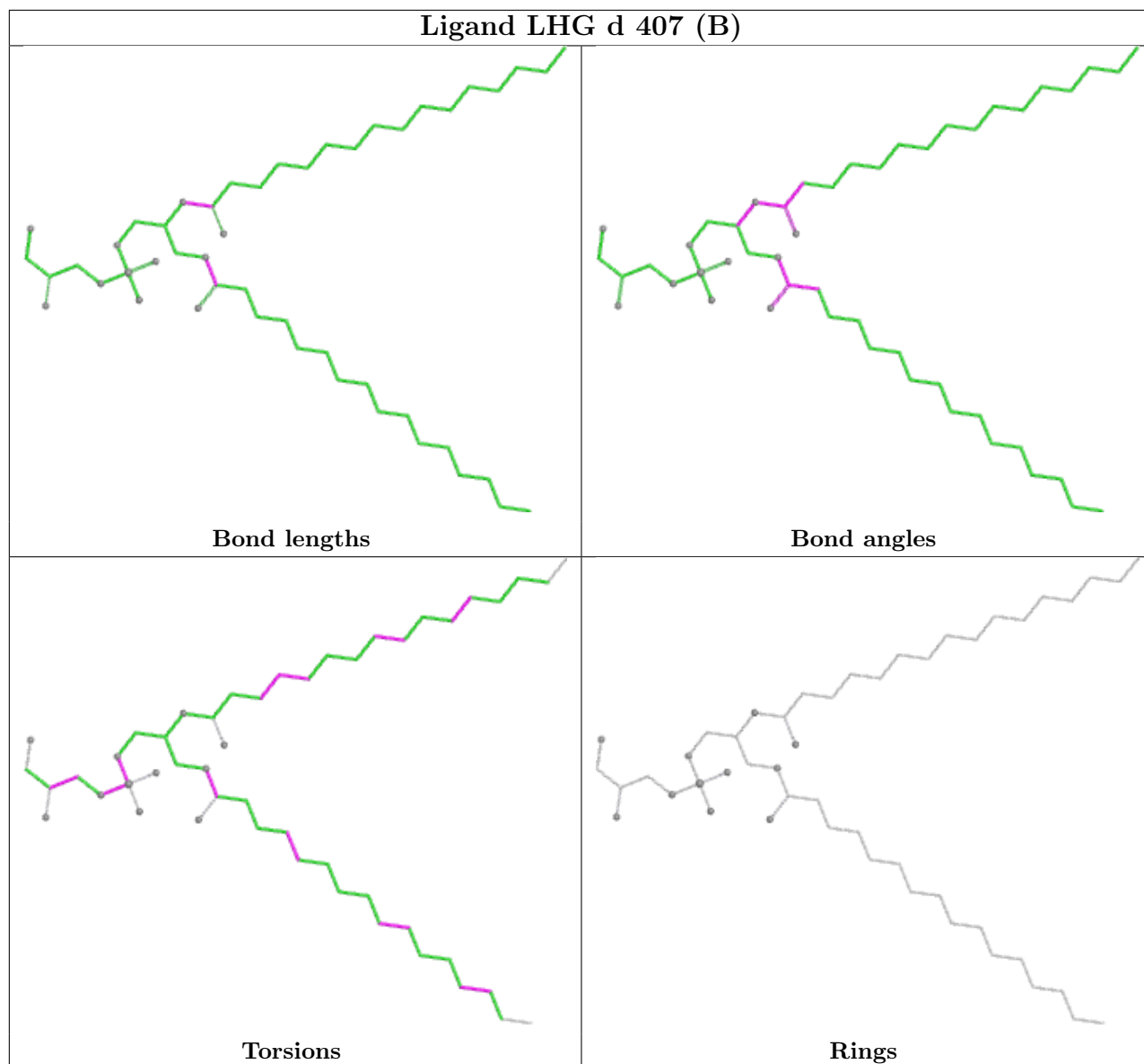




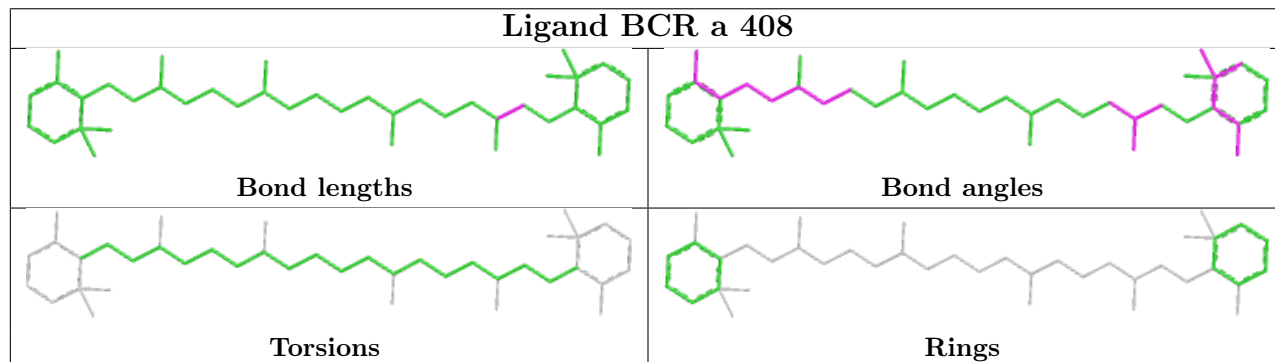


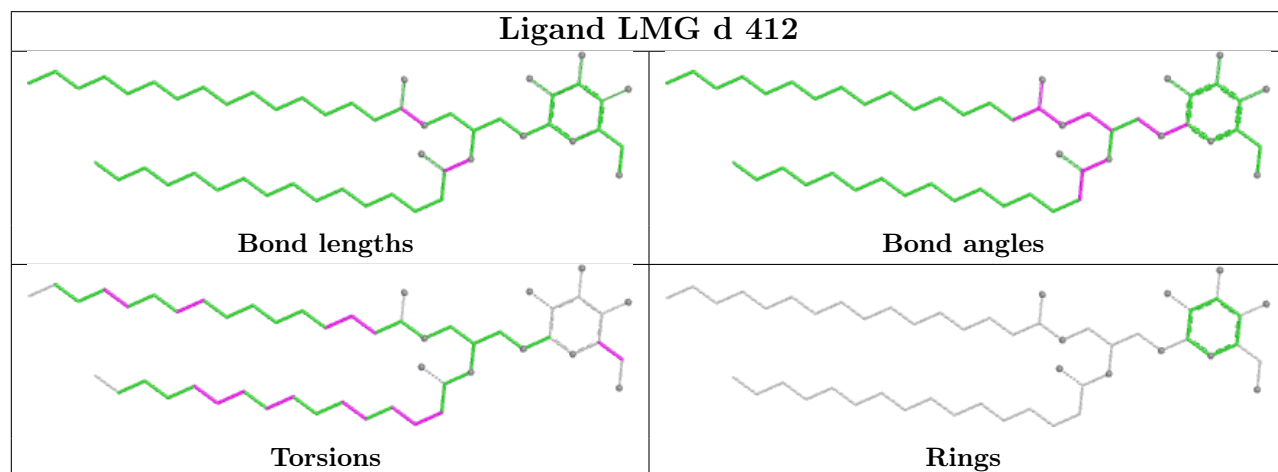
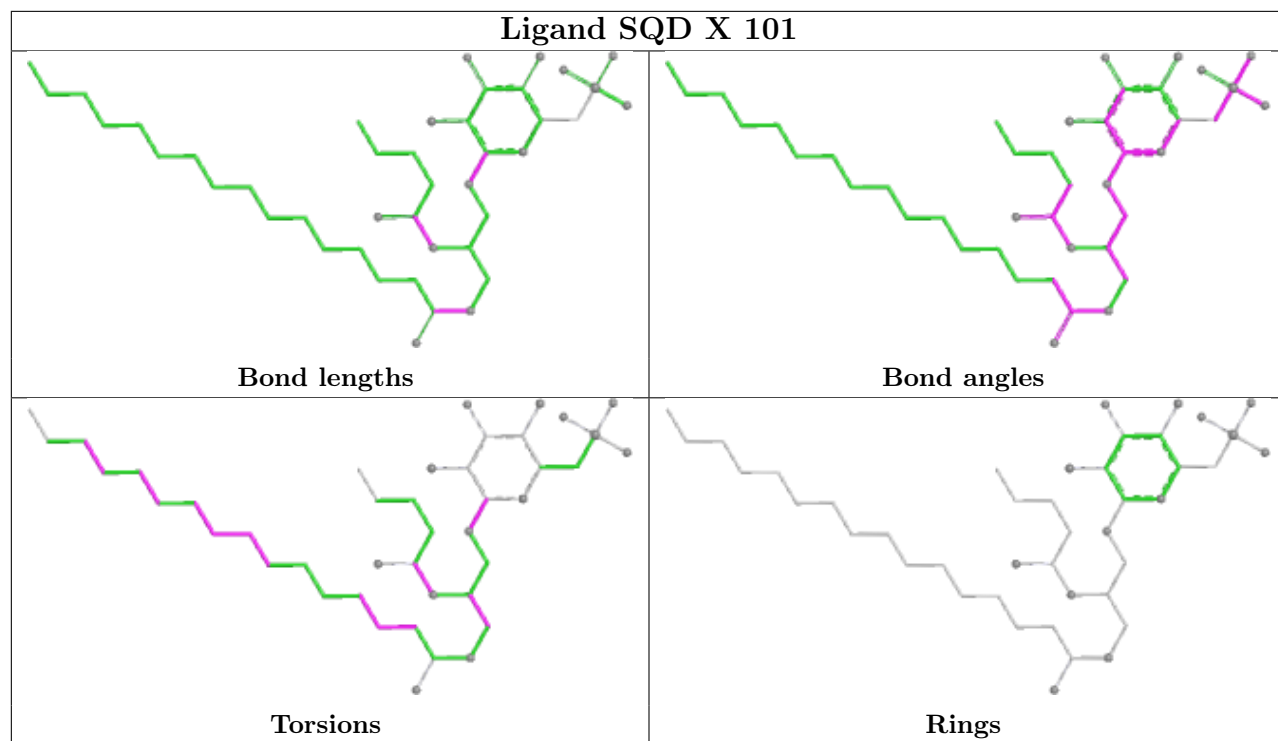
**Ligand CLA a 404 (B)****Ligand CLA B 606**

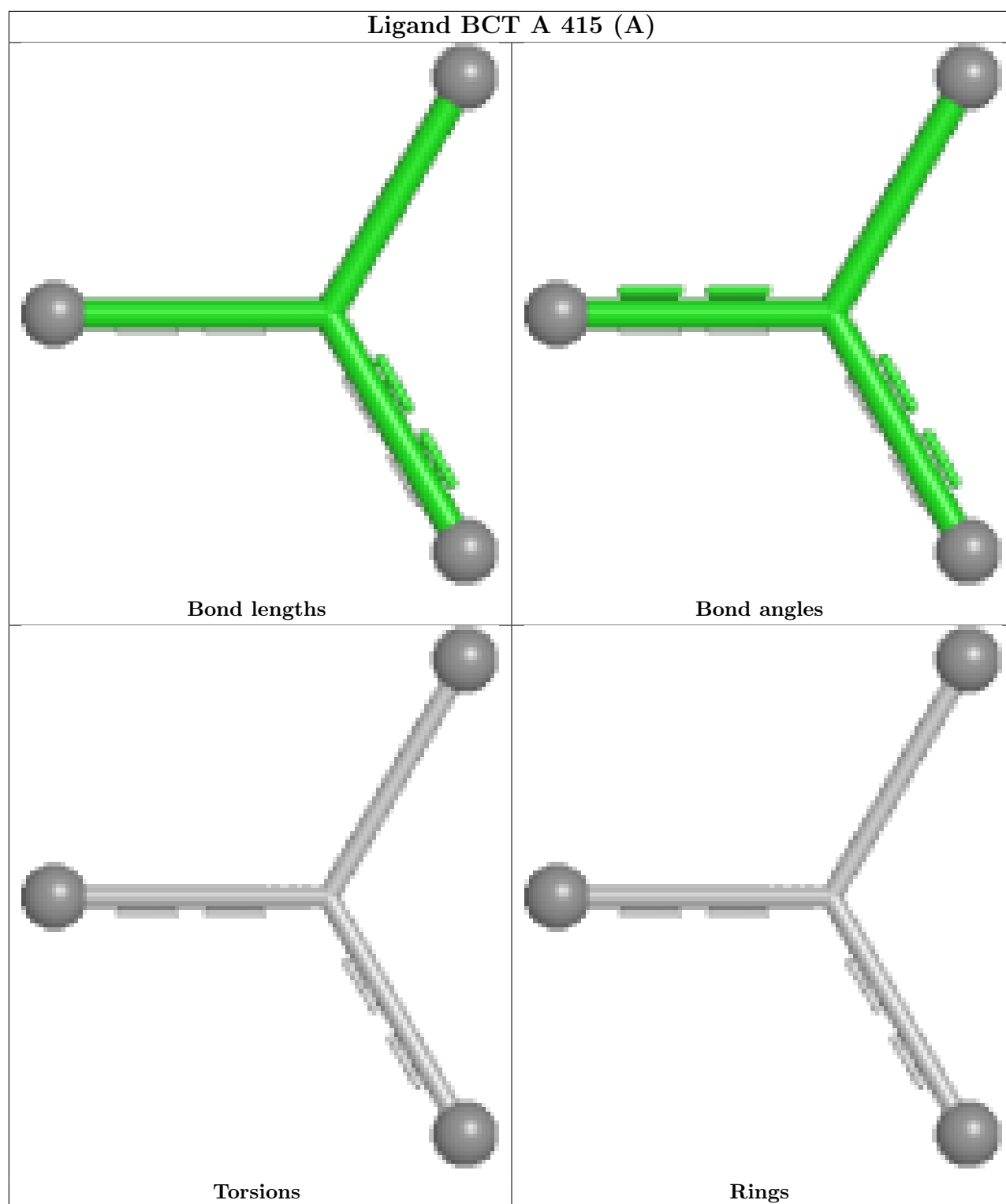
## Ligand LHG d 407 (B)

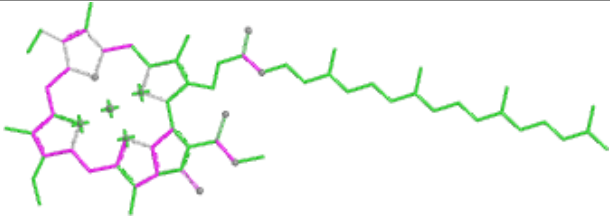
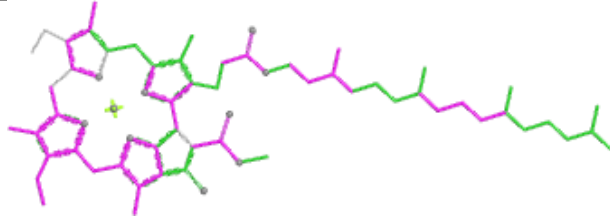
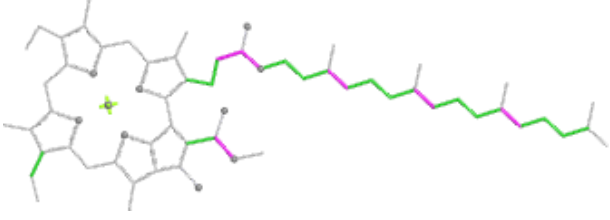
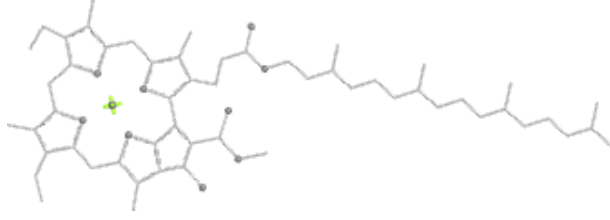
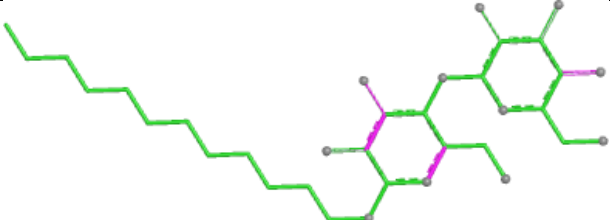
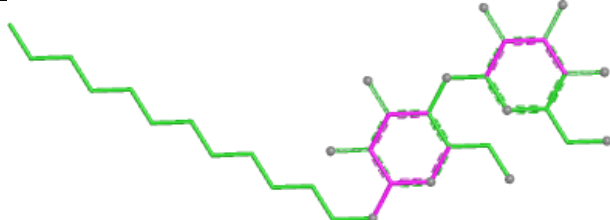
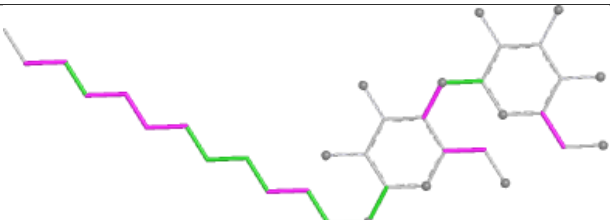
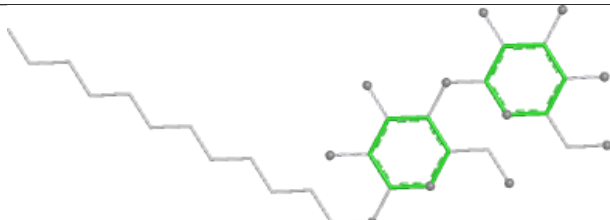
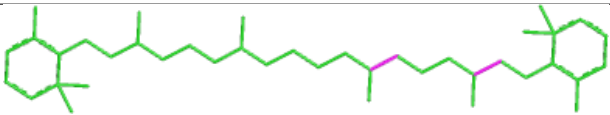
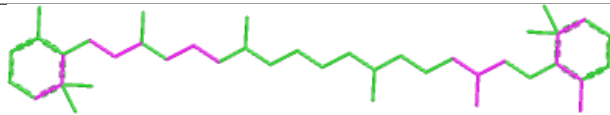
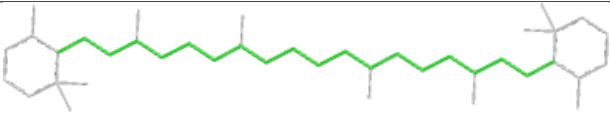
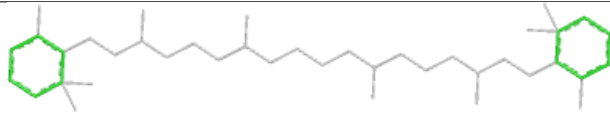


## Ligand BCR a 408

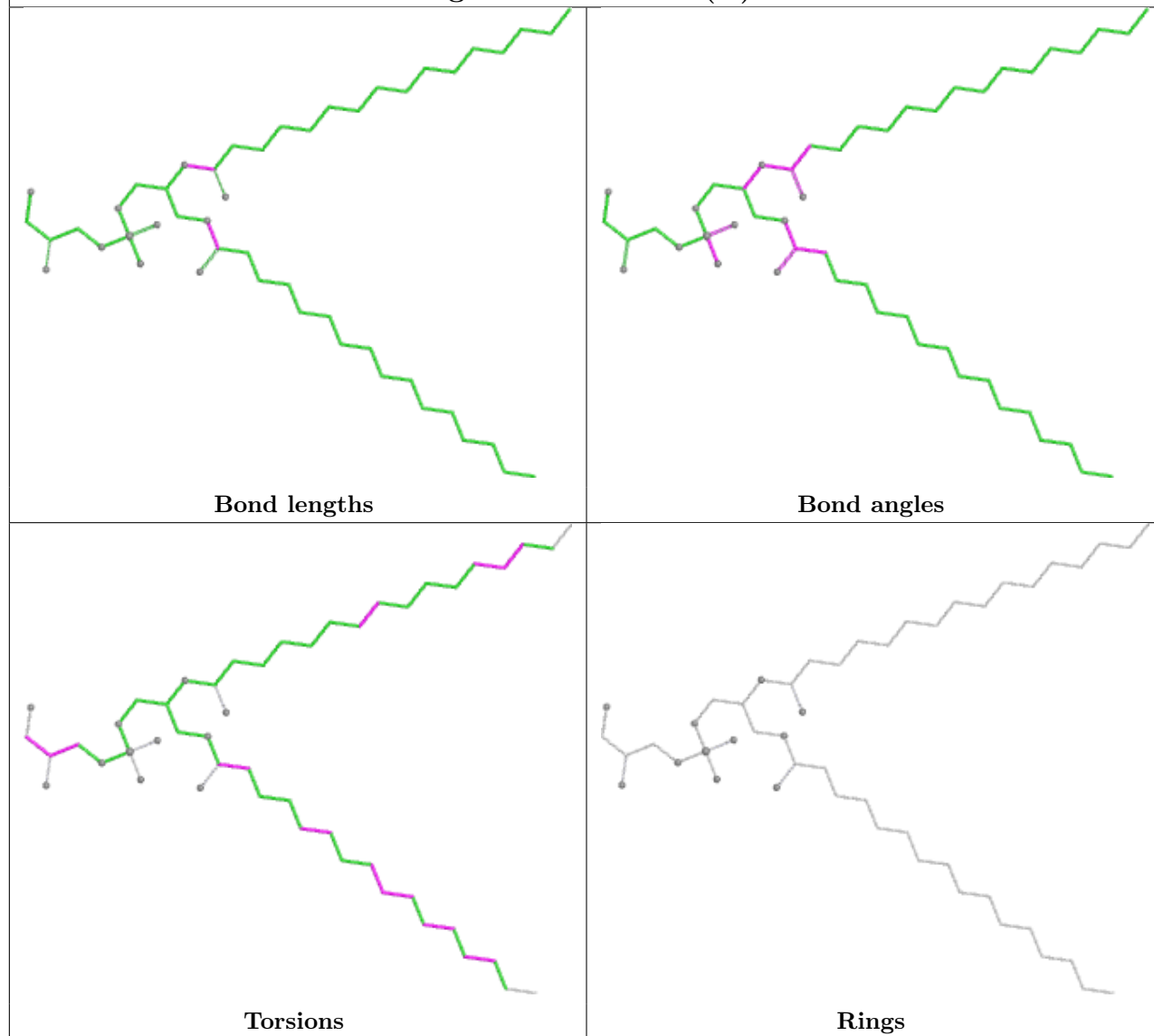




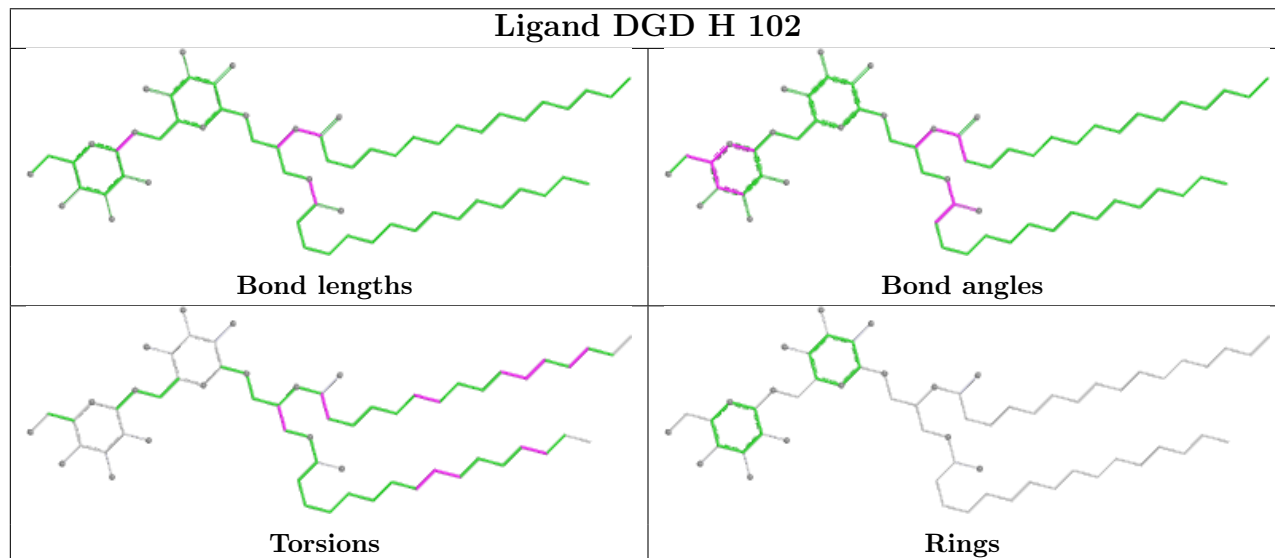


| Ligand CLA c 511                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMT B 626                                                                                        |                                                                                                         |
|  <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>       |

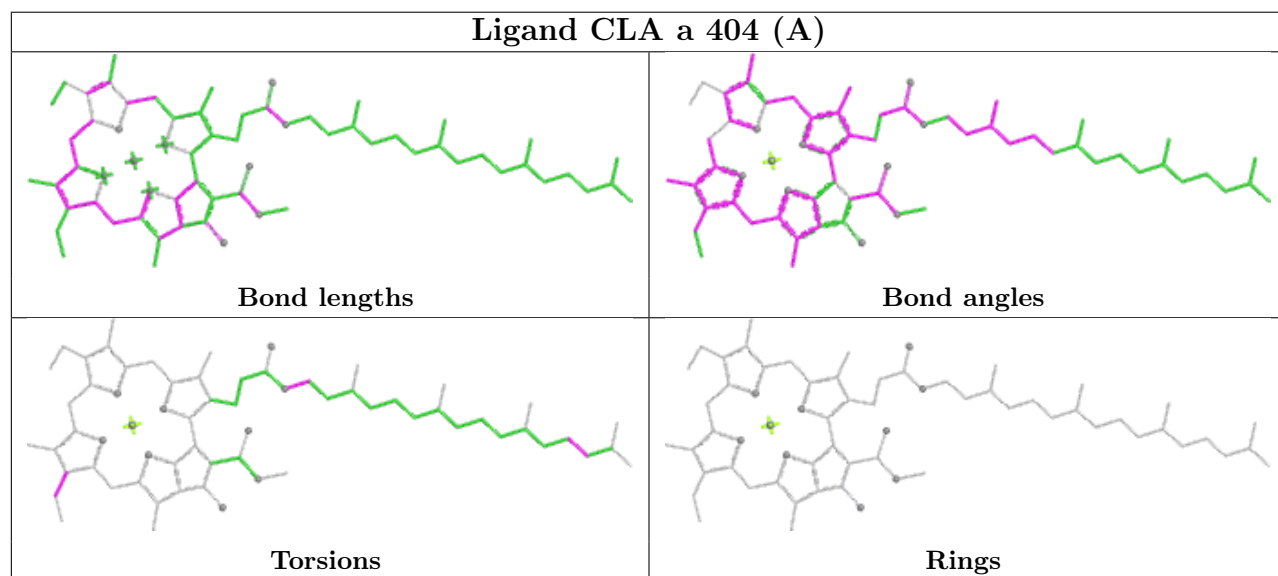
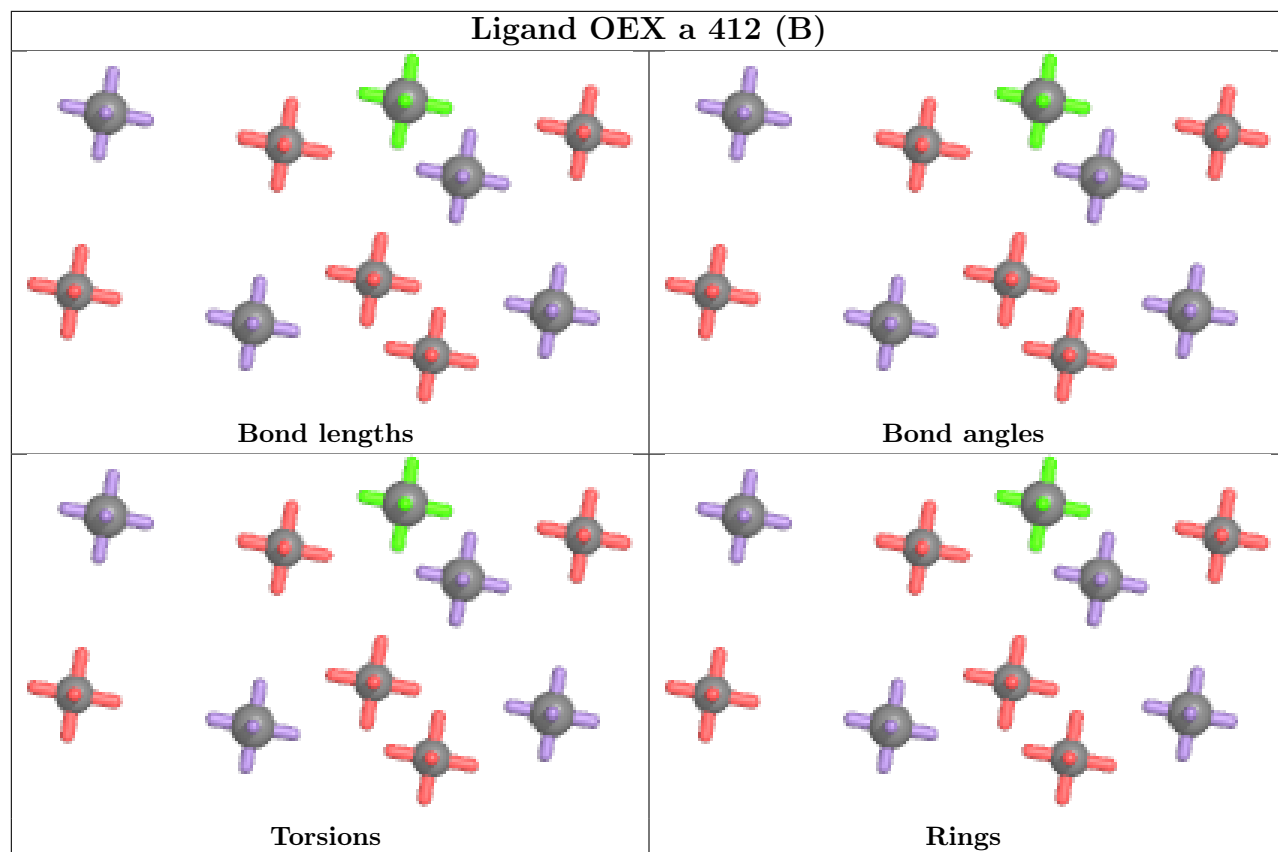
## Ligand LHG A 418 (A)

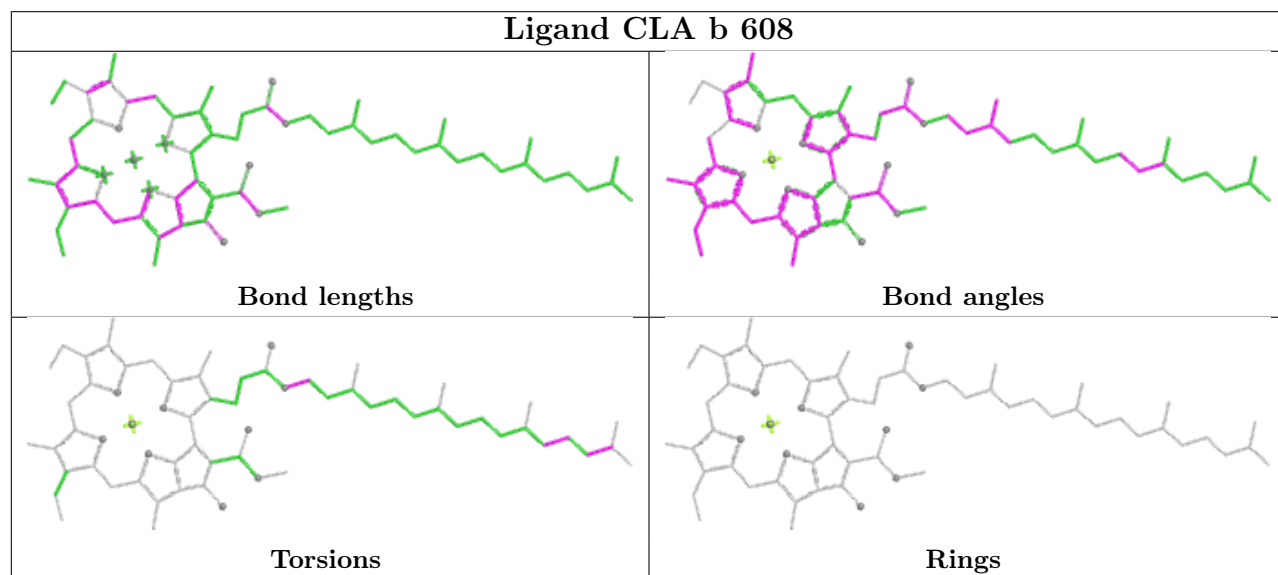
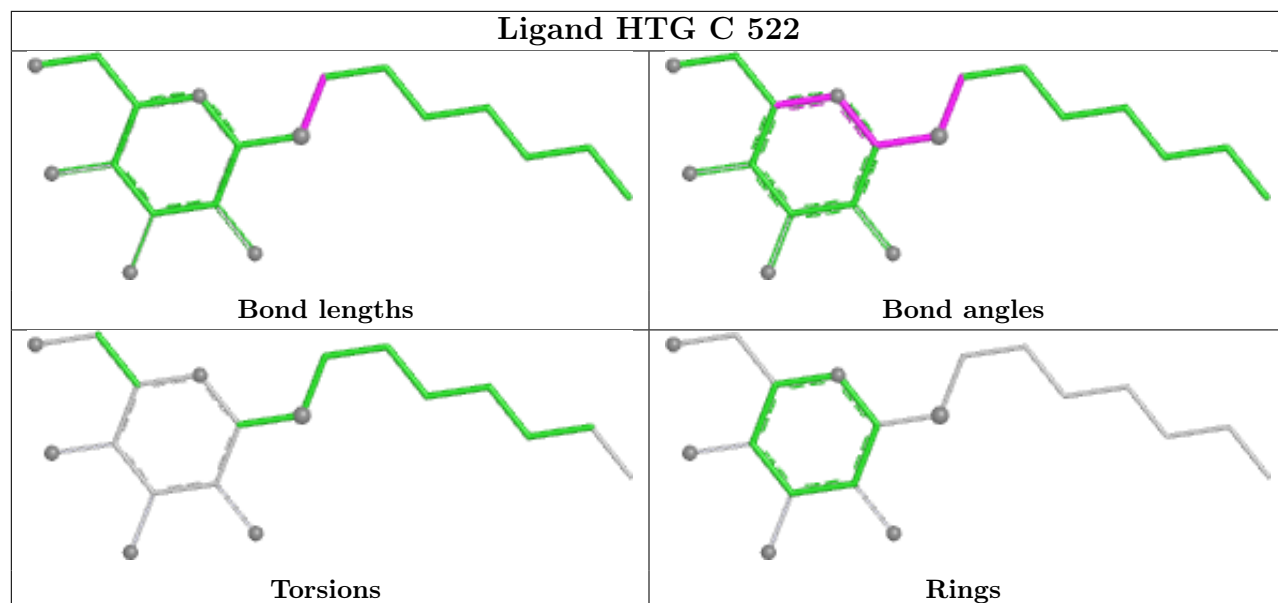


## Ligand DGD H 102

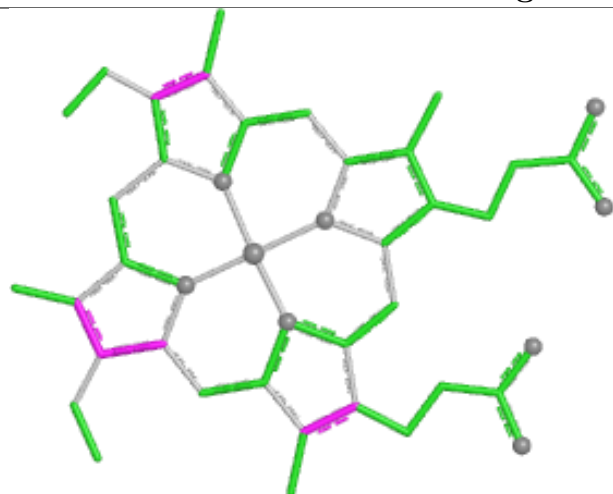




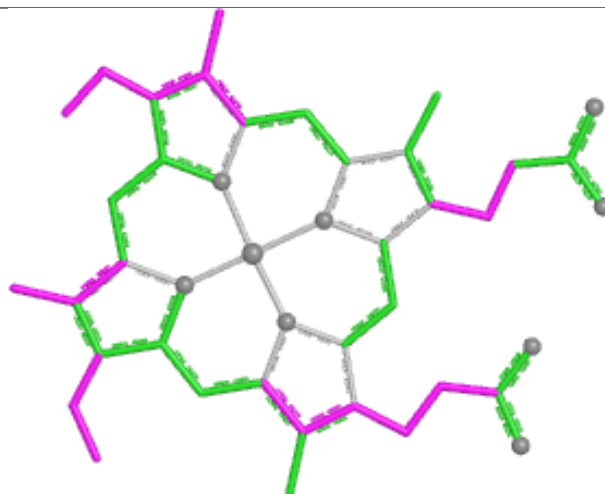




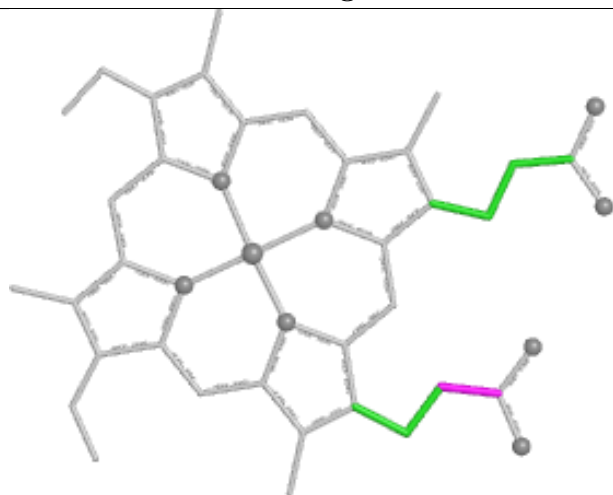
## Ligand HEC v 201



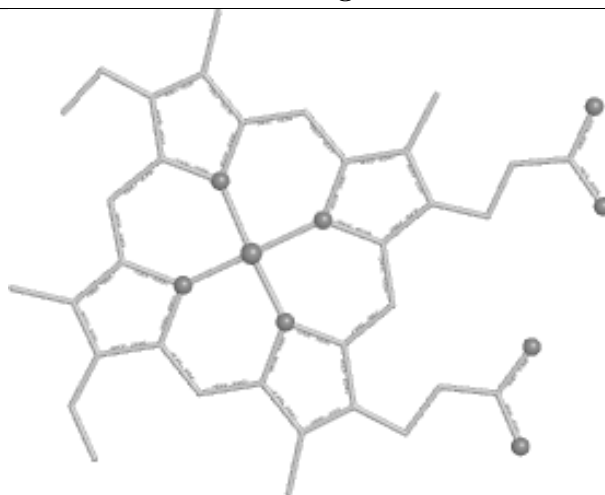
Bond lengths



Bond angles

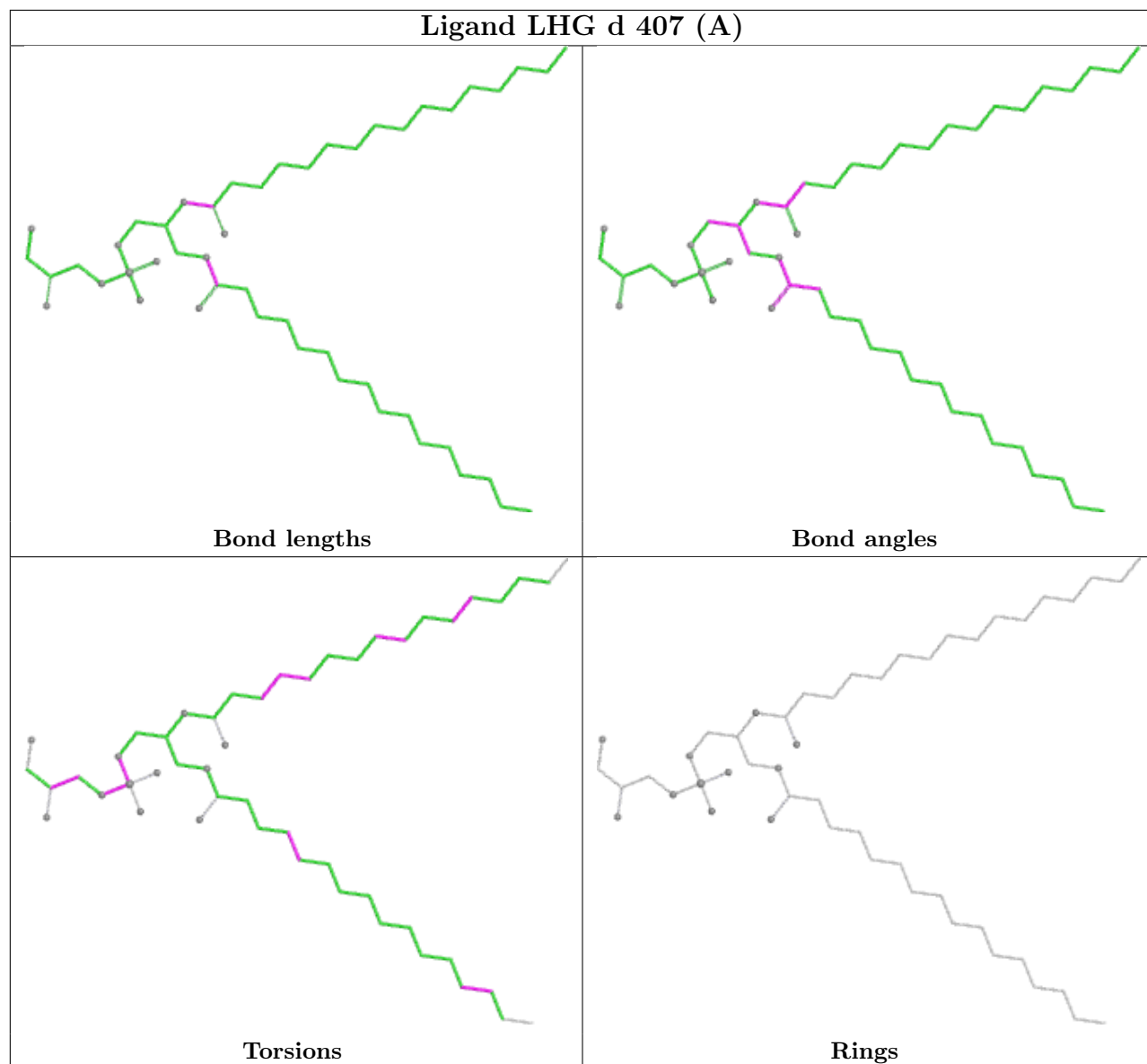


Torsions

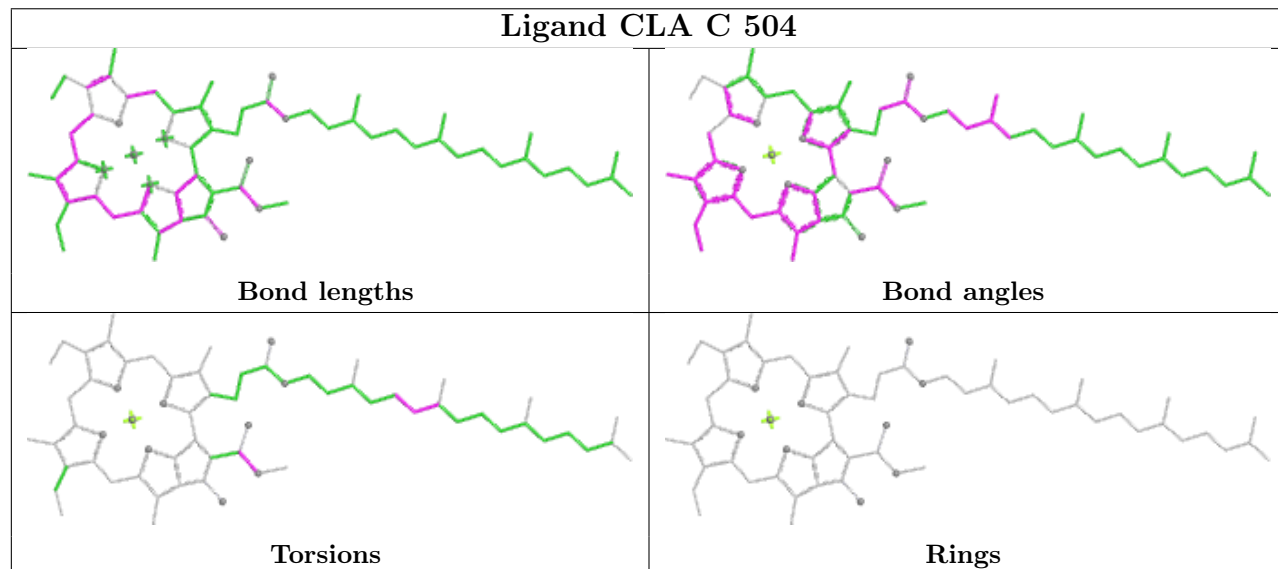


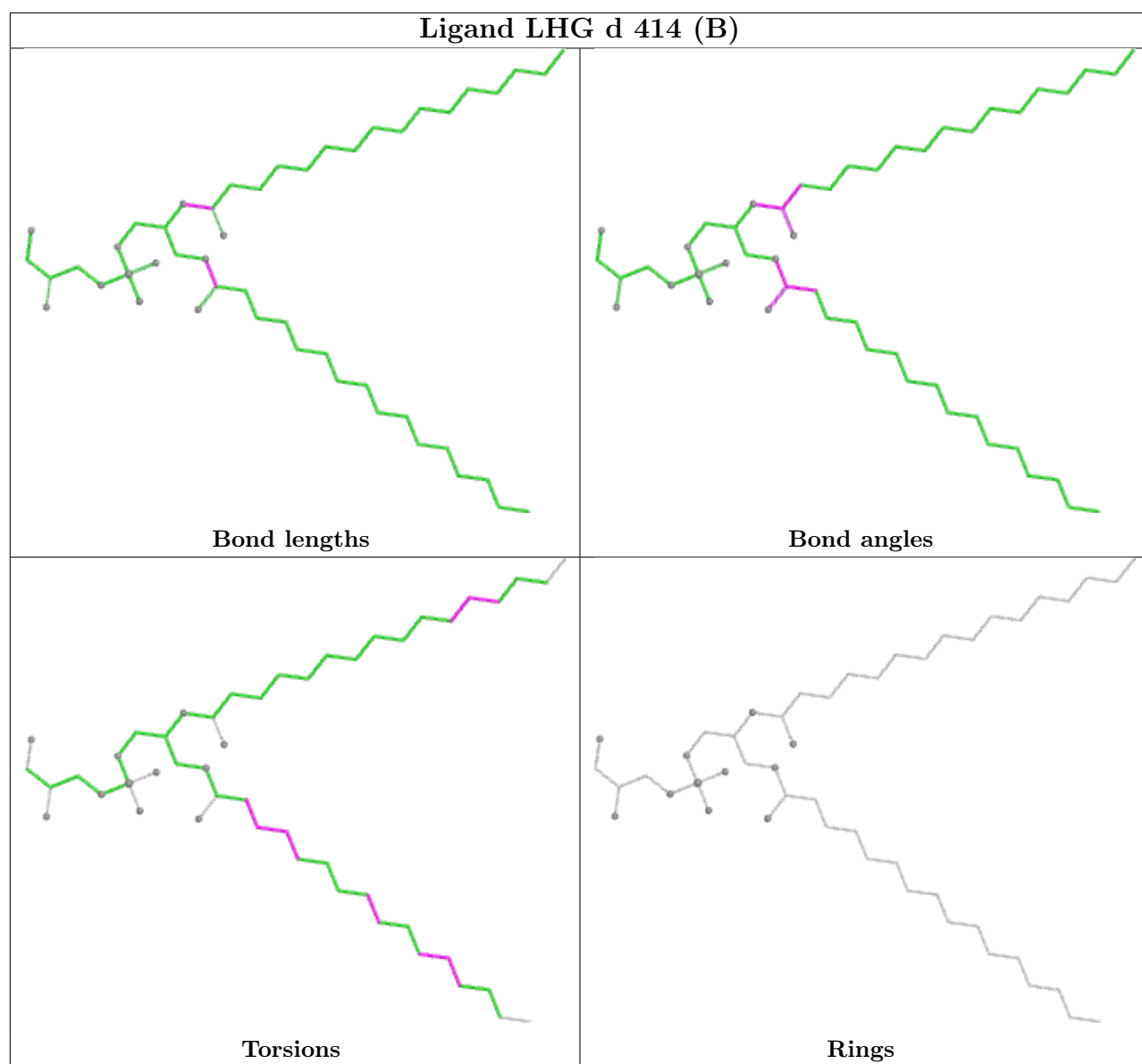
Rings

## Ligand LHG d 407 (A)

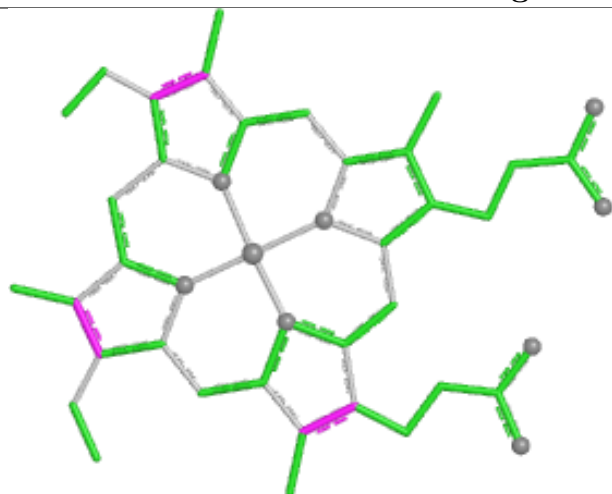


## Ligand CLA C 504

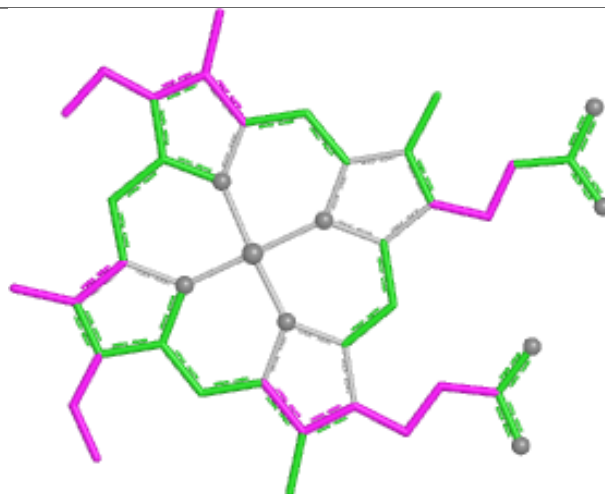




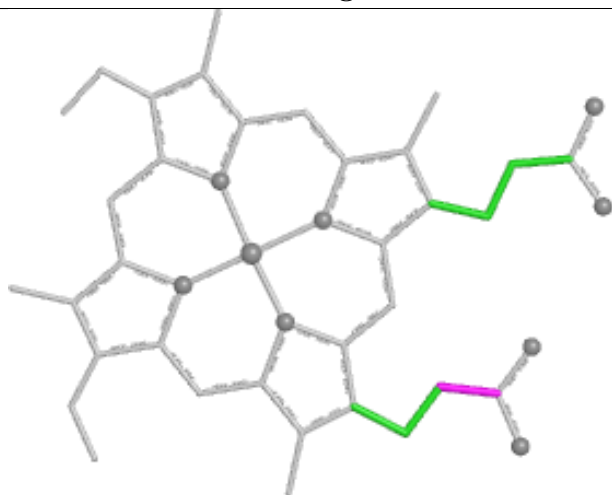
## Ligand HEC V 201



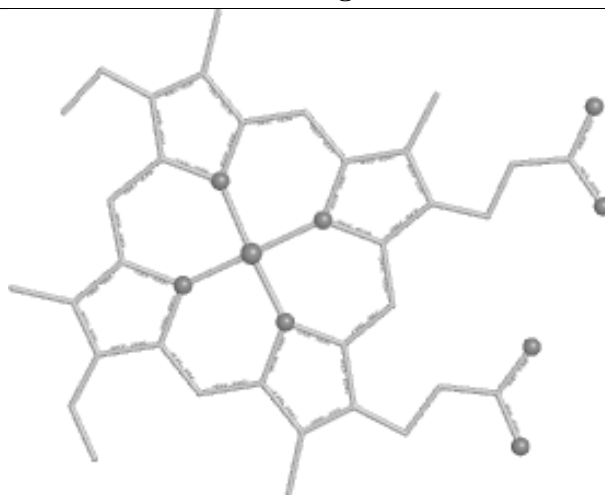
Bond lengths



Bond angles

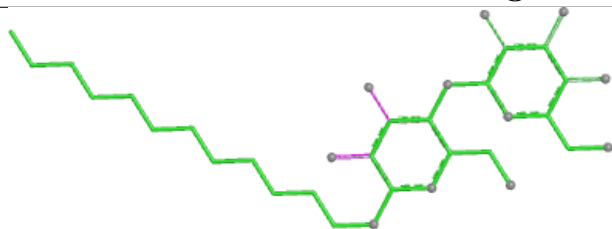


Torsions

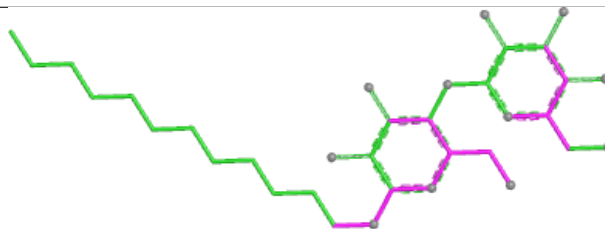


Rings

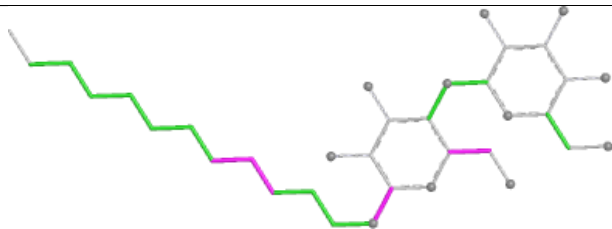
## Ligand LMT M 101



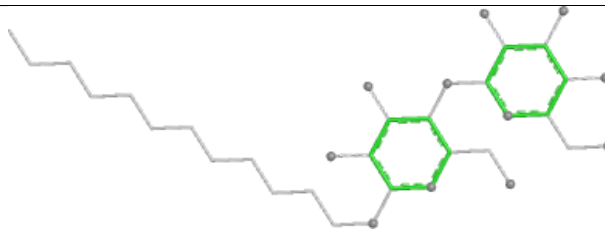
Bond lengths



Bond angles

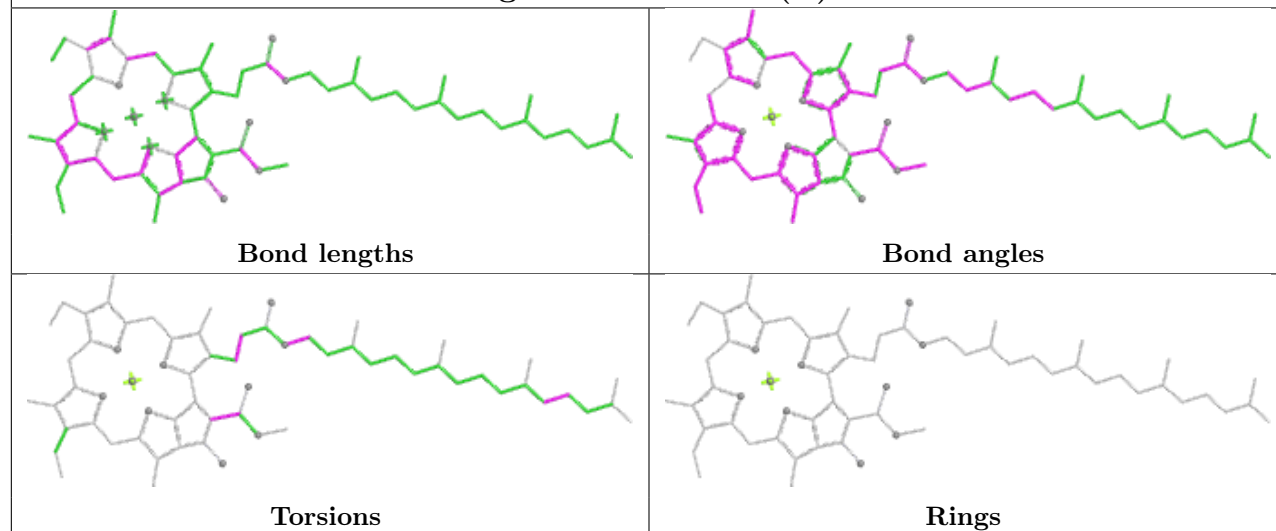


Torsions

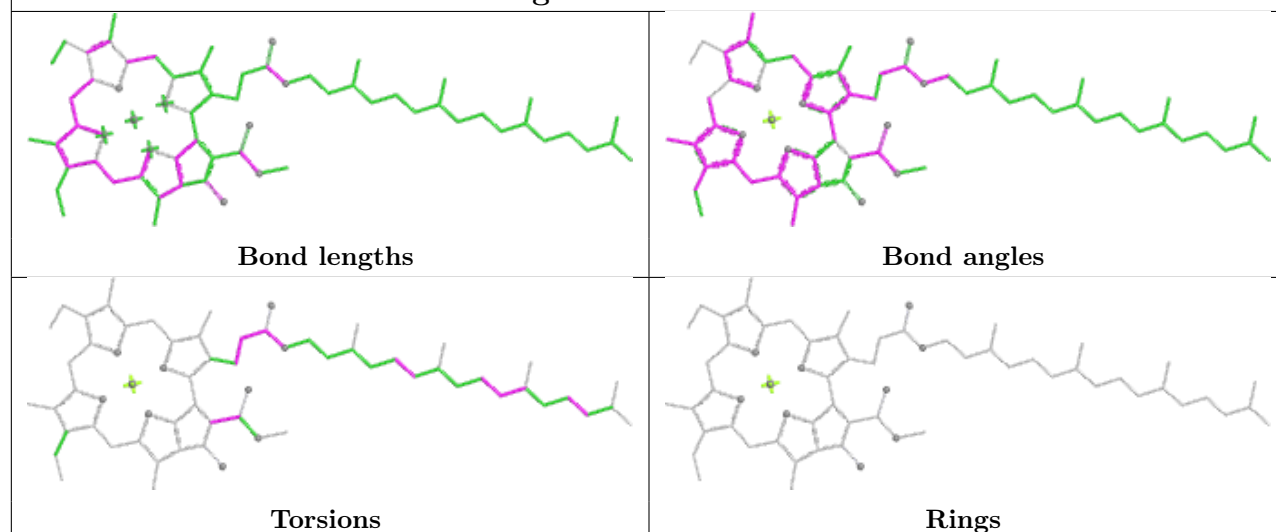


Rings

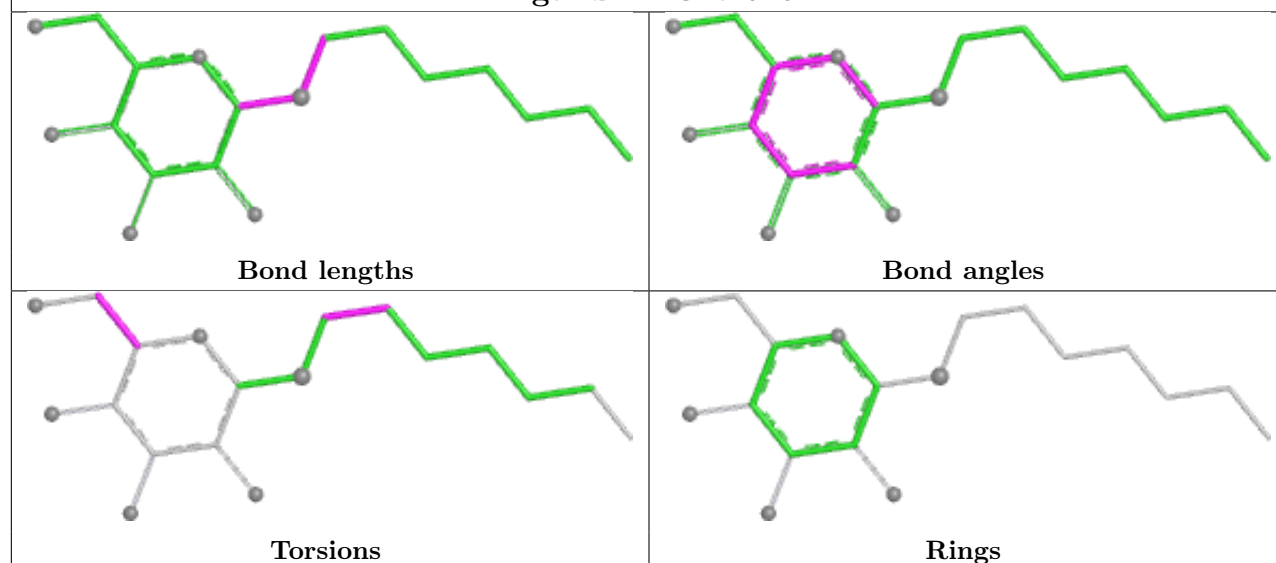
## Ligand CLA A 404 (B)

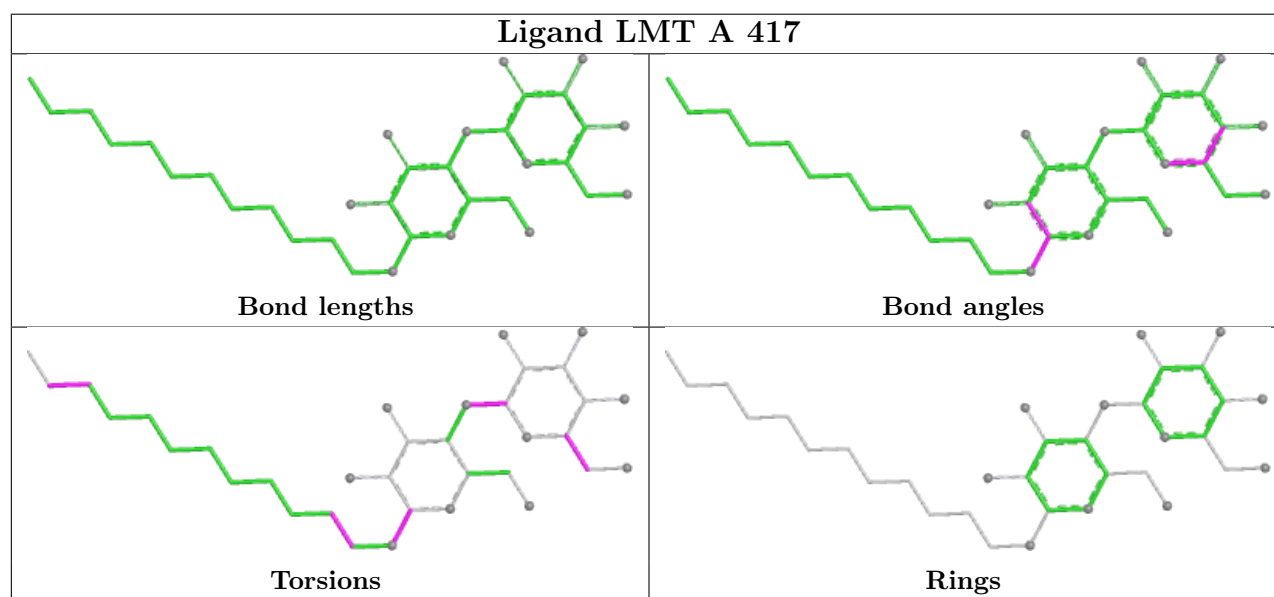
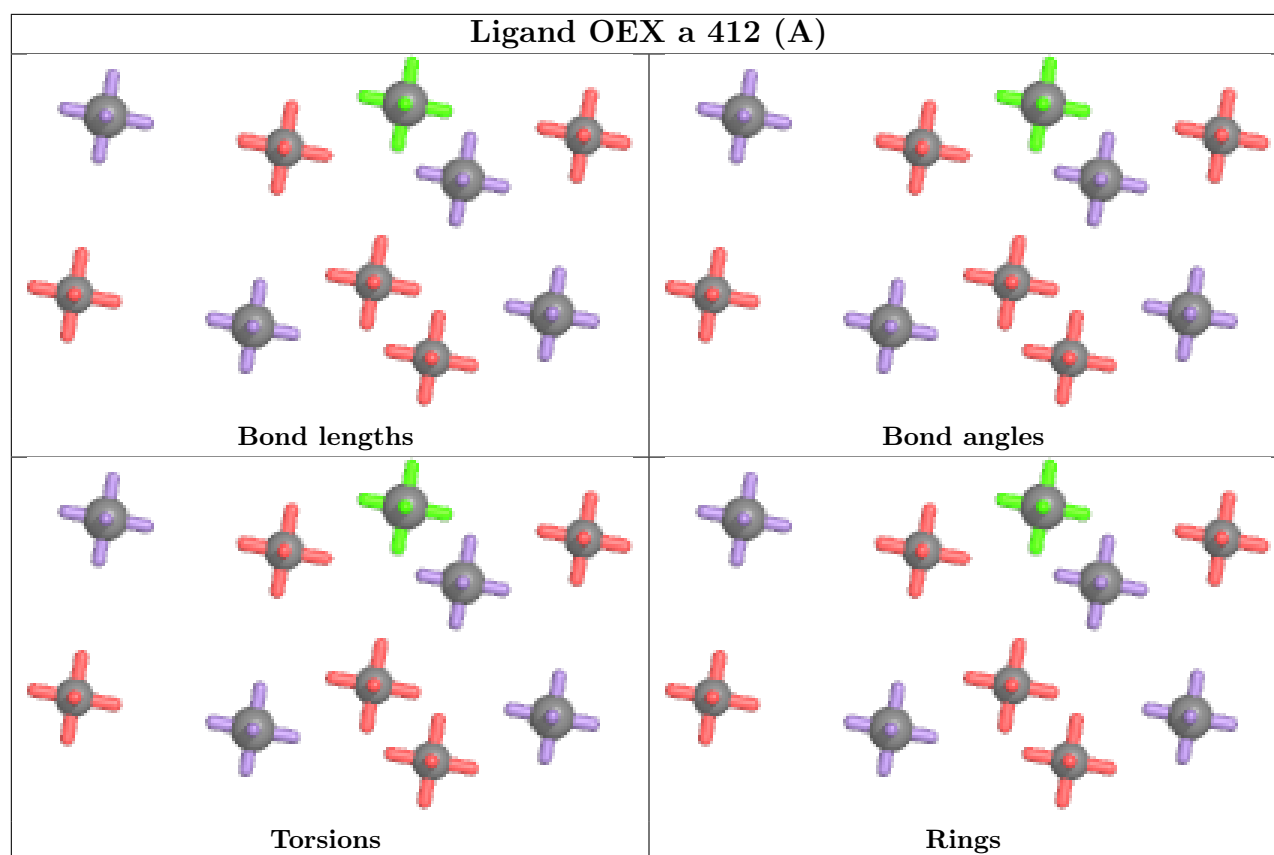


## Ligand CLA B 601

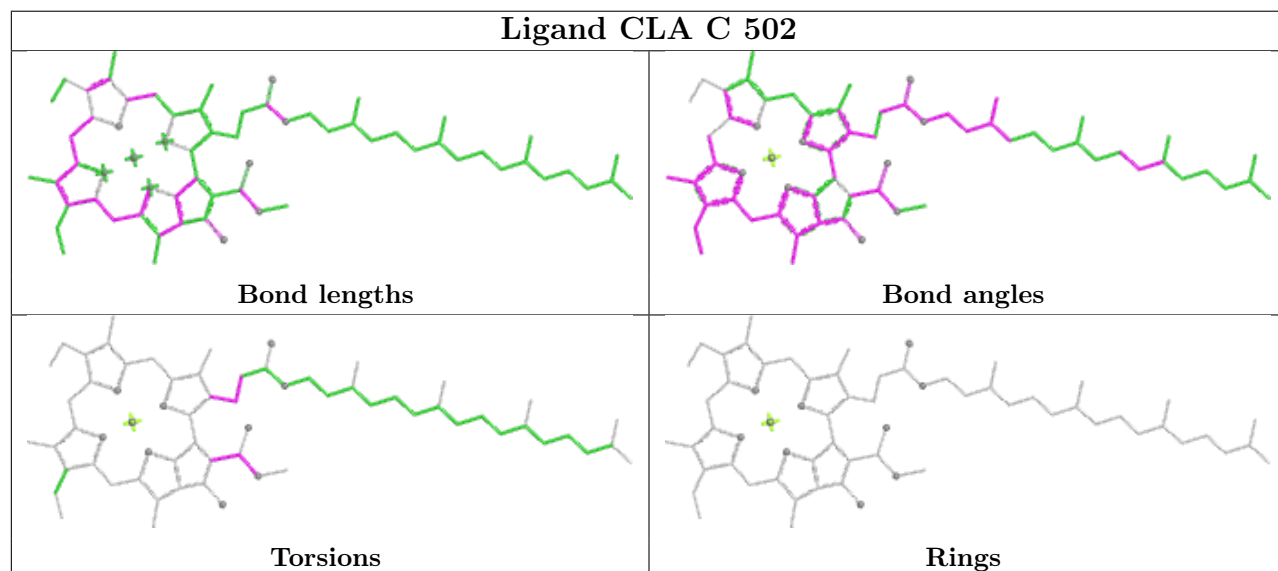
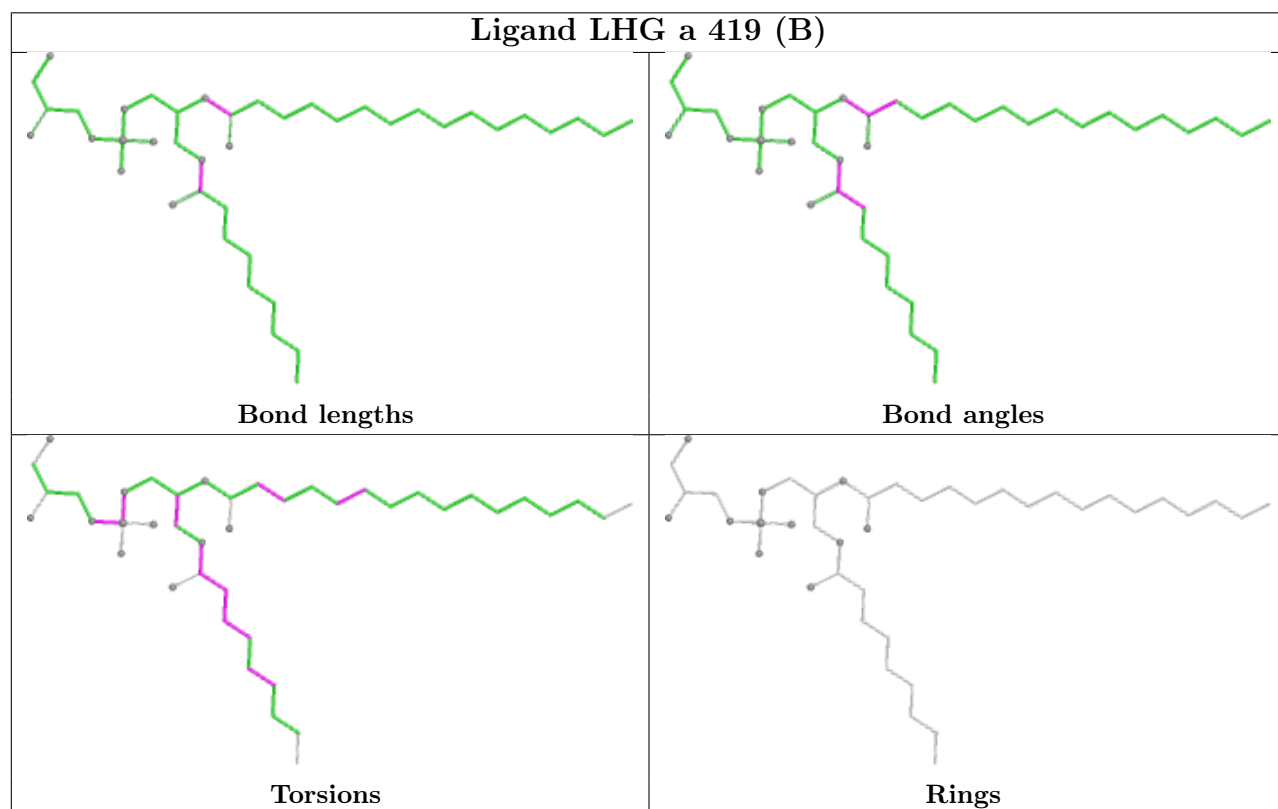
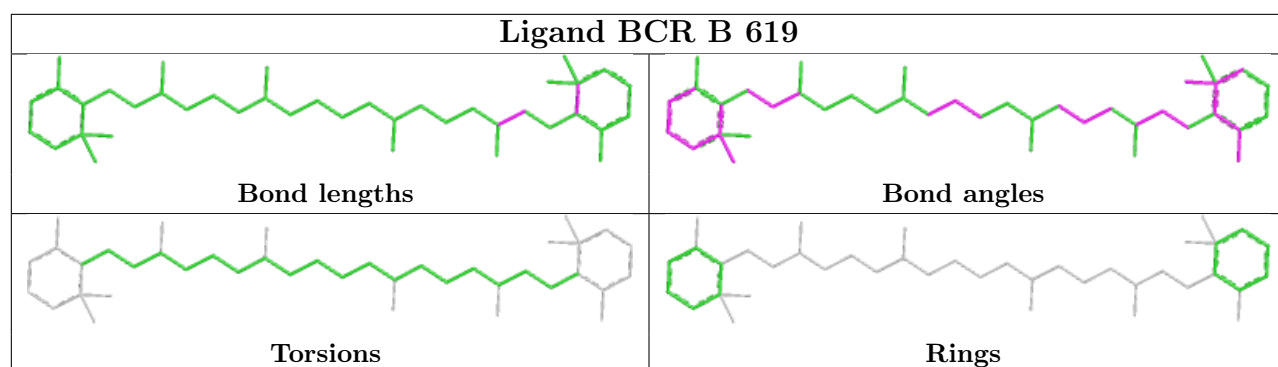


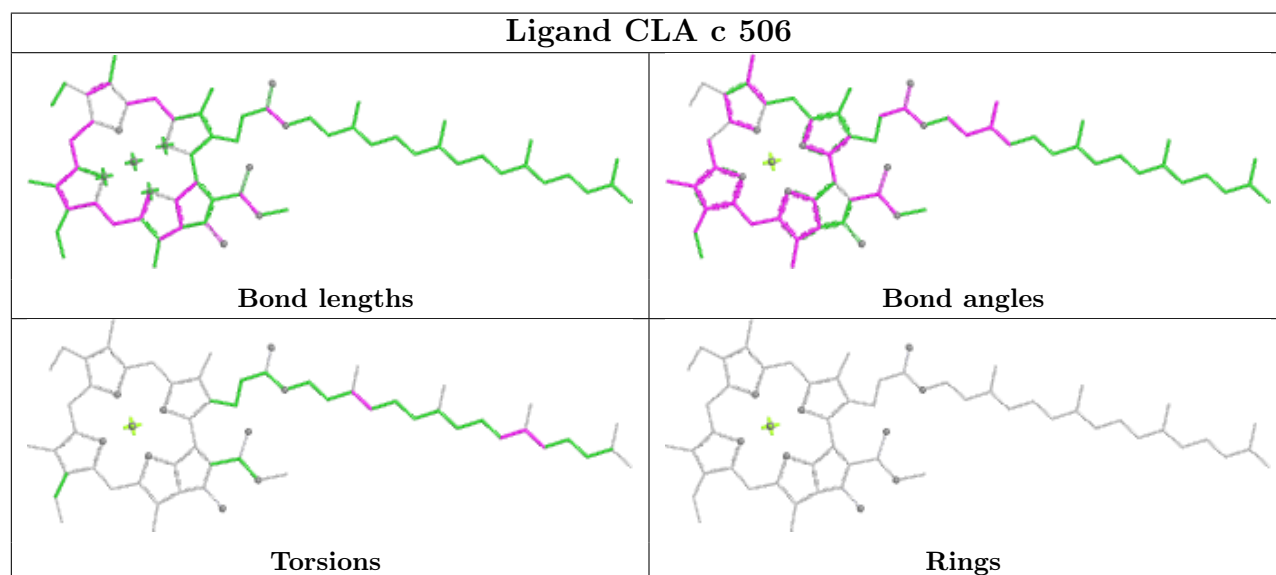
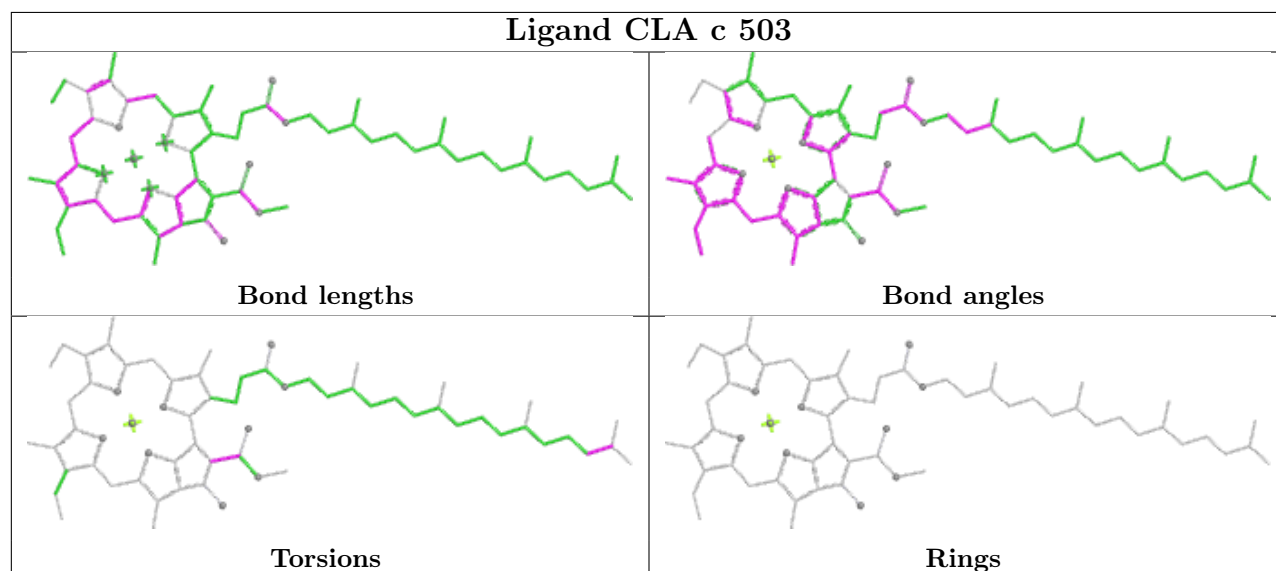
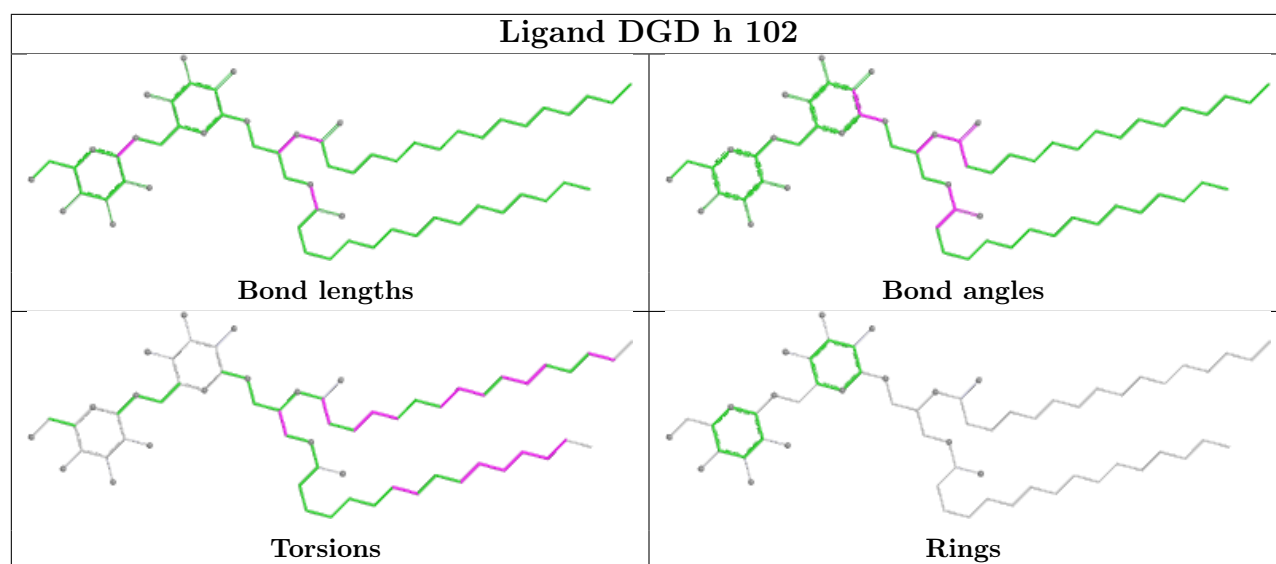
## Ligand HTG b 625



