



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:17 PM UTC

PDB ID : 8IRB / pdb\_00008irb  
Title : XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 5-millisecond 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 : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

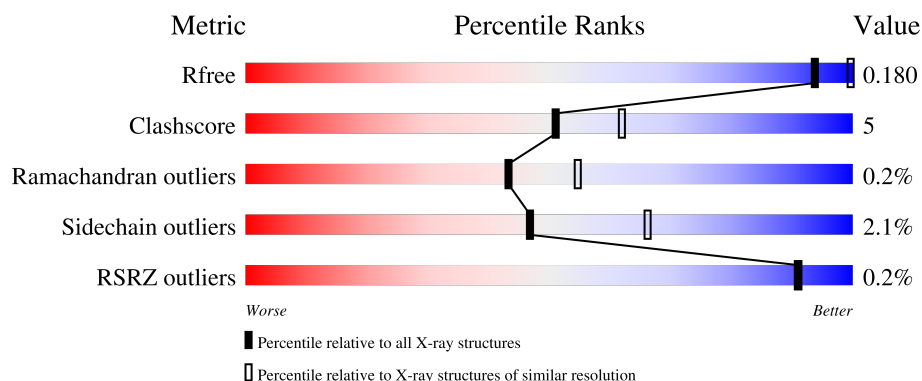
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

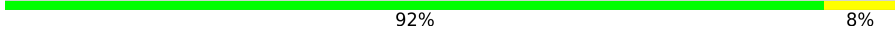
The reported resolution of this entry is 2.30 Å.

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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 6319 (2.30-2.30)                                      |
| Clashscore            | 190562                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |
| RSRZ outliers         | 180081                      | 6325 (2.30-2.30)                                      |

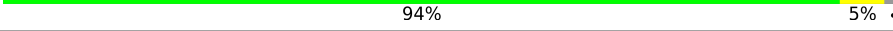
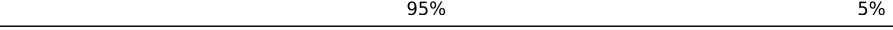
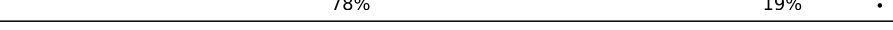
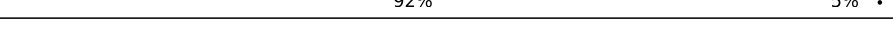
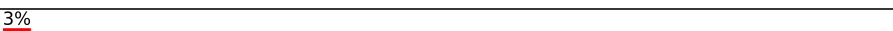
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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    | <br>88% 9% .  |
| 1   | a     | 344    | <br>86% 11% . |
| 2   | B     | 505    | <br>92% 8%    |
| 2   | b     | 505    | <br>89% 10% . |
| 3   | C     | 455    | <br>90% 9% .  |

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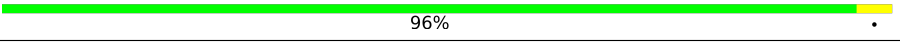


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| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 3   | c     | 455    |  89% 10% .       |
| 4   | D     | 342    |  89% 11%         |
| 4   | d     | 342    |  91% 8%          |
| 5   | E     | 84     |  80% 17% .       |
| 5   | e     | 84     |  83% 11% 6%      |
| 6   | F     | 44     |  68% 9% 23%      |
| 6   | f     | 44     |  64% 7% 30%      |
| 7   | H     | 65     |  94% 5% .        |
| 7   | h     | 65     |  86% 12% .       |
| 8   | I     | 38     |  76% 16% 8%      |
| 8   | i     | 38     |  95% 5%          |
| 9   | J     | 39     |  82% 10% 5% .   |
| 9   | j     | 39     |  85% 15%       |
| 10  | K     | 37     |  78% 19% .     |
| 10  | k     | 37     |  78% 19% .     |
| 11  | L     | 37     |  92% 5% .      |
| 11  | l     | 37     |  81% 16% .     |
| 12  | M     | 36     |  78% 11% . 8%  |
| 12  | m     | 36     |  78% 14% . 6%  |
| 13  | O     | 244    |  87% 13%       |
| 13  | o     | 244    |  90% 9%        |
| 14  | T     | 32     |  78% 16% 6%    |
| 14  | t     | 32     |  3% 81% 12% 6% |
| 15  | U     | 104    |  83% 10% 8%    |
| 15  | u     | 104    |  88% . . 7%    |

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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 16  | V     | 137    |  96% .        |
| 16  | v     | 137    |  89% 10% .    |
| 17  | X     | 40     |  85% 10% 5%   |
| 17  | x     | 40     |  90% 5% 5%    |
| 18  | Y     | 30     |  87% 10% .    |
| 18  | y     | 30     |  63% 33% .    |
| 19  | Z     | 62     |  89% 10% .    |
| 19  | z     | 62     |  77% 23%      |
| 20  | R     | 34     |  6% 76% 21% . |

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[B] | X         | -        | -       | -                |
| 23  | CLA  | A     | 408    | 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         | -        | -       | -                |

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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     | 702[A] | X         | -        | -       | -                |
| 23  | CLA  | D     | 702[B] | X         | -        | -       | -                |
| 23  | CLA  | D     | 703    | X         | -        | -       | -                |
| 23  | CLA  | a     | 405[A] | X         | -        | -       | -                |
| 23  | CLA  | a     | 405[B] | X         | -        | -       | -                |
| 23  | CLA  | a     | 406[A] | X         | -        | -       | -                |
| 23  | CLA  | a     | 406[B] | 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         | -        | -       | -                |

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| Mol | Type | Chain | Res    | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 23  | CLA  | c     | 512    | X         | -        | -       | -                |
| 23  | CLA  | c     | 513    | X         | -        | -       | -                |
| 23  | CLA  | c     | 514    | X         | -        | -       | -                |
| 23  | CLA  | d     | 401[A] | X         | -        | -       | -                |
| 23  | CLA  | d     | 401[B] | X         | -        | -       | -                |
| 23  | CLA  | d     | 402    | X         | -        | -       | -                |
| 27  | GOL  | D     | 701    | -         | -        | X       | -                |
| 27  | GOL  | D     | 712    | -         | X        | -       | -                |

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62674 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       | 220     | 0     |
|     |       |          | 4318  | 2821 | 715 | 757 | 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       | 22      | 0     |
|     |       |          | 4166  | 2735 | 694 | 724 | 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       | 99      | 0     |
|     |       |          | 4272  | 2796 | 715 | 743 | 18 |         |         |       |
| 3   | c     | 455      | Total | C    | N   | O   | S  | 0       | 101     | 0     |
|     |       |          | 4316  | 2827 | 720 | 751 | 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       | 115     | 0     |
|     |       |          | 3625  | 2390 | 597 | 623 | 15 |         |         |       |
| 4   | d     | 341      | Total | C    | N   | O   | S  | 0       | 119     | 0     |
|     |       |          | 3658  | 2412 | 605 | 626 | 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       | 5       | 0     |
|     |       |          | 815   | 519 | 135 | 161 |  |         |         |       |

- 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).

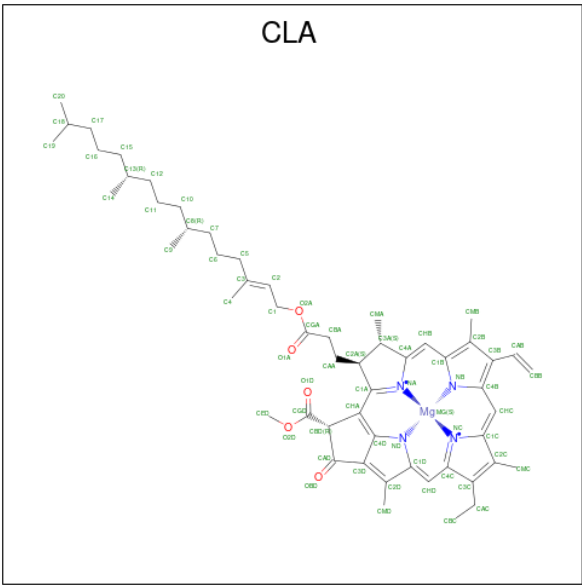
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22  | A     | 2        | Total | Cl | 0       | 2       |
|     |       |          | 4     | 4  |         |         |

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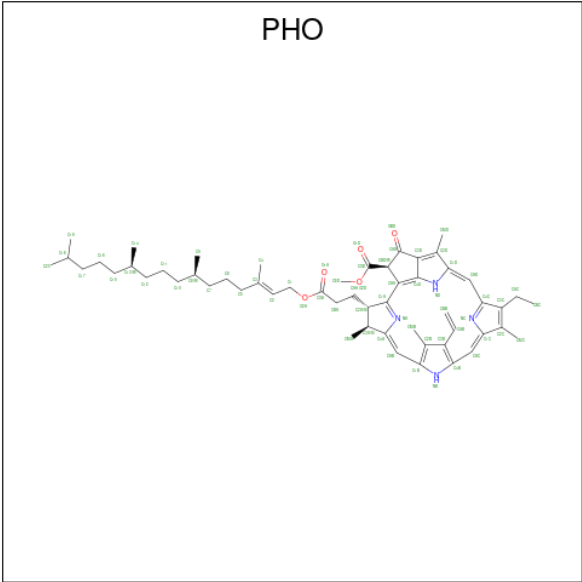
| Mol | Chain | Residues | Atoms        |          |         |        |         | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|--------|---------|---------|---------|
| 23  | C     | 1        | Total<br>65  | C<br>55  | Mg<br>1 | N<br>4 | O<br>5  | 0       | 0   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

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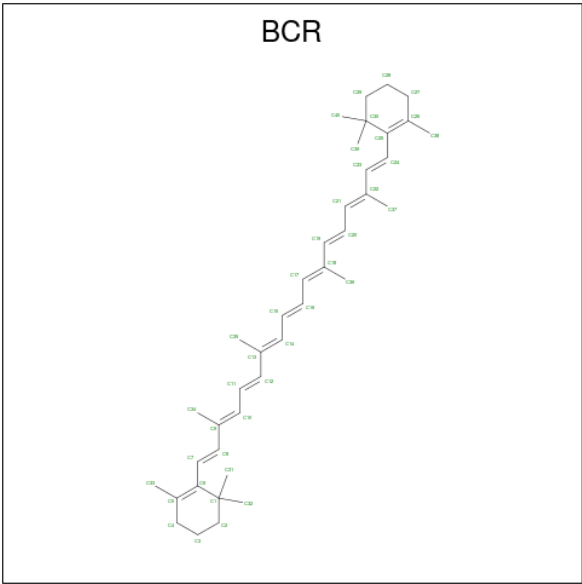
| Mol | Chain | Residues | Atoms |     |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|----|---|----|---------|---------|
| 23  | b     | 1        | Total | C   | Mg | N | O  | 0       | 0       |
|     |       |          | 65    | 55  | 1  | 4 | 5  |         |         |
|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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



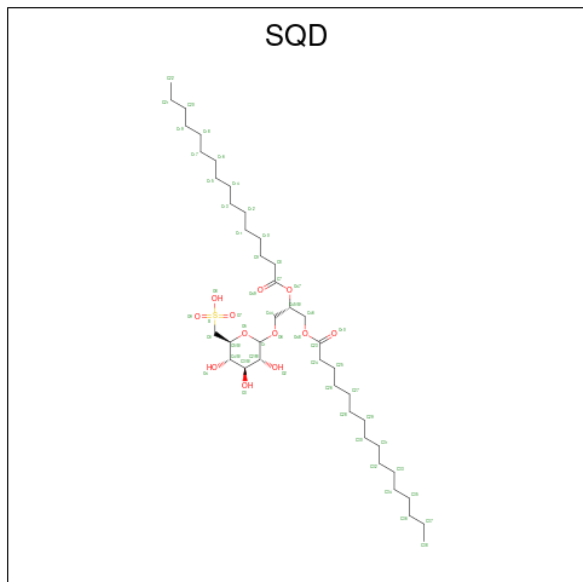
| Mol | Chain | Residues | Atoms |     |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---|----|---------|---------|
| 24  | A     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |
| 24  | A     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |
| 24  | a     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |
| 24  | a     | 1        | Total | C   | N | O  | 0       | 1       |
|     |       |          | 128   | 110 | 8 | 10 |         |         |

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 25  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | D     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | T     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | Y     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | a     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | d     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | h     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | k     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | t     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | y     | 1        | Total C<br>40 40 | 0       | 0       |

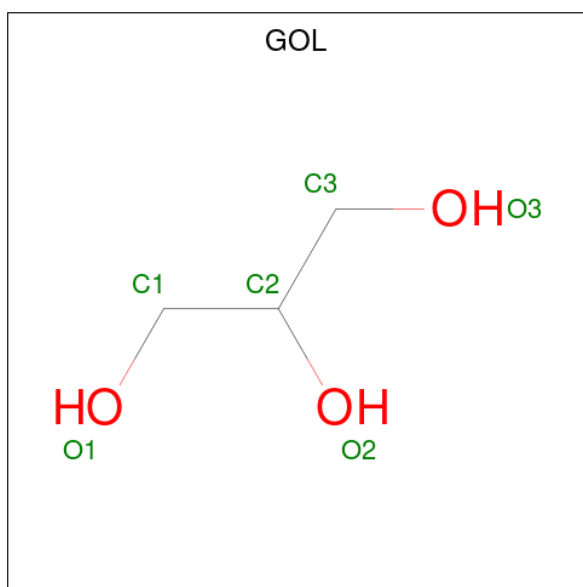
- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26  | A     | 1        | Total | C  | O  | S | 0       | 1       |
|     |       |          | 108   | 82 | 24 | 2 |         |         |
| 26  | A     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 26  | B     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 26  | X     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |
| 26  | a     | 1        | Total | C  | O  | S | 0       | 1       |
|     |       |          | 108   | 82 | 24 | 2 |         |         |
| 26  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 26  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 26  | f     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).





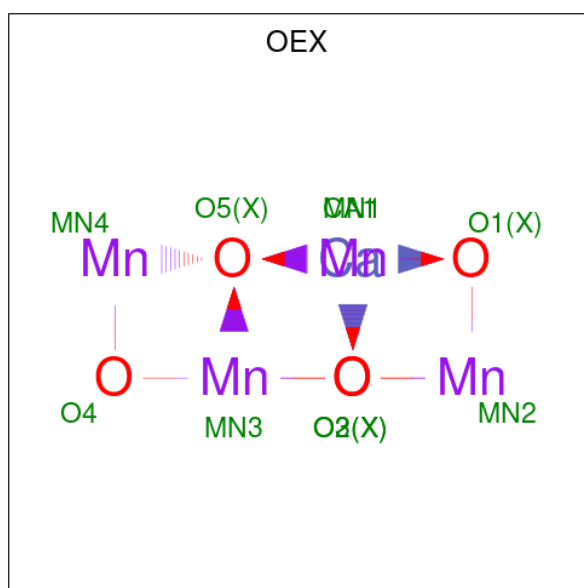
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 27  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | C     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |
| 27  | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | O     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | O     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | V     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |
| 27  | a     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | a     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | b     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | b     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 27  | c     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |
| 27  | c     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | d     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | l     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |
| 27  | o     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | o     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 27  | v     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 12    | 6 | 6 |         |         |

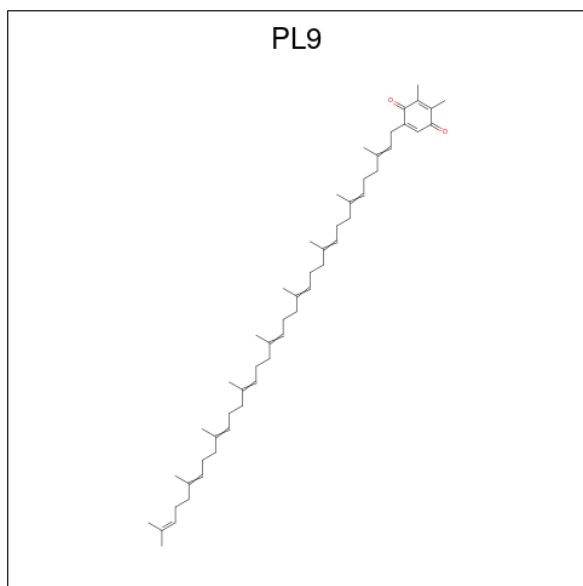
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 28  | A     | 1        | Total | Ca | Mn | O  | 0       | 1       |
|     |       |          | 20    | 2  | 8  | 10 |         |         |
| 28  | a     | 1        | Total | Ca | Mn | O  | 0       | 1       |
|     |       |          | 20    | 2  | 8  | 10 |         |         |

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ )

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



| Mol | Chain | Residues | Atoms |     |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---|---------|---------|
| 29  | A     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |
| 29  | D     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |
| 29  | a     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |
| 29  | d     | 1        | Total | C   | O | 0       | 1       |
|     |       |          | 110   | 106 | 4 |         |         |

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

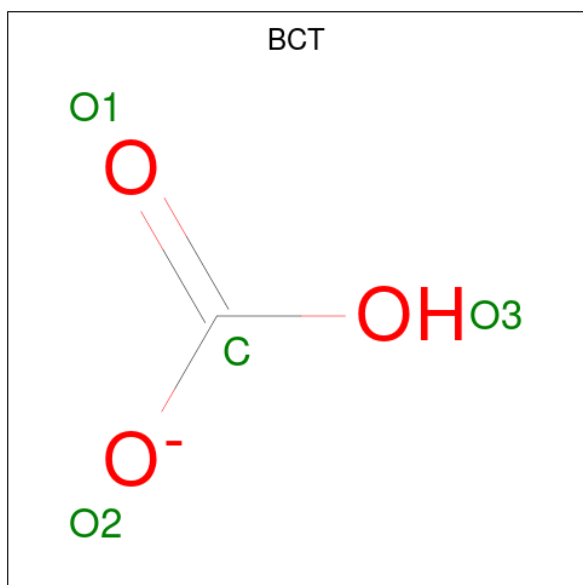
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 30  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 28    | 23 | 5  |         |         |
| 30  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 28 | 5  |         |         |
| 30  | D     | 2        | Total | C  | O  | 0       | 0       |
|     |       |          | 57    | 51 | 6  |         |         |
| 30  | I     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 40    | 35 | 5  |         |         |
| 30  | J     | 1        | Total | C  |    | 0       | 0       |
|     |       |          | 10    | 10 |    |         |         |
| 30  | K     | 1        | Total | C  | O  | 0       | 1       |
|     |       |          | 68    | 58 | 10 |         |         |
| 30  | X     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 18    | 16 | 2  |         |         |

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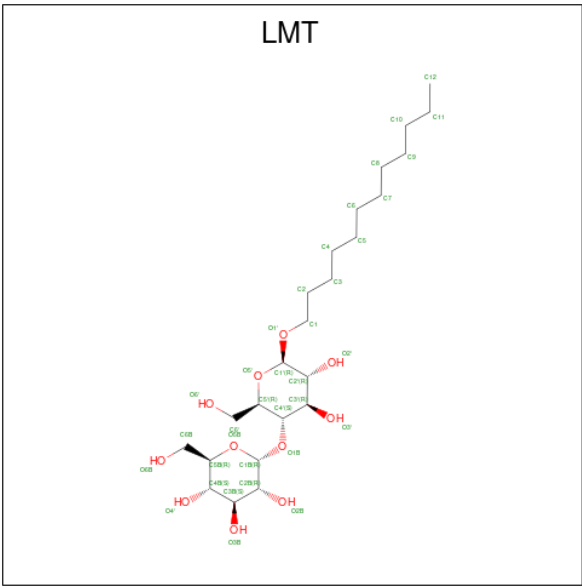
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 30  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 30    | 25 | 5  |         |         |
| 30  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 28 | 5  |         |         |
| 30  | c     | 1        | Total | C  | O  | 0       | 1       |
|     |       |          | 64    | 54 | 10 |         |         |
| 30  | d     | 2        | Total | C  | O  | 0       | 0       |
|     |       |          | 53    | 47 | 6  |         |         |
| 30  | i     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 40    | 35 | 5  |         |         |
| 30  | j     | 1        | Total | C  |    | 0       | 0       |
|     |       |          | 10    | 10 |    |         |         |
| 30  | l     | 1        | Total | C  |    | 0       | 0       |
|     |       |          | 10    | 10 |    |         |         |
| 30  | m     | 1        | Total | C  |    | 0       | 0       |
|     |       |          | 10    | 10 |    |         |         |
| 30  | x     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 18    | 16 | 2  |         |         |

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 31  | A     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 8     | 2 | 6 |         |         |
| 31  | a     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 8     | 2 | 6 |         |         |

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



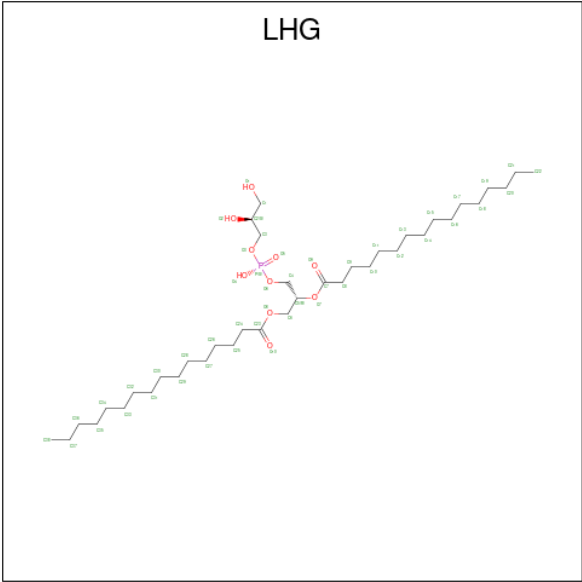
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 32  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 32  | A     | 1        | Total | C  | O  | 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 |         |         |
| 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 |         |         |

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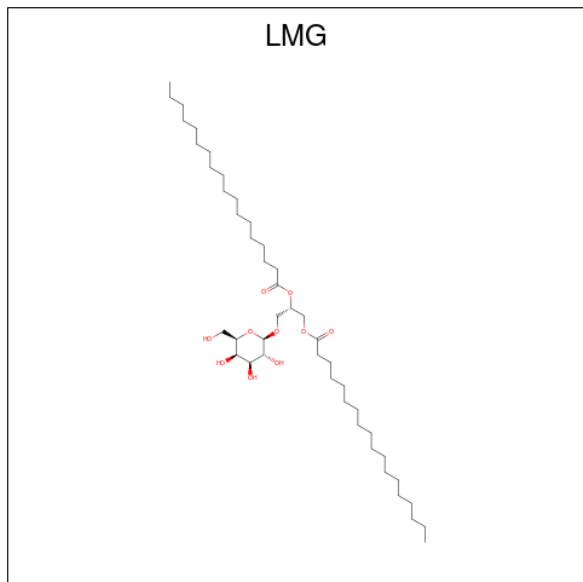
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 32  | t     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 26    | 19 | 7 |         |         |

- 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).



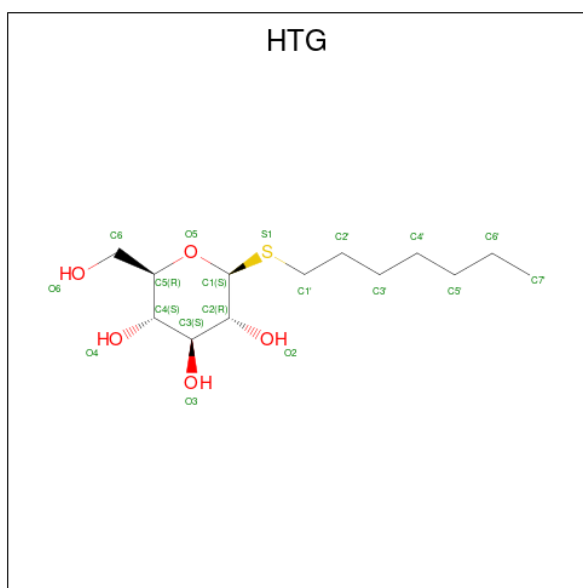
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 33  | A     | 1        | Total | C  | O  | P | 0       | 1       |
|     |       |          | 98    | 76 | 20 | 2 |         |         |
| 33  | D     | 1       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

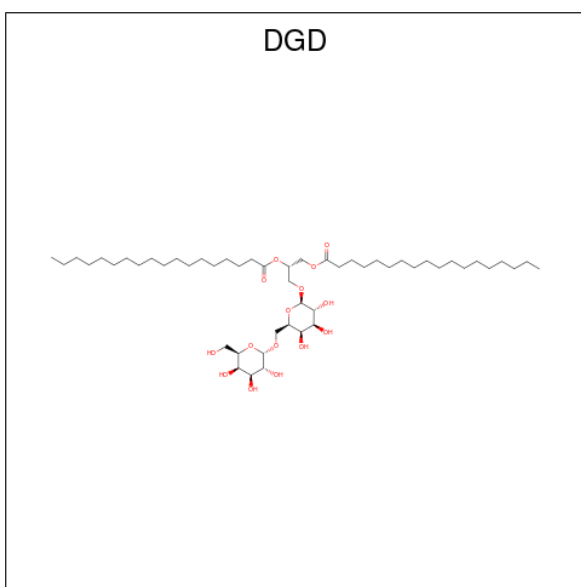
- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



| 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 |         |         |
| 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 |         |         |
| 36  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 36  | h     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |

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

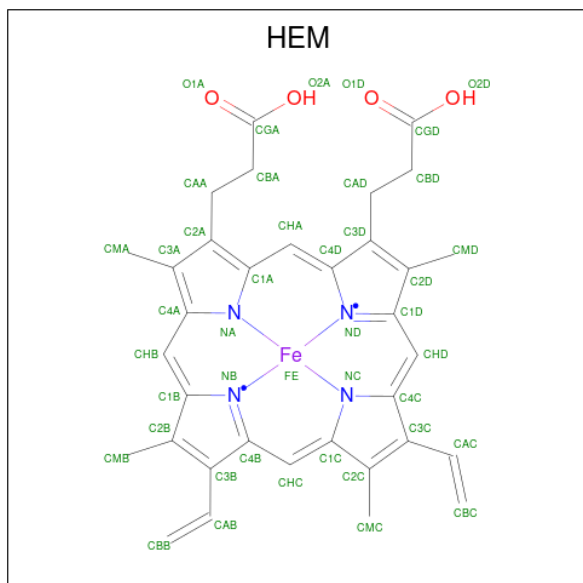
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 37  | C     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 37  | F     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 37  | O     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 37  | c     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

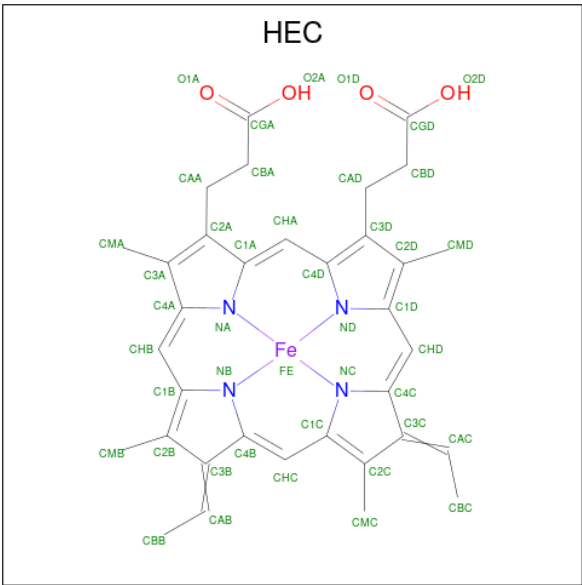
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| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 37  | f     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 37  | o     | 1        | Total Ca<br>1 1 | 0       | 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 |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 40  | V     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 40  | v     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 41 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 41  | A     | 138      | Total | O   | 0       | 86      |
|     |       |          | 223   | 223 |         |         |
| 41  | B     | 188      | Total | O   | 0       | 2       |
|     |       |          | 190   | 190 |         |         |
| 41  | C     | 167      | Total | O   | 0       | 38      |
|     |       |          | 204   | 204 |         |         |
| 41  | D     | 121      | Total | O   | 0       | 35      |
|     |       |          | 156   | 156 |         |         |
| 41  | E     | 16       | Total | O   | 0       | 0       |
|     |       |          | 16    | 16  |         |         |
| 41  | F     | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 41  | H     | 21       | Total | O   | 0       | 0       |
|     |       |          | 21    | 21  |         |         |
| 41  | I     | 5        | Total | O   | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 41  | J     | 7        | Total | O   | 0       | 0       |
|     |       |          | 7     | 7   |         |         |
| 41  | K     | 5        | Total | O   | 0       | 0       |
|     |       |          | 5     | 5   |         |         |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 41  | L     | 8        | Total O<br>9 9     | 0       | 1       |
| 41  | M     | 6        | Total O<br>6 6     | 0       | 0       |
| 41  | O     | 105      | Total O<br>109 109 | 0       | 4       |
| 41  | T     | 11       | Total O<br>14 14   | 0       | 3       |
| 41  | U     | 46       | Total O<br>48 48   | 0       | 2       |
| 41  | V     | 79       | Total O<br>80 80   | 0       | 1       |
| 41  | X     | 9        | Total O<br>9 9     | 0       | 0       |
| 41  | a     | 134      | Total O<br>215 215 | 0       | 82      |
| 41  | b     | 199      | Total O<br>202 202 | 0       | 3       |
| 41  | c     | 160      | Total O<br>193 193 | 0       | 34      |
| 41  | d     | 116      | Total O<br>147 147 | 0       | 31      |
| 41  | e     | 9        | Total O<br>9 9     | 0       | 0       |
| 41  | f     | 3        | Total O<br>3 3     | 0       | 0       |
| 41  | h     | 18       | Total O<br>18 18   | 0       | 0       |
| 41  | i     | 2        | Total O<br>2 2     | 0       | 0       |
| 41  | j     | 2        | Total O<br>2 2     | 0       | 0       |
| 41  | k     | 3        | Total O<br>3 3     | 0       | 0       |
| 41  | l     | 8        | Total O<br>10 10   | 0       | 2       |
| 41  | m     | 13       | Total O<br>13 13   | 0       | 0       |
| 41  | o     | 99       | Total O<br>103 103 | 0       | 4       |
| 41  | t     | 6        | Total O<br>9 9     | 0       | 3       |

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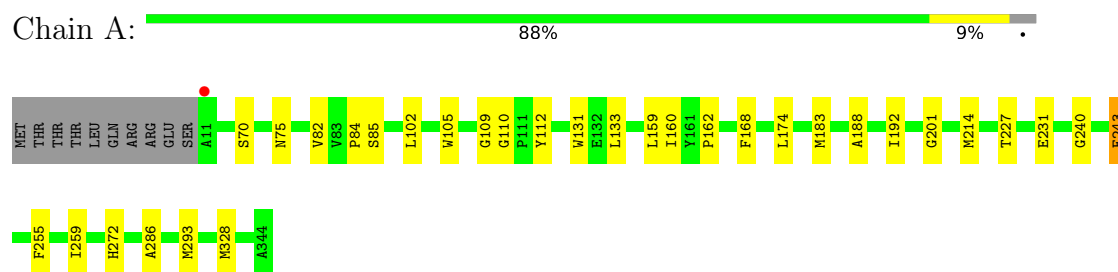
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 41  | u     | 50       | Total<br>51 | O<br>51 | 0       | 1       |
| 41  | v     | 57       | Total<br>59 | O<br>59 | 0       | 2       |
| 41  | x     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 41  | y     | 2        | Total<br>2  | O<br>2  | 0       | 0       |

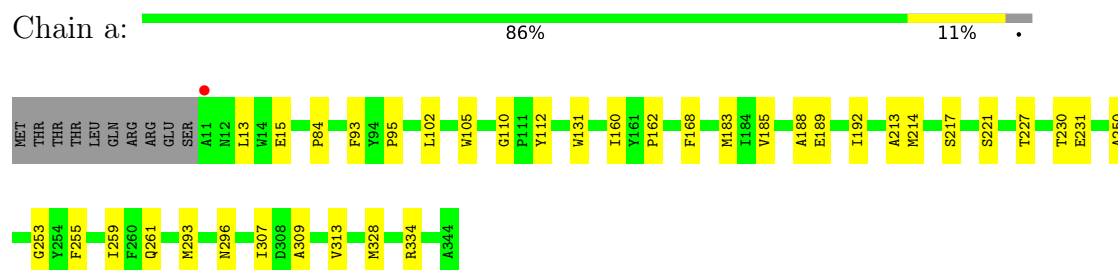
### 3 Residue-property plots

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.

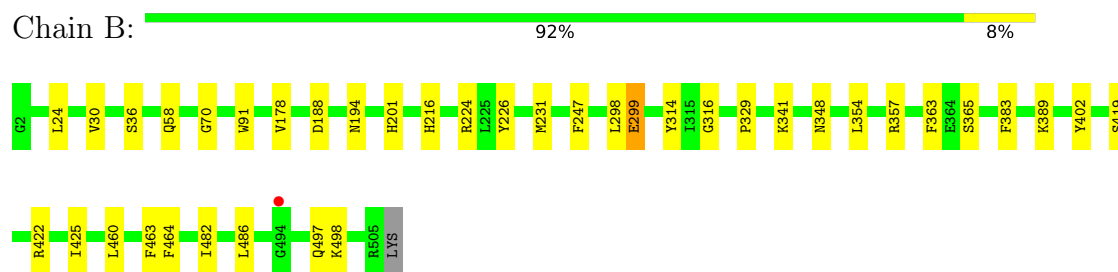
- Molecule 1: Photosystem II protein D1



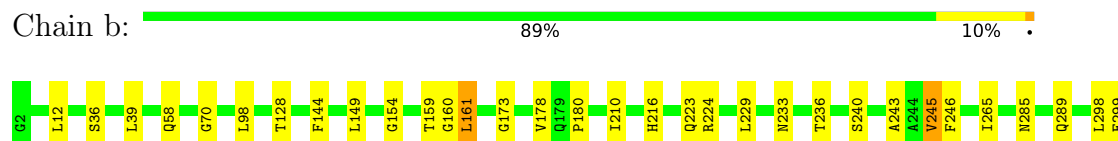
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



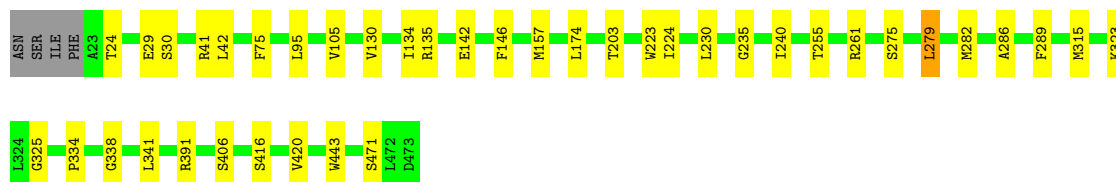
- Molecule 2: Photosystem II CP47 reaction center protein





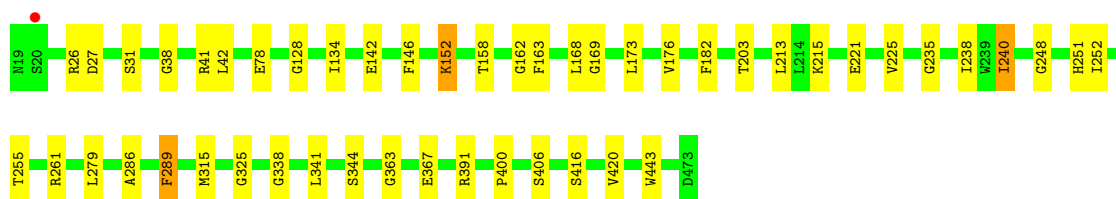
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 90% 9% .