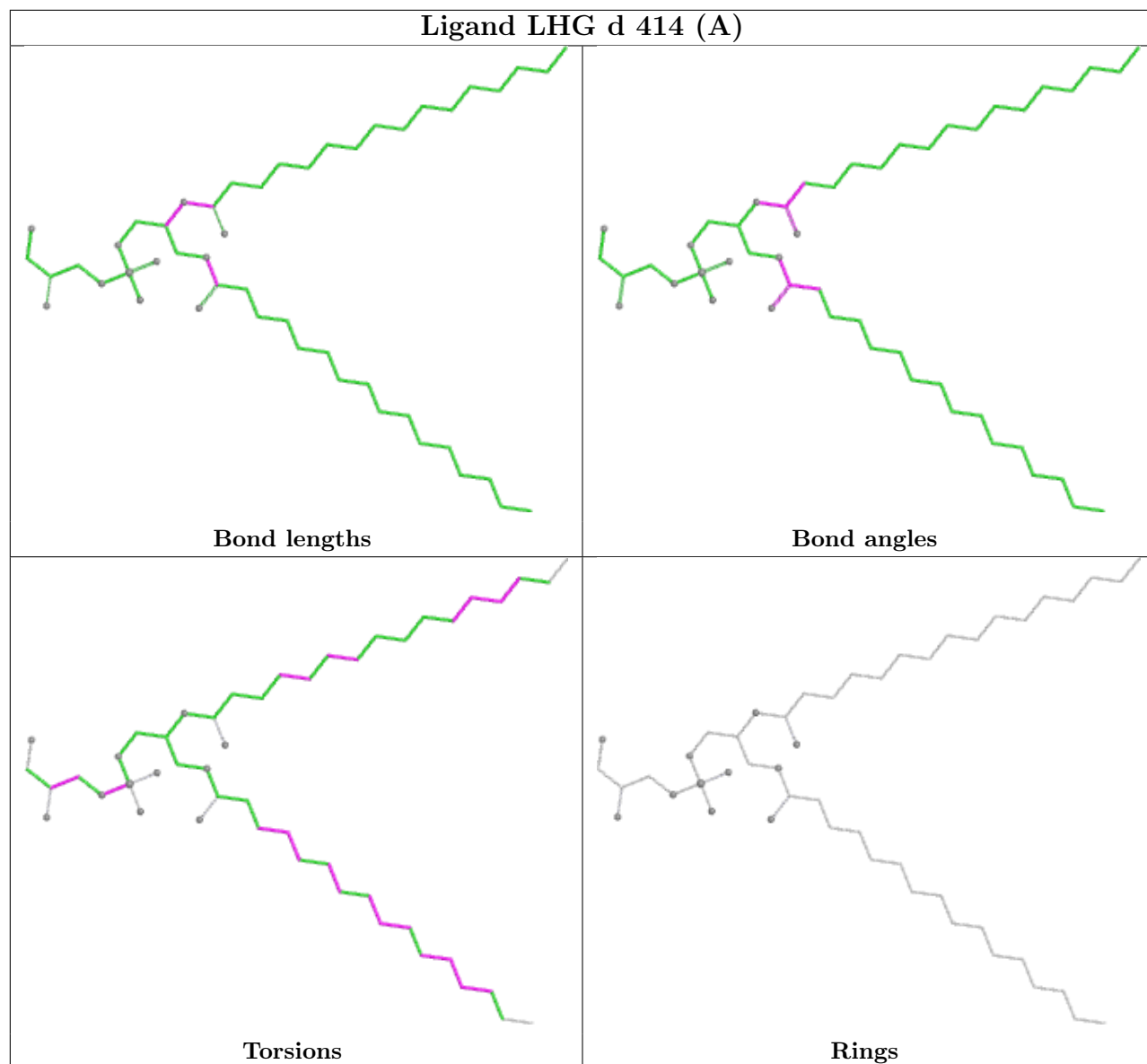




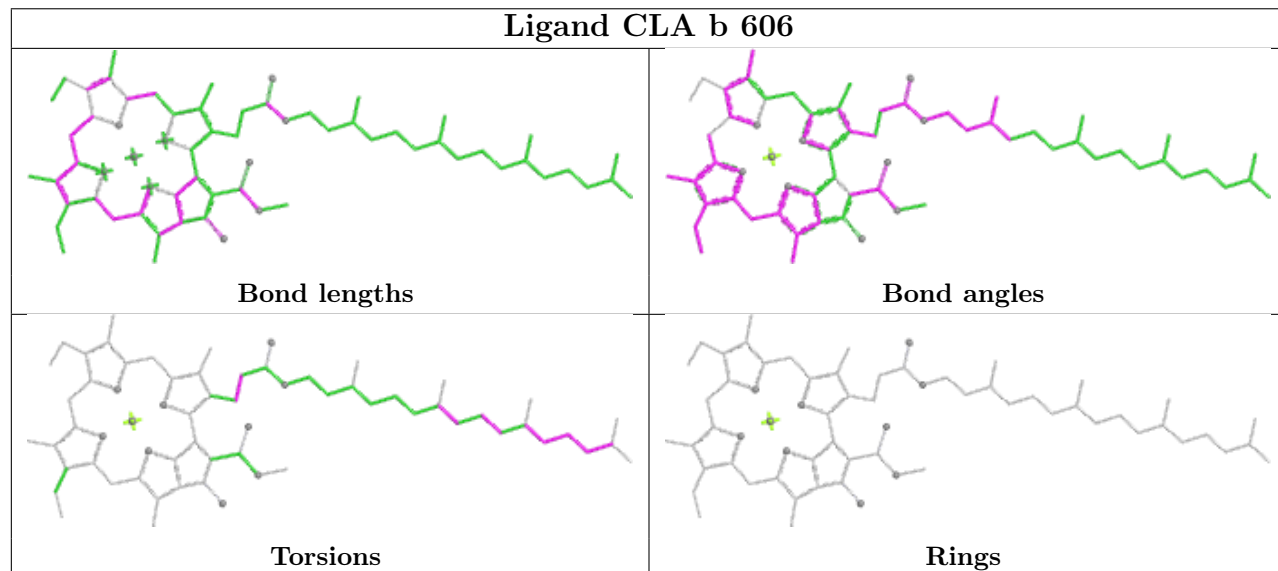


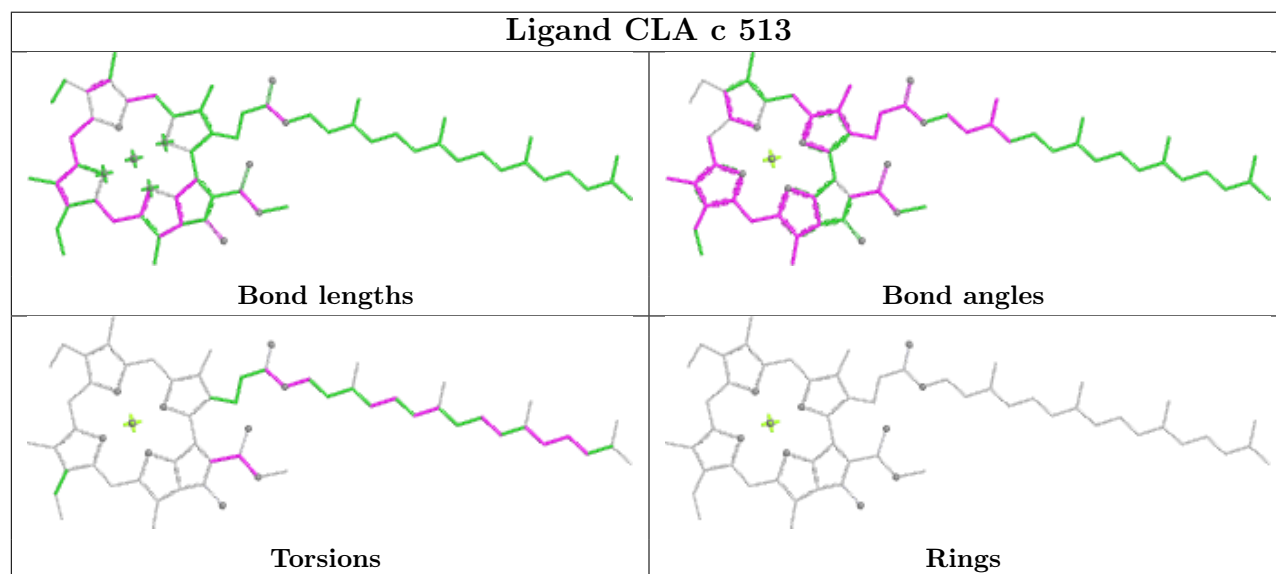
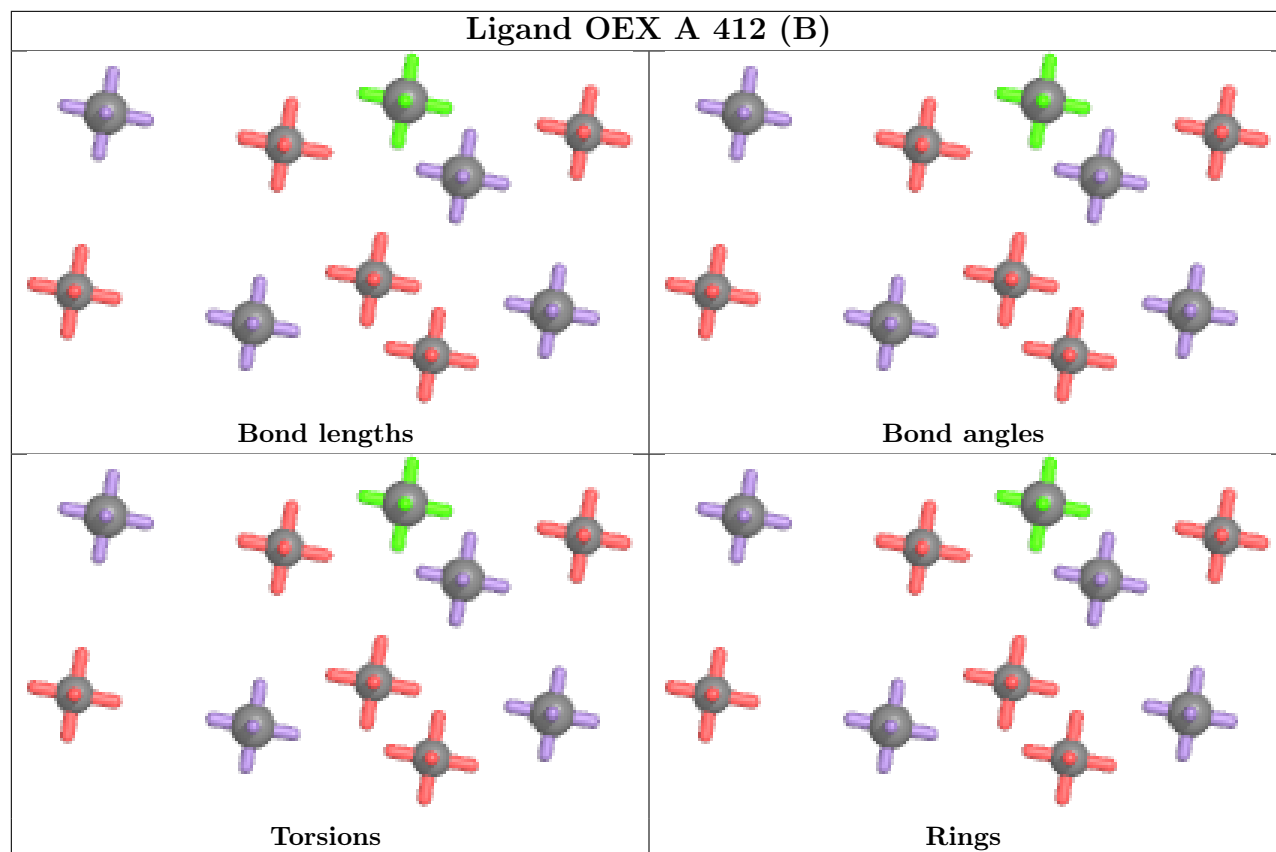


## Ligand LHG d 414 (A)

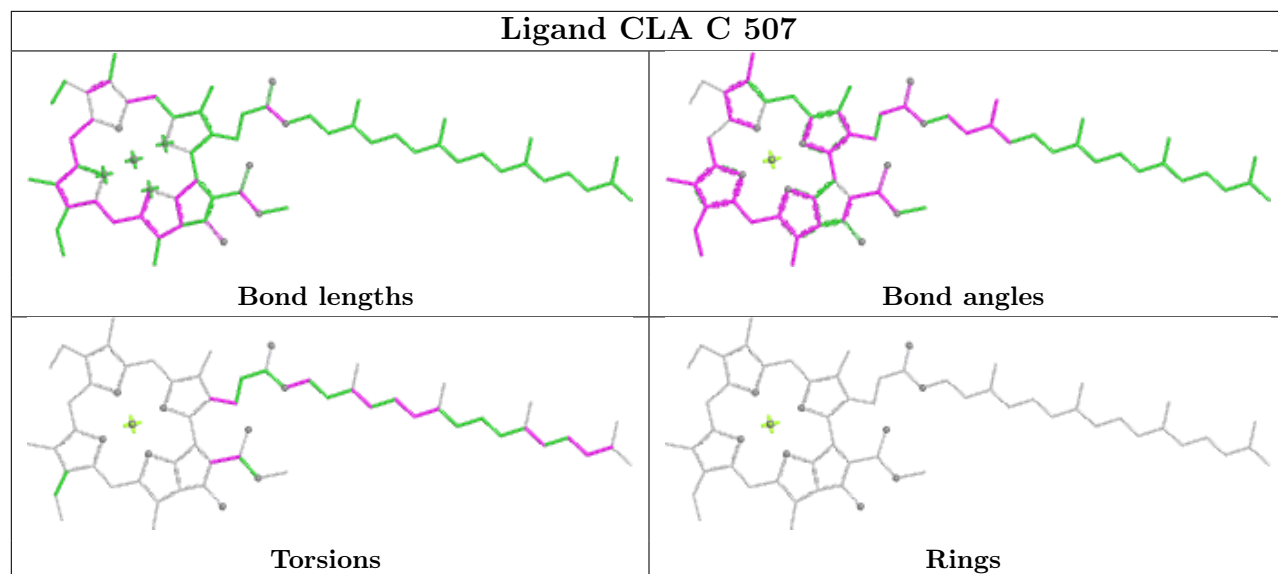


## Ligand CLA b 606

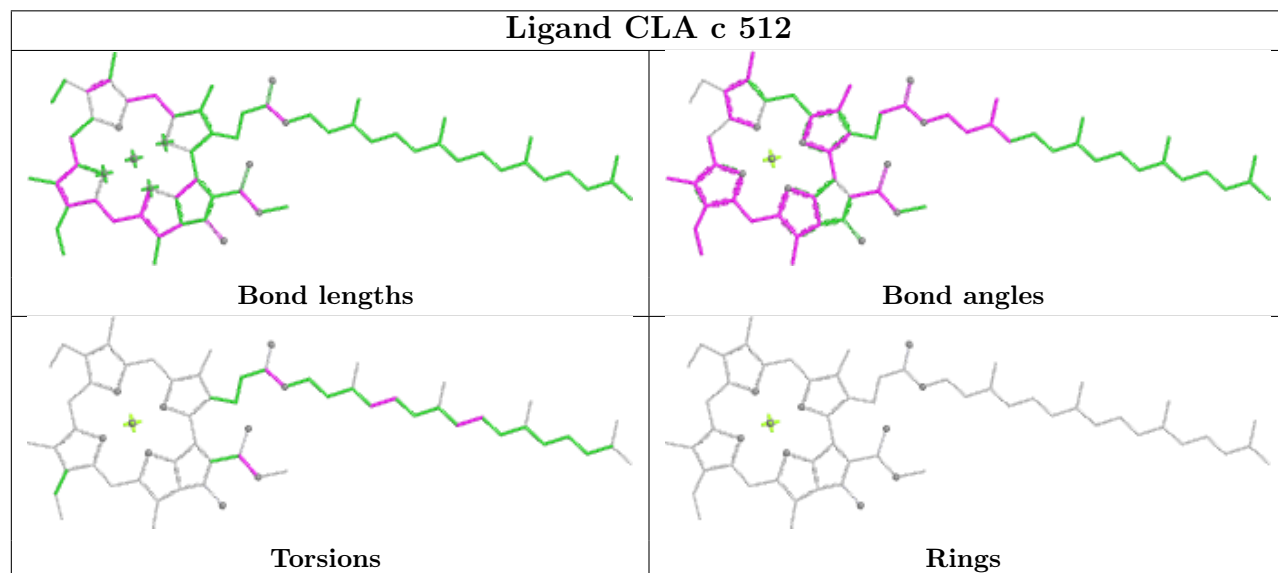




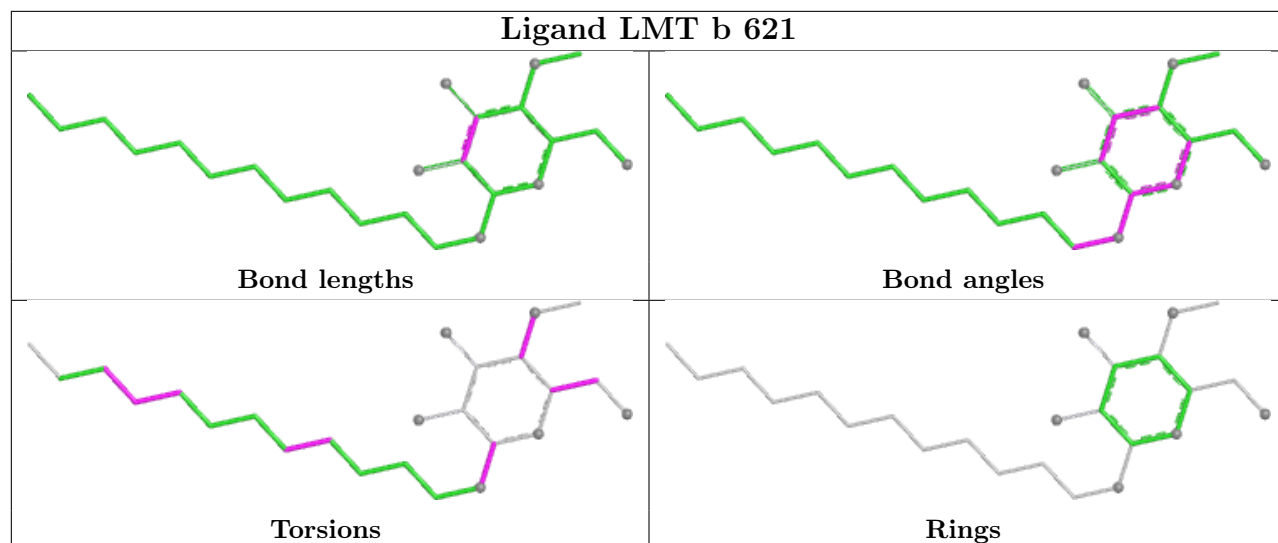
## Ligand CLA C 507

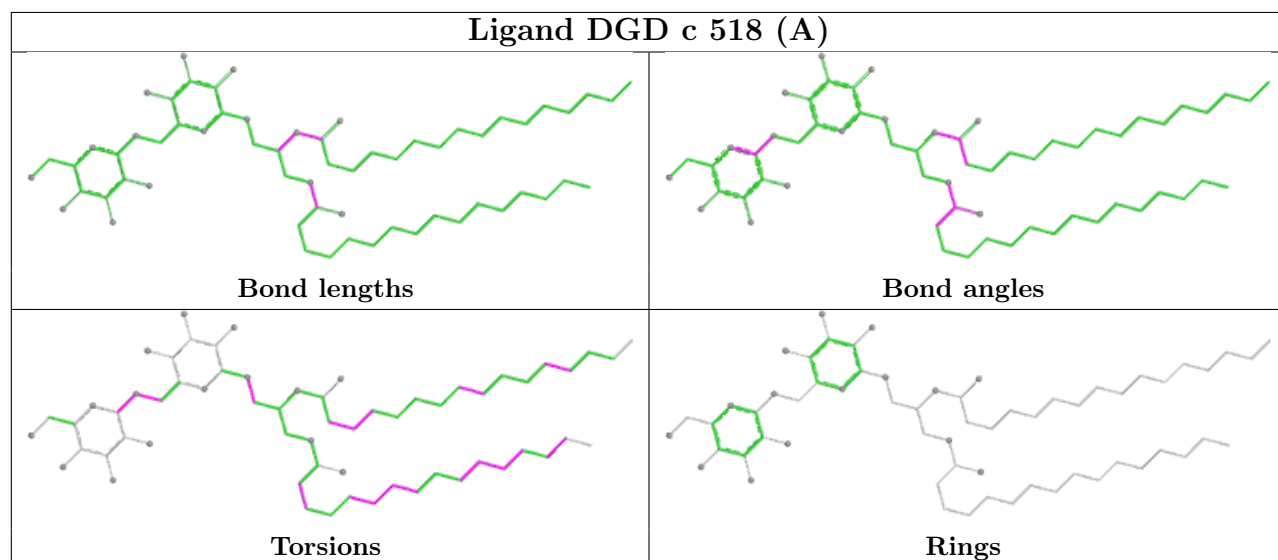
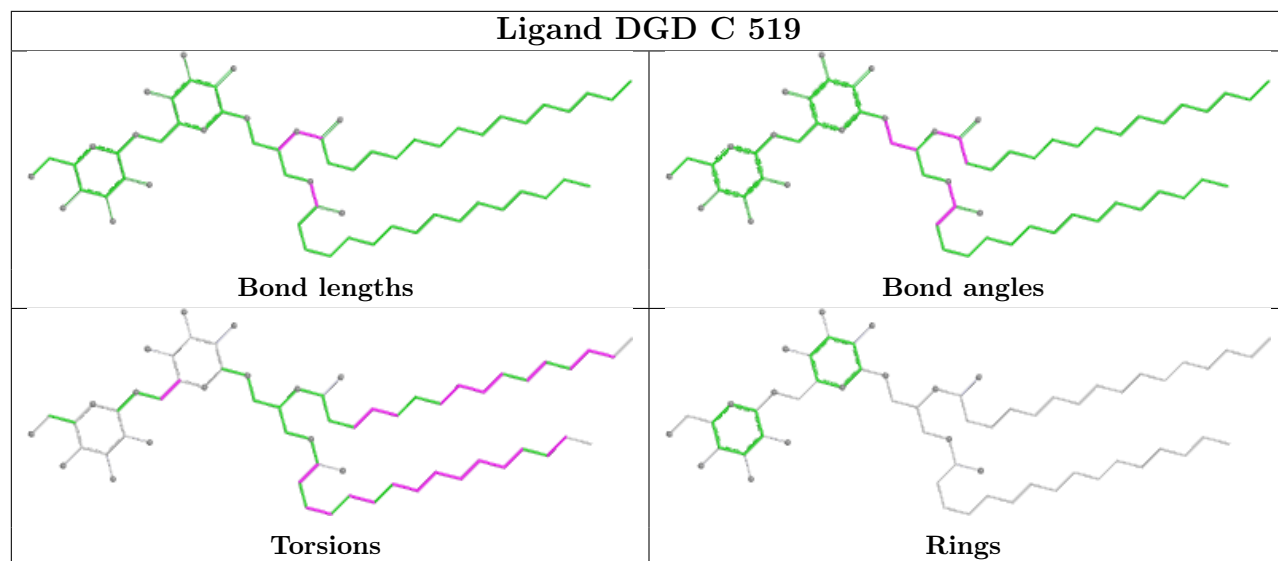


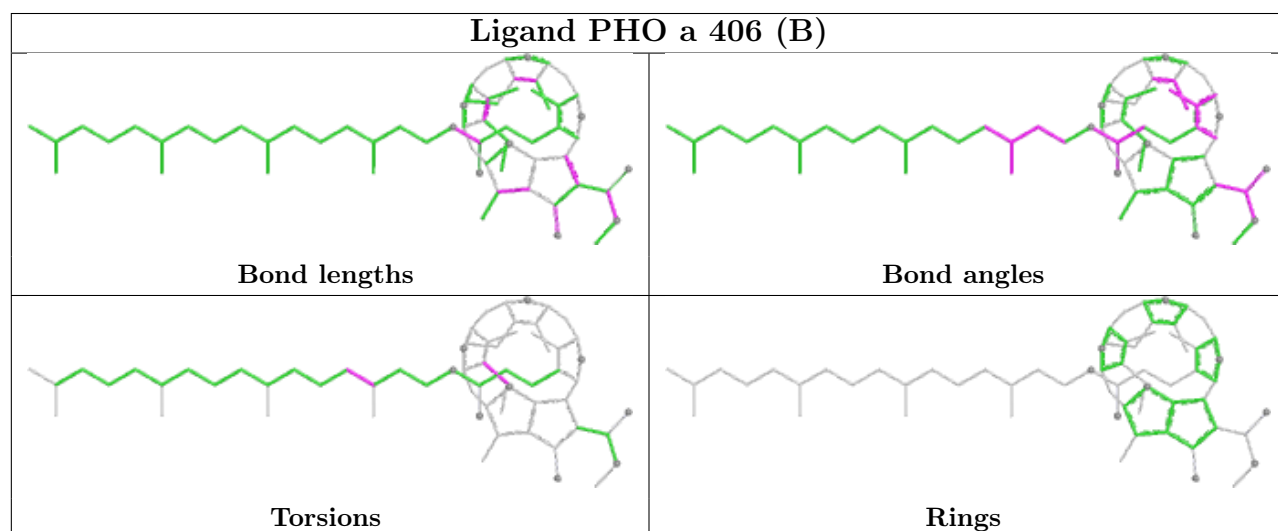
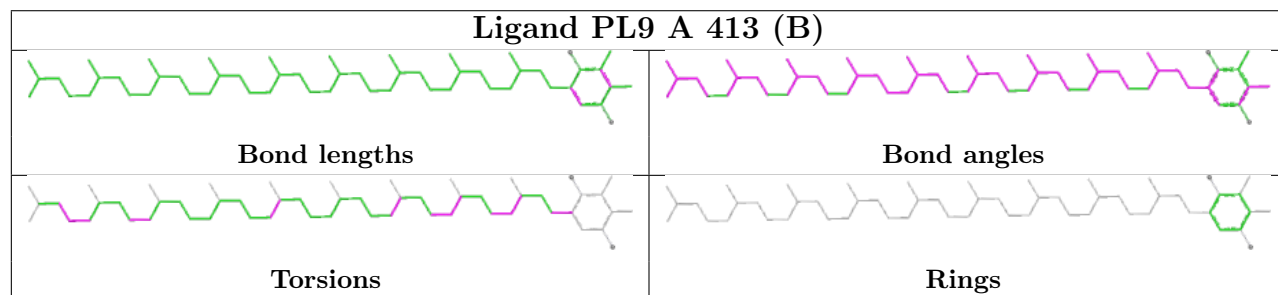
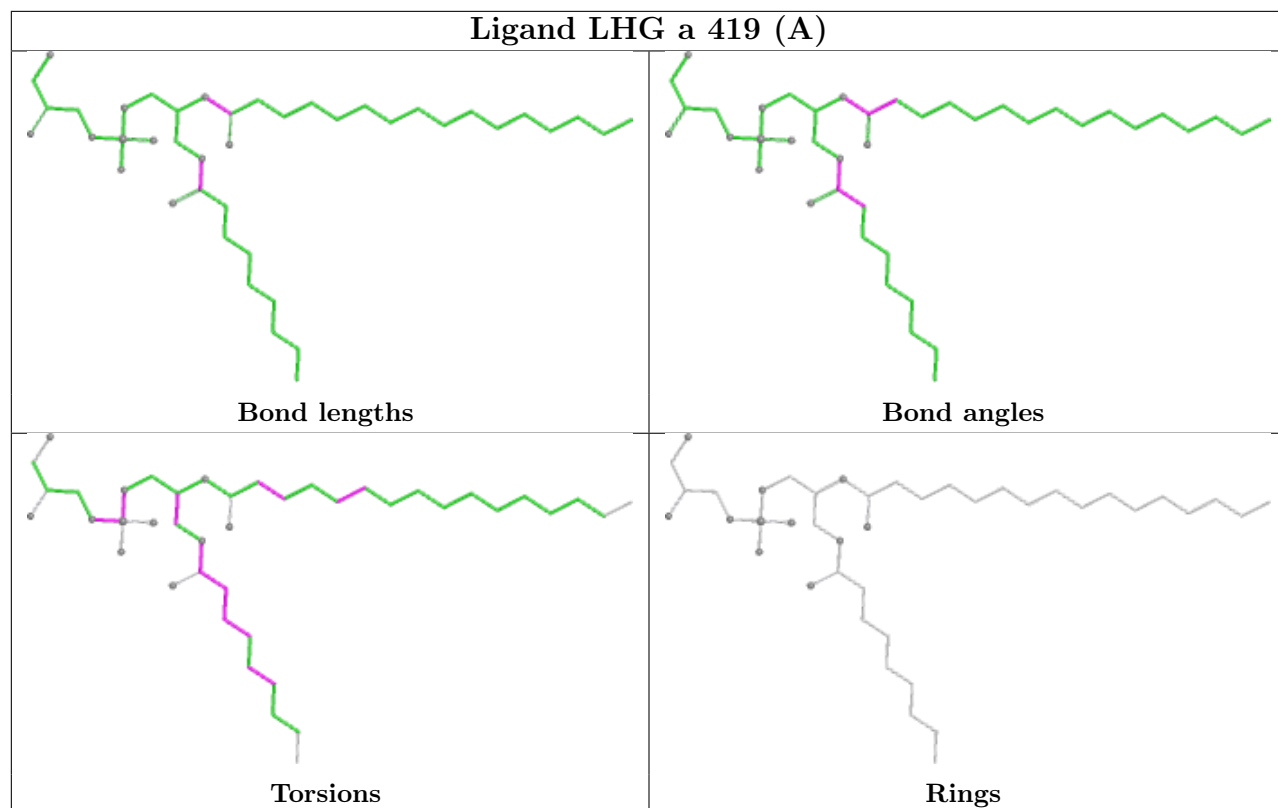
## Ligand CLA c 512



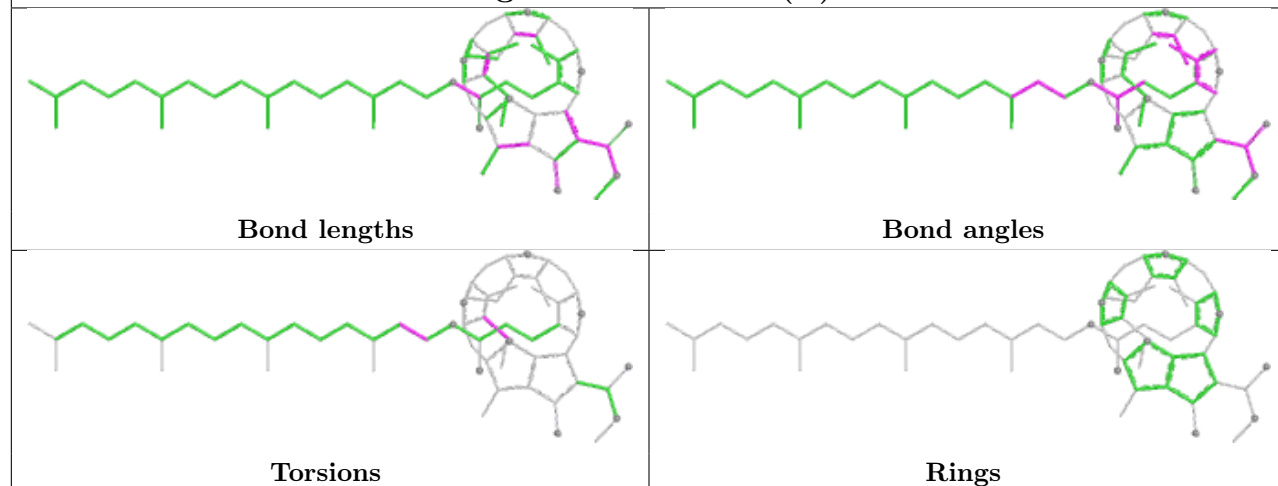
## Ligand LMT b 621



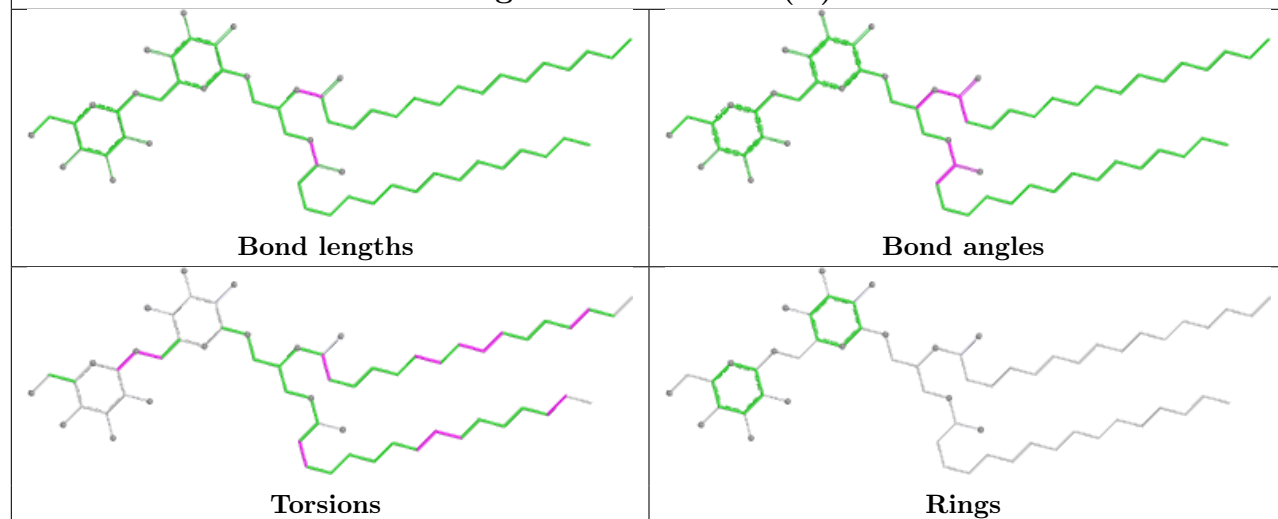




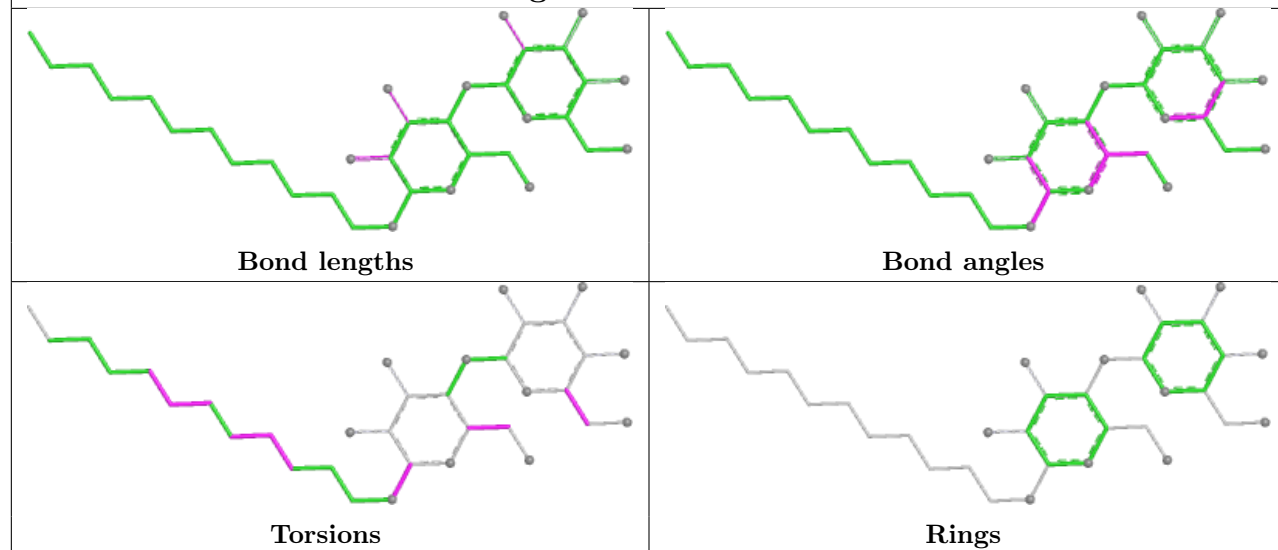
## Ligand PHO D 401 (B)



## Ligand DGD C 518 (B)

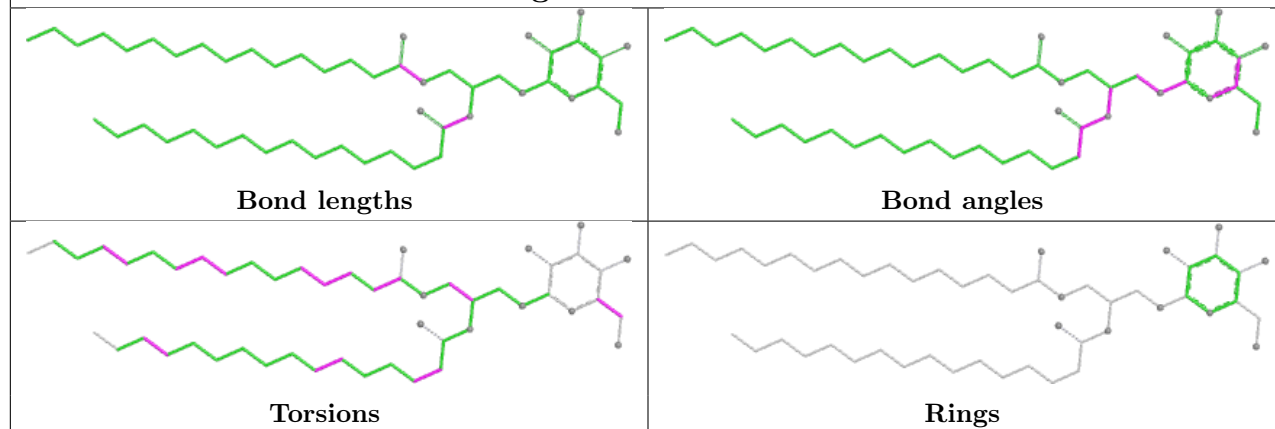


## Ligand LMT B 627

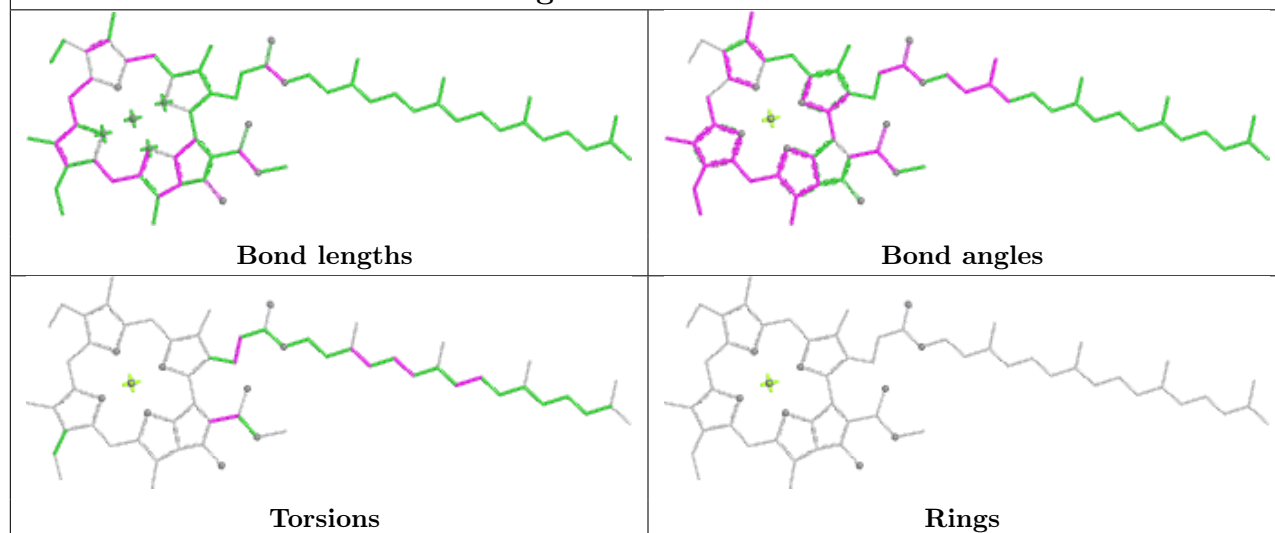




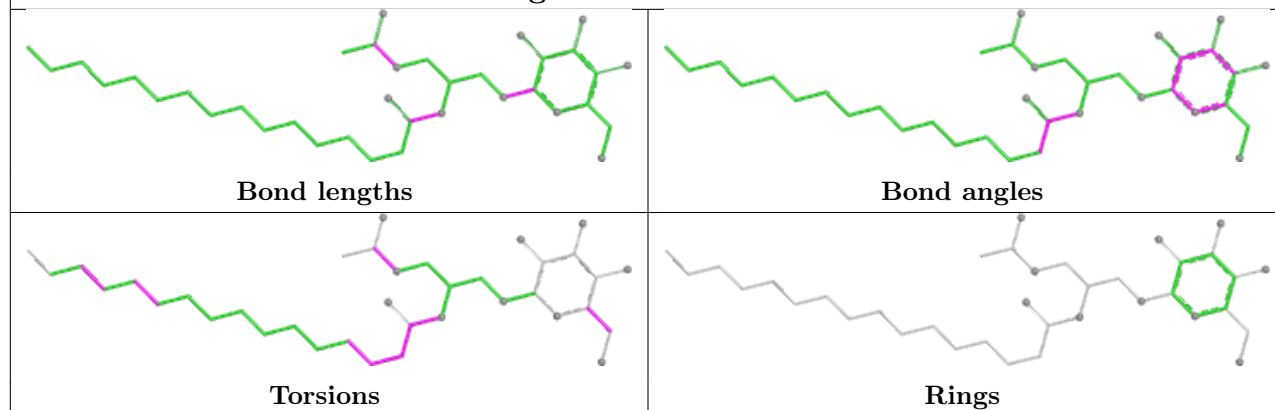
## Ligand LMG c 501

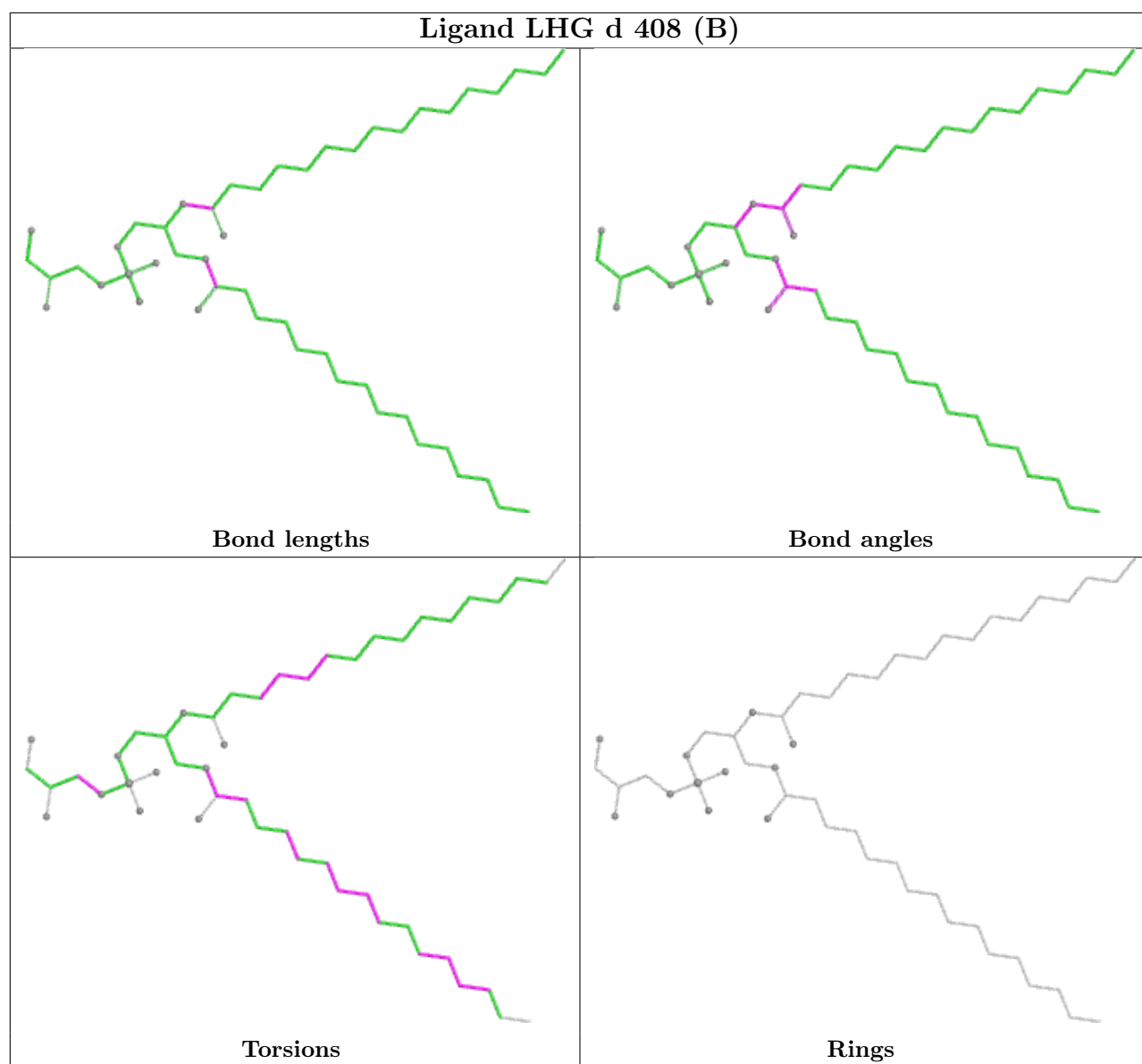


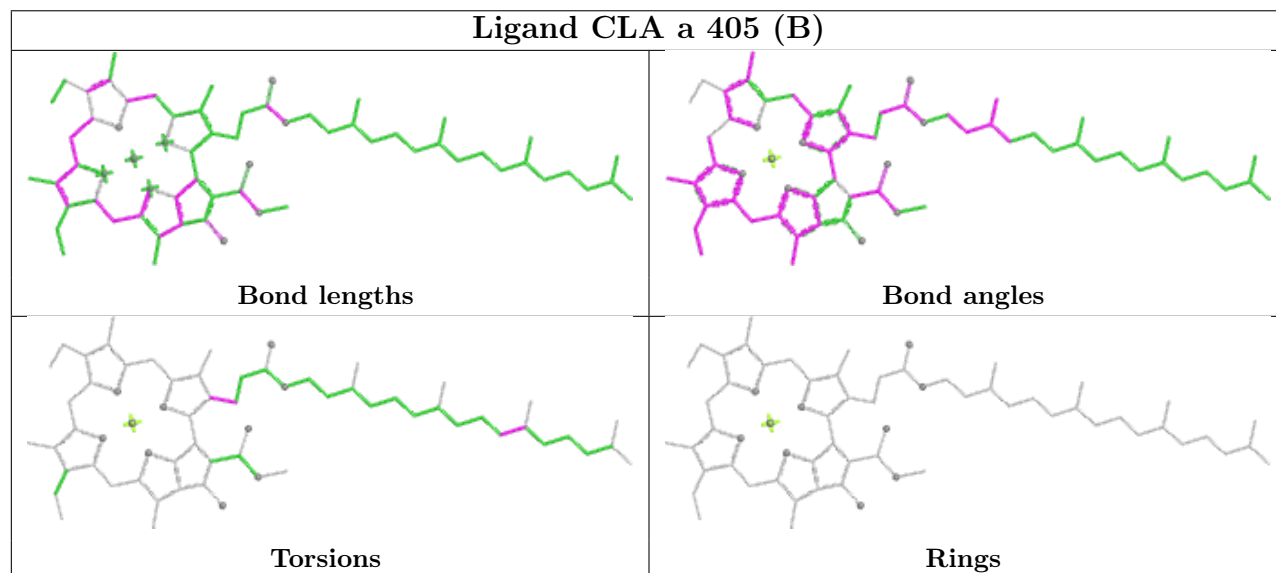
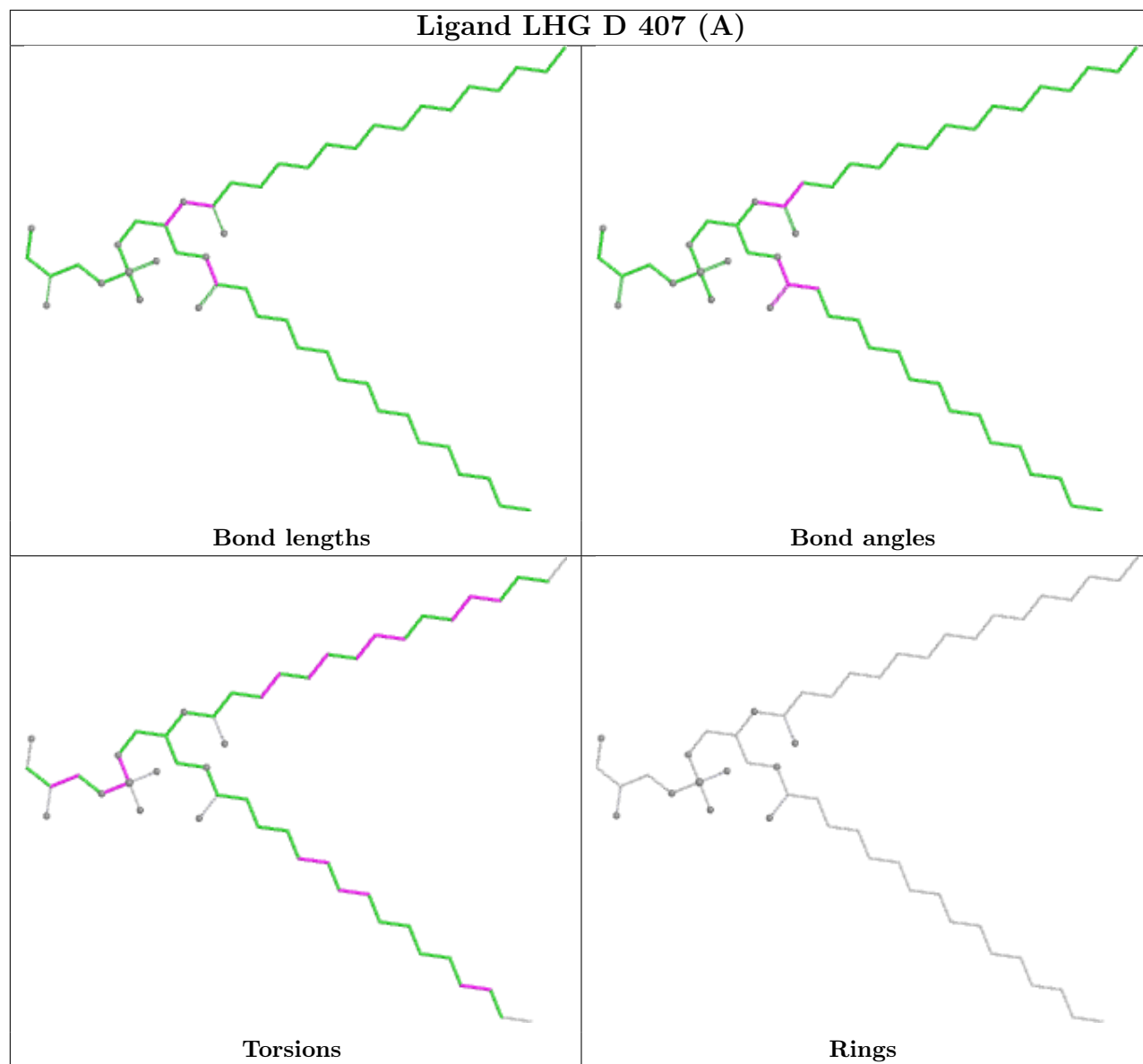
## Ligand CLA c 508

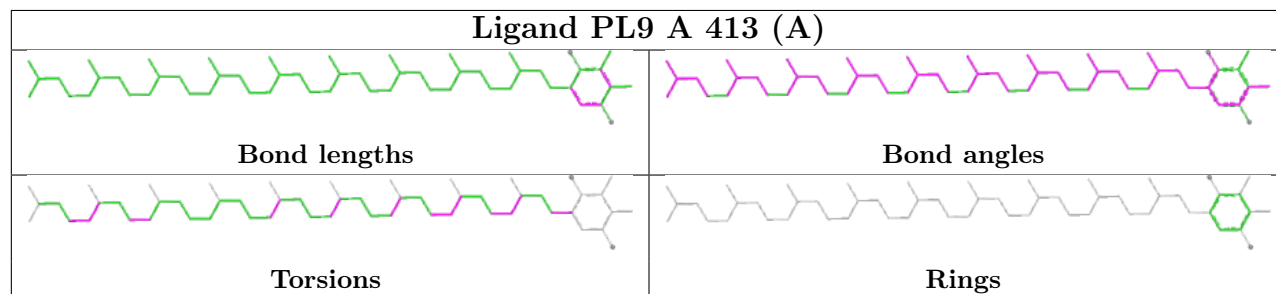
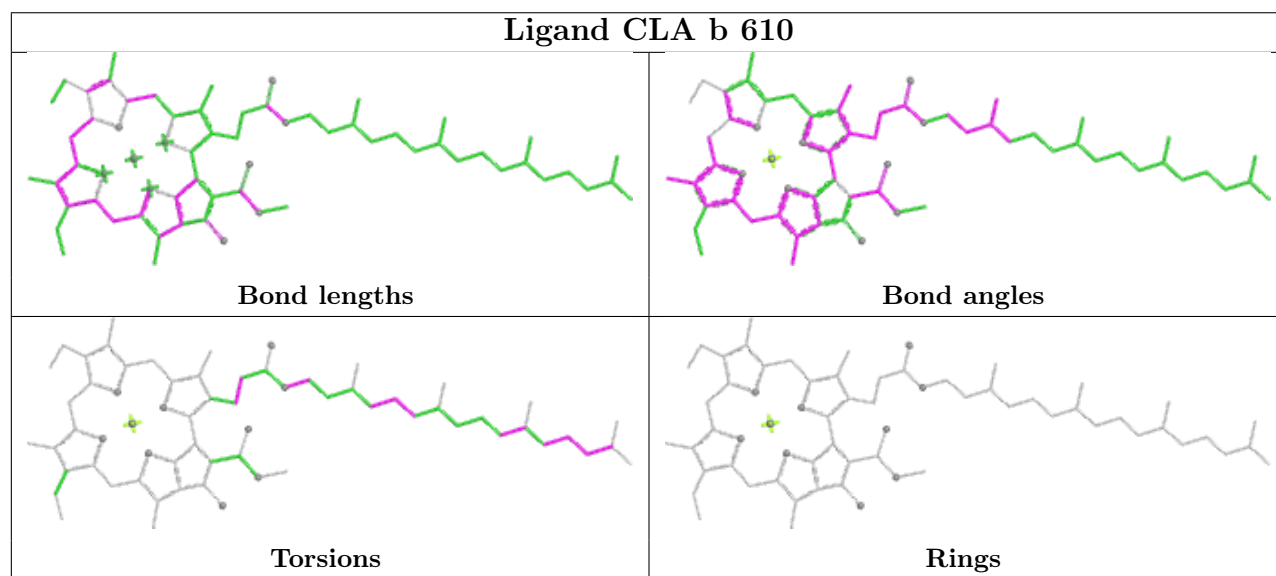
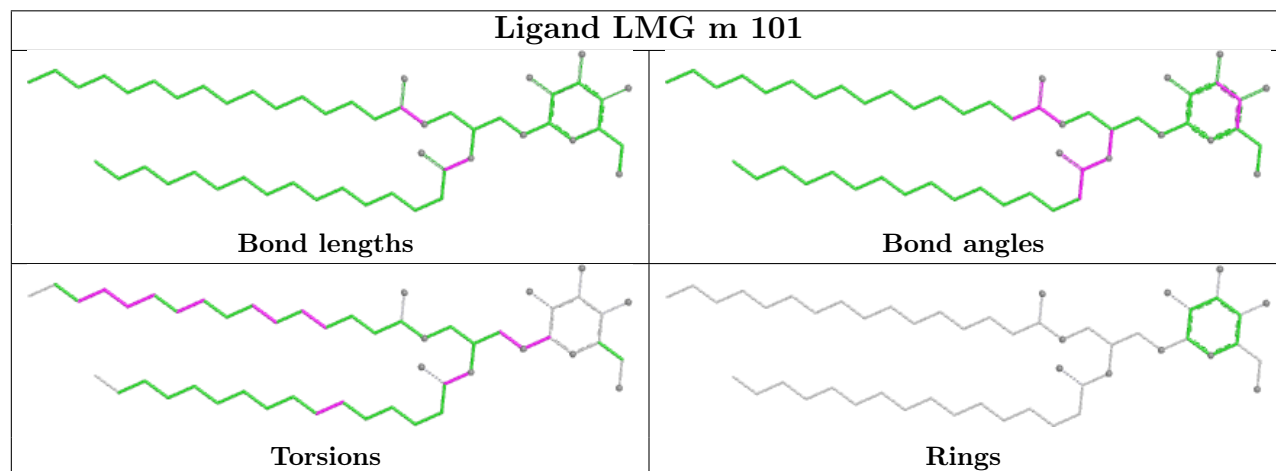
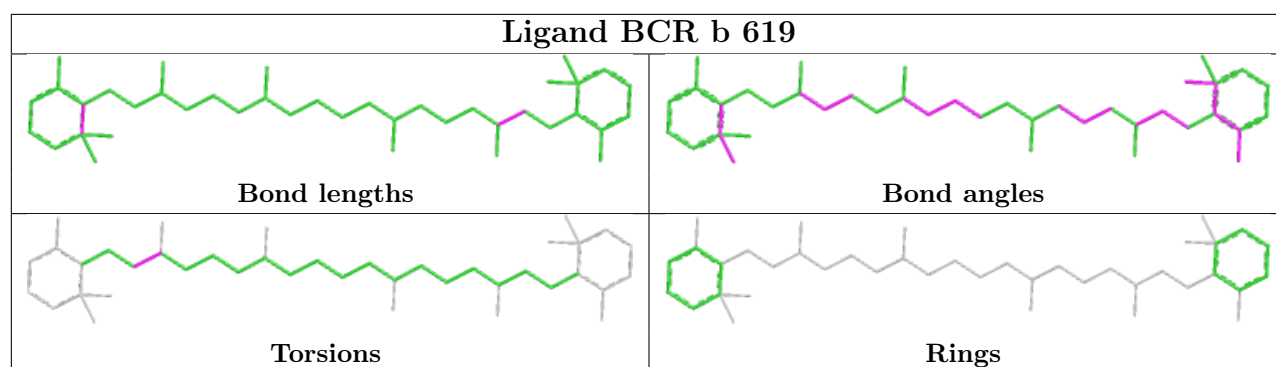


## Ligand LMG Z 101

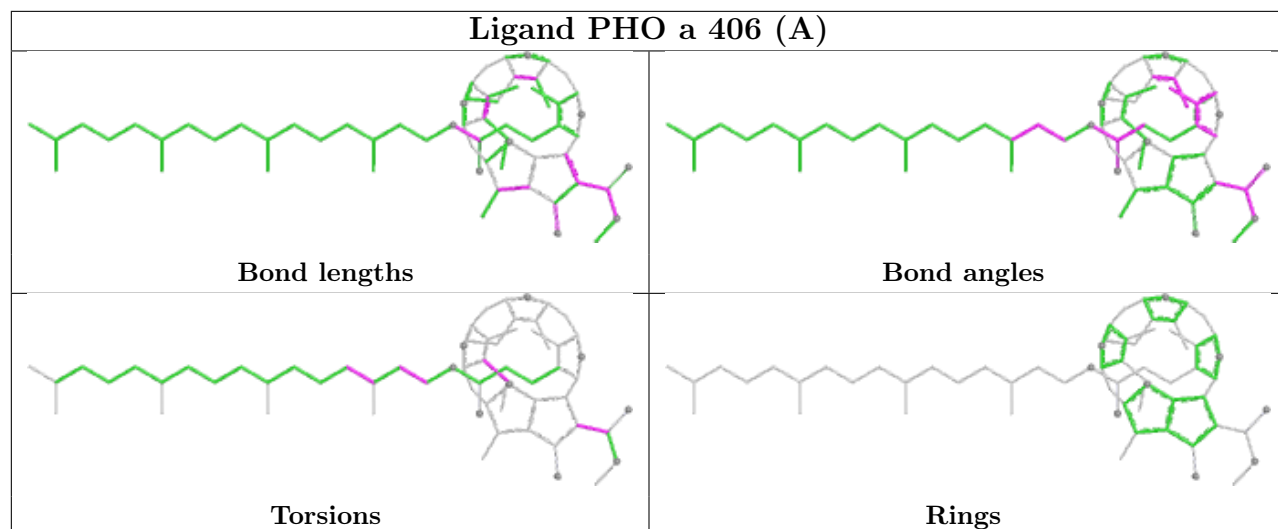




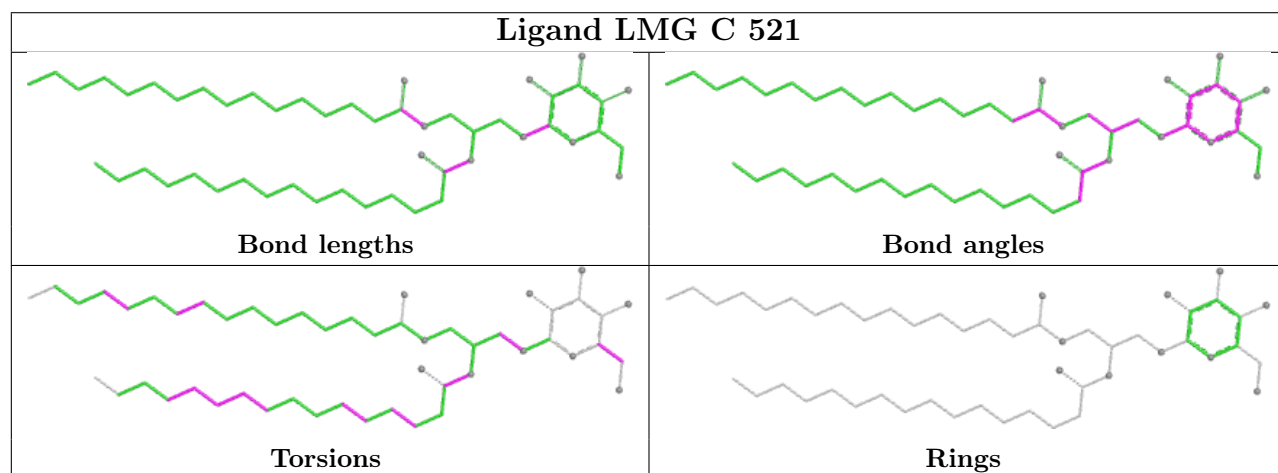




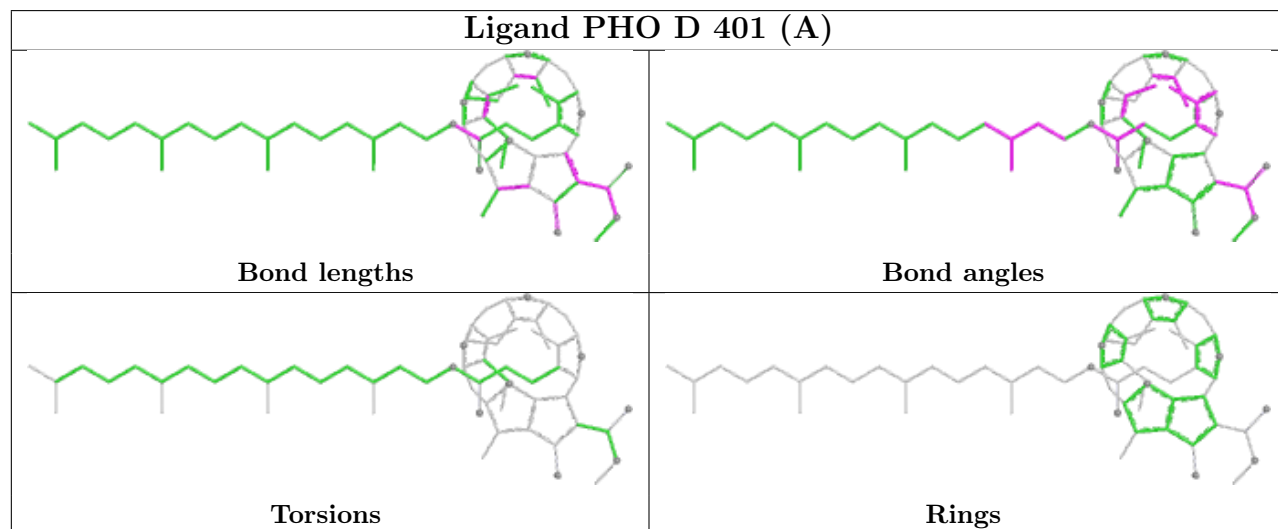
## Ligand PHO a 406 (A)

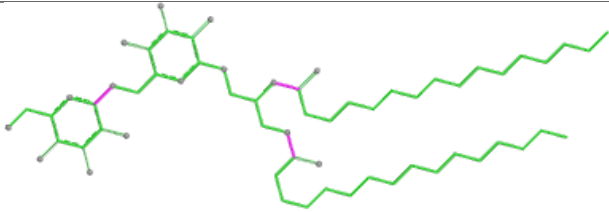
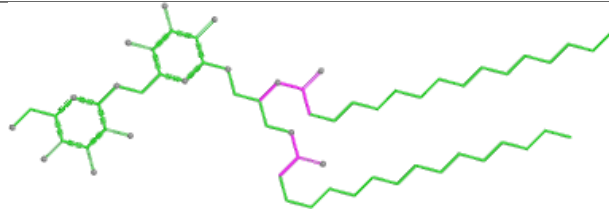
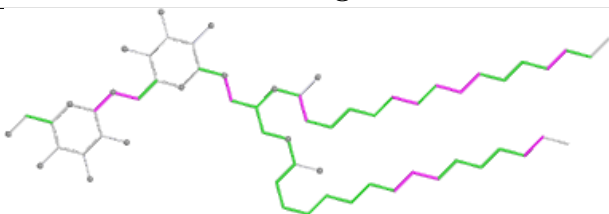
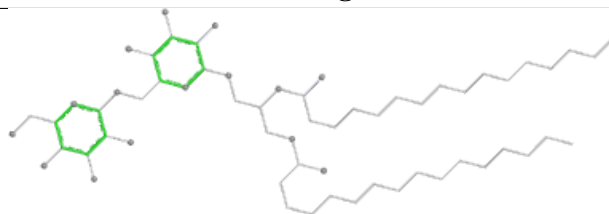


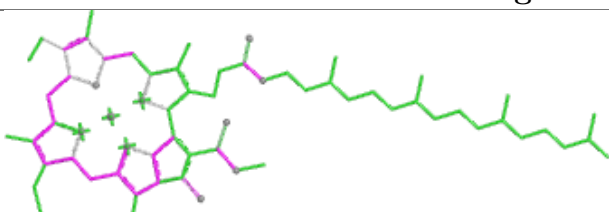
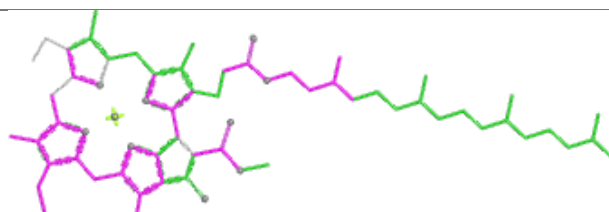
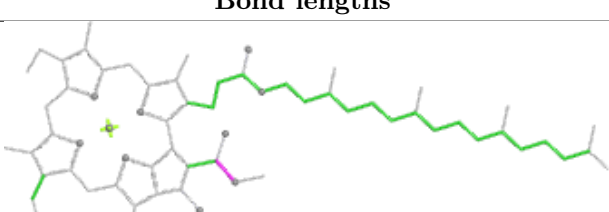
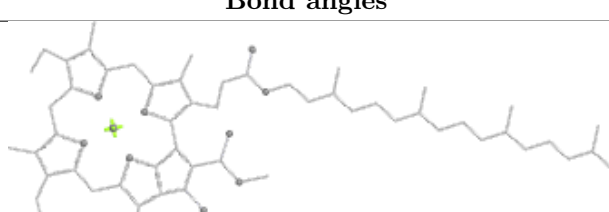
## Ligand LMG C 521

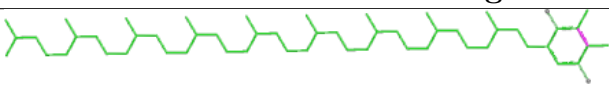
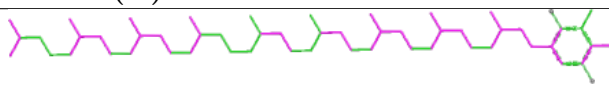
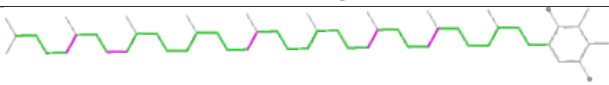
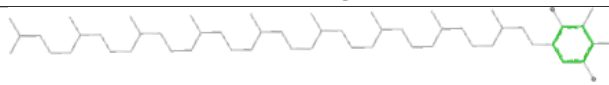


## Ligand PHO D 401 (A)

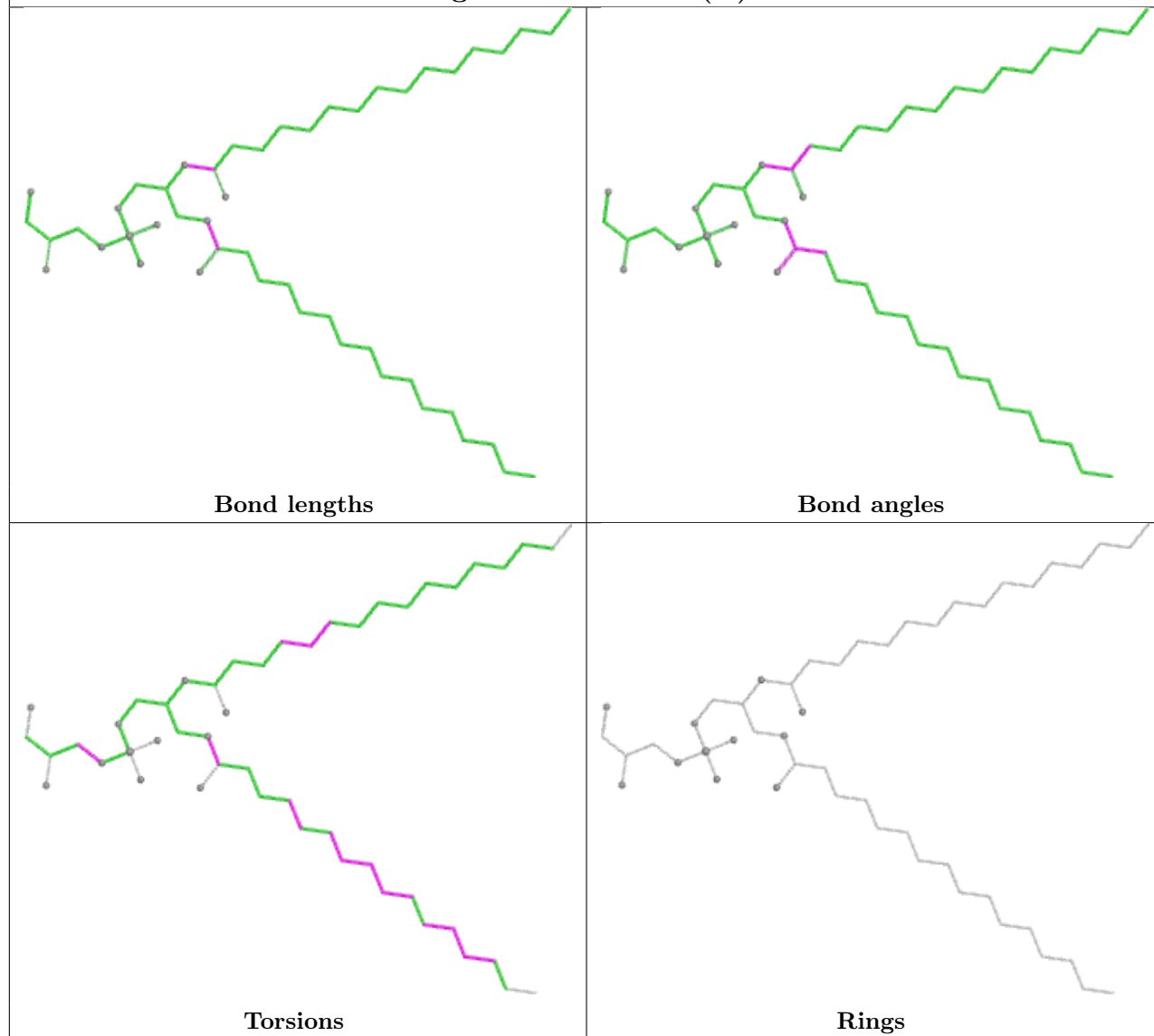


| Ligand DGD C 518 (A)                                                              |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

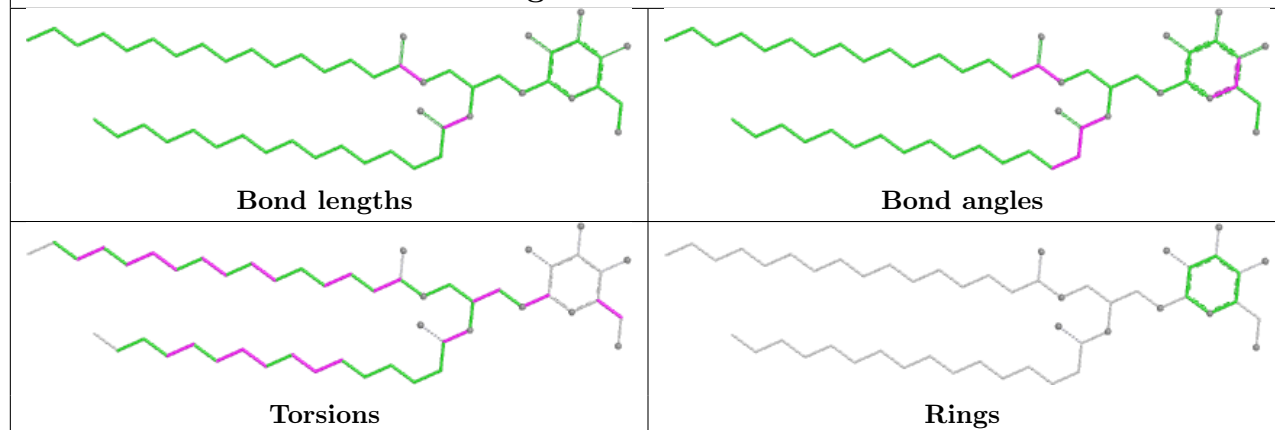
| Ligand CLA c 502                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

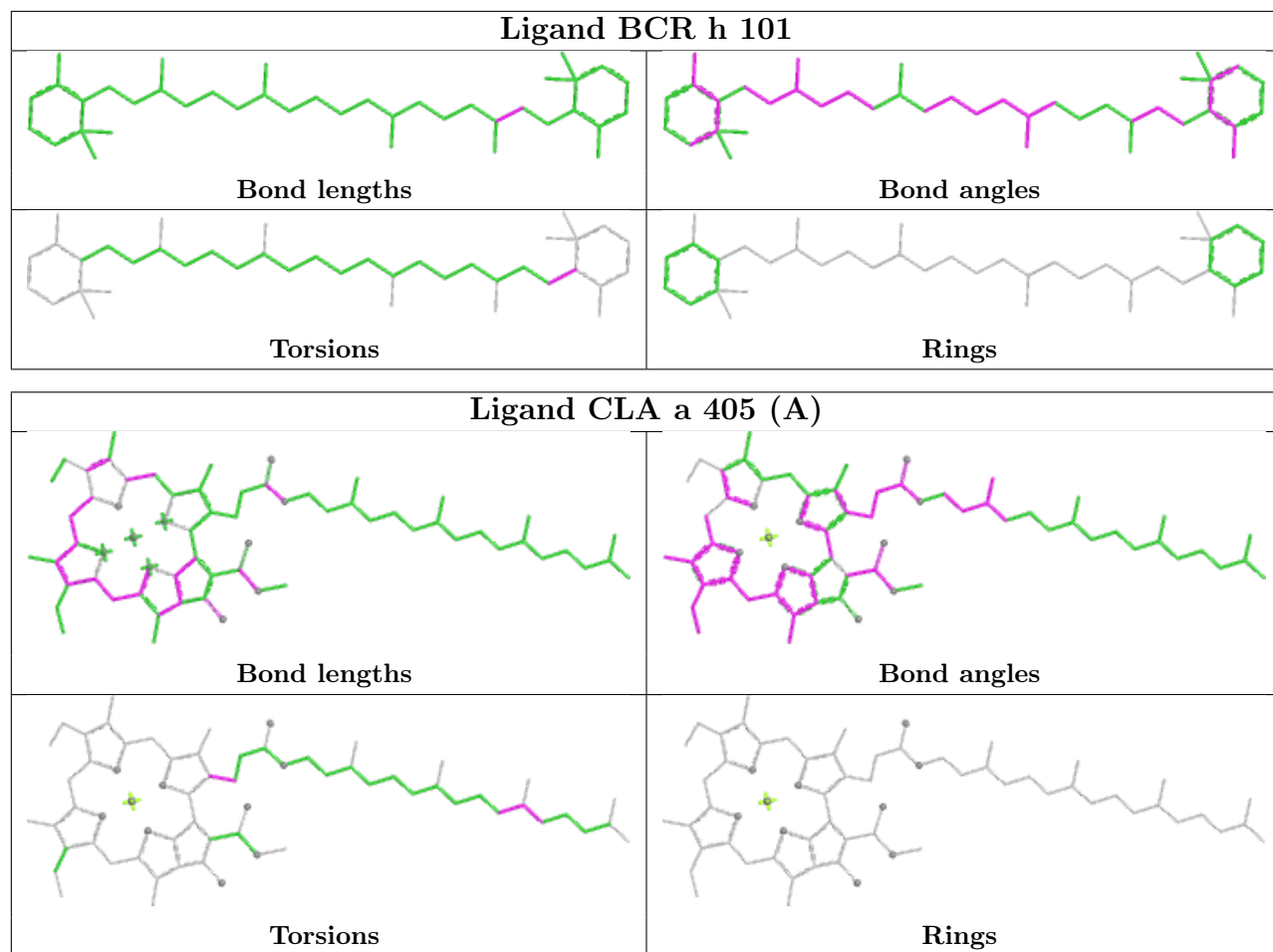
| Ligand PL9 d 406 (B)                                                                |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

## Ligand LHG d 408 (A)



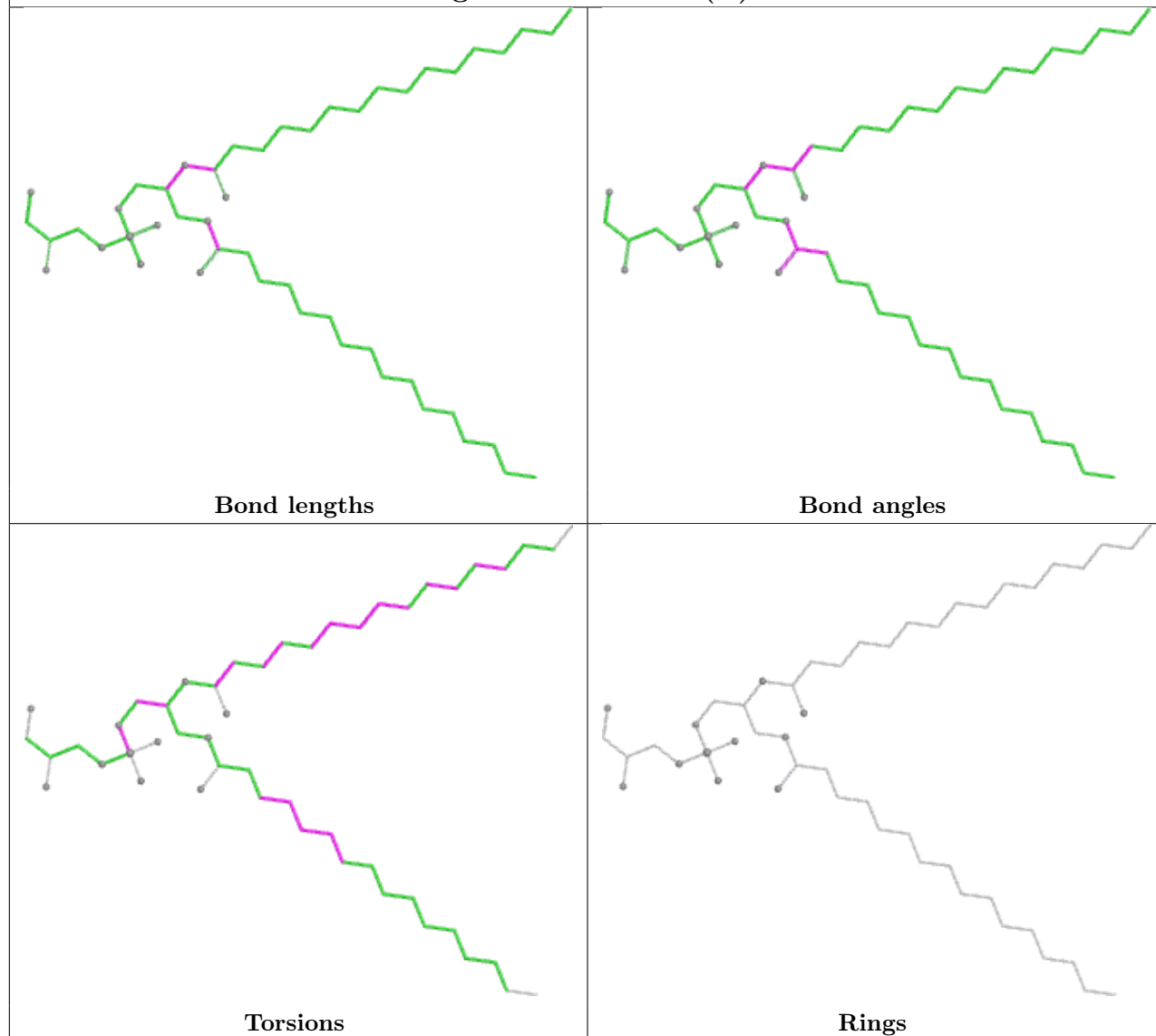
## Ligand LMG B 620



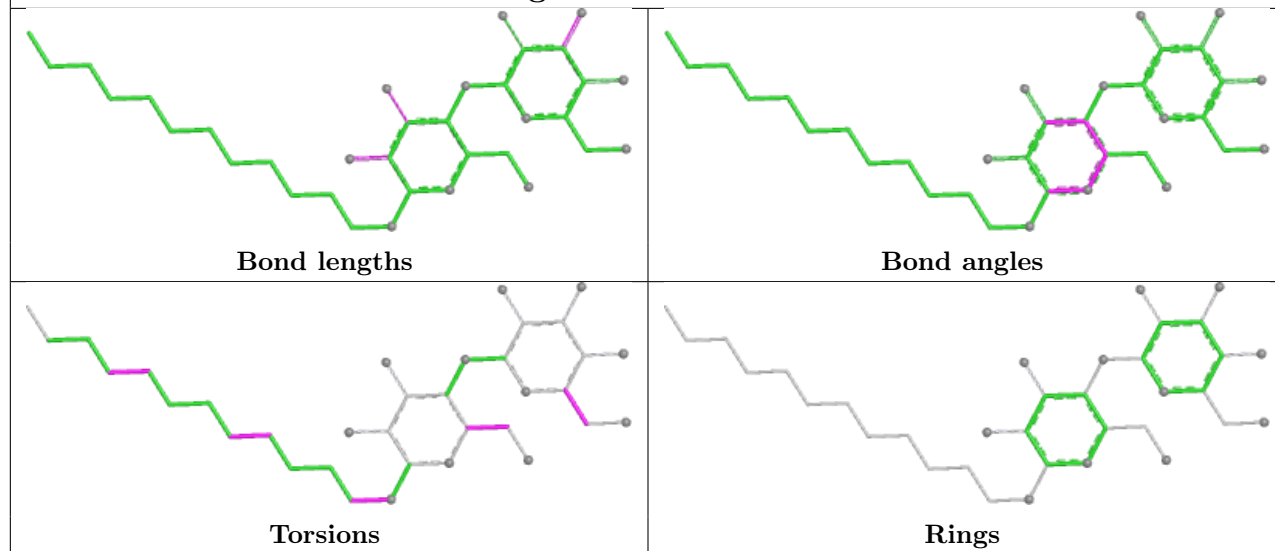




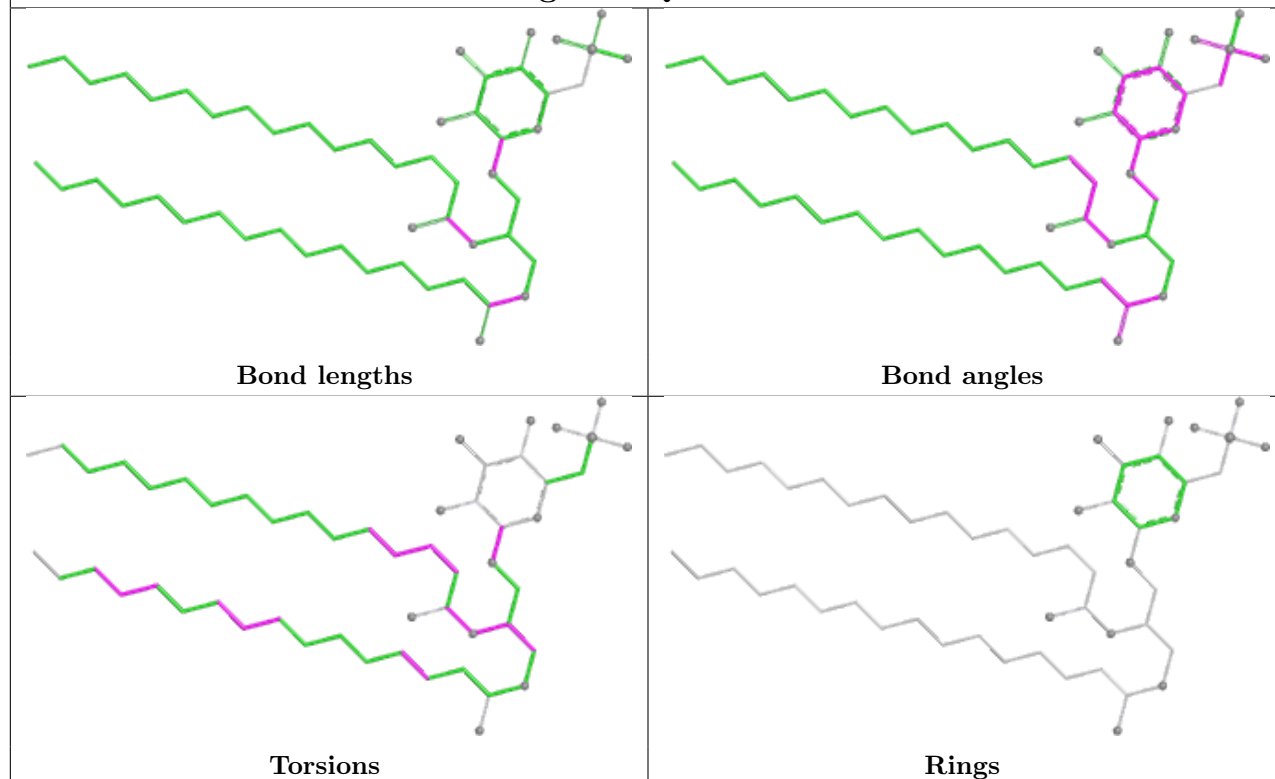
## Ligand LHG L 101 (B)



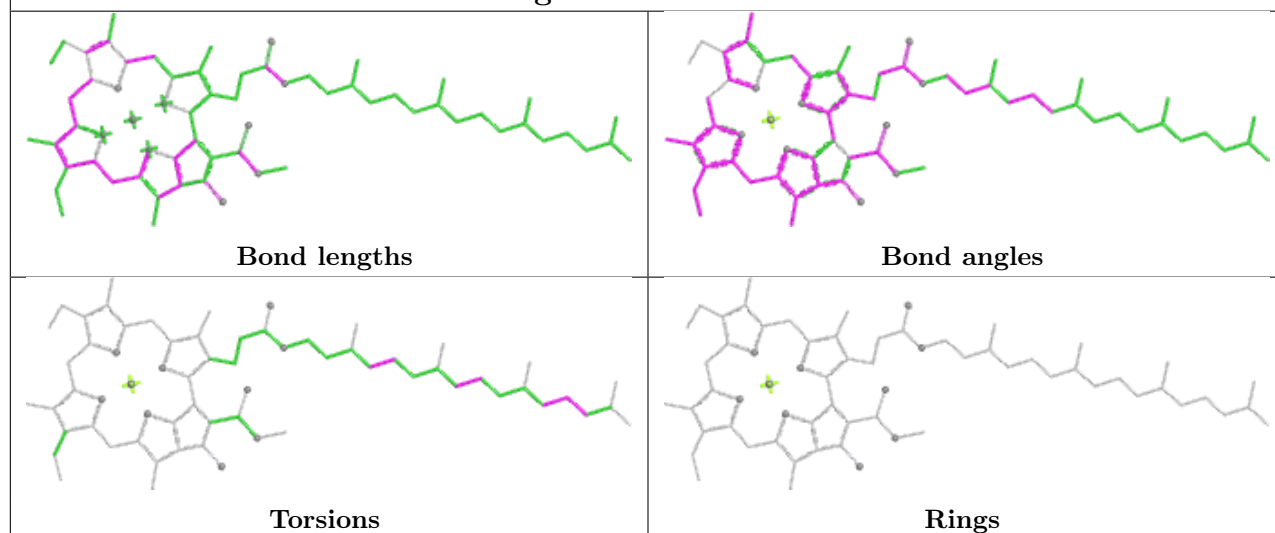
## Ligand LMT T 101

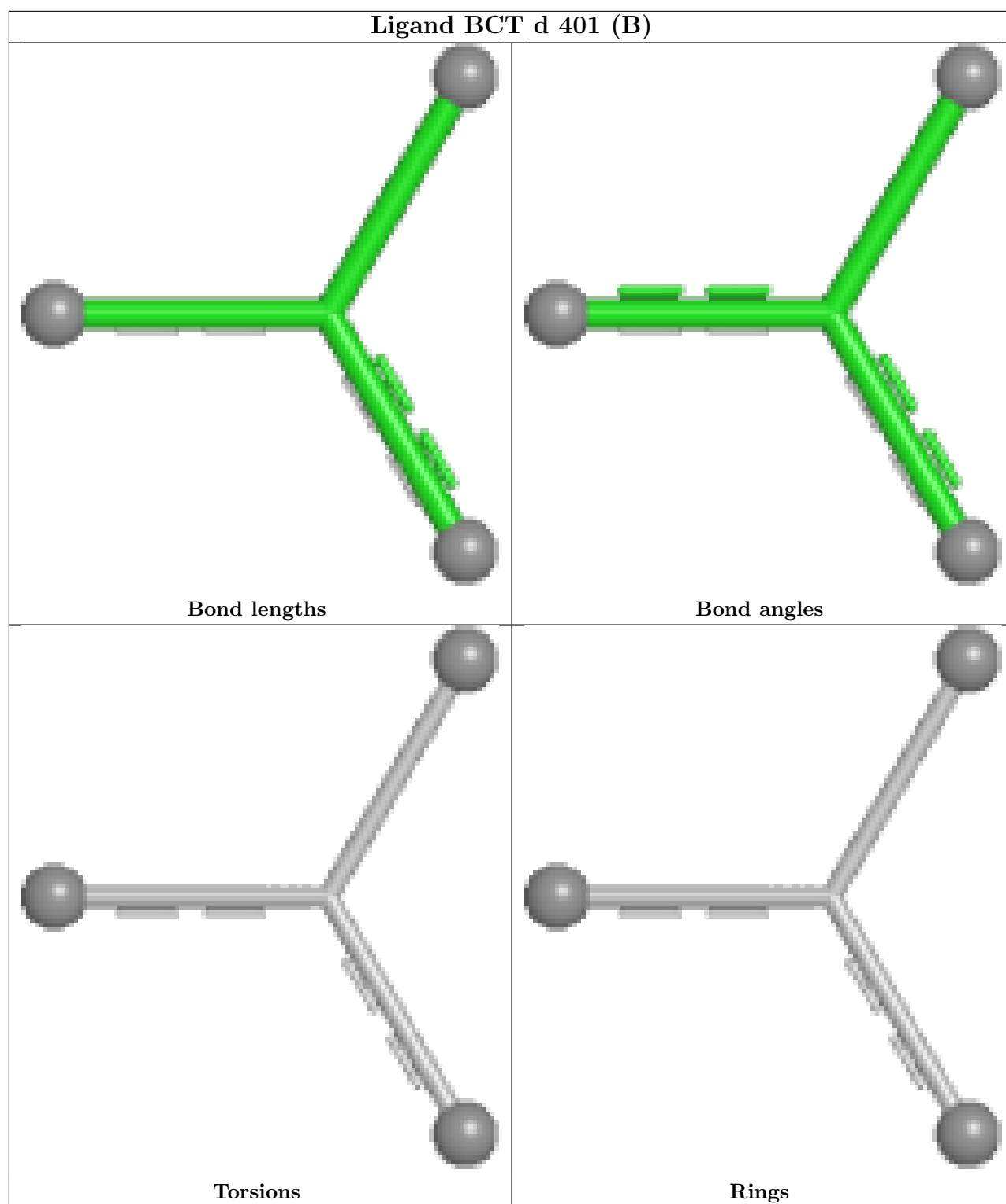


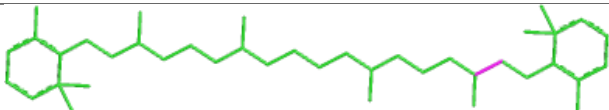
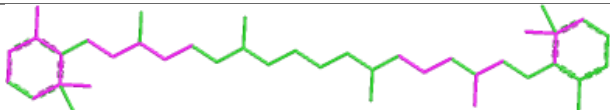
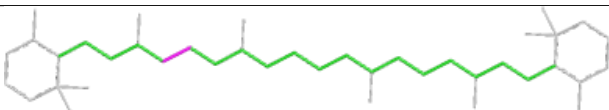
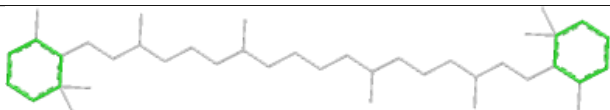
## Ligand SQD l 101

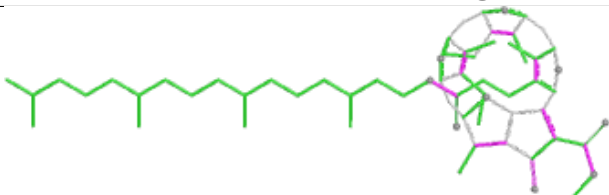
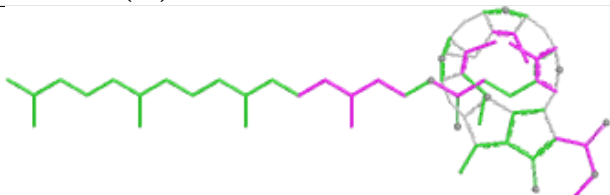
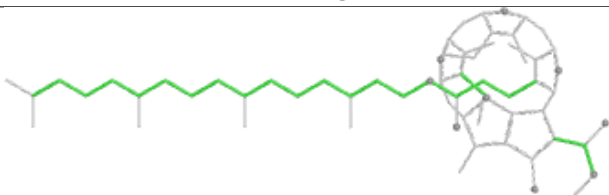
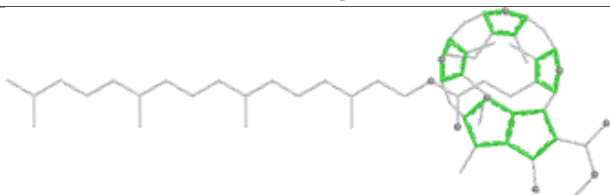


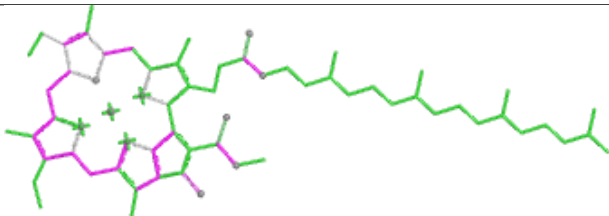
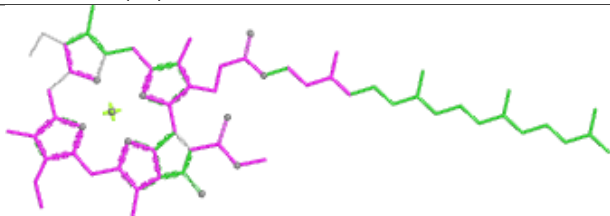
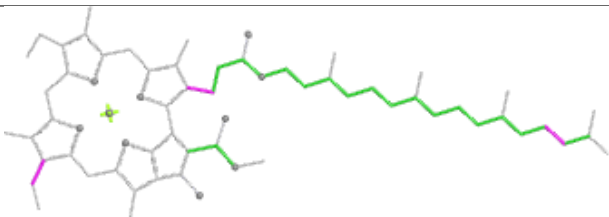
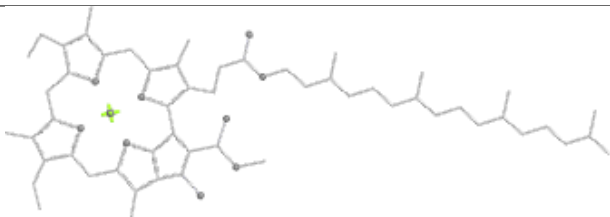
## Ligand CLA b 611



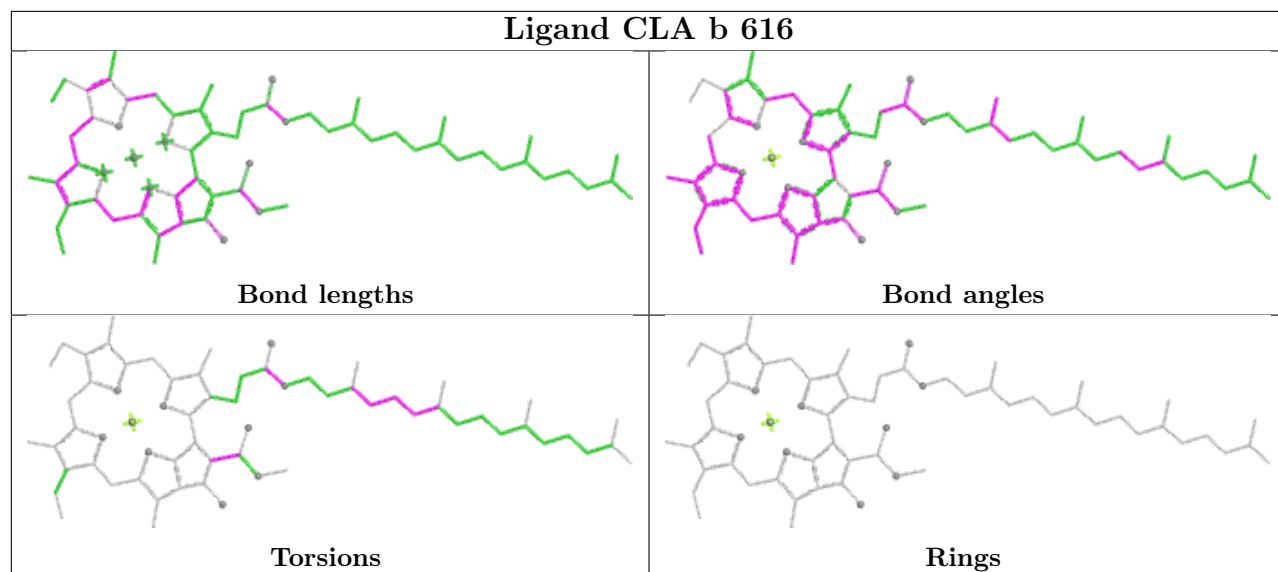


| Ligand BCR C 516                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|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

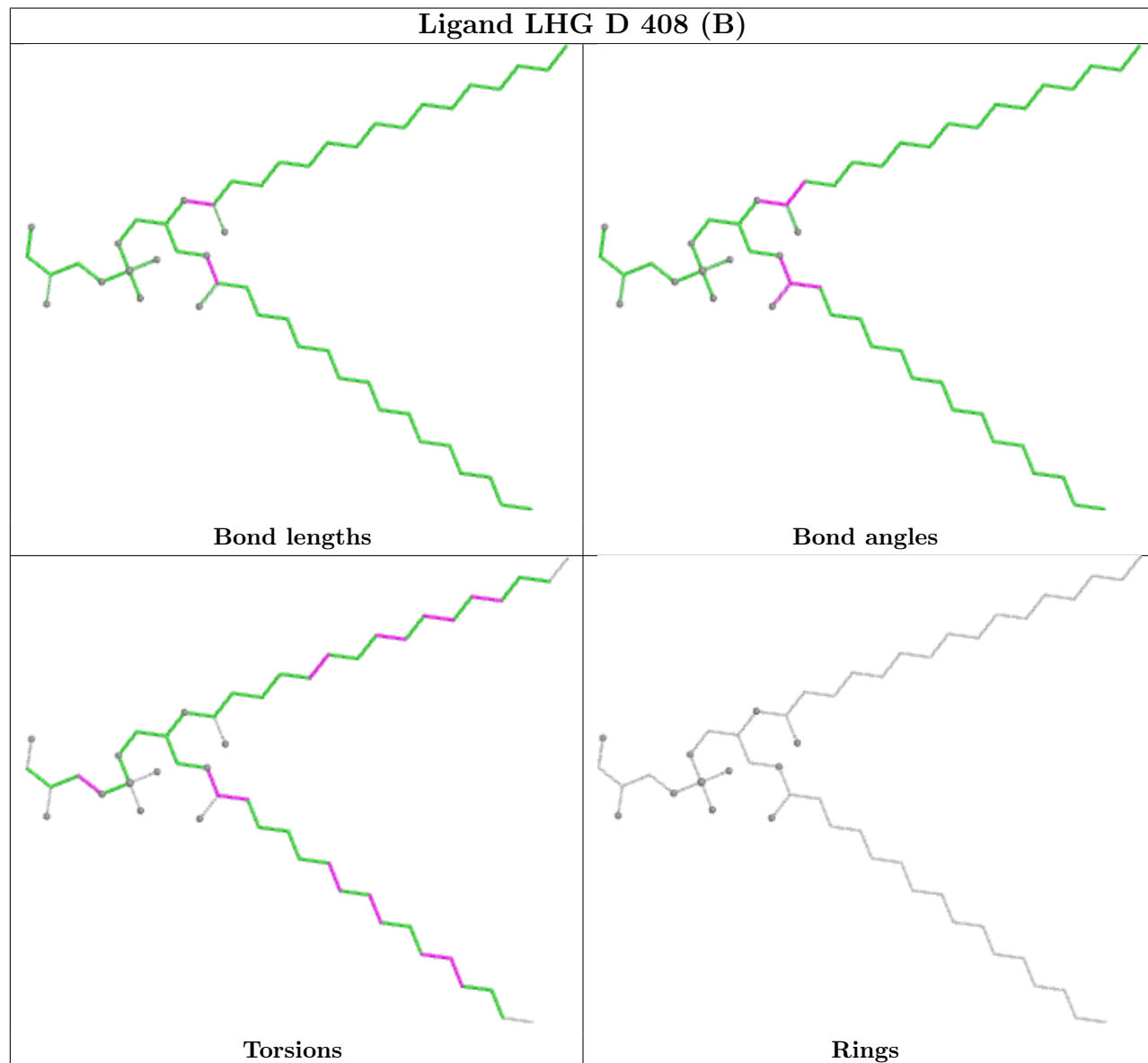
| Ligand PHO A 416 (B)                                                               |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

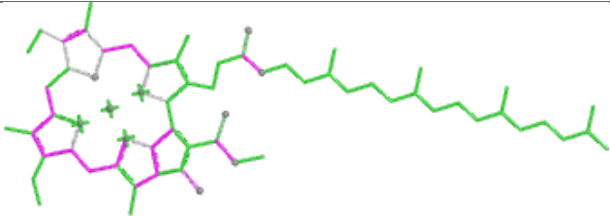
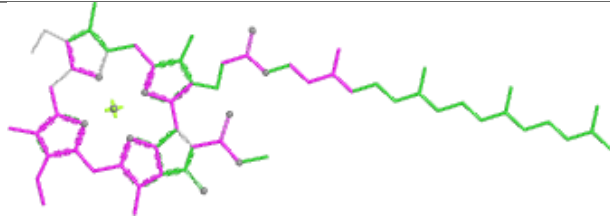
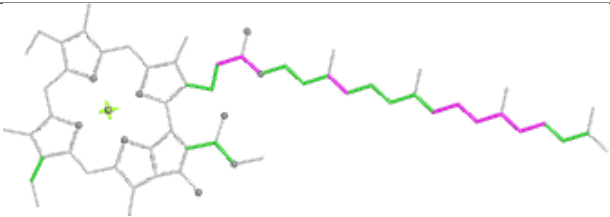
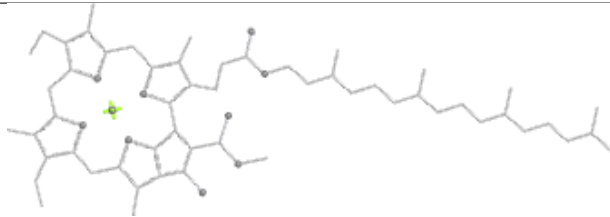
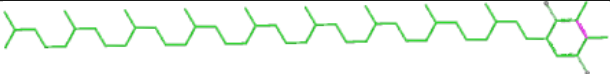
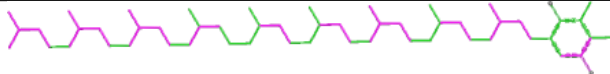
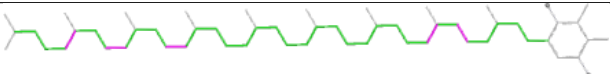
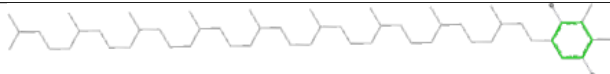
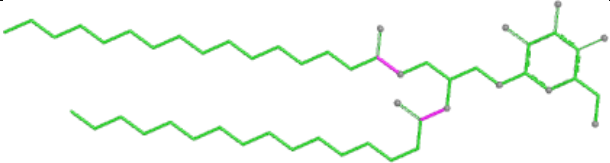
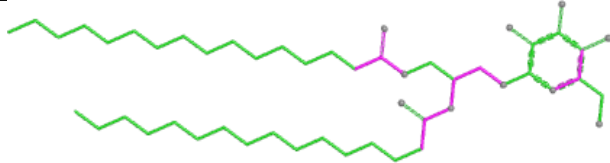
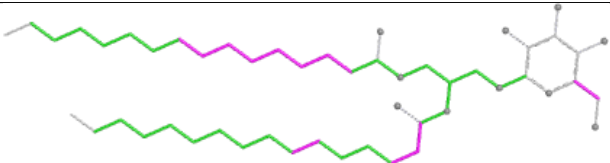
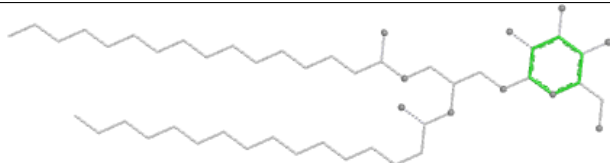
| Ligand CLA A 405 (B)                                                                |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

## Ligand CLA b 616

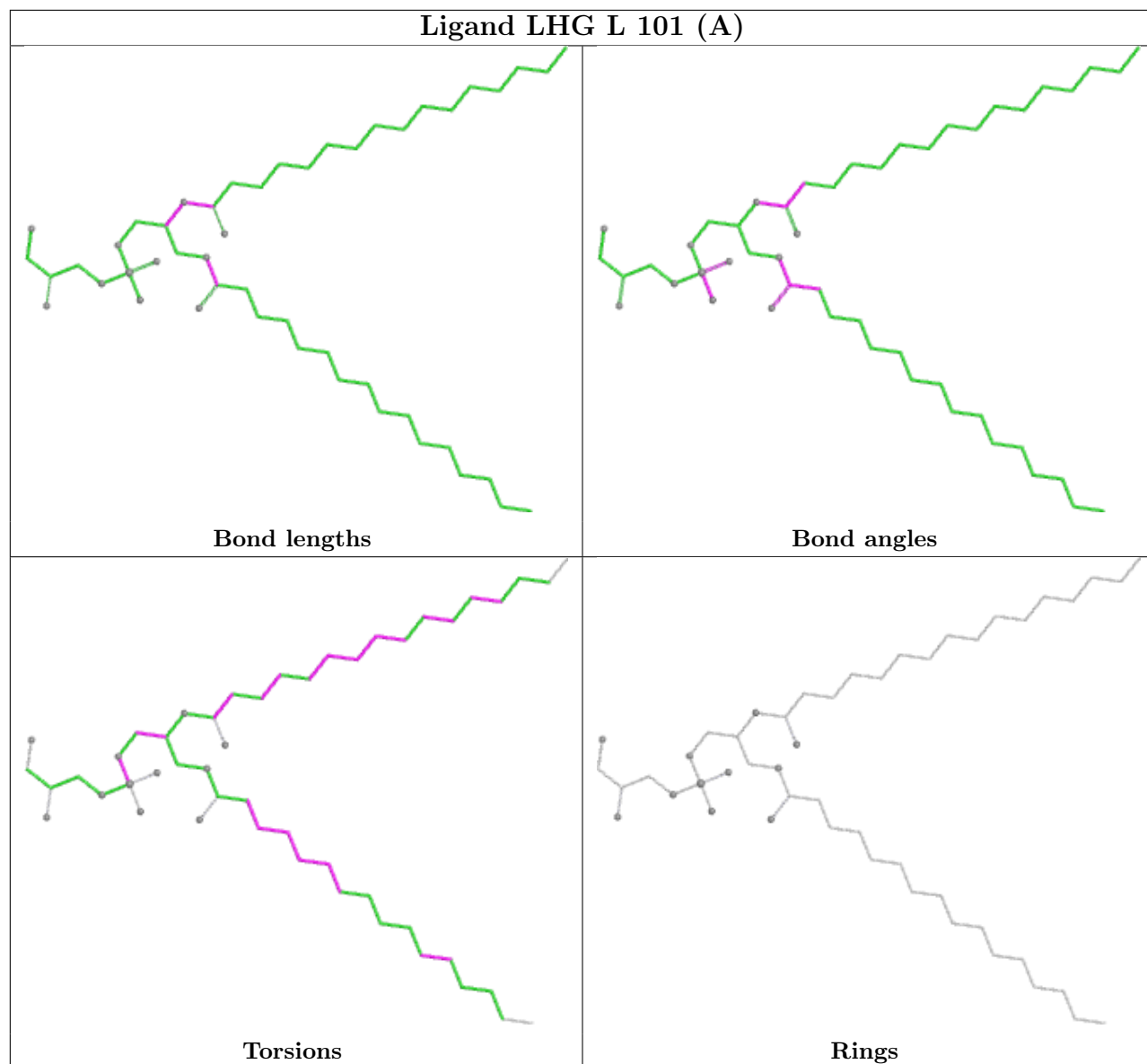


## Ligand LHG D 408 (B)

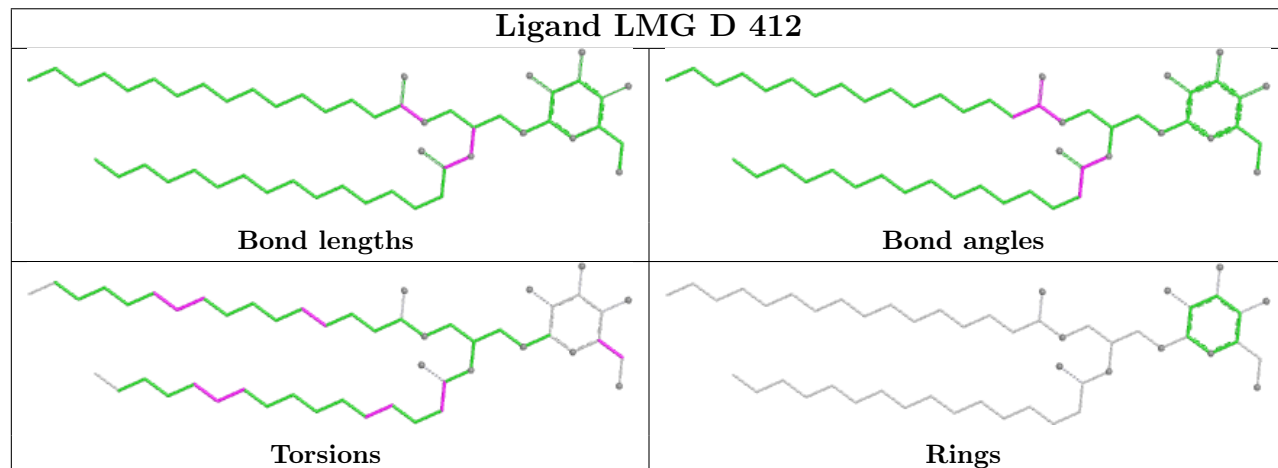


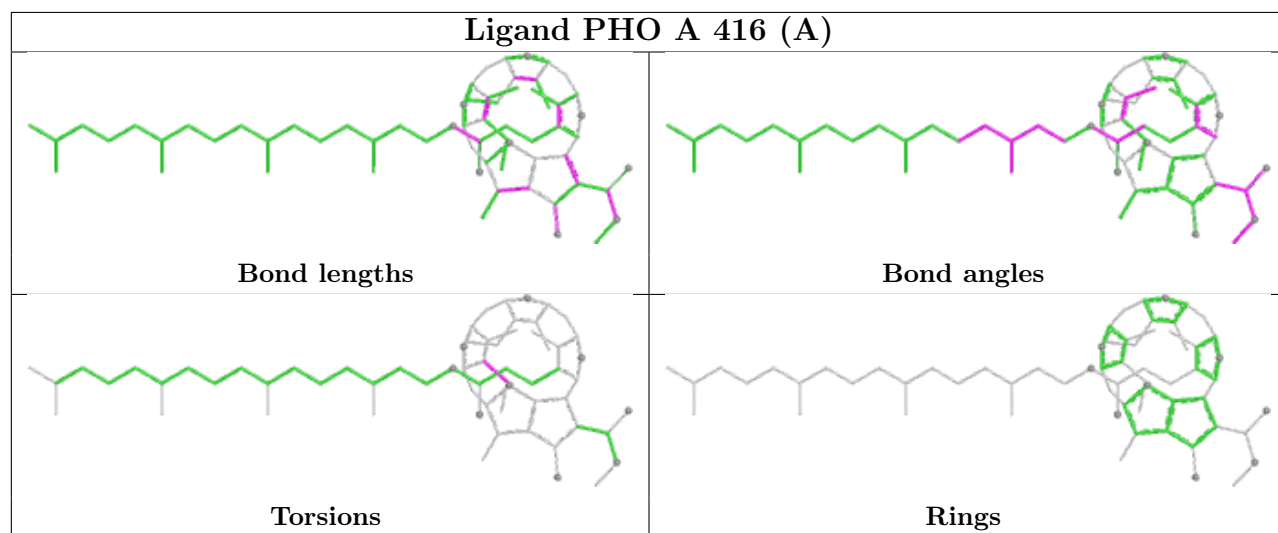
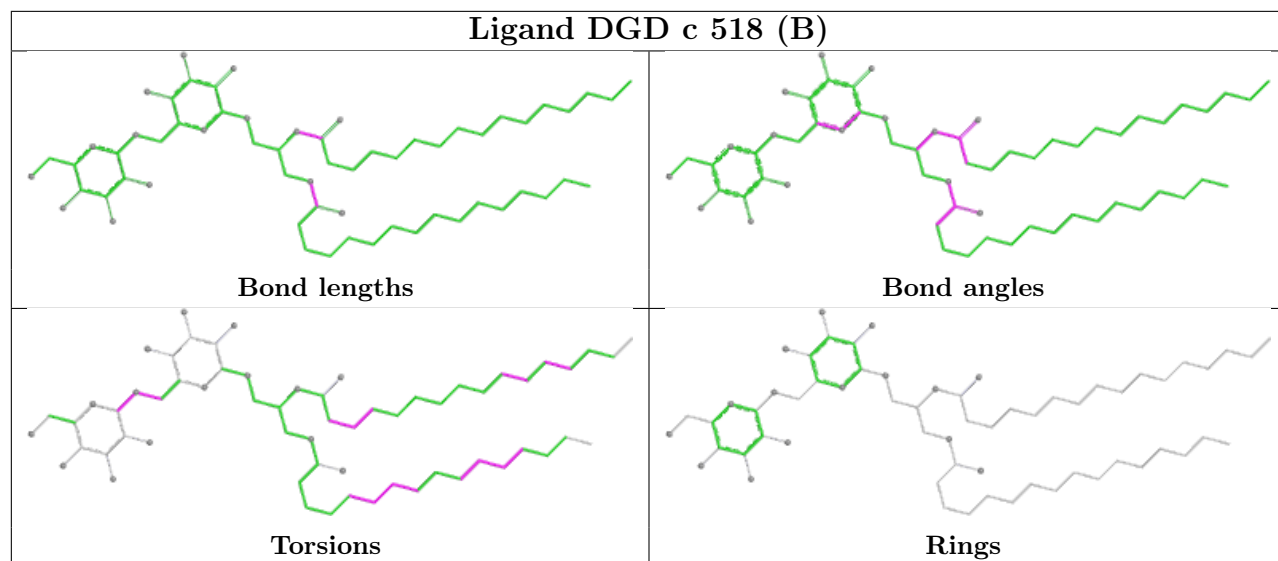
| Ligand CLA C 511                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand PL9 d 406 (A)                                                                                    |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMG c 520                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

## Ligand LHG L 101 (A)

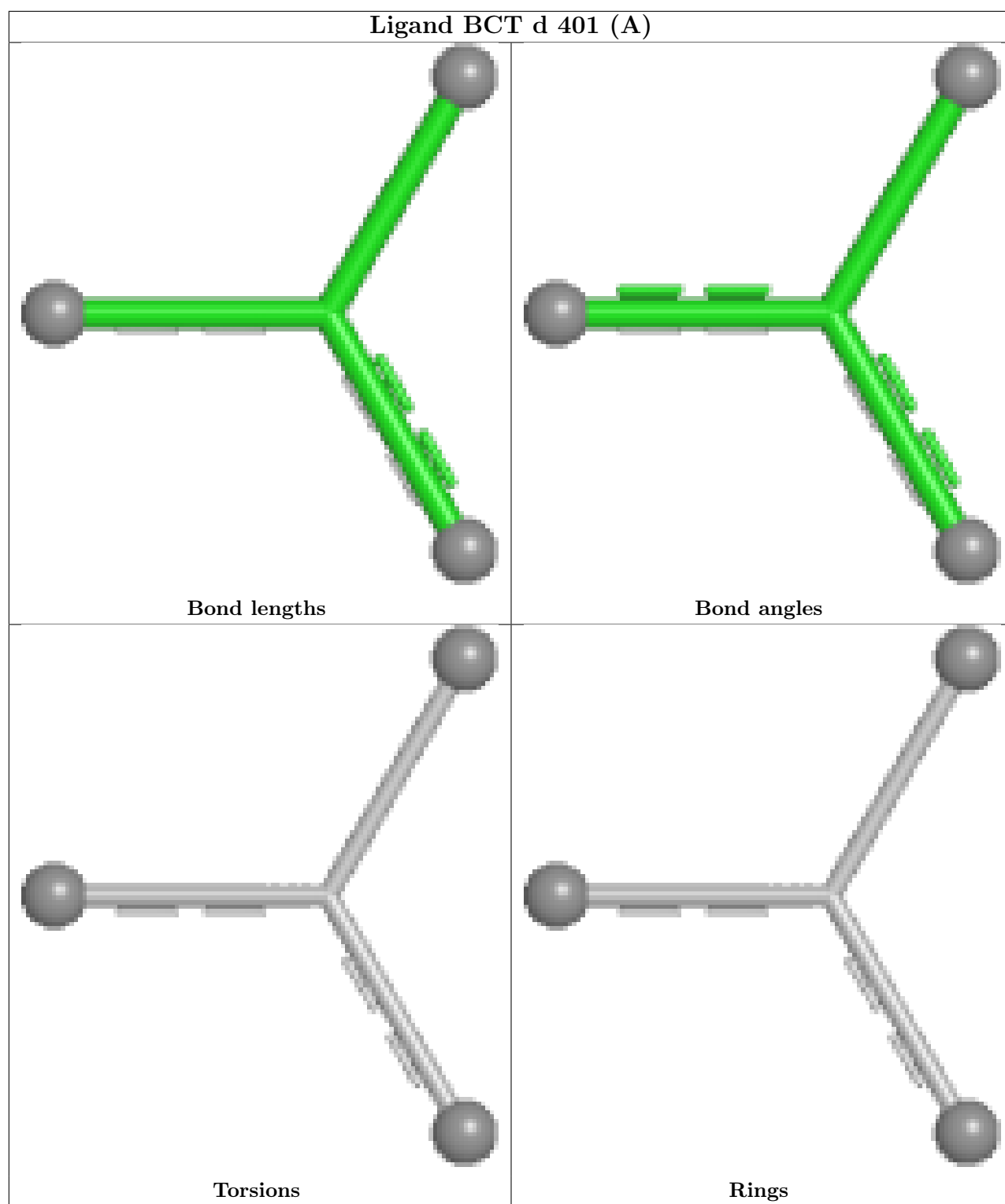


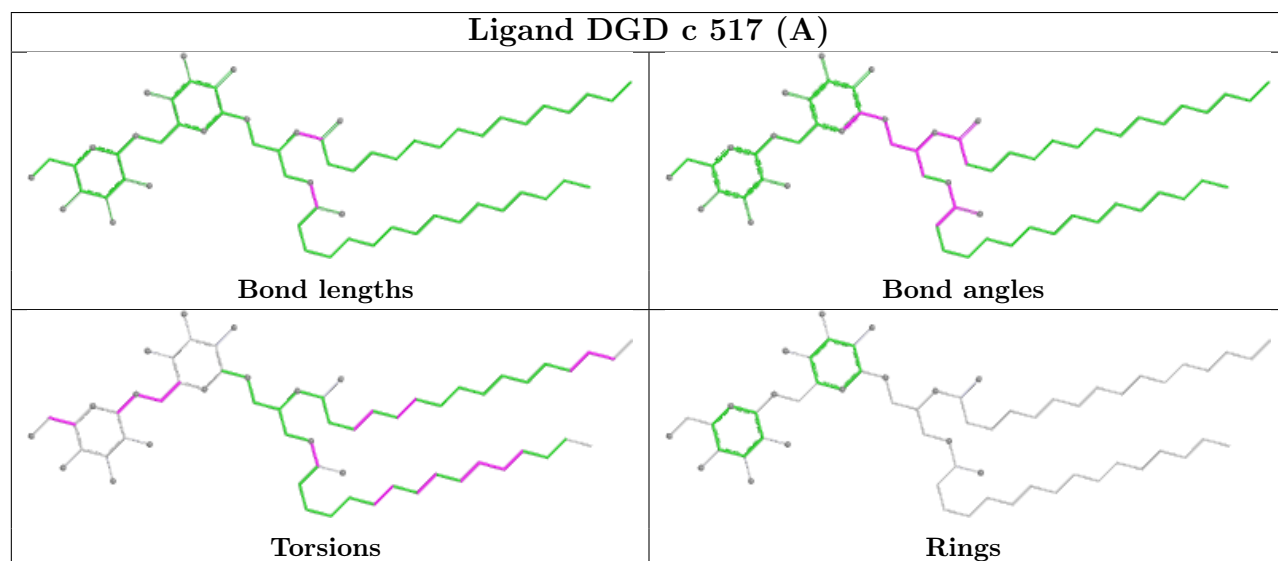
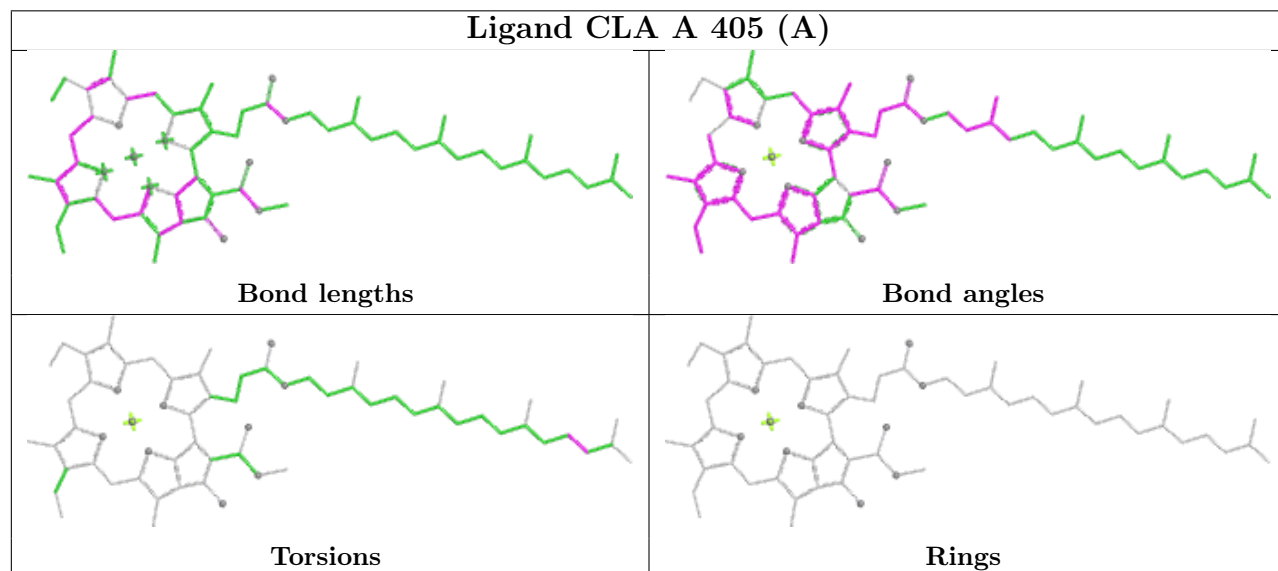
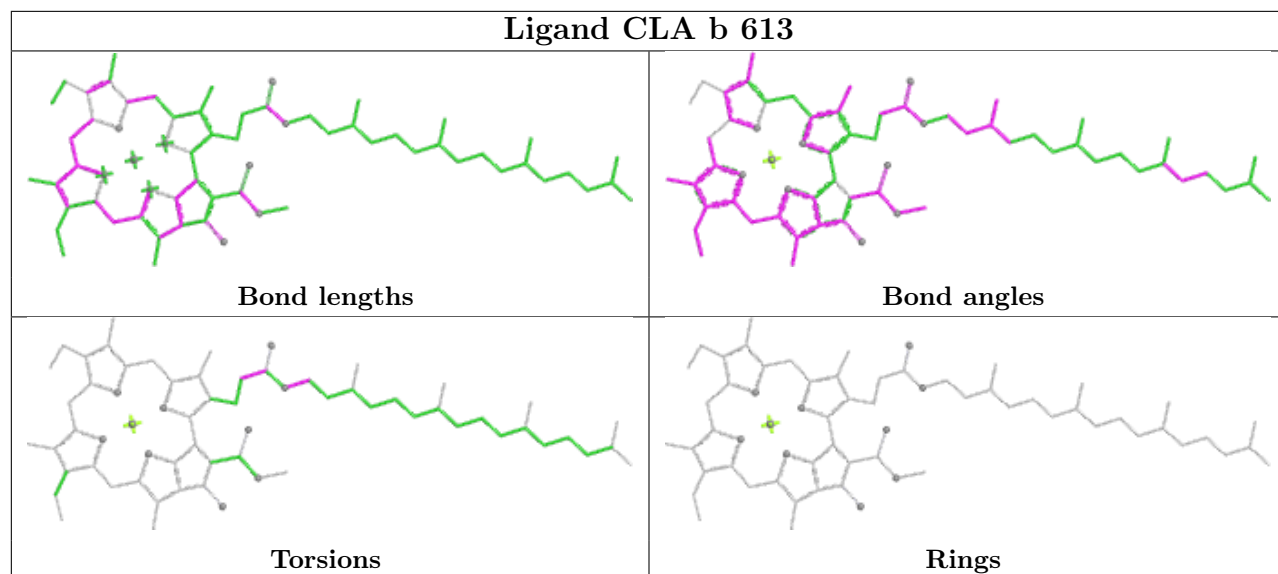
## Ligand LMG D 412



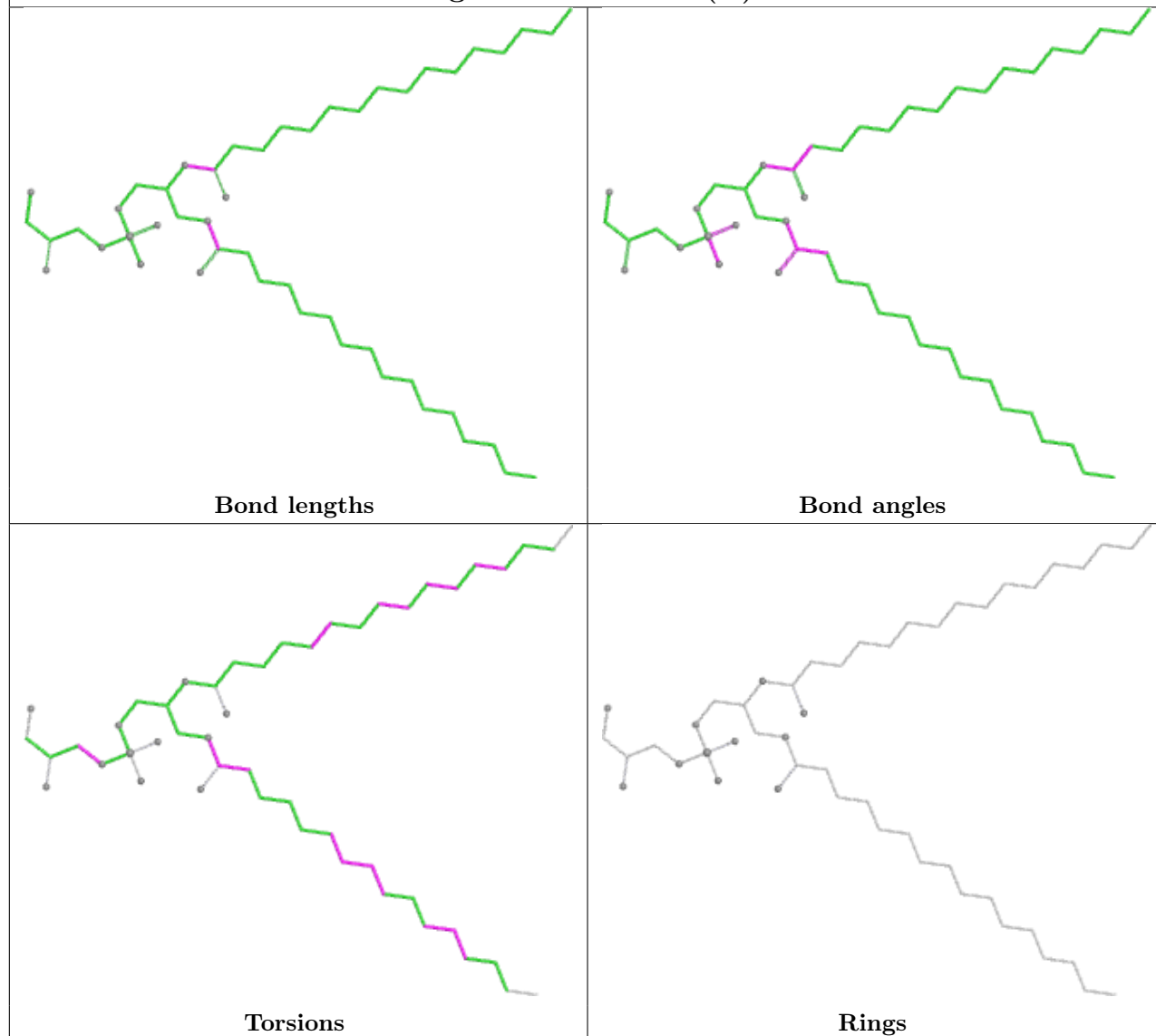




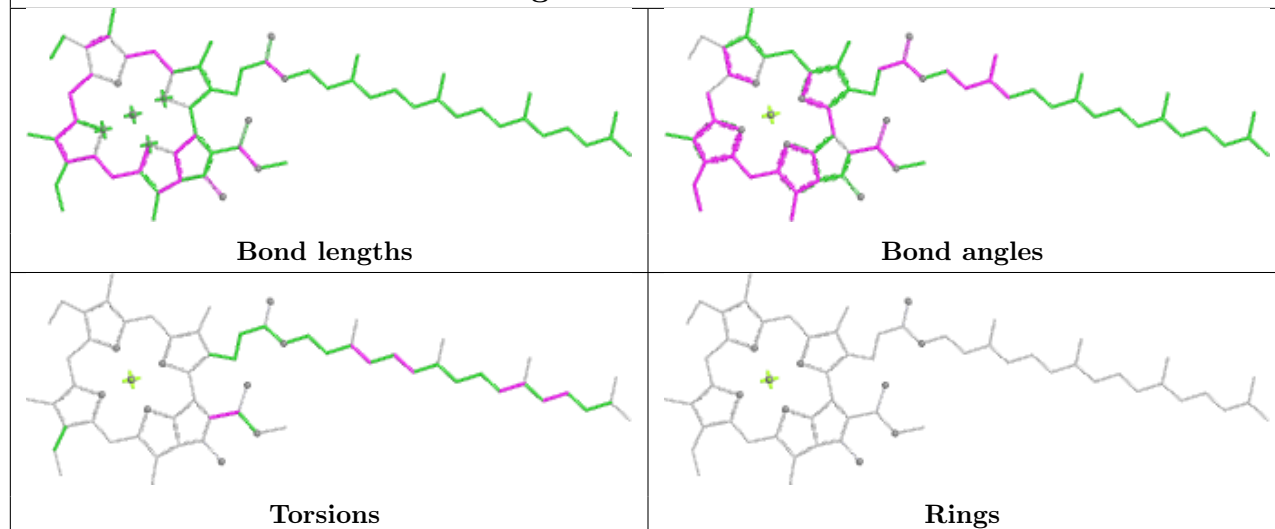




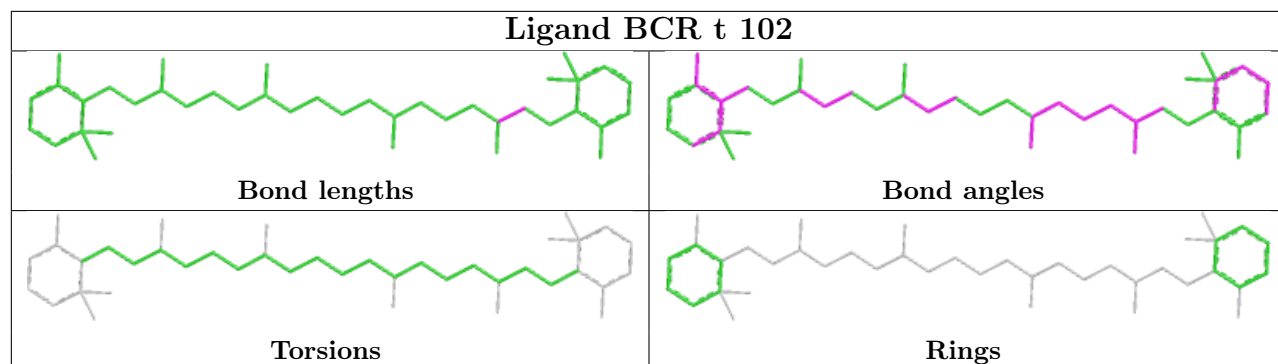
## Ligand LHG D 408 (A)



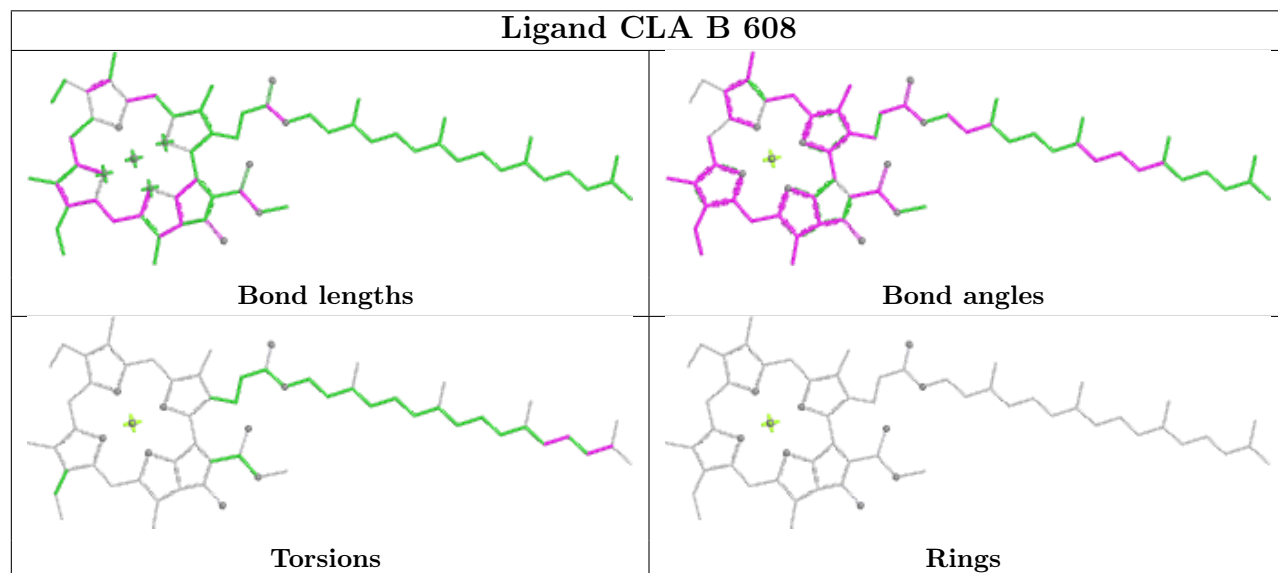
## Ligand CLA C 508



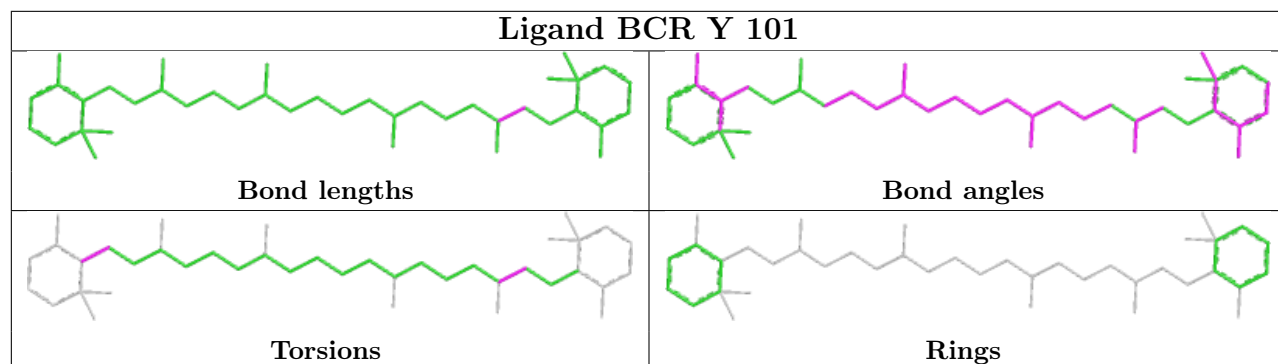
## Ligand BCR t 102

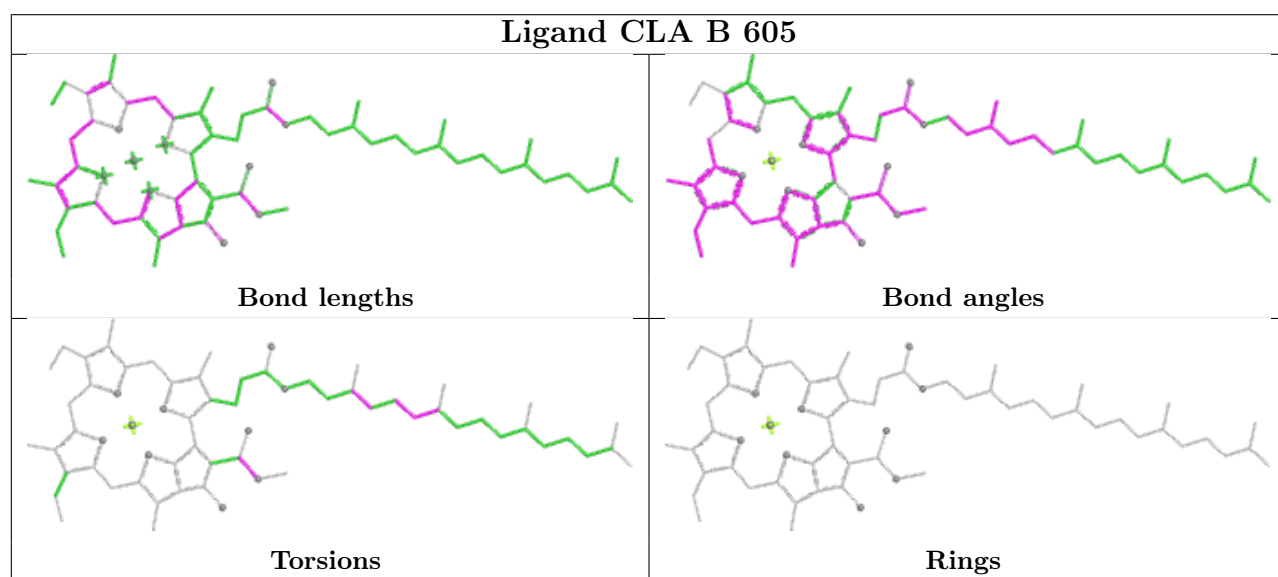
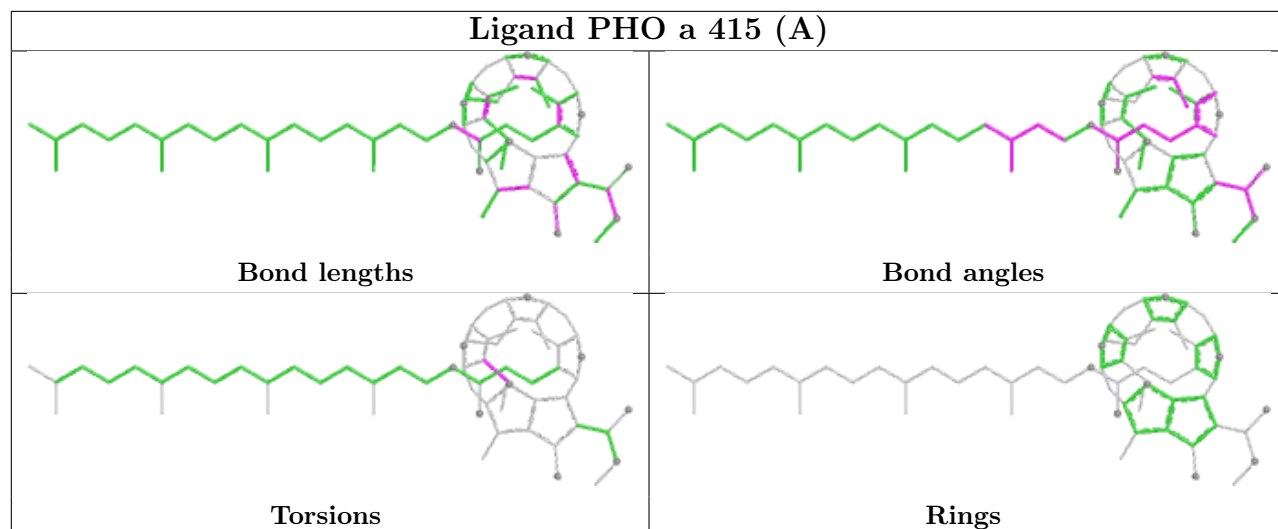


## Ligand CLA B 608

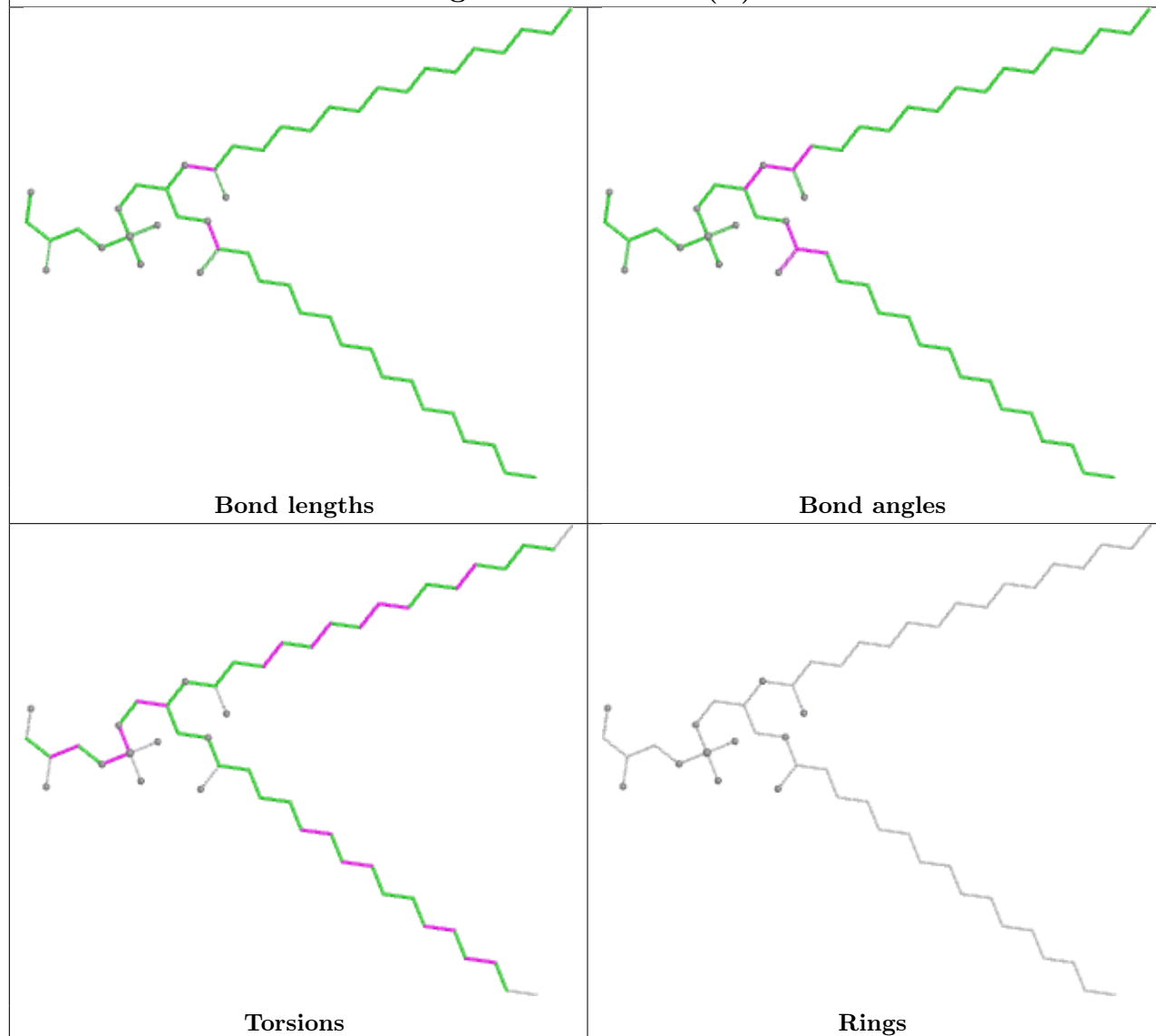


## Ligand BCR Y 101

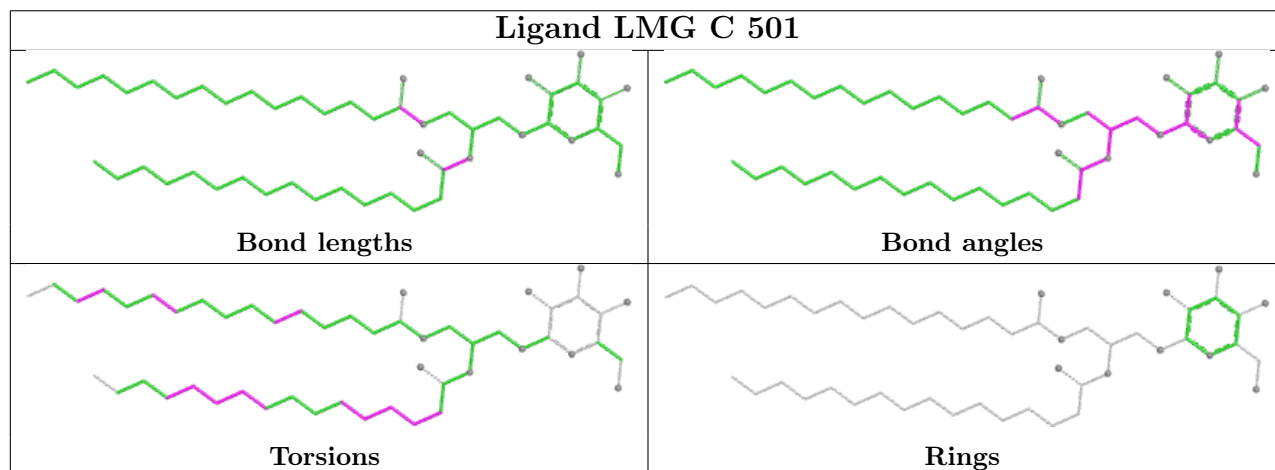


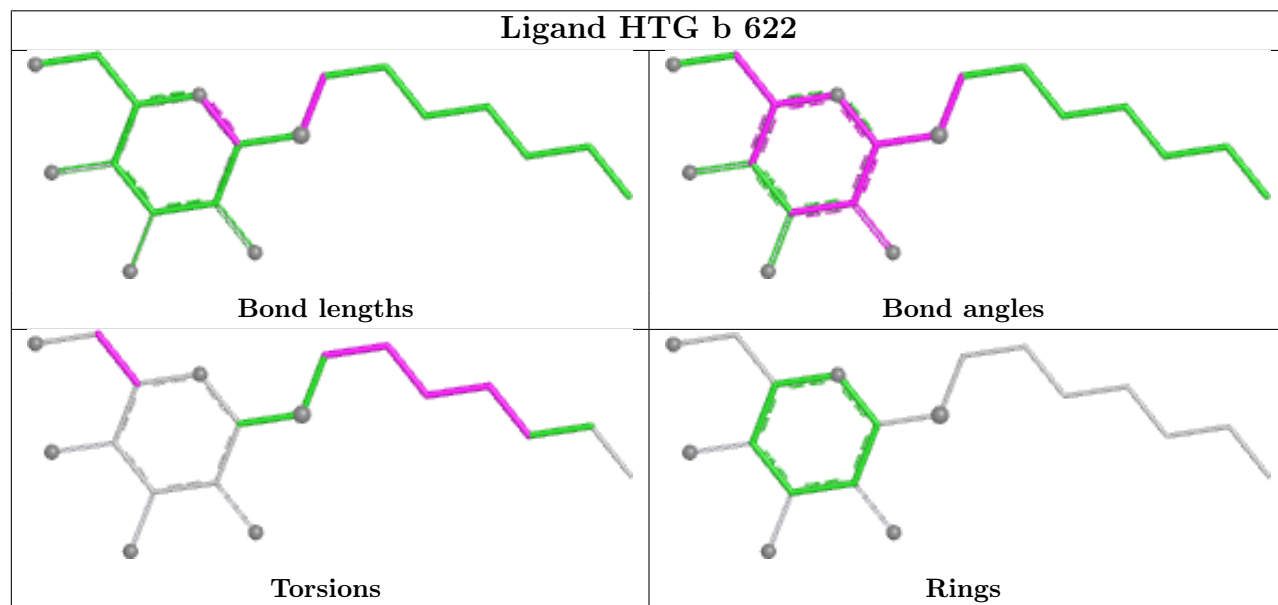
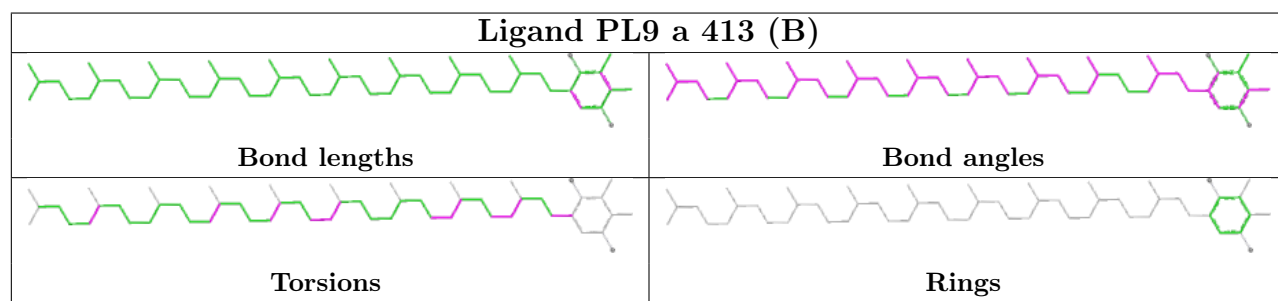
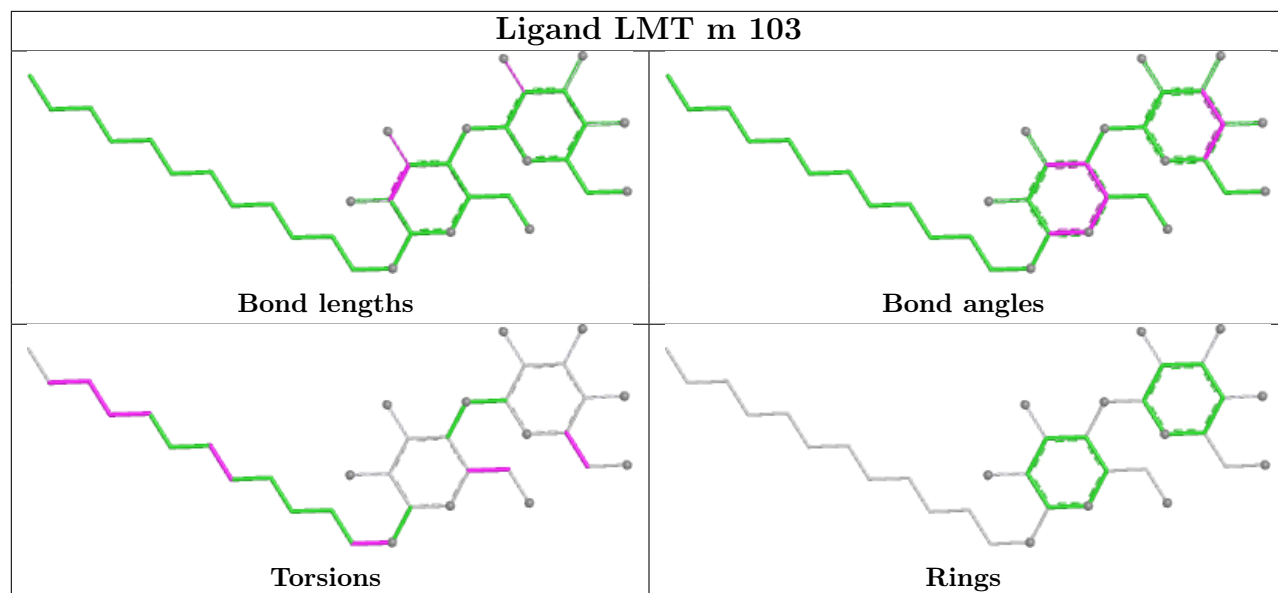


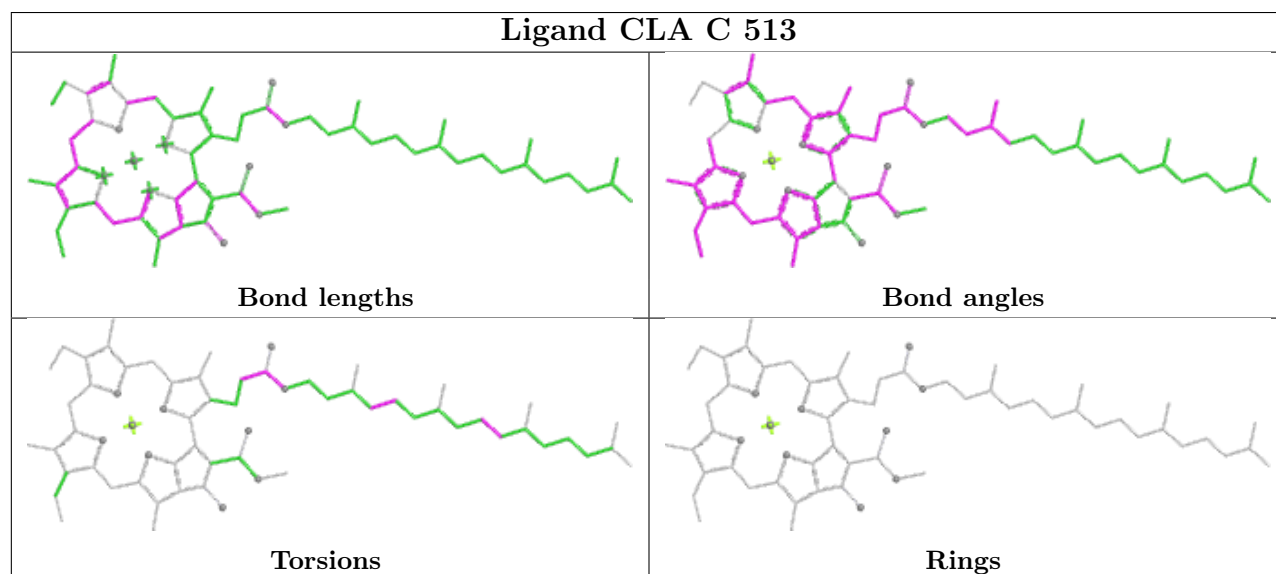
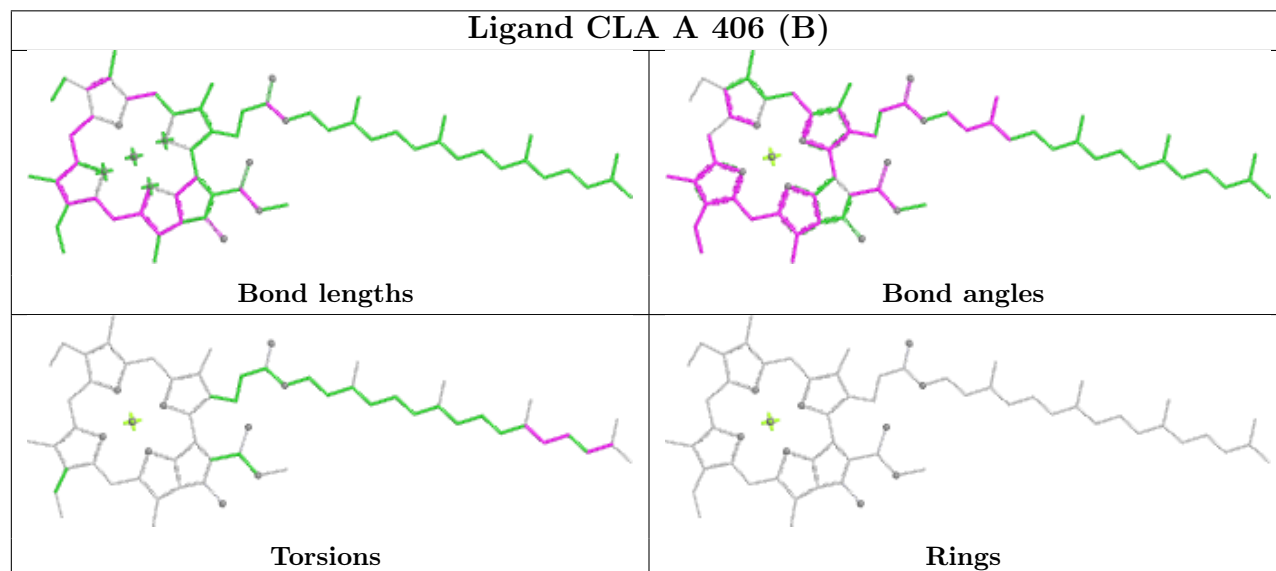
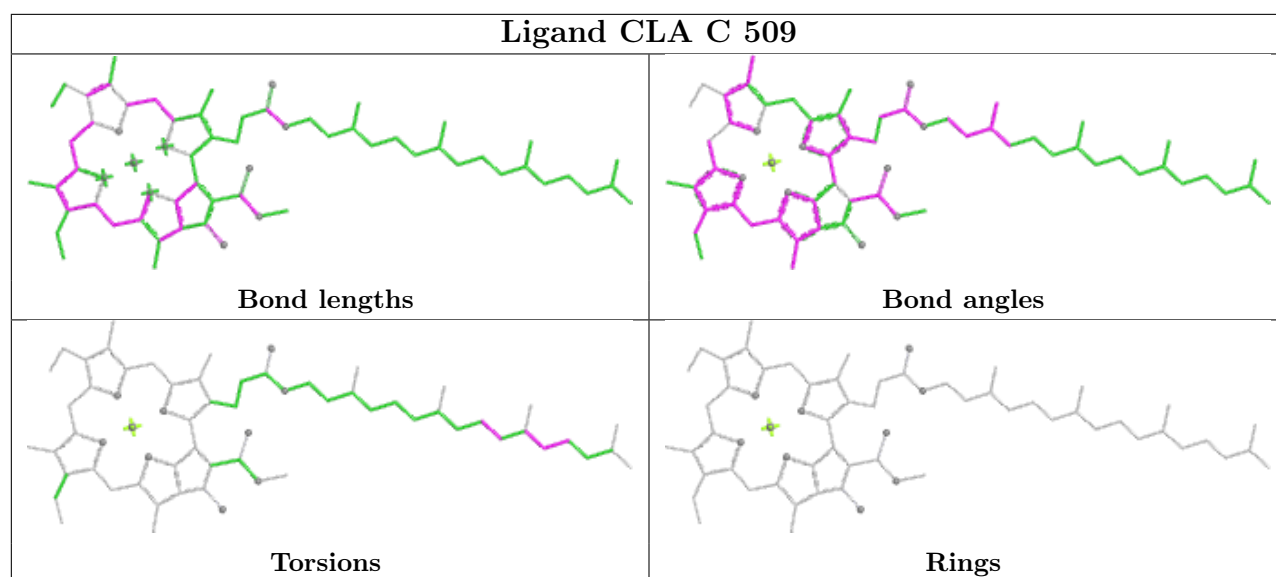
## Ligand LHG D 407 (B)



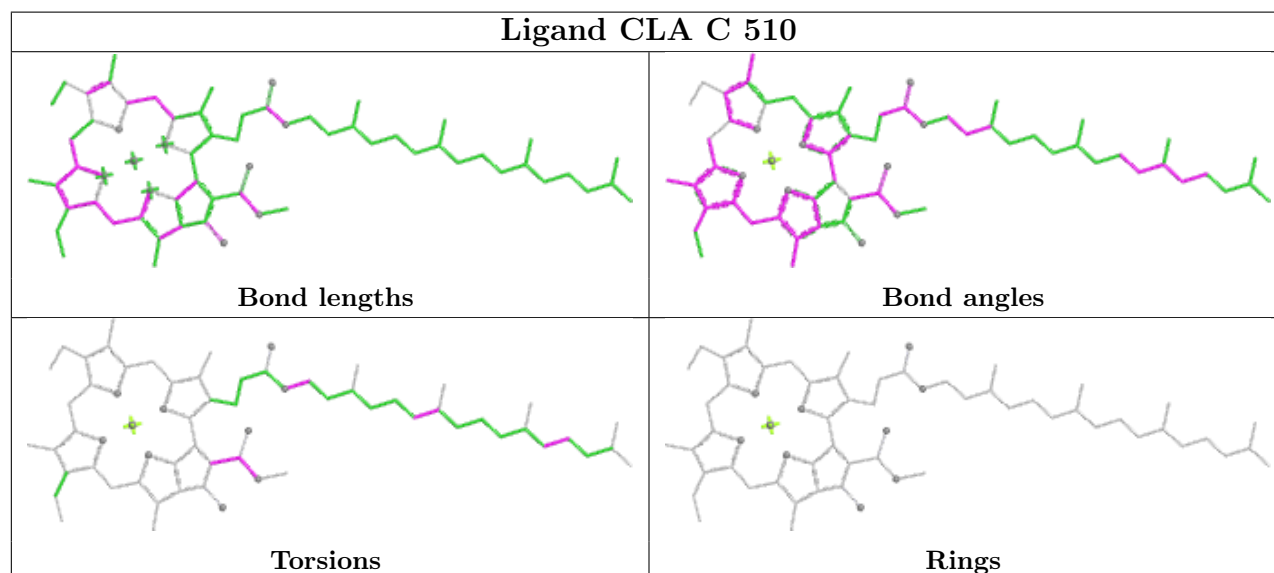
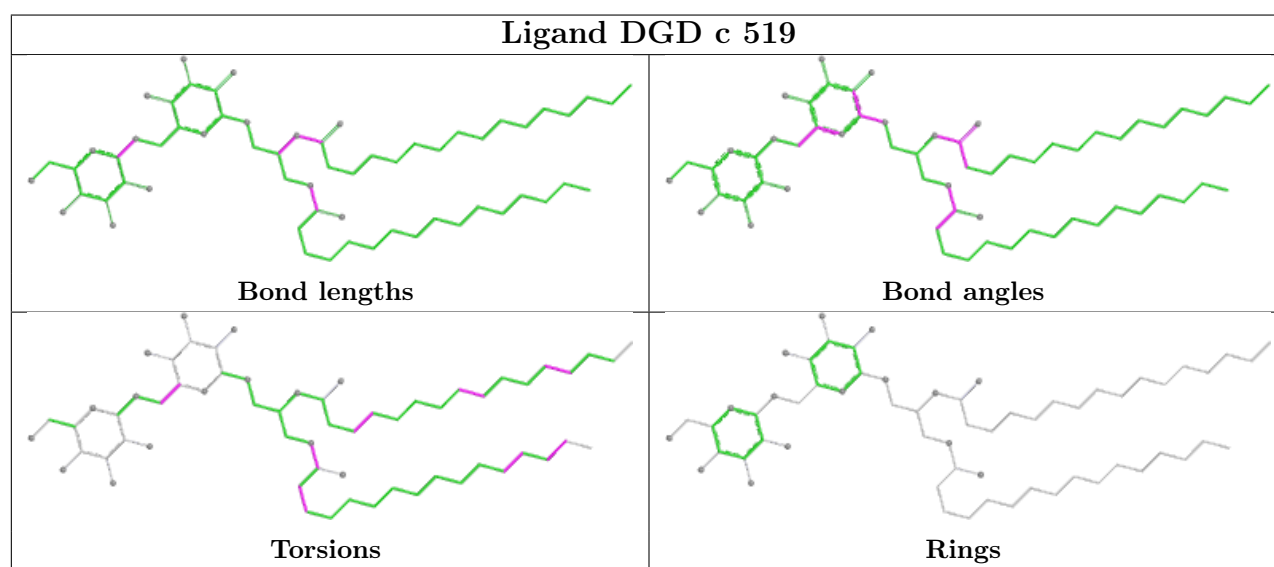
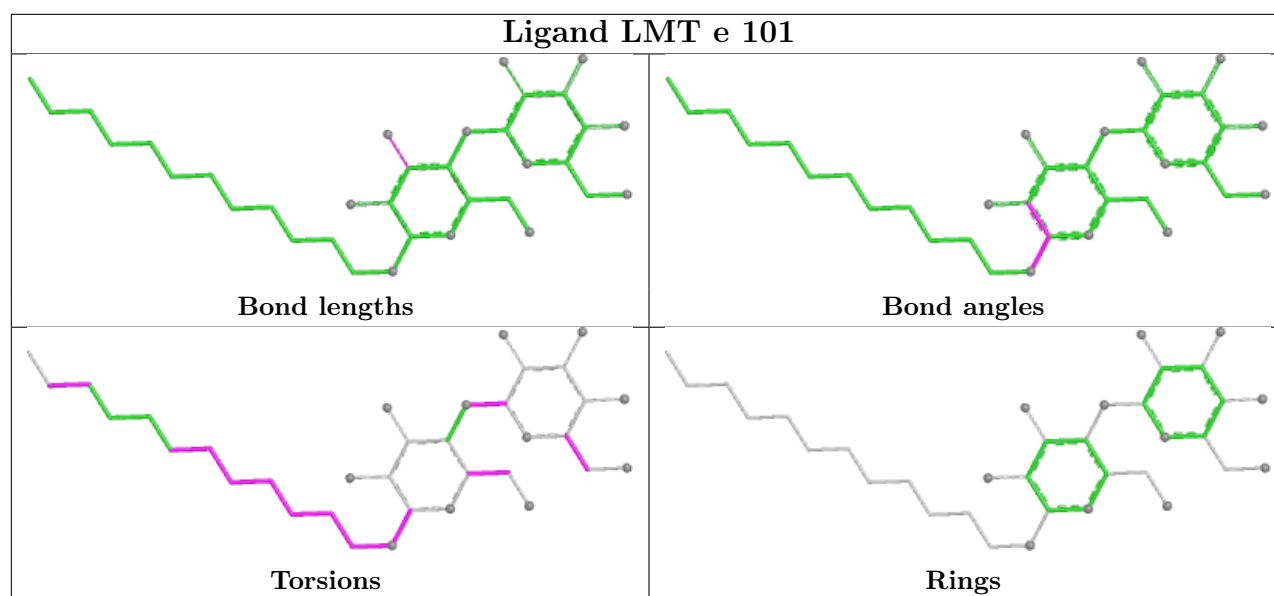
## Ligand LMG C 501