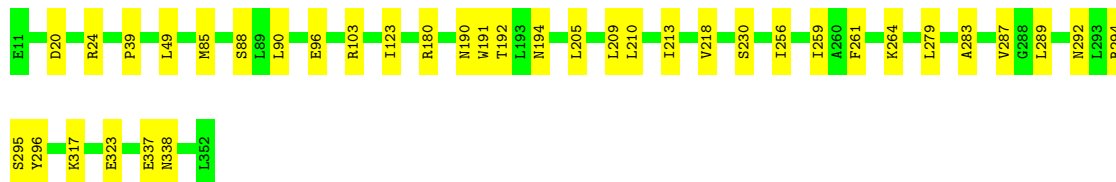
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 10% .



• Molecule 4: Photosystem II D2 protein

Chain D: 89% 11%



• Molecule 4: Photosystem II D2 protein

Chain d: 91% 8%

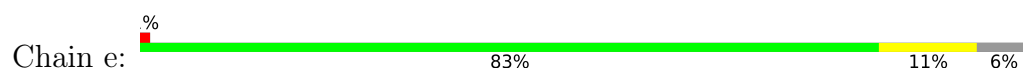


• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 80% 17% .



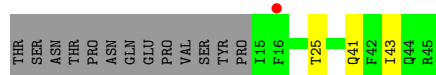
• Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



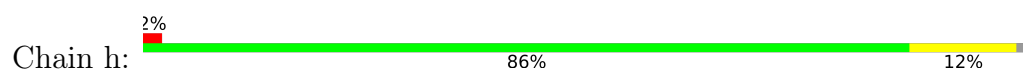
- Molecule 6: Cytochrome b559 subunit beta



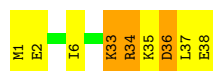
- Molecule 7: Photosystem II reaction center protein H



- 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

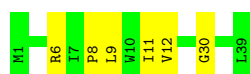


Chain J:  82% 10% 5% .



- Molecule 9: Photosystem II reaction center protein J

Chain j:  85% 15%



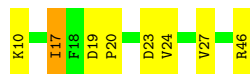
- Molecule 10: Photosystem II reaction center protein K

Chain K:  78% 19% .

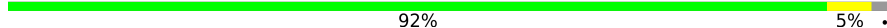


- Molecule 10: Photosystem II reaction center protein K

Chain k:  78% 19% .



- 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% 11% . 8%



- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 14% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  87% 13%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  90% 9%



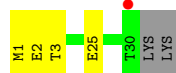
- Molecule 14: Photosystem II reaction center protein T

Chain T:  78% 16% 6%



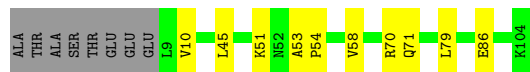
- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 81% 12% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  83% 10% 8%

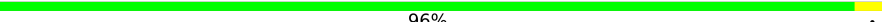


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  88% 7% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



- Molecule 16: Cytochrome c-550

Chain v:  89% 10% .



- Molecule 17: Photosystem II reaction center protein X

Chain X:  85% 10% 5% .



- Molecule 17: Photosystem II reaction center protein X

Chain x:  90% 5% 5% .



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  87% 10% .



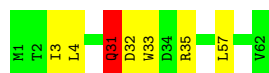
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  63% 33% .



- Molecule 19: Photosystem II reaction center protein Z

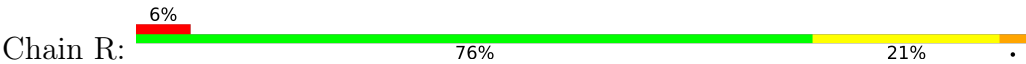
Chain Z:  89% 10% .



- 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, $\alpha$ , $\beta$ , $\gamma$                | 125.75Å 231.60Å 288.28Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 19.98 – 2.30<br>19.98 – 2.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (19.98-2.30)<br>99.7 (19.98-2.30)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.14 (at 2.30Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.19.2_4158: ???)                                   | Depositor        |
| R, $R_{free}$                                                           | 0.139 , 0.180<br>0.145 , 0.180                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 21187 reflections (2.60%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 50.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.541                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 69.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.98                                                        | EDS              |
| Total number of atoms                                                   | 62674                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 65.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.27         | 0/4478  | 0.45        | 0/6098  |
| 1   | a     | 0.25         | 0/4457  | 0.41        | 0/6069  |
| 2   | B     | 0.35         | 0/4314  | 0.49        | 0/5879  |
| 2   | b     | 0.33         | 0/4285  | 0.48        | 0/5841  |
| 3   | C     | 0.27         | 0/4416  | 0.42        | 0/6013  |
| 3   | c     | 0.28         | 0/4467  | 0.42        | 0/6082  |
| 4   | D     | 0.32         | 0/3746  | 0.47        | 0/5102  |
| 4   | d     | 0.30         | 0/3780  | 0.44        | 0/5147  |
| 5   | E     | 0.32         | 0/681   | 0.50        | 0/928   |
| 5   | e     | 0.29         | 0/690   | 0.46        | 0/939   |
| 6   | F     | 0.30         | 0/284   | 0.46        | 0/387   |
| 6   | f     | 0.29         | 0/269   | 0.45        | 0/365   |
| 7   | H     | 0.30         | 0/519   | 0.47        | 0/708   |
| 7   | h     | 0.30         | 0/530   | 0.48        | 0/722   |
| 8   | I     | 0.29         | 0/311   | 0.42        | 0/419   |
| 8   | i     | 0.32         | 0/311   | 0.45        | 0/419   |
| 9   | J     | 0.33         | 0/278   | 0.45        | 0/376   |
| 9   | j     | 0.27         | 0/283   | 0.43        | 0/383   |
| 10  | K     | 0.32         | 0/303   | 0.48        | 0/416   |
| 10  | k     | 0.34         | 0/303   | 0.47        | 0/416   |
| 11  | L     | 0.36         | 0/318   | 0.46        | 0/433   |
| 11  | l     | 0.37         | 0/318   | 0.45        | 0/433   |
| 12  | M     | 0.37         | 0/261   | 0.50        | 0/357   |
| 12  | m     | 0.30         | 0/279   | 0.47        | 0/380   |
| 13  | O     | 0.34         | 0/1991  | 0.52        | 0/2698  |
| 13  | o     | 0.32         | 0/1966  | 0.50        | 0/2665  |
| 14  | T     | 0.33         | 0/310   | 0.43        | 0/419   |
| 14  | t     | 0.32         | 0/301   | 0.41        | 0/406   |
| 15  | U     | 0.36         | 0/811   | 0.54        | 0/1095  |
| 15  | u     | 0.35         | 0/826   | 0.55        | 0/1116  |
| 16  | V     | 0.34         | 0/1142  | 0.48        | 0/1545  |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 16  | v     | 0.30         | 0/1139  | 0.46        | 0/1542  |
| 17  | X     | 0.22         | 0/292   | 0.33        | 0/395   |
| 17  | x     | 0.23         | 0/284   | 0.36        | 0/384   |
| 18  | Y     | 0.24         | 0/216   | 0.42        | 0/289   |
| 18  | y     | 0.25         | 0/216   | 0.40        | 0/289   |
| 19  | Z     | 0.23         | 0/490   | 0.37        | 0/669   |
| 19  | z     | 0.22         | 0/490   | 0.33        | 0/669   |
| 20  | R     | 0.27         | 0/279   | 0.35        | 0/383   |
| All | All   | 0.30         | 0/50634 | 0.46        | 0/68876 |