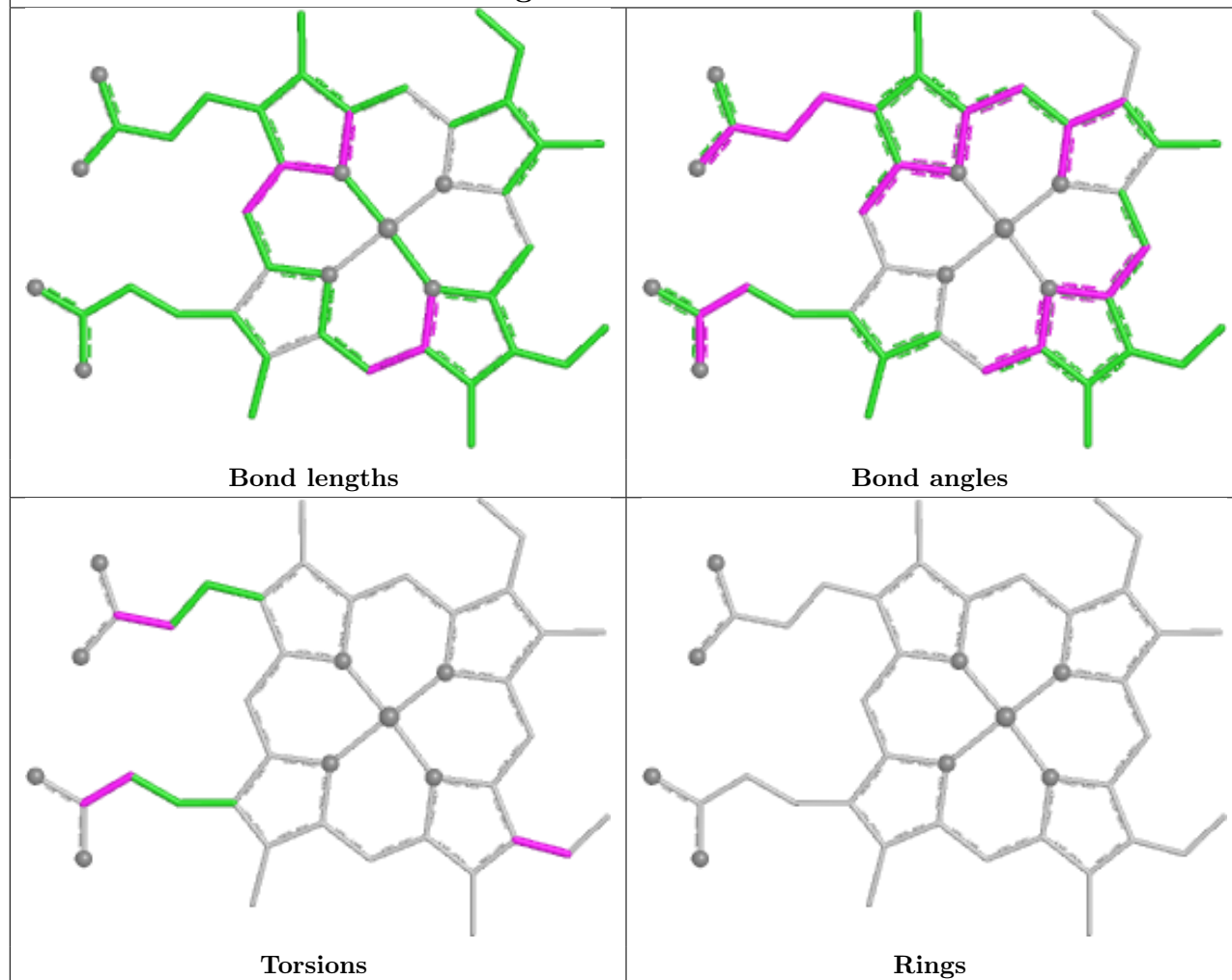




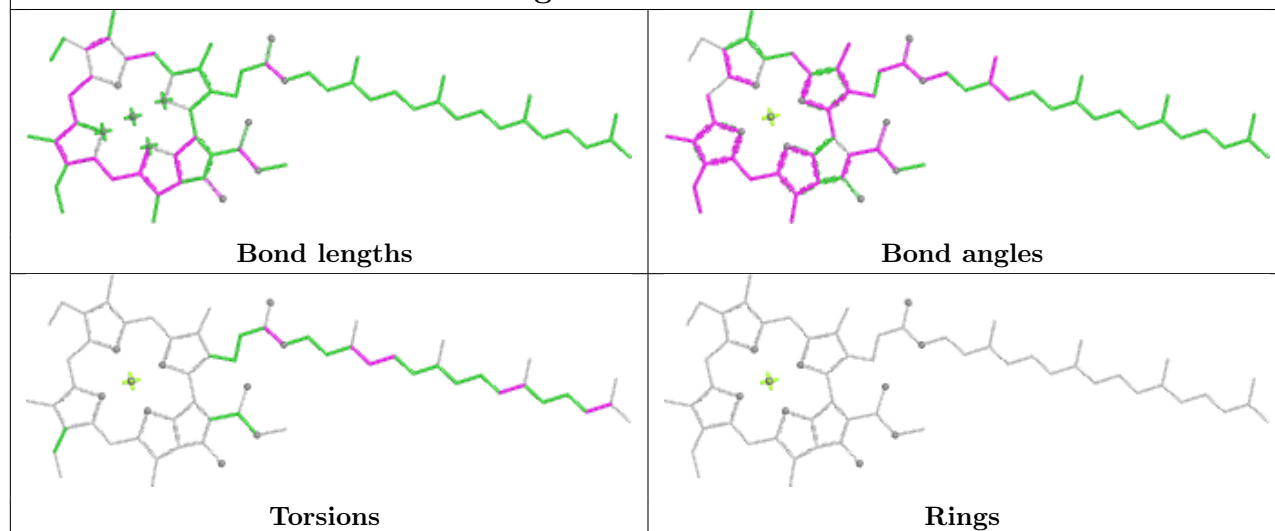


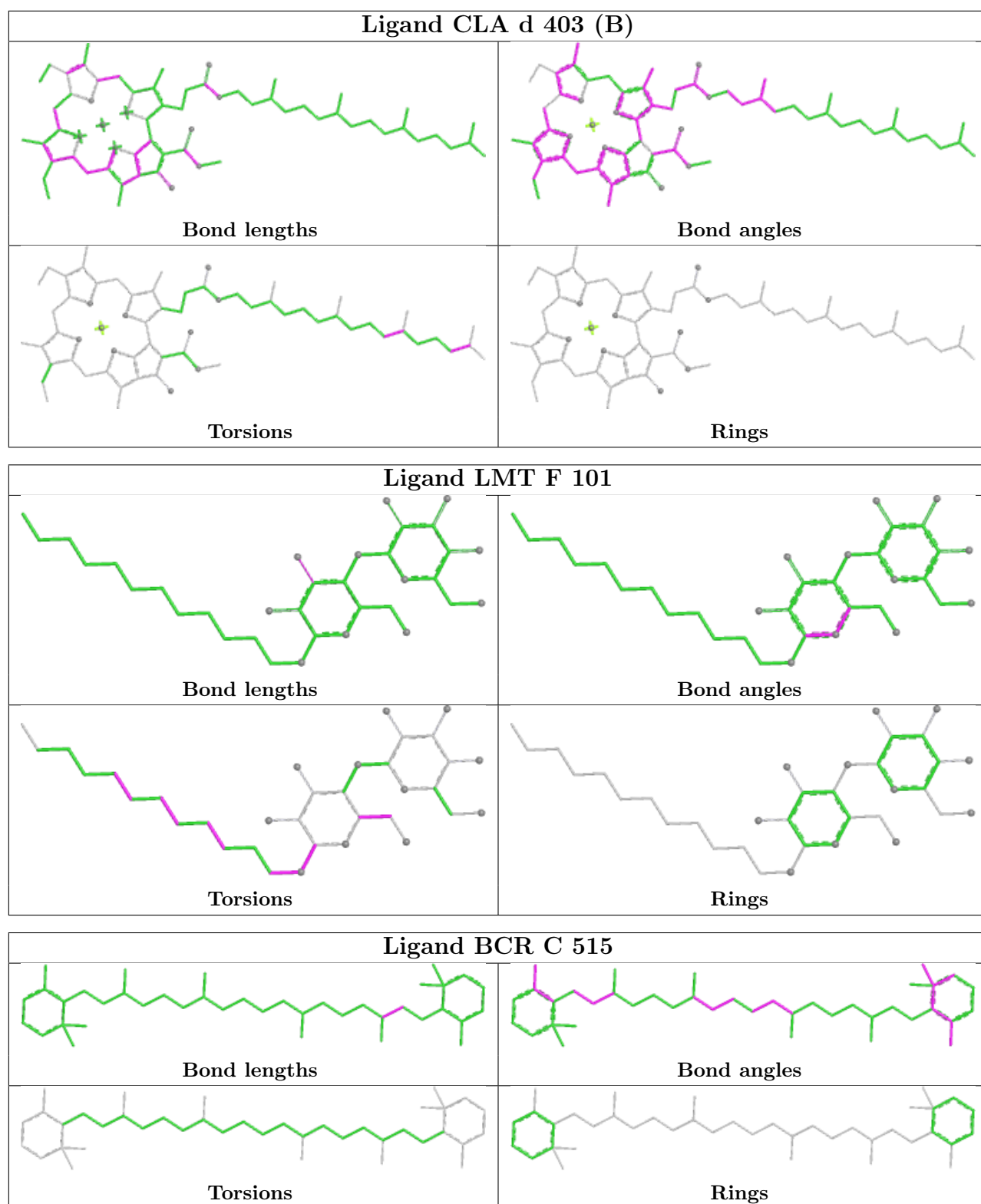


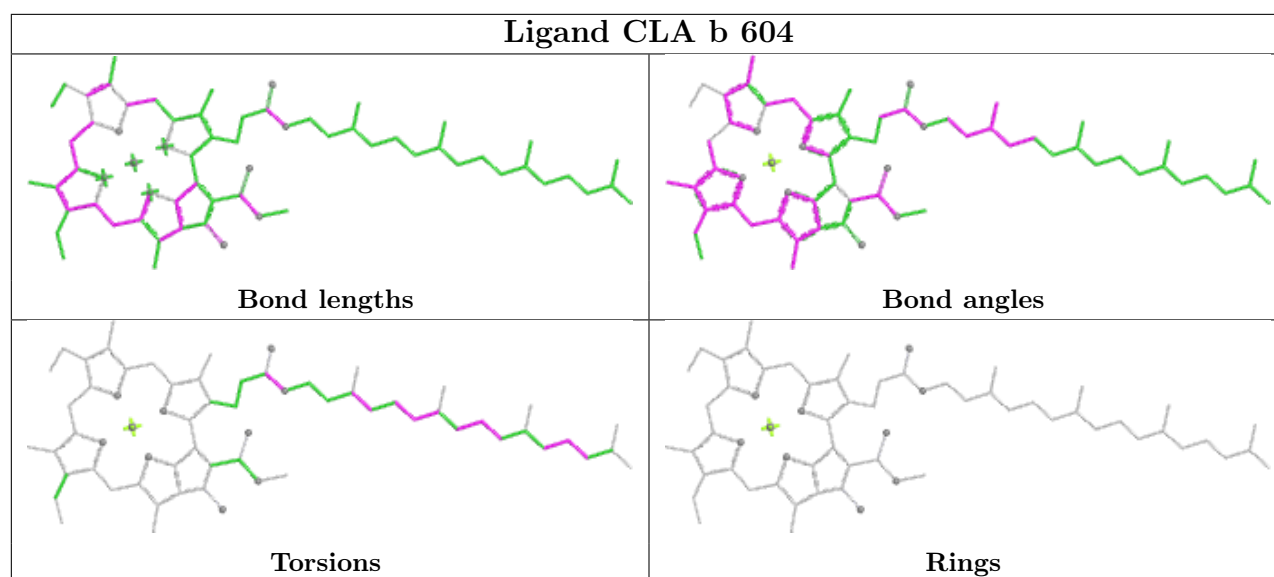
## Ligand HEM f 101



## Ligand CLA d 404







## 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%)  | -0.79  | 1 (0%) 90 90 | 19, 25, 59, 119       | 222 (66%) |
| 1   | a     | 334/344 (97%)  | -0.74  | 1 (0%) 90 90 | 20, 28, 64, 128       | 221 (66%) |
| 2   | B     | 504/505 (99%)  | -0.69  | 0 100 100    | 21, 52, 82, 116       | 20 (3%)   |
| 2   | b     | 504/505 (99%)  | -0.61  | 0 100 100    | 23, 57, 98, 150       | 19 (3%)   |
| 3   | C     | 451/455 (99%)  | -0.69  | 0 100 100    | 21, 59, 82, 134       | 97 (21%)  |
| 3   | c     | 455/455 (100%) | -0.60  | 1 (0%) 92 92 | 24, 65, 87, 128       | 100 (21%) |
| 4   | D     | 342/342 (100%) | -0.83  | 0 100 100    | 19, 44, 64, 127       | 114 (33%) |
| 4   | d     | 341/342 (99%)  | -0.82  | 0 100 100    | 21, 49, 73, 128       | 116 (34%) |
| 5   | E     | 81/84 (96%)    | -0.47  | 0 100 100    | 51, 69, 96, 147       | 0         |
| 5   | e     | 79/84 (94%)    | -0.48  | 1 (1%) 74 75 | 31, 74, 116, 142      | 2 (2%)    |
| 6   | F     | 34/44 (77%)    | -0.65  | 0 100 100    | 52, 59, 89, 110       | 0         |
| 6   | f     | 31/44 (70%)    | -0.39  | 1 (3%) 50 52 | 53, 66, 94, 132       | 1 (3%)    |
| 7   | H     | 64/65 (98%)    | -0.45  | 1 (1%) 70 71 | 53, 62, 88, 108       | 0         |
| 7   | h     | 64/65 (98%)    | -0.48  | 0 100 100    | 39, 72, 93, 105       | 1 (1%)    |
| 8   | I     | 37/38 (97%)    | -0.29  | 0 100 100    | 55, 65, 117, 143      | 0         |
| 8   | i     | 37/38 (97%)    | -0.46  | 0 100 100    | 53, 64, 111, 130      | 0         |
| 9   | J     | 38/39 (97%)    | -0.50  | 0 100 100    | 49, 67, 118, 153      | 0         |
| 9   | j     | 39/39 (100%)   | -0.41  | 0 100 100    | 56, 77, 124, 150      | 0         |
| 10  | K     | 37/37 (100%)   | -0.75  | 0 100 100    | 57, 66, 85, 105       | 0         |
| 10  | k     | 37/37 (100%)   | -0.62  | 0 100 100    | 67, 74, 95, 111       | 0         |
| 11  | L     | 36/37 (97%)    | -0.81  | 0 100 100    | 22, 45, 110, 128      | 2 (5%)    |
| 11  | l     | 36/37 (97%)    | -0.70  | 0 100 100    | 23, 46, 104, 118      | 2 (5%)    |
| 12  | M     | 32/36 (88%)    | -0.81  | 0 100 100    | 25, 47, 76, 125       | 1 (3%)    |
| 12  | m     | 33/36 (91%)    | -0.75  | 0 100 100    | 23, 48, 71, 137       | 2 (6%)    |

*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%)   | -0.64  | 0       | 100 | 100 | 20, 64, 118, 161      | 10 (4%)   |
| 13  | o     | 243/244 (99%)   | -0.58  | 0       | 100 | 100 | 22, 68, 121, 153      | 8 (3%)    |
| 14  | T     | 29/32 (90%)     | -0.75  | 0       | 100 | 100 | 25, 45, 54, 65        | 6 (20%)   |
| 14  | t     | 29/32 (90%)     | -0.75  | 1 (3%)  | 48  | 50  | 26, 46, 59, 72        | 5 (17%)   |
| 15  | U     | 96/104 (92%)    | -0.73  | 0       | 100 | 100 | 24, 57, 87, 101       | 4 (4%)    |
| 15  | u     | 97/104 (93%)    | -0.80  | 0       | 100 | 100 | 28, 60, 80, 121       | 4 (4%)    |
| 16  | V     | 137/137 (100%)  | -0.84  | 0       | 100 | 100 | 23, 56, 81, 103       | 6 (4%)    |
| 16  | v     | 137/137 (100%)  | -0.67  | 0       | 100 | 100 | 26, 70, 99, 131       | 6 (4%)    |
| 17  | X     | 38/40 (95%)     | -0.34  | 0       | 100 | 100 | 34, 73, 92, 111       | 1 (2%)    |
| 17  | x     | 38/40 (95%)     | -0.20  | 0       | 100 | 100 | 67, 80, 118, 151      | 0         |
| 18  | Y     | 29/30 (96%)     | -0.25  | 0       | 100 | 100 | 67, 81, 117, 120      | 0         |
| 18  | y     | 29/30 (96%)     | -0.33  | 0       | 100 | 100 | 77, 88, 110, 112      | 0         |
| 19  | Z     | 62/62 (100%)    | -0.43  | 0       | 100 | 100 | 67, 81, 130, 150      | 0         |
| 19  | z     | 62/62 (100%)    | -0.02  | 0       | 100 | 100 | 80, 94, 137, 165      | 0         |
| 20  | R     | 34/34 (100%)    | 0.41   | 1 (2%)  | 54  | 55  | 87, 110, 132, 143     | 0         |
| All | All   | 5283/5384 (98%) | -0.65  | 8 (0%)  | 92  | 92  | 19, 57, 100, 165      | 970 (18%) |

All (8) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 7   | H     | 65     | LEU  | 3.7  |
| 5   | e     | 79[A]  | PHE  | 3.4  |
| 6   | f     | 16[A]  | PHE  | 2.9  |
| 3   | c     | 245[A] | ILE  | 2.1  |
| 1   | A     | 11     | ALA  | 2.1  |
| 1   | a     | 11     | ALA  | 2.1  |
| 20  | R     | 28     | VAL  | 2.1  |
| 14  | t     | 30[A]  | THR  | 2.0  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 8   | FME  | I     | 1   | 10/11 | 0.95 | 0.07 | 60,70,83,88                 | 0     |
| 14  | FME  | T     | 1   | 10/11 | 0.96 | 0.07 | 43,53,70,79                 | 0     |
| 14  | FME  | t     | 1   | 10/11 | 0.96 | 0.07 | 41,46,62,73                 | 0     |
| 12  | FME  | m     | 1   | 10/11 | 0.97 | 0.07 | 50,61,88,116                | 0     |
| 8   | FME  | i     | 1   | 10/11 | 0.97 | 0.07 | 54,70,80,85                 | 0     |
| 12  | FME  | M     | 1   | 10/11 | 0.98 | 0.06 | 43,55,88,98                 | 0     |

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 26  | GOL  | a     | 417    | 6/6   | 0.61 | 0.17 | 79,98,105,108               | 0     |
| 32  | LMT  | F     | 101    | 35/35 | 0.69 | 0.15 | 91,127,168,174              | 0     |
| 32  | LMT  | e     | 101    | 35/35 | 0.69 | 0.14 | 100,141,180,182             | 0     |
| 29  | UNL  | A     | 414    | 28/-  | 0.70 | 0.14 | 81,103,122,140              | 0     |
| 29  | UNL  | a     | 414    | 30/-  | 0.70 | 0.12 | 80,106,129,138              | 0     |
| 29  | UNL  | j     | 101    | 10/-  | 0.71 | 0.19 | 73,87,102,104               | 0     |
| 32  | LMT  | A     | 419    | 35/35 | 0.71 | 0.12 | 89,125,143,156              | 0     |
| 29  | UNL  | K     | 101[B] | 34/-  | 0.72 | 0.14 | 72,97,111,114               | 34    |
| 32  | LMT  | B     | 627    | 35/35 | 0.72 | 0.14 | 62,116,137,153              | 0     |
| 29  | UNL  | I     | 101    | 40/-  | 0.72 | 0.15 | 73,100,150,155              | 0     |
| 29  | UNL  | K     | 101[A] | 34/-  | 0.72 | 0.14 | 72,97,111,114               | 34    |
| 29  | UNL  | m     | 102    | 10/-  | 0.73 | 0.19 | 61,71,91,93                 | 0     |
| 32  | LMT  | A     | 417    | 35/35 | 0.73 | 0.12 | 59,109,132,137              | 0     |
| 25  | SQD  | f     | 102    | 43/54 | 0.74 | 0.13 | 94,125,167,177              | 0     |
| 29  | UNL  | J     | 101    | 10/-  | 0.74 | 0.22 | 60,75,83,91                 | 0     |
| 35  | HTG  | C     | 522    | 19/19 | 0.74 | 0.12 | 99,119,131,131              | 0     |
| 32  | LMT  | a     | 416    | 35/35 | 0.75 | 0.12 | 107,126,147,155             | 0     |
| 33  | LHG  | a     | 419[A] | 42/49 | 0.76 | 0.11 | 85,125,144,152              | 42    |
| 33  | LHG  | a     | 419[B] | 42/49 | 0.76 | 0.11 | 85,125,144,152              | 42    |
| 29  | UNL  | l     | 102    | 10/-  | 0.76 | 0.16 | 63,77,90,92                 | 0     |
| 29  | UNL  | B     | 628    | 40/-  | 0.78 | 0.13 | 71,99,149,159               | 0     |
| 29  | UNL  | b     | 626    | 33/-  | 0.79 | 0.13 | 63,94,149,161               | 0     |
| 29  | UNL  | c     | 525[B] | 32/-  | 0.80 | 0.14 | 86,104,116,126              | 32    |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 26  | GOL  | B     | 625    | 6/6   | 0.80 | 0.14 | 68,88,99,112                | 0     |
| 29  | UNL  | c     | 525[A] | 32/-  | 0.80 | 0.14 | 86,104,116,126              | 32    |
| 35  | HTG  | B     | 621    | 19/19 | 0.80 | 0.14 | 60,90,112,112               | 0     |
| 32  | LMT  | b     | 621    | 25/35 | 0.80 | 0.12 | 78,103,153,161              | 0     |
| 34  | LMG  | C     | 521    | 51/55 | 0.81 | 0.11 | 56,115,150,170              | 0     |
| 26  | GOL  | o     | 303    | 6/6   | 0.81 | 0.15 | 79,100,105,111              | 0     |
| 26  | GOL  | o     | 304    | 6/6   | 0.81 | 0.14 | 76,87,97,97                 | 0     |
| 35  | HTG  | D     | 411    | 16/19 | 0.81 | 0.12 | 88,102,126,149              | 0     |
| 35  | HTG  | c     | 522    | 19/19 | 0.81 | 0.10 | 103,120,141,142             | 0     |
| 26  | GOL  | d     | 413    | 6/6   | 0.82 | 0.21 | 49,63,77,82                 | 0     |
| 29  | UNL  | D     | 410    | 40/-  | 0.82 | 0.12 | 62,90,136,141               | 0     |
| 35  | HTG  | b     | 623    | 19/19 | 0.82 | 0.12 | 79,124,158,158              | 0     |
| 26  | GOL  | O     | 302    | 6/6   | 0.82 | 0.09 | 79,87,104,108               | 0     |
| 32  | LMT  | T     | 101    | 35/35 | 0.83 | 0.10 | 61,120,165,176              | 0     |
| 28  | PL9  | A     | 413[A] | 55/55 | 0.83 | 0.14 | 61,85,102,106               | 55    |
| 28  | PL9  | A     | 413[B] | 55/55 | 0.83 | 0.14 | 61,85,102,106               | 55    |
| 32  | LMT  | B     | 626    | 35/35 | 0.83 | 0.11 | 66,102,146,152              | 0     |
| 26  | GOL  | A     | 410    | 6/6   | 0.83 | 0.13 | 63,79,84,85                 | 0     |
| 26  | GOL  | O     | 303    | 6/6   | 0.83 | 0.13 | 69,83,99,99                 | 0     |
| 28  | PL9  | a     | 413[A] | 55/55 | 0.84 | 0.13 | 72,95,109,116               | 55    |
| 32  | LMT  | B     | 629    | 25/35 | 0.84 | 0.12 | 56,84,135,159               | 0     |
| 29  | UNL  | d     | 410    | 36/-  | 0.84 | 0.10 | 65,96,131,136               | 0     |
| 28  | PL9  | a     | 413[B] | 55/55 | 0.84 | 0.13 | 72,95,109,117               | 55    |
| 25  | SQD  | a     | 411    | 54/54 | 0.84 | 0.10 | 63,90,135,145               | 0     |
| 34  | LMG  | Z     | 101    | 37/55 | 0.85 | 0.13 | 66,115,142,163              | 0     |
| 29  | UNL  | B     | 624    | 33/-  | 0.85 | 0.13 | 54,104,138,148              | 0     |
| 32  | LMT  | m     | 103    | 35/35 | 0.85 | 0.10 | 54,88,104,115               | 0     |
| 26  | GOL  | v     | 202[B] | 6/6   | 0.85 | 0.11 | 60,72,79,80                 | 6     |
| 35  | HTG  | b     | 622    | 19/19 | 0.85 | 0.12 | 60,90,115,118               | 0     |
| 26  | GOL  | b     | 624    | 6/6   | 0.85 | 0.14 | 84,98,100,109               | 0     |
| 26  | GOL  | v     | 202[A] | 6/6   | 0.85 | 0.11 | 60,72,80,80                 | 6     |
| 35  | HTG  | d     | 411    | 16/19 | 0.85 | 0.11 | 89,124,140,154              | 0     |
| 34  | LMG  | z     | 101    | 39/55 | 0.86 | 0.12 | 72,125,150,157              | 0     |
| 25  | SQD  | A     | 411    | 54/54 | 0.86 | 0.10 | 57,86,128,153               | 0     |
| 34  | LMG  | c     | 521    | 51/55 | 0.86 | 0.10 | 74,126,157,185              | 0     |
| 32  | LMT  | t     | 101    | 26/35 | 0.86 | 0.11 | 64,98,139,140               | 0     |
| 37  | CA   | F     | 103    | 1/1   | 0.86 | 0.23 | 122,122,122,122             | 0     |
| 35  | HTG  | V     | 202    | 11/19 | 0.87 | 0.09 | 78,108,125,127              | 0     |
| 32  | LMT  | M     | 101    | 35/35 | 0.87 | 0.10 | 57,93,120,130               | 0     |
| 32  | LMT  | b     | 627    | 25/35 | 0.87 | 0.12 | 51,88,142,153               | 0     |
| 25  | SQD  | X     | 101    | 43/54 | 0.88 | 0.11 | 72,103,125,141              | 0     |
| 26  | GOL  | l     | 103[A] | 6/6   | 0.88 | 0.15 | 61,91,98,100                | 6     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 26  | GOL  | l     | 103[B] | 6/6   | 0.88 | 0.15 | 61,91,98,100                | 6     |
| 26  | GOL  | c     | 527    | 6/6   | 0.88 | 0.14 | 89,98,113,115               | 0     |
| 23  | CLA  | b     | 601    | 65/65 | 0.89 | 0.10 | 59,90,123,154               | 0     |
| 29  | UNL  | D     | 409    | 17/-  | 0.89 | 0.11 | 62,72,103,109               | 0     |
| 25  | SQD  | l     | 101    | 54/54 | 0.89 | 0.09 | 59,87,139,148               | 0     |
| 25  | SQD  | b     | 620    | 54/54 | 0.89 | 0.09 | 55,94,121,128               | 0     |
| 33  | LHG  | E     | 101[A] | 42/49 | 0.89 | 0.10 | 71,96,111,117               | 42    |
| 33  | LHG  | E     | 101[B] | 42/49 | 0.89 | 0.10 | 71,96,111,117               | 42    |
| 26  | GOL  | a     | 410    | 6/6   | 0.89 | 0.12 | 70,73,91,93                 | 0     |
| 35  | HTG  | o     | 301    | 19/19 | 0.90 | 0.11 | 58,83,117,119               | 0     |
| 35  | HTG  | B     | 623    | 19/19 | 0.90 | 0.08 | 64,77,94,103                | 0     |
| 26  | GOL  | V     | 203[A] | 6/6   | 0.91 | 0.11 | 56,65,67,73                 | 6     |
| 26  | GOL  | V     | 203[B] | 6/6   | 0.91 | 0.11 | 56,65,67,73                 | 6     |
| 26  | GOL  | D     | 413    | 6/6   | 0.91 | 0.14 | 45,64,71,91                 | 0     |
| 26  | GOL  | B     | 622    | 6/6   | 0.91 | 0.13 | 66,76,84,85                 | 0     |
| 26  | GOL  | a     | 418    | 6/6   | 0.91 | 0.21 | 54,74,79,80                 | 0     |
| 34  | LMG  | C     | 501    | 51/55 | 0.91 | 0.09 | 64,89,114,133               | 0     |
| 23  | CLA  | B     | 601    | 65/65 | 0.91 | 0.09 | 56,80,112,156               | 0     |
| 37  | CA   | f     | 103    | 1/1   | 0.91 | 0.10 | 117,117,117,117             | 0     |
| 23  | CLA  | c     | 514    | 65/65 | 0.92 | 0.09 | 68,96,126,148               | 0     |
| 34  | LMG  | C     | 520    | 51/55 | 0.92 | 0.09 | 54,81,114,130               | 0     |
| 26  | GOL  | D     | 402    | 6/6   | 0.92 | 0.24 | 47,72,77,80                 | 0     |
| 34  | LMG  | c     | 501    | 51/55 | 0.92 | 0.08 | 69,91,107,113               | 0     |
| 34  | LMG  | c     | 520    | 51/55 | 0.92 | 0.09 | 59,90,127,156               | 0     |
| 34  | LMG  | B     | 620    | 51/55 | 0.92 | 0.07 | 49,66,89,112                | 0     |
| 34  | LMG  | m     | 101    | 51/55 | 0.92 | 0.08 | 48,72,97,107                | 0     |
| 25  | SQD  | A     | 409[A] | 54/54 | 0.93 | 0.09 | 56,78,109,113               | 54    |
| 29  | UNL  | d     | 409    | 17/-  | 0.93 | 0.09 | 67,80,117,121               | 0     |
| 25  | SQD  | A     | 409[B] | 54/54 | 0.93 | 0.09 | 56,78,109,113               | 54    |
| 23  | CLA  | c     | 513    | 65/65 | 0.93 | 0.09 | 59,80,117,144               | 0     |
| 23  | CLA  | C     | 514    | 65/65 | 0.93 | 0.08 | 63,87,112,119               | 0     |
| 24  | BCR  | C     | 515    | 40/40 | 0.93 | 0.08 | 55,73,87,93                 | 0     |
| 24  | BCR  | D     | 405    | 40/40 | 0.93 | 0.08 | 41,56,98,102                | 0     |
| 24  | BCR  | T     | 102    | 40/40 | 0.93 | 0.07 | 43,58,70,78                 | 0     |
| 34  | LMG  | D     | 412    | 51/55 | 0.93 | 0.08 | 46,67,120,132               | 0     |
| 24  | BCR  | d     | 405    | 40/40 | 0.93 | 0.08 | 48,64,98,104                | 0     |
| 24  | BCR  | t     | 102    | 40/40 | 0.93 | 0.07 | 40,58,79,85                 | 0     |
| 33  | LHG  | A     | 418[A] | 49/49 | 0.93 | 0.08 | 46,60,79,84                 | 49    |
| 36  | DGD  | C     | 518[A] | 62/66 | 0.93 | 0.08 | 50,63,110,114               | 62    |
| 36  | DGD  | C     | 518[B] | 62/66 | 0.93 | 0.08 | 50,63,110,114               | 62    |
| 34  | LMG  | d     | 412    | 51/55 | 0.93 | 0.08 | 54,68,116,145               | 0     |
| 33  | LHG  | A     | 418[B] | 49/49 | 0.93 | 0.08 | 46,60,79,84                 | 49    |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 24  | BCR  | c     | 515    | 40/40 | 0.94 | 0.08 | 66,82,95,96                 | 0     |
| 23  | CLA  | C     | 507    | 65/65 | 0.94 | 0.08 | 54,70,117,136               | 0     |
| 26  | GOL  | b     | 628    | 6/6   | 0.94 | 0.08 | 75,79,82,86                 | 0     |
| 23  | CLA  | B     | 614    | 65/65 | 0.94 | 0.07 | 35,49,100,116               | 0     |
| 33  | LHG  | D     | 408[A] | 49/49 | 0.94 | 0.09 | 43,58,107,110               | 49    |
| 33  | LHG  | D     | 408[B] | 49/49 | 0.94 | 0.09 | 43,58,107,110               | 49    |
| 23  | CLA  | d     | 404    | 65/65 | 0.94 | 0.09 | 54,68,124,147               | 0     |
| 26  | GOL  | C     | 523[A] | 6/6   | 0.94 | 0.09 | 53,56,61,68                 | 6     |
| 26  | GOL  | C     | 523[B] | 6/6   | 0.94 | 0.09 | 54,58,61,68                 | 6     |
| 24  | BCR  | B     | 619    | 40/40 | 0.94 | 0.08 | 46,58,90,104                | 0     |
| 33  | LHG  | d     | 414[A] | 49/49 | 0.94 | 0.08 | 48,65,80,87                 | 49    |
| 33  | LHG  | d     | 414[B] | 49/49 | 0.94 | 0.08 | 48,66,80,87                 | 49    |
| 35  | HTG  | b     | 625    | 19/19 | 0.94 | 0.07 | 61,79,95,108                | 0     |
| 23  | CLA  | C     | 505    | 65/65 | 0.94 | 0.07 | 40,56,98,131                | 0     |
| 23  | CLA  | b     | 616    | 65/65 | 0.94 | 0.08 | 50,63,122,134               | 0     |
| 25  | SQD  | a     | 409[A] | 54/54 | 0.94 | 0.09 | 60,81,112,118               | 54    |
| 25  | SQD  | a     | 409[B] | 54/54 | 0.94 | 0.09 | 60,80,112,118               | 54    |
| 24  | BCR  | K     | 102    | 40/40 | 0.94 | 0.09 | 54,65,80,91                 | 0     |
| 36  | DGD  | c     | 517[A] | 62/66 | 0.94 | 0.08 | 49,65,100,108               | 62    |
| 36  | DGD  | c     | 517[B] | 62/66 | 0.94 | 0.08 | 49,65,100,108               | 62    |
| 36  | DGD  | c     | 518[A] | 62/66 | 0.94 | 0.07 | 53,67,118,128               | 62    |
| 36  | DGD  | c     | 518[B] | 62/66 | 0.94 | 0.07 | 53,68,118,128               | 62    |
| 36  | DGD  | c     | 519    | 62/66 | 0.94 | 0.07 | 48,63,100,128               | 0     |
| 23  | CLA  | c     | 507    | 65/65 | 0.94 | 0.08 | 47,70,117,134               | 0     |
| 24  | BCR  | Y     | 101    | 40/40 | 0.94 | 0.08 | 54,63,80,89                 | 0     |
| 37  | CA   | o     | 302    | 1/1   | 0.94 | 0.07 | 113,113,113,113             | 0     |
| 26  | GOL  | c     | 526[B] | 6/6   | 0.95 | 0.08 | 64,66,71,74                 | 6     |
| 23  | CLA  | A     | 407    | 65/65 | 0.95 | 0.08 | 39,52,127,140               | 0     |
| 24  | BCR  | A     | 408    | 40/40 | 0.95 | 0.07 | 40,51,64,65                 | 0     |
| 29  | UNL  | d     | 415    | 18/-  | 0.95 | 0.09 | 66,79,126,127               | 0     |
| 24  | BCR  | B     | 618    | 40/40 | 0.95 | 0.06 | 37,54,69,79                 | 0     |
| 23  | CLA  | a     | 405[A] | 65/65 | 0.95 | 0.07 | 38,52,118,133               | 65    |
| 23  | CLA  | a     | 405[B] | 65/65 | 0.95 | 0.07 | 38,52,118,133               | 65    |
| 30  | BCT  | d     | 401[A] | 4/4   | 0.95 | 0.07 | 53,60,61,76                 | 4     |
| 30  | BCT  | d     | 401[B] | 4/4   | 0.95 | 0.07 | 54,60,61,77                 | 4     |
| 23  | CLA  | a     | 407    | 65/65 | 0.95 | 0.10 | 42,55,139,160               | 0     |
| 24  | BCR  | H     | 101    | 40/40 | 0.95 | 0.08 | 50,64,84,89                 | 0     |
| 23  | CLA  | B     | 616    | 65/65 | 0.95 | 0.08 | 46,59,129,139               | 0     |
| 23  | CLA  | b     | 606    | 65/65 | 0.95 | 0.07 | 42,62,115,119               | 0     |
| 23  | CLA  | b     | 614    | 65/65 | 0.95 | 0.07 | 39,50,98,113                | 0     |
| 28  | PL9  | D     | 406[A] | 55/55 | 0.95 | 0.07 | 35,47,55,65                 | 55    |
| 28  | PL9  | D     | 406[B] | 55/55 | 0.95 | 0.07 | 35,47,55,64                 | 55    |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 24  | BCR  | b     | 617    | 40/40 | 0.95 | 0.06 | 41,52,64,66                 | 0     |
| 24  | BCR  | b     | 618    | 40/40 | 0.95 | 0.06 | 42,57,76,84                 | 0     |
| 24  | BCR  | b     | 619    | 40/40 | 0.95 | 0.07 | 48,61,90,95                 | 0     |
| 23  | CLA  | B     | 603    | 65/65 | 0.95 | 0.08 | 43,53,73,87                 | 0     |
| 24  | BCR  | c     | 516    | 40/40 | 0.95 | 0.07 | 57,66,80,82                 | 0     |
| 23  | CLA  | c     | 505    | 65/65 | 0.95 | 0.07 | 46,64,108,137               | 0     |
| 24  | BCR  | h     | 101    | 40/40 | 0.95 | 0.09 | 54,69,91,98                 | 0     |
| 24  | BCR  | k     | 101    | 40/40 | 0.95 | 0.08 | 56,72,84,86                 | 0     |
| 23  | CLA  | B     | 606    | 65/65 | 0.95 | 0.08 | 41,57,108,129               | 0     |
| 24  | BCR  | y     | 101    | 40/40 | 0.95 | 0.07 | 58,72,85,96                 | 0     |
| 23  | CLA  | c     | 508    | 65/65 | 0.95 | 0.09 | 49,68,83,90                 | 0     |
| 36  | DGD  | C     | 519    | 62/66 | 0.95 | 0.07 | 41,56,101,115               | 0     |
| 29  | UNL  | X     | 102    | 18/-  | 0.95 | 0.09 | 52,68,103,105               | 0     |
| 23  | CLA  | C     | 509    | 65/65 | 0.95 | 0.07 | 44,55,117,141               | 0     |
| 23  | CLA  | C     | 513    | 65/65 | 0.95 | 0.08 | 57,75,108,121               | 0     |
| 26  | GOL  | c     | 526[A] | 6/6   | 0.95 | 0.08 | 65,66,71,74                 | 6     |
| 33  | LHG  | b     | 629[A] | 49/49 | 0.95 | 0.07 | 45,57,70,81                 | 49    |
| 36  | DGD  | h     | 102    | 62/66 | 0.95 | 0.07 | 51,65,80,90                 | 0     |
| 33  | LHG  | b     | 629[B] | 49/49 | 0.95 | 0.07 | 45,57,70,82                 | 49    |
| 33  | LHG  | d     | 408[A] | 49/49 | 0.95 | 0.09 | 49,63,108,129               | 49    |
| 33  | LHG  | d     | 408[B] | 49/49 | 0.95 | 0.09 | 49,63,108,129               | 49    |
| 23  | CLA  | c     | 504    | 65/65 | 0.96 | 0.06 | 51,71,85,88                 | 0     |
| 28  | PL9  | d     | 406[A] | 55/55 | 0.96 | 0.06 | 37,49,59,65                 | 55    |
| 28  | PL9  | d     | 406[B] | 55/55 | 0.96 | 0.06 | 37,49,59,65                 | 55    |
| 23  | CLA  | C     | 508    | 65/65 | 0.96 | 0.07 | 52,64,85,95                 | 0     |
| 23  | CLA  | c     | 506    | 65/65 | 0.96 | 0.07 | 47,65,92,105                | 0     |
| 23  | CLA  | A     | 406[B] | 65/65 | 0.96 | 0.06 | 36,45,110,121               | 65    |
| 23  | CLA  | C     | 510    | 65/65 | 0.96 | 0.08 | 44,59,84,91                 | 0     |
| 23  | CLA  | c     | 509    | 65/65 | 0.96 | 0.07 | 47,62,121,152               | 0     |
| 23  | CLA  | c     | 512    | 65/65 | 0.96 | 0.07 | 54,70,85,101                | 0     |
| 23  | CLA  | B     | 607    | 65/65 | 0.96 | 0.06 | 32,46,73,77                 | 0     |
| 23  | CLA  | B     | 611    | 65/65 | 0.96 | 0.06 | 32,44,65,72                 | 0     |
| 23  | CLA  | D     | 404    | 65/65 | 0.96 | 0.07 | 49,58,120,137               | 0     |
| 23  | CLA  | B     | 613    | 65/65 | 0.96 | 0.06 | 38,46,99,109                | 0     |
| 23  | CLA  | A     | 404[A] | 65/65 | 0.96 | 0.06 | 35,41,54,66                 | 65    |
| 23  | CLA  | A     | 404[B] | 65/65 | 0.96 | 0.06 | 35,41,56,66                 | 65    |
| 23  | CLA  | C     | 502    | 65/65 | 0.96 | 0.06 | 49,60,75,82                 | 0     |
| 24  | BCR  | C     | 516    | 40/40 | 0.96 | 0.06 | 49,64,75,83                 | 0     |
| 23  | CLA  | B     | 602    | 65/65 | 0.96 | 0.07 | 46,56,75,88                 | 0     |
| 23  | CLA  | b     | 607    | 65/65 | 0.96 | 0.06 | 36,46,77,84                 | 0     |
| 23  | CLA  | b     | 609    | 65/65 | 0.96 | 0.07 | 51,66,83,88                 | 0     |
| 36  | DGD  | C     | 517[A] | 62/66 | 0.96 | 0.06 | 46,59,101,106               | 62    |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 36  | DGD  | C     | 517[B] | 62/66 | 0.96 | 0.06 | 46,59,101,107               | 62    |
| 23  | CLA  | b     | 612    | 65/65 | 0.96 | 0.07 | 38,53,67,76                 | 0     |
| 23  | CLA  | b     | 613    | 65/65 | 0.96 | 0.06 | 41,50,85,95                 | 0     |
| 24  | BCR  | a     | 408    | 40/40 | 0.96 | 0.06 | 40,54,63,75                 | 0     |
| 36  | DGD  | H     | 102    | 62/66 | 0.96 | 0.07 | 44,61,75,90                 | 0     |
| 33  | LHG  | d     | 407[A] | 49/49 | 0.96 | 0.07 | 47,54,69,75                 | 49    |
| 33  | LHG  | d     | 407[B] | 49/49 | 0.96 | 0.07 | 47,54,69,75                 | 49    |
| 23  | CLA  | C     | 506    | 65/65 | 0.96 | 0.07 | 50,60,91,105                | 0     |
| 23  | CLA  | A     | 406[A] | 65/65 | 0.96 | 0.06 | 36,46,110,121               | 65    |
| 31  | PHO  | A     | 416[A] | 64/64 | 0.96 | 0.06 | 38,48,54,58                 | 64    |
| 31  | PHO  | A     | 416[B] | 64/64 | 0.96 | 0.06 | 38,48,54,57                 | 64    |
| 37  | CA   | C     | 524    | 1/1   | 0.96 | 0.05 | 75,75,75,75                 | 0     |
| 31  | PHO  | a     | 415[A] | 64/64 | 0.96 | 0.06 | 45,55,62,66                 | 64    |
| 37  | CA   | O     | 301    | 1/1   | 0.96 | 0.04 | 106,106,106,106             | 0     |
| 31  | PHO  | a     | 415[B] | 64/64 | 0.96 | 0.06 | 45,55,62,67                 | 64    |
| 23  | CLA  | c     | 502    | 65/65 | 0.96 | 0.07 | 56,67,81,88                 | 0     |
| 23  | CLA  | A     | 405[A] | 65/65 | 0.97 | 0.05 | 32,42,54,66                 | 65    |
| 23  | CLA  | c     | 510    | 65/65 | 0.97 | 0.07 | 41,60,86,100                | 0     |
| 31  | PHO  | D     | 401[A] | 64/64 | 0.97 | 0.04 | 38,44,51,55                 | 64    |
| 31  | PHO  | D     | 401[B] | 64/64 | 0.97 | 0.04 | 38,44,51,55                 | 64    |
| 31  | PHO  | a     | 406[A] | 64/64 | 0.97 | 0.05 | 40,46,53,60                 | 64    |
| 31  | PHO  | a     | 406[B] | 64/64 | 0.97 | 0.05 | 40,46,53,60                 | 64    |
| 23  | CLA  | c     | 511    | 65/65 | 0.97 | 0.06 | 47,61,79,83                 | 0     |
| 23  | CLA  | C     | 504    | 65/65 | 0.97 | 0.06 | 49,62,72,83                 | 0     |
| 23  | CLA  | A     | 405[B] | 65/65 | 0.97 | 0.05 | 32,42,54,66                 | 65    |
| 23  | CLA  | B     | 609    | 65/65 | 0.97 | 0.06 | 45,59,72,76                 | 0     |
| 23  | CLA  | d     | 402[A] | 65/65 | 0.97 | 0.05 | 36,43,61,73                 | 65    |
| 23  | CLA  | d     | 402[B] | 65/65 | 0.97 | 0.05 | 36,43,61,73                 | 65    |
| 23  | CLA  | d     | 403[A] | 65/65 | 0.97 | 0.06 | 33,45,71,89                 | 65    |
| 23  | CLA  | d     | 403[B] | 65/65 | 0.97 | 0.06 | 33,45,71,89                 | 65    |
| 23  | CLA  | b     | 602    | 65/65 | 0.97 | 0.07 | 51,61,81,87                 | 0     |
| 23  | CLA  | b     | 603    | 65/65 | 0.97 | 0.06 | 44,57,75,91                 | 0     |
| 24  | BCR  | B     | 617    | 40/40 | 0.97 | 0.05 | 39,51,60,67                 | 0     |
| 23  | CLA  | b     | 604    | 65/65 | 0.97 | 0.06 | 42,52,94,121                | 0     |
| 23  | CLA  | b     | 605    | 65/65 | 0.97 | 0.06 | 38,50,74,80                 | 0     |
| 23  | CLA  | B     | 610    | 65/65 | 0.97 | 0.07 | 41,52,68,84                 | 0     |
| 22  | CL   | a     | 403[A] | 1/1   | 0.97 | 0.07 | 52,52,52,52                 | 1     |
| 23  | CLA  | b     | 608    | 65/65 | 0.97 | 0.05 | 37,56,78,98                 | 0     |
| 23  | CLA  | B     | 612    | 65/65 | 0.97 | 0.06 | 35,49,60,75                 | 0     |
| 23  | CLA  | b     | 610    | 65/65 | 0.97 | 0.07 | 47,59,71,75                 | 0     |
| 33  | LHG  | D     | 407[A] | 49/49 | 0.97 | 0.06 | 45,53,65,73                 | 49    |
| 33  | LHG  | D     | 407[B] | 49/49 | 0.97 | 0.06 | 45,53,65,73                 | 49    |

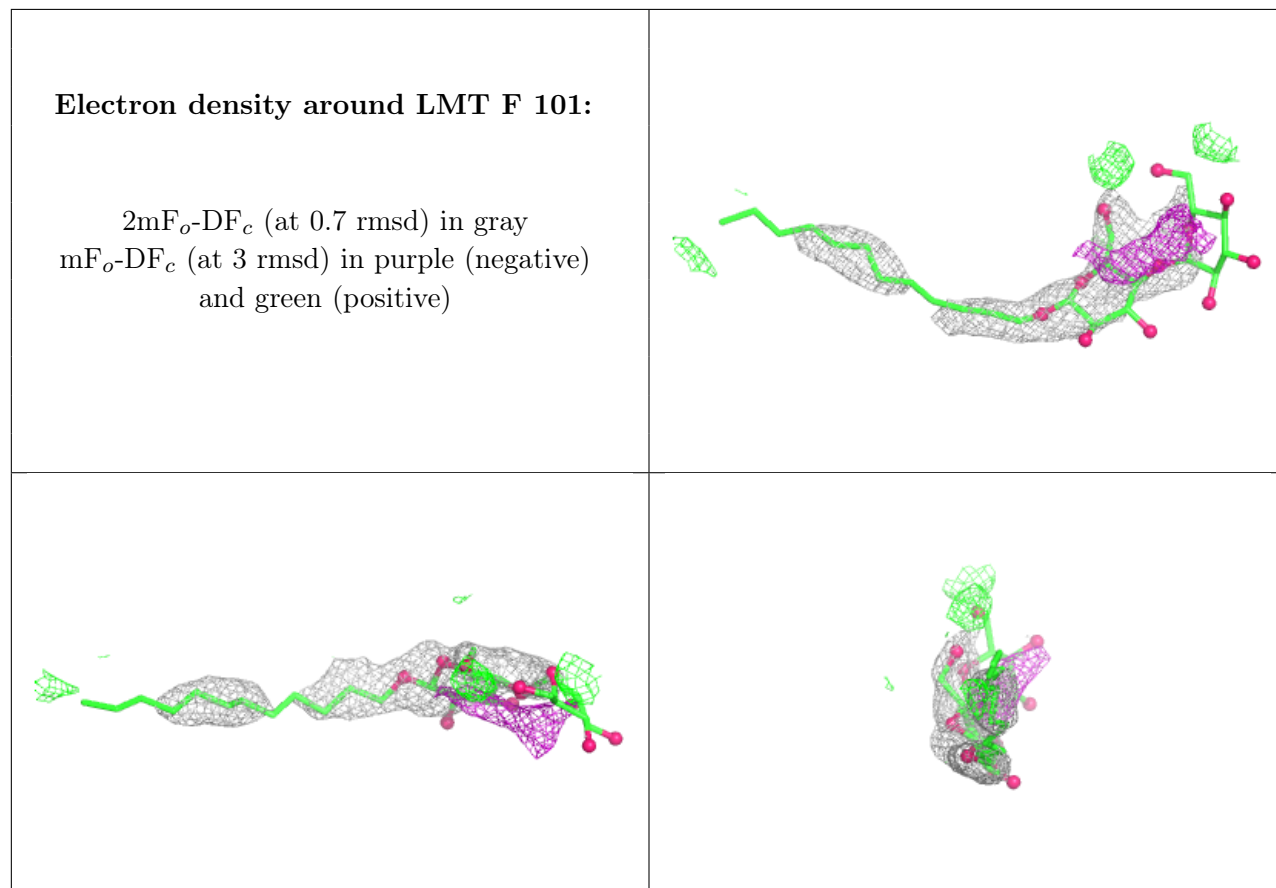
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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 23  | CLA  | b     | 611    | 65/65 | 0.97 | 0.06 | 36,48,67,85                 | 0     |
| 22  | CL   | a     | 403[B] | 1/1   | 0.97 | 0.07 | 51,51,51,51                 | 1     |
| 23  | CLA  | C     | 511    | 65/65 | 0.97 | 0.05 | 44,56,76,87                 | 0     |
| 23  | CLA  | C     | 512    | 65/65 | 0.97 | 0.07 | 52,63,82,92                 | 0     |
| 33  | LHG  | L     | 101[A] | 49/49 | 0.97 | 0.06 | 46,54,64,85                 | 49    |
| 33  | LHG  | L     | 101[B] | 49/49 | 0.97 | 0.06 | 46,54,63,85                 | 49    |
| 23  | CLA  | b     | 615    | 65/65 | 0.97 | 0.06 | 45,62,85,90                 | 0     |
| 23  | CLA  | B     | 604    | 65/65 | 0.97 | 0.06 | 35,47,105,134               | 0     |
| 23  | CLA  | B     | 615    | 65/65 | 0.97 | 0.05 | 42,53,77,94                 | 0     |
| 23  | CLA  | c     | 503    | 65/65 | 0.97 | 0.06 | 42,57,87,101                | 0     |
| 23  | CLA  | D     | 403[A] | 65/65 | 0.97 | 0.06 | 32,42,67,73                 | 65    |
| 23  | CLA  | D     | 403[B] | 65/65 | 0.97 | 0.06 | 32,42,67,73                 | 65    |
| 23  | CLA  | B     | 605    | 65/65 | 0.97 | 0.06 | 38,48,63,77                 | 0     |
| 37  | CA   | c     | 523    | 1/1   | 0.97 | 0.06 | 78,78,78,78                 | 0     |
| 23  | CLA  | a     | 404[A] | 65/65 | 0.97 | 0.06 | 36,44,61,73                 | 65    |
| 23  | CLA  | a     | 404[B] | 65/65 | 0.97 | 0.06 | 37,44,61,73                 | 65    |
| 23  | CLA  | B     | 608    | 65/65 | 0.98 | 0.05 | 35,48,69,73                 | 0     |
| 30  | BCT  | A     | 415[A] | 4/4   | 0.98 | 0.05 | 53,53,57,67                 | 4     |
| 30  | BCT  | A     | 415[B] | 4/4   | 0.98 | 0.05 | 53,53,57,67                 | 4     |
| 23  | CLA  | C     | 503    | 65/65 | 0.98 | 0.06 | 38,55,79,86                 | 0     |
| 38  | HEM  | f     | 101    | 43/43 | 0.98 | 0.07 | 60,84,110,124               | 0     |
| 40  | HEC  | V     | 201    | 43/43 | 0.98 | 0.06 | 39,52,68,71                 | 0     |
| 40  | HEC  | v     | 201    | 43/43 | 0.98 | 0.07 | 50,61,70,75                 | 0     |
| 27  | OEX  | A     | 412[A] | 10/10 | 0.99 | 0.03 | 37,44,51,55                 | 10    |
| 27  | OEX  | A     | 412[B] | 10/10 | 0.99 | 0.03 | 37,44,51,55                 | 10    |
| 22  | CL   | A     | 402[A] | 1/1   | 0.99 | 0.07 | 40,40,40,40                 | 1     |
| 37  | CA   | c     | 524    | 1/1   | 0.99 | 0.05 | 81,81,81,81                 | 0     |
| 22  | CL   | A     | 402[B] | 1/1   | 0.99 | 0.07 | 40,40,40,40                 | 1     |
| 22  | CL   | A     | 403[A] | 1/1   | 0.99 | 0.05 | 45,45,45,45                 | 1     |
| 38  | HEM  | F     | 102    | 43/43 | 0.99 | 0.06 | 52,68,86,92                 | 0     |
| 22  | CL   | A     | 403[B] | 1/1   | 0.99 | 0.05 | 45,45,45,45                 | 1     |
| 39  | MG   | J     | 102    | 1/1   | 0.99 | 0.04 | 57,57,57,57                 | 0     |
| 39  | MG   | j     | 102    | 1/1   | 0.99 | 0.04 | 64,64,64,64                 | 0     |
| 22  | CL   | a     | 402[A] | 1/1   | 0.99 | 0.07 | 47,47,47,47                 | 1     |
| 22  | CL   | a     | 402[B] | 1/1   | 0.99 | 0.07 | 47,47,47,47                 | 1     |
| 21  | FE2  | A     | 401[A] | 1/1   | 1.00 | 0.01 | 49,49,49,49                 | 1     |
| 21  | FE2  | A     | 401[B] | 1/1   | 1.00 | 0.01 | 50,50,50,50                 | 1     |
| 27  | OEX  | a     | 412[A] | 10/10 | 1.00 | 0.02 | 47,49,54,54                 | 10    |
| 27  | OEX  | a     | 412[B] | 10/10 | 1.00 | 0.02 | 46,49,53,54                 | 10    |
| 21  | FE2  | a     | 401[A] | 1/1   | 1.00 | 0.01 | 52,52,52,52                 | 1     |
| 21  | FE2  | a     | 401[B] | 1/1   | 1.00 | 0.01 | 52,52,52,52                 | 1     |

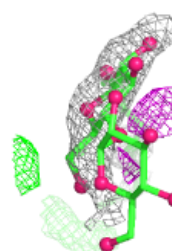
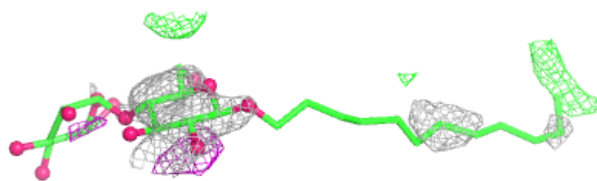
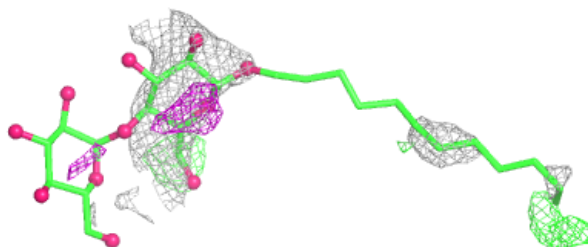
The following is a graphical depiction of the model fit to experimental electron density of all

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.

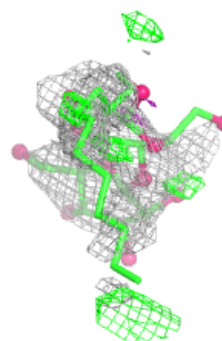
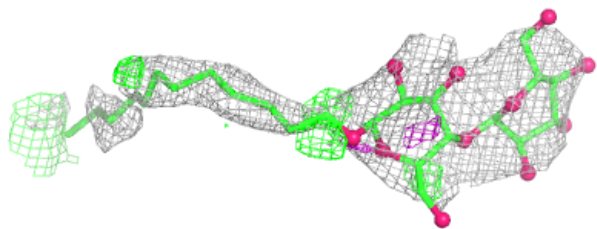
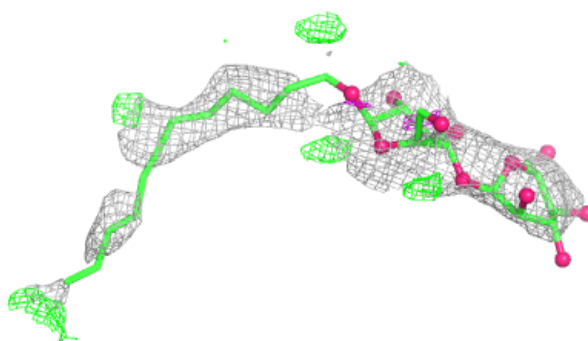


**Electron density around LMT e 101:**

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

**Electron density around LMT A 419:**

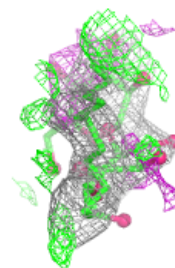
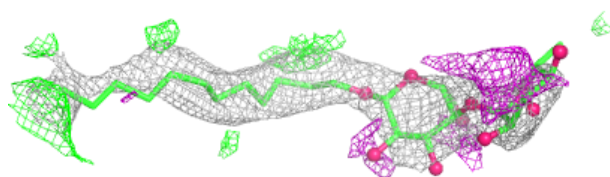
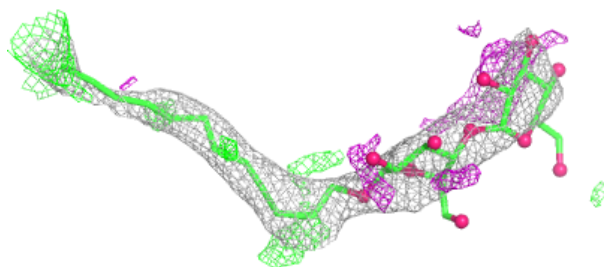
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



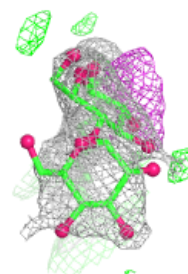
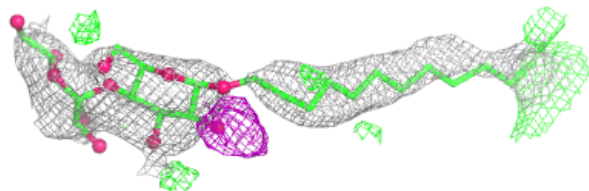
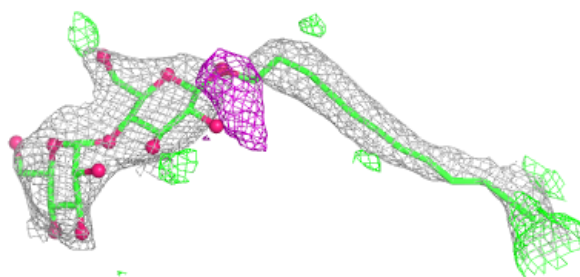


**Electron density around LMT B 627:**

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

**Electron density around LMT A 417:**

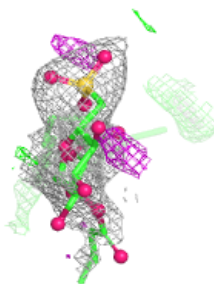
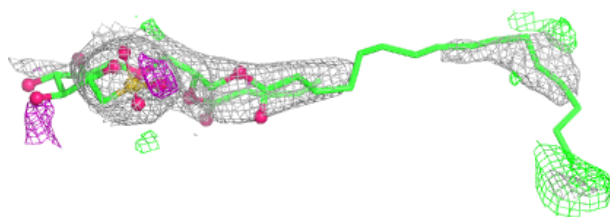
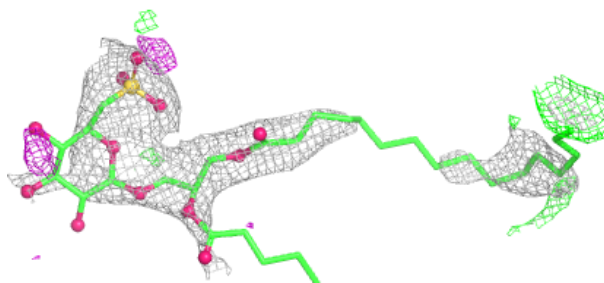
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



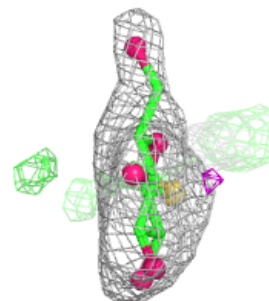
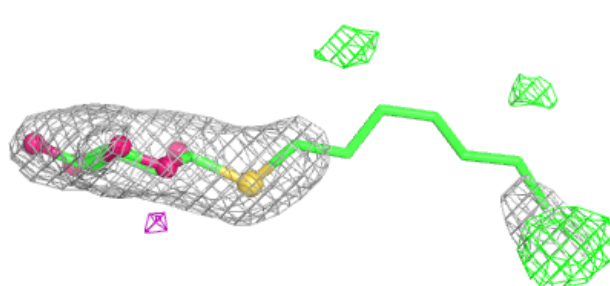
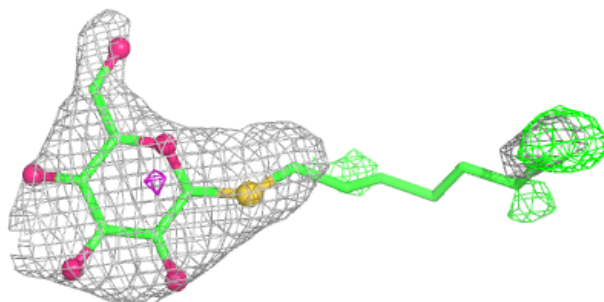


**Electron density around SQD f 102:**

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

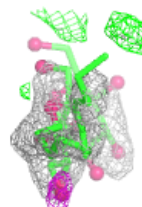
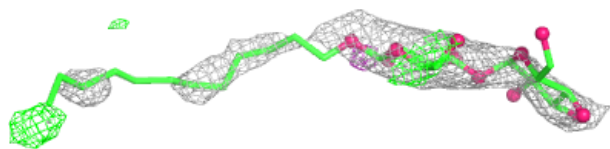
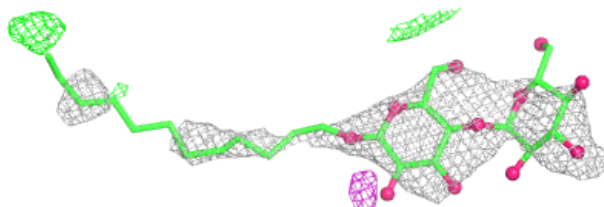
**Electron density around HTG C 522:**

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

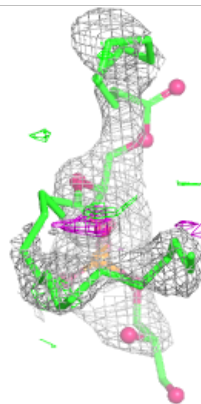
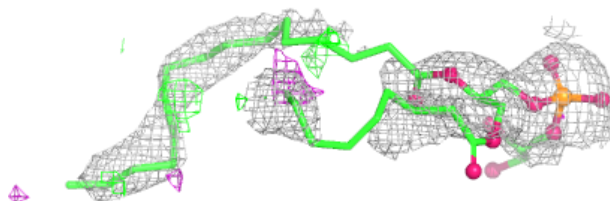
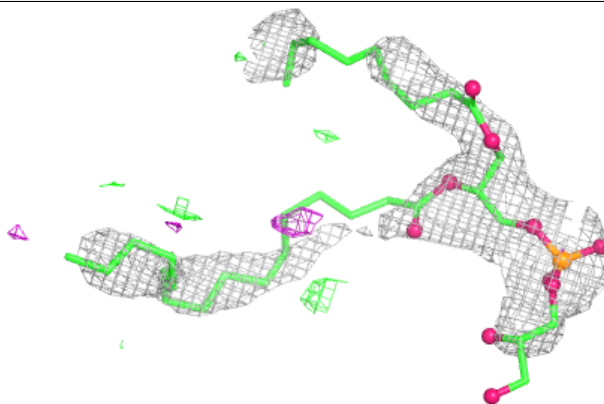


**Electron density around LMT a 416:**

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

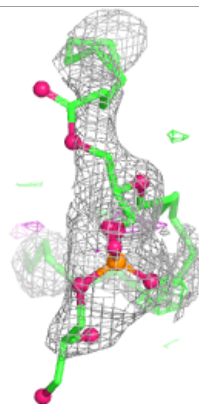
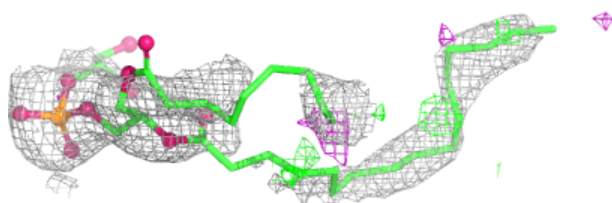
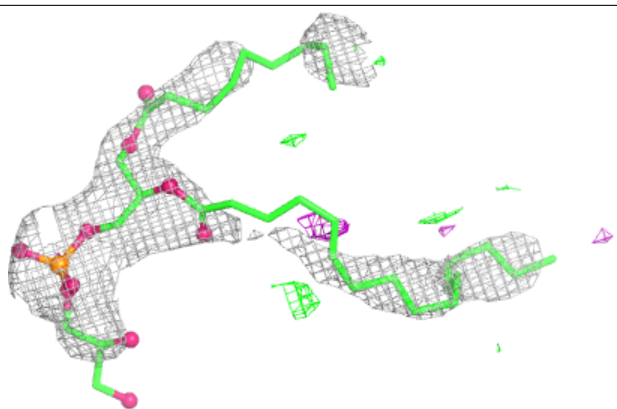
**Electron density around LHG a 419 (A):**

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

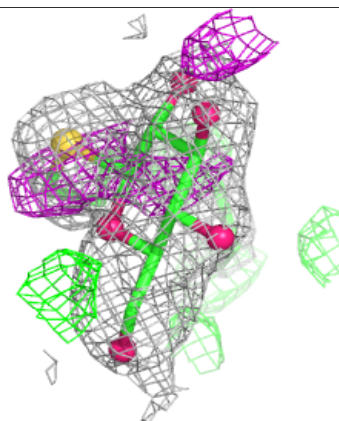
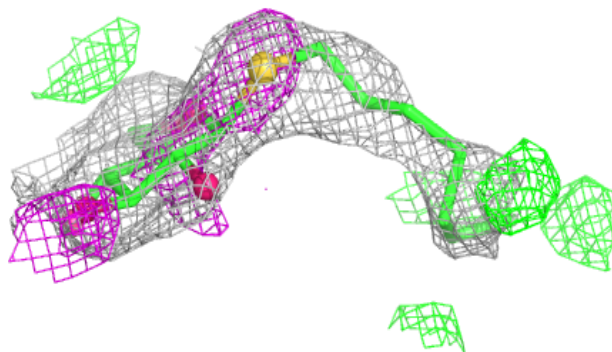
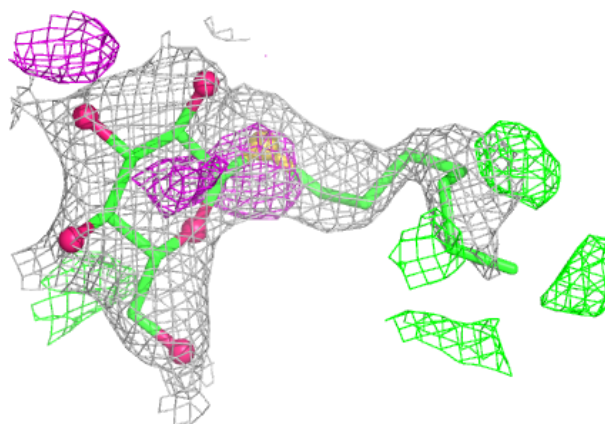


**Electron density around LHG a 419 (B):**

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

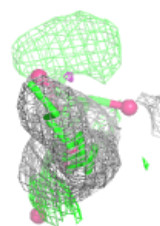
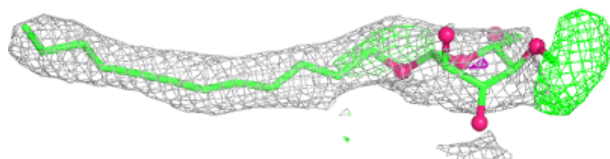
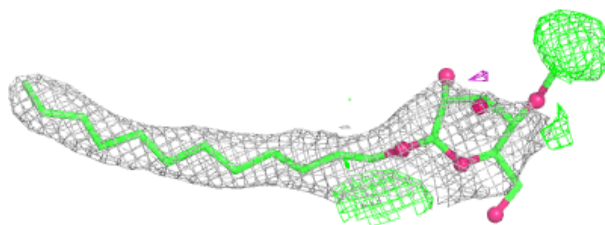
**Electron density around HTG B 621:**

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

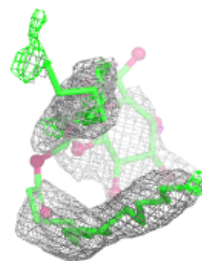
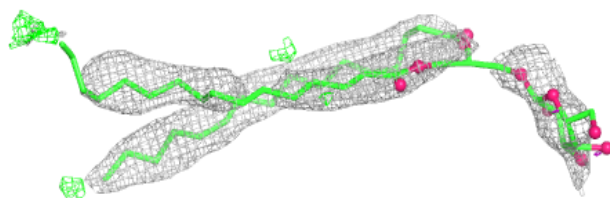
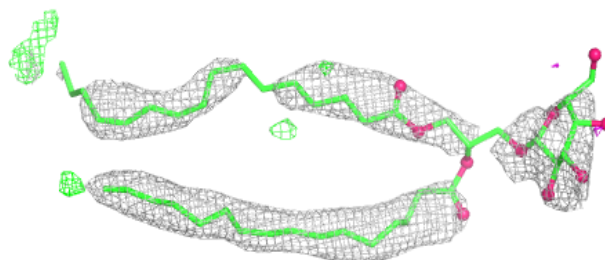


**Electron density around LMT b 621:**

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

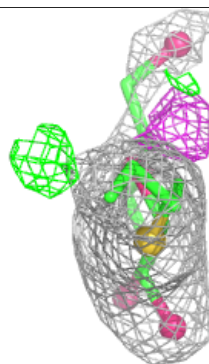
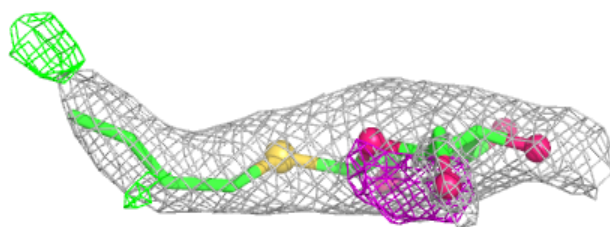
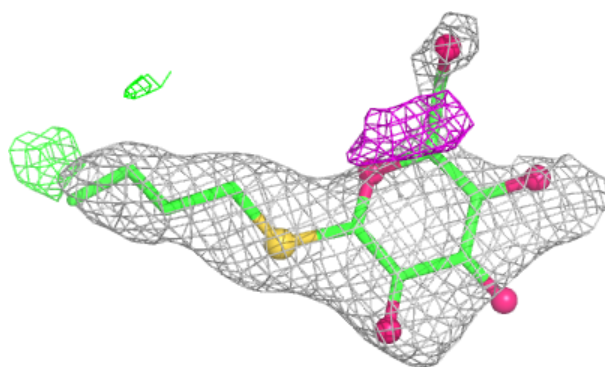
**Electron density around LMG C 521:**

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

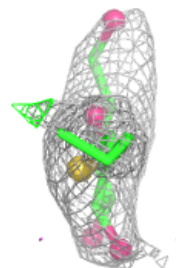
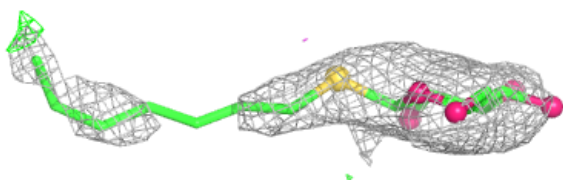
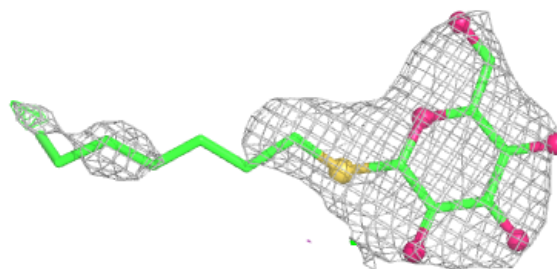


**Electron density around HTG D 411:**

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

**Electron density around HTG c 522:**

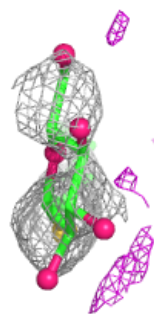
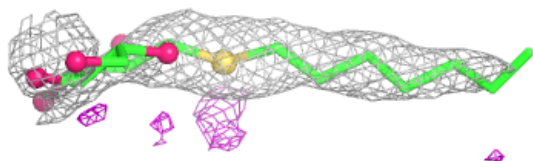
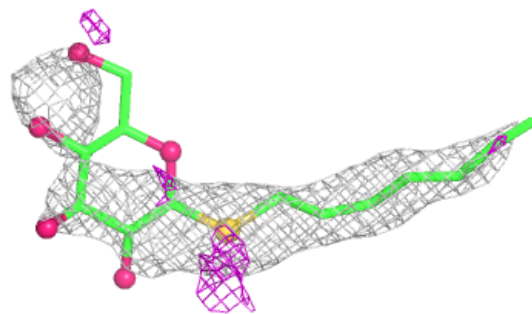
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



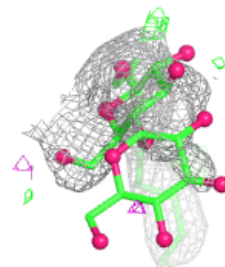
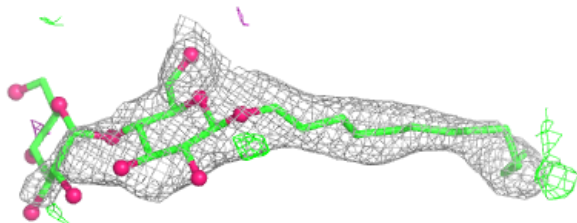
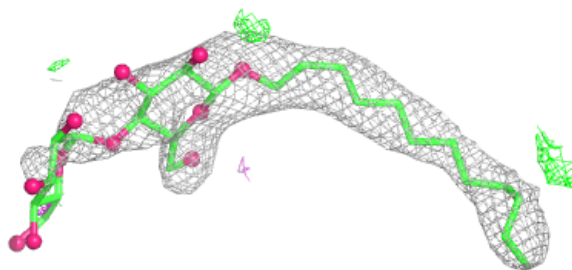


**Electron density around HTG b 623:**

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

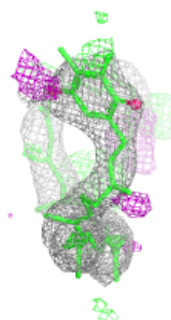
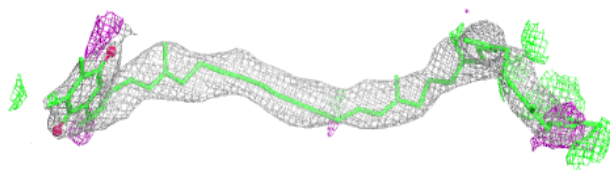
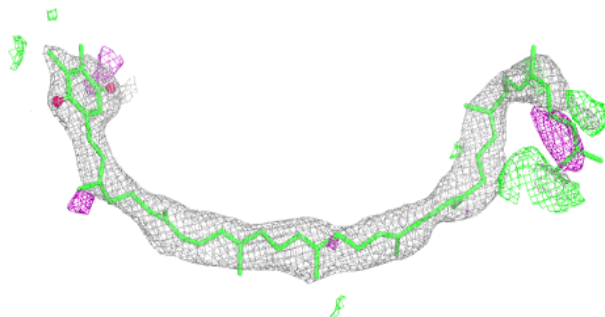
**Electron density around LMT T 101:**

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

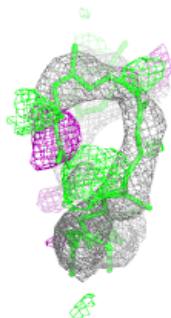
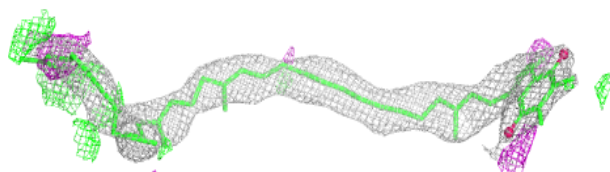
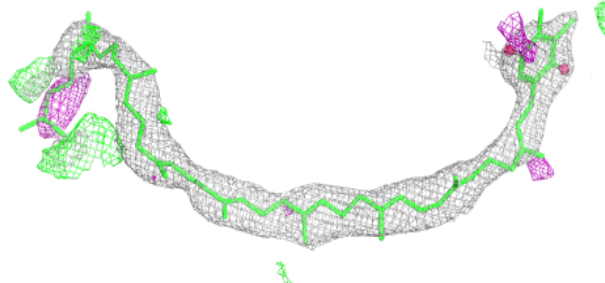


**Electron density around PL9 A 413 (A):**

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

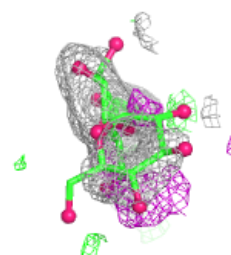
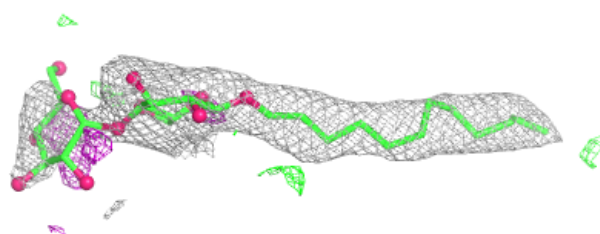
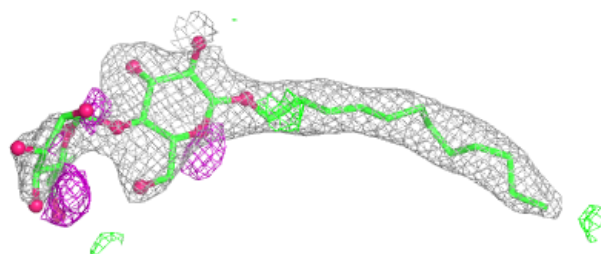
**Electron density around PL9 A 413 (B):**

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

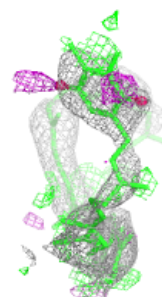
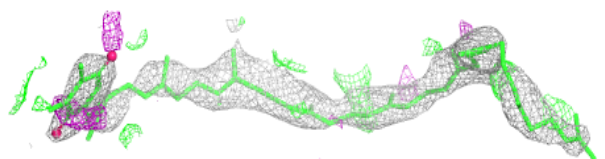
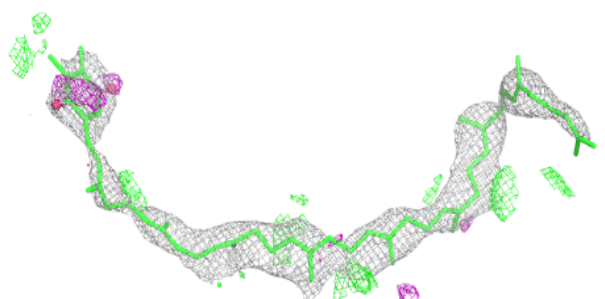


**Electron density around LMT B 626:**

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

**Electron density around PL9 a 413 (A):**

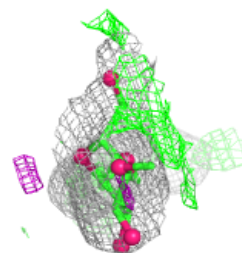
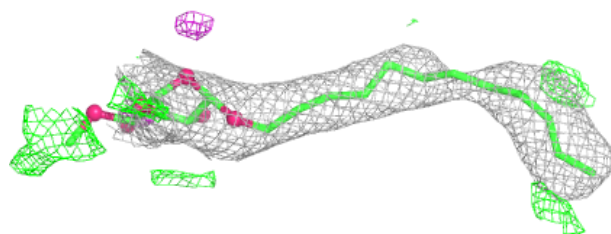
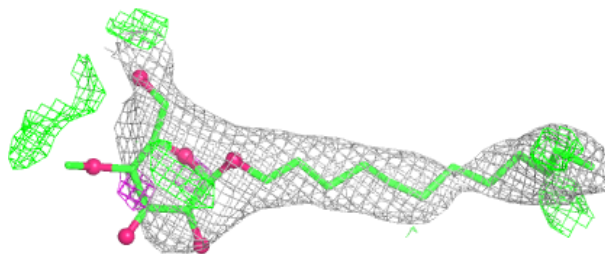
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



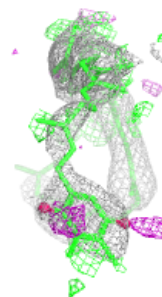
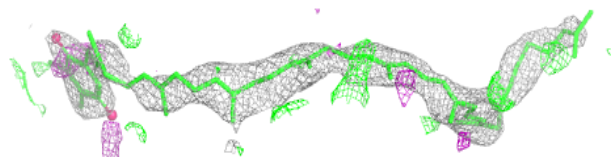
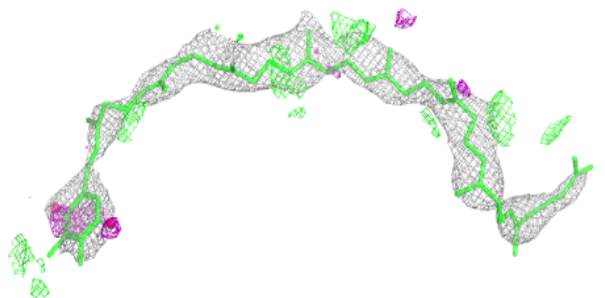