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     | 26      | 0            |
| 1   | a     | 4318  | 0        | 4124     | 42      | 0            |
| 2   | B     | 4166  | 0        | 3999     | 31      | 0            |
| 2   | b     | 4134  | 0        | 3976     | 48      | 0            |
| 3   | C     | 4272  | 0        | 4138     | 28      | 0            |
| 3   | c     | 4316  | 0        | 4183     | 37      | 0            |
| 4   | D     | 3625  | 0        | 3489     | 36      | 0            |
| 4   | d     | 3658  | 0        | 3522     | 28      | 0            |
| 5   | E     | 662   | 0        | 648      | 10      | 0            |
| 5   | e     | 670   | 0        | 655      | 7       | 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      | 6       | 0            |
| 8   | I     | 314   | 0        | 328      | 5       | 0            |
| 8   | i     | 314   | 0        | 328      | 1       | 0            |
| 9   | J     | 272   | 0        | 279      | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | j     | 277   | 0        | 284      | 4       | 0            |
| 10  | K     | 293   | 0        | 305      | 5       | 0            |
| 10  | k     | 293   | 0        | 305      | 6       | 0            |
| 11  | L     | 311   | 0        | 320      | 2       | 0            |
| 11  | l     | 311   | 0        | 320      | 5       | 0            |
| 12  | M     | 268   | 0        | 285      | 5       | 0            |
| 12  | m     | 286   | 0        | 305      | 7       | 0            |
| 13  | O     | 1958  | 0        | 1920     | 20      | 0            |
| 13  | o     | 1933  | 0        | 1900     | 12      | 0            |
| 14  | T     | 311   | 0        | 318      | 3       | 0            |
| 14  | t     | 302   | 0        | 311      | 4       | 0            |
| 15  | U     | 800   | 0        | 796      | 5       | 0            |
| 15  | u     | 815   | 0        | 817      | 4       | 0            |
| 16  | V     | 1120  | 0        | 1122     | 3       | 0            |
| 16  | v     | 1117  | 0        | 1131     | 9       | 0            |
| 17  | X     | 289   | 0        | 322      | 4       | 0            |
| 17  | x     | 281   | 0        | 312      | 2       | 0            |
| 18  | Y     | 215   | 0        | 246      | 2       | 0            |
| 18  | y     | 215   | 0        | 246      | 6       | 0            |
| 19  | Z     | 479   | 0        | 516      | 5       | 0            |
| 19  | z     | 479   | 0        | 516      | 3       | 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      | 20      | 0            |
| 23  | B     | 1040  | 0        | 1152     | 29      | 0            |
| 23  | C     | 845   | 0        | 936      | 41      | 0            |
| 23  | D     | 195   | 0        | 216      | 6       | 0            |
| 23  | a     | 455   | 0        | 504      | 21      | 0            |
| 23  | b     | 1040  | 0        | 1152     | 28      | 0            |
| 23  | c     | 845   | 0        | 936      | 37      | 0            |
| 23  | d     | 195   | 0        | 216      | 7       | 0            |
| 24  | A     | 256   | 0        | 296      | 7       | 0            |
| 24  | a     | 256   | 0        | 296      | 4       | 0            |
| 25  | A     | 40    | 0        | 56       | 1       | 0            |
| 25  | B     | 120   | 0        | 168      | 6       | 0            |
| 25  | C     | 80    | 0        | 112      | 3       | 0            |
| 25  | D     | 40    | 0        | 56       | 1       | 0            |
| 25  | H     | 40    | 0        | 56       | 1       | 0            |
| 25  | K     | 40    | 0        | 56       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25  | T     | 40    | 0        | 56       | 6       | 0            |
| 25  | Y     | 40    | 0        | 56       | 1       | 0            |
| 25  | a     | 40    | 0        | 56       | 1       | 0            |
| 25  | b     | 120   | 0        | 168      | 8       | 0            |
| 25  | c     | 80    | 0        | 112      | 4       | 0            |
| 25  | d     | 40    | 0        | 56       | 3       | 0            |
| 25  | h     | 40    | 0        | 56       | 4       | 0            |
| 25  | k     | 40    | 0        | 56       | 1       | 0            |
| 25  | t     | 40    | 0        | 56       | 5       | 0            |
| 25  | y     | 40    | 0        | 56       | 2       | 0            |
| 26  | A     | 162   | 0        | 232      | 5       | 0            |
| 26  | B     | 54    | 0        | 78       | 2       | 0            |
| 26  | X     | 43    | 0        | 53       | 2       | 0            |
| 26  | a     | 162   | 0        | 232      | 10      | 0            |
| 26  | b     | 54    | 0        | 78       | 2       | 0            |
| 26  | f     | 43    | 0        | 53       | 1       | 0            |
| 27  | A     | 6     | 0        | 8        | 0       | 0            |
| 27  | B     | 18    | 0        | 24       | 2       | 0            |
| 27  | C     | 12    | 0        | 16       | 0       | 0            |
| 27  | D     | 12    | 0        | 15       | 6       | 0            |
| 27  | O     | 12    | 0        | 16       | 4       | 0            |
| 27  | V     | 12    | 0        | 16       | 0       | 0            |
| 27  | a     | 12    | 0        | 16       | 5       | 0            |
| 27  | b     | 12    | 0        | 16       | 2       | 0            |
| 27  | c     | 18    | 0        | 24       | 1       | 0            |
| 27  | d     | 6     | 0        | 8        | 0       | 0            |
| 27  | l     | 12    | 0        | 16       | 2       | 0            |
| 27  | o     | 12    | 0        | 16       | 0       | 0            |
| 27  | v     | 12    | 0        | 16       | 2       | 0            |
| 28  | A     | 20    | 0        | 0        | 0       | 0            |
| 28  | a     | 20    | 0        | 0        | 0       | 0            |
| 29  | A     | 110   | 0        | 160      | 18      | 0            |
| 29  | D     | 110   | 0        | 160      | 0       | 0            |
| 29  | a     | 110   | 0        | 160      | 9       | 0            |
| 29  | d     | 110   | 0        | 160      | 1       | 0            |
| 30  | A     | 28    | 0        | 0        | 0       | 0            |
| 30  | B     | 33    | 0        | 0        | 1       | 0            |
| 30  | D     | 57    | 0        | 0        | 0       | 0            |
| 30  | I     | 40    | 0        | 0        | 0       | 0            |
| 30  | J     | 10    | 0        | 0        | 0       | 0            |
| 30  | K     | 68    | 0        | 0        | 0       | 0            |
| 30  | X     | 18    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30  | a     | 30    | 0        | 0        | 0       | 0            |
| 30  | b     | 33    | 0        | 0        | 0       | 0            |
| 30  | c     | 64    | 0        | 0        | 0       | 0            |
| 30  | d     | 53    | 0        | 0        | 0       | 0            |
| 30  | i     | 40    | 0        | 0        | 0       | 0            |
| 30  | j     | 10    | 0        | 0        | 0       | 0            |
| 30  | l     | 10    | 0        | 0        | 0       | 0            |
| 30  | m     | 10    | 0        | 0        | 0       | 0            |
| 30  | x     | 18    | 0        | 0        | 0       | 0            |
| 31  | A     | 8     | 0        | 0        | 0       | 0            |
| 31  | a     | 8     | 0        | 0        | 0       | 0            |
| 32  | A     | 70    | 0        | 92       | 2       | 0            |
| 32  | B     | 95    | 0        | 127      | 3       | 0            |
| 32  | F     | 35    | 0        | 46       | 0       | 0            |
| 32  | M     | 35    | 0        | 46       | 1       | 0            |
| 32  | T     | 35    | 0        | 46       | 1       | 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        | 35       | 2       | 0            |
| 33  | A     | 98    | 0        | 148      | 3       | 0            |
| 33  | D     | 196   | 0        | 296      | 13      | 0            |
| 33  | E     | 84    | 0        | 114      | 7       | 0            |
| 33  | L     | 98    | 0        | 148      | 0       | 0            |
| 33  | a     | 84    | 0        | 114      | 8       | 0            |
| 33  | b     | 98    | 0        | 148      | 1       | 0            |
| 33  | d     | 294   | 0        | 444      | 26      | 0            |
| 34  | B     | 51    | 0        | 72       | 1       | 0            |
| 34  | C     | 153   | 0        | 216      | 2       | 0            |
| 34  | D     | 51    | 0        | 72       | 0       | 0            |
| 34  | Z     | 37    | 0        | 44       | 2       | 0            |
| 34  | c     | 153   | 0        | 216      | 2       | 0            |
| 34  | d     | 51    | 0        | 72       | 3       | 0            |
| 34  | m     | 51    | 0        | 72       | 2       | 0            |
| 34  | z     | 39    | 0        | 48       | 2       | 0            |
| 35  | B     | 38    | 0        | 52       | 3       | 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            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | d     | 16    | 0        | 17       | 1       | 0            |
| 35  | o     | 19    | 0        | 26       | 2       | 0            |
| 36  | C     | 310   | 0        | 410      | 9       | 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       | 0       | 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       | 1       | 0            |
| 40  | v     | 43    | 0        | 30       | 0       | 0            |
| 41  | A     | 223   | 0        | 0        | 0       | 0            |
| 41  | B     | 190   | 0        | 0        | 1       | 0            |
| 41  | C     | 204   | 0        | 0        | 3       | 0            |
| 41  | D     | 156   | 0        | 0        | 5       | 0            |
| 41  | E     | 16    | 0        | 0        | 1       | 0            |
| 41  | F     | 6     | 0        | 0        | 0       | 0            |
| 41  | H     | 21    | 0        | 0        | 0       | 0            |
| 41  | I     | 5     | 0        | 0        | 0       | 0            |
| 41  | J     | 7     | 0        | 0        | 0       | 0            |
| 41  | K     | 5     | 0        | 0        | 0       | 0            |
| 41  | L     | 9     | 0        | 0        | 0       | 0            |
| 41  | M     | 6     | 0        | 0        | 0       | 0            |
| 41  | O     | 109   | 0        | 0        | 1       | 0            |
| 41  | T     | 14    | 0        | 0        | 0       | 0            |
| 41  | U     | 48    | 0        | 0        | 0       | 0            |
| 41  | V     | 80    | 0        | 0        | 0       | 0            |
| 41  | X     | 9     | 0        | 0        | 0       | 0            |
| 41  | a     | 215   | 0        | 0        | 3       | 0            |
| 41  | b     | 202   | 0        | 0        | 0       | 0            |
| 41  | c     | 193   | 0        | 0        | 5       | 0            |
| 41  | d     | 147   | 0        | 0        | 1       | 0            |
| 41  | e     | 9     | 0        | 0        | 0       | 0            |
| 41  | f     | 3     | 0        | 0        | 0       | 0            |
| 41  | h     | 18    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41  | i     | 2     | 0        | 0        | 0       | 0            |
| 41  | j     | 2     | 0        | 0        | 0       | 0            |
| 41  | k     | 3     | 0        | 0        | 0       | 0            |
| 41  | l     | 10    | 0        | 0        | 0       | 0            |
| 41  | m     | 13    | 0        | 0        | 0       | 0            |
| 41  | o     | 103   | 0        | 0        | 1       | 0            |
| 41  | t     | 9     | 0        | 0        | 1       | 0            |
| 41  | u     | 51    | 0        | 0        | 1       | 0            |
| 41  | v     | 59    | 0        | 0        | 0       | 0            |
| 41  | x     | 6     | 0        | 0        | 0       | 0            |
| 41  | y     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 62674 | 0        | 61527    | 641     | 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 (641) 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                     | 0.98              |
| 27:D:701:GOL:H11     | 12:M:1:FME:HG2       | 1.46                     | 0.97              |
| 1:a:250[B]:ALA:HA    | 2:b:491[B]:VAL:HG11  | 1.52                     | 0.92              |
| 1:a:250[A]:ALA:HA    | 2:b:491[A]:VAL:HG11  | 1.53                     | 0.88              |
| 23:B:601:CLA:H12     | 23:B:601:CLA:H71     | 1.60                     | 0.81              |
| 23:c:504:CLA:HBB1    | 23:c:513:CLA:H41     | 1.64                     | 0.80              |
| 4:d:192[A]:THR:HG23  | 23:d:401[A]:CLA:HBC2 | 1.64                     | 0.80              |
| 25:t:102:BCR:HC8     | 25:t:102:BCR:H321    | 1.66                     | 0.77              |
| 23:A:406[A]:CLA:H152 | 29:A:414[A]:PL9:H252 | 1.67                     | 0.76              |
| 25:b:619:BCR:H331    | 25:b:619:BCR:HC8     | 1.69                     | 0.74              |
| 4:d:192[B]:THR:HG23  | 23:d:401[B]:CLA:HBC2 | 1.70                     | 0.73              |
| 23:c:506:CLA:HHC     | 23:c:506:CLA:HBB1    | 1.70                     | 0.73              |
| 23:A:406[B]:CLA:H152 | 29:A:414[B]:PL9:H252 | 1.72                     | 0.72              |
| 23:C:502:CLA:H193    | 23:C:508:CLA:HBB1    | 1.72                     | 0.72              |
| 33:D:707[A]:LHG:H382 | 33:D:707[A]:LHG:H112 | 1.74                     | 0.70              |
| 23:B:605:CLA:HHC     | 23:B:605:CLA:HBB1    | 1.73                     | 0.69              |
| 1:a:253[A]:GLY:HA3   | 2:b:491[A]:VAL:HG12  | 1.74                     | 0.69              |
| 23:C:506:CLA:CMD     | 23:C:508:CLA:HAB     | 2.22                     | 0.69              |
| 13:O:42:ARG:HH12     | 27:O:302:GOL:H12     | 1.55                     | 0.69              |
| 23:A:408:CLA:H193    | 23:C:507:CLA:H101    | 1.75                     | 0.68              |
| 33:D:707[B]:LHG:H382 | 33:D:707[B]:LHG:H112 | 1.75                     | 0.68              |
| 23:a:409:CLA:H192    | 23:c:506:CLA:H142    | 1.76                     | 0.68              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 4:D:85:MET:HE1       | 4:D:96:GLU:HG2       | 1.76                     | 0.68              |
| 3:c:261:ARG:NH1      | 8:i:38:GLU:OE2       | 2.27                     | 0.67              |
| 25:y:101:BCR:H321    | 25:y:101:BCR:HC8     | 1.77                     | 0.67              |
| 3:c:134[B]:ILE:HD13  | 23:c:512:CLA:H43     | 1.76                     | 0.67              |
| 23:c:503:CLA:H61     | 23:c:513:CLA:H42     | 1.74                     | 0.67              |
| 27:a:418:GOL:H32     | 12:m:1:FME:HG3       | 1.77                     | 0.67              |
| 1:a:253[B]:GLY:HA3   | 2:b:491[B]:VAL:HG12  | 1.78                     | 0.66              |
| 23:C:507:CLA:H142    | 36:C:517[A]:DGD:HAF2 | 1.78                     | 0.66              |
| 27:D:701:GOL:O2      | 41:D:801:HOH:O       | 2.13                     | 0.66              |
| 2:B:357[B]:ARG:NH2   | 4:D:337:GLU:O        | 2.26                     | 0.65              |
| 29:A:414[A]:PL9:H262 | 33:E:101[A]:LHG:H223 | 1.80                     | 0.64              |
| 23:a:409:CLA:H152    | 23:c:507:CLA:H142    | 1.80                     | 0.64              |
| 34:z:101:LMG:H302    | 34:z:101:LMG:H141    | 1.80                     | 0.64              |
| 4:d:85:MET:HE1       | 4:d:96:GLU:HG2       | 1.80                     | 0.63              |
| 25:Y:101:BCR:H321    | 25:Y:101:BCR:HC8     | 1.81                     | 0.63              |
| 3:c:213:LEU:HD13     | 23:c:507:CLA:H202    | 1.80                     | 0.63              |
| 16:v:78:ASN:OD1      | 16:v:96:ARG:NH1      | 2.29                     | 0.63              |
| 4:D:123:ILE:HD11     | 36:H:102:DGD:HAH2    | 1.80                     | 0.62              |
| 23:b:605:CLA:HHC     | 23:b:605:CLA:HBB1    | 1.80                     | 0.62              |
| 29:A:414[B]:PL9:H262 | 33:E:101[B]:LHG:H223 | 1.79                     | 0.62              |
| 23:c:512:CLA:H191    | 34:z:101:LMG:H241    | 1.80                     | 0.62              |
| 2:b:482[A]:ILE:HD12  | 2:b:486[A]:LEU:HD12  | 1.82                     | 0.62              |
| 10:K:17:ILE:H        | 10:K:17:ILE:HD13     | 1.65                     | 0.62              |
| 23:C:506:CLA:HHC     | 23:C:506:CLA:HBB1    | 1.82                     | 0.62              |
| 23:C:511:CLA:H192    | 23:C:511:CLA:HBC3    | 1.80                     | 0.62              |
| 26:a:411[B]:SQD:H141 | 33:d:406[B]:LHG:H152 | 1.80                     | 0.61              |
| 3:C:325:GLY:O        | 15:U:51:LYS:NZ       | 2.30                     | 0.60              |
| 3:c:78:GLU:OE2       | 16:v:106:ASN:ND2     | 2.34                     | 0.60              |
| 26:a:411[B]:SQD:H152 | 33:d:406[B]:LHG:H172 | 1.84                     | 0.60              |
| 16:v:134[A]:LYS:HE2  | 27:v:202[A]:GOL:H32  | 1.83                     | 0.60              |
| 10:k:23:ASP:OD2      | 18:y:21:GLN:NE2      | 2.34                     | 0.60              |
| 4:D:85:MET:HE2       | 4:D:90:LEU:HD21      | 1.84                     | 0.59              |
| 23:b:601:CLA:H72     | 23:b:601:CLA:H2      | 1.82                     | 0.59              |
| 23:C:514:CLA:H202    | 34:C:521:LMG:H402    | 1.83                     | 0.59              |
| 1:A:102:LEU:HD12     | 35:b:625:HTG:H61     | 1.85                     | 0.59              |
| 23:B:615:CLA:H2      | 23:B:616:CLA:HBB2    | 1.83                     | 0.59              |
| 2:b:98:LEU:HB2       | 35:b:622:HTG:H7'1    | 1.84                     | 0.59              |
| 23:c:506:CLA:CMD     | 23:c:508:CLA:HAB     | 2.33                     | 0.59              |
| 10:k:17:ILE:HD13     | 10:k:17:ILE:H        | 1.67                     | 0.59              |
| 23:c:506:CLA:HMD1    | 23:c:508:CLA:HAB     | 1.85                     | 0.59              |
| 23:C:507:CLA:H142    | 36:C:517[B]:DGD:HAF2 | 1.83                     | 0.59              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:a:406[A]:CLA:HHC  | 23:a:406[A]:CLA:HBB1 | 1.85                     | 0.58              |
| 27:a:419:GOL:O2      | 41:a:501:HOH:O       | 2.09                     | 0.58              |
| 26:a:411[A]:SQD:H152 | 33:d:406[A]:LHG:H172 | 1.86                     | 0.58              |
| 27:a:419:GOL:O3      | 14:t:2:GLU:OE1       | 2.21                     | 0.58              |
| 2:b:285:ASN:O        | 2:b:289:GLN:HG2      | 2.03                     | 0.58              |
| 1:a:334[B]:ARG:NH2   | 41:a:503[B]:HOH:O    | 2.37                     | 0.58              |
| 2:B:226:TYR:HA       | 2:B:231:MET:HG3      | 1.84                     | 0.58              |
| 34:c:520:LMG:H181    | 10:k:27:VAL:HG11     | 1.85                     | 0.58              |
| 15:U:86[B]:GLU:H     | 15:U:86[B]:GLU:CD    | 2.12                     | 0.58              |
| 13:O:169:ASP:H       | 27:O:303:GOL:H12     | 1.67                     | 0.58              |
| 1:a:221[B]:SER:HB2   | 4:d:139[B]:ARG:O     | 2.03                     | 0.57              |
| 27:a:419:GOL:H11     | 12:m:1:FME:HE3       | 1.86                     | 0.57              |
| 32:e:101:LMT:H6'1    | 6:f:43:ILE:HG12      | 1.85                     | 0.57              |
| 23:C:502:CLA:C3D     | 23:C:504:CLA:H2      | 2.34                     | 0.57              |
| 23:C:509:CLA:HBC3    | 23:C:511:CLA:H71     | 1.85                     | 0.57              |
| 32:A:418:LMT:H71     | 2:b:39:LEU:HD13      | 1.87                     | 0.57              |
| 23:a:405[B]:CLA:H201 | 33:d:405[B]:LHG:H161 | 1.86                     | 0.56              |
| 23:c:502:CLA:C4D     | 23:c:504:CLA:H2      | 2.36                     | 0.56              |
| 1:a:221[A]:SER:HB2   | 4:d:139[A]:ARG:O     | 2.06                     | 0.56              |
| 26:a:411[A]:SQD:H141 | 33:d:406[A]:LHG:H152 | 1.86                     | 0.56              |
| 12:M:33:GLN:HB2      | 12:m:33:GLN:HG3      | 1.87                     | 0.56              |
| 19:z:9:LEU:HD13      | 19:z:54:VAL:HG11     | 1.87                     | 0.56              |
| 1:A:188[B]:ALA:HB2   | 1:A:328[B]:MET:HB2   | 1.88                     | 0.56              |
| 1:a:160[B]:ILE:HD11  | 36:c:517[B]:DGD:HBT1 | 1.88                     | 0.56              |
| 2:b:216:HIS:HE1      | 23:b:609:CLA:C1A     | 2.18                     | 0.56              |
| 23:B:616:CLA:HED2    | 23:B:616:CLA:H43     | 1.88                     | 0.55              |
| 4:D:24:ARG:HD3       | 17:X:37:VAL:HG22     | 1.86                     | 0.55              |
| 2:b:482[B]:ILE:HD12  | 2:b:486[B]:LEU:HD12  | 1.89                     | 0.55              |
| 33:d:405[B]:LHG:HC62 | 11:l:15[B]:THR:HG23  | 1.89                     | 0.55              |
| 32:B:629:LMT:H52     | 35:o:301:HTG:H4'1    | 1.87                     | 0.55              |
| 3:c:134[B]:ILE:HD11  | 23:c:512:CLA:H71     | 1.88                     | 0.55              |
| 2:B:224:ARG:HD3      | 7:H:25:TRP:CE2       | 2.42                     | 0.54              |
| 1:A:84[B]:PRO:HA     | 1:A:112[B]:TYR:CG    | 2.42                     | 0.54              |
| 23:C:502:CLA:C4D     | 23:C:504:CLA:H2      | 2.37                     | 0.54              |
| 3:c:338[B]:GLY:HA3   | 3:c:341[B]:LEU:O     | 2.07                     | 0.54              |
| 27:c:526[B]:GOL:O1   | 41:c:601[B]:HOH:O    | 2.18                     | 0.54              |
| 1:A:82[B]:VAL:HB     | 1:A:174[B]:LEU:HB2   | 1.87                     | 0.54              |
| 23:a:407[A]:CLA:H191 | 33:a:420[A]:LHG:H111 | 1.88                     | 0.54              |
| 2:b:224:ARG:HD3      | 7:h:25:TRP:CE2       | 2.42                     | 0.54              |
| 29:A:414[B]:PL9:H253 | 23:D:702[B]:CLA:H141 | 1.88                     | 0.54              |
| 1:a:183[B]:MET:HA    | 23:a:405[B]:CLA:HMD1 | 1.90                     | 0.54              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 4:D:323[A]:GLU:O     | 27:D:712:GOL:O2      | 2.26                     | 0.54              |
| 1:a:183[A]:MET:HA    | 23:a:405[A]:CLA:HMD1 | 1.90                     | 0.54              |
| 24:a:416[B]:PHO:HBC3 | 4:d:279:LEU:HD22     | 1.89                     | 0.54              |
| 27:l:102[A]:GOL:H32  | 14:t:25:GLU:HB2      | 1.89                     | 0.54              |
| 5:E:77:GLU:O         | 5:E:81:GLU:HG2       | 2.08                     | 0.53              |
| 2:B:299:GLU:HG3      | 2:B:402:TYR:HD1      | 1.73                     | 0.53              |
| 3:c:338[A]:GLY:HA3   | 3:c:341[A]:LEU:O     | 2.08                     | 0.53              |
| 1:A:227[B]:THR:HB    | 1:A:231:GLU:HG3      | 1.91                     | 0.53              |
| 25:b:619:BCR:H331    | 25:b:619:BCR:C8      | 2.35                     | 0.53              |
| 15:u:10[A]:VAL:HG12  | 41:u:245:HOH:O       | 2.08                     | 0.53              |
| 23:A:405[B]:CLA:HHC  | 23:A:405[B]:CLA:HBB1 | 1.91                     | 0.53              |
| 23:B:613:CLA:HBB1    | 23:B:613:CLA:HMB1    | 1.91                     | 0.53              |
| 4:D:192[A]:THR:HG23  | 23:D:702[A]:CLA:HBC2 | 1.90                     | 0.53              |
| 2:B:383[A]:PHE:CZ    | 13:O:167:GLY:HA2     | 2.44                     | 0.53              |
| 4:D:85:MET:CE        | 4:D:96:GLU:HG2       | 2.39                     | 0.53              |
| 4:D:192[B]:THR:HG23  | 23:D:702[B]:CLA:HBC2 | 1.91                     | 0.53              |
| 24:A:407[B]:PHO:HAB  | 4:D:205[B]:LEU:HD13  | 1.90                     | 0.53              |
| 25:T:102:BCR:H19C    | 25:b:618:BCR:H363    | 1.91                     | 0.53              |
| 19:Z:32:ASP:OD2      | 19:Z:35:ARG:HB3      | 2.09                     | 0.53              |
| 17:X:31:ILE:HD11     | 26:X:101:SQD:H102    | 1.89                     | 0.52              |
| 23:b:609:CLA:HMD1    | 7:h:27:THR:HB        | 1.90                     | 0.52              |
| 29:d:404[B]:PL9:H401 | 33:d:405[B]:LHG:H223 | 1.91                     | 0.52              |
| 6:f:41:GLN:OE1       | 9:j:30:GLY:HA3       | 2.09                     | 0.52              |
| 24:A:417[B]:PHO:H3A  | 23:D:702[B]:CLA:H142 | 1.92                     | 0.52              |
| 25:T:102:BCR:H321    | 25:T:102:BCR:HC8     | 1.92                     | 0.52              |
| 29:a:414[B]:PL9:H28  | 33:a:420[B]:LHG:H222 | 1.92                     | 0.52              |
| 36:c:517[B]:DGD:HG11 | 41:c:605[B]:HOH:O    | 2.09                     | 0.52              |
| 33:A:419[B]:LHG:H361 | 23:B:613:CLA:H51     | 1.92                     | 0.52              |
| 2:B:216:HIS:HE1      | 23:B:609:CLA:C1A     | 2.22                     | 0.52              |
| 23:C:504:CLA:HBB1    | 23:C:513:CLA:H41     | 1.90                     | 0.52              |
| 1:a:188[A]:ALA:HB2   | 1:a:328[A]:MET:HB2   | 1.92                     | 0.52              |
| 2:b:383[B]:PHE:CZ    | 13:o:167:GLY:HA2     | 2.44                     | 0.52              |
| 23:b:604:CLA:H42     | 23:b:605:CLA:H2      | 1.91                     | 0.52              |
| 23:b:613:CLA:HBB1    | 23:b:613:CLA:HMB1    | 1.91                     | 0.52              |
| 3:c:42:LEU:HD21      | 23:c:512:CLA:H2A     | 1.92                     | 0.52              |
| 32:B:630:LMT:H6E     | 32:t:101:LMT:H6D     | 1.92                     | 0.51              |
| 1:a:84[A]:PRO:HA     | 1:a:112[A]:TYR:CG    | 2.45                     | 0.51              |
| 23:a:407[B]:CLA:H191 | 33:a:420[B]:LHG:H111 | 1.91                     | 0.51              |
| 3:c:406:SER:HA       | 3:c:420[B]:VAL:HG23  | 1.92                     | 0.51              |
| 19:Z:4:LEU:HD22      | 19:Z:57:LEU:HD11     | 1.91                     | 0.51              |
| 24:A:407[A]:PHO:HAB  | 4:D:205[A]:LEU:HD13  | 1.91                     | 0.51              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:A:84[A]:PRO:HA     | 1:A:112[A]:TYR:CG    | 2.46                     | 0.51              |
| 2:B:224:ARG:HD3      | 7:H:25:TRP:CD2       | 2.45                     | 0.51              |
| 23:a:406[B]:CLA:HBB1 | 23:a:406[B]:CLA:HHC  | 1.93                     | 0.51              |
| 29:a:414[A]:PL9:H28  | 33:a:420[A]:LHG:H222 | 1.92                     | 0.51              |
| 23:b:606:CLA:H72     | 25:b:619:BCR:HC7     | 1.93                     | 0.51              |
| 2:b:144:PHE:CE1      | 2:b:210:ILE:HG23     | 2.46                     | 0.51              |
| 23:B:615:CLA:H2      | 23:B:616:CLA:CBB     | 2.41                     | 0.51              |
| 23:c:514:CLA:HBB1    | 25:c:515:BCR:H24C    | 1.93                     | 0.51              |
| 3:c:279:LEU:HD22     | 23:c:510:CLA:HED2    | 1.92                     | 0.50              |
| 2:B:70:GLY:HA2       | 2:B:178:VAL:HG21     | 1.92                     | 0.50              |
| 33:d:406[B]:LHG:H342 | 33:d:406[B]:LHG:H151 | 1.93                     | 0.50              |
| 18:y:20:ALA:O        | 18:y:24:MET:HG2      | 2.12                     | 0.50              |
| 29:A:414[A]:PL9:H253 | 23:D:702[A]:CLA:H141 | 1.92                     | 0.50              |
| 4:d:244[B]:TYR:OH    | 4:d:264[B]:LYS:HE3   | 2.11                     | 0.50              |
| 33:d:405[A]:LHG:HC62 | 11:l:15[A]:THR:HG23  | 1.94                     | 0.50              |
| 26:A:410[B]:SQD:H361 | 10:K:34:ALA:HA       | 1.93                     | 0.50              |
| 33:a:420[A]:LHG:HC31 | 5:e:9:PRO:HA         | 1.92                     | 0.50              |
| 25:h:101:BCR:H331    | 25:h:101:BCR:C8      | 2.41                     | 0.50              |
| 25:B:618:BCR:H363    | 25:t:102:BCR:H19C    | 1.92                     | 0.50              |
| 15:u:58:VAL:HG12     | 15:u:79:LEU:HD22     | 1.93                     | 0.50              |
| 3:c:286:ALA:HB2      | 23:c:503:CLA:HMD1    | 1.94                     | 0.50              |
| 12:m:5[B]:GLN:H      | 12:m:5[B]:GLN:NE2    | 2.10                     | 0.50              |
| 26:a:411[A]:SQD:H321 | 23:c:509:CLA:H102    | 1.94                     | 0.49              |
| 2:B:383[B]:PHE:CZ    | 13:O:167:GLY:HA2     | 2.47                     | 0.49              |
| 3:C:203:THR:O        | 3:C:235:GLY:HA3      | 2.12                     | 0.49              |
| 4:D:323[B]:GLU:O     | 27:D:712:GOL:O2      | 2.30                     | 0.49              |
| 1:a:227[B]:THR:HB    | 1:a:231:GLU:HG3      | 1.94                     | 0.49              |
| 1:A:133:LEU:HD23     | 4:D:256[A]:ILE:HG12  | 1.95                     | 0.49              |
| 13:O:40:ILE:HD12     | 13:O:95:PHE:CD1      | 2.47                     | 0.49              |
| 29:a:414[A]:PL9:H351 | 6:f:25:THR:OG1       | 2.12                     | 0.49              |
| 41:E:204:HOH:O       | 9:J:6:ARG:HG3        | 2.12                     | 0.49              |
| 1:a:84[B]:PRO:HA     | 1:a:112[B]:TYR:CG    | 2.48                     | 0.49              |
| 33:A:419[A]:LHG:H361 | 23:B:613:CLA:H51     | 1.93                     | 0.49              |
| 2:b:379:ALA:HA       | 2:b:390:TYR:HB3      | 1.94                     | 0.49              |
| 4:d:85:MET:CE        | 4:d:96:GLU:HG2       | 2.41                     | 0.49              |
| 13:o:205:ASP:OD2     | 13:o:207:ARG:NH2     | 2.46                     | 0.49              |
| 23:a:405[A]:CLA:H201 | 33:d:405[A]:LHG:H161 | 1.95                     | 0.49              |
| 16:v:126:LEU:HB3     | 16:v:129:LYS:HB2     | 1.93                     | 0.49              |
| 3:C:95:LEU:HD21      | 23:C:502:CLA:OBD     | 2.13                     | 0.49              |
| 23:c:505:CLA:H62     | 36:c:519:DGD:HB62    | 1.95                     | 0.49              |
| 3:C:42:LEU:HD21      | 23:C:512:CLA:H2A     | 1.95                     | 0.49              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 13:O:42:ARG:O        | 13:O:241:ALA:HA      | 2.13                     | 0.49              |
| 1:a:192[B]:ILE:HG13  | 1:a:293[B]:MET:HE1   | 1.95                     | 0.49              |
| 33:a:420[B]:LHG:HC31 | 5:e:9:PRO:HA         | 1.93                     | 0.49              |
| 26:a:411[B]:SQD:H321 | 23:c:509:CLA:H102    | 1.95                     | 0.48              |
| 4:D:103:ARG:HG3      | 5:E:73:LYS:HG3       | 1.94                     | 0.48              |
| 2:b:173:GLY:HA3      | 2:b:265:ILE:HD11     | 1.95                     | 0.48              |
| 33:d:406[A]:LHG:H331 | 33:d:406[A]:LHG:H361 | 1.55                     | 0.48              |
| 12:m:5[B]:GLN:H      | 12:m:5[B]:GLN:CD     | 2.19                     | 0.48              |
| 23:B:615:CLA:H71     | 23:B:616:CLA:H172    | 1.94                     | 0.48              |
| 27:O:303:GOL:O1      | 41:O:401:HOH:O       | 2.20                     | 0.48              |
| 23:B:602:CLA:H203    | 23:B:602:CLA:H162    | 1.66                     | 0.48              |
| 3:C:174:LEU:HB3      | 23:C:503:CLA:H152    | 1.96                     | 0.48              |
| 25:t:102:BCR:H382    | 25:t:102:BCR:H23C    | 1.95                     | 0.48              |
| 3:C:406:SER:HA       | 3:C:420[B]:VAL:HG23  | 1.95                     | 0.48              |
| 4:D:317[B]:LYS:NZ    | 41:D:812[B]:HOH:O    | 2.47                     | 0.48              |
| 33:D:707[A]:LHG:H382 | 33:D:707[A]:LHG:H132 | 1.96                     | 0.48              |
| 2:B:24:LEU:HD21      | 23:B:616:CLA:CAB     | 2.42                     | 0.48              |
| 13:O:25:THR:O        | 13:O:27:ARG:N        | 2.47                     | 0.48              |
| 2:B:357[A]:ARG:HD2   | 41:B:736:HOH:O       | 2.12                     | 0.48              |
| 23:B:606:CLA:H202    | 26:a:412:SQD:H302    | 1.96                     | 0.48              |
| 33:D:707[B]:LHG:H382 | 33:D:707[B]:LHG:H132 | 1.96                     | 0.48              |
| 23:b:605:CLA:H41     | 23:b:605:CLA:H62     | 1.55                     | 0.48              |
| 33:d:406[A]:LHG:H122 | 33:d:406[A]:LHG:C38  | 2.44                     | 0.48              |
| 25:T:102:BCR:H351    | 26:b:620:SQD:H211    | 1.96                     | 0.48              |
| 4:d:194:ASN:HA       | 4:d:295[B]:SER:OG    | 2.14                     | 0.48              |
| 2:b:491[B]:VAL:HG13  | 4:d:136[B]:VAL:HG13  | 1.96                     | 0.47              |
| 33:d:406[B]:LHG:H122 | 33:d:406[B]:LHG:C38  | 2.44                     | 0.47              |
| 23:A:405[A]:CLA:H203 | 23:A:405[A]:CLA:H162 | 1.74                     | 0.47              |
| 23:B:615:CLA:HHC     | 23:B:615:CLA:HBB1    | 1.96                     | 0.47              |
| 2:b:233:ASN:O        | 2:b:236:THR:HG22     | 2.14                     | 0.47              |
| 1:A:240[A]:GLY:HA3   | 14:T:29[A]:ILE:HG23  | 1.96                     | 0.47              |
| 3:C:41:ARG:NH1       | 23:C:512:CLA:HMD1    | 2.29                     | 0.47              |
| 5:E:12:ASP:OD1       | 9:J:4:GLY:HA3        | 2.15                     | 0.47              |
| 3:c:363:GLY:O        | 3:c:367:GLU:HG2      | 2.14                     | 0.47              |
| 2:B:58:GLN:C         | 2:B:329:PRO:HB3      | 2.39                     | 0.47              |
| 23:C:511:CLA:H52     | 33:D:707[B]:LHG:H371 | 1.95                     | 0.47              |
| 4:D:49:LEU:HD13      | 25:D:704:BCR:C15     | 2.44                     | 0.47              |
| 13:O:137:THR:C       | 13:O:139:SER:H       | 2.23                     | 0.47              |
| 1:a:160[A]:ILE:HD11  | 36:c:517[A]:DGD:HBT1 | 1.96                     | 0.47              |
| 20:R:18:TRP:O        | 20:R:22:ASN:ND2      | 2.39                     | 0.47              |
| 2:B:498:LYS:HE3      | 4:D:20:ASP:HA        | 1.95                     | 0.47              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 4:D:88:SER:HB2       | 5:E:69:ARG:CZ        | 2.44                     | 0.47              |
| 8:I:35:LYS:O         | 8:I:37:LEU:N         | 2.47                     | 0.47              |
| 23:a:406[B]:CLA:HBA1 | 23:a:406[B]:CLA:C4A  | 2.43                     | 0.47              |
| 26:A:410[A]:SQD:H152 | 26:A:410[A]:SQD:H122 | 1.54                     | 0.47              |
| 1:a:217[B]:SER:O     | 1:a:221[B]:SER:HB3   | 2.15                     | 0.47              |
| 2:b:36:SER:OG        | 25:b:618:BCR:H362    | 2.15                     | 0.47              |
| 3:c:26:ARG:NH2       | 18:y:46:LEU:OXT      | 2.37                     | 0.47              |
| 1:A:240[B]:GLY:HA3   | 14:T:29[B]:ILE:HG23  | 1.97                     | 0.47              |
| 23:B:613:CLA:H162    | 23:B:613:CLA:H121    | 1.60                     | 0.47              |
| 23:C:511:CLA:H112    | 23:C:511:CLA:H152    | 1.45                     | 0.47              |
| 10:K:26:PRO:O        | 10:K:29:PRO:HD2      | 2.15                     | 0.47              |
| 25:b:617:BCR:H24C    | 25:b:617:BCR:H371    | 1.69                     | 0.47              |
| 1:A:214[A]:MET:HE2   | 1:A:255[A]:PHE:CE1   | 2.49                     | 0.47              |
| 36:c:519:DGD:HBH2    | 33:d:406[B]:LHG:H211 | 1.97                     | 0.47              |
| 4:D:180:ARG:HD3      | 4:D:180:ARG:C        | 2.40                     | 0.47              |
| 23:a:405[B]:CLA:H203 | 23:a:405[B]:CLA:H162 | 1.77                     | 0.47              |
| 33:d:406[A]:LHG:H332 | 33:d:406[A]:LHG:H302 | 1.77                     | 0.47              |
| 1:A:272[B]:HIS:CD2   | 4:D:218[B]:VAL:HG21  | 2.50                     | 0.46              |
| 29:a:414[B]:PL9:H171 | 29:a:414[B]:PL9:H151 | 1.53                     | 0.46              |
| 2:b:314:TYR:CE2      | 2:b:316:GLY:HA3      | 2.50                     | 0.46              |
| 13:o:138:THR:HG23    | 41:o:401:HOH:O       | 2.14                     | 0.46              |
| 3:C:279:LEU:HD12     | 3:C:282:MET:HE3      | 1.98                     | 0.46              |
| 23:C:506:CLA:H93     | 23:C:506:CLA:H111    | 1.72                     | 0.46              |
| 1:a:192[A]:ILE:HG13  | 1:a:293[A]:MET:HE1   | 1.97                     | 0.46              |
| 26:B:620:SQD:H1      | 26:B:620:SQD:H462    | 1.97                     | 0.46              |
| 23:b:606:CLA:H122    | 23:b:606:CLA:H162    | 1.82                     | 0.46              |
| 3:C:261:ARG:NH1      | 8:I:38:GLU:OE2       | 2.48                     | 0.46              |
| 6:F:21:VAL:O         | 6:F:25:THR:HG23      | 2.15                     | 0.46              |
| 29:a:414[A]:PL9:H151 | 29:a:414[A]:PL9:H171 | 1.57                     | 0.46              |
| 27:a:418:GOL:H12     | 41:t:201:HOH:O       | 2.15                     | 0.46              |
| 2:b:422:ARG:NH2      | 13:o:169:ASP:OD2     | 2.41                     | 0.46              |
| 3:c:27:ASP:HB3       | 10:k:46:ARG:HG3      | 1.98                     | 0.46              |
| 11:l:20:GLY:O        | 11:l:24:ILE:HG12     | 2.14                     | 0.46              |
| 23:B:609:CLA:HHC     | 23:B:609:CLA:HBB1    | 1.96                     | 0.46              |
| 3:C:443[B]:TRP:CE2   | 23:C:509:CLA:HMD2    | 2.51                     | 0.46              |
| 25:K:102:BCR:H24C    | 25:K:102:BCR:H371    | 1.71                     | 0.46              |
| 2:b:160:GLY:HA3      | 2:b:180:PRO:HB3      | 1.97                     | 0.46              |
| 4:d:103:ARG:HG3      | 5:e:73:LYS:HG3       | 1.96                     | 0.46              |
| 36:h:102:DGD:HB62    | 36:h:102:DGD:HB32    | 1.80                     | 0.46              |
| 4:D:283:ALA:O        | 4:D:287:VAL:HG23     | 2.16                     | 0.46              |
| 1:a:93[A]:PHE:CD2    | 1:a:95:PRO:HD3       | 2.51                     | 0.46              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:A:404[B]:CLA:HBB1 | 23:A:404[B]:CLA:HMB3 | 1.98                     | 0.46              |
| 26:A:410[B]:SQD:H122 | 26:A:410[B]:SQD:H152 | 1.60                     | 0.46              |
| 2:B:482[B]:ILE:HD12  | 2:B:486[B]:LEU:HD22  | 1.97                     | 0.46              |
| 3:C:334[B]:PRO:HA    | 13:O:153:THR:OG1     | 2.16                     | 0.46              |
| 23:C:506:CLA:HMD3    | 23:C:508:CLA:HAB     | 1.96                     | 0.46              |
| 23:a:409:CLA:H203    | 23:c:507:CLA:H101    | 1.97                     | 0.46              |
| 3:c:443[B]:TRP:CE2   | 23:c:509:CLA:HMD2    | 2.51                     | 0.46              |
| 34:c:521:LMG:H232    | 34:c:521:LMG:H391    | 1.98                     | 0.46              |
| 19:Z:33:TRP:HZ2      | 34:Z:101:LMG:HC61    | 1.81                     | 0.46              |
| 2:b:243:ALA:HA       | 2:b:246:PHE:CE2      | 2.51                     | 0.46              |
| 27:b:628:GOL:O3      | 27:b:628:GOL:O1      | 2.25                     | 0.46              |
| 9:j:6:ARG:NH1        | 9:j:6:ARG:HA         | 2.30                     | 0.46              |
| 29:A:414[B]:PL9:H322 | 29:A:414[B]:PL9:H301 | 1.75                     | 0.46              |
| 2:B:36[B]:SER:OG     | 25:B:618:BCR:H362    | 2.16                     | 0.46              |
| 23:C:502:CLA:HHC     | 23:C:502:CLA:HBB1    | 1.97                     | 0.46              |
| 13:O:58:ASN:HD21     | 13:O:61:GLN:HG3      | 1.80                     | 0.46              |
| 15:U:58:VAL:HG12     | 15:U:79:LEU:HD22     | 1.96                     | 0.46              |
| 2:B:341:LYS:NZ       | 35:B:622:HTG:O2      | 2.31                     | 0.45              |
| 2:B:422:ARG:O        | 2:B:425:ILE:HG12     | 2.16                     | 0.45              |
| 23:B:615:CLA:H172    | 23:B:615:CLA:H13     | 1.78                     | 0.45              |
| 13:O:130:GLN:H       | 13:O:130:GLN:CD      | 2.22                     | 0.45              |
| 23:a:406[A]:CLA:HBA1 | 23:a:406[A]:CLA:C4A  | 2.45                     | 0.45              |
| 3:c:391[B]:ARG:NH2   | 41:c:610:HOH:O       | 2.48                     | 0.45              |
| 14:t:2:GLU:HG2       | 14:t:3:THR:N         | 2.31                     | 0.45              |
| 3:C:275:SER:HB3      | 23:C:510:CLA:HED3    | 1.97                     | 0.45              |
| 33:E:101[A]:LHG:O2   | 6:F:19:ARG:NH1       | 2.49                     | 0.45              |
| 24:a:416[A]:PHO:HBC3 | 4:d:279:LEU:HD22     | 1.97                     | 0.45              |
| 1:A:133:LEU:HD23     | 4:D:256[B]:ILE:HG12  | 1.99                     | 0.45              |
| 5:E:18:ARG:H         | 9:J:2:SER:N          | 2.14                     | 0.45              |
| 23:A:408:CLA:H18     | 23:C:506:CLA:H142    | 1.98                     | 0.45              |
| 32:T:101:LMT:H2'     | 34:m:101:LMG:HC5     | 1.98                     | 0.45              |
| 15:U:45:LEU:HD21     | 15:U:71:GLN:HB3      | 1.98                     | 0.45              |
| 29:A:414[A]:PL9:H472 | 4:D:39:PRO:HD3       | 1.99                     | 0.45              |
| 29:A:414[B]:PL9:H171 | 29:A:414[B]:PL9:H151 | 1.50                     | 0.45              |
| 2:b:224:ARG:HH21     | 32:b:621:LMT:H1'     | 1.81                     | 0.45              |
| 23:c:513:CLA:H121    | 23:c:514:CLA:H142    | 1.99                     | 0.45              |
| 29:A:414[A]:PL9:H503 | 26:X:101:SQD:H341    | 1.98                     | 0.45              |
| 3:C:230:LEU:HD23     | 3:C:230:LEU:HA       | 1.81                     | 0.45              |
| 23:C:502:CLA:H42     | 23:C:503:CLA:HMD3    | 1.99                     | 0.45              |
| 1:a:214[B]:MET:HB3   | 29:a:414[B]:PL9:H103 | 1.97                     | 0.45              |
| 3:c:215:LYS:HD3      | 3:c:221:GLU:O        | 2.17                     | 0.45              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 33:d:406[B]:LHG:H331 | 33:d:406[B]:LHG:H361 | 1.53                     | 0.45              |
| 5:e:57:ALA:HB3       | 5:e:60:GLN:HG2       | 1.99                     | 0.45              |
| 13:O:51:LEU:HD12     | 13:O:234:LYS:HG2     | 1.97                     | 0.45              |
| 23:b:612:CLA:HBB1    | 23:b:612:CLA:HMB1    | 1.99                     | 0.45              |
| 23:b:615:CLA:H91     | 23:b:615:CLA:H112    | 1.73                     | 0.45              |
| 3:c:176:VAL:HG21     | 3:c:238:ILE:HG13     | 1.99                     | 0.45              |
| 5:e:14:ILE:HD12      | 9:j:12:VAL:HG11      | 1.99                     | 0.45              |
| 2:B:314:TYR:CE2      | 2:B:316:GLY:HA3      | 2.52                     | 0.45              |
| 26:a:411[A]:SQD:H271 | 33:d:406[A]:LHG:H141 | 1.98                     | 0.45              |
| 2:b:70:GLY:HA2       | 2:b:178:VAL:HG21     | 1.98                     | 0.45              |
| 33:d:406[A]:LHG:H342 | 33:d:406[A]:LHG:H151 | 1.99                     | 0.45              |
| 25:A:409:BCR:H24C    | 25:A:409:BCR:H371    | 1.75                     | 0.45              |
| 2:B:247:PHE:CE2      | 23:B:602:CLA:H102    | 2.52                     | 0.45              |
| 5:E:56:TYR:HA        | 5:E:60:GLN:HE21      | 1.81                     | 0.45              |
| 2:b:245:VAL:HG22     | 23:b:612:CLA:H202    | 1.99                     | 0.45              |
| 2:b:363:PHE:HB3      | 2:b:365:SER:O        | 2.17                     | 0.45              |
| 25:d:403:BCR:H15C    | 25:d:403:BCR:H351    | 1.78                     | 0.45              |
| 26:f:102:SQD:O7      | 26:f:102:SQD:H462    | 2.17                     | 0.45              |
| 1:A:85[B]:SER:HA     | 1:A:109[B]:GLY:HA3   | 1.99                     | 0.45              |
| 5:E:40:THR:HB        | 20:R:4:ARG:HG2       | 1.98                     | 0.45              |
| 1:a:214[A]:MET:HE2   | 1:a:255[A]:PHE:CE1   | 2.52                     | 0.45              |
| 25:t:102:BCR:HC7     | 25:t:102:BCR:H331    | 1.68                     | 0.45              |
| 3:C:130:VAL:O        | 3:C:134:ILE:HG12     | 2.17                     | 0.44              |
| 13:O:66:VAL:HG21     | 13:O:110:MET:HE3     | 1.98                     | 0.44              |
| 16:V:41:HIS:CD2      | 40:V:201:HEC:NB      | 2.85                     | 0.44              |
| 23:b:609:CLA:NC      | 25:h:101:BCR:H332    | 2.32                     | 0.44              |
| 4:d:286:VAL:HG21     | 23:d:401[A]:CLA:HED2 | 1.99                     | 0.44              |
| 18:Y:23:THR:HB       | 18:Y:24:MET:HE2      | 2.00                     | 0.44              |
| 2:b:413:ASP:O        | 2:b:417:VAL:HG23     | 2.17                     | 0.44              |
| 13:o:58:ASN:HD22     | 13:o:61:GLN:HG3      | 1.81                     | 0.44              |
| 23:a:405[A]:CLA:H203 | 23:a:405[A]:CLA:H162 | 1.80                     | 0.44              |
| 23:b:613:CLA:H18     | 33:d:412[B]:LHG:H201 | 1.99                     | 0.44              |
| 23:b:614:CLA:H112    | 23:b:614:CLA:H72     | 1.66                     | 0.44              |
| 16:v:45[B]:ILE:HD13  | 27:v:202[B]:GOL:H11  | 1.99                     | 0.44              |
| 1:A:227[A]:THR:HB    | 1:A:231:GLU:HG3      | 1.98                     | 0.44              |
| 32:A:420:LMT:O3'     | 32:A:420:LMT:H6'2    | 2.18                     | 0.44              |
| 23:C:507:CLA:H18     | 23:C:507:CLA:H152    | 1.49                     | 0.44              |
| 36:C:519:DGD:HBE2    | 36:C:519:DGD:HB81    | 1.89                     | 0.44              |
| 4:D:261[A]:PHE:CZ    | 33:D:706[A]:LHG:HC81 | 2.52                     | 0.44              |
| 23:c:509:CLA:H18     | 36:c:518[A]:DGD:HAT2 | 1.98                     | 0.44              |
| 4:d:266[A]:TRP:CD1   | 33:d:405[A]:LHG:HC31 | 2.52                     | 0.44              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 32:t:101:LMT:H112    | 32:t:101:LMT:H81     | 1.55                     | 0.44              |
| 18:y:30:ILE:HD12     | 18:y:30:ILE:HA       | 1.92                     | 0.44              |
| 1:A:160[B]:ILE:HD11  | 36:C:517[B]:DGD:HBT2 | 2.00                     | 0.44              |
| 25:T:102:BCR:H24C    | 25:T:102:BCR:H371    | 1.82                     | 0.44              |
| 2:b:497:GLN:HB2      | 2:b:504:THR:HB       | 1.98                     | 0.44              |
| 25:k:101:BCR:H371    | 25:k:101:BCR:H24C    | 1.69                     | 0.44              |
| 33:E:101[A]:LHG:H241 | 33:E:101[A]:LHG:HC61 | 1.85                     | 0.44              |
| 1:a:227[A]:THR:HB    | 1:a:231:GLU:HG3      | 1.98                     | 0.44              |
| 33:a:420[B]:LHG:H241 | 33:a:420[B]:LHG:HC61 | 1.87                     | 0.44              |
| 7:h:38:PHE:HB2       | 25:h:101:BCR:C10     | 2.47                     | 0.44              |
| 9:j:8:PRO:HG2        | 9:j:11:ILE:HD12      | 1.98                     | 0.44              |
| 13:o:58:ASN:C        | 13:o:60:ARG:H        | 2.25                     | 0.44              |
| 4:D:261[B]:PHE:CZ    | 33:D:706[B]:LHG:HC81 | 2.53                     | 0.44              |
| 3:c:406:SER:HA       | 3:c:420[A]:VAL:HG23  | 2.00                     | 0.44              |
| 23:c:502:CLA:C3D     | 23:c:504:CLA:H2      | 2.48                     | 0.44              |
| 1:A:192[B]:ILE:HG13  | 1:A:293[B]:MET:HE1   | 2.00                     | 0.44              |
| 29:A:414[A]:PL9:H322 | 29:A:414[A]:PL9:H301 | 1.77                     | 0.44              |
| 3:C:240:ILE:HD13     | 3:C:240:ILE:HA       | 1.90                     | 0.44              |
| 23:C:505:CLA:H41     | 23:C:505:CLA:H62     | 1.70                     | 0.44              |
| 27:D:701:GOL:H31     | 12:M:1:FME:HE3       | 1.98                     | 0.44              |
| 10:K:24:VAL:HG13     | 18:Y:25:ILE:HD13     | 1.99                     | 0.44              |
| 33:A:419[A]:LHG:H252 | 2:B:464:PHE:CZ       | 2.53                     | 0.44              |
| 1:a:131:TRP:CH2      | 23:c:506:CLA:HAA2    | 2.53                     | 0.44              |
| 2:b:243:ALA:HA       | 2:b:246:PHE:CD2      | 2.53                     | 0.44              |
| 23:d:401[A]:CLA:HAA2 | 23:d:401[A]:CLA:HBD  | 2.00                     | 0.44              |
| 26:B:620:SQD:H381    | 32:m:103:LMT:H121    | 2.00                     | 0.43              |
| 23:C:511:CLA:H52     | 33:D:707[A]:LHG:H371 | 1.98                     | 0.43              |
| 25:C:516:BCR:H371    | 25:C:516:BCR:H24C    | 1.71                     | 0.43              |
| 1:a:214[B]:MET:HE2   | 1:a:255[B]:PHE:CE1   | 2.52                     | 0.43              |
| 3:c:38:GLY:HA3       | 23:c:512:CLA:HMD2    | 1.99                     | 0.43              |
| 36:c:517[A]:DGD:HG11 | 41:c:605[A]:HOH:O    | 2.18                     | 0.43              |
| 4:d:54:PHE:HB3       | 5:e:47:PHE:CD2       | 2.52                     | 0.43              |
| 23:B:610:CLA:H122    | 23:B:615:CLA:HAA1    | 2.00                     | 0.43              |
| 4:D:230[A]:SER:HB2   | 41:D:861:HOH:O       | 2.17                     | 0.43              |
| 1:a:188[B]:ALA:HB2   | 1:a:328[B]:MET:HB2   | 1.99                     | 0.43              |
| 3:c:225:VAL:HG13     | 3:c:289:PHE:HA       | 1.99                     | 0.43              |
| 18:y:22:LEU:HA       | 18:y:25:ILE:HG22     | 1.99                     | 0.43              |
| 34:Z:101:LMG:H141    | 34:Z:101:LMG:H111    | 1.77                     | 0.43              |
| 2:B:357[A]:ARG:HH12  | 27:B:623:GOL:C3      | 2.30                     | 0.43              |
| 25:B:619:BCR:H24C    | 25:B:619:BCR:H371    | 1.72                     | 0.43              |
| 1:a:105:TRP:CE2      | 1:a:110[A]:GLY:HA3   | 2.53                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 29:a:414[A]:PL9:H503 | 17:x:24:THR:OG1      | 2.18                     | 0.43              |
| 4:d:332[A]:GLN:NE2   | 41:d:504:HOH:O       | 2.50                     | 0.43              |
| 5:e:68:ASP:O         | 5:e:72:ALA:HB2       | 2.18                     | 0.43              |
| 25:B:617:BCR:H11C    | 25:B:617:BCR:H341    | 1.89                     | 0.43              |
| 25:C:515:BCR:H20C    | 25:C:515:BCR:H361    | 1.85                     | 0.43              |
| 4:D:264[B]:LYS:NZ    | 41:D:817[B]:HOH:O    | 2.51                     | 0.43              |
| 5:E:9:PRO:HA         | 33:E:101[A]:LHG:HC31 | 2.00                     | 0.43              |
| 8:I:33:LYS:HB3       | 8:I:34:ARG:H         | 1.65                     | 0.43              |
| 23:c:513:CLA:H142    | 23:c:513:CLA:H111    | 1.89                     | 0.43              |
| 23:A:404[A]:CLA:H143 | 24:A:407[A]:PHO:H61  | 2.01                     | 0.43              |
| 23:A:408:CLA:H41     | 23:A:408:CLA:H61     | 1.63                     | 0.43              |
| 24:A:417[B]:PHO:HBC3 | 4:D:279:LEU:HD22     | 2.00                     | 0.43              |
| 4:D:210[B]:LEU:HA    | 4:D:213[B]:ILE:HG22  | 2.00                     | 0.43              |
| 4:D:230[B]:SER:HB2   | 41:D:861:HOH:O       | 2.17                     | 0.43              |
| 33:E:101[B]:LHG:H241 | 33:E:101[B]:LHG:HC61 | 1.77                     | 0.43              |
| 2:b:216:HIS:CE1      | 23:b:609:CLA:NA      | 2.86                     | 0.43              |
| 33:d:406[A]:LHG:H242 | 33:d:406[A]:LHG:H272 | 1.86                     | 0.43              |
| 13:o:216:GLU:CD      | 13:o:234:LYS:HD2     | 2.43                     | 0.43              |
| 33:D:706[A]:LHG:HC62 | 11:L:15[A]:THR:HG23  | 2.00                     | 0.43              |
| 1:a:334[B]:ARG:HD3   | 4:d:320[B]:LEU:HD13  | 2.00                     | 0.43              |
| 19:Z:31:GLN:CD       | 19:Z:31:GLN:H        | 2.26                     | 0.43              |
| 1:A:183[B]:MET:HA    | 23:A:404[B]:CLA:HMD1 | 2.00                     | 0.43              |
| 23:A:404[A]:CLA:HBB1 | 23:A:404[A]:CLA:HMB3 | 2.01                     | 0.43              |
| 2:B:357[A]:ARG:HH12  | 27:B:623:GOL:H32     | 1.83                     | 0.43              |
| 23:C:503:CLA:HBD     | 23:C:503:CLA:HAA1    | 2.01                     | 0.43              |
| 23:C:506:CLA:HAA1    | 23:C:506:CLA:HBD     | 2.00                     | 0.43              |
| 36:C:517[A]:DGD:HG11 | 41:C:601[A]:HOH:O    | 2.18                     | 0.43              |
| 36:C:518[A]:DGD:HAT1 | 36:C:519:DGD:HBE1    | 2.00                     | 0.43              |
| 5:E:20:TRP:CD1       | 9:J:7:ILE:HD12       | 2.54                     | 0.43              |
| 6:F:41:GLN:OE1       | 9:J:30:GLY:HA3       | 2.18                     | 0.43              |
| 1:a:15:GLU:HG3       | 32:a:417:LMT:O4'     | 2.19                     | 0.43              |
| 1:a:185[B]:VAL:O     | 1:a:189[B]:GLU:HG3   | 2.19                     | 0.43              |
| 25:a:410:BCR:H24C    | 25:a:410:BCR:H371    | 1.73                     | 0.43              |
| 3:c:152:LYS:HD2      | 41:c:742:HOH:O       | 2.16                     | 0.43              |
| 26:a:412:SQD:H1      | 41:a:623:HOH:O       | 2.18                     | 0.43              |
| 33:b:629[B]:LHG:H112 | 4:d:273[B]:PHE:CZ    | 2.54                     | 0.43              |
| 3:c:240:ILE:HD13     | 3:c:240:ILE:HA       | 1.77                     | 0.43              |
| 3:c:325:GLY:O        | 15:u:51:LYS:NZ       | 2.49                     | 0.43              |
| 4:d:12:ARG:NE        | 4:d:12:ARG:HA        | 2.34                     | 0.43              |
| 23:A:405[A]:CLA:HHC  | 23:A:405[A]:CLA:HBB1 | 2.01                     | 0.43              |
| 29:A:414[B]:PL9:HC8  | 29:A:414[B]:PL9:HC2  | 1.76                     | 0.43              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 24:A:417[A]:PHO:H3A  | 23:D:702[A]:CLA:H142 | 1.99                     | 0.43              |
| 2:B:30:VAL:HG12      | 23:B:605:CLA:HHD     | 2.00                     | 0.43              |
| 3:C:391[B]:ARG:HA    | 3:C:391[B]:ARG:HD3   | 1.81                     | 0.43              |
| 4:d:12:ARG:HA        | 4:d:12:ARG:HE        | 1.84                     | 0.43              |
| 2:b:383[A]:PHE:CZ    | 13:o:167:GLY:HA2     | 2.53                     | 0.43              |
| 26:b:620:SQD:H341    | 26:b:620:SQD:H311    | 1.70                     | 0.43              |
| 25:d:403:BCR:C8      | 25:d:403:BCR:H331    | 2.49                     | 0.43              |
| 10:k:20:PRO:HB3      | 18:y:21:GLN:HG3      | 2.01                     | 0.43              |
| 1:A:131:TRP:CD2      | 1:A:131:TRP:C        | 2.95                     | 0.42              |
| 34:B:621:LMG:H112    | 34:B:621:LMG:H141    | 1.84                     | 0.42              |
| 25:C:516:BCR:H11C    | 25:C:516:BCR:H341    | 1.90                     | 0.42              |
| 24:a:408[B]:PHO:HAB  | 4:d:205[B]:LEU:HD13  | 2.00                     | 0.42              |
| 2:b:491[A]:VAL:HG13  | 4:d:136[A]:VAL:HG13  | 2.02                     | 0.42              |
| 2:B:363:PHE:HB3      | 2:B:365:SER:O        | 2.18                     | 0.42              |
| 23:B:601:CLA:H92     | 23:B:601:CLA:H62     | 1.88                     | 0.42              |
| 4:D:191:TRP:CE3      | 4:D:289:LEU:HD11     | 2.53                     | 0.42              |
| 16:V:126:LEU:HB3     | 16:V:129:LYS:HB2     | 2.01                     | 0.42              |
| 33:a:420[A]:LHG:H241 | 33:a:420[A]:LHG:HC61 | 1.89                     | 0.42              |
| 23:b:615:CLA:H92     | 23:b:615:CLA:H61     | 1.74                     | 0.42              |
| 4:d:14:TRP:CD1       | 35:d:409:HTG:H61     | 2.53                     | 0.42              |
| 25:h:101:BCR:H24C    | 25:h:101:BCR:H371    | 1.71                     | 0.42              |
| 3:C:157:MET:HE2      | 3:C:157:MET:HA       | 2.00                     | 0.42              |
| 3:C:443[A]:TRP:CE2   | 23:C:509:CLA:HMD2    | 2.53                     | 0.42              |
| 4:D:292:ASN:O        | 4:D:294:ARG:HG3      | 2.18                     | 0.42              |
| 13:O:110:MET:HE2     | 13:O:110:MET:HB3     | 1.92                     | 0.42              |
| 1:a:261[B]:GLN:HG3   | 2:b:493[B]:TRP:CH2   | 2.55                     | 0.42              |
| 33:d:406[B]:LHG:H242 | 33:d:406[B]:LHG:H272 | 1.89                     | 0.42              |
| 10:k:19:ASP:HB3      | 10:k:20:PRO:HD3      | 2.00                     | 0.42              |
| 25:t:102:BCR:H11C    | 25:t:102:BCR:H341    | 1.87                     | 0.42              |
| 29:A:414[A]:PL9:H171 | 29:A:414[A]:PL9:H151 | 1.53                     | 0.42              |
| 23:B:614:CLA:HAA1    | 23:B:614:CLA:HBD     | 2.02                     | 0.42              |
| 15:U:53:ALA:HB1      | 15:U:54:PRO:HA       | 2.01                     | 0.42              |
| 1:a:105:TRP:CE2      | 1:a:110[B]:GLY:HA3   | 2.54                     | 0.42              |
| 1:a:162[B]:PRO:HB3   | 1:a:168[B]:PHE:HA    | 2.02                     | 0.42              |
| 23:c:505:CLA:H151    | 23:c:509:CLA:H143    | 2.02                     | 0.42              |
| 23:c:505:CLA:ND      | 36:c:518[A]:DGD:HB32 | 2.35                     | 0.42              |
| 23:c:513:CLA:HMB2    | 23:c:513:CLA:H192    | 2.01                     | 0.42              |
| 19:z:26:ALA:HB1      | 19:z:36:SER:HB3      | 2.00                     | 0.42              |
| 3:C:338[A]:GLY:HA3   | 3:C:341[A]:LEU:O     | 2.20                     | 0.42              |
| 23:C:509:CLA:H142    | 23:C:509:CLA:H111    | 1.83                     | 0.42              |
| 23:C:510:CLA:H192    | 23:C:510:CLA:H162    | 1.83                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 23:C:514:CLA:H161    | 34:C:521:LMG:H421    | 2.01                     | 0.42              |
| 27:D:701:GOL:H12     | 14:T:2:GLU:OE1       | 2.19                     | 0.42              |
| 23:b:611:CLA:H72     | 23:b:611:CLA:H112    | 1.84                     | 0.42              |
| 3:c:146:PHE:HZ       | 23:c:513:CLA:HBB2    | 1.84                     | 0.42              |
| 25:c:515:BCR:H351    | 25:c:515:BCR:H15C    | 1.77                     | 0.42              |
| 27:l:102[B]:GOL:H32  | 14:t:25:GLU:HB2      | 2.00                     | 0.42              |
| 20:R:8:VAL:O         | 20:R:11:PRO:HD2      | 2.20                     | 0.42              |
| 3:C:75:PHE:HZ        | 3:C:105:VAL:HG21     | 1.84                     | 0.42              |
| 3:C:334[A]:PRO:HA    | 13:O:153:THR:OG1     | 2.19                     | 0.42              |
| 3:C:443[B]:TRP:CD2   | 23:C:509:CLA:HMD2    | 2.54                     | 0.42              |
| 36:C:517[B]:DGD:HG11 | 41:C:601[B]:HOH:O    | 2.18                     | 0.42              |
| 33:D:707[A]:LHG:H332 | 33:D:707[A]:LHG:H302 | 1.85                     | 0.42              |
| 11:L:9:PRO:HA        | 32:m:103:LMT:H6D     | 2.01                     | 0.42              |
| 12:M:25:LEU:HD23     | 12:M:25:LEU:HA       | 1.85                     | 0.42              |
| 23:b:605:CLA:HAA1    | 23:b:605:CLA:HBD     | 2.01                     | 0.42              |
| 3:c:168:LEU:HD23     | 3:c:168:LEU:HA       | 1.89                     | 0.42              |
| 1:A:70:SER:O         | 1:A:75:ASN:HB2       | 2.19                     | 0.42              |
| 1:A:183[A]:MET:HA    | 23:A:404[A]:CLA:HMD1 | 2.01                     | 0.42              |
| 24:A:417[A]:PHO:HBC3 | 4:D:279:LEU:HD22     | 2.02                     | 0.42              |
| 13:O:23:ASP:OD1      | 13:O:24:ASP:N        | 2.52                     | 0.42              |
| 1:a:230:THR:HG21     | 11:l:8:GLN:HE22      | 1.85                     | 0.42              |
| 23:a:405[B]:CLA:H122 | 23:a:405[B]:CLA:H161 | 1.89                     | 0.42              |
| 2:b:149[B]:LEU:HD11  | 23:b:604:CLA:H122    | 2.02                     | 0.42              |
| 4:d:191:TRP:CE3      | 4:d:289:LEU:HD11     | 2.55                     | 0.42              |
| 16:v:41:HIS:HA       | 16:v:45[A]:ILE:O     | 2.20                     | 0.42              |
| 23:B:605:CLA:HAA1    | 23:B:605:CLA:HBD     | 2.02                     | 0.42              |
| 1:a:213[B]:ALA:HB2   | 4:d:275[B]:PRO:HG2   | 2.02                     | 0.42              |
| 1:a:296[B]:ASN:HB2   | 3:c:400[B]:PRO:O     | 2.19                     | 0.42              |
| 23:a:407[B]:CLA:HMB2 | 23:d:401[B]:CLA:H122 | 2.02                     | 0.42              |
| 2:b:358:ARG:HB2      | 27:b:628:GOL:H31     | 2.02                     | 0.42              |
| 23:b:606:CLA:H151    | 23:b:616:CLA:H112    | 2.00                     | 0.42              |
| 25:c:515:BCR:H11C    | 25:c:515:BCR:H341    | 1.78                     | 0.42              |
| 36:h:102:DGD:HB61    | 36:h:102:DGD:HB91    | 1.81                     | 0.42              |
| 23:A:405[A]:CLA:HBA1 | 23:A:405[A]:CLA:C4A  | 2.50                     | 0.42              |
| 23:C:503:CLA:H151    | 23:C:504:CLA:HMB2    | 2.01                     | 0.42              |
| 33:D:707[A]:LHG:H382 | 33:D:707[A]:LHG:C11  | 2.45                     | 0.42              |
| 5:E:57:ALA:HB3       | 5:E:60:GLN:HG2       | 2.02                     | 0.42              |
| 1:a:261[B]:GLN:HG3   | 2:b:493[B]:TRP:CZ3   | 2.54                     | 0.42              |
| 2:b:98:LEU:HB2       | 35:b:622:HTG:C7'     | 2.50                     | 0.42              |
| 2:b:216:HIS:CE1      | 23:b:609:CLA:C1A     | 3.02                     | 0.42              |
| 25:b:618:BCR:C8      | 25:b:618:BCR:H331    | 2.50                     | 0.42              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 2:B:497:GLN:HB2      | 17:X:37:VAL:HG13     | 2.02                     | 0.41              |
| 3:C:286:ALA:HB2      | 23:C:503:CLA:HMD2    | 2.01                     | 0.41              |
| 16:V:72:LEU:HD23     | 16:V:72:LEU:HA       | 1.93                     | 0.41              |
| 23:a:405[B]:CLA:CBD  | 23:a:406[B]:CLA:HAC2 | 2.50                     | 0.41              |
| 23:a:407[A]:CLA:H203 | 34:d:410:LMG:H412    | 2.01                     | 0.41              |
| 7:h:43:LEU:O         | 7:h:47:GLU:HG3       | 2.20                     | 0.41              |
| 25:y:101:BCR:H15C    | 25:y:101:BCR:H351    | 1.92                     | 0.41              |
| 1:A:105:TRP:CE2      | 1:A:110[A]:GLY:HA3   | 2.56                     | 0.41              |
| 23:A:404[A]:CLA:H192 | 23:A:404[A]:CLA:H161 | 1.80                     | 0.41              |
| 26:A:412:SQD:H222    | 26:A:412:SQD:H192    | 1.77                     | 0.41              |
| 33:D:707[A]:LHG:H362 | 33:D:707[A]:LHG:H331 | 1.86                     | 0.41              |
| 2:b:161:LEU:HD12     | 2:b:161:LEU:HA       | 1.83                     | 0.41              |
| 2:b:229:LEU:HD23     | 2:b:229:LEU:HA       | 1.91                     | 0.41              |
| 23:b:607:CLA:H42     | 34:m:101:LMG:H311    | 2.01                     | 0.41              |
| 3:c:169:GLY:O        | 3:c:173:LEU:HG       | 2.19                     | 0.41              |
| 29:A:414[B]:PL9:H221 | 29:A:414[B]:PL9:H201 | 1.88                     | 0.41              |
| 3:C:223:TRP:CG       | 3:C:224:ILE:H        | 2.38                     | 0.41              |
| 1:a:261[A]:GLN:HG3   | 2:b:493[A]:TRP:CH2   | 2.56                     | 0.41              |
| 26:a:411[B]:SQD:H302 | 23:c:509:CLA:H71     | 2.02                     | 0.41              |
| 23:d:402:CLA:H162    | 7:h:37:LEU:HD21      | 2.02                     | 0.41              |
| 2:B:188:ASP:OD2      | 2:B:194:ASN:ND2      | 2.46                     | 0.41              |
| 33:D:707[B]:LHG:H382 | 33:D:707[B]:LHG:C11  | 2.47                     | 0.41              |
| 8:I:2:GLU:O          | 8:I:6:ILE:HG12       | 2.20                     | 0.41              |
| 1:a:214[A]:MET:HB3   | 29:a:414[A]:PL9:H103 | 2.01                     | 0.41              |
| 24:a:416[A]:PHO:H42  | 24:a:416[A]:PHO:H11  | 1.92                     | 0.41              |
| 23:b:602:CLA:H111    | 23:b:602:CLA:H91     | 1.89                     | 0.41              |
| 26:A:410[A]:SQD:H361 | 10:K:34:ALA:HA       | 2.03                     | 0.41              |
| 29:A:414[B]:PL9:H451 | 17:X:28:LEU:HD11     | 2.01                     | 0.41              |
| 35:B:624:HTG:H61     | 1:a:102:LEU:HD12     | 2.01                     | 0.41              |
| 3:C:135:ARG:HA       | 3:C:135:ARG:HD2      | 1.95                     | 0.41              |
| 4:D:190:ASN:HB2      | 4:D:296:TYR:CD1      | 2.56                     | 0.41              |
| 13:O:39[B]:ARG:NH1   | 13:O:244:GLU:OE2     | 2.51                     | 0.41              |
| 1:a:307:ILE:HG22     | 1:a:313:VAL:HA       | 2.01                     | 0.41              |
| 2:b:154:GLY:O        | 2:b:159:THR:HG23     | 2.21                     | 0.41              |
| 2:b:224:ARG:HD3      | 7:h:25:TRP:CD2       | 2.56                     | 0.41              |
| 3:c:158:THR:O        | 3:c:251:HIS:HB3      | 2.20                     | 0.41              |
| 4:d:148[A]:ALA:HB3   | 4:d:149[A]:PRO:HD3   | 2.03                     | 0.41              |
| 33:d:406[A]:LHG:H142 | 33:d:406[A]:LHG:H372 | 2.03                     | 0.41              |
| 34:d:410:LMG:H392    | 34:d:410:LMG:H362    | 1.94                     | 0.41              |
| 17:x:23:LEU:HD23     | 17:x:23:LEU:HA       | 1.88                     | 0.41              |
| 19:Z:57:LEU:HA       | 19:Z:57:LEU:HD23     | 1.86                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:A:162[B]:PRO:HB3   | 1:A:168[B]:PHE:HA    | 2.02                     | 0.41              |
| 23:A:405[B]:CLA:C4A  | 23:A:405[B]:CLA:HBA1 | 2.49                     | 0.41              |
| 25:B:618:BCR:H15C    | 25:B:618:BCR:H351    | 1.91                     | 0.41              |
| 23:C:508:CLA:H92     | 23:C:508:CLA:H61     | 1.92                     | 0.41              |
| 36:C:518[B]:DGD:HAE2 | 36:C:518[B]:DGD:HA81 | 1.85                     | 0.41              |
| 1:a:93[B]:PHE:CD2    | 1:a:95:PRO:HD3       | 2.54                     | 0.41              |
| 29:a:414[B]:PL9:H351 | 6:f:25:THR:OG1       | 2.19                     | 0.41              |
| 16:v:6:GLU:CD        | 16:v:6:GLU:H         | 2.29                     | 0.41              |
| 1:A:85[A]:SER:HA     | 1:A:109[A]:GLY:HA3   | 2.03                     | 0.41              |
| 1:A:201:GLY:HA3      | 1:A:286[B]:ALA:HB2   | 2.03                     | 0.41              |
| 23:A:404[B]:CLA:CBD  | 23:A:405[B]:CLA:HAC2 | 2.51                     | 0.41              |
| 3:C:146:PHE:HZ       | 23:C:513:CLA:HBB2    | 1.85                     | 0.41              |
| 8:I:36:ASP:OD1       | 8:I:36:ASP:N         | 2.52                     | 0.41              |
| 12:M:20:VAL:HG22     | 12:m:20:VAL:HG11     | 2.02                     | 0.41              |
| 2:b:299:GLU:HG2      | 2:b:402:TYR:HD2      | 1.86                     | 0.41              |
| 25:d:403:BCR:H11C    | 25:d:403:BCR:H341    | 1.99                     | 0.41              |
| 32:B:629:LMT:H21     | 35:o:301:HTG:O2      | 2.21                     | 0.41              |
| 3:C:323:LYS:NZ       | 41:C:603:HOH:O       | 2.35                     | 0.41              |
| 33:E:101[A]:LHG:H291 | 33:E:101[A]:LHG:H261 | 1.75                     | 0.41              |
| 25:T:102:BCR:H331    | 25:T:102:BCR:HC7     | 1.55                     | 0.41              |
| 23:b:615:CLA:H111    | 23:b:615:CLA:H152    | 1.89                     | 0.41              |
| 3:c:162:GLY:HA2      | 3:c:248:GLY:HA2      | 2.02                     | 0.41              |
| 4:d:20:ASP:O         | 4:d:24:ARG:HG2       | 2.21                     | 0.41              |
| 15:u:75:LEU:HD23     | 15:u:75:LEU:HA       | 1.92                     | 0.41              |
| 23:A:408:CLA:H171    | 23:C:507:CLA:H121    | 2.01                     | 0.41              |
| 2:B:298:LEU:HA       | 2:B:298:LEU:HD12     | 1.84                     | 0.41              |
| 2:B:460:LEU:O        | 2:B:463:PHE:HB3      | 2.20                     | 0.41              |
| 23:B:606:CLA:H151    | 23:B:616:CLA:H122    | 2.03                     | 0.41              |
| 25:B:618:BCR:C8      | 25:B:618:BCR:H331    | 2.51                     | 0.41              |
| 4:D:209[A]:LEU:C     | 4:D:209[A]:LEU:HD23  | 2.46                     | 0.41              |
| 13:O:169:ASP:OD1     | 27:O:303:GOL:H12     | 2.21                     | 0.41              |
| 25:T:102:BCR:H11C    | 25:T:102:BCR:H341    | 1.82                     | 0.41              |
| 2:b:298:LEU:HD12     | 2:b:298:LEU:HA       | 1.93                     | 0.41              |
| 23:b:603:CLA:H3A     | 23:b:603:CLA:CGA     | 2.51                     | 0.41              |
| 3:c:128:GLY:HA3      | 23:c:514:CLA:C3C     | 2.51                     | 0.41              |
| 3:c:163:PHE:CD1      | 3:c:252:ILE:HD11     | 2.56                     | 0.41              |
| 3:c:182:PHE:HA       | 35:c:522:HTG:H61     | 2.03                     | 0.41              |
| 23:d:402:CLA:H61     | 23:d:402:CLA:H41     | 1.69                     | 0.41              |
| 33:d:412[B]:LHG:H211 | 12:m:18:PRO:HG3      | 2.03                     | 0.41              |
| 23:B:606:CLA:H161    | 23:B:606:CLA:H122    | 1.87                     | 0.41              |
| 23:C:509:CLA:H122    | 23:C:509:CLA:H162    | 1.88                     | 0.41              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 32:M:101:LMT:H6D     | 11:l:9:PRO:HA        | 2.03                     | 0.41              |
| 23:b:613:CLA:H203    | 23:b:613:CLA:H161    | 1.92                     | 0.41              |
| 3:c:344[B]:SER:O     | 13:o:75:THR:HG22     | 2.21                     | 0.41              |
| 19:z:37:LYS:HE2      | 19:z:41:PHE:HE2      | 1.86                     | 0.41              |
| 1:A:243[A]:GLU:CD    | 1:A:243[A]:GLU:H     | 2.27                     | 0.40              |
| 23:A:404[A]:CLA:CBD  | 23:A:405[A]:CLA:HAC2 | 2.51                     | 0.40              |
| 35:B:622:HTG:H7'3    | 35:B:622:HTG:H4'2    | 1.94                     | 0.40              |
| 3:C:406:SER:HA       | 3:C:420[A]:VAL:HG23  | 2.02                     | 0.40              |
| 13:O:93:LEU:O        | 13:O:128:SER:HA      | 2.20                     | 0.40              |
| 3:c:203:THR:O        | 3:c:235:GLY:HA3      | 2.21                     | 0.40              |
| 23:c:509:CLA:H18     | 36:c:518[B]:DGD:HAT2 | 2.03                     | 0.40              |
| 4:d:148[B]:ALA:HB3   | 4:d:149[B]:PRO:HD3   | 2.03                     | 0.40              |
| 13:o:92:SER:HB3      | 13:o:131:PRO:HA      | 2.02                     | 0.40              |
| 20:R:24:LEU:N        | 20:R:25:PRO:HD2      | 2.35                     | 0.40              |
| 23:A:404[B]:CLA:H192 | 23:A:404[B]:CLA:H161 | 1.81                     | 0.40              |
| 29:A:414[A]:PL9:H121 | 29:A:414[A]:PL9:HC8  | 1.78                     | 0.40              |
| 2:B:91:TRP:HE1       | 30:B:625:UNL:C10     | 2.34                     | 0.40              |
| 23:B:612:CLA:HMB1    | 23:B:612:CLA:HBB1    | 2.03                     | 0.40              |
| 23:a:407[B]:CLA:H203 | 34:d:410:LMG:H412    | 2.01                     | 0.40              |
| 25:c:516:BCR:H20C    | 25:c:516:BCR:H361    | 1.98                     | 0.40              |
| 13:o:42:ARG:O        | 13:o:241:ALA:HA      | 2.22                     | 0.40              |
| 1:A:159[B]:LEU:C     | 1:A:162[B]:PRO:HD2   | 2.46                     | 0.40              |
| 25:H:101:BCR:H24C    | 25:H:101:BCR:H371    | 1.80                     | 0.40              |
| 2:b:58:GLN:C         | 2:b:329:PRO:HB3      | 2.46                     | 0.40              |
| 2:b:413:ASP:HA       | 2:b:414:PRO:HD3      | 1.95                     | 0.40              |
| 23:c:513:CLA:H122    | 23:c:513:CLA:H162    | 1.81                     | 0.40              |
| 33:d:406[B]:LHG:H332 | 33:d:406[B]:LHG:H302 | 1.73                     | 0.40              |
| 16:v:63:THR:HA       | 16:v:64:PRO:HA       | 1.94                     | 0.40              |
| 29:A:414[A]:PL9:HC8  | 29:A:414[A]:PL9:HC2  | 1.71                     | 0.40              |
| 2:B:348:ASN:HB3      | 2:B:354:LEU:HD11     | 2.04                     | 0.40              |
| 13:O:27:ARG:NH1      | 13:O:203:LYS:HG2     | 2.36                     | 0.40              |
| 2:b:12:LEU:HB2       | 23:b:612:CLA:HMC2    | 2.03                     | 0.40              |
| 25:b:619:BCR:HC7     | 25:b:619:BCR:H311    | 1.63                     | 0.40              |
| 3:c:31:SER:CB        | 3:c:41:ARG:HG2       | 2.51                     | 0.40              |
| 3:c:443[A]:TRP:CE2   | 23:c:509:CLA:HMD2    | 2.55                     | 0.40              |
| 23:c:509:CLA:H162    | 23:c:509:CLA:H122    | 1.73                     | 0.40              |
| 13:o:120:PHE:CD1     | 13:o:235:ILE:HD13    | 2.56                     | 0.40              |
| 29:A:414[A]:PL9:H221 | 29:A:414[A]:PL9:H201 | 1.86                     | 0.40              |
| 2:B:201:HIS:HB2      | 23:B:602:CLA:C1B     | 2.52                     | 0.40              |
| 23:B:615:CLA:H91     | 23:B:615:CLA:H112    | 1.86                     | 0.40              |
| 36:C:518[A]:DGD:HAE2 | 36:C:518[A]:DGD:HA81 | 1.86                     | 0.40              |