**Electron density around LMT B 629:**

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

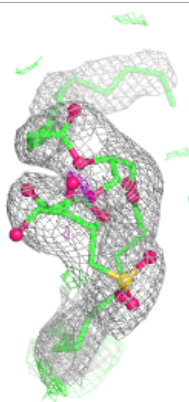
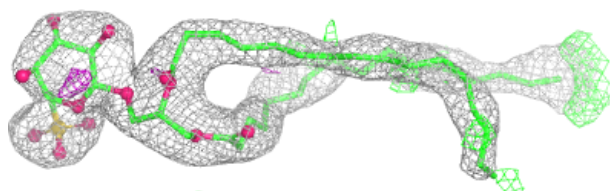
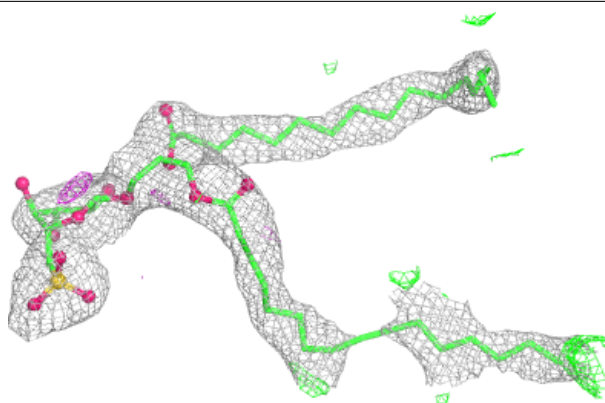
**Electron density around PL9 a 413 (B):**

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

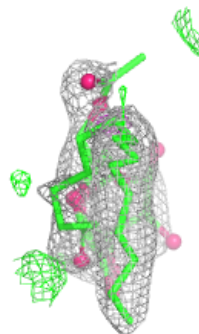
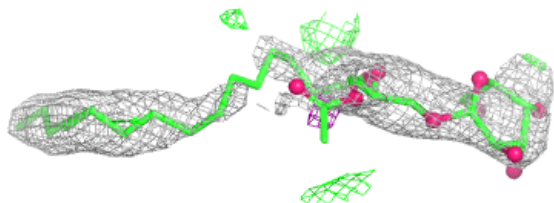
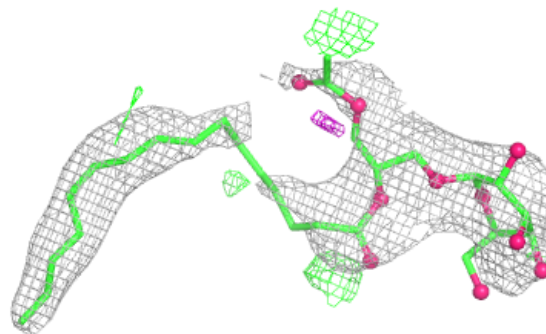


**Electron density around SQD a 411:**

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

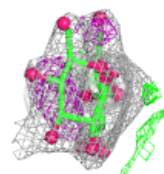
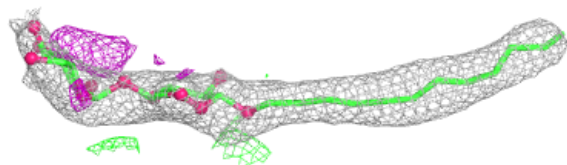
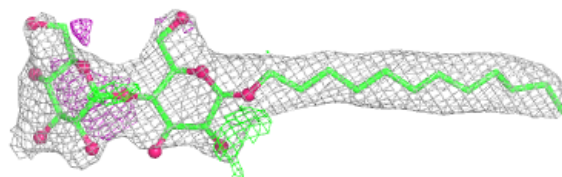
**Electron density around LMG Z 101:**

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

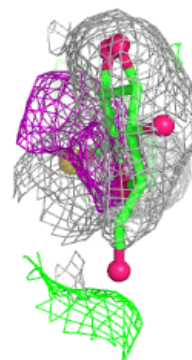
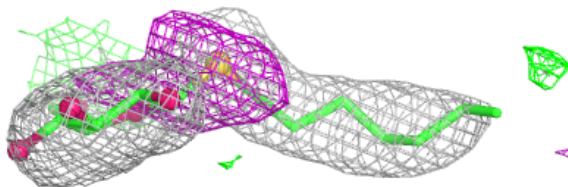
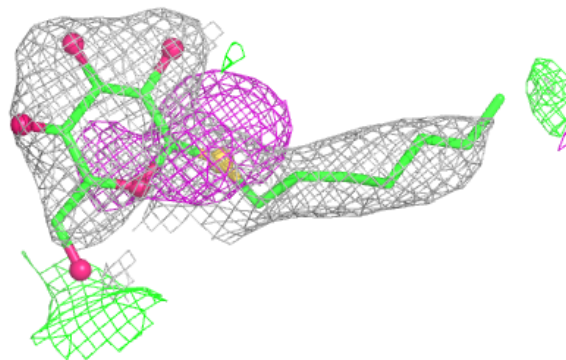


**Electron density around LMT m 103:**

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

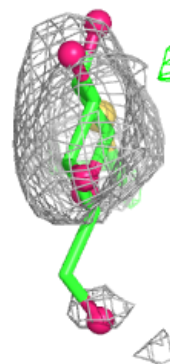
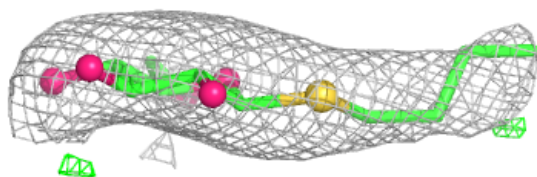
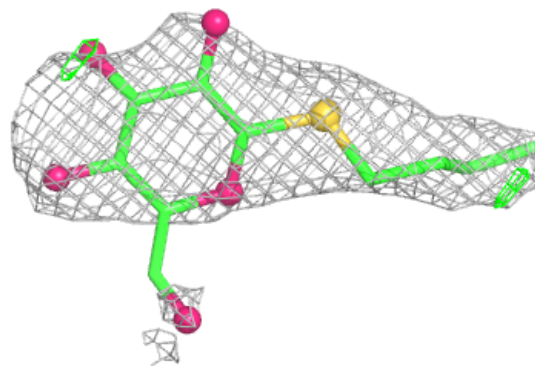
**Electron density around HTG b 622:**

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

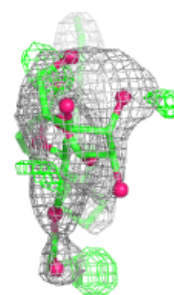
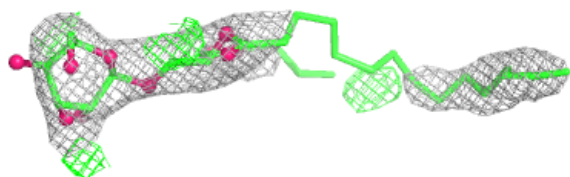
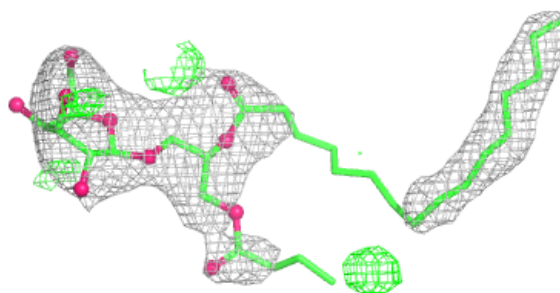


**Electron density around HTG d 411:**

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

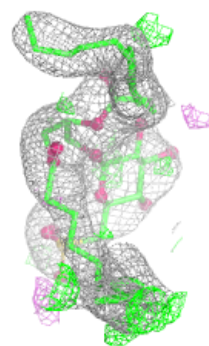
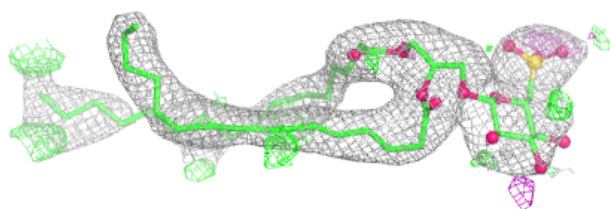
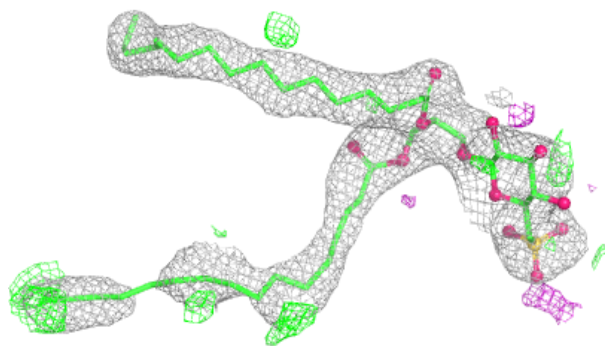
**Electron density around LMG z 101:**

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

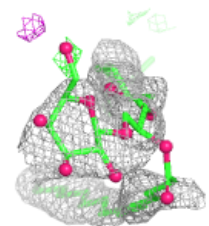
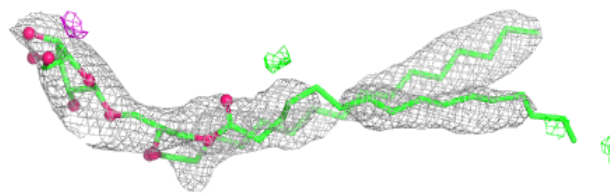
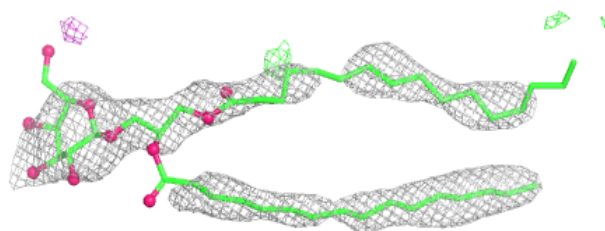


**Electron density around SQD A 411:**

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

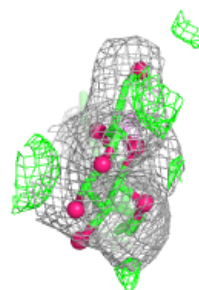
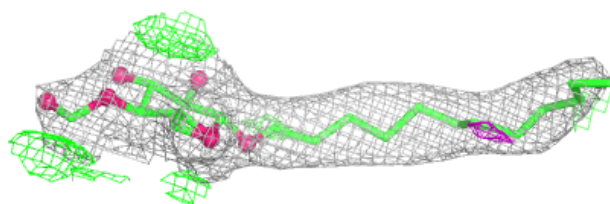
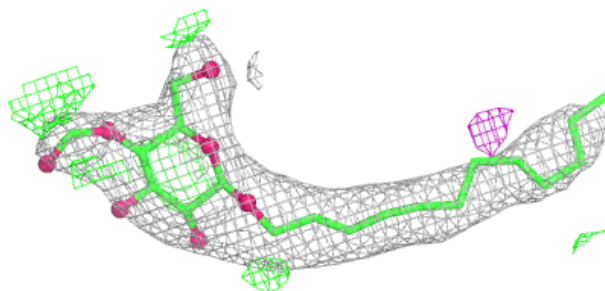
**Electron density around LMG c 521:**

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



**Electron density around LMT t 101:**

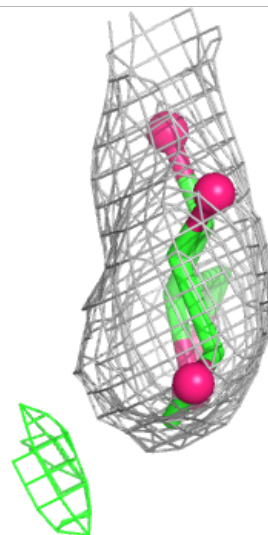
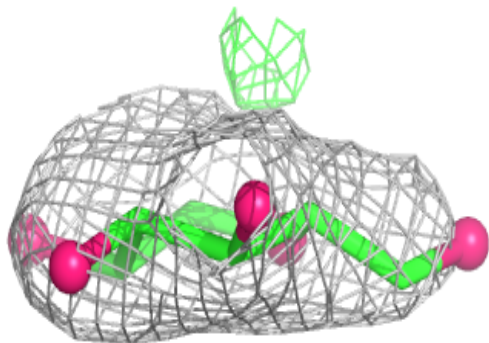
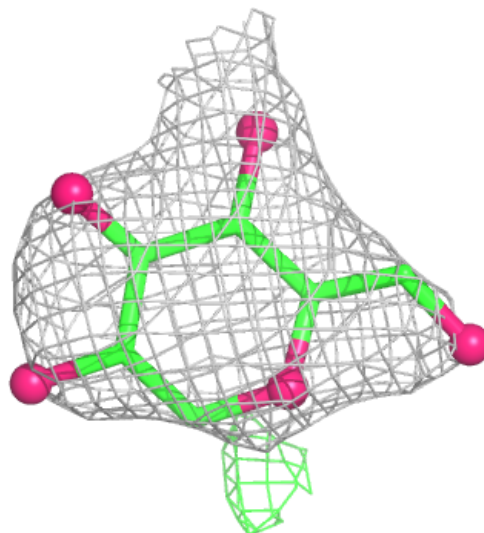
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





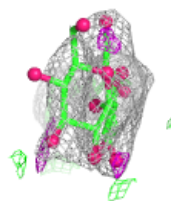
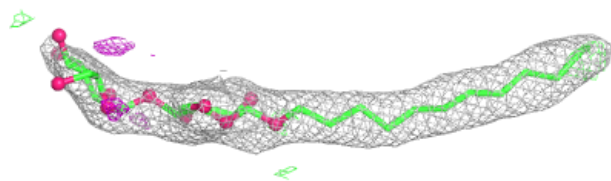
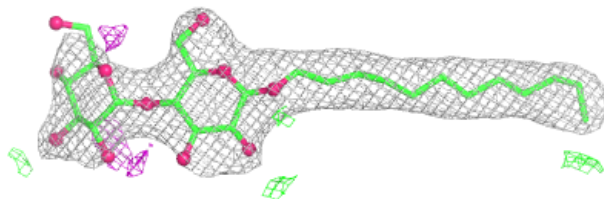
**Electron density around HTG V 202:**

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

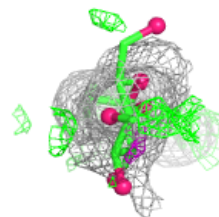
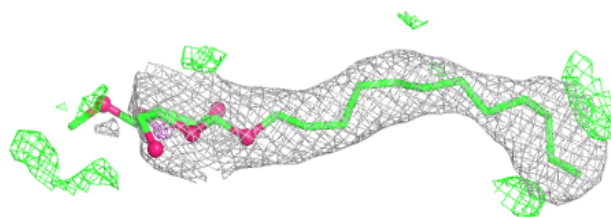
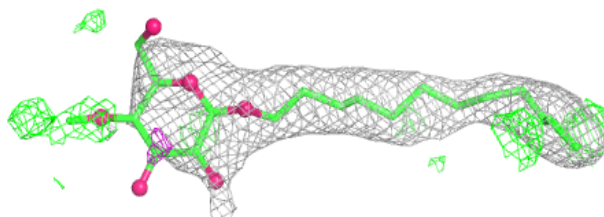


**Electron density around LMT M 101:**

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

**Electron density around LMT b 627:**

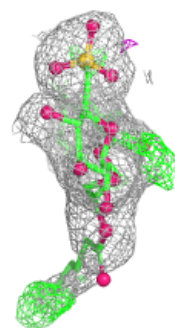
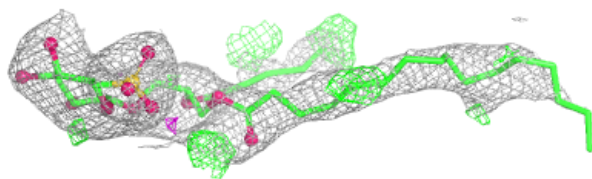
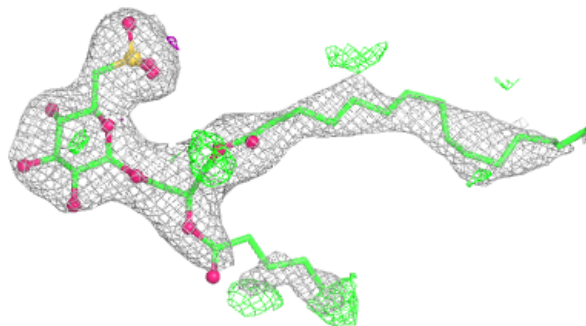
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



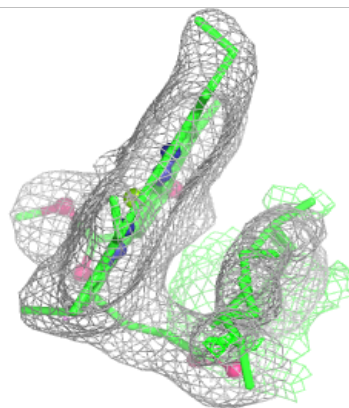
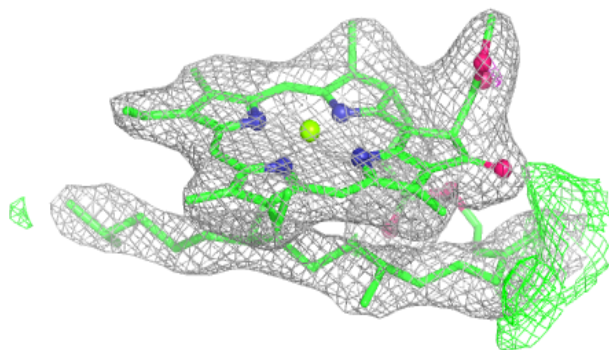
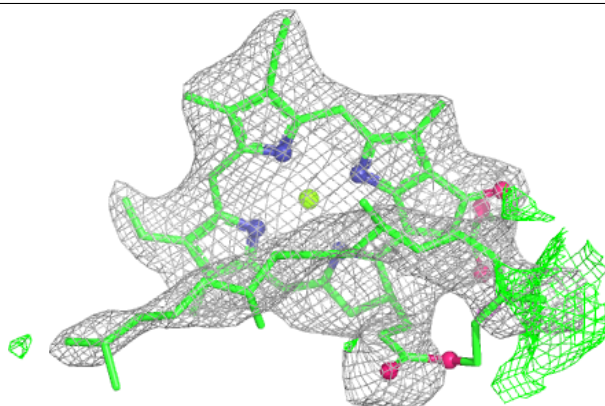


**Electron density around SQD X 101:**

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

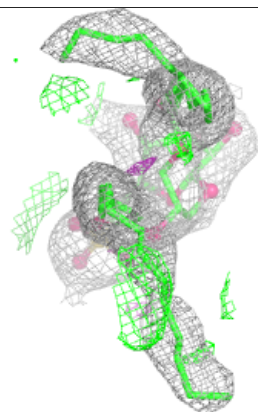
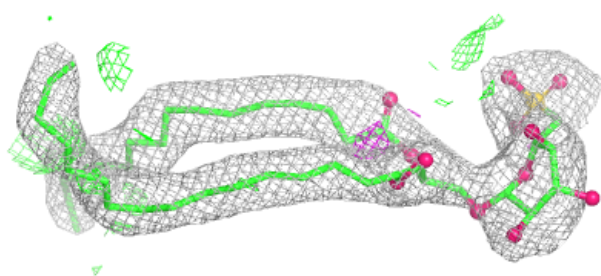
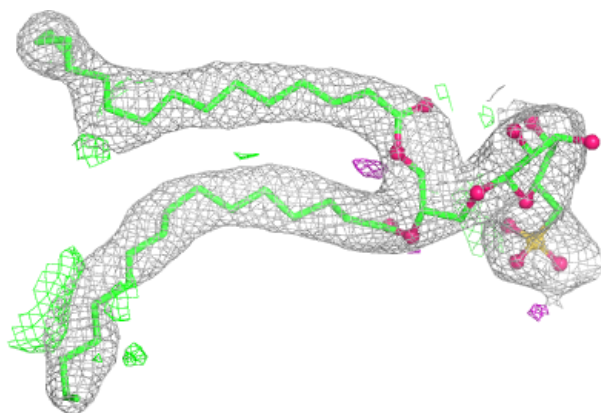
**Electron density around CLA b 601:**

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

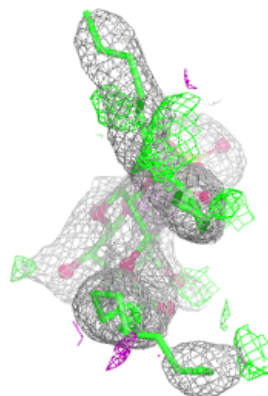
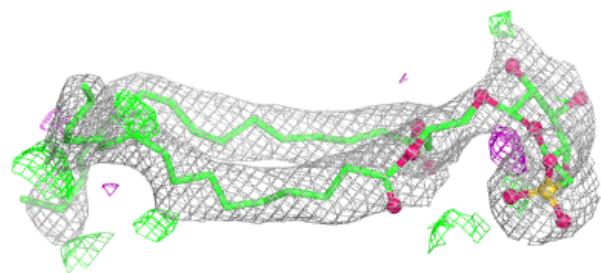
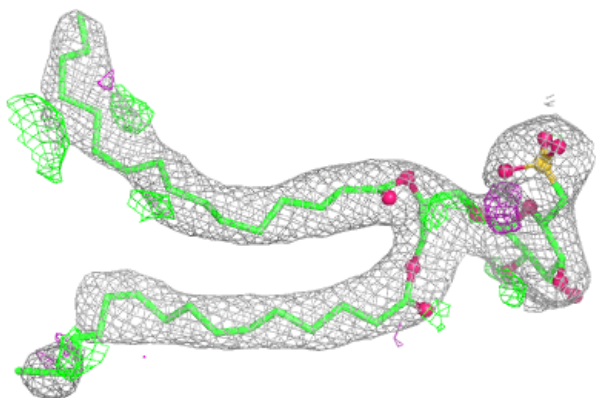


**Electron density around SQD 1 101:**

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

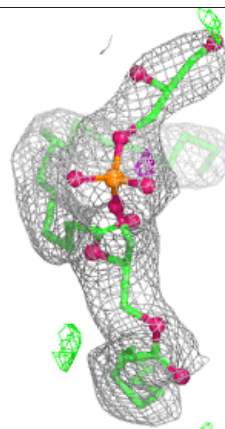
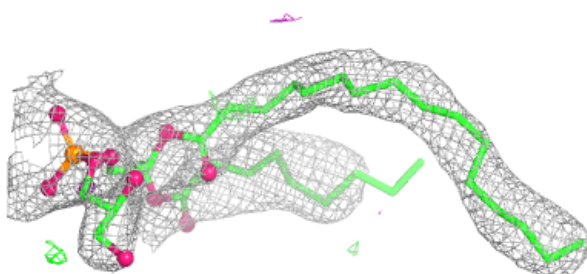
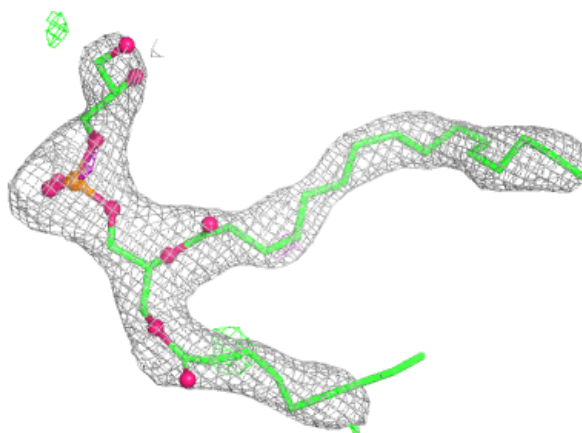
**Electron density around SQD b 620:**

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



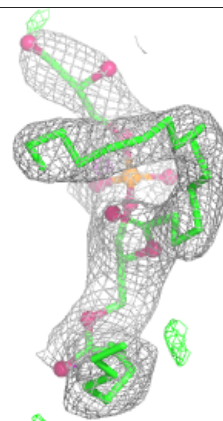
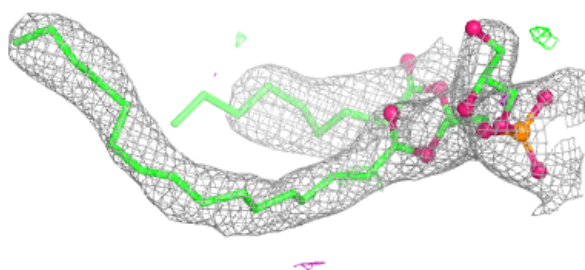
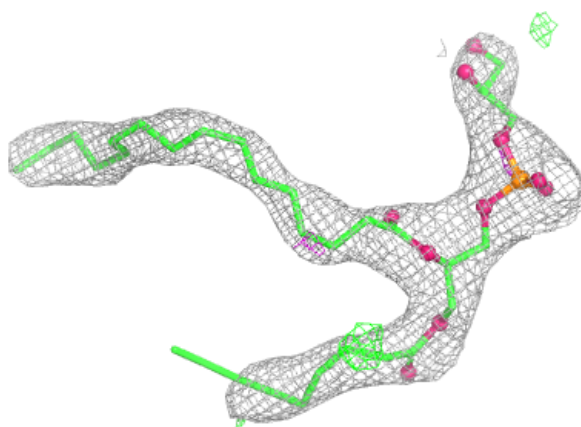
**Electron density around LHG E 101 (A):**

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

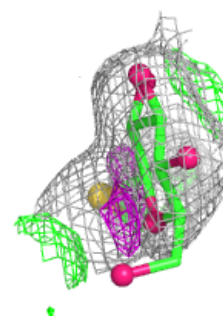
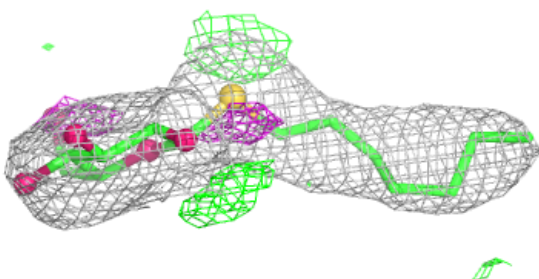
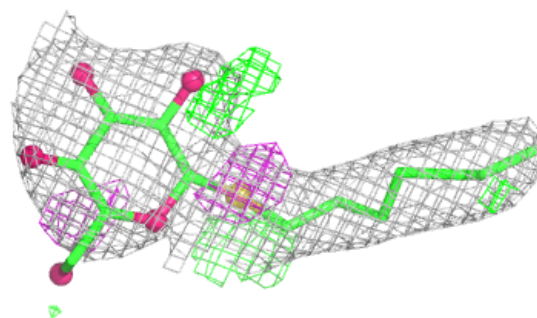


**Electron density around LHG E 101 (B):**

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

**Electron density around HTG o 301:**

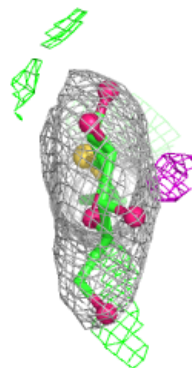
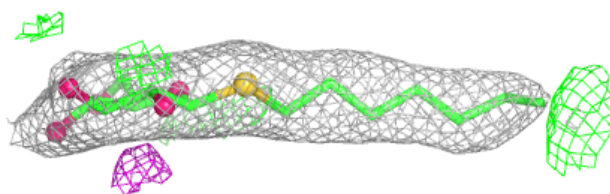
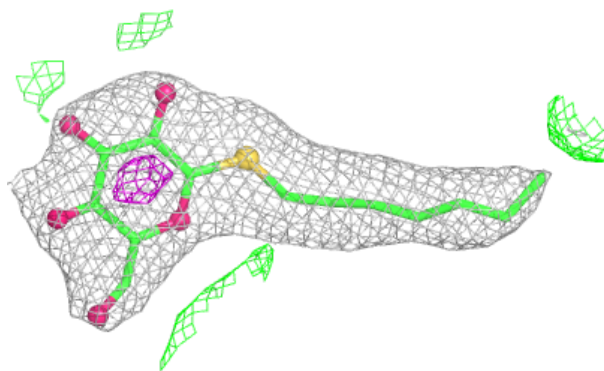
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



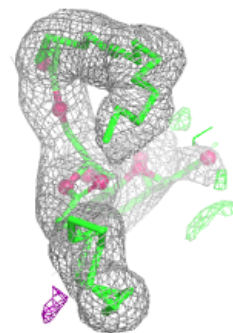
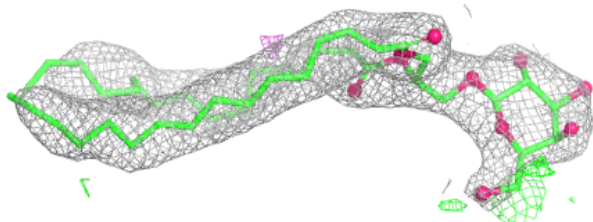
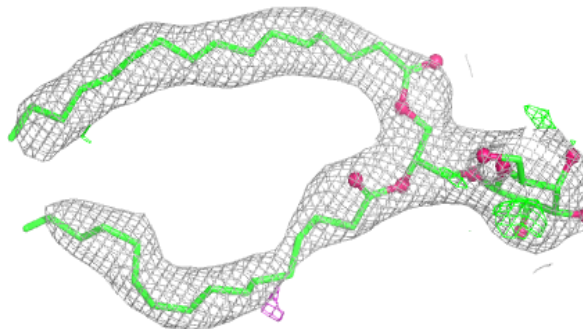


**Electron density around HTG B 623:**

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

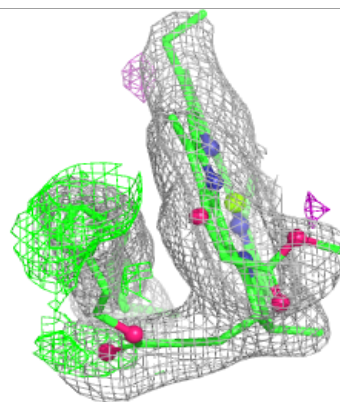
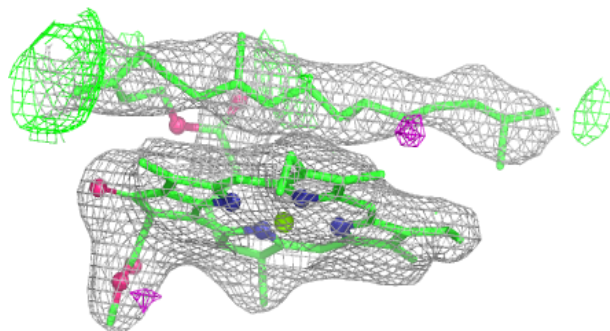
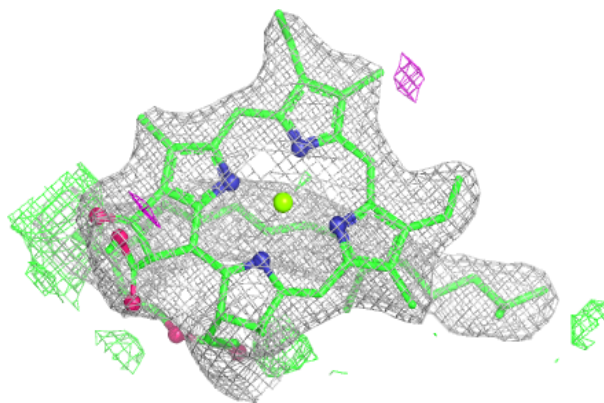
**Electron density around LMG C 501:**

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

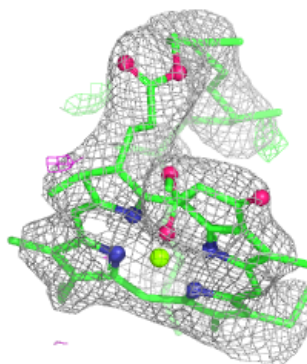
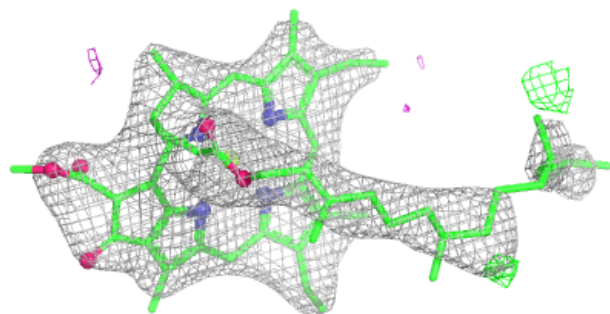
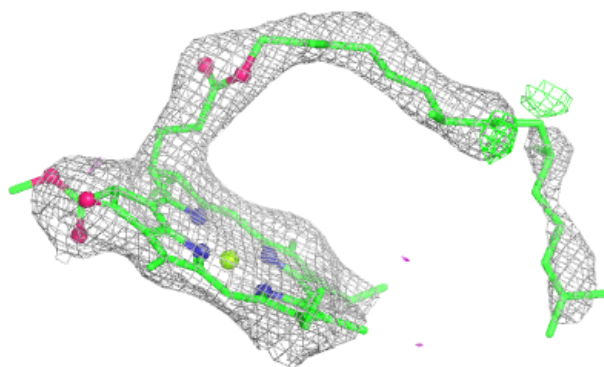


**Electron density around CLA B 601:**

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

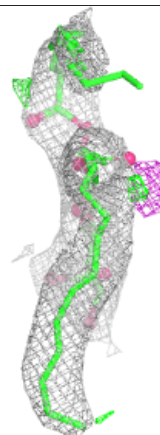
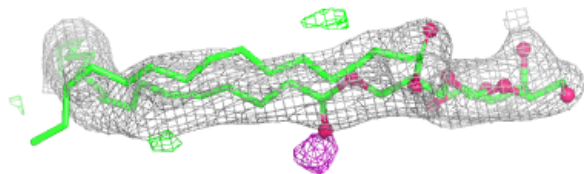
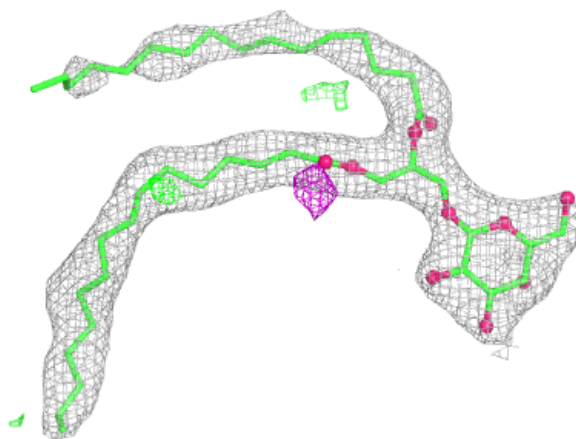
**Electron density around CLA c 514:**

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

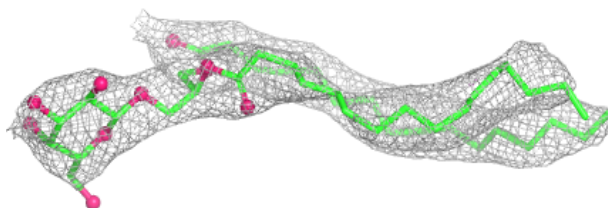
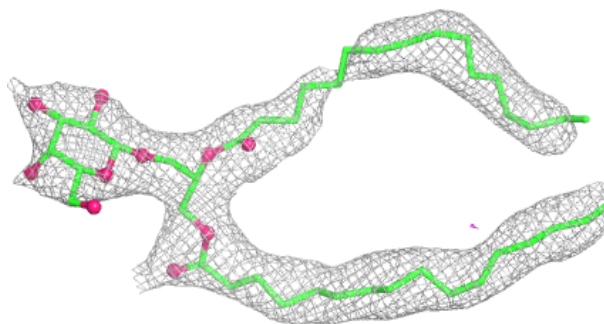


**Electron density around LMG C 520:**

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

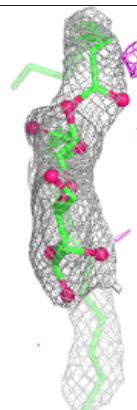
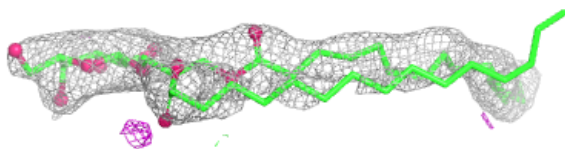
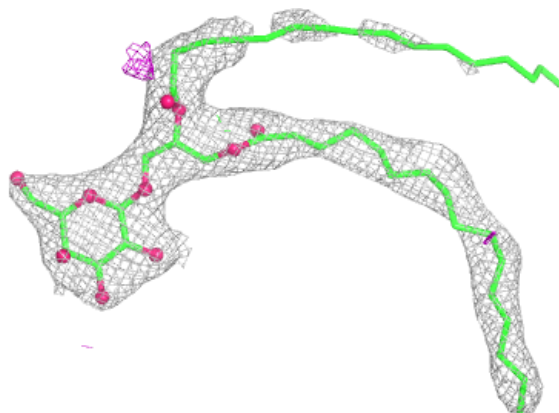
**Electron density around LMG c 501:**

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



**Electron density around LMG c 520:**

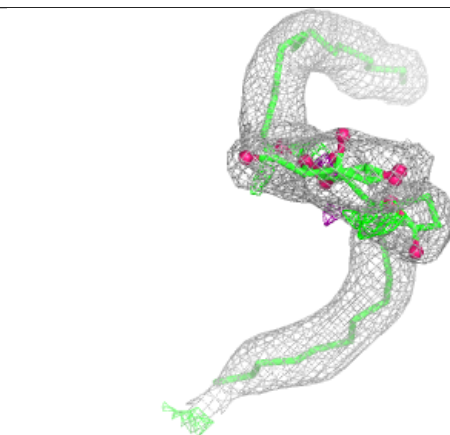
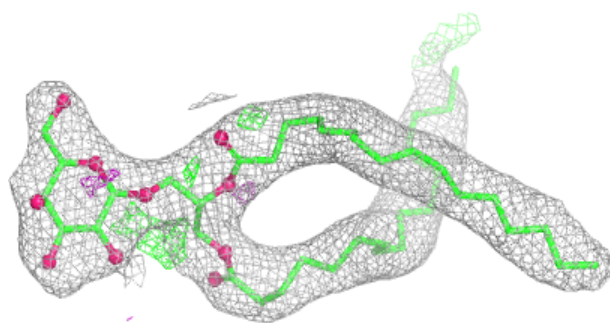
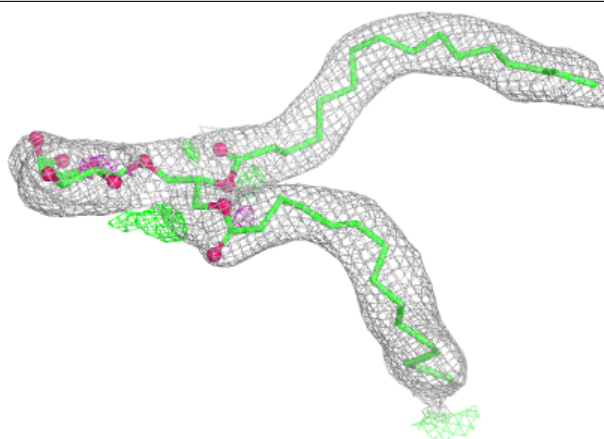
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



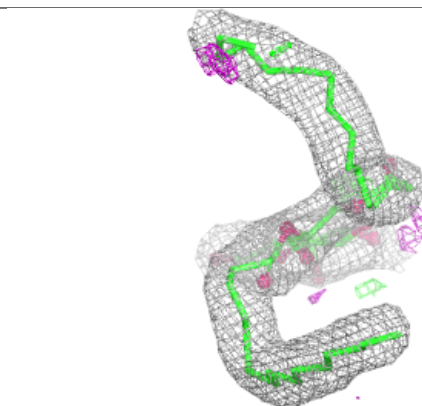
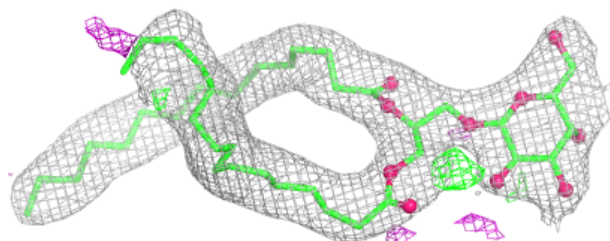
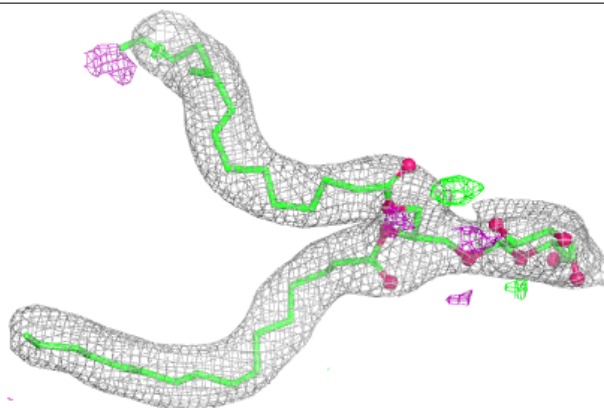


**Electron density around LMG B 620:**

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

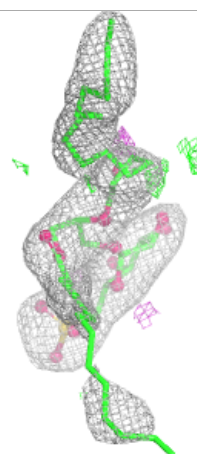
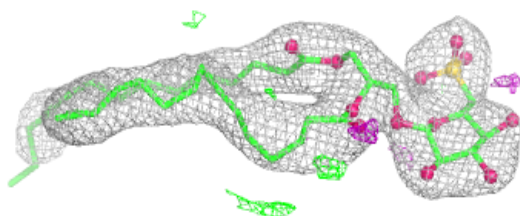
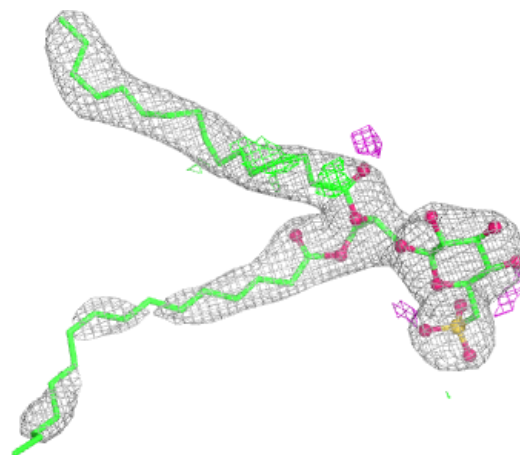
**Electron density around LMG m 101:**

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



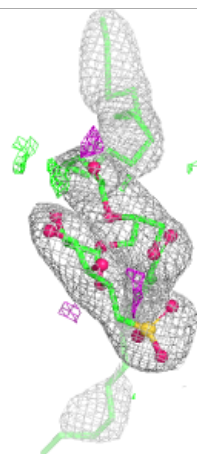
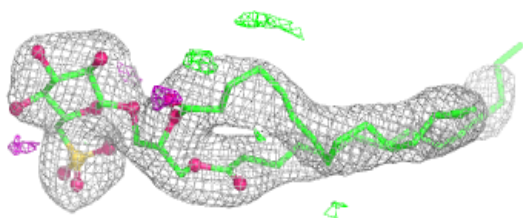
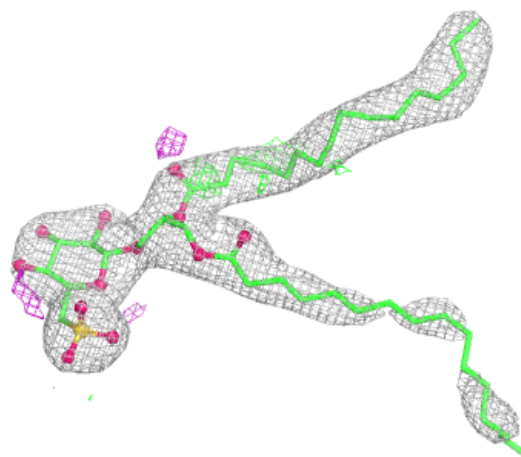
**Electron density around SQD A 409 (A):**

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



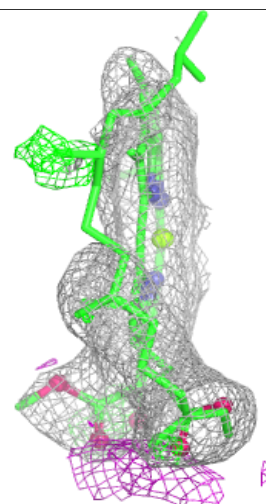
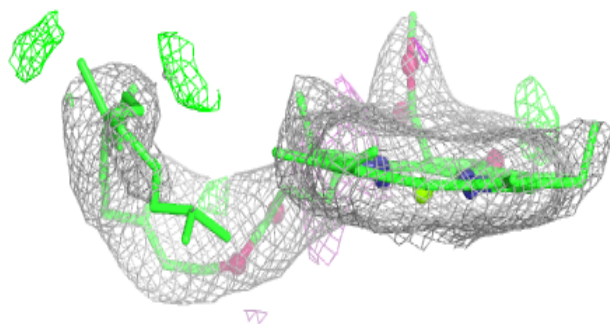
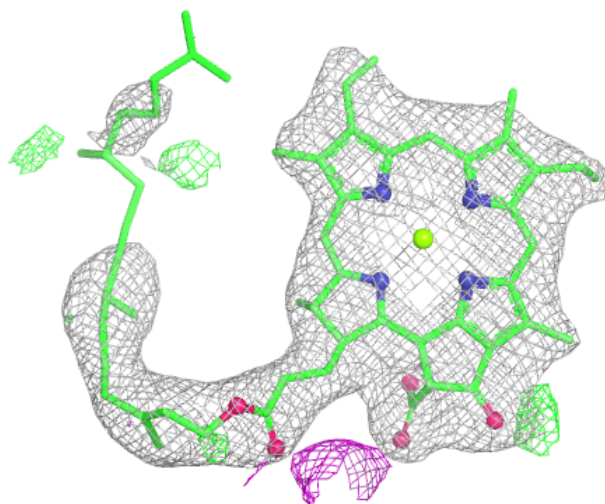
**Electron density around SQD A 409 (B):**

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



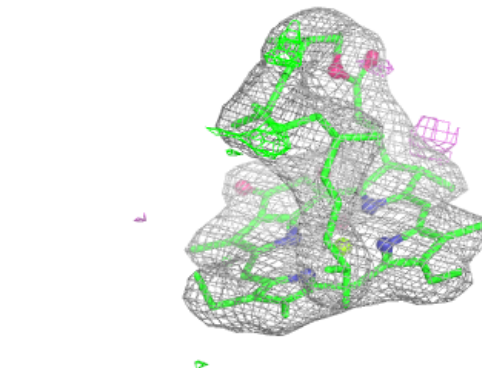
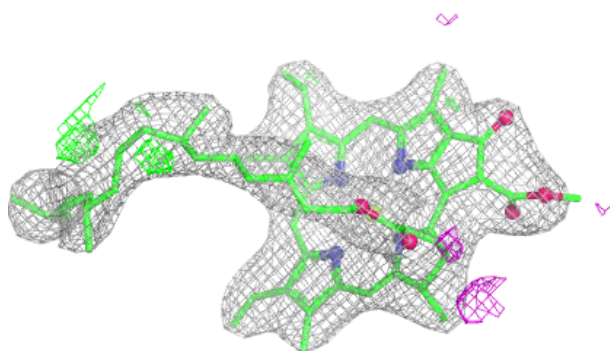
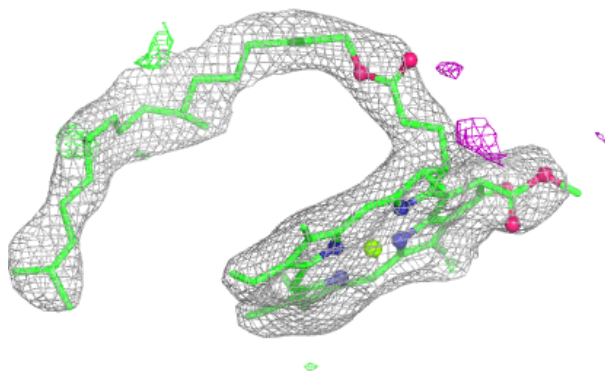
**Electron density around CLA c 513:**

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

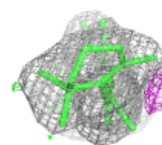
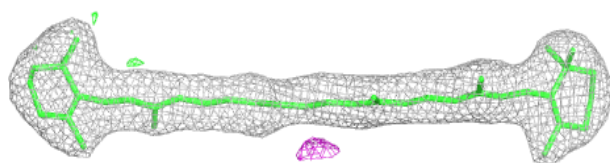
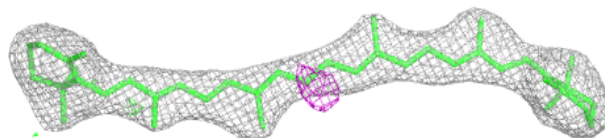


**Electron density around CLA C 514:**

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

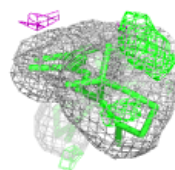
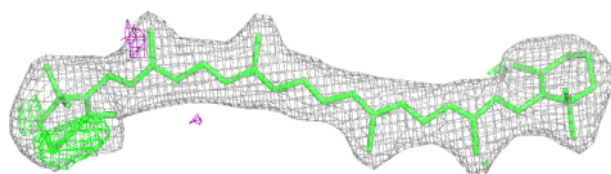
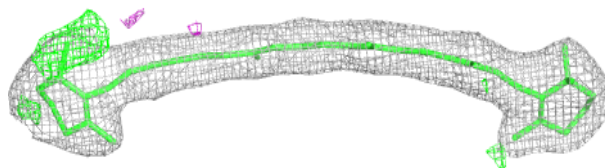
**Electron density around BCR C 515:**

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

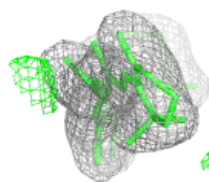
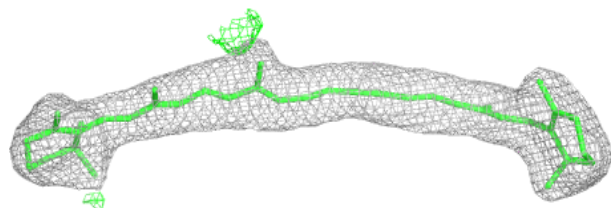
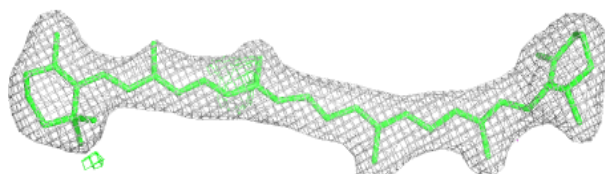


**Electron density around BCR D 405:**

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

**Electron density around BCR T 102:**

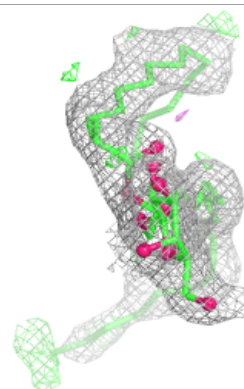
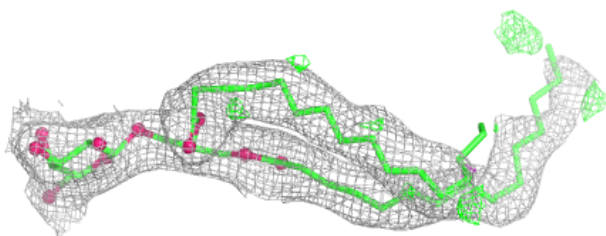
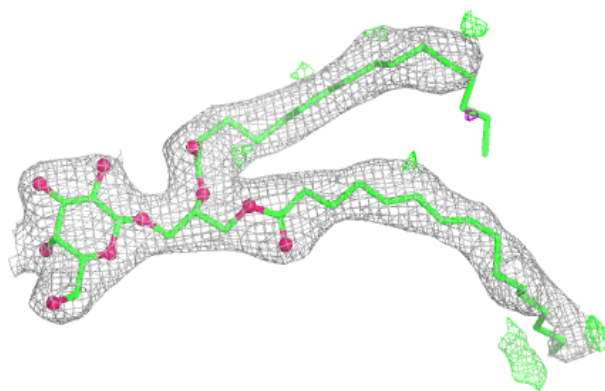
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



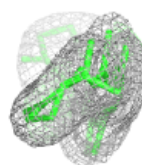
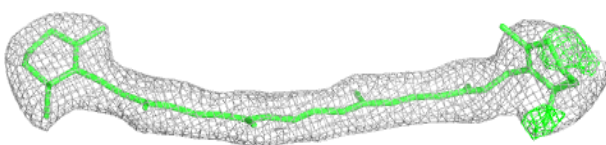
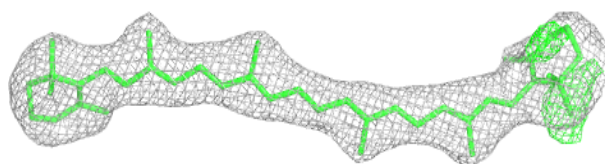


**Electron density around LMG D 412:**

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

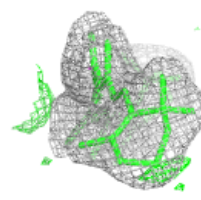
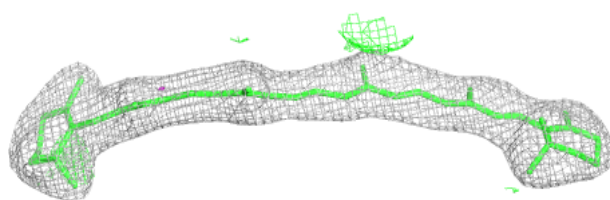
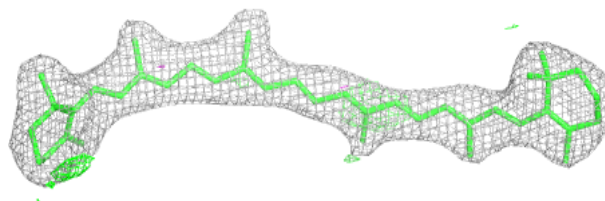
**Electron density around BCR d 405:**

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

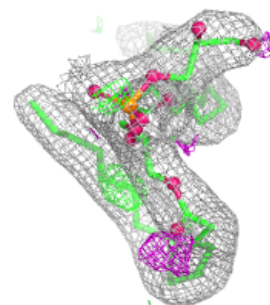
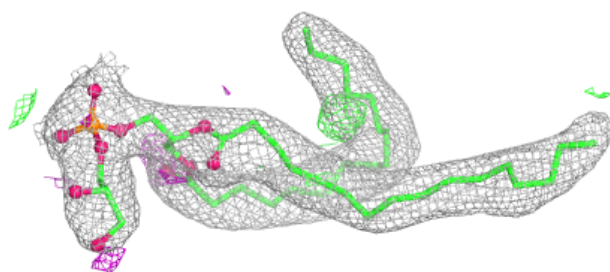
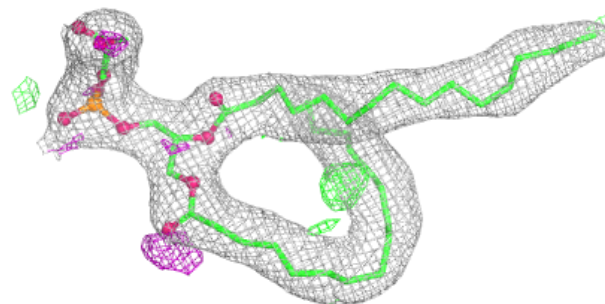


**Electron density around BCR t 102:**

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

**Electron density around LHG A 418 (A):**

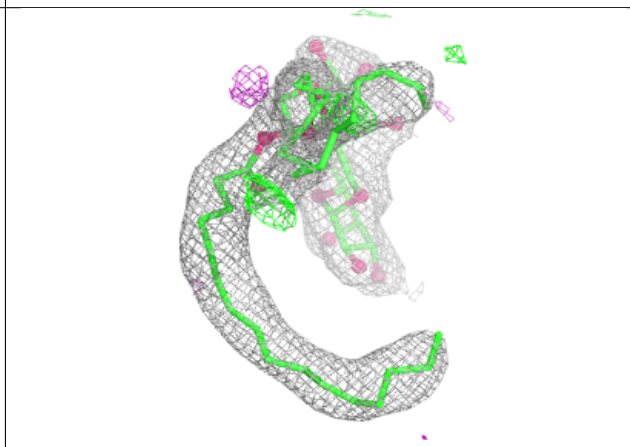
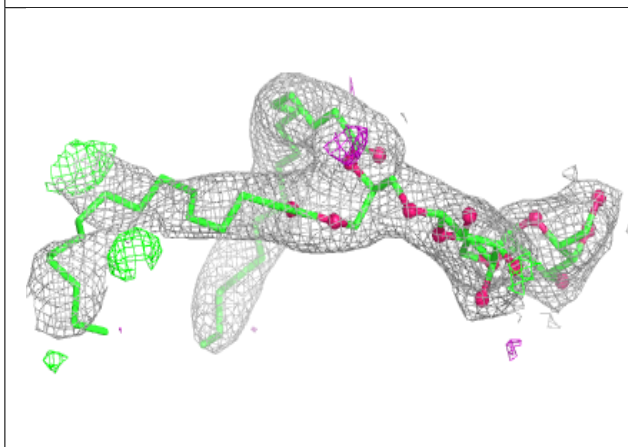
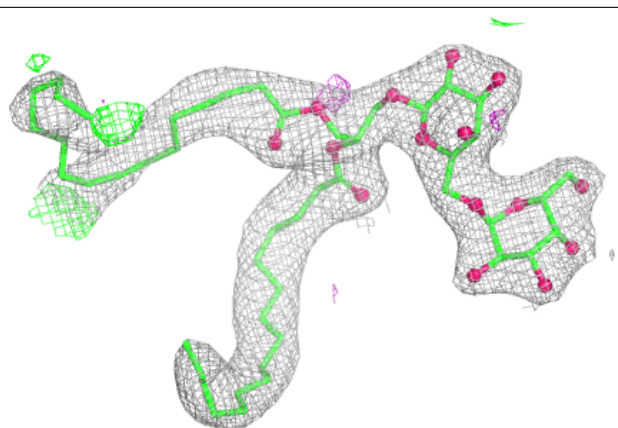
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





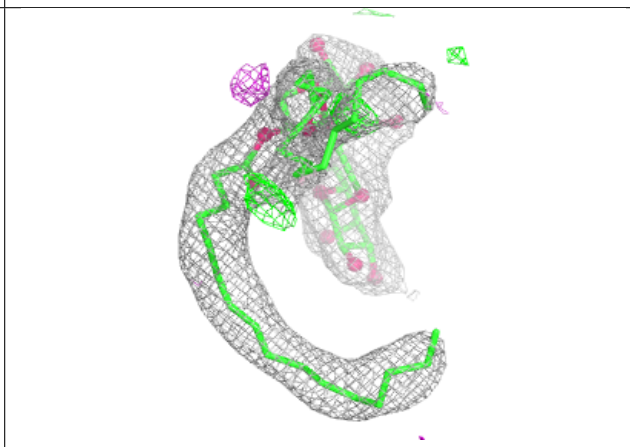
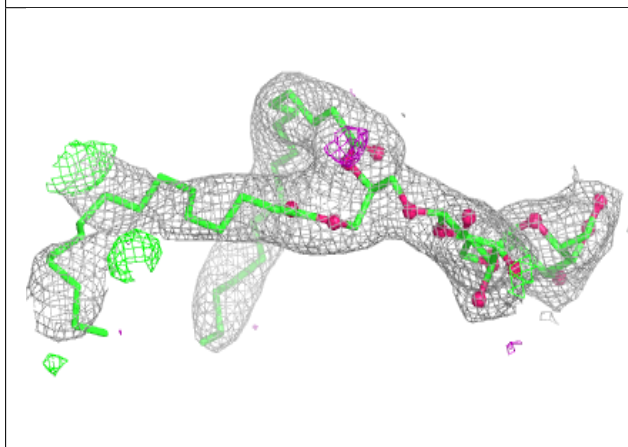
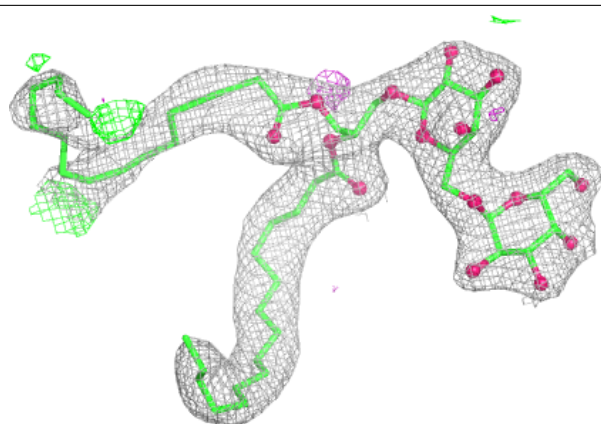
**Electron density around DGD C 518 (A):**

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



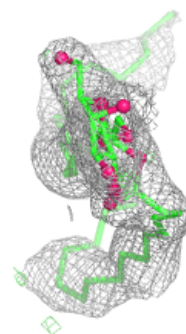
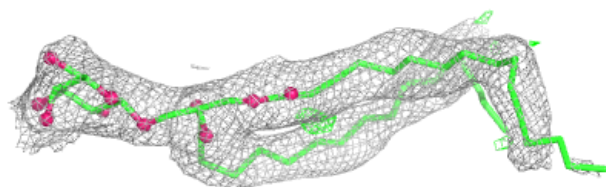
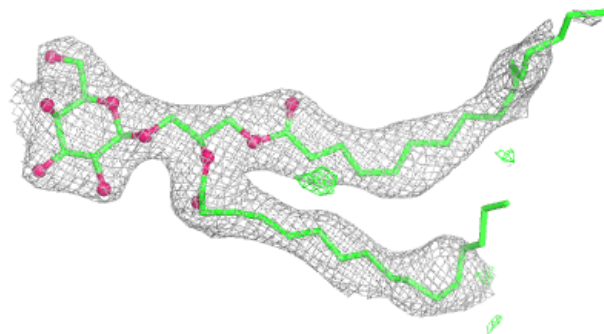
**Electron density around DGD C 518 (B):**

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

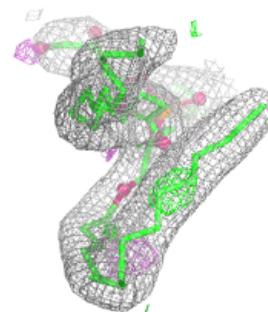
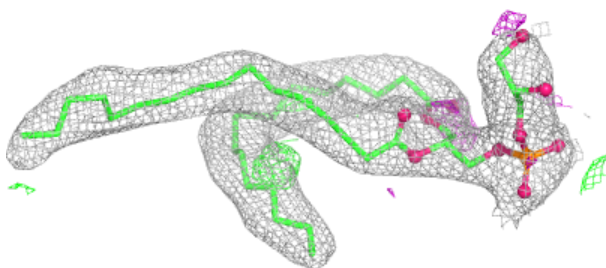
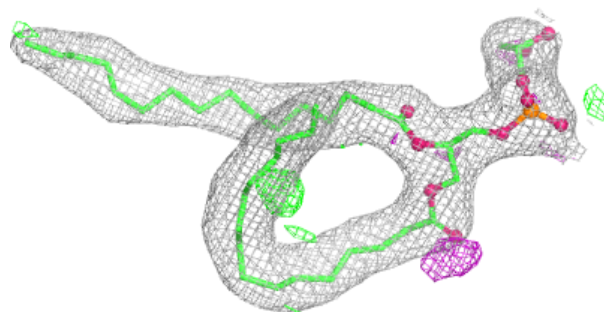


**Electron density around LMG d 412:**

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

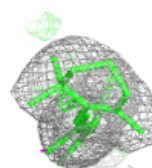
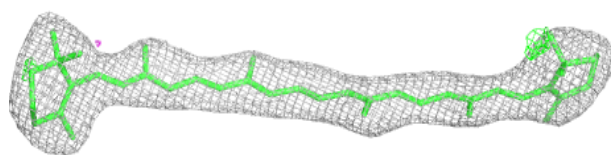
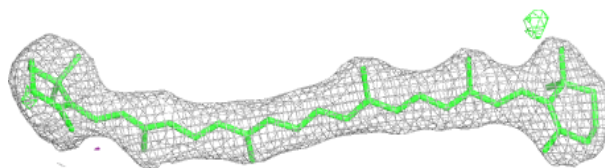
**Electron density around LHG A 418 (B):**

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

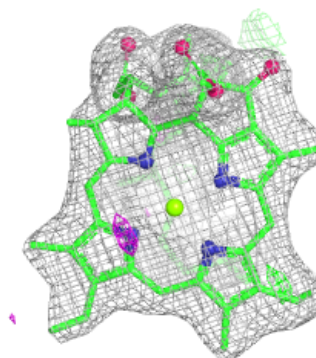
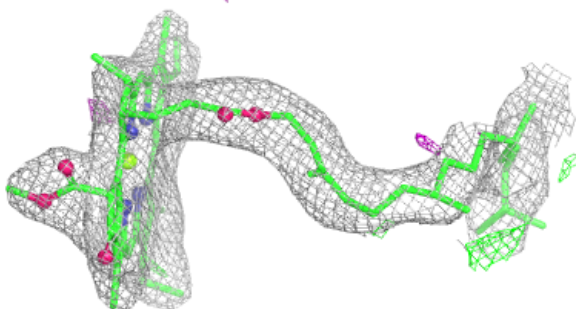
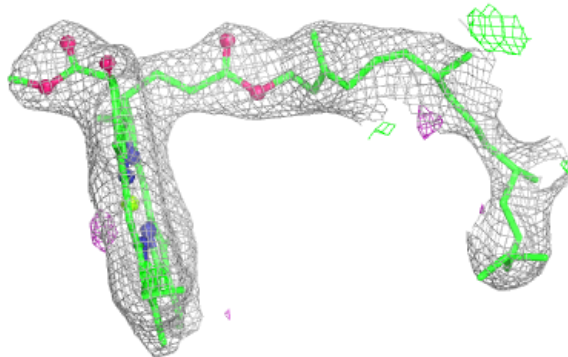


**Electron density around BCR c 515:**

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

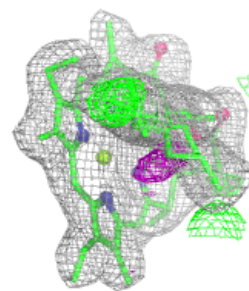
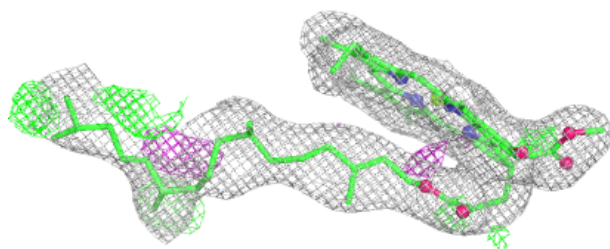
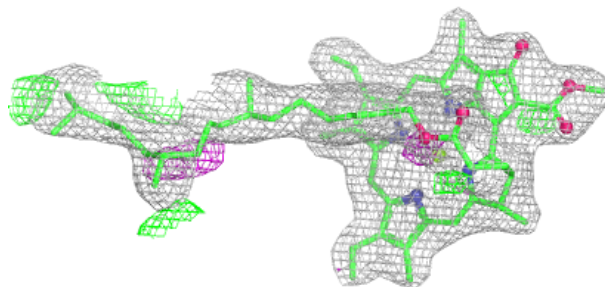
**Electron density around CLA C 507:**

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

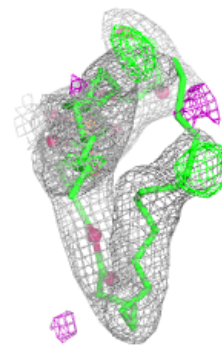
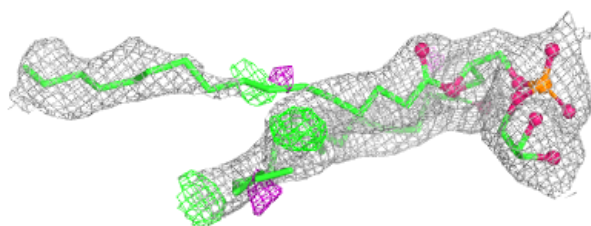
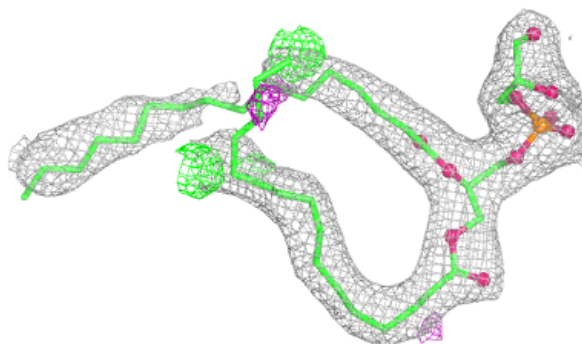


**Electron density around CLA B 614:**

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

**Electron density around LHG D 408 (A):**

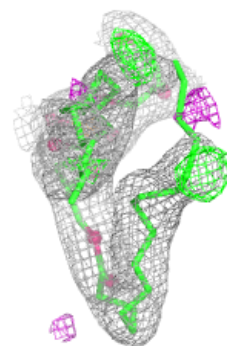
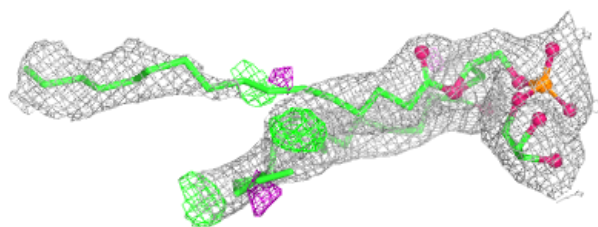
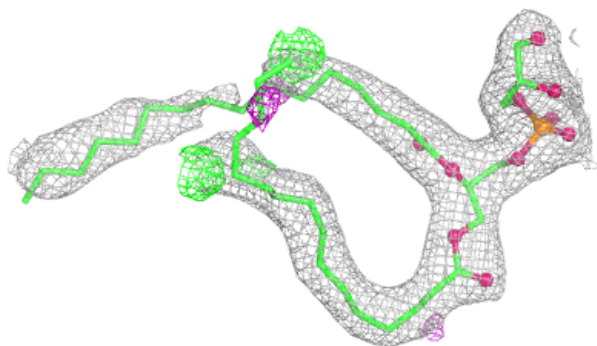
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



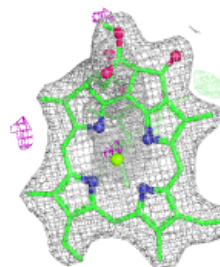
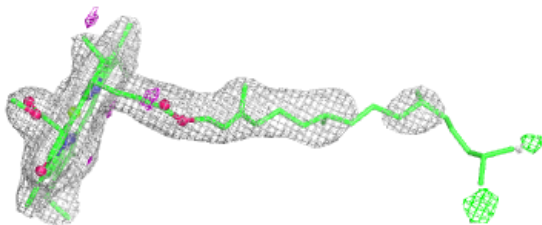
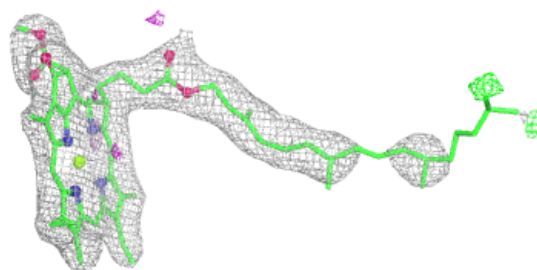


**Electron density around LHG D 408 (B):**

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

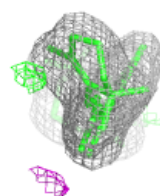
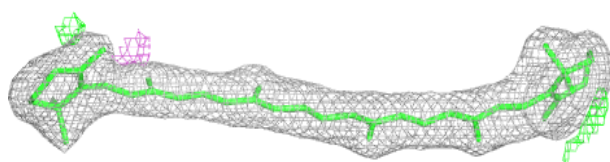
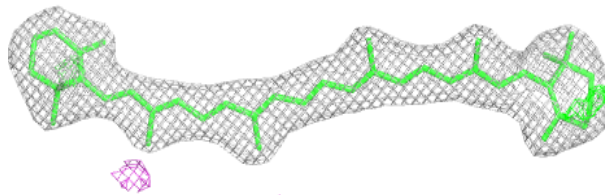
**Electron density around CLA d 404:**

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

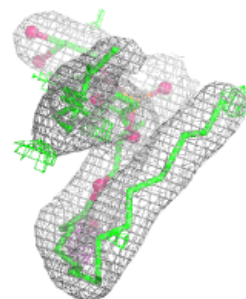
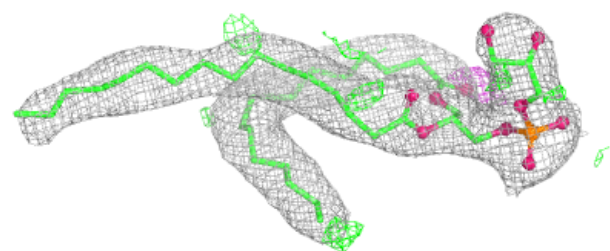
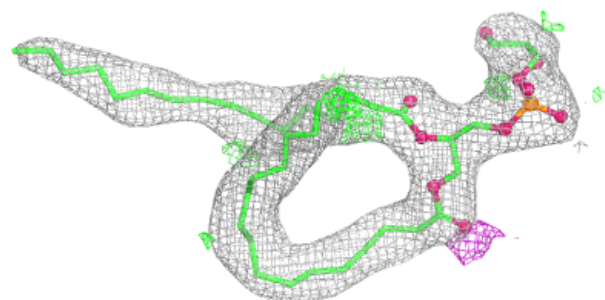


**Electron density around BCR B 619:**

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

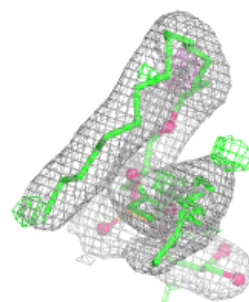
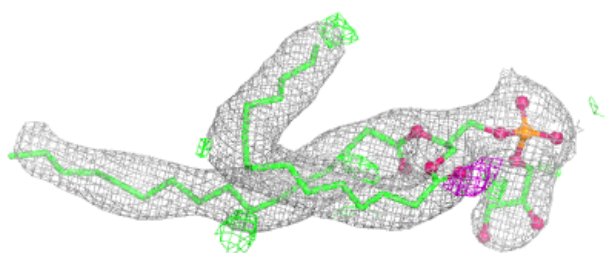
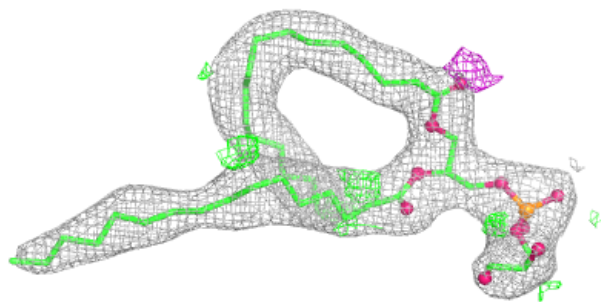
**Electron density around LHG d 414 (A):**

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

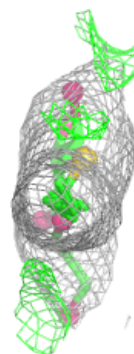
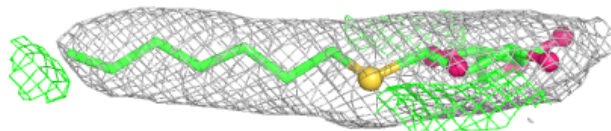
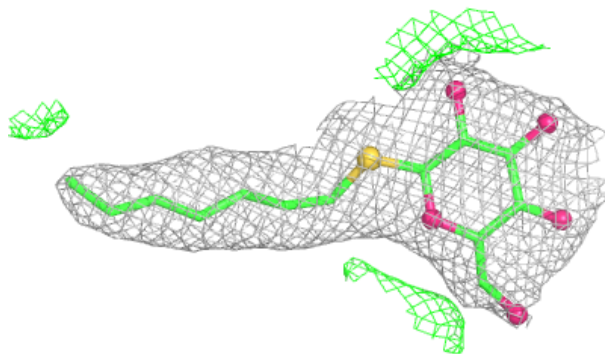


**Electron density around LHG d 414 (B):**

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

**Electron density around HTG b 625:**

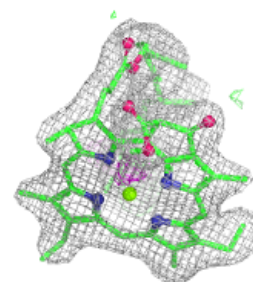
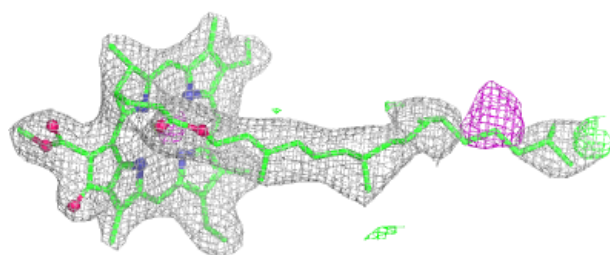
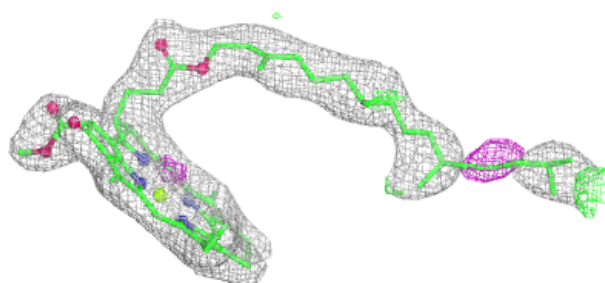
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





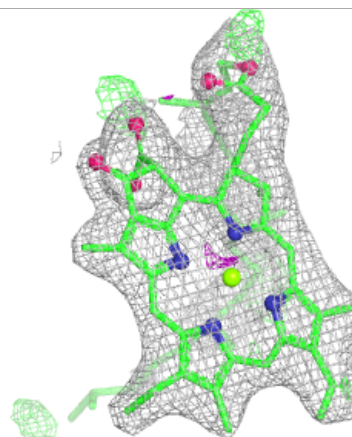
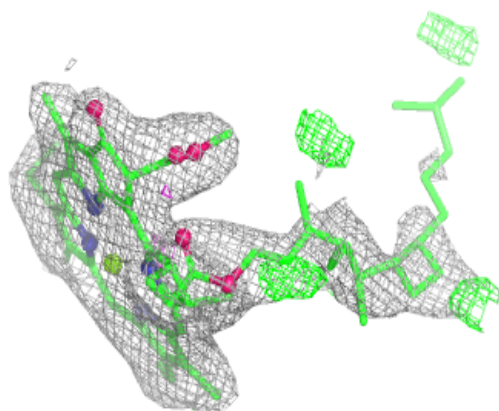
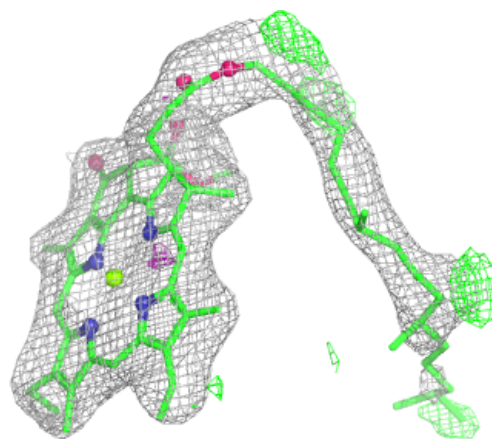
**Electron density around CLA C 505:**

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



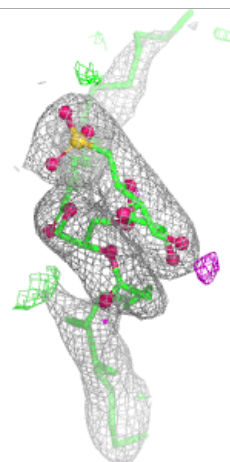
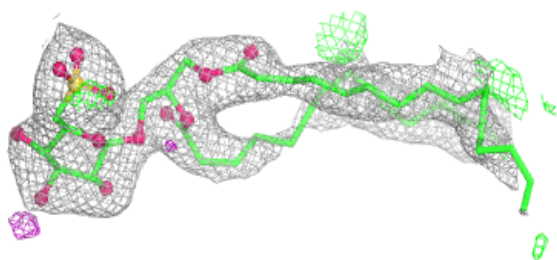
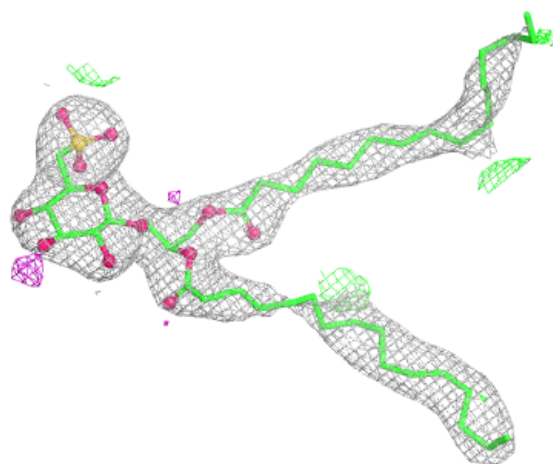
**Electron density around CLA b 616:**

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



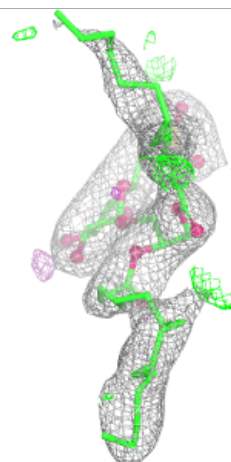
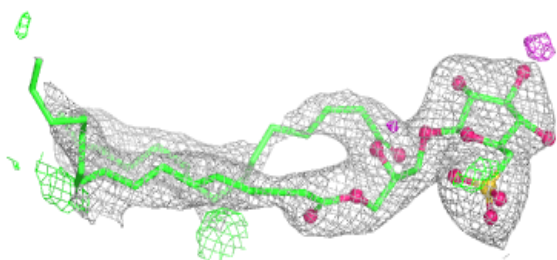
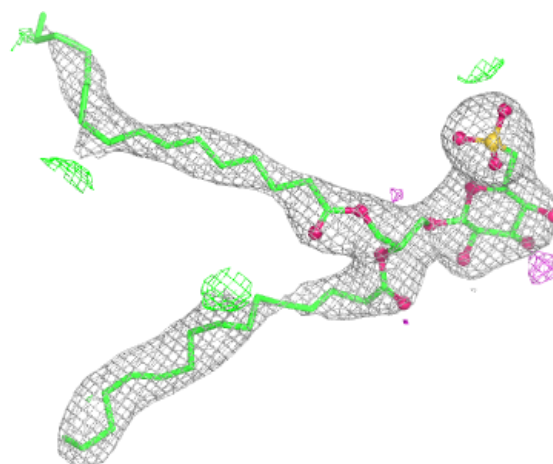
**Electron density around SQD a 409 (A):**