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| Atom-1            | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------------|--------------------------|-------------------|
| 4:D:194:ASN:HA    | 4:D:295[B]:SER:OG    | 2.21                     | 0.40              |
| 1:a:309:ALA:HB3   | 16:v:1:ALA:O         | 2.21                     | 0.40              |
| 23:a:409:CLA:H102 | 23:a:409:CLA:H61     | 1.84                     | 0.40              |
| 36:c:519:DGD:HBH2 | 33:d:406[A]:LHG:H211 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 553/344 (161%) | 546 (99%) | 5 (1%)  | 2 (0%)   | 30          | 38  |
| 1   | a     | 551/344 (160%) | 544 (99%) | 5 (1%)  | 2 (0%)   | 30          | 38  |
| 2   | B     | 524/505 (104%) | 514 (98%) | 10 (2%) | 0        | 100         | 100 |
| 2   | b     | 521/505 (103%) | 510 (98%) | 11 (2%) | 0        | 100         | 100 |
| 3   | C     | 548/455 (120%) | 539 (98%) | 8 (2%)  | 1 (0%)   | 43          | 55  |
| 3   | c     | 554/455 (122%) | 542 (98%) | 11 (2%) | 1 (0%)   | 43          | 55  |
| 4   | D     | 454/342 (133%) | 437 (96%) | 17 (4%) | 0        | 100         | 100 |
| 4   | d     | 457/342 (134%) | 445 (97%) | 12 (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%)    | 61 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 7   | h     | 63/65 (97%)    | 58 (92%)  | 4 (6%)  | 1 (2%)   | 7           | 7   |
| 8   | I     | 36/38 (95%)    | 34 (94%)  | 1 (3%)  | 1 (3%)   | 4           | 2   |
| 8   | i     | 36/38 (95%)    | 32 (89%)  | 4 (11%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 9   | J     | 36/39 (92%)      | 33 (92%)   | 3 (8%)   | 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%)      | 34 (97%)   | 1 (3%)   | 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%)   | 244 (98%)  | 5 (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     | 99/104 (95%)     | 96 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 16  | V     | 140/137 (102%)   | 137 (98%)  | 3 (2%)   | 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%)      | 25 (93%)   | 2 (7%)   | 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   | 6180/5384 (115%) | 6040 (98%) | 128 (2%) | 12 (0%)  | 43          | 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  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 7   | h     | 63     | LYS  |
| 13  | O     | 138    | THR  |
| 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%) | 442 (100%) | 2 (0%)   | 81          | 90  |
| 1   | a     | 442/279 (158%) | 441 (100%) | 1 (0%)   | 87          | 94  |
| 2   | B     | 423/403 (105%) | 420 (99%)  | 3 (1%)   | 76          | 87  |
| 2   | b     | 420/403 (104%) | 410 (98%)  | 10 (2%)  | 43          | 62  |
| 3   | C     | 431/356 (121%) | 421 (98%)  | 10 (2%)  | 44          | 63  |
| 3   | c     | 437/356 (123%) | 430 (98%)  | 7 (2%)   | 55          | 73  |
| 4   | D     | 368/277 (133%) | 365 (99%)  | 3 (1%)   | 73          | 86  |
| 4   | d     | 372/277 (134%) | 368 (99%)  | 4 (1%)   | 65          | 81  |
| 5   | E     | 72/73 (99%)    | 70 (97%)   | 2 (3%)   | 38          | 56  |
| 5   | e     | 72/73 (99%)    | 71 (99%)   | 1 (1%)   | 59          | 76  |
| 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%)   | 30          | 45  |
| 7   | h     | 55/54 (102%)   | 54 (98%)   | 1 (2%)   | 51          | 70  |
| 8   | I     | 34/34 (100%)   | 32 (94%)   | 2 (6%)   | 18          | 26  |
| 8   | i     | 34/34 (100%)   | 33 (97%)   | 1 (3%)   | 37          | 55  |
| 9   | J     | 26/27 (96%)    | 23 (88%)   | 3 (12%)  | 5           | 6   |
| 9   | j     | 26/27 (96%)    | 25 (96%)   | 1 (4%)   | 29          | 44  |
| 10  | K     | 30/30 (100%)   | 26 (87%)   | 4 (13%)  | 4           | 4   |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 10  | k     | 30/30 (100%)     | 27 (90%)   | 3 (10%)  | 7           | 9   |
| 11  | L     | 36/35 (103%)     | 36 (100%)  | 0        | 100         | 100 |
| 11  | l     | 36/35 (103%)     | 35 (97%)   | 1 (3%)   | 38          | 56  |
| 12  | M     | 30/32 (94%)      | 28 (93%)   | 2 (7%)   | 15          | 21  |
| 12  | m     | 32/32 (100%)     | 30 (94%)   | 2 (6%)   | 16          | 23  |
| 13  | O     | 216/207 (104%)   | 211 (98%)  | 5 (2%)   | 44          | 63  |
| 13  | o     | 213/207 (103%)   | 206 (97%)  | 7 (3%)   | 33          | 50  |
| 14  | T     | 32/28 (114%)     | 28 (88%)   | 4 (12%)  | 4           | 5   |
| 14  | t     | 31/28 (111%)     | 31 (100%)  | 0        | 100         | 100 |
| 15  | U     | 86/89 (97%)      | 84 (98%)   | 2 (2%)   | 44          | 63  |
| 15  | u     | 88/89 (99%)      | 86 (98%)   | 2 (2%)   | 44          | 63  |
| 16  | V     | 123/117 (105%)   | 122 (99%)  | 1 (1%)   | 73          | 86  |
| 16  | v     | 123/117 (105%)   | 119 (97%)  | 4 (3%)   | 33          | 50  |
| 17  | X     | 32/33 (97%)      | 31 (97%)   | 1 (3%)   | 35          | 52  |
| 17  | x     | 31/33 (94%)      | 31 (100%)  | 0        | 100         | 100 |
| 18  | Y     | 22/23 (96%)      | 22 (100%)  | 0        | 100         | 100 |
| 18  | y     | 22/23 (96%)      | 19 (86%)   | 3 (14%)  | 3           | 4   |
| 19  | Z     | 52/52 (100%)     | 50 (96%)   | 2 (4%)   | 29          | 44  |
| 19  | z     | 52/52 (100%)     | 45 (86%)   | 7 (14%)  | 4           | 4   |
| 20  | R     | 29/29 (100%)     | 27 (93%)   | 2 (7%)   | 14          | 20  |
| All | All   | 5110/4403 (116%) | 5005 (98%) | 105 (2%) | 47          | 66  |