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



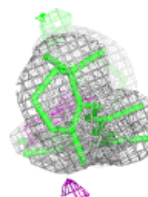
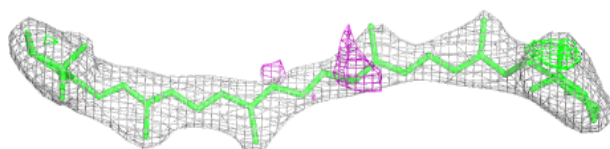
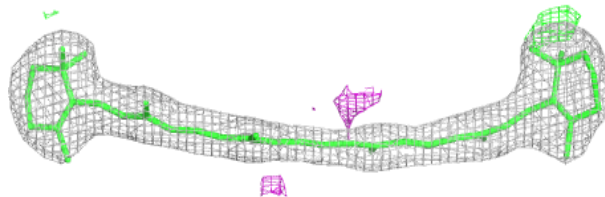
**Electron density around SQD a 409 (B):**

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

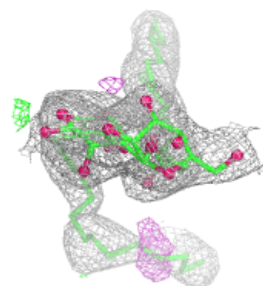
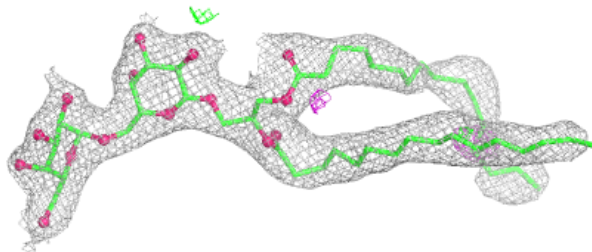
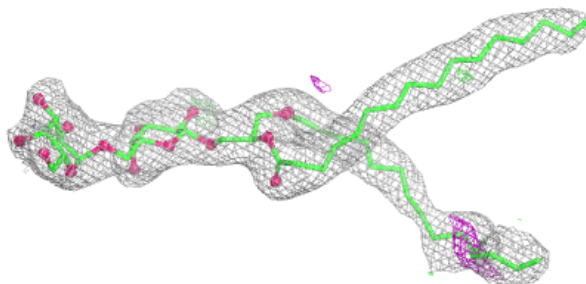


**Electron density around BCR K 102:**

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

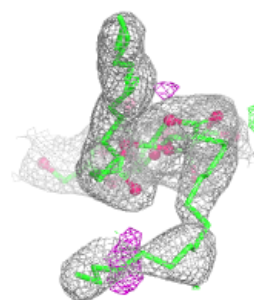
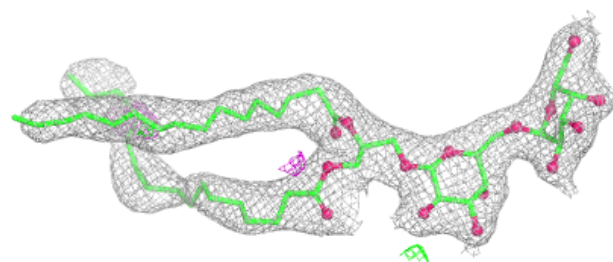
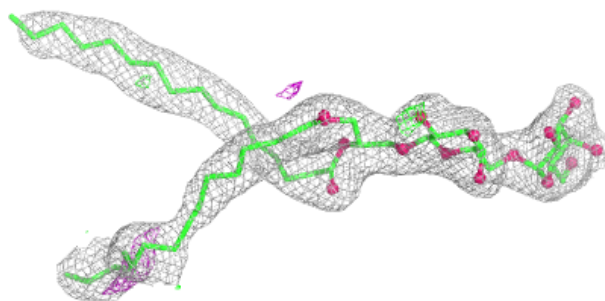
**Electron density around DGD c 517 (A):**

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

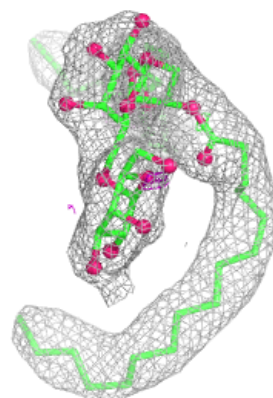
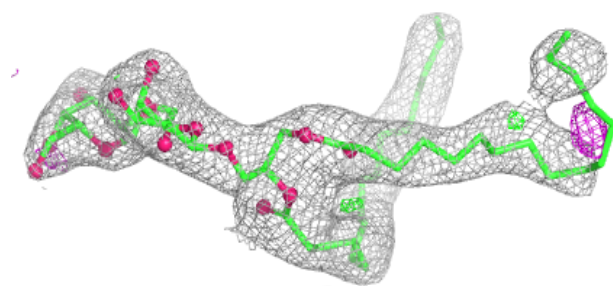
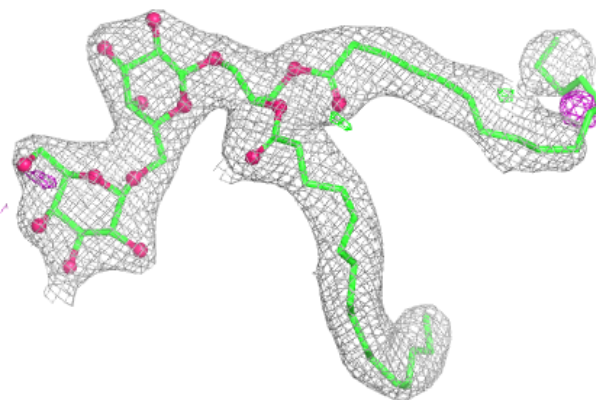


**Electron density around DGD c 517 (B):**

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

**Electron density around DGD c 518 (A):**

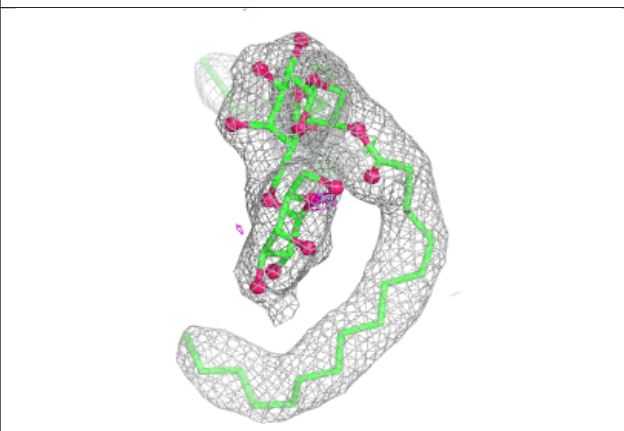
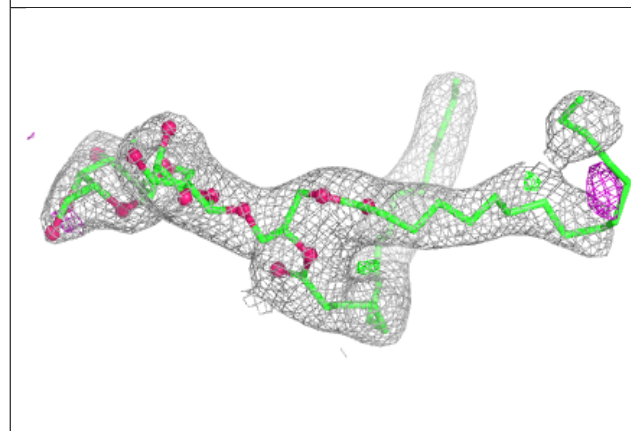
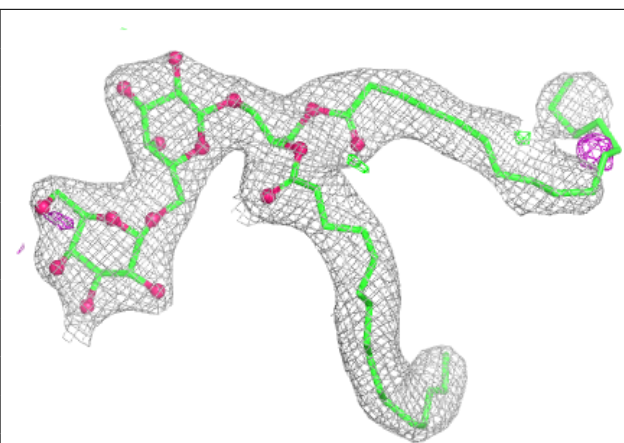
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



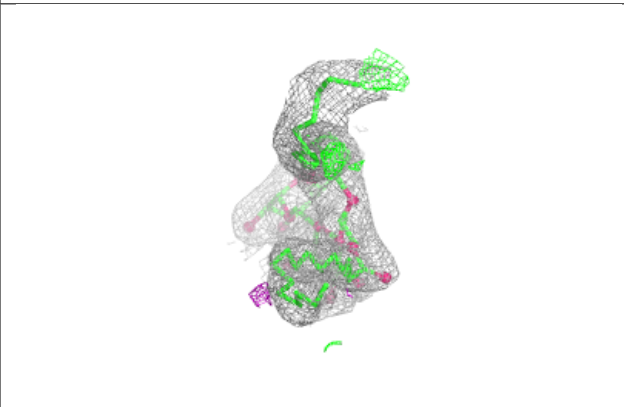
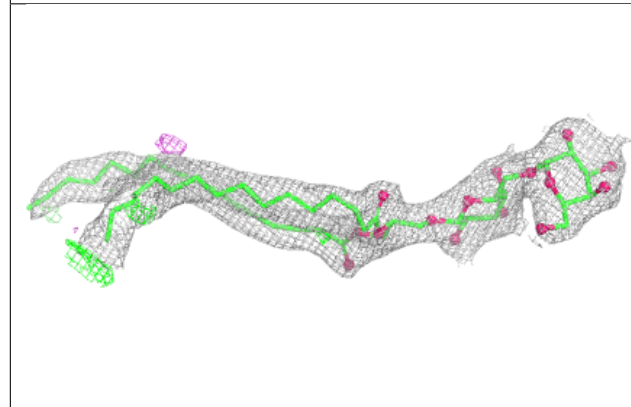
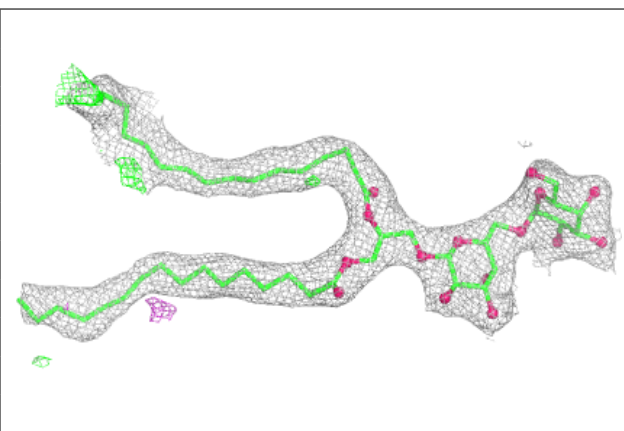


**Electron density around DGD c 518 (B):**

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

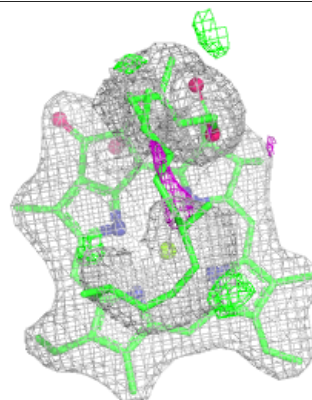
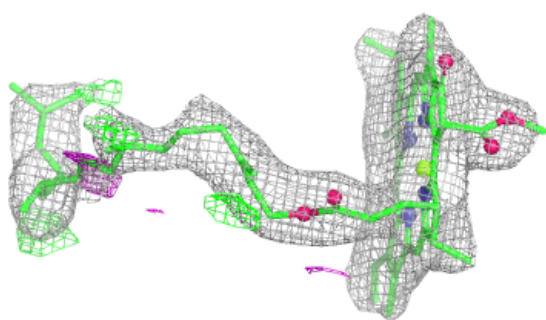
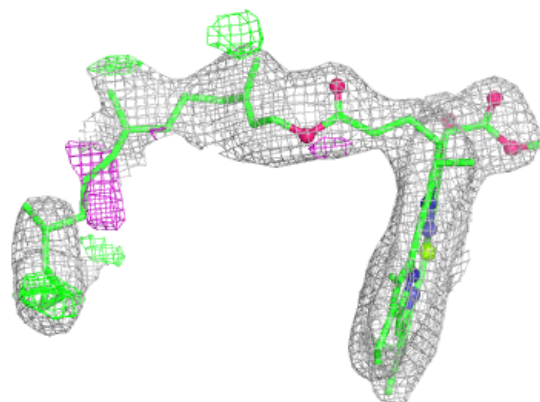
**Electron density around DGD c 519:**

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

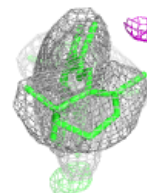
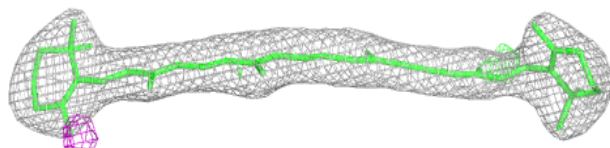
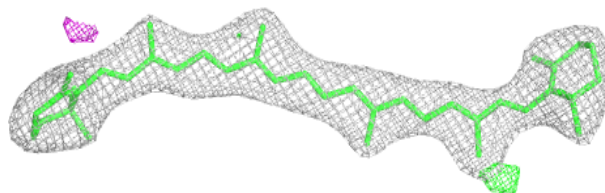


**Electron density around CLA c 507:**

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

**Electron density around BCR Y 101:**

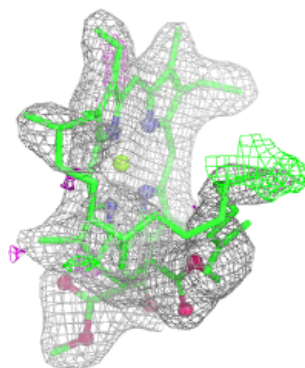
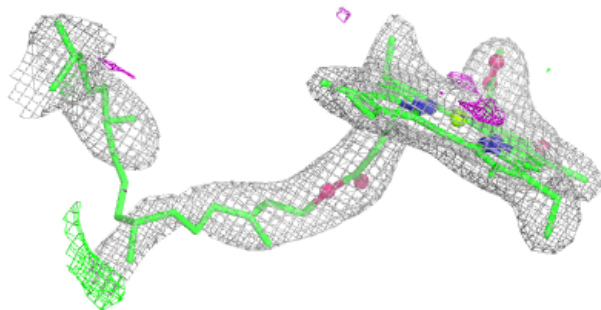
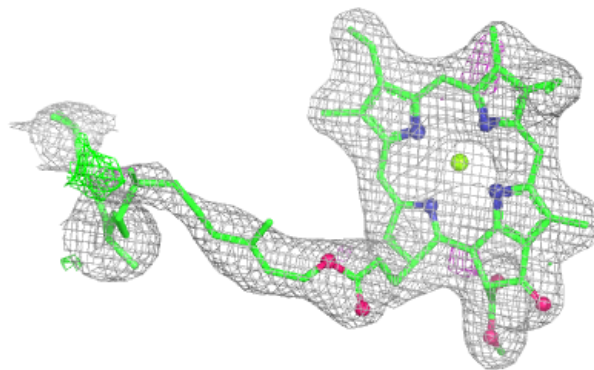
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



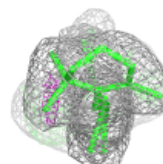
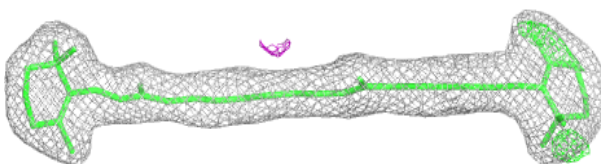
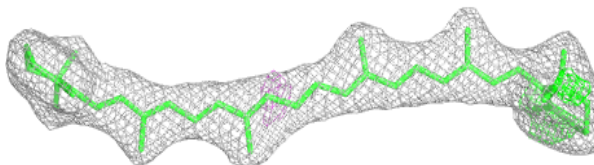


**Electron density around CLA A 407:**

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

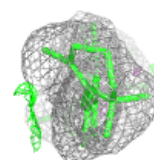
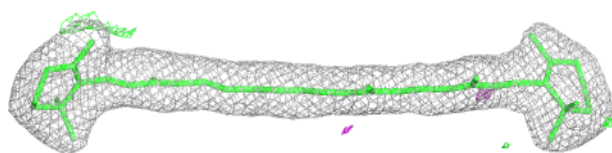
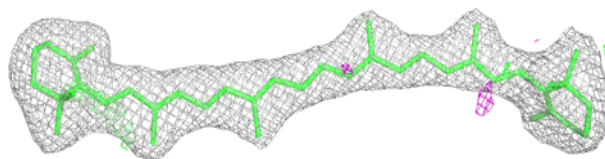
**Electron density around BCR A 408:**

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

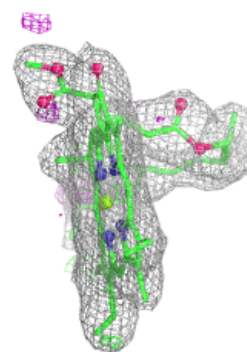
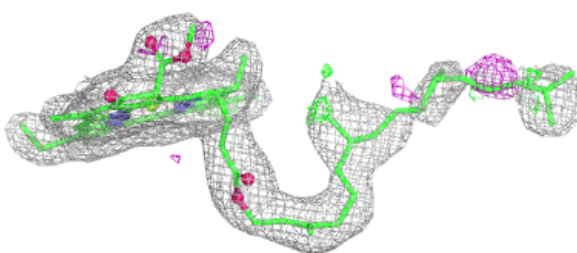
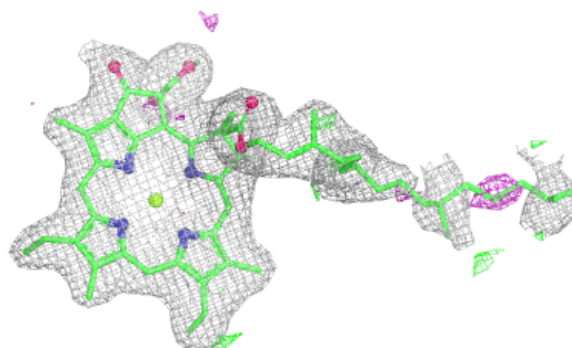


**Electron density around BCR B 618:**

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

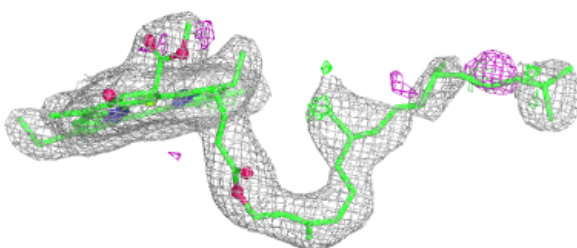
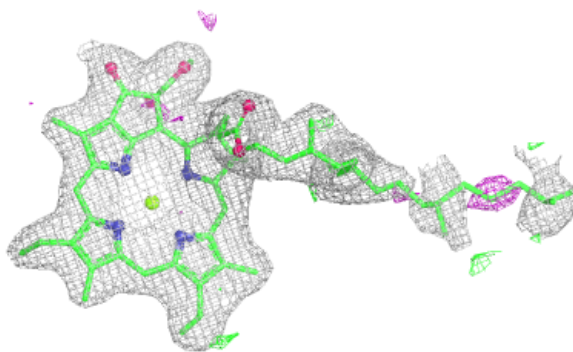
**Electron density around CLA a 405 (A):**

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



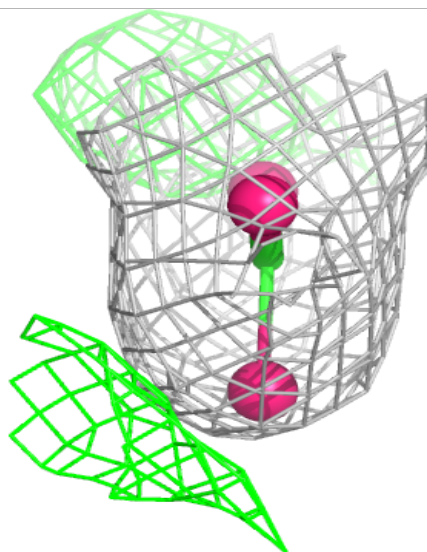
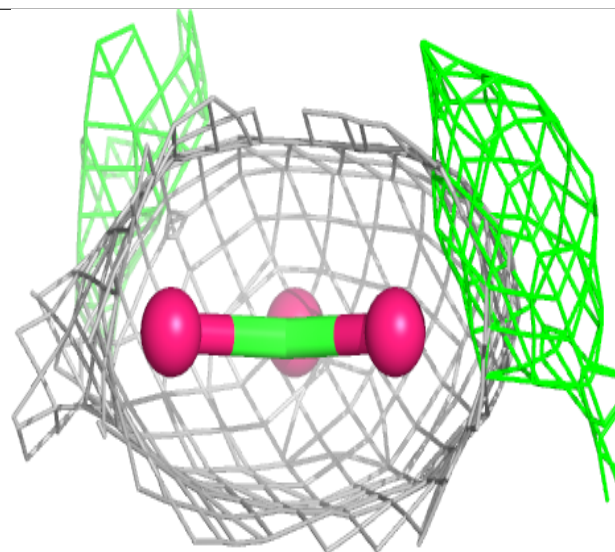
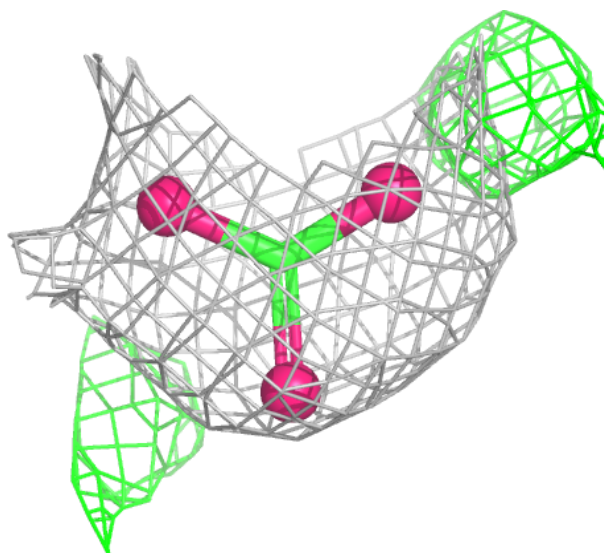
**Electron density around CLA a 405 (B):**

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



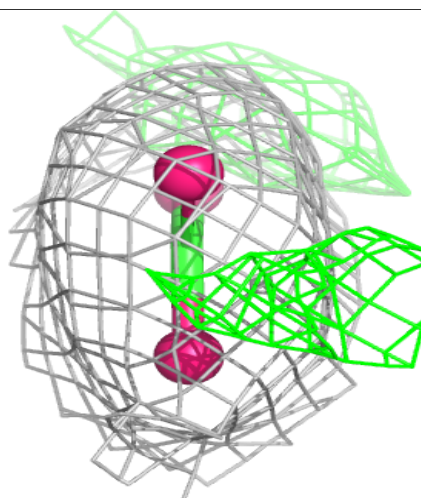
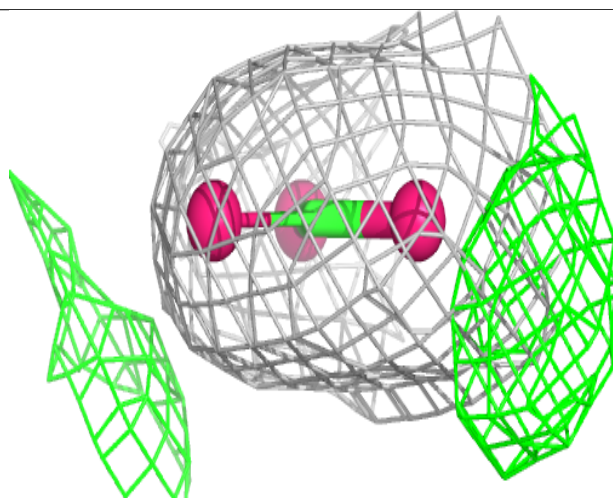
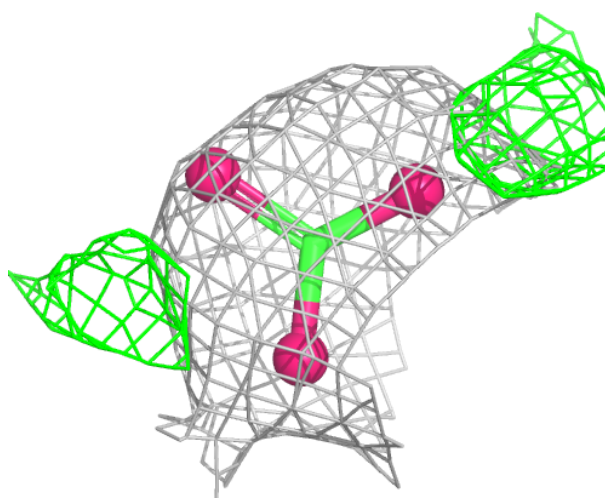
**Electron density around BCT d 401 (A):**

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



**Electron density around BCT d 401 (B):**

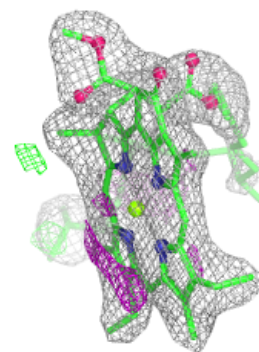
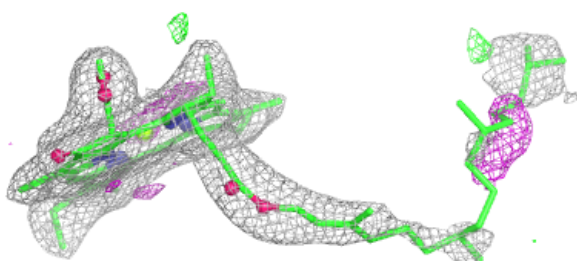
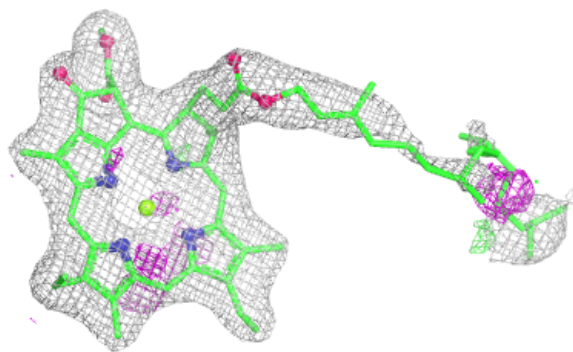
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



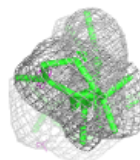
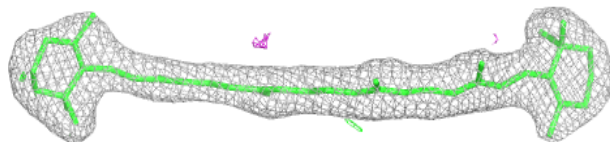
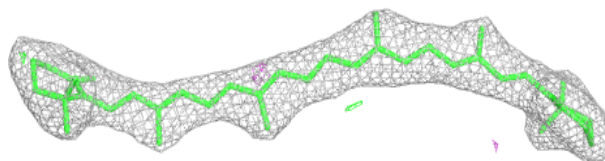


**Electron density around CLA a 407:**

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

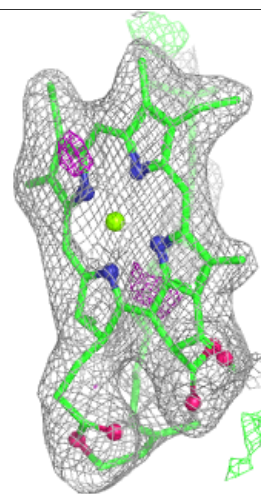
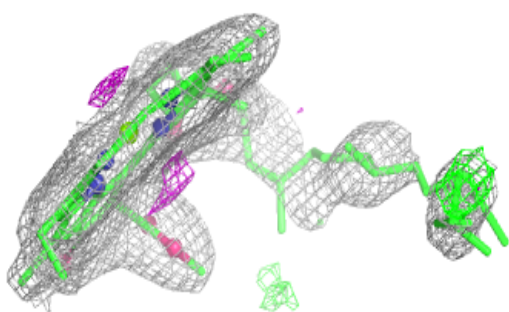
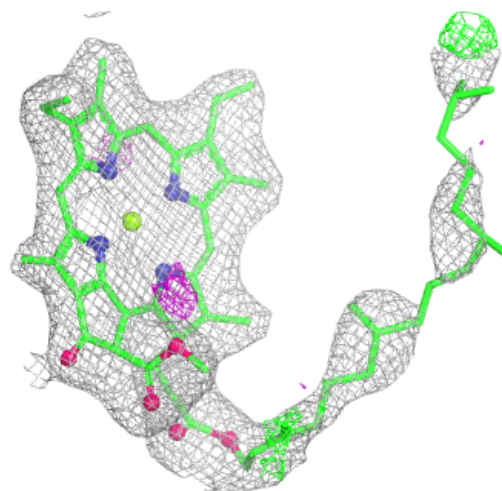
**Electron density around BCR H 101:**

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



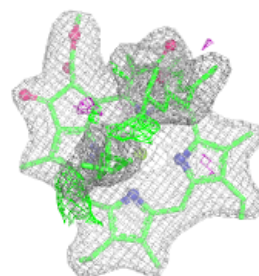
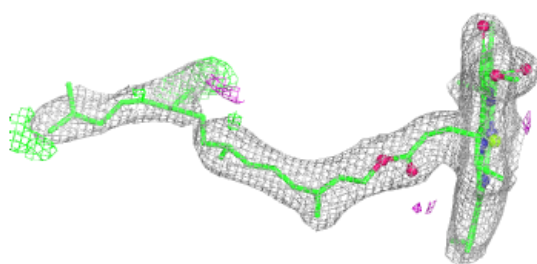
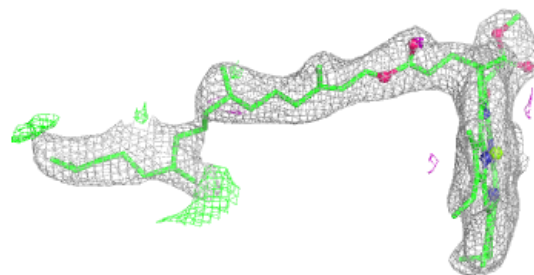
**Electron density around CLA B 616:**

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

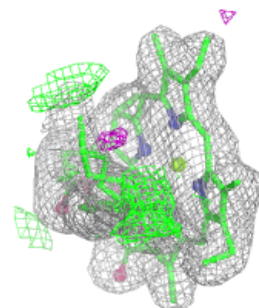
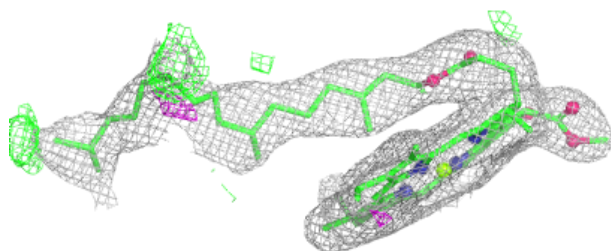
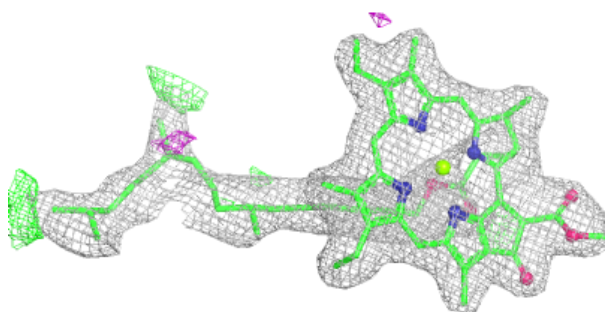


**Electron density around CLA b 606:**

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

**Electron density around CLA b 614:**

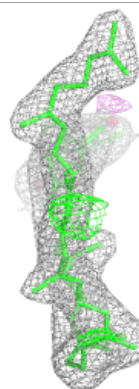
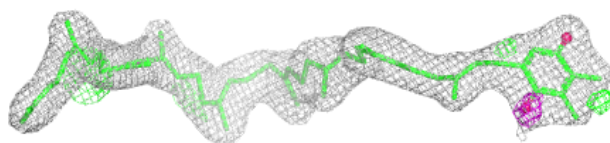
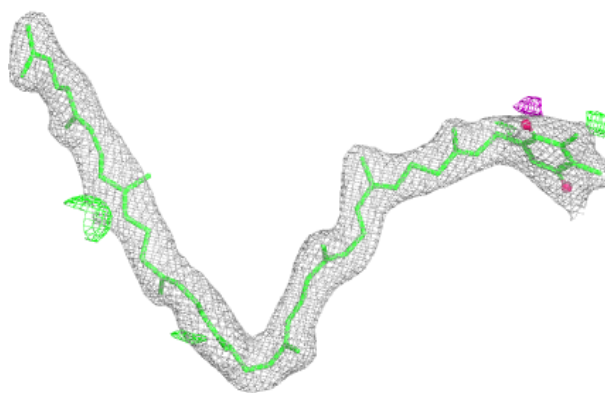
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



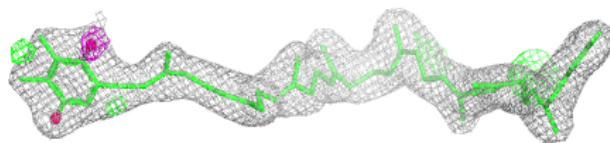
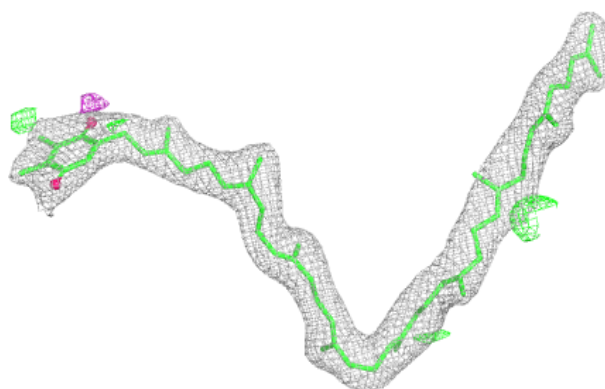


**Electron density around PL9 D 406 (A):**

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

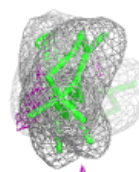
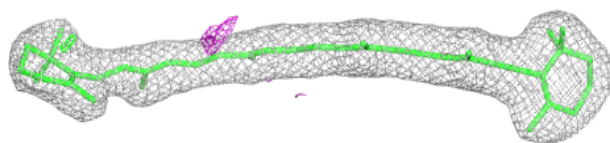
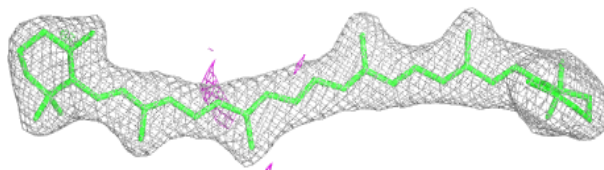
**Electron density around PL9 D 406 (B):**

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

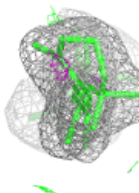
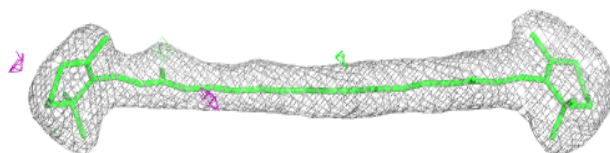
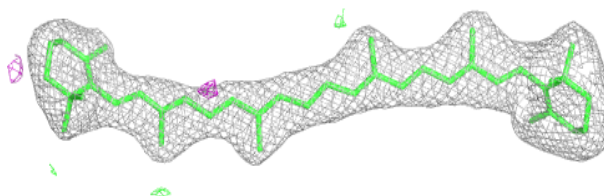


**Electron density around BCR b 617:**

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

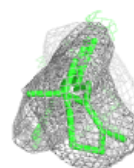
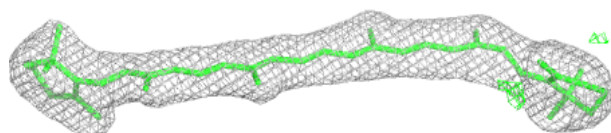
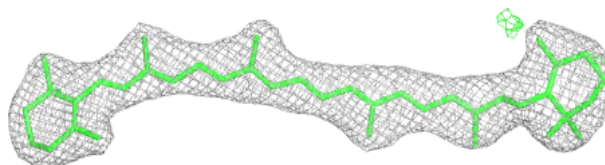
**Electron density around BCR b 618:**

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

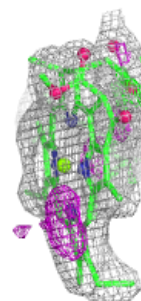
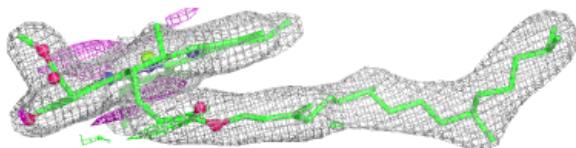
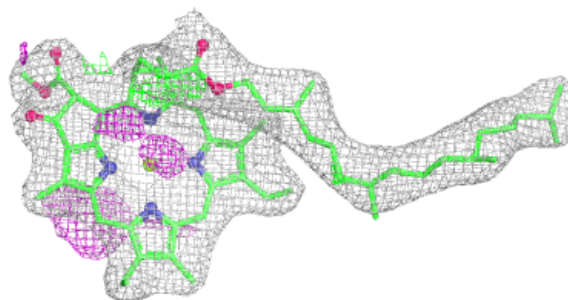


**Electron density around BCR b 619:**

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

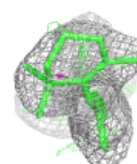
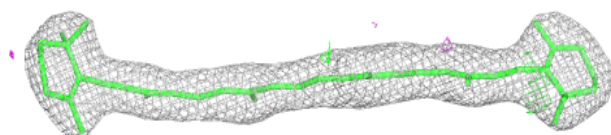
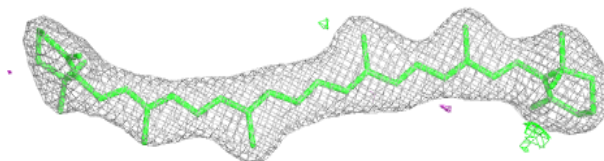
**Electron density around CLA B 603:**

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

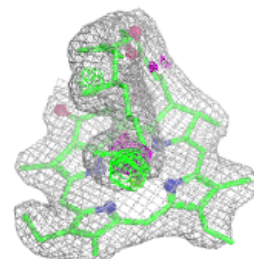
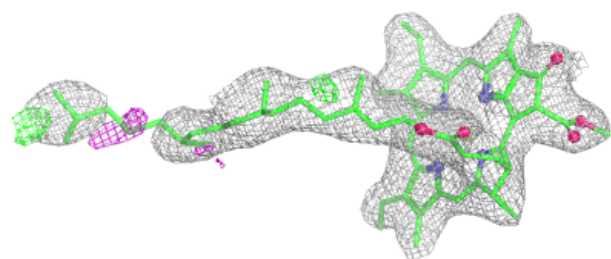
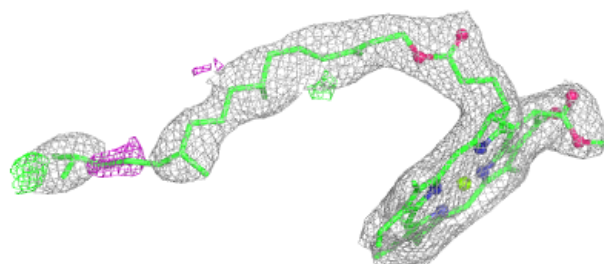


**Electron density around BCR c 516:**

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

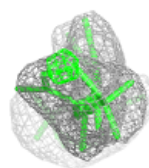
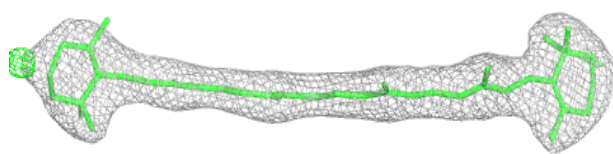
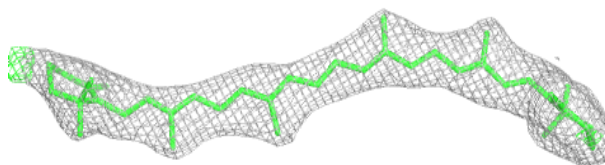
**Electron density around CLA c 505:**

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

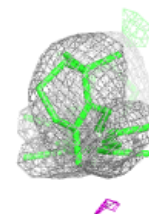
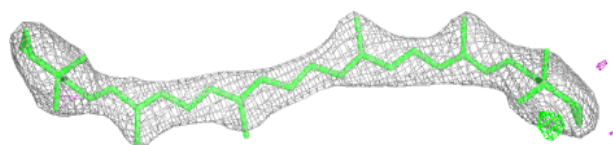
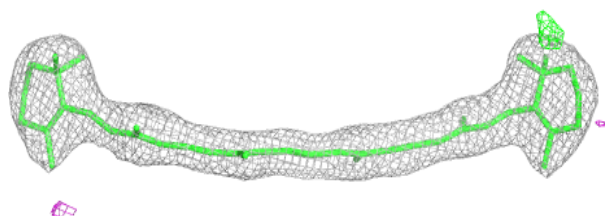


**Electron density around BCR h 101:**

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

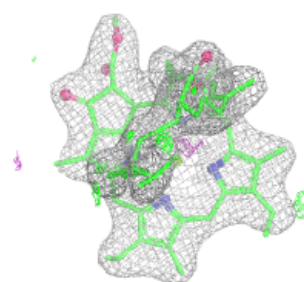
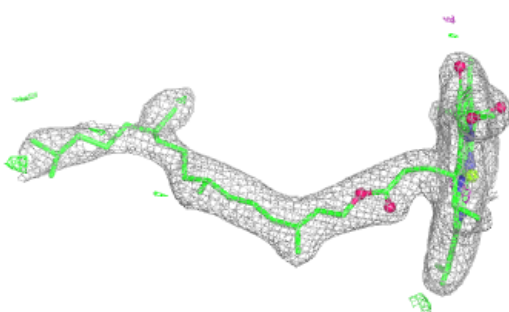
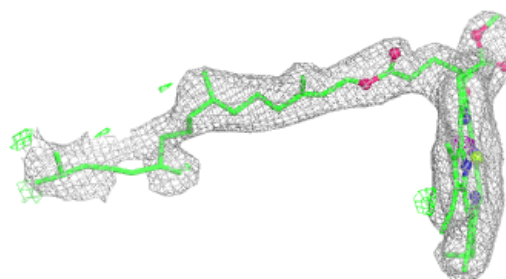
**Electron density around BCR k 101:**

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

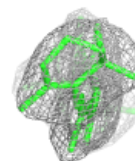
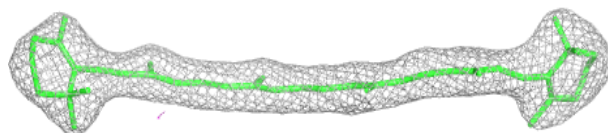
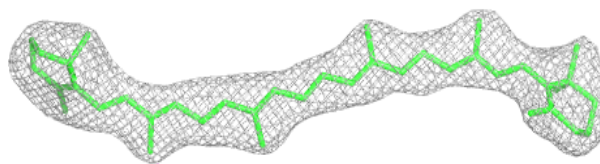


**Electron density around CLA B 606:**

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

**Electron density around BCR y 101:**

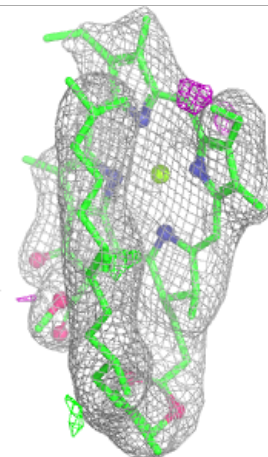
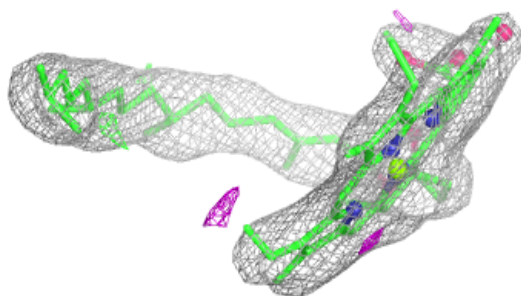
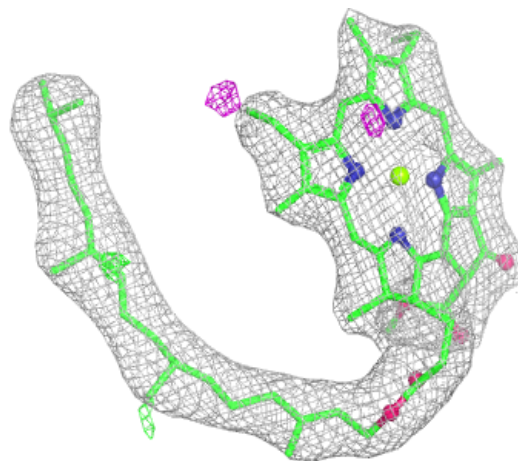
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





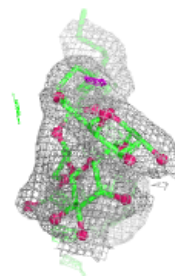
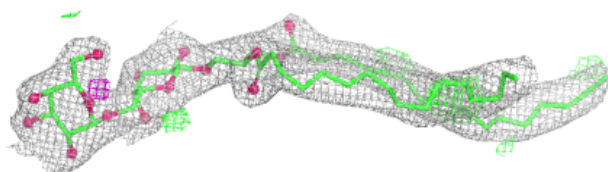
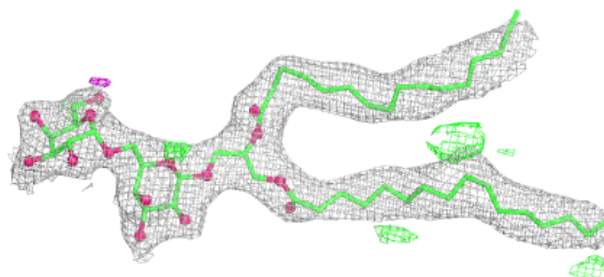
**Electron density around CLA c 508:**

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

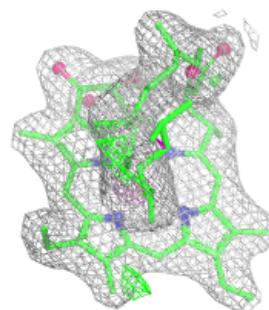
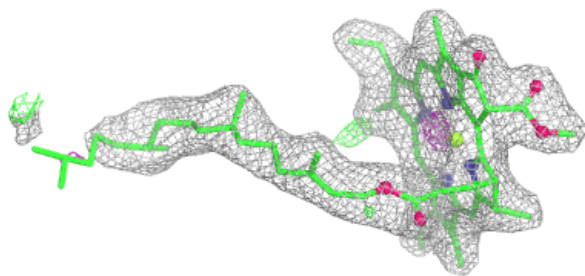
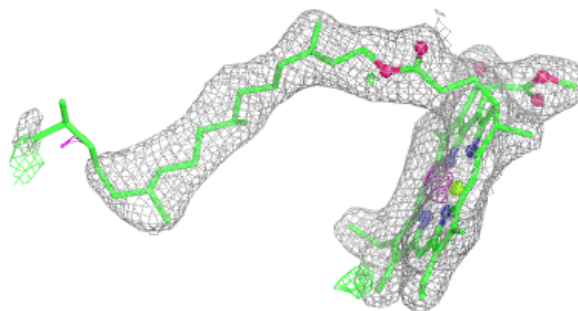


**Electron density around DGD C 519:**

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

**Electron density around CLA C 509:**

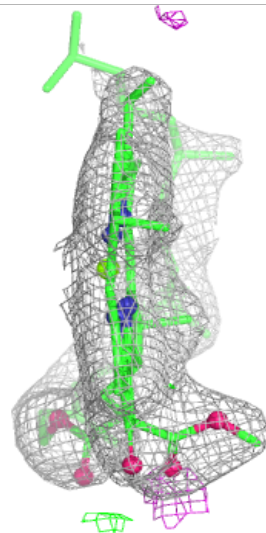
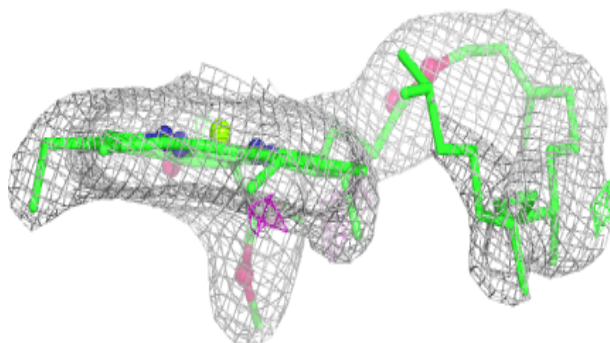
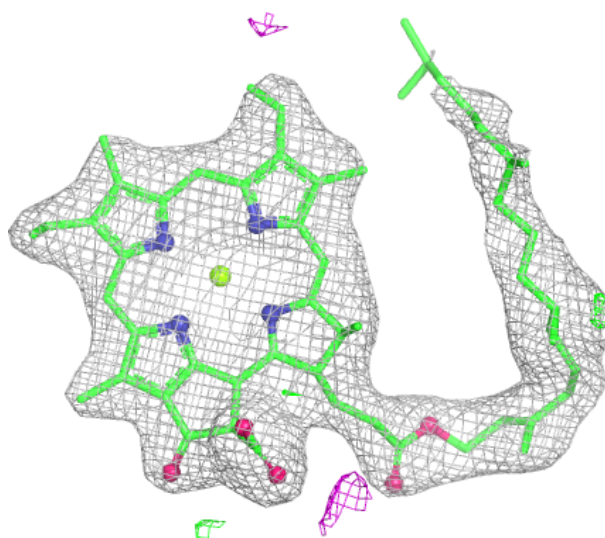
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





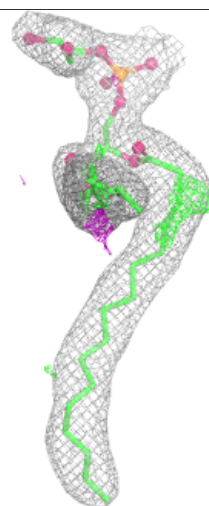
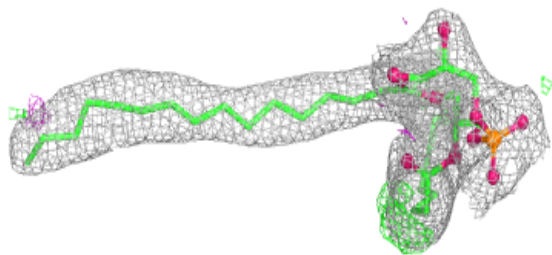
**Electron density around CLA C 513:**

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



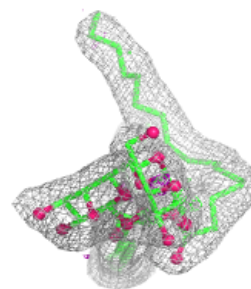
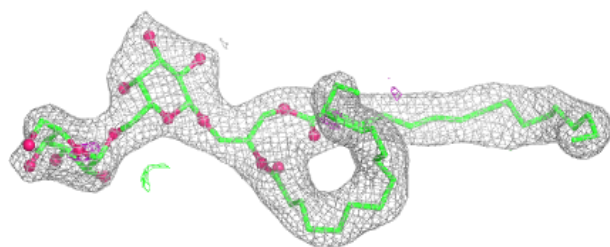
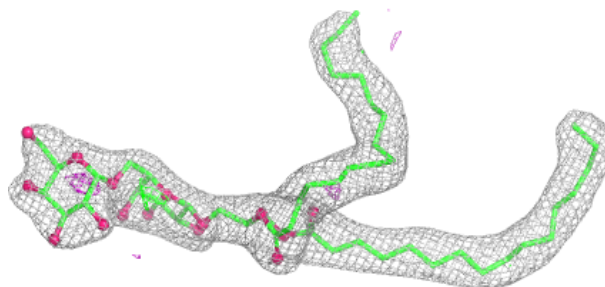
**Electron density around LHG b 629 (A):**

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



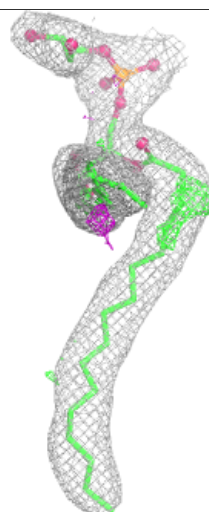
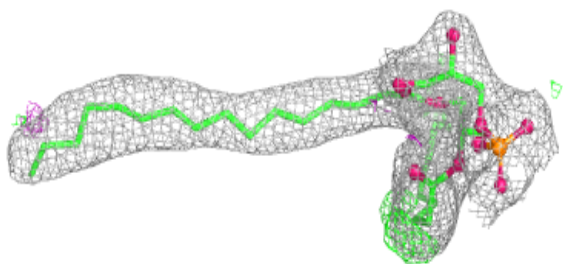
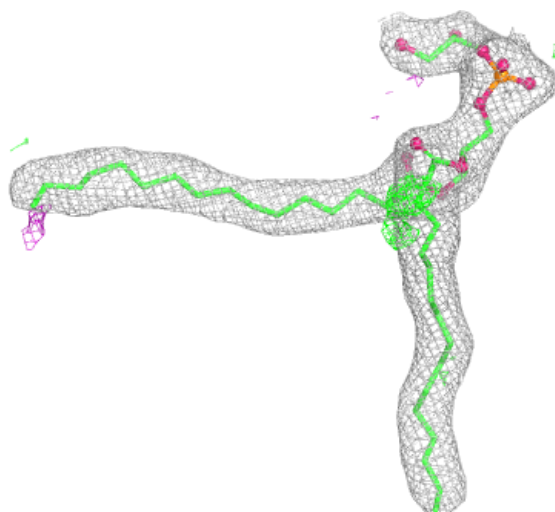
**Electron density around DGD h 102:**

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



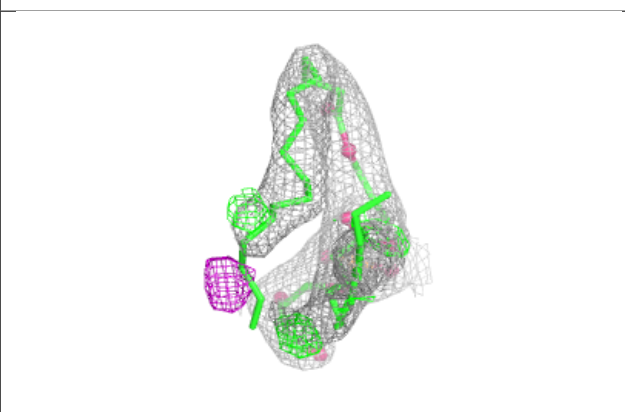
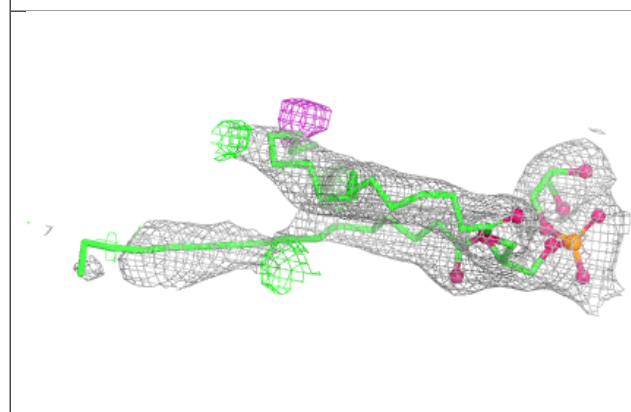
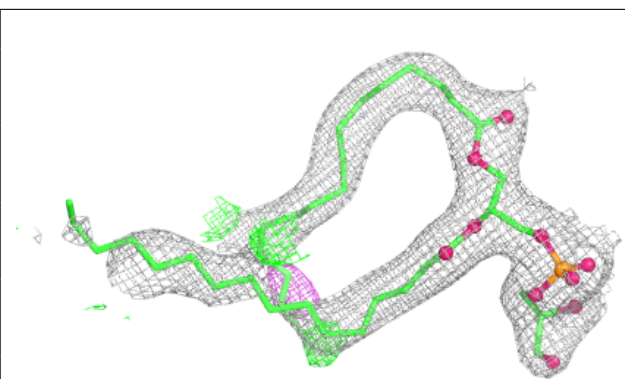
**Electron density around LHG b 629 (B):**

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

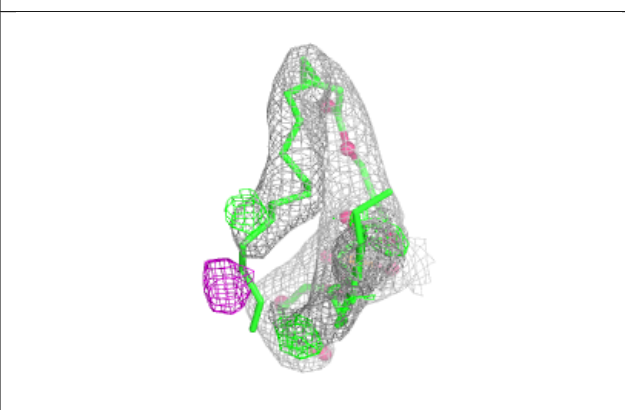
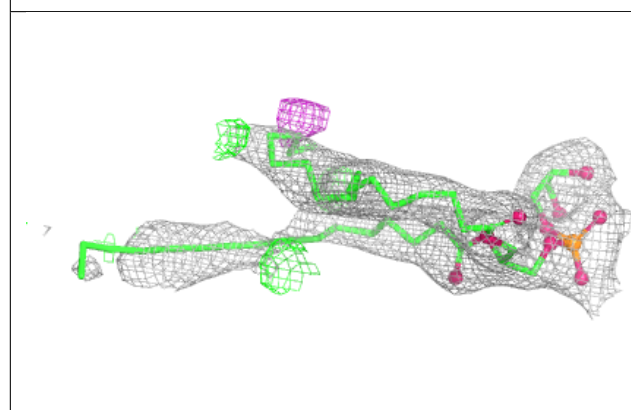
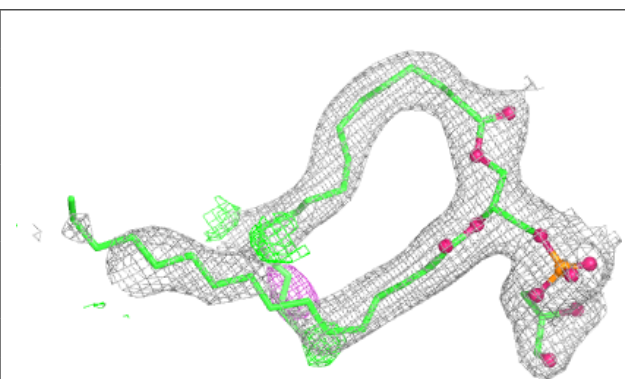


**Electron density around LHG d 408 (A):**

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

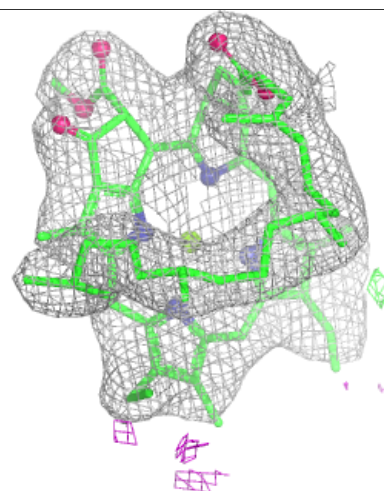
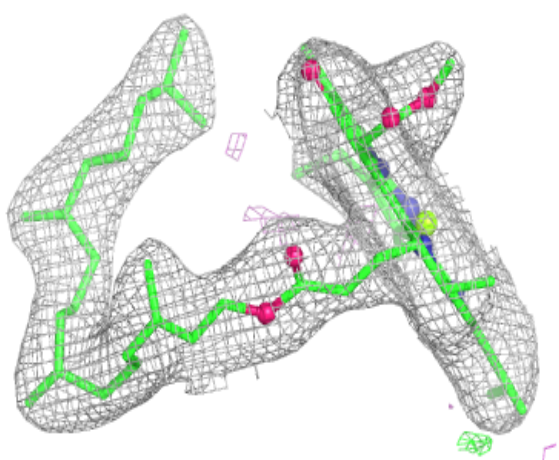
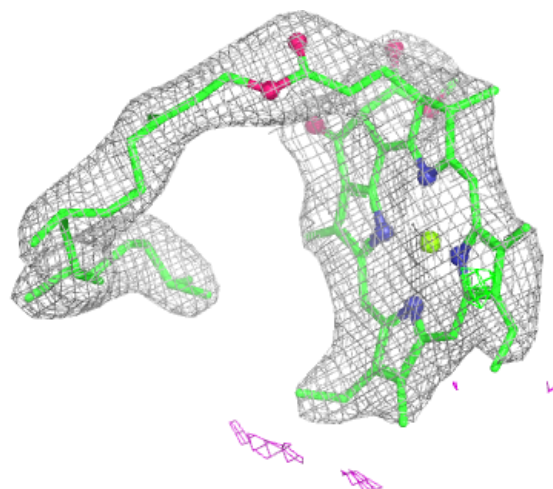
**Electron density around LHG d 408 (B):**

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



**Electron density around CLA c 504:**

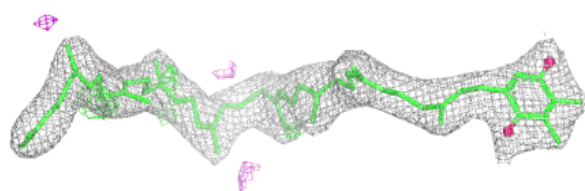
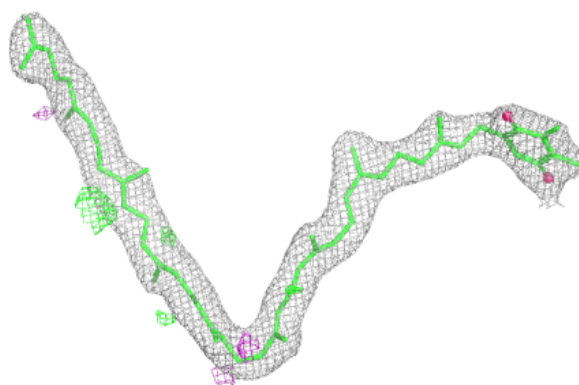
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



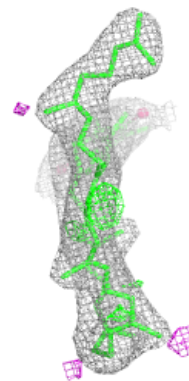
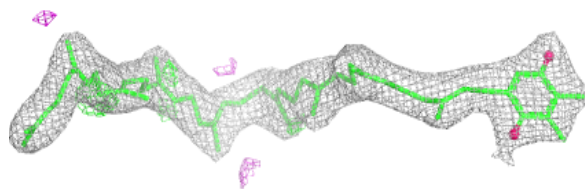
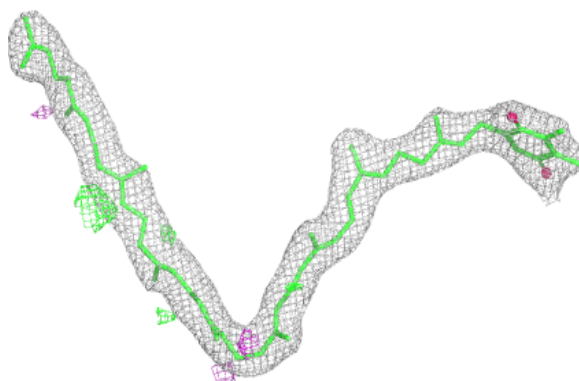


**Electron density around PL9 d 406 (A):**

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

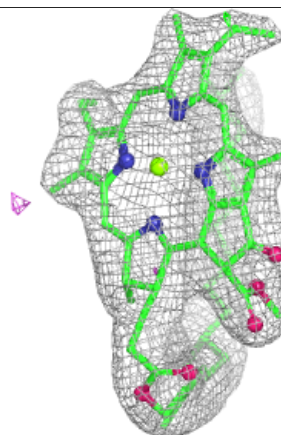
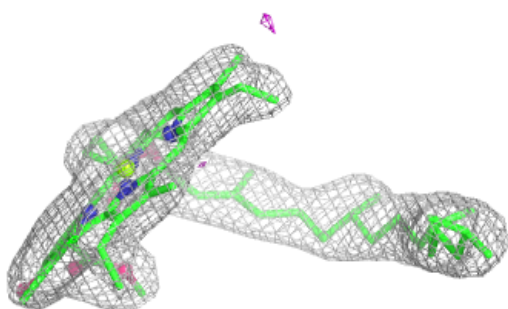
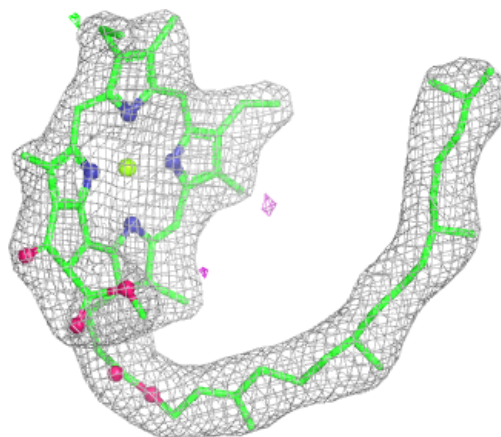
**Electron density around PL9 d 406 (B):**

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



**Electron density around CLA C 508:**

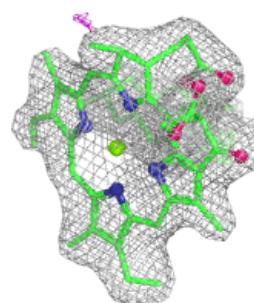
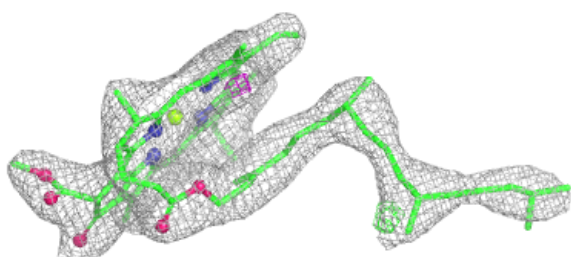
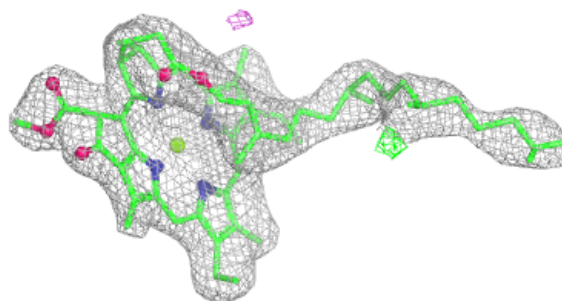
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



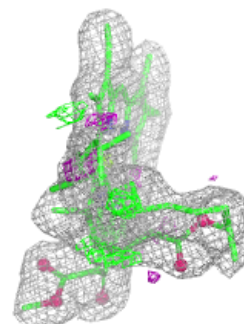
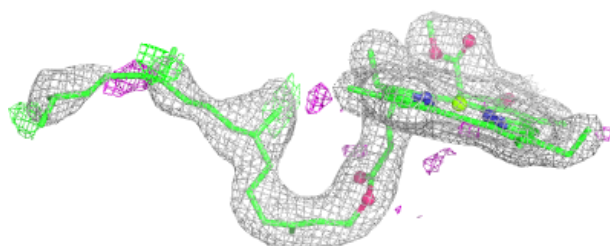
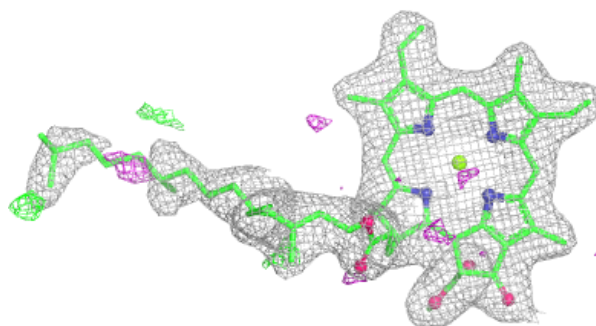


**Electron density around CLA c 506:**

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

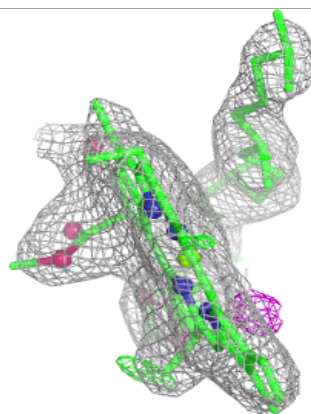
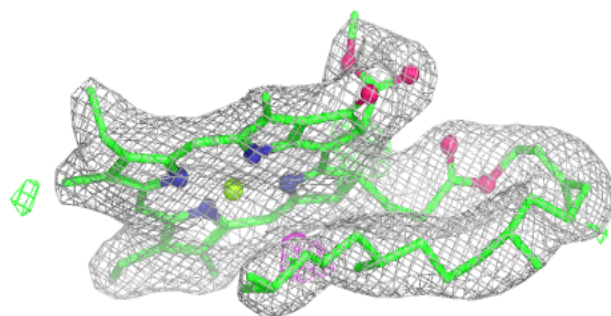
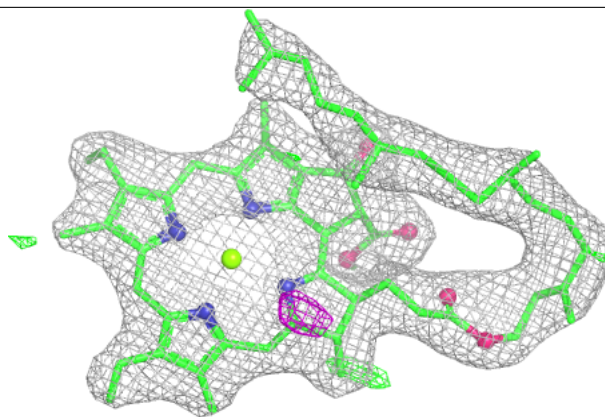
**Electron density around CLA A 406 (B):**

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

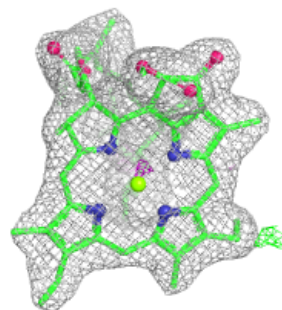
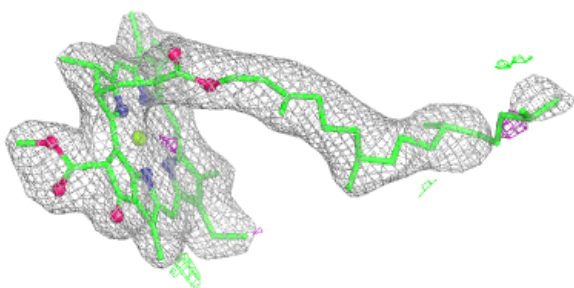
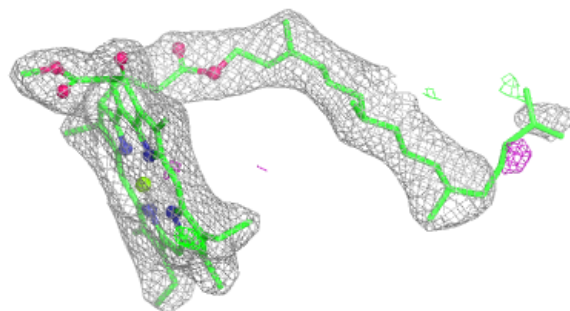


**Electron density around CLA C 510:**

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

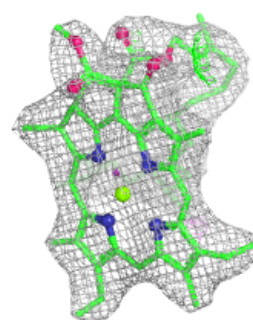
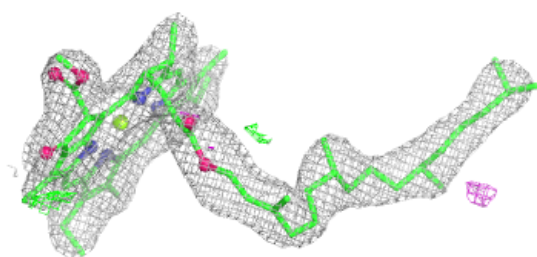
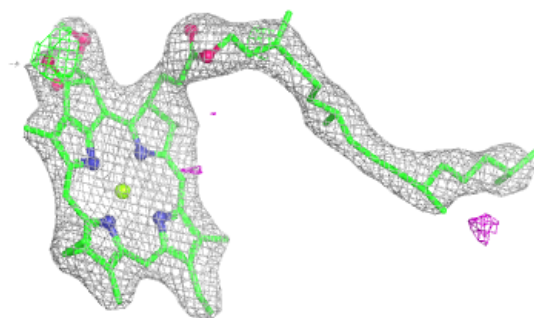
**Electron density around CLA c 509:**

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

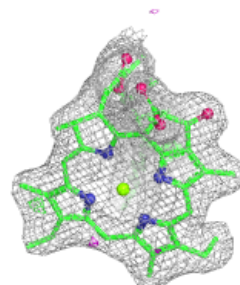
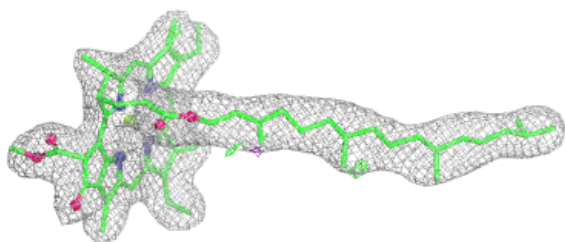
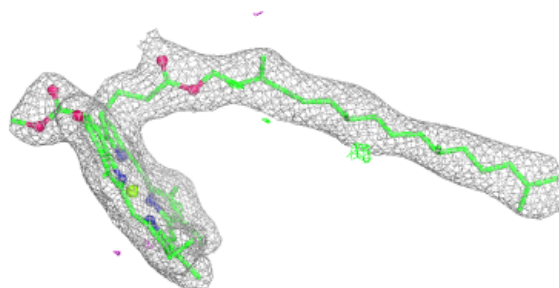


**Electron density around CLA c 512:**

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

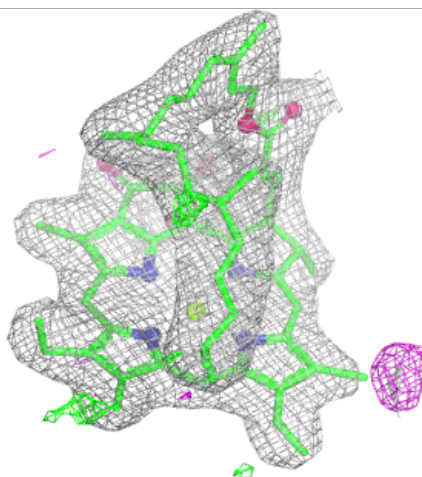
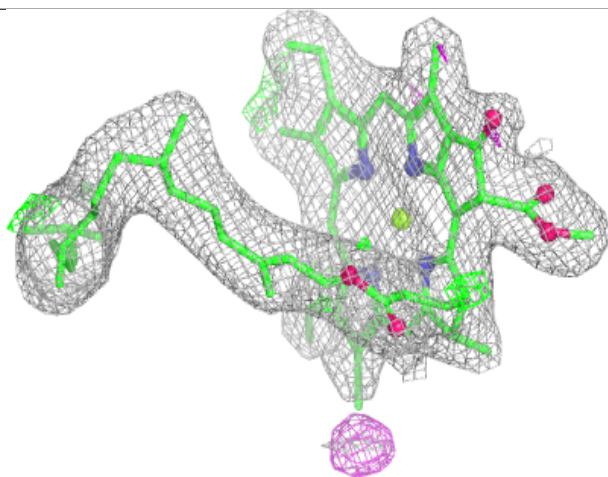
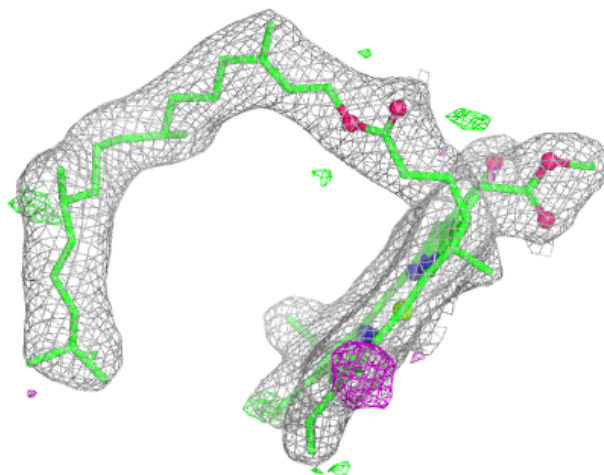
**Electron density around CLA B 607:**

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



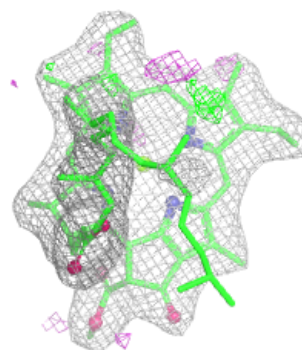
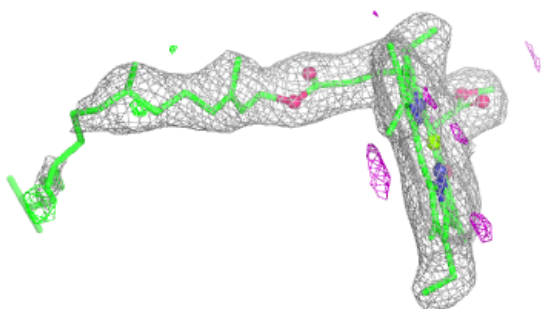
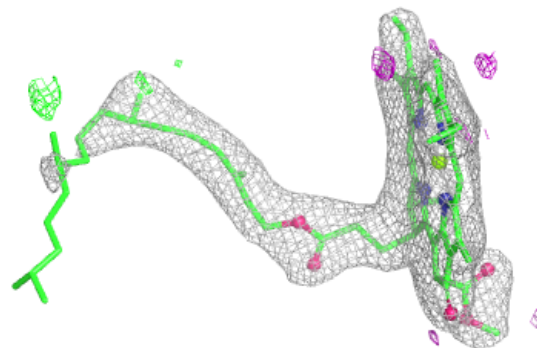
**Electron density around CLA B 611:**

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



**Electron density around CLA D 404:**

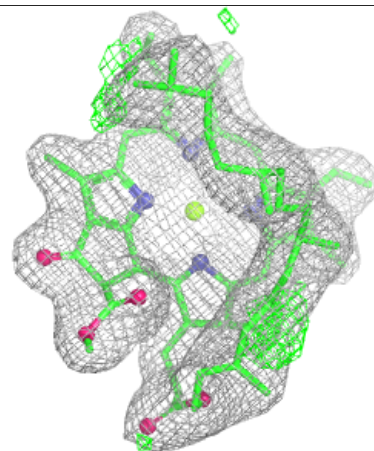
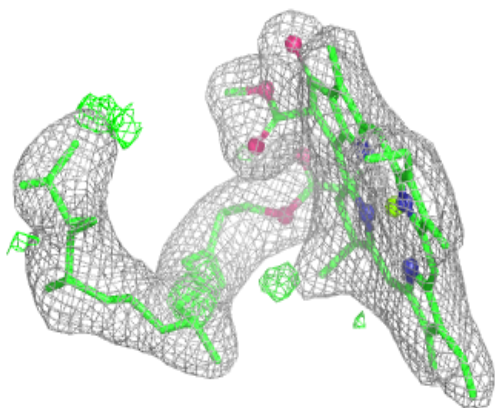
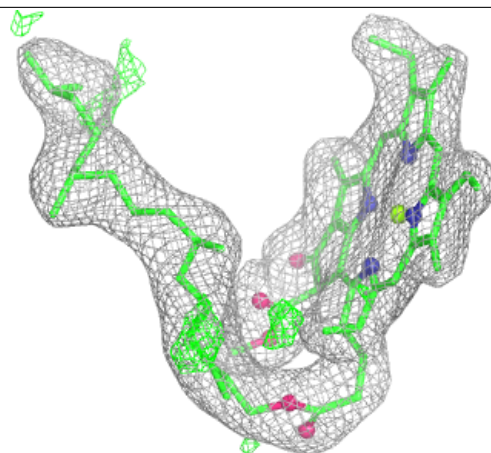
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





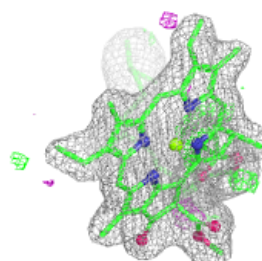
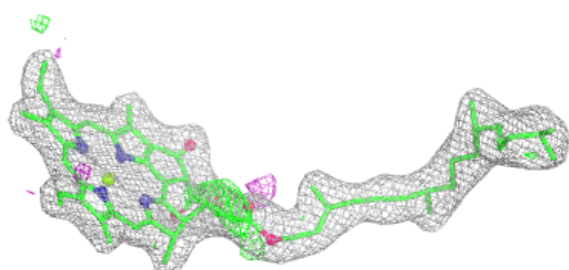
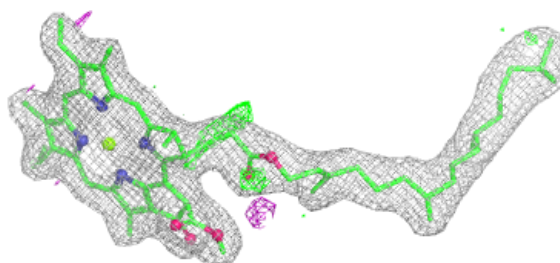
**Electron density around CLA B 613:**

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

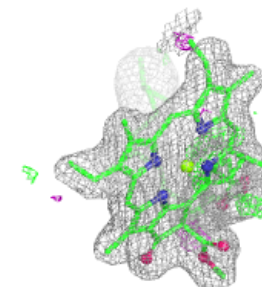
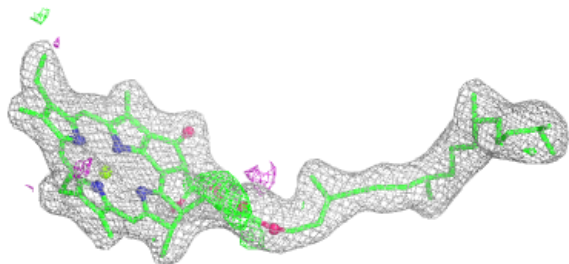
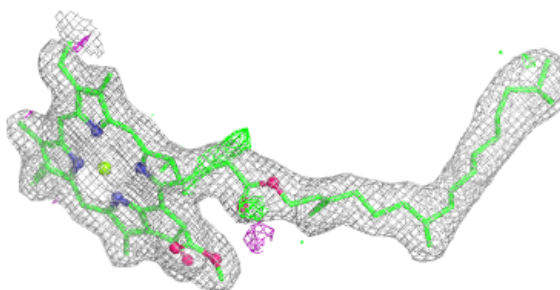