All (105) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 243[A] | GLU  |
| 1   | A     | 243[B] | GLU  |
| 2   | B     | 299    | GLU  |
| 2   | B     | 389    | LYS  |
| 2   | B     | 419    | SER  |
| 3   | C     | 24     | THR  |
| 3   | C     | 29     | GLU  |
| 3   | C     | 30     | SER  |
| 3   | C     | 142    | GLU  |
| 3   | C     | 255    | THR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 3   | C     | 279    | LEU  |
| 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     | 4      | THR  |
| 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     | 7      | ILE  |
| 9   | J     | 9      | LEU  |
| 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  |
| 13  | O     | 49     | THR  |
| 13  | O     | 55     | GLU  |
| 13  | O     | 98[A]  | GLU  |
| 13  | O     | 98[B]  | GLU  |
| 13  | O     | 118    | LEU  |
| 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  |
| 17  | X     | 14     | LEU  |
| 1   | a     | 13     | LEU  |
| 2   | b     | 128    | THR  |
| 2   | b     | 161    | LEU  |
| 2   | b     | 223    | GLN  |
| 2   | b     | 240    | SER  |
| 2   | b     | 245    | VAL  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 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     | 142    | GLU  |
| 3   | c     | 152    | LYS  |
| 3   | c     | 240    | ILE  |
| 3   | c     | 255    | THR  |
| 3   | c     | 289    | PHE  |
| 3   | c     | 315[A] | MET  |
| 3   | c     | 315[B] | MET  |
| 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     | 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     | 106    | ASN  |
| 18  | y     | 18     | VAL  |
| 18  | y     | 19     | ILE  |
| 18  | y     | 45     | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | Z     | 3   | ILE  |
| 19  | Z     | 31  | GLN  |
| 20  | R     | 4   | ARG  |
| 20  | R     | 29  | LYS  |
| 19  | z     | 2   | THR  |
| 19  | z     | 3   | ILE  |
| 19  | z     | 4   | LEU  |
| 19  | z     | 7   | LEU  |
| 19  | z     | 21  | ILE  |
| 19  | z     | 32  | ASP  |
| 19  | z     | 42  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 44  | ASN  |
| 3   | C     | 322 | GLN  |
| 3   | C     | 415 | ASN  |
| 5   | E     | 60  | GLN  |
| 13  | O     | 231 | HIS  |
| 15  | U     | 78  | ASN  |
| 17  | X     | 38  | GLN  |
| 2   | b     | 14  | ASN  |
| 2   | b     | 53  | ASN  |
| 2   | b     | 331 | ASN  |
| 3   | c     | 201 | ASN  |
| 11  | l     | 8   | GLN  |
| 13  | o     | 58  | ASN  |
| 15  | u     | 78  | ASN  |
| 18  | y     | 45  | ASN  |
| 19  | Z     | 31  | 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$ |
| 14  | FME  | T     | 1   | 14   | 8,9,10       | 0.68 | 0           | 8,9,11      | 1.97 | 4 (50%)     |
| 8   | FME  | I     | 1   | 8    | 8,9,10       | 0.55 | 0           | 8,9,11      | 1.15 | 1 (12%)     |
| 14  | FME  | t     | 1   | 14   | 8,9,10       | 0.78 | 0           | 8,9,11      | 1.56 | 2 (25%)     |
| 12  | FME  | m     | 1   | 12   | 8,9,10       | 0.50 | 0           | 8,9,11      | 1.47 | 2 (25%)     |
| 8   | FME  | i     | 1   | 8    | 8,9,10       | 0.71 | 0           | 8,9,11      | 1.26 | 0           |
| 12  | FME  | M     | 1   | 12   | 8,9,10       | 0.66 | 0           | 8,9,11      | 1.24 | 2 (25%)     |