**Electron density around CLA A 404 (A):**

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

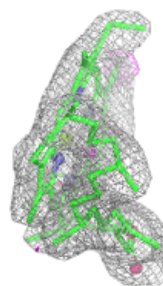
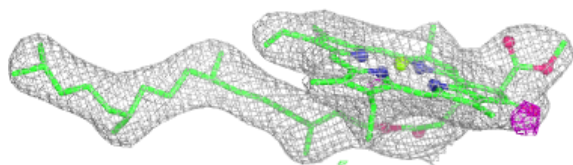
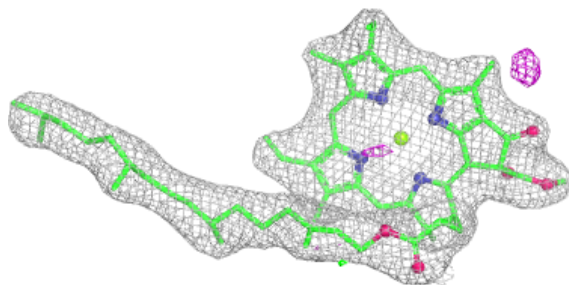
**Electron density around CLA A 404 (B):**

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

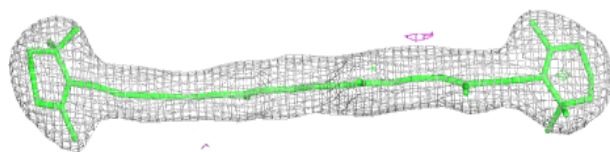
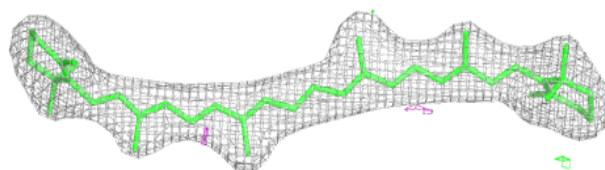


**Electron density around CLA C 502:**

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

**Electron density around BCR C 516:**

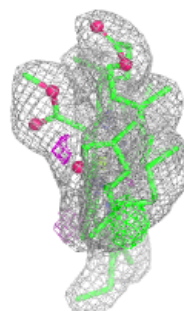
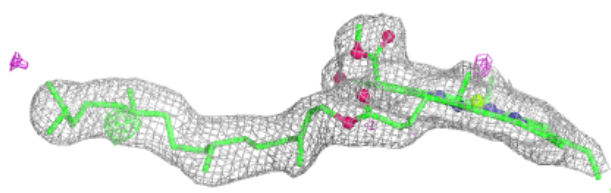
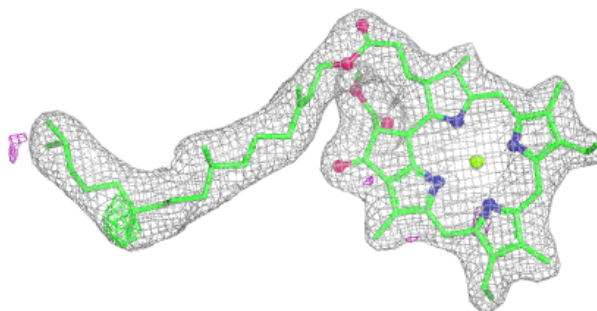
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



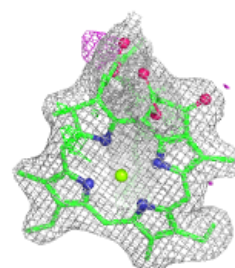
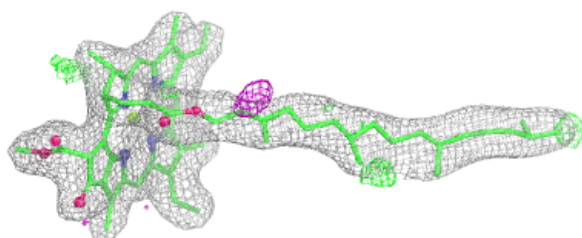
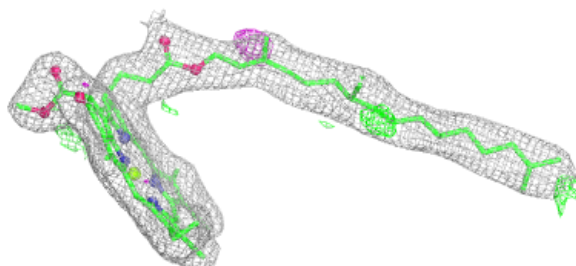


**Electron density around CLA B 602:**

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

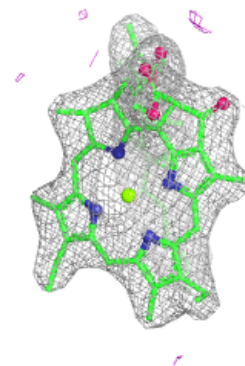
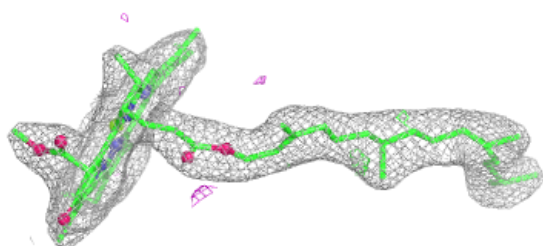
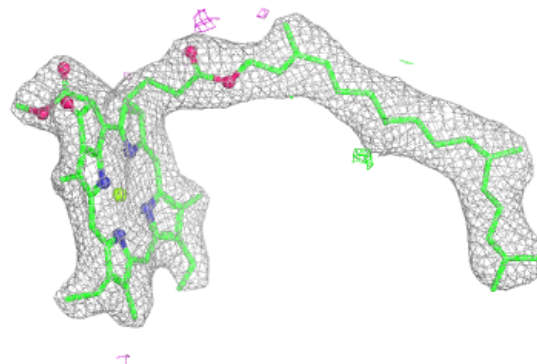
**Electron density around CLA b 607:**

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

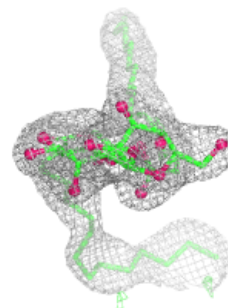
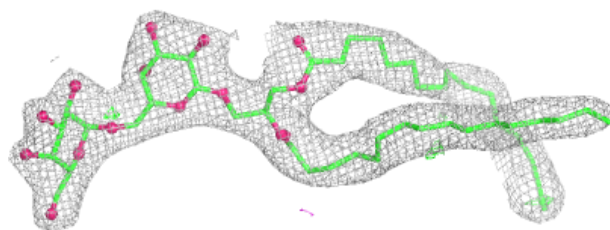
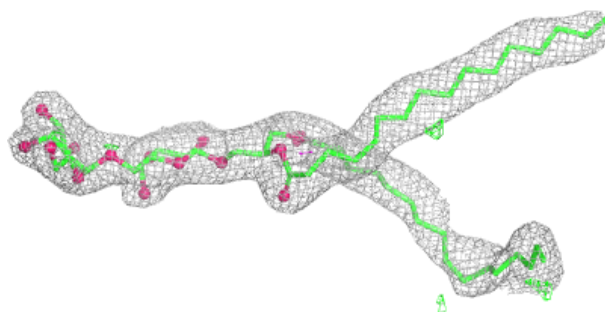


**Electron density around CLA b 609:**

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

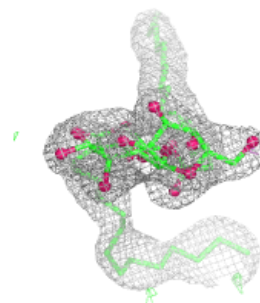
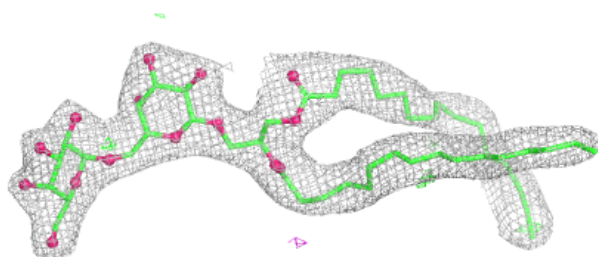
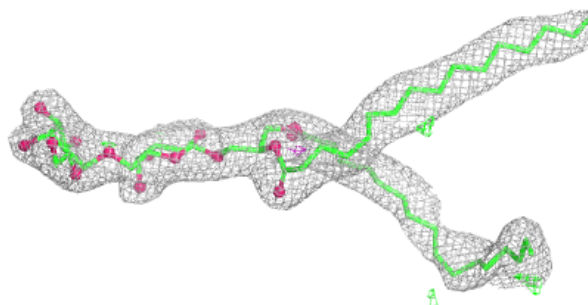
**Electron density around DGD C 517 (A):**

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

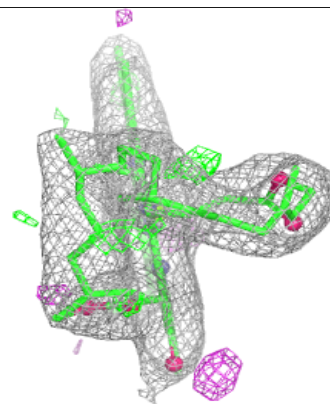
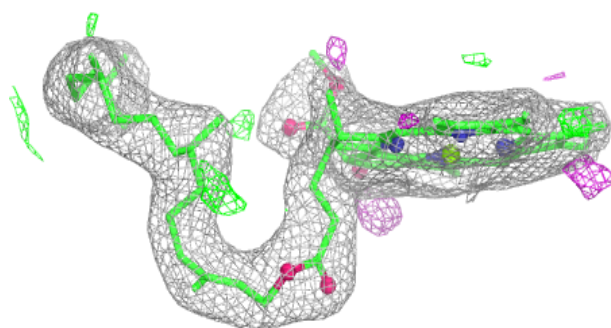
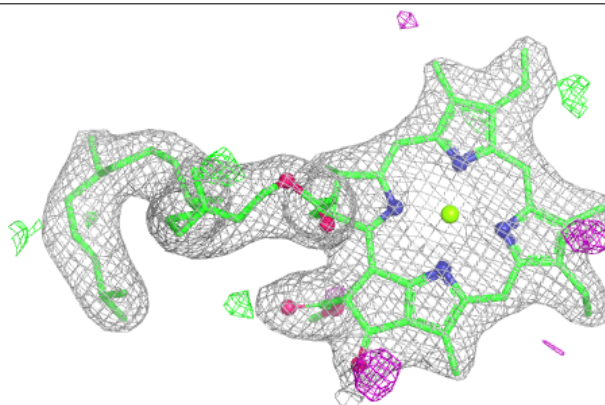


**Electron density around DGD C 517 (B):**

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

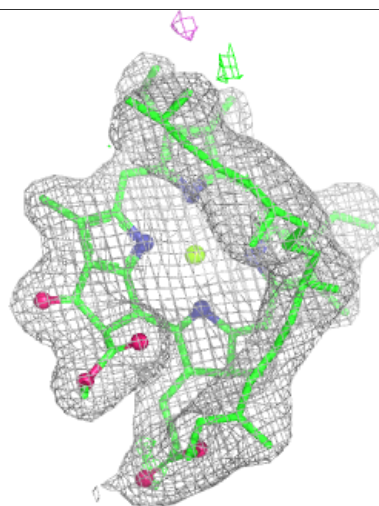
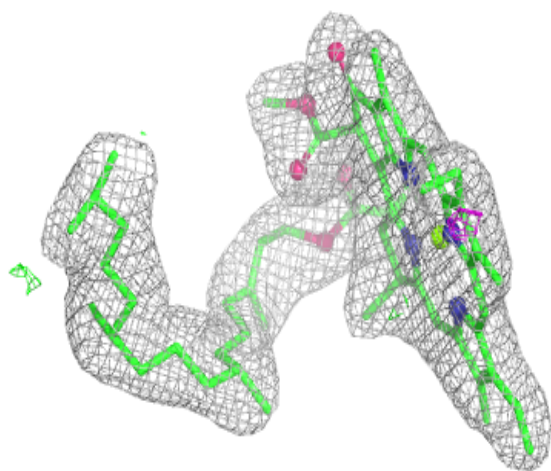
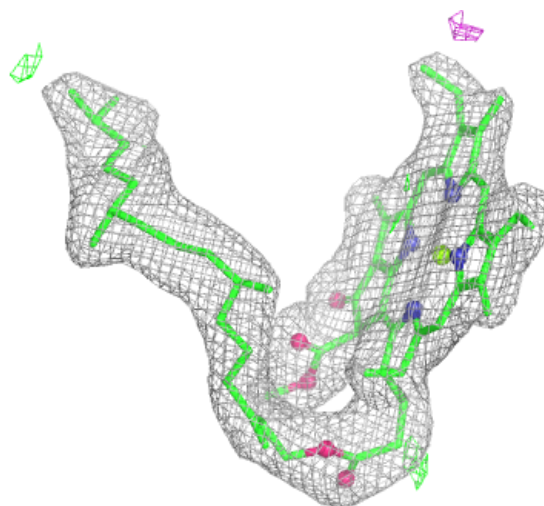
**Electron density around CLA b 612:**

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



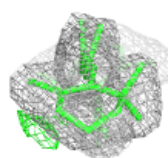
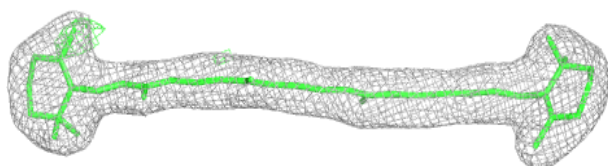
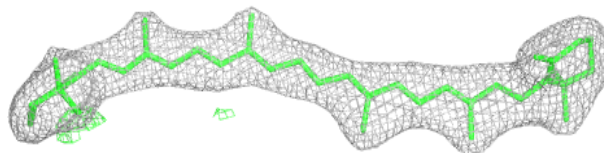
**Electron density around CLA b 613:**

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

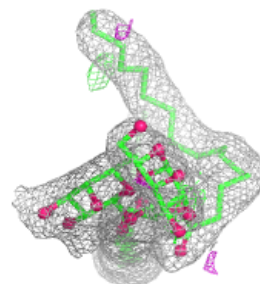
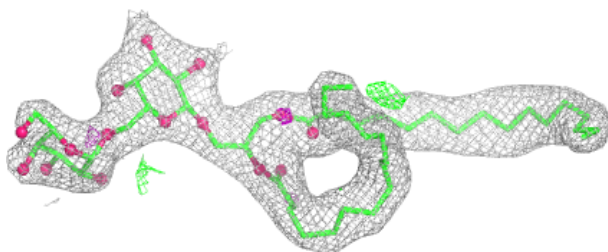
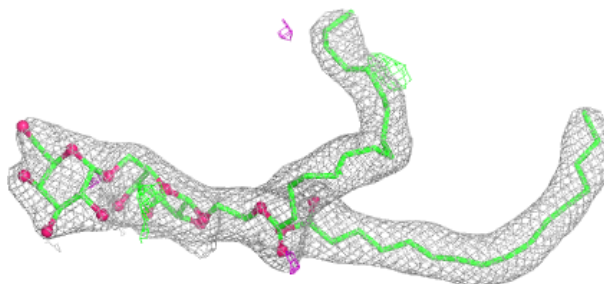


**Electron density around BCR a 408:**

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

**Electron density around DGD H 102:**

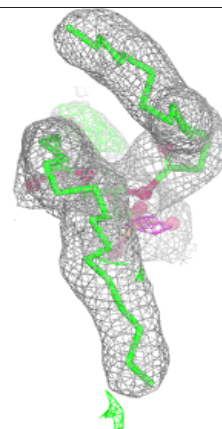
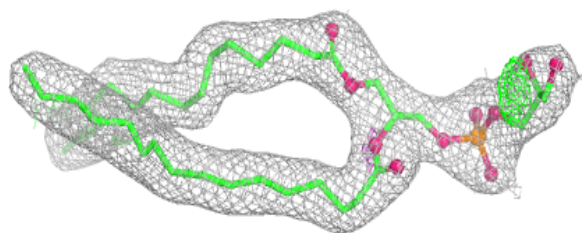
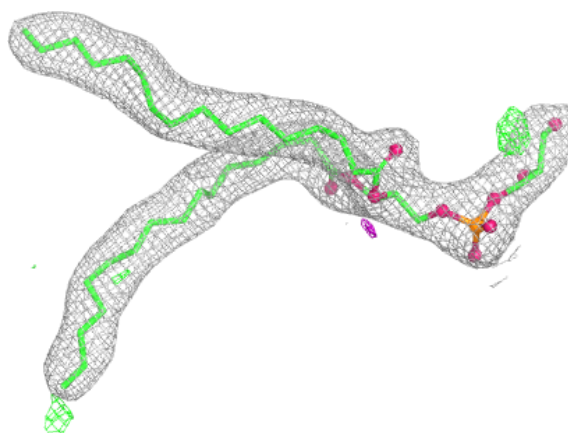
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





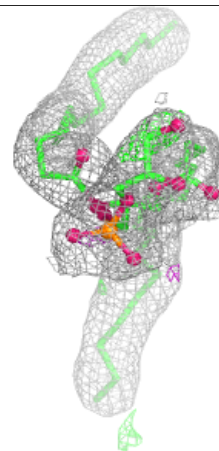
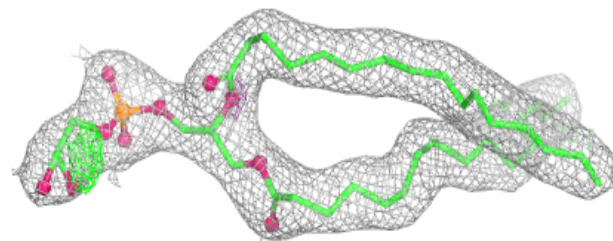
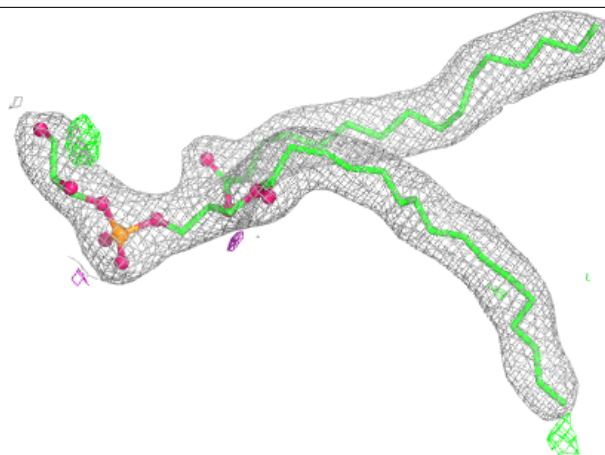
**Electron density around LHG d 407 (A):**

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



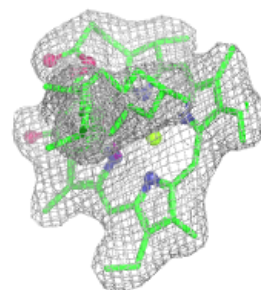
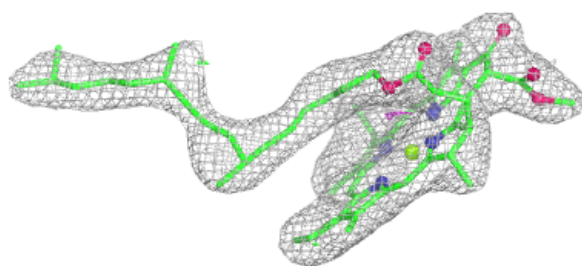
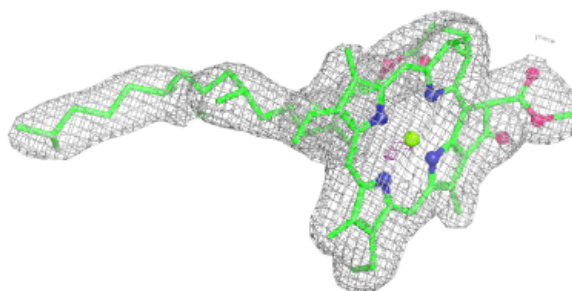
**Electron density around LHG d 407 (B):**

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

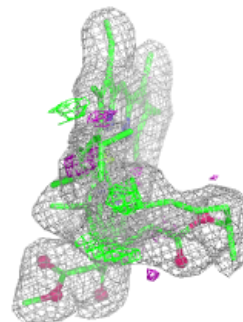
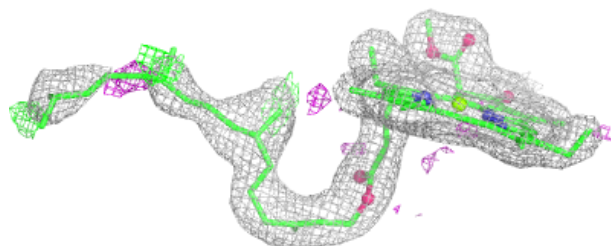
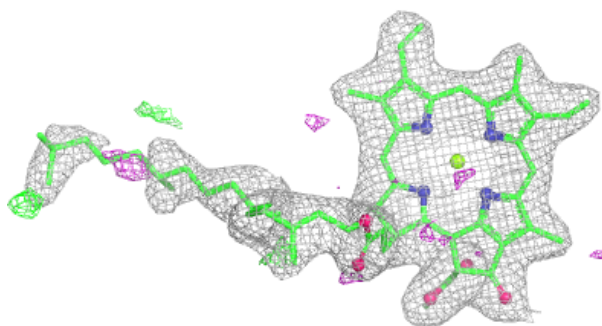


**Electron density around CLA C 506:**

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

**Electron density around CLA A 406 (A):**

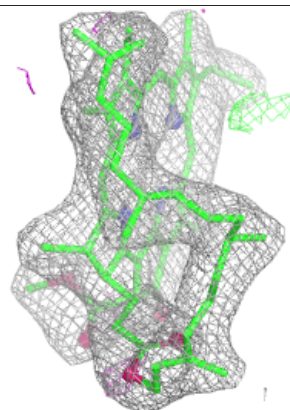
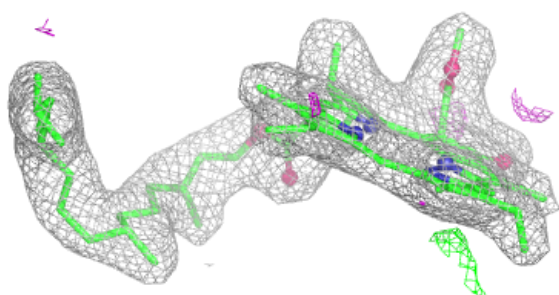
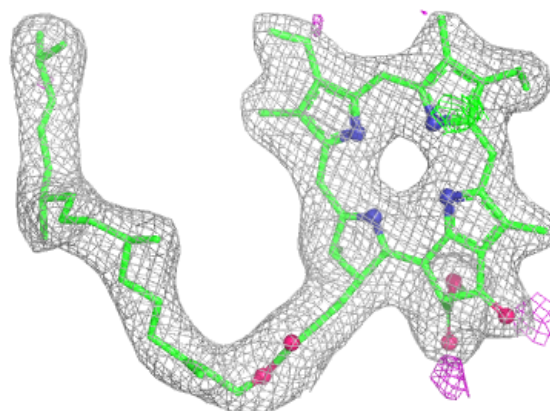
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



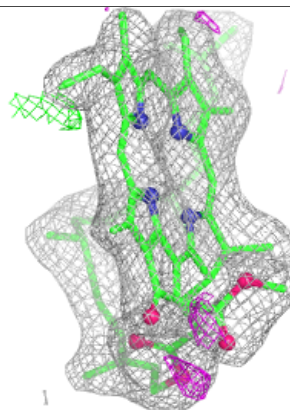
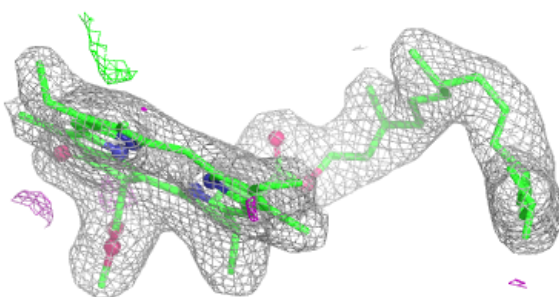
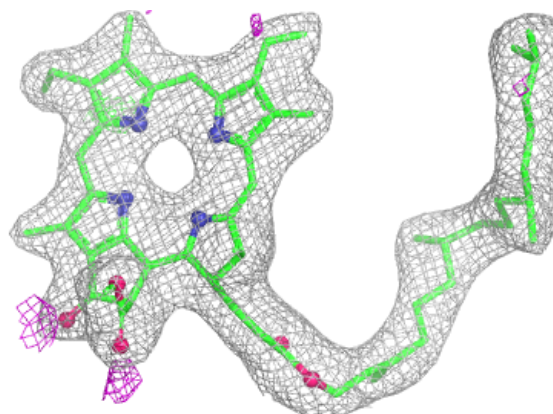


**Electron density around PHO A 416 (A):**

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

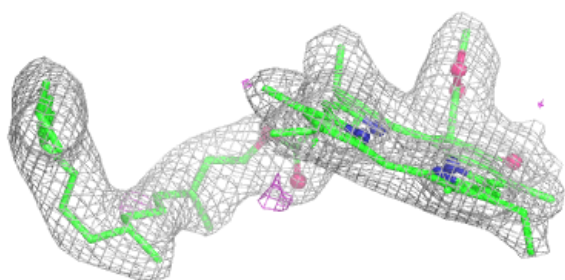
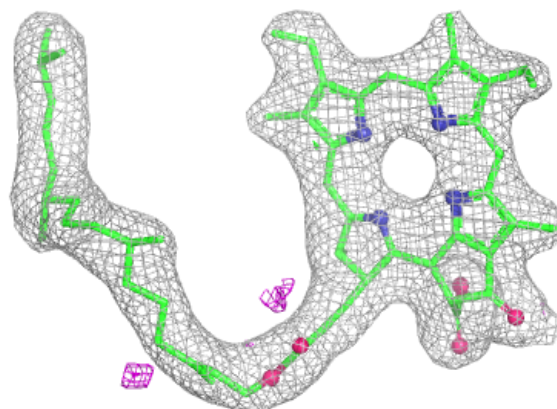
**Electron density around PHO A 416 (B):**

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

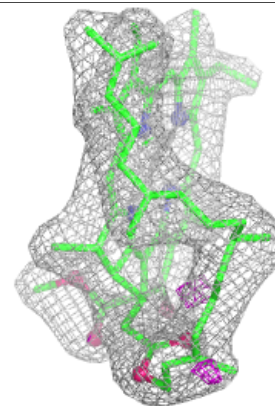
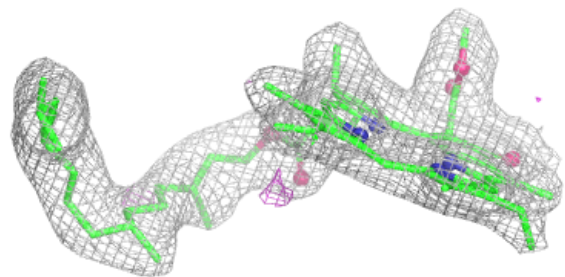
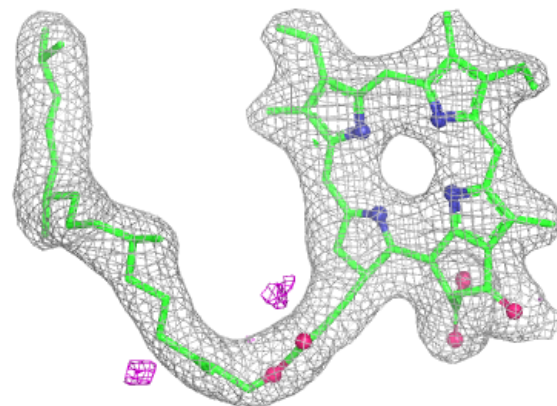


**Electron density around PHO a 415 (A):**

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

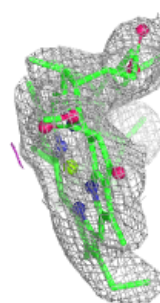
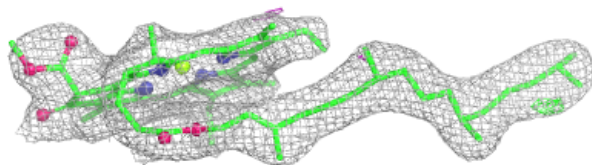
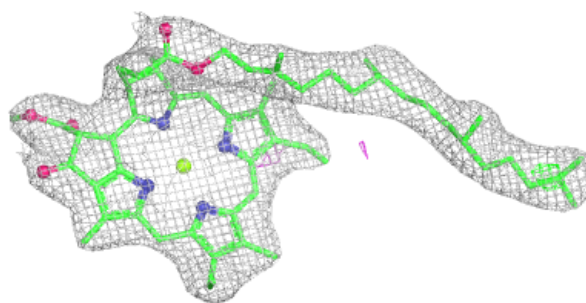
**Electron density around PHO a 415 (B):**

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

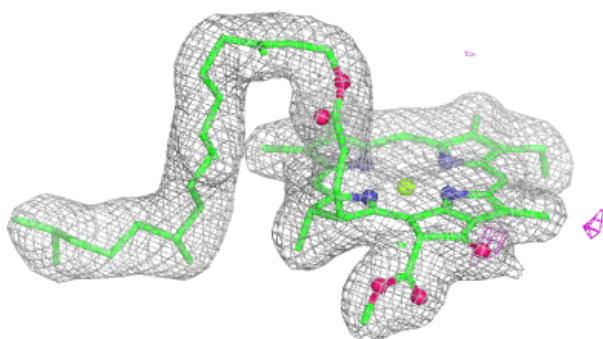
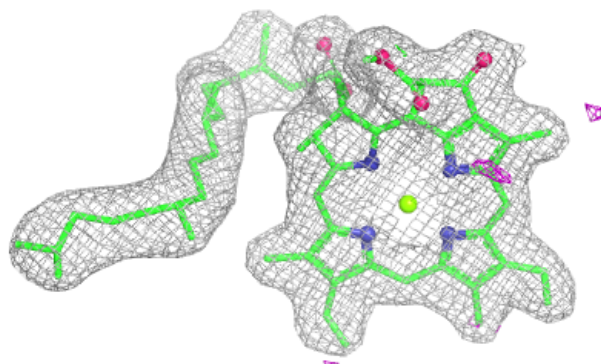


**Electron density around CLA c 502:**

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

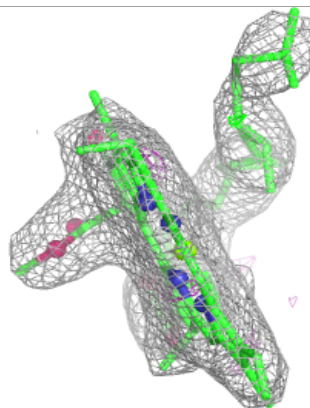
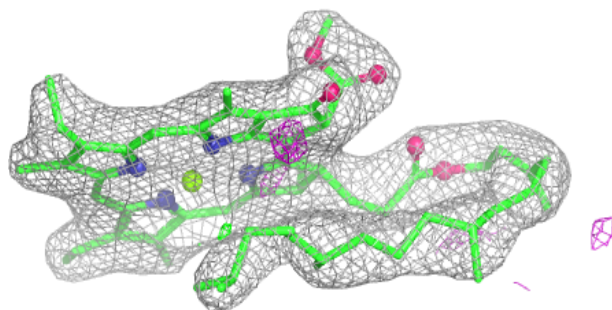
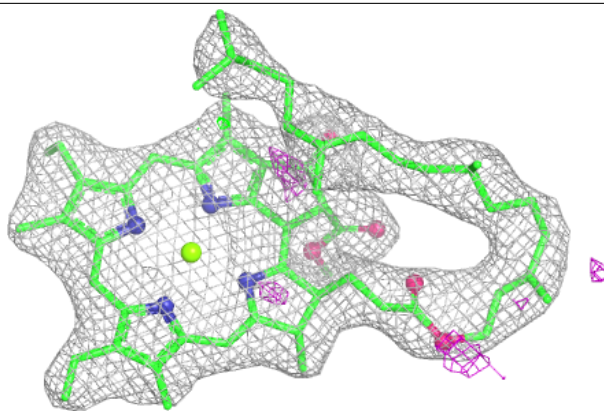
**Electron density around CLA A 405 (A):**

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



**Electron density around CLA c 510:**

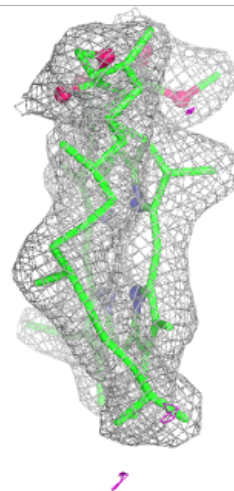
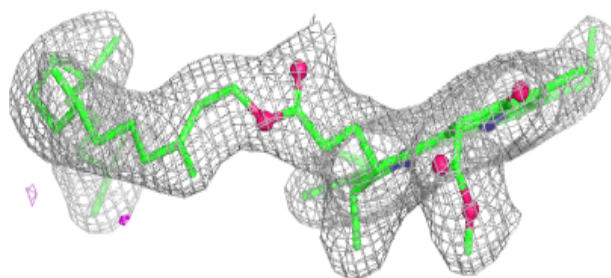
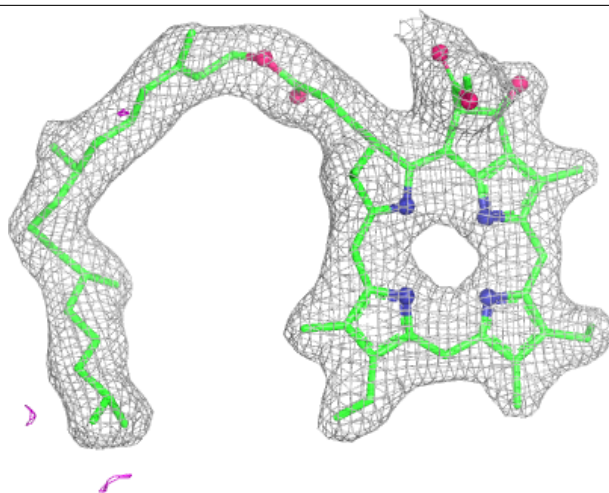
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





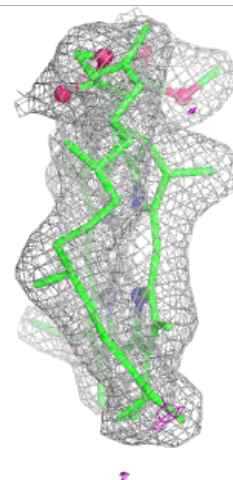
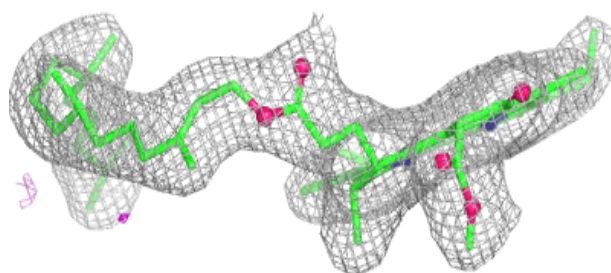
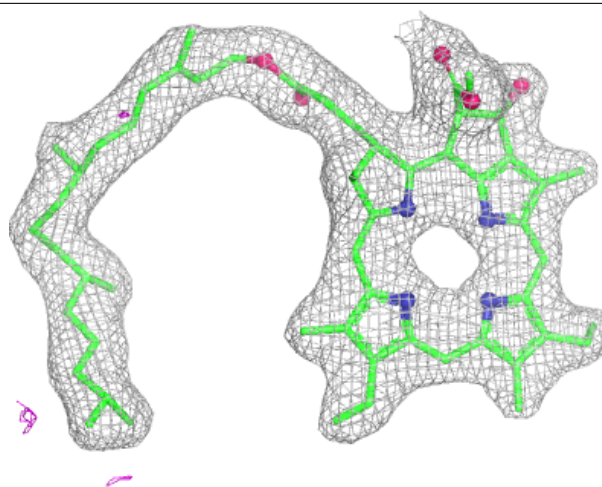
**Electron density around PHO D 401 (A):**

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



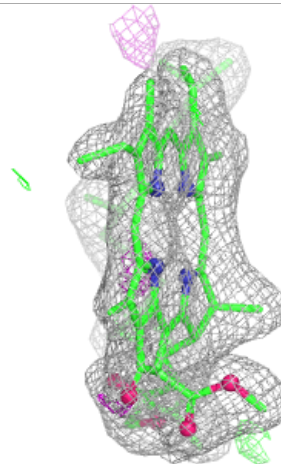
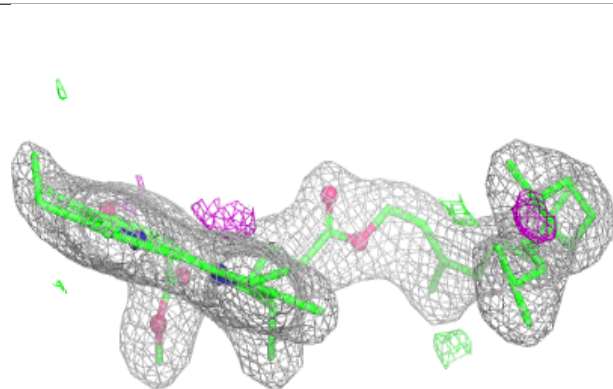
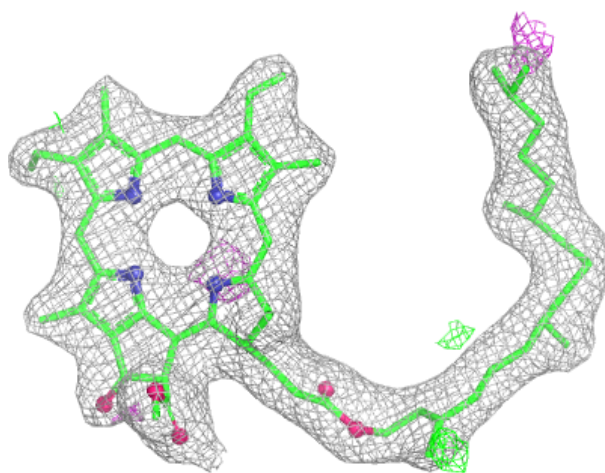
**Electron density around PHO D 401 (B):**

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



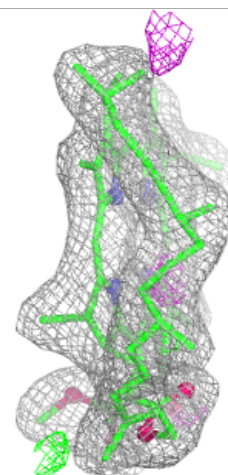
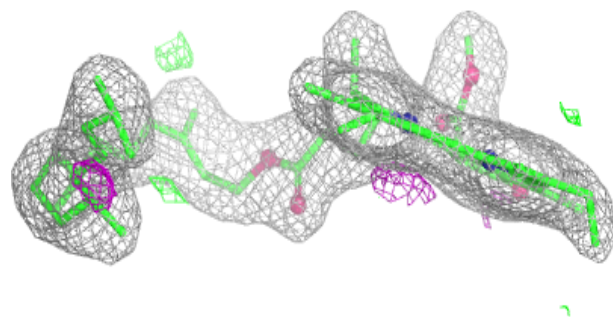
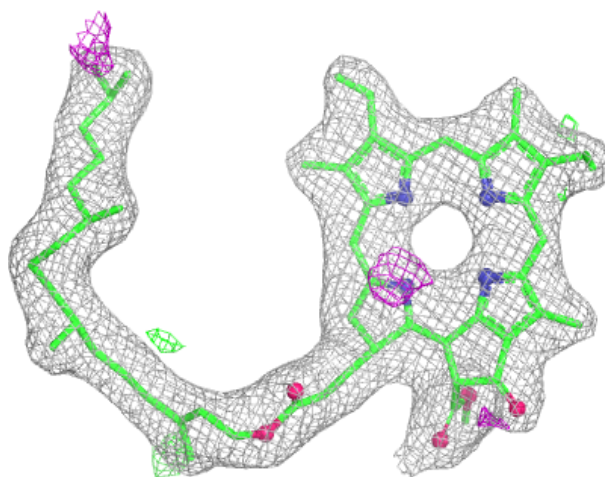
**Electron density around PHO a 406 (A):**

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



**Electron density around PHO a 406 (B):**

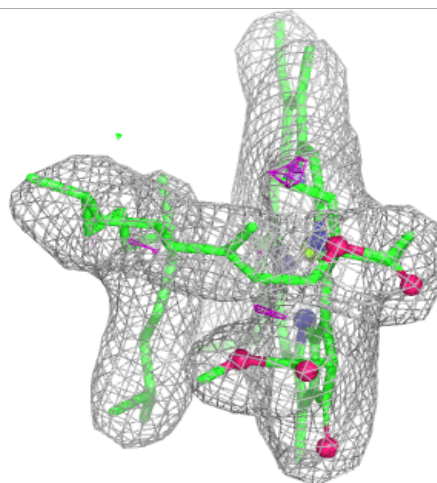
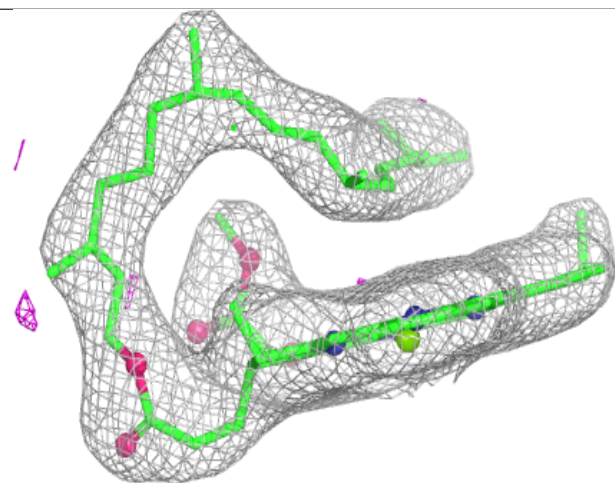
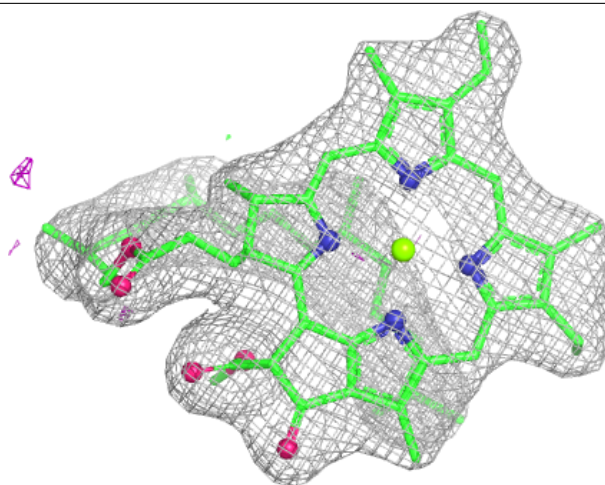
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





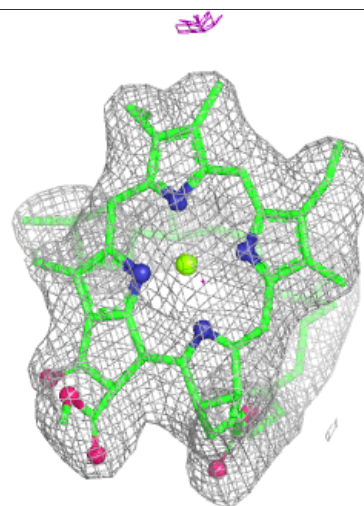
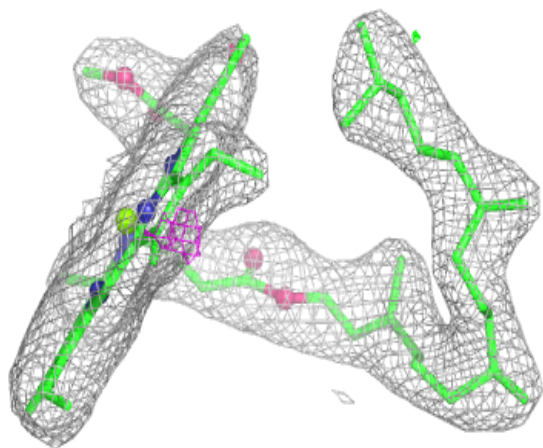
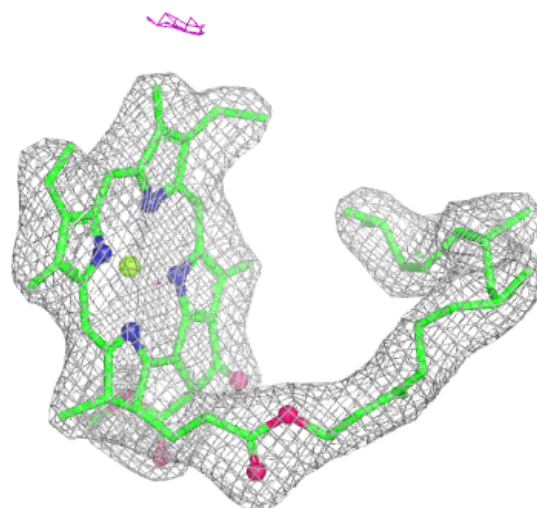
**Electron density around CLA c 511:**

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



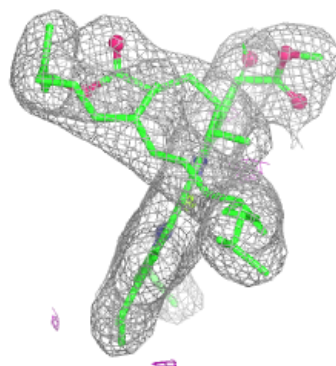
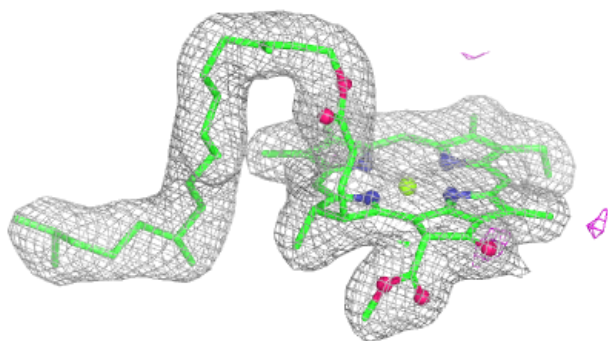
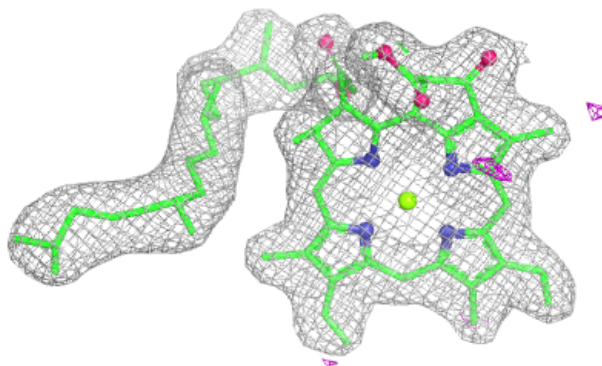
**Electron density around CLA C 504:**

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

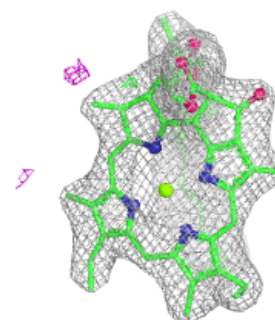
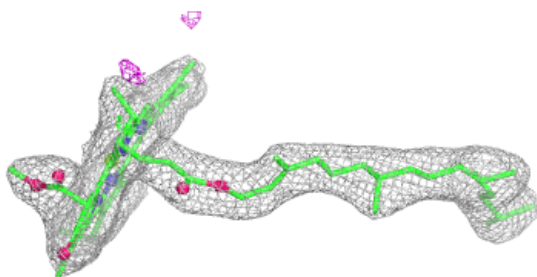
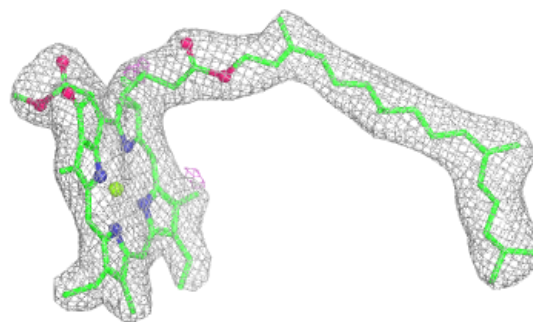


**Electron density around CLA A 405 (B):**

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

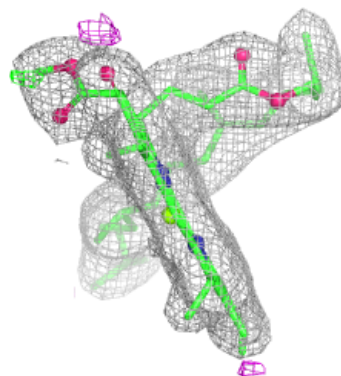
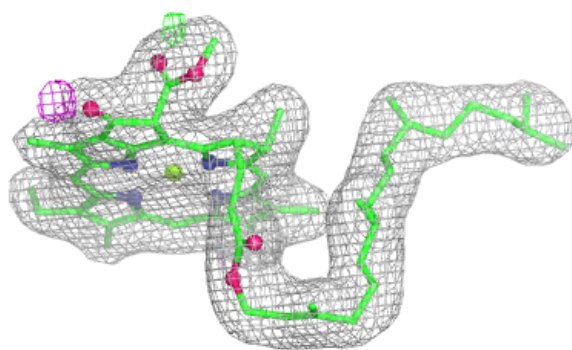
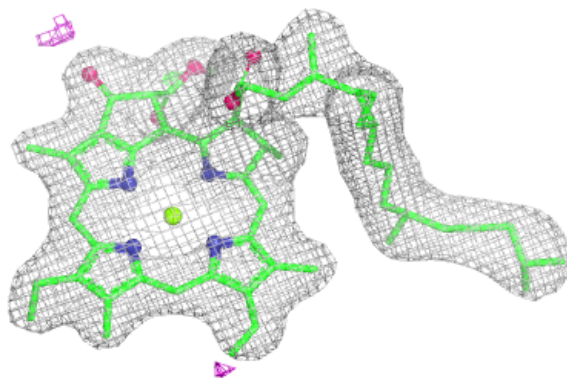
**Electron density around CLA B 609:**

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

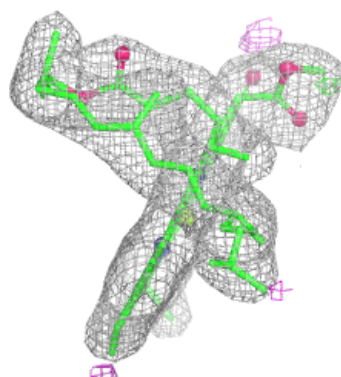
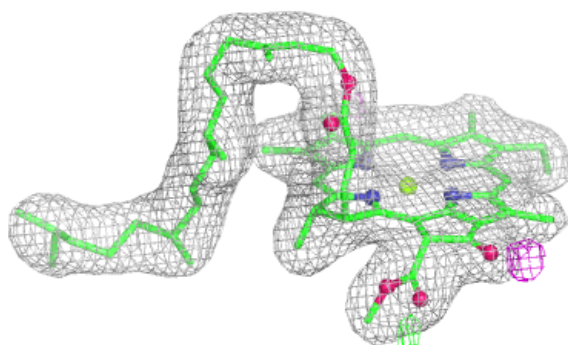
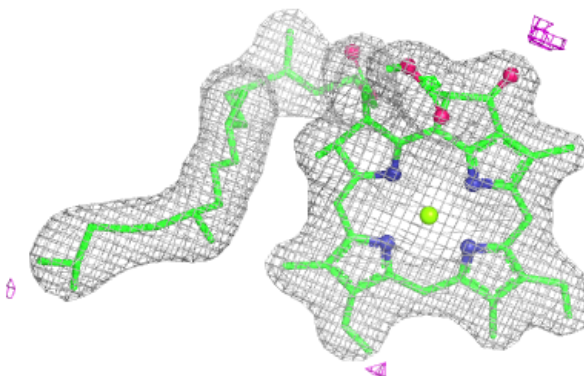


**Electron density around CLA d 402 (A):**

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

**Electron density around CLA d 402 (B):**

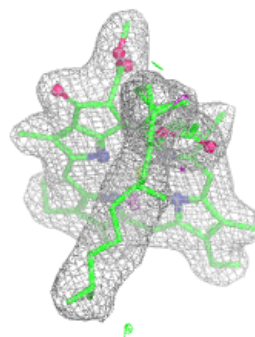
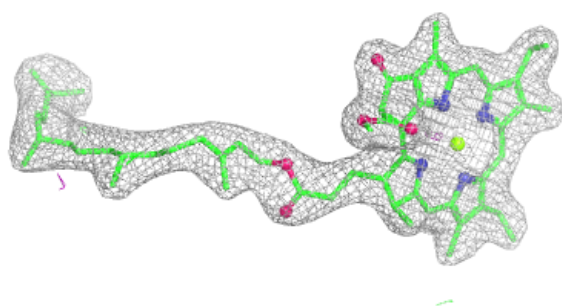
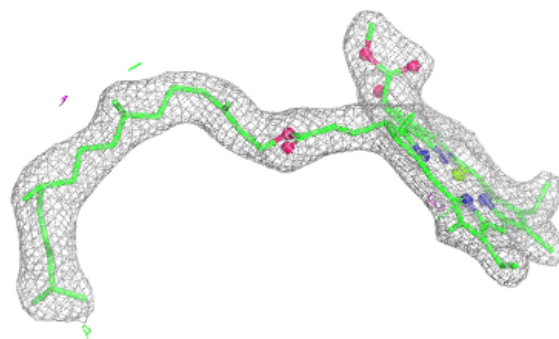
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



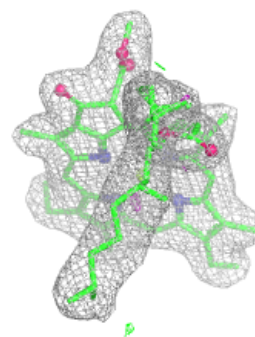
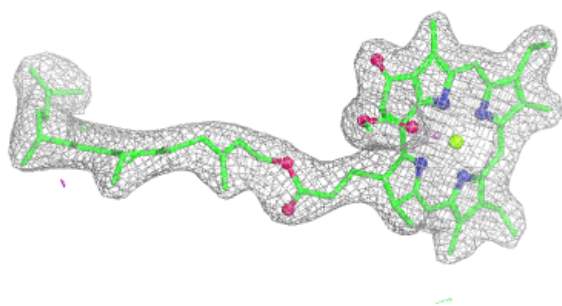
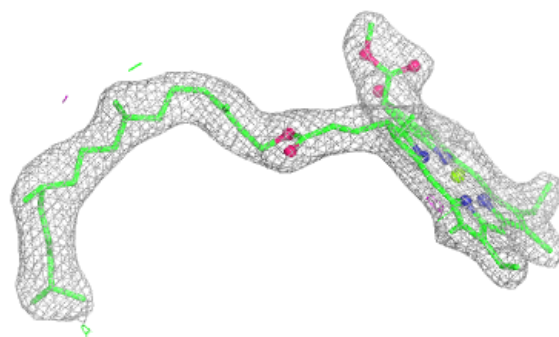


**Electron density around CLA d 403 (A):**

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

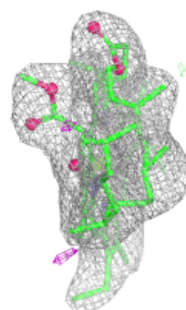
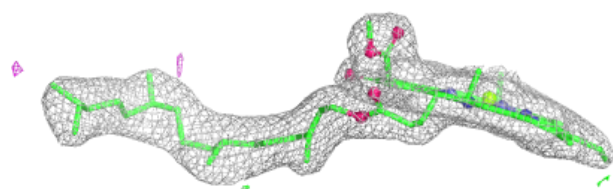
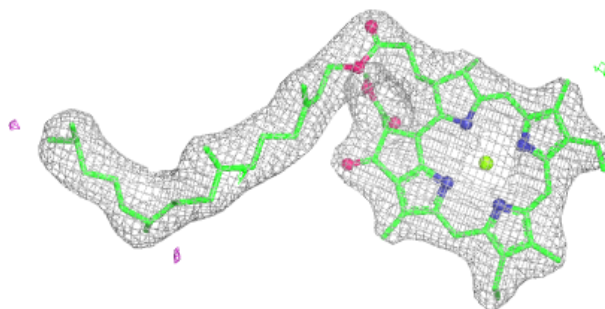
**Electron density around CLA d 403 (B):**

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

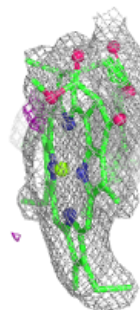
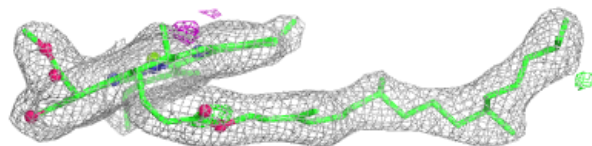
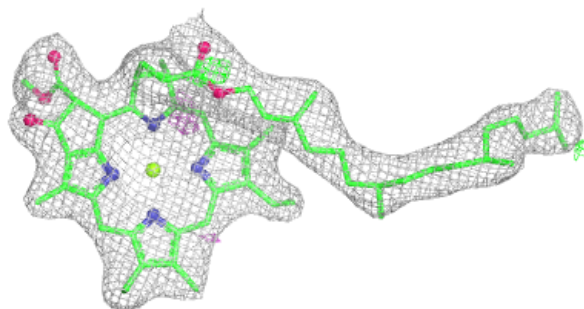


**Electron density around CLA b 602:**

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

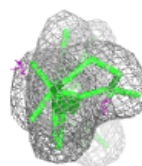
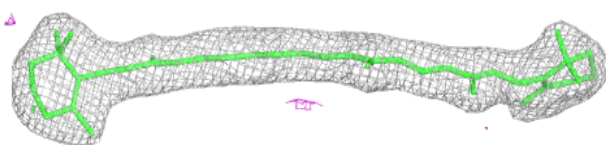
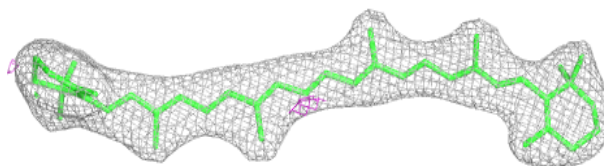
**Electron density around CLA b 603:**

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

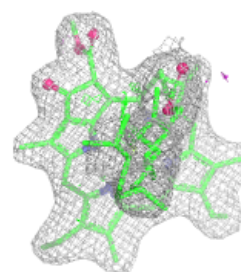
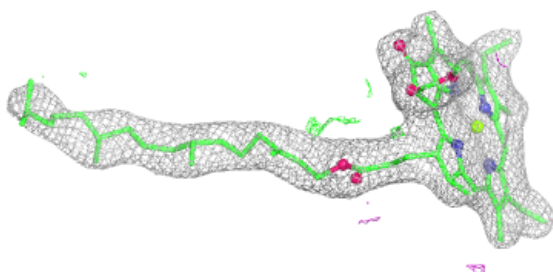
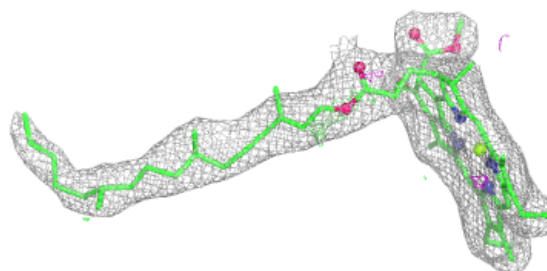


**Electron density around BCR B 617:**

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

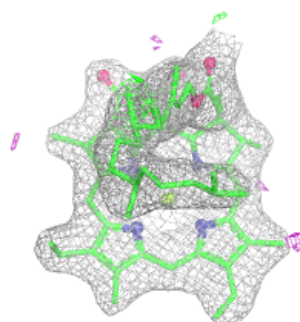
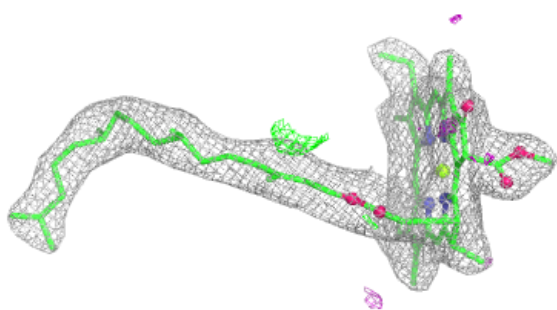
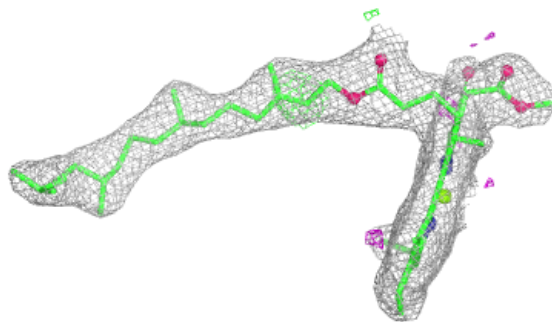
**Electron density around CLA b 604:**

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



**Electron density around CLA b 605:**

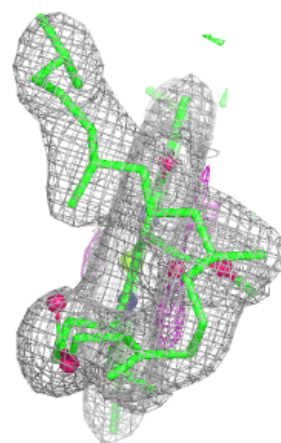
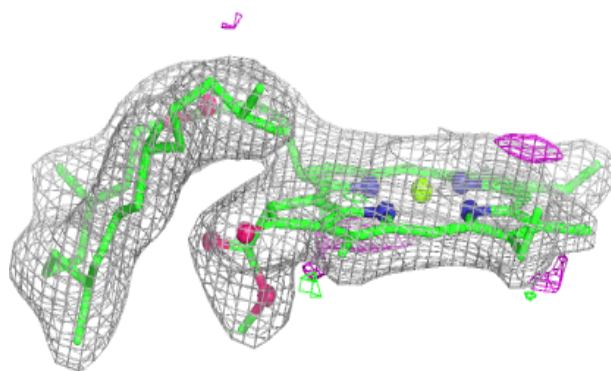
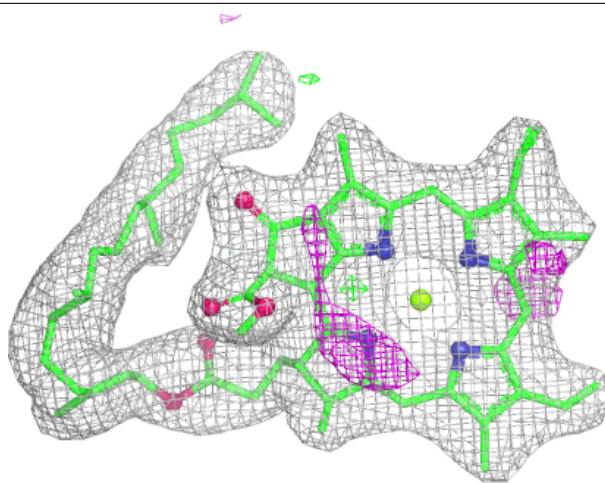
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





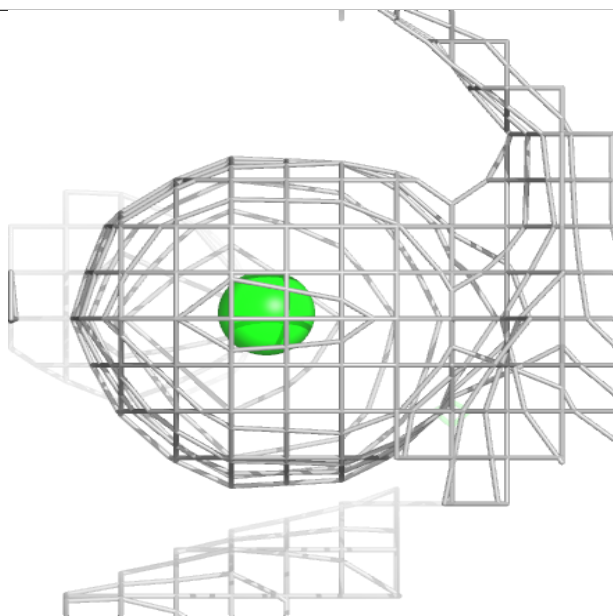
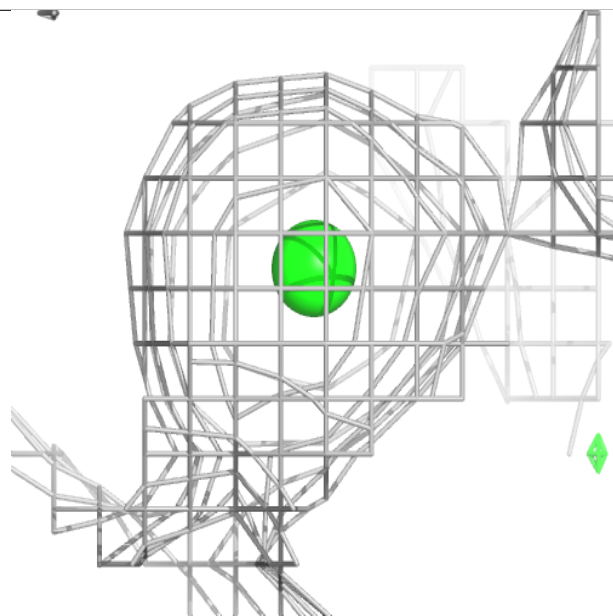
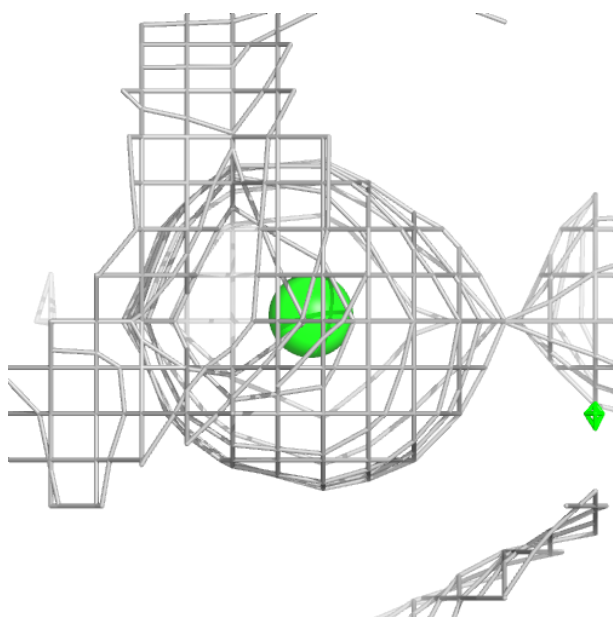
**Electron density around CLA B 610:**

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



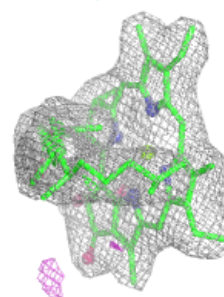
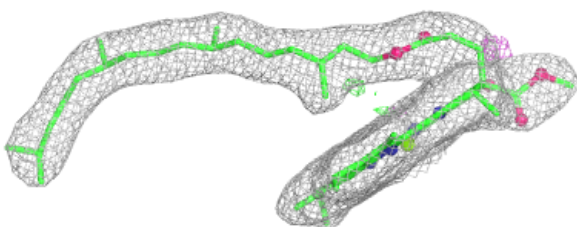
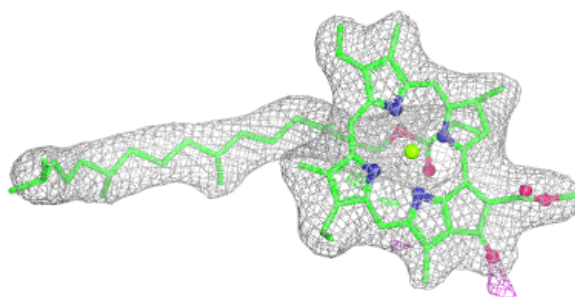
**Electron density around CL a 403 (A):**

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

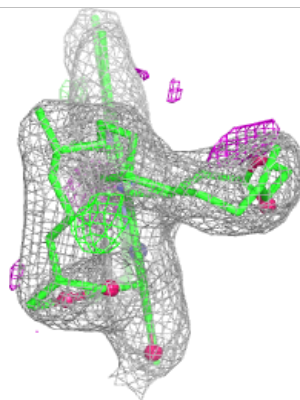
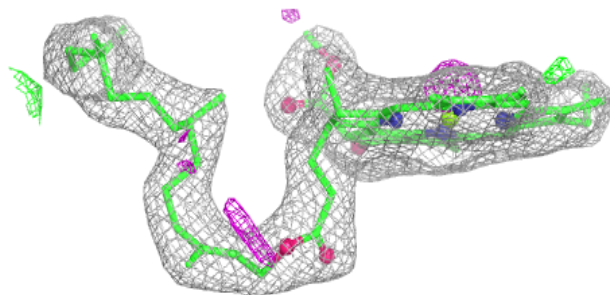
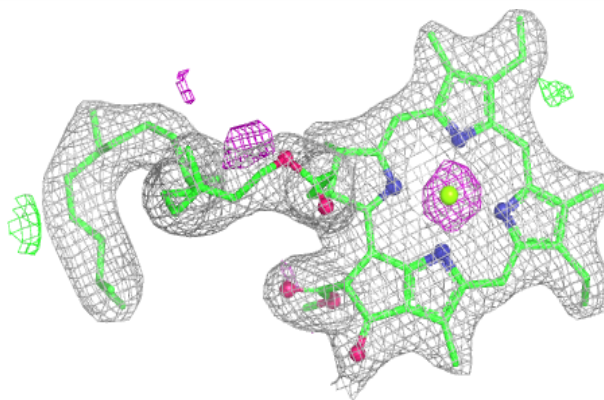


**Electron density around CLA b 608:**

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

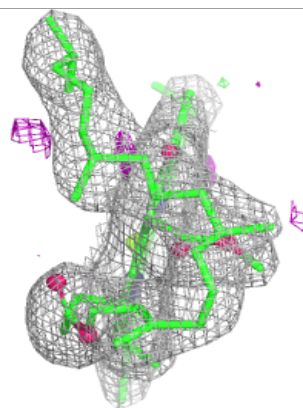
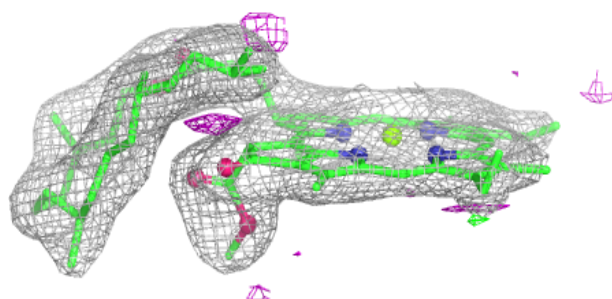
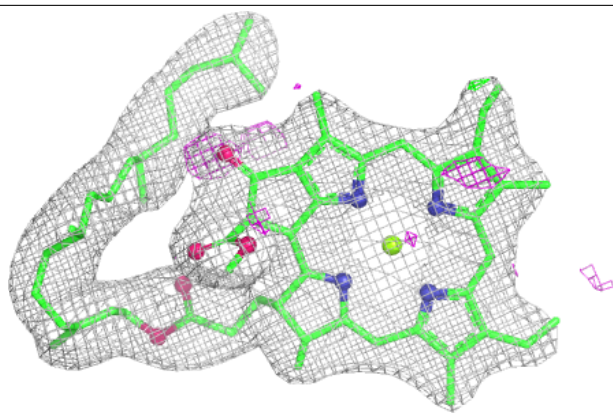
**Electron density around CLA B 612:**

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



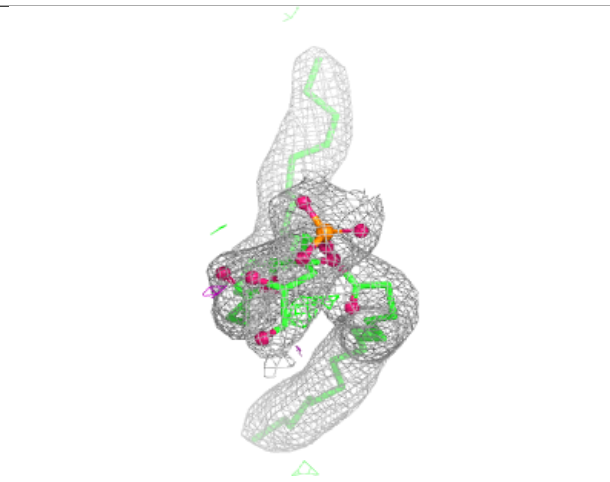
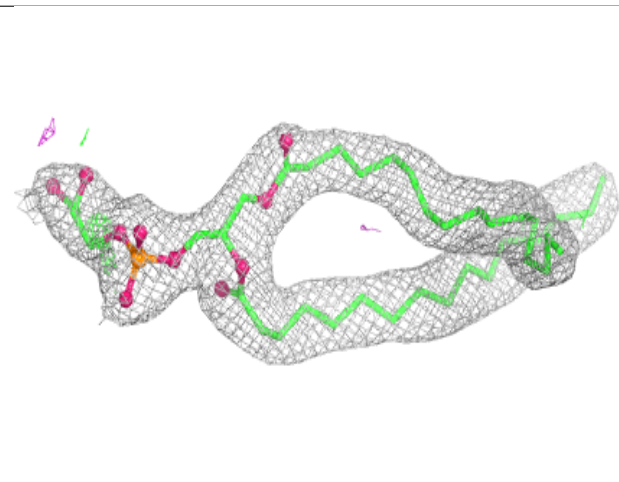
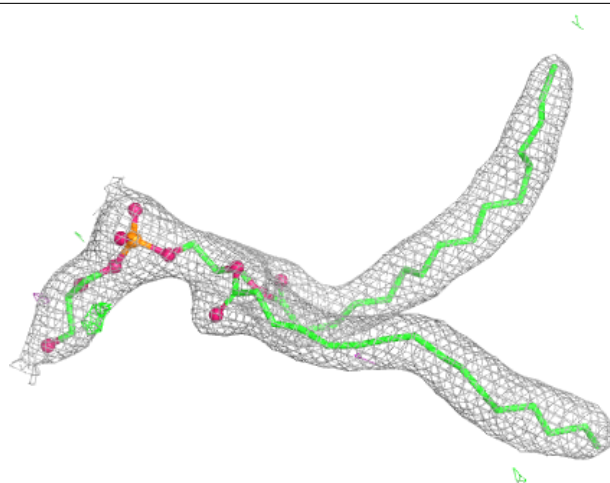
**Electron density around CLA b 610:**

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



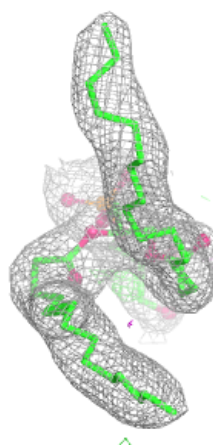
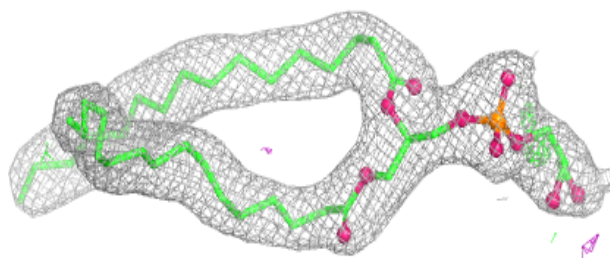
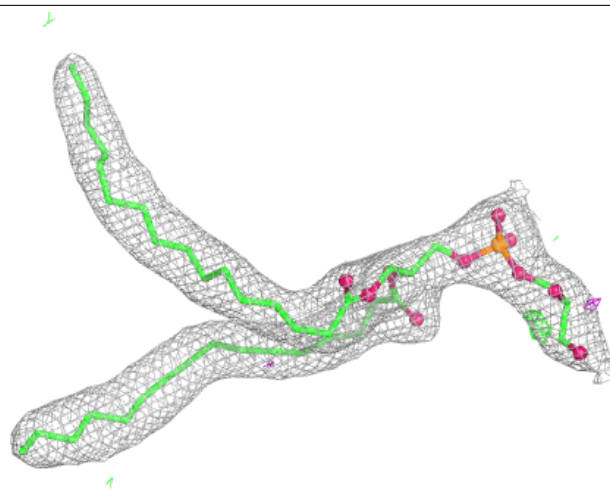
**Electron density around LHG D 407 (A):**

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



**Electron density around LHG D 407 (B):**

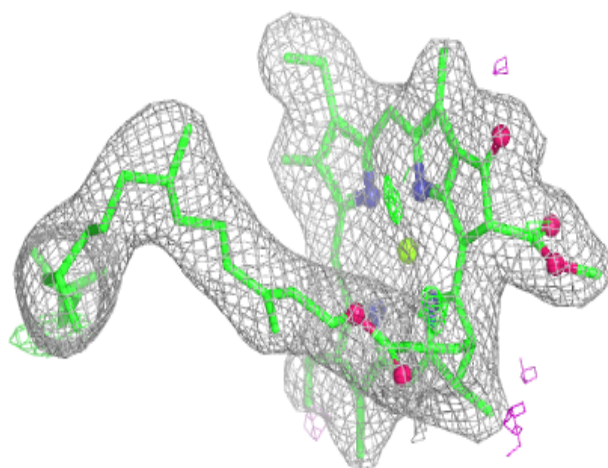
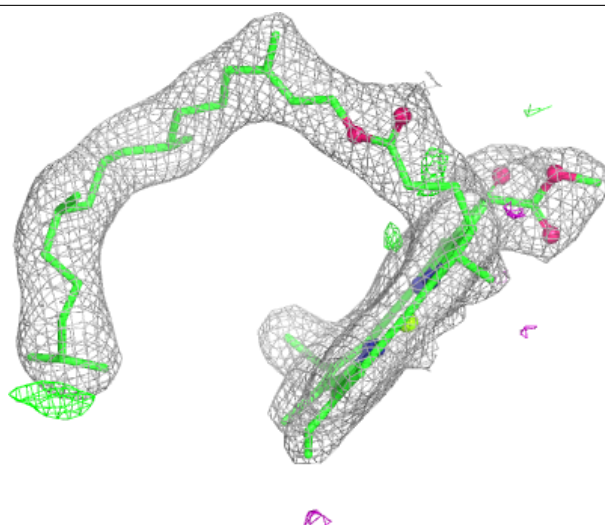
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA b 611:**

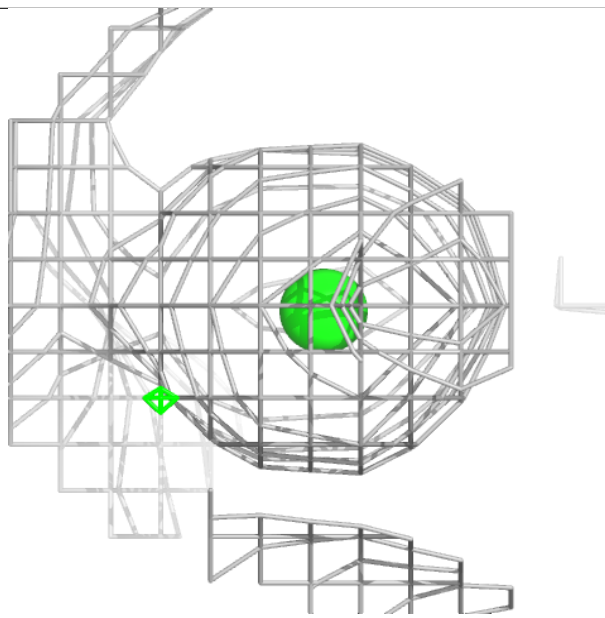
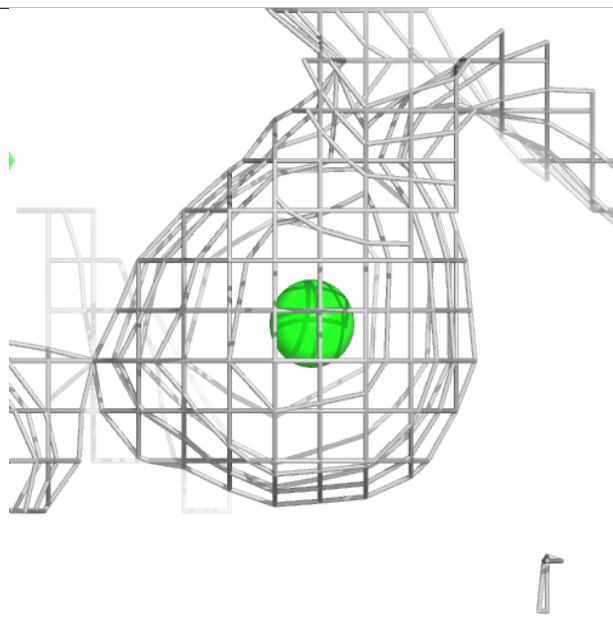
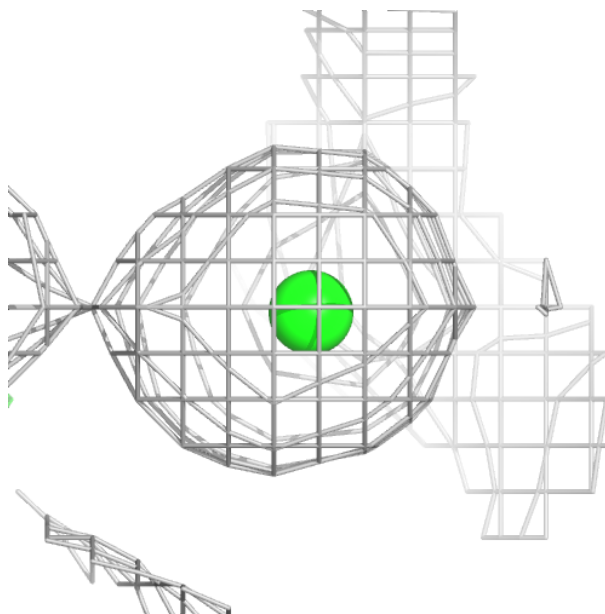
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





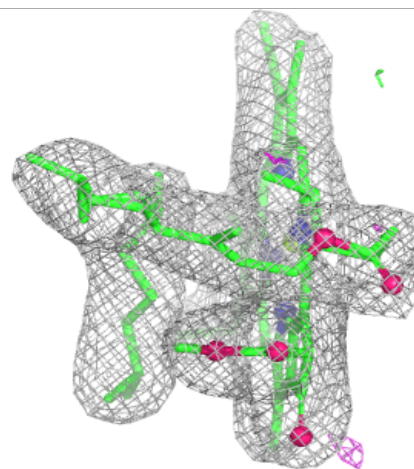
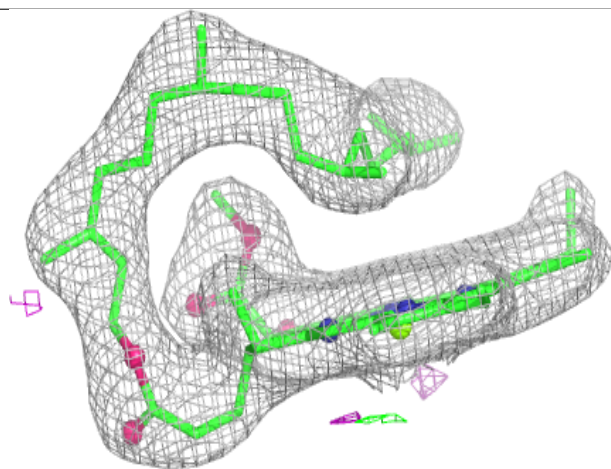
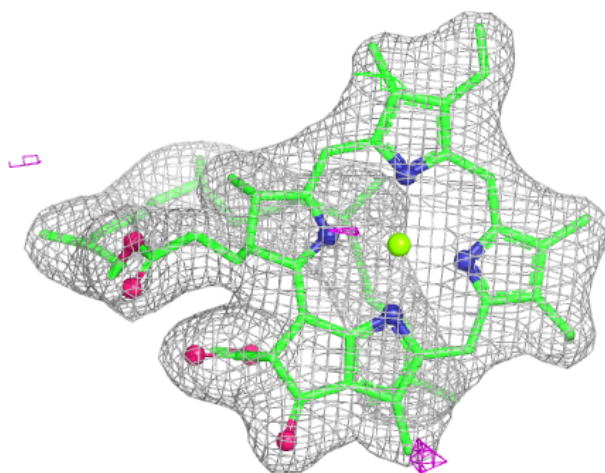
**Electron density around CL a 403 (B):**

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



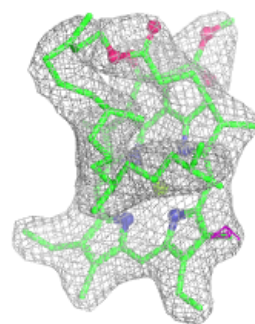
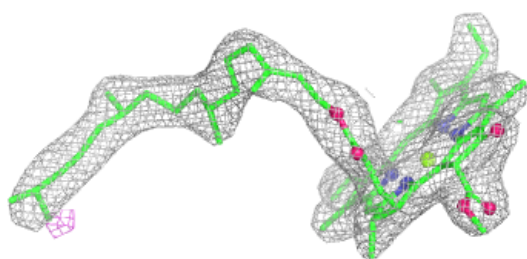
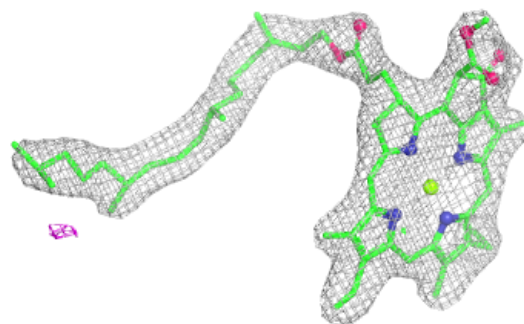
**Electron density around CLA C 511:**

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



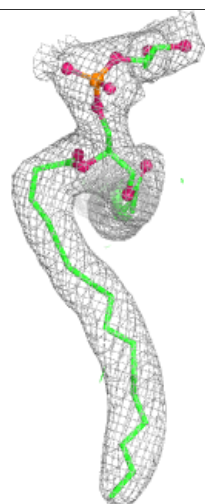
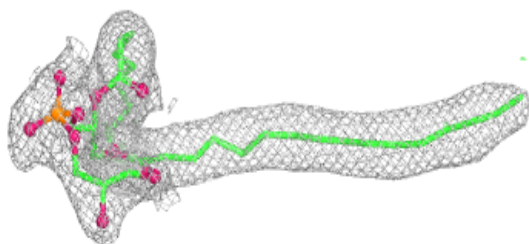
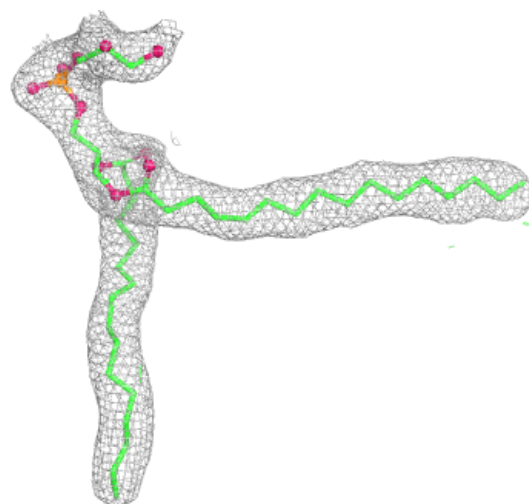
**Electron density around CLA C 512:**

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



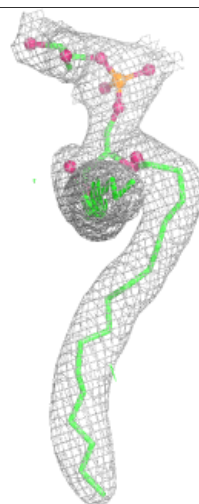
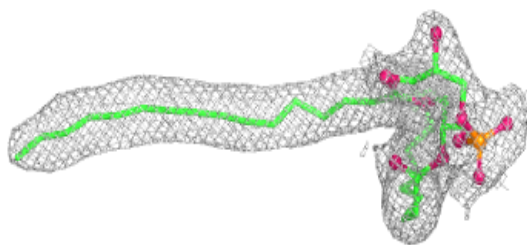
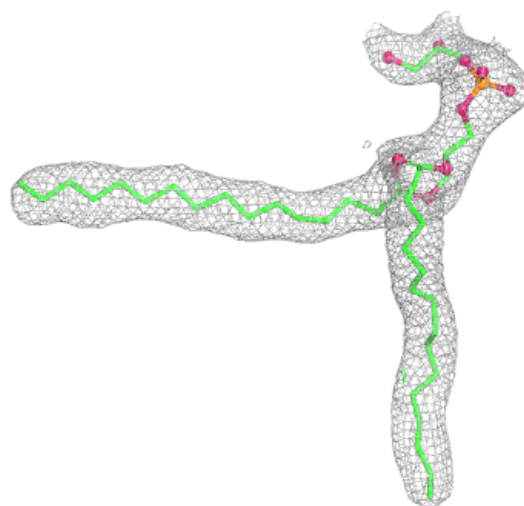
**Electron density around LHG L 101 (A):**

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



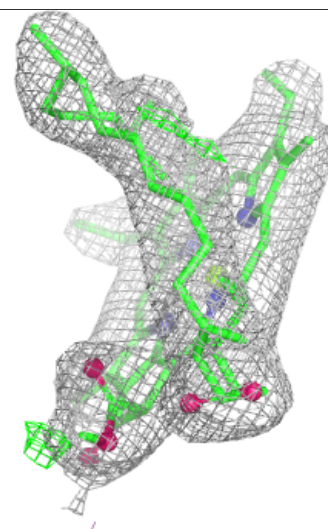
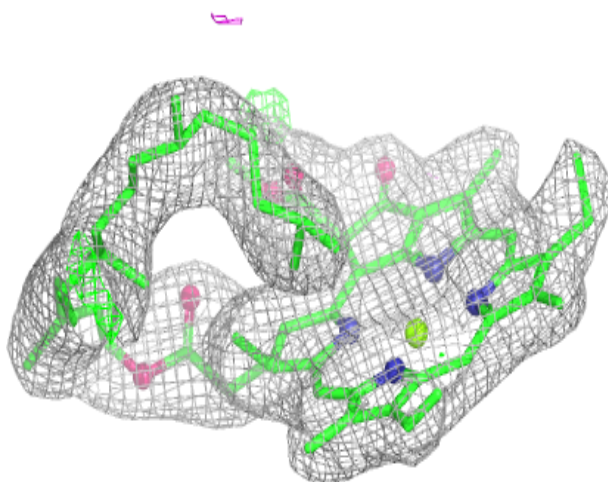
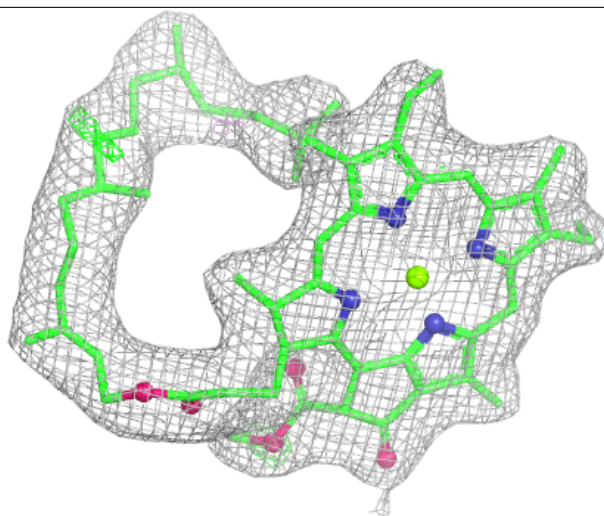
**Electron density around LHG L 101 (B):**

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



**Electron density around CLA b 615:**

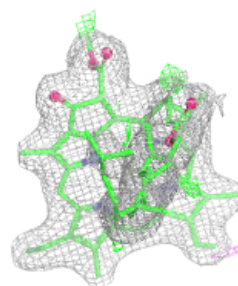
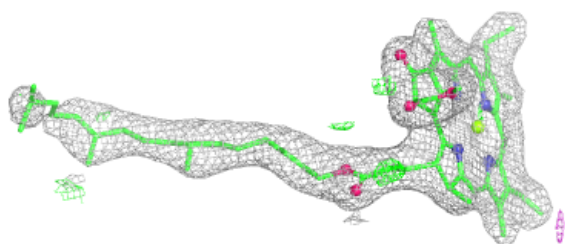
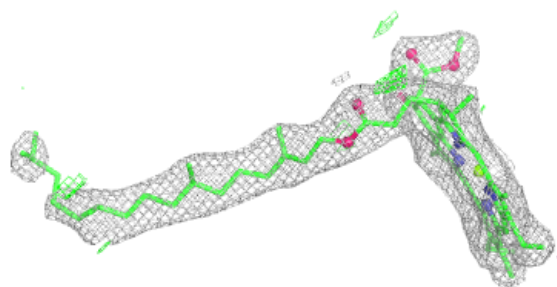
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



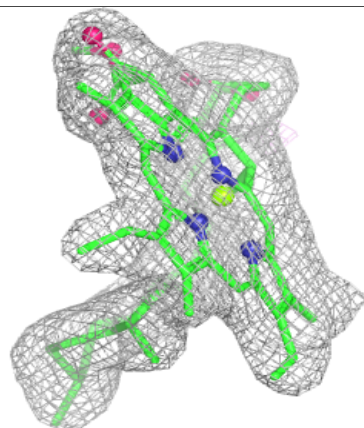
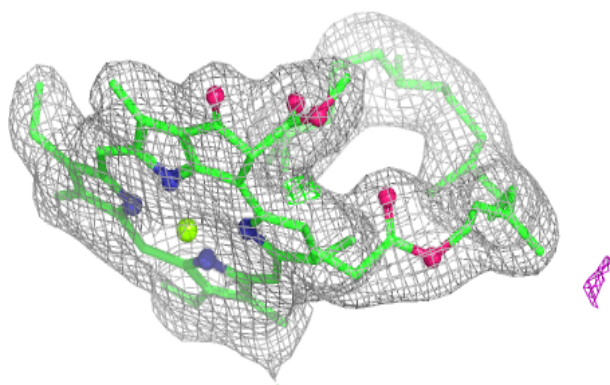
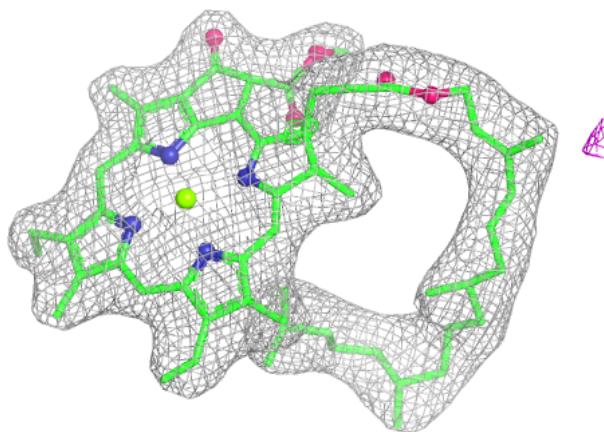


**Electron density around CLA B 604:**

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

**Electron density around CLA B 615:**

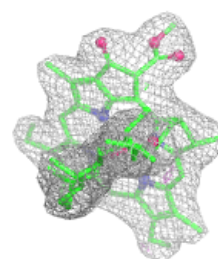
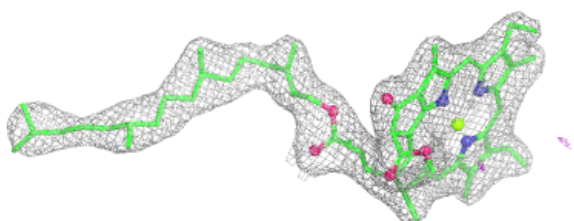
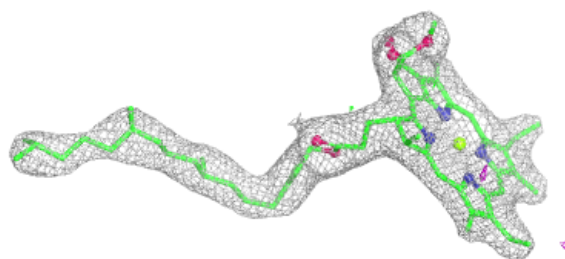
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



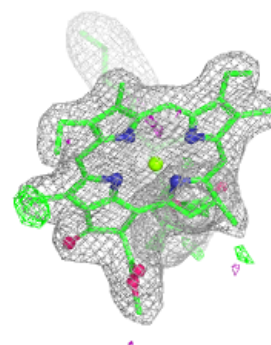
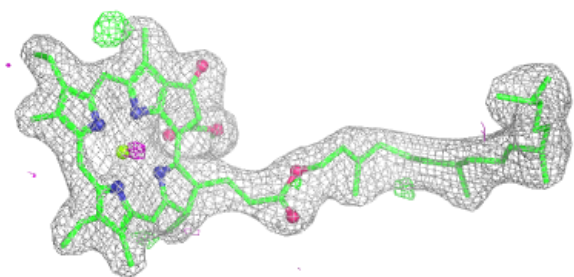
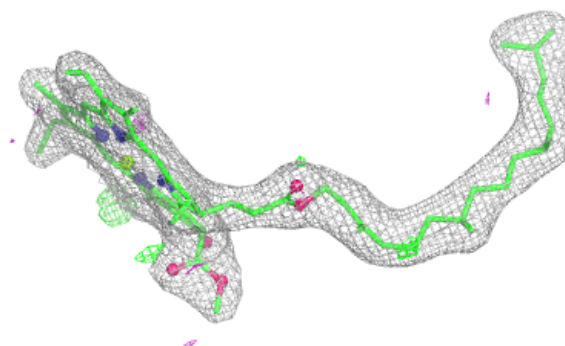


**Electron density around CLA c 503:**

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

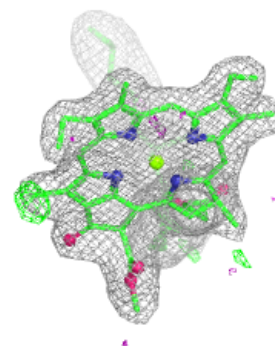
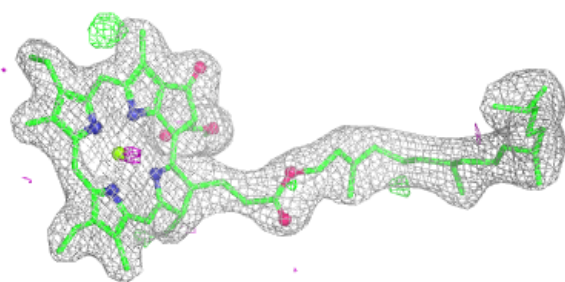
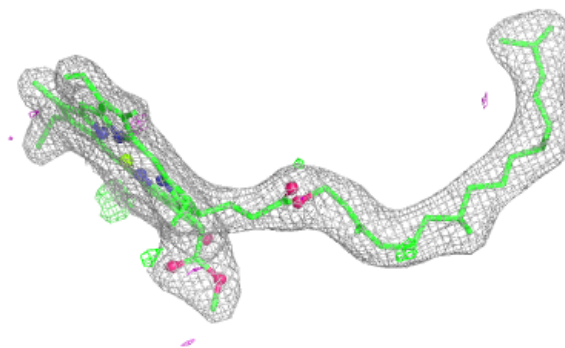
**Electron density around CLA D 403 (A):**

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

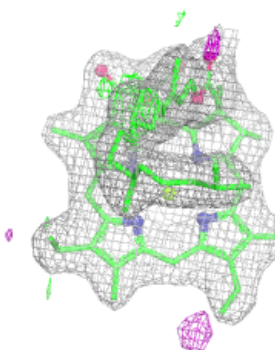
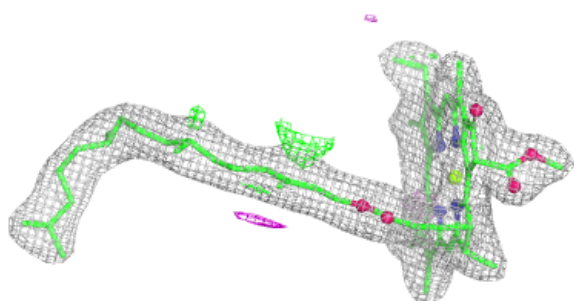
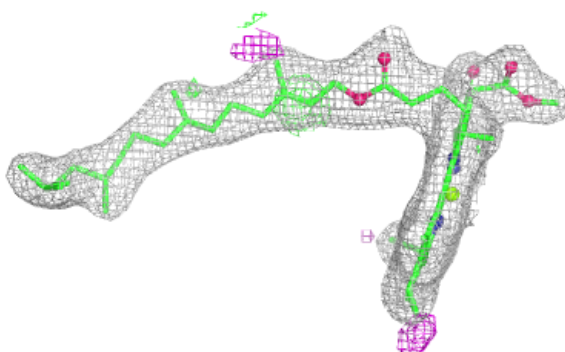


**Electron density around CLA D 403 (B):**

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

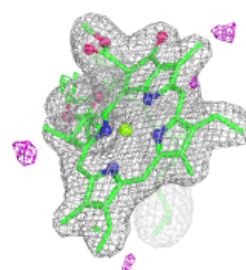
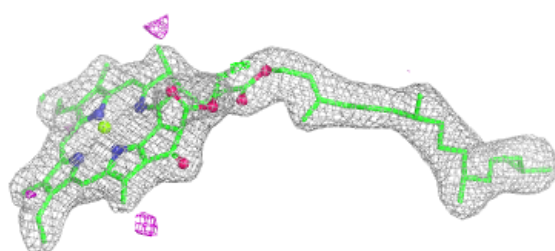
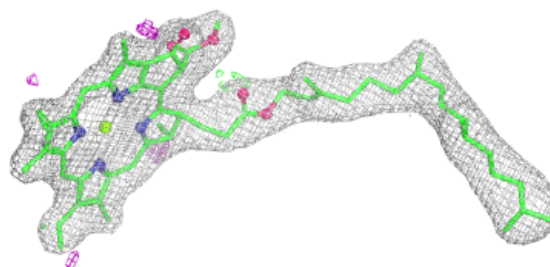
**Electron density around CLA B 605:**

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

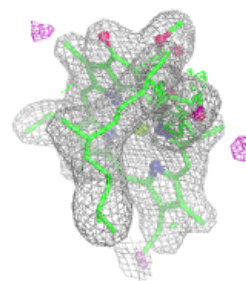
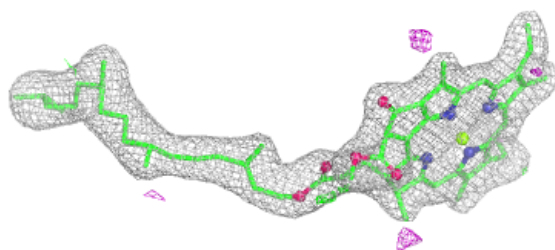
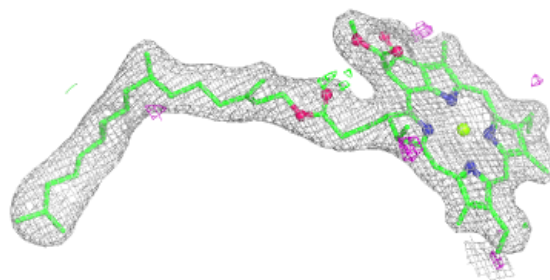


**Electron density around CLA a 404 (A):**

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

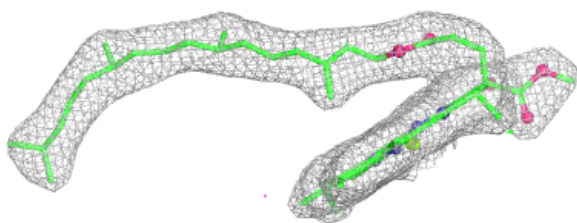
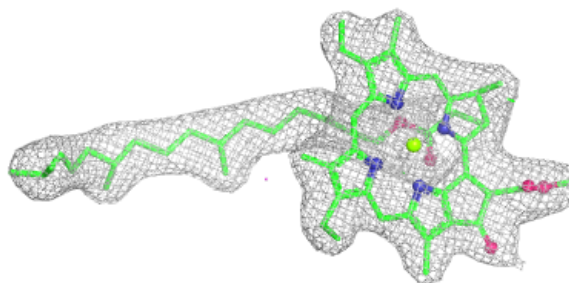
**Electron density around CLA a 404 (B):**

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



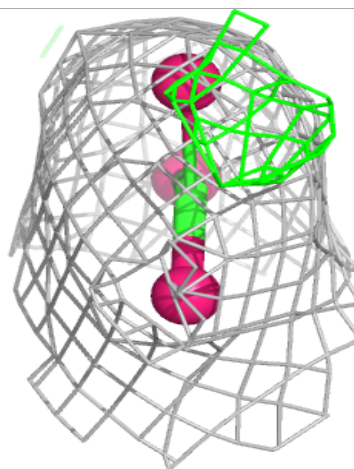
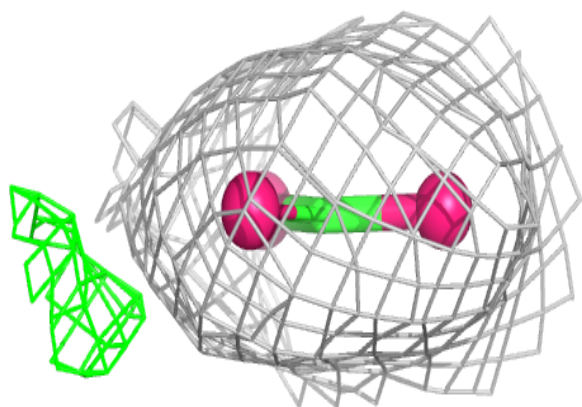
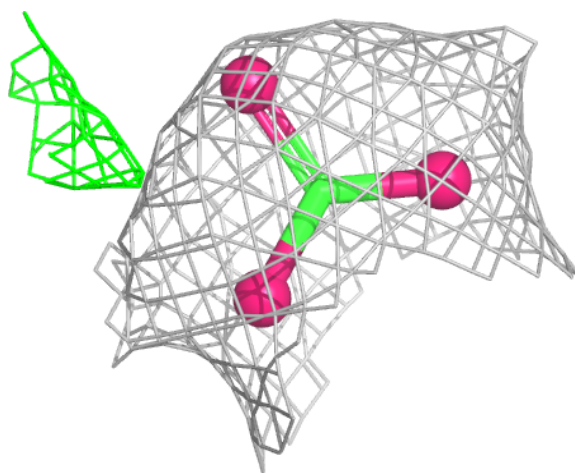
**Electron density around CLA B 608:**

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



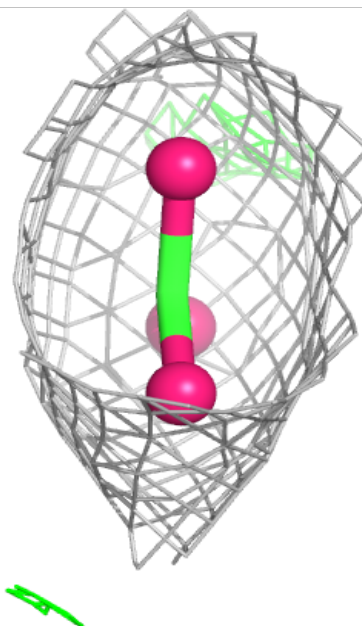
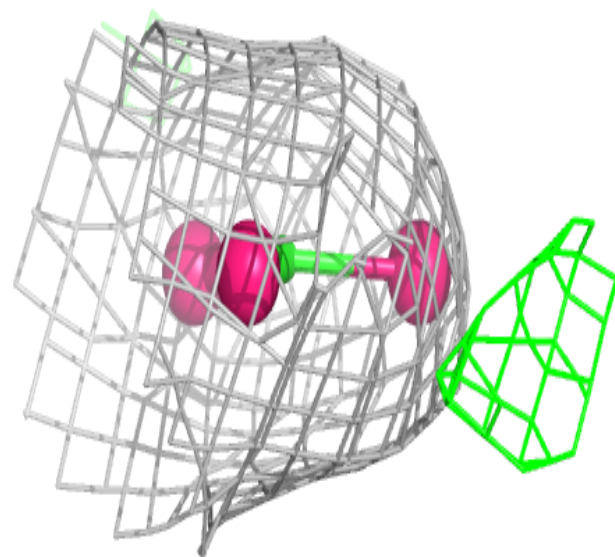
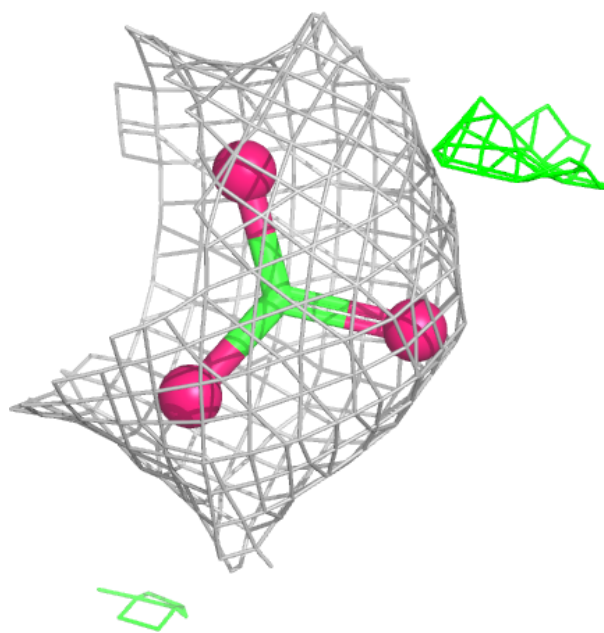
**Electron density around BCT A 415 (A):**

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



**Electron density around BCT A 415 (B):**

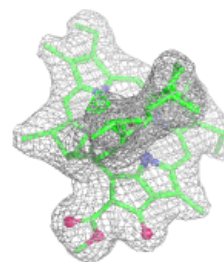
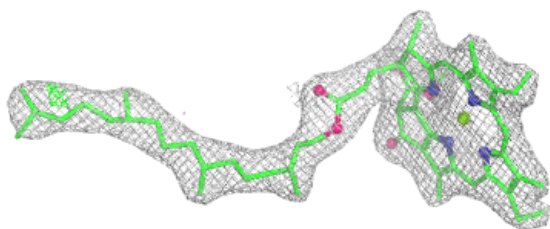
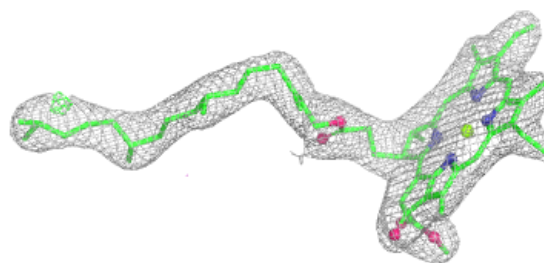
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA C 503:**

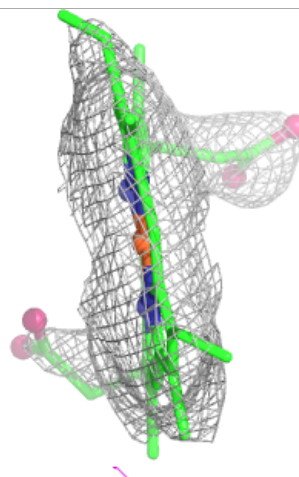
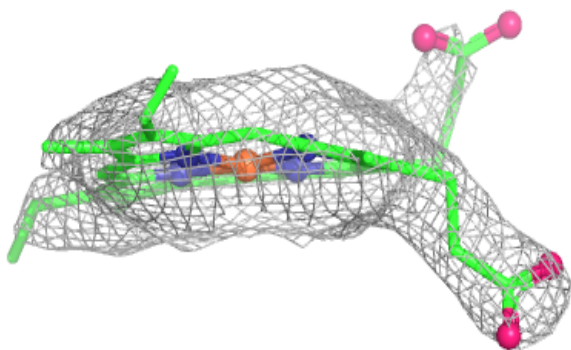
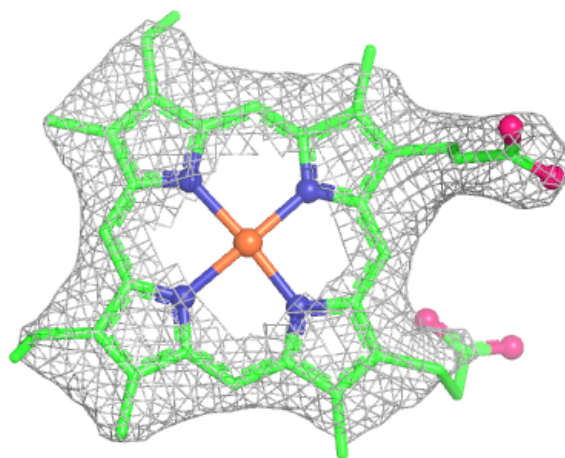
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





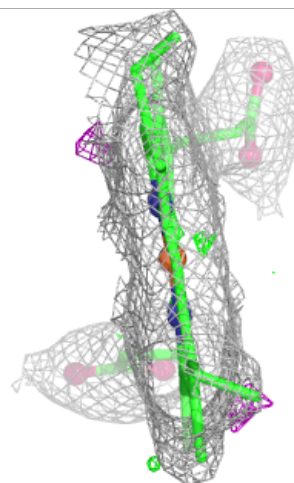
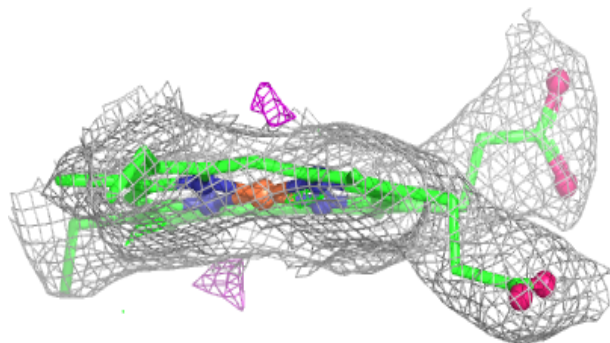
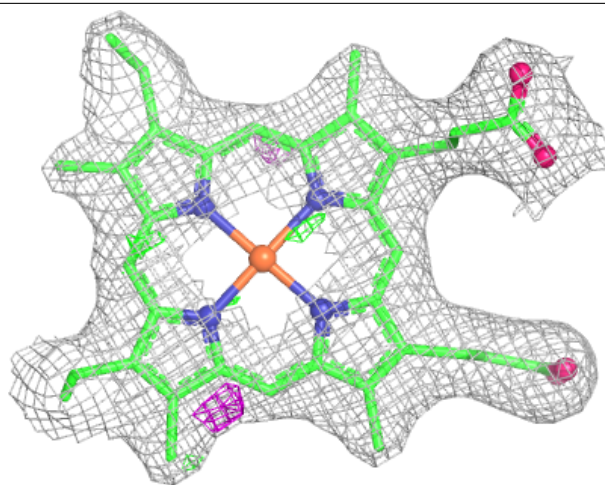
**Electron density around HEM f 101:**

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



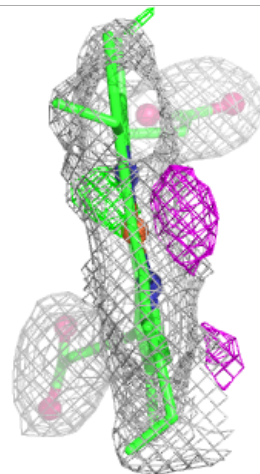
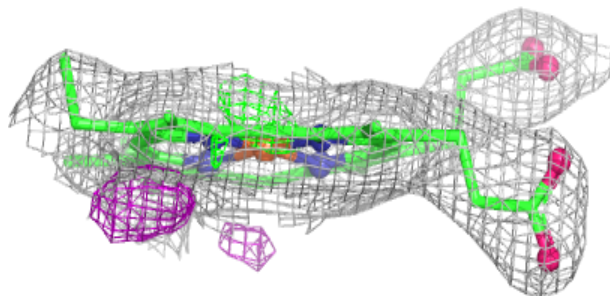
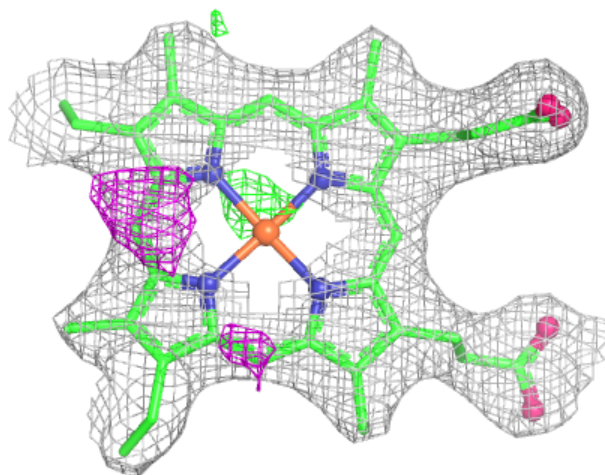
**Electron density around HEC V 201:**

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



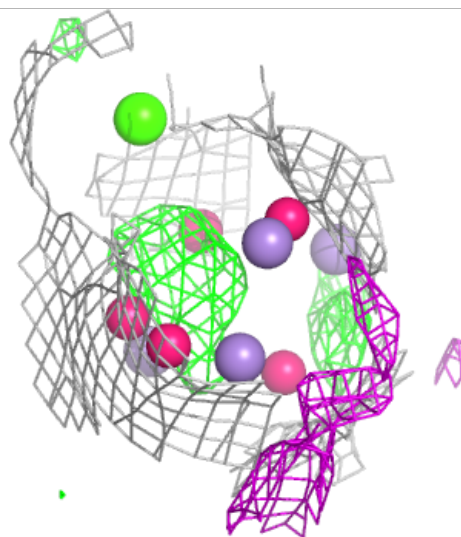
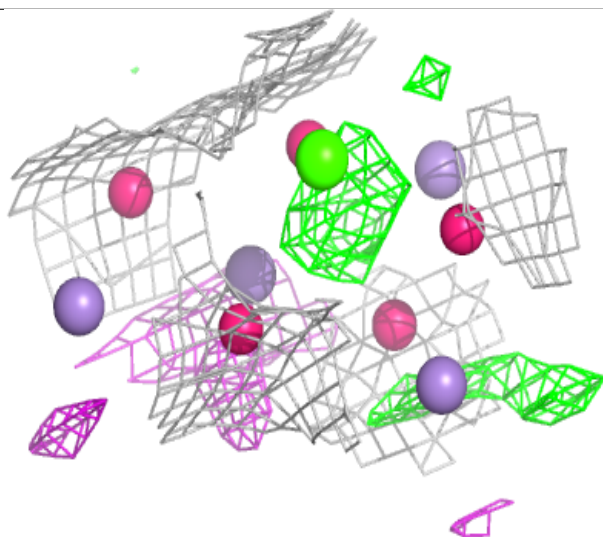
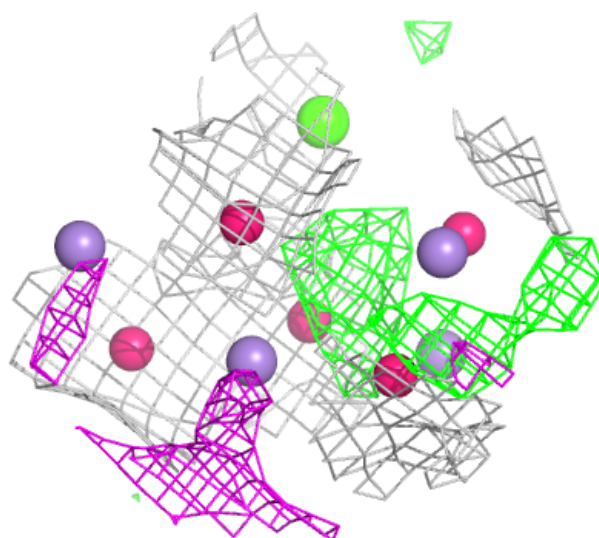
**Electron density around HEC v 201:**

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



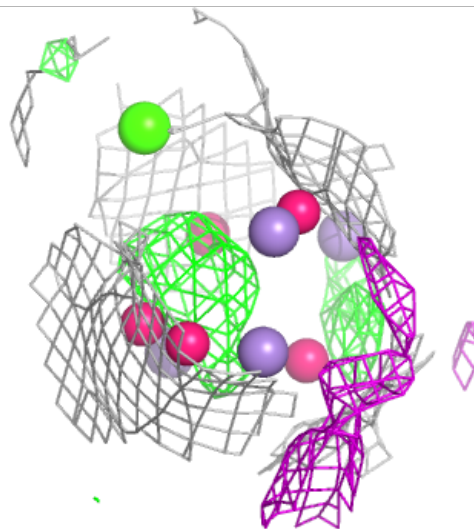
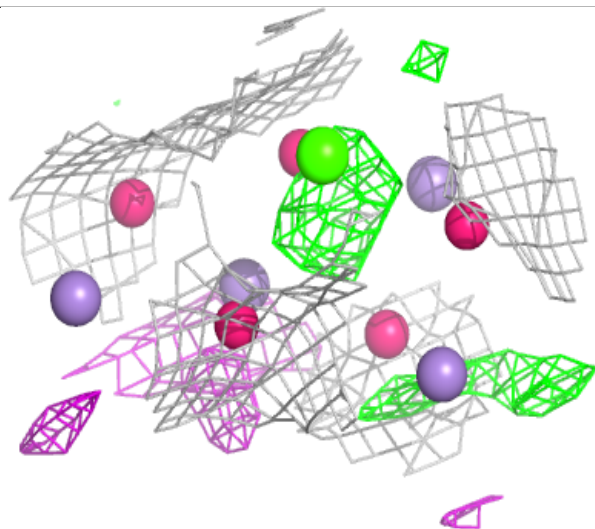
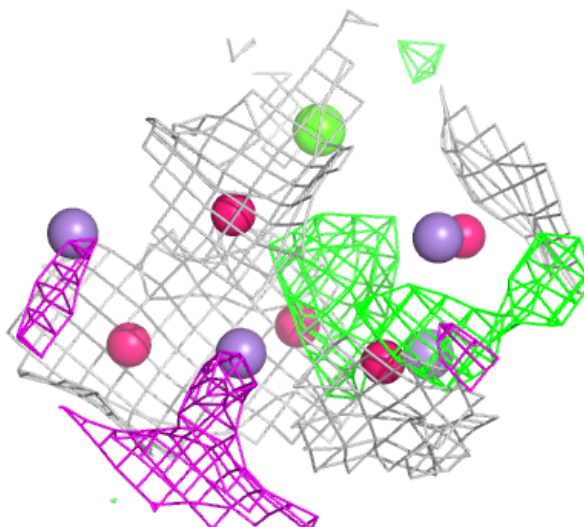
**Electron density around OEX A 412 (A):**

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



**Electron density around OEX A 412 (B):**

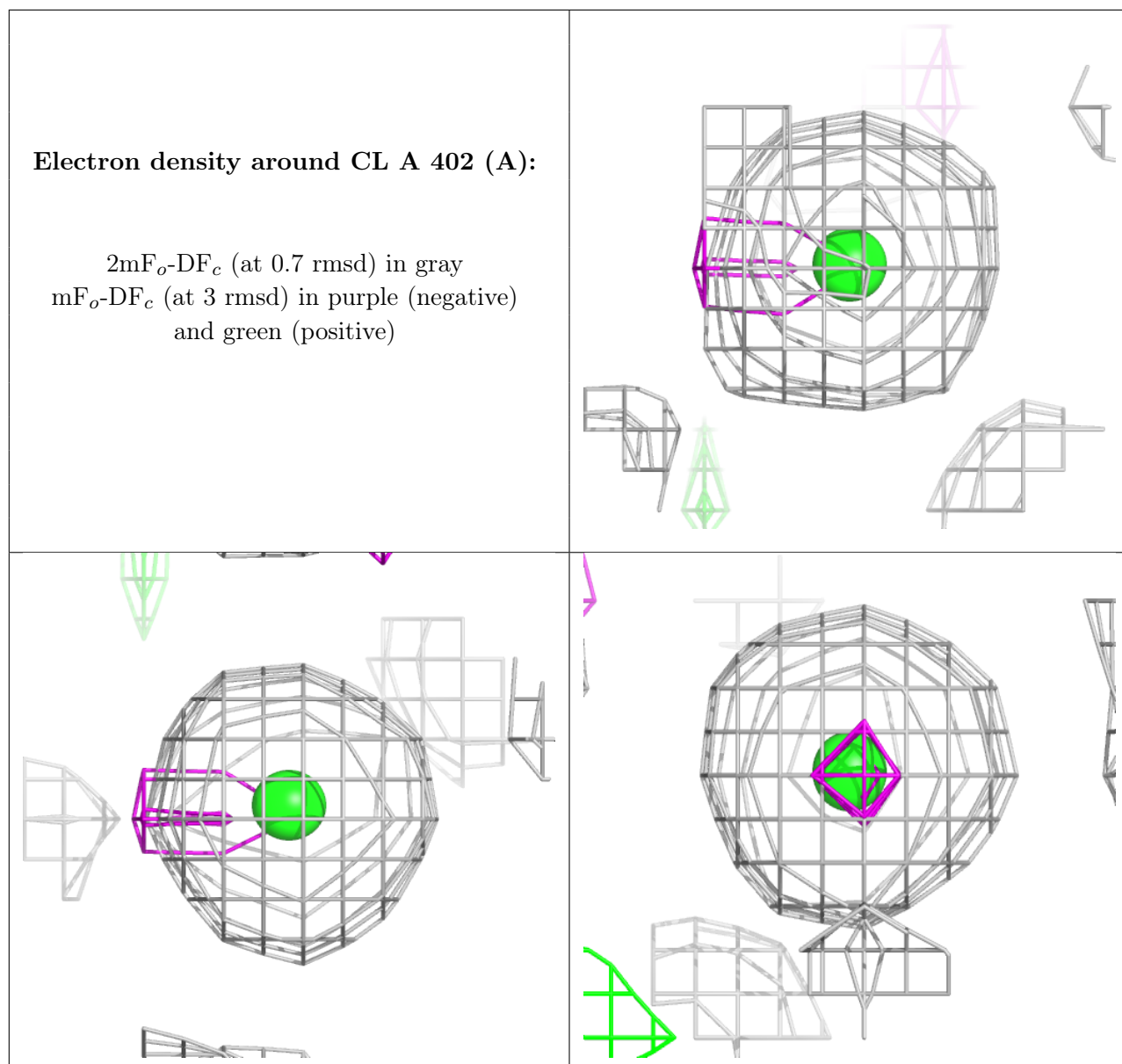
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





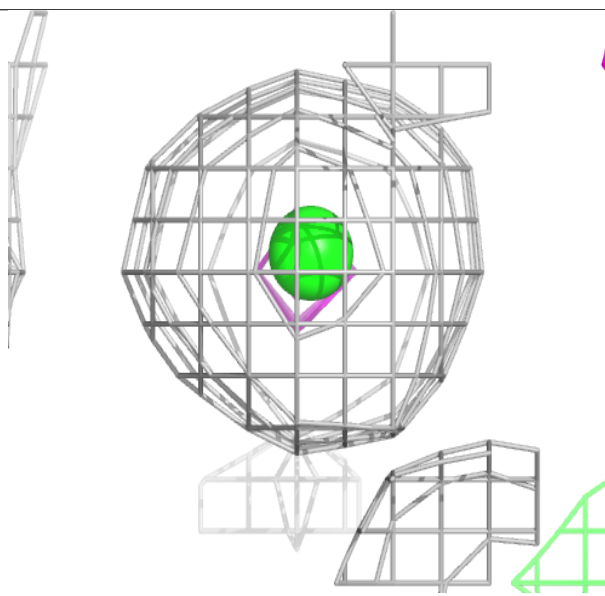
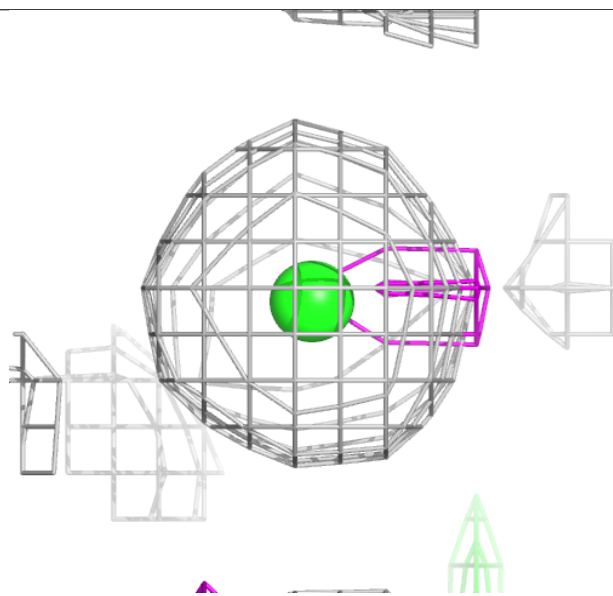
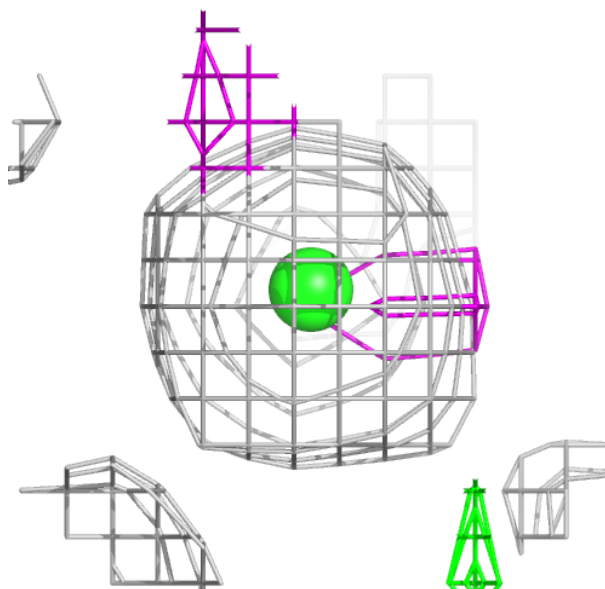
**Electron density around CL A 402 (A):**

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



**Electron density around CL A 402 (B):**

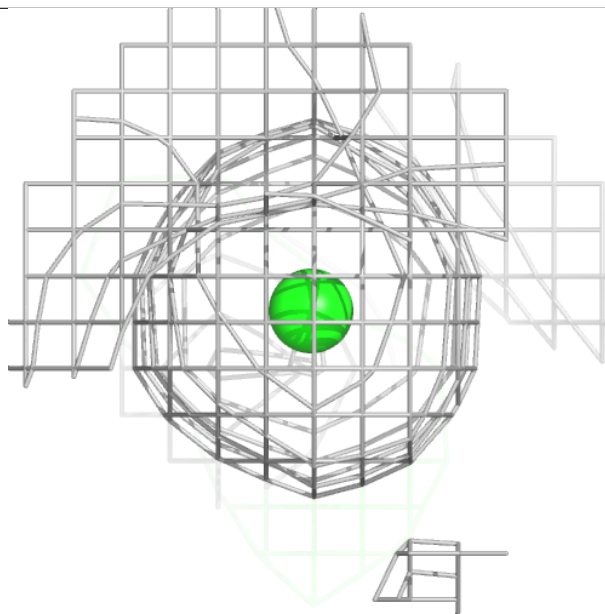
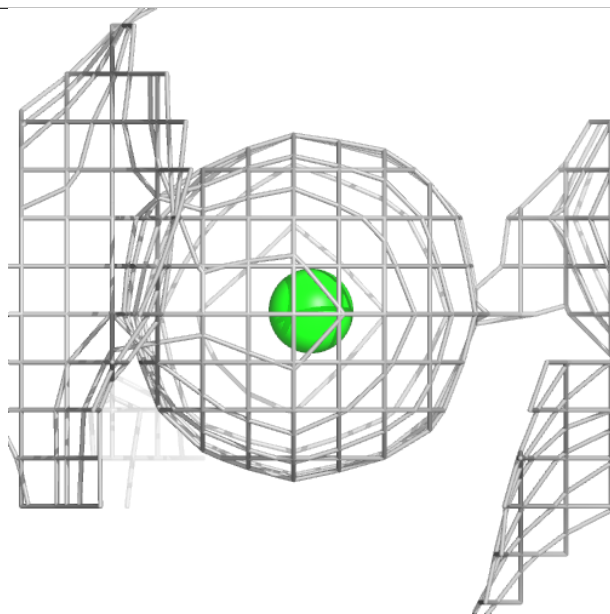
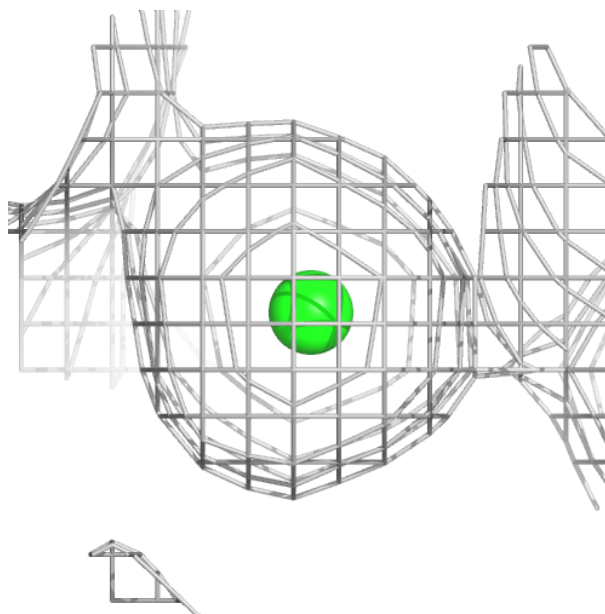
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





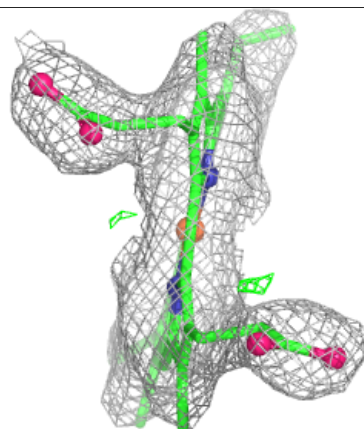
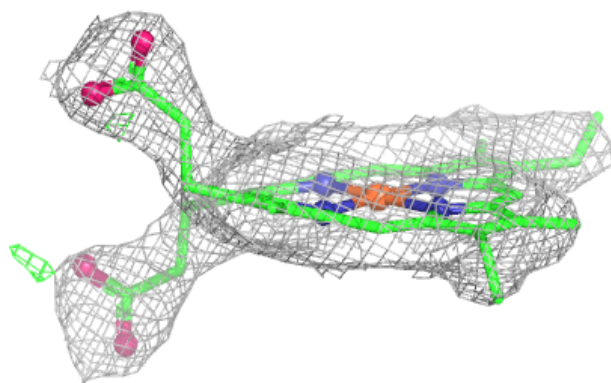
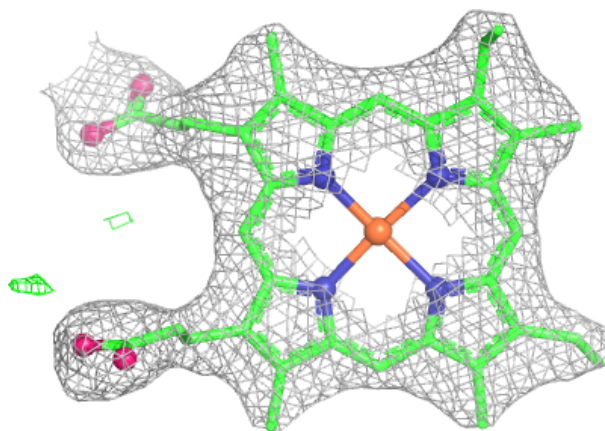
**Electron density around CL A 403 (A):**

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



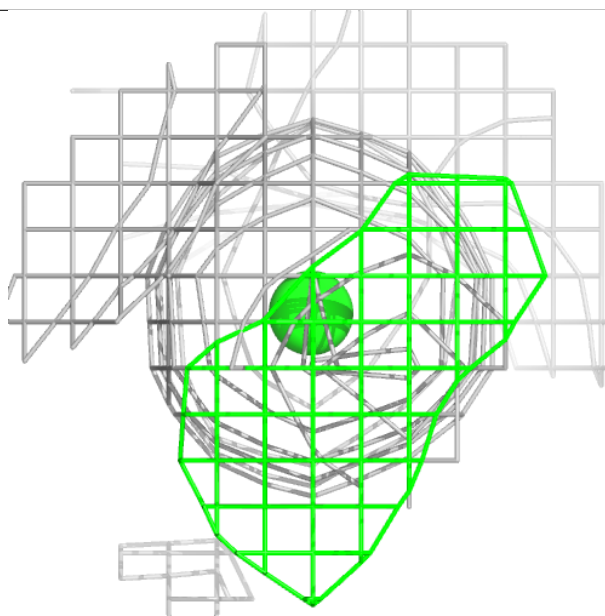
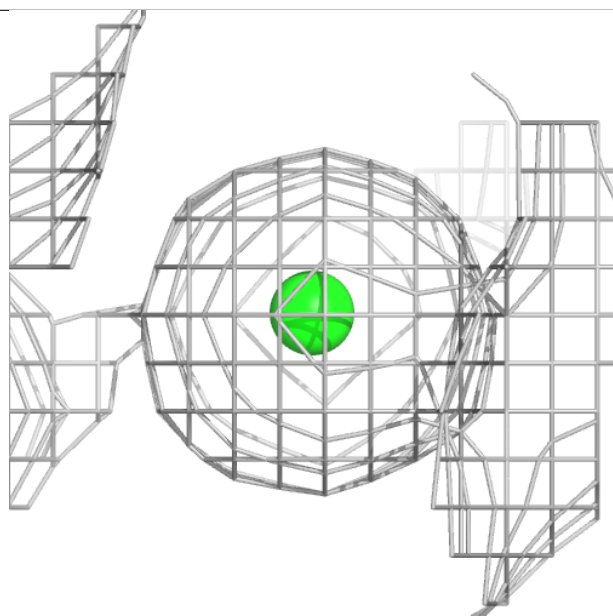
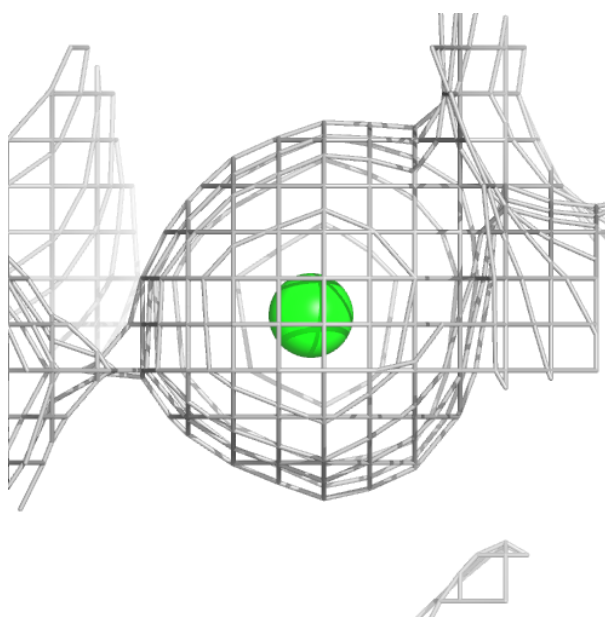
**Electron density around HEM F 102:**

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



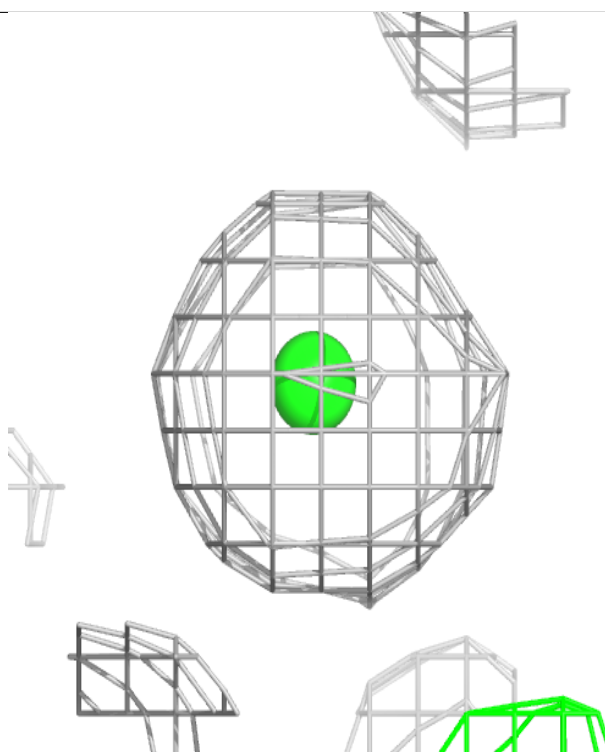
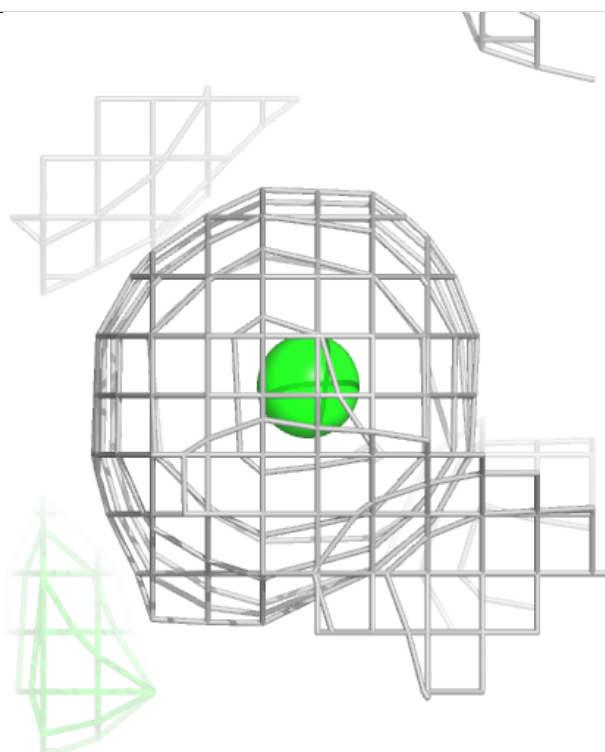
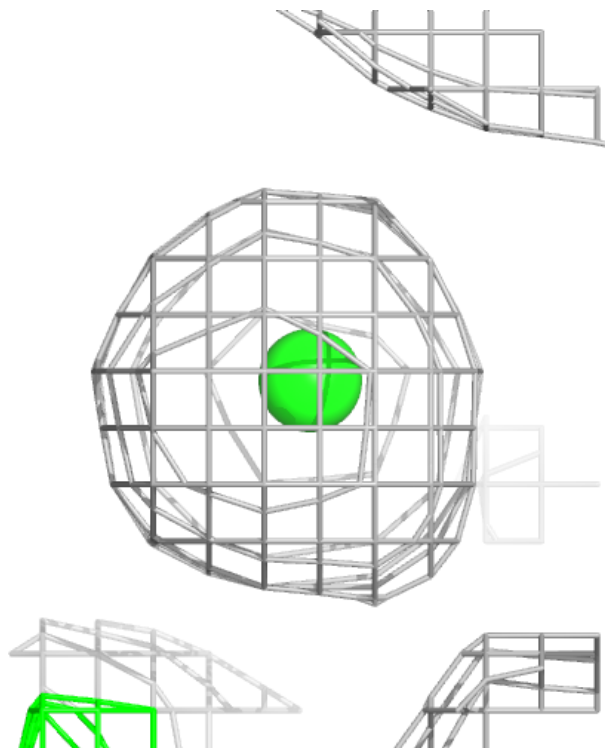
**Electron density around CL A 403 (B):**

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



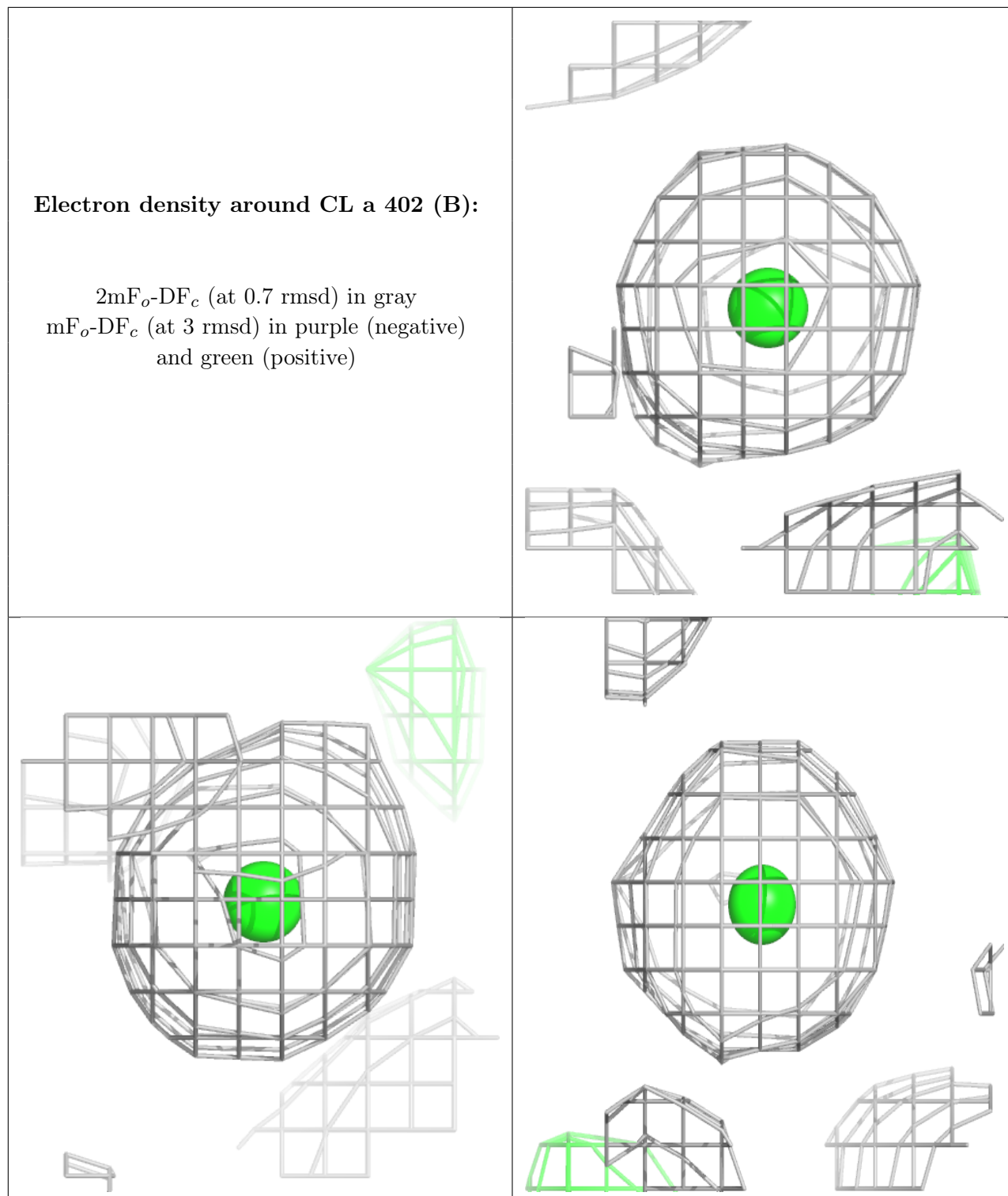
**Electron density around CL a 402 (A):**

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



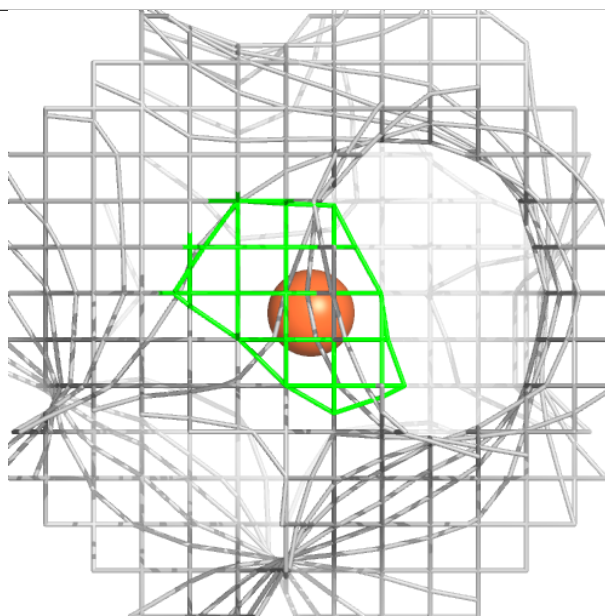
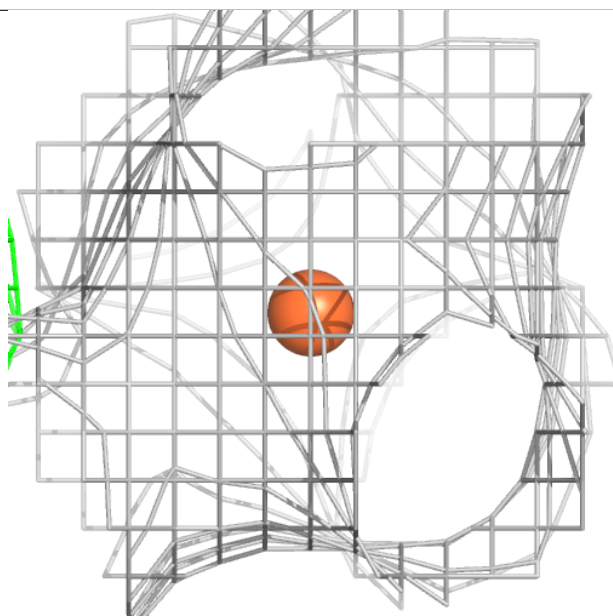
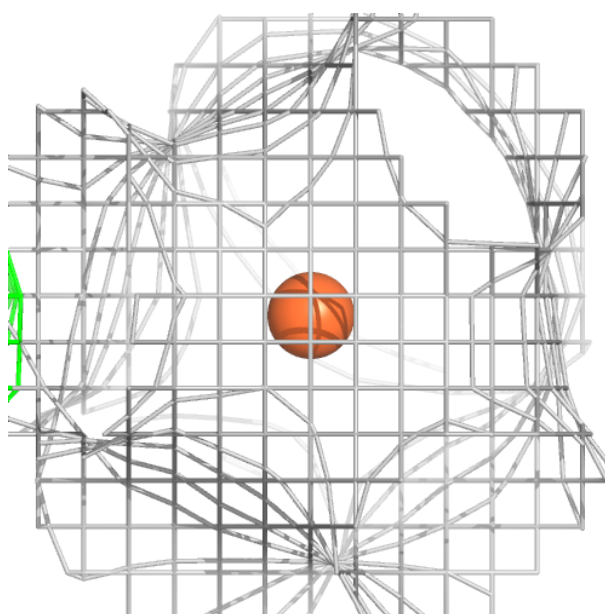
**Electron density around CL a 402 (B):**

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



**Electron density around FE2 A 401 (A):**

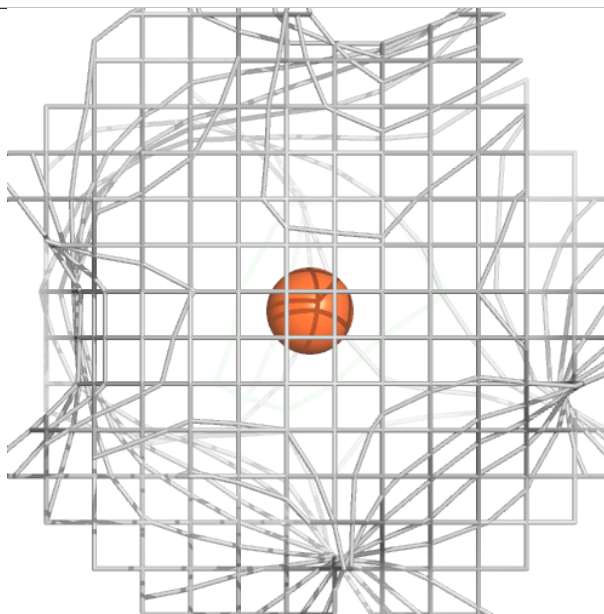
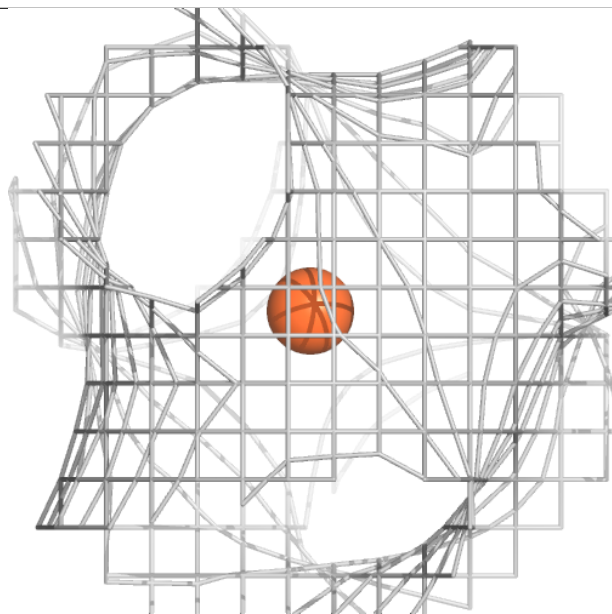
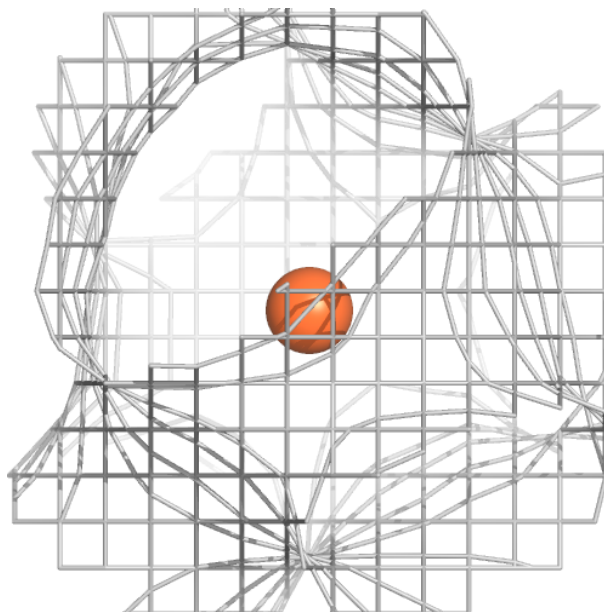
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FE2 A 401 (B):**

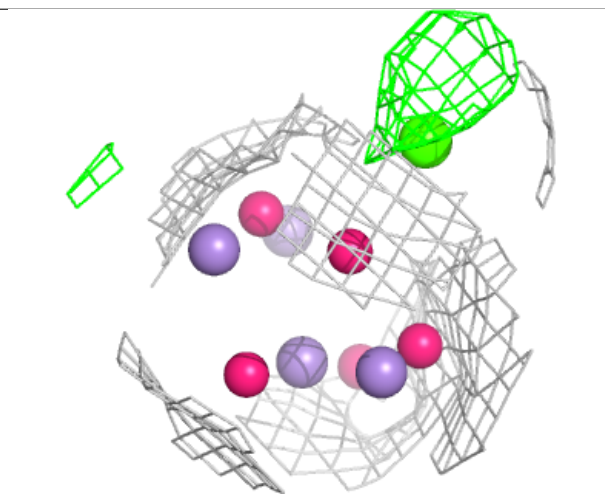
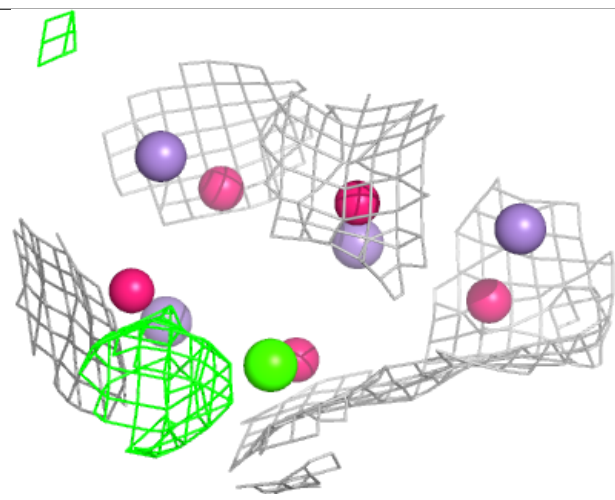
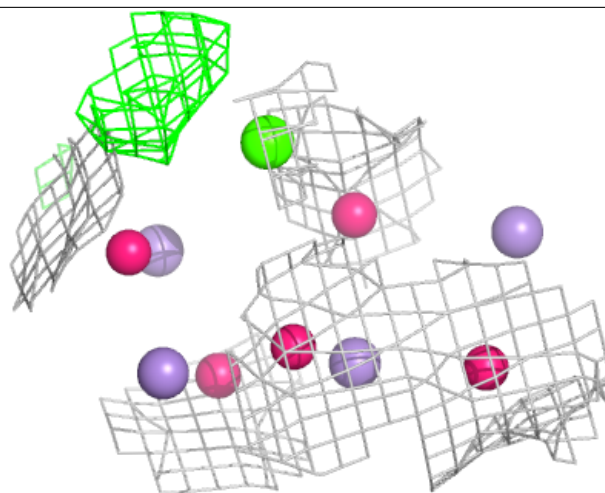
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





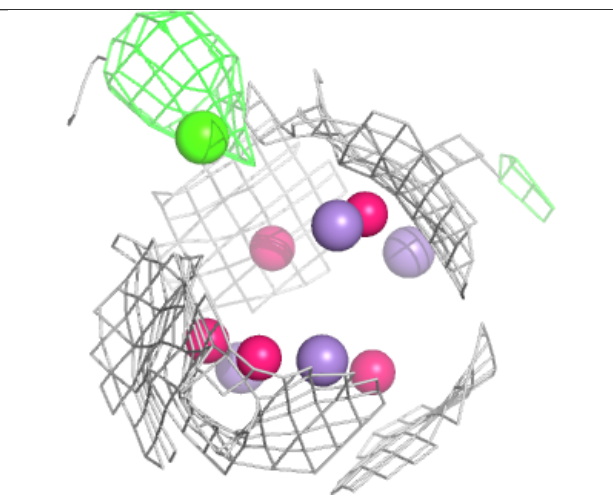
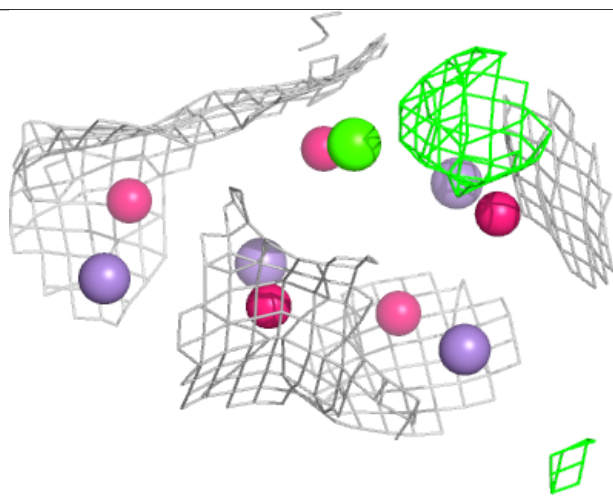
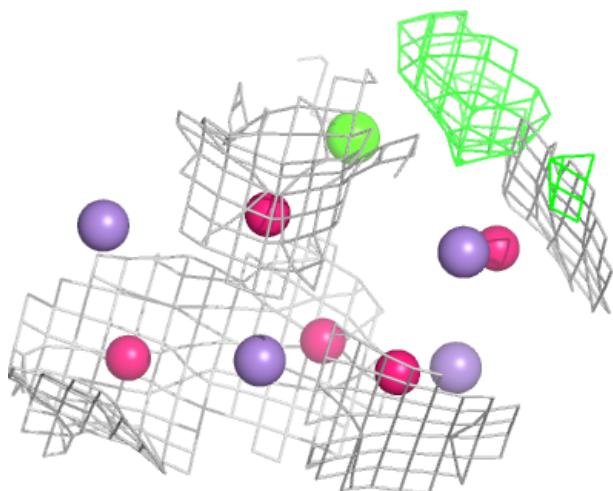
**Electron density around OEX a 412 (A):**

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



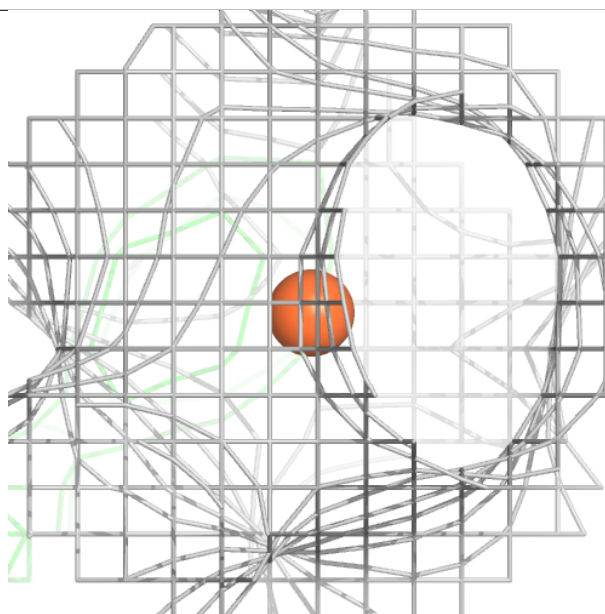
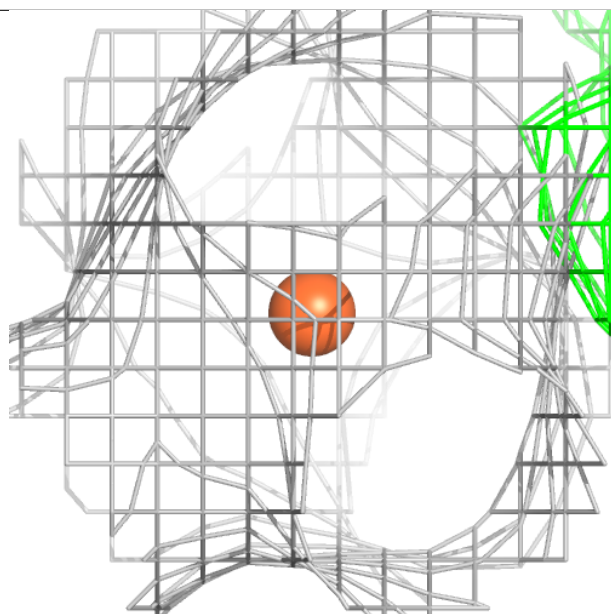
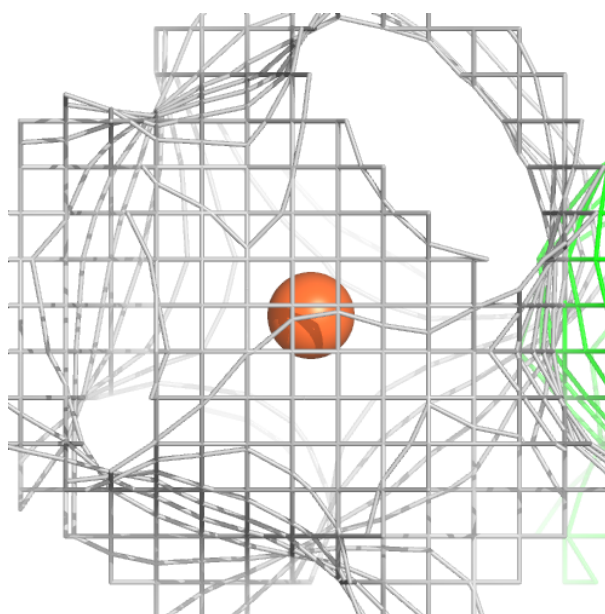
**Electron density around OEX a 412 (B):**

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



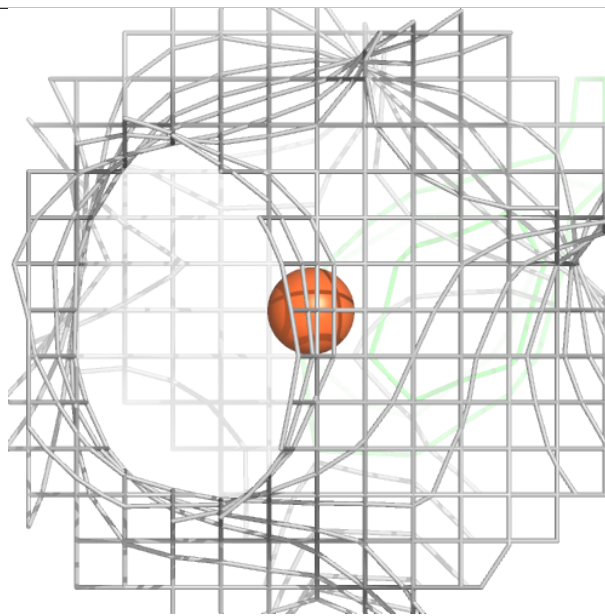
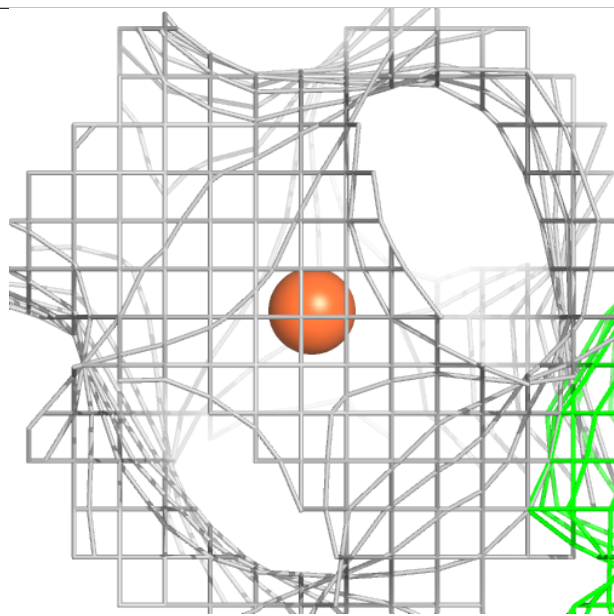
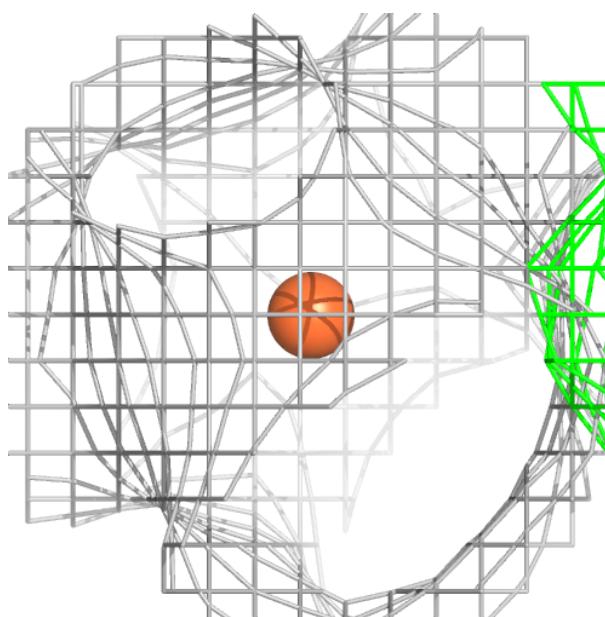
**Electron density around FE2 a 401 (A):**

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



**Electron density around FE2 a 401 (B):**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.