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | T     | 1   | FME  | CB-CA-N | -3.18 | 104.73      | 110.52   |
| 14  | T     | 1   | FME  | CA-N-CN | 2.47  | 126.62      | 122.82   |
| 12  | m     | 1   | FME  | O1-CN-N | -2.47 | 118.93      | 125.32   |
| 14  | t     | 1   | FME  | O-C-CA  | -2.47 | 118.43      | 124.77   |
| 12  | m     | 1   | FME  | CA-N-CN | -2.45 | 119.06      | 122.82   |
| 14  | t     | 1   | FME  | CA-N-CN | -2.41 | 119.12      | 122.82   |
| 12  | M     | 1   | FME  | O-C-CA  | -2.27 | 118.93      | 124.77   |
| 8   | I     | 1   | FME  | O-C-CA  | -2.18 | 119.17      | 124.77   |
| 14  | T     | 1   | FME  | C-CA-N  | 2.16  | 113.67      | 109.50   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 14  | T     | 1   | FME  | CG-CB-CA | 2.15  | 119.44      | 112.87   |
| 12  | M     | 1   | FME  | O1-CN-N  | -2.00 | 120.15      | 125.32   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | m     | 1   | FME  | 2       | 0            |
| 12  | M     | 1   | FME  | 2       | 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 | $\# Z  > 2$ |
| 27  | GOL  | v     | 202[B] | -    | 5,5,5        | 1.12 | 0           | 5,5,5       | 0.91 | 0           |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | CLA  | C     | 504    | -    | 69,73,73     | 1.99 | 19 (27%) | 82,113,113  | 2.76 | 30 (36%) |
| 34  | LMG  | c     | 521    | -    | 51,51,55     | 1.02 | 3 (5%)   | 59,59,63    | 1.38 | 7 (11%)  |
| 23  | CLA  | b     | 615    | -    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.70 | 33 (40%) |
| 34  | LMG  | c     | 520    | -    | 51,51,55     | 0.91 | 2 (3%)   | 59,59,63    | 1.18 | 6 (10%)  |
| 33  | LHG  | D     | 706[A] | -    | 48,48,48     | 0.86 | 3 (6%)   | 51,54,54    | 1.00 | 4 (7%)   |
| 27  | GOL  | C     | 523[A] | -    | 5,5,5        | 1.24 | 0        | 5,5,5       | 0.89 | 0        |
| 25  | BCR  | b     | 617    | -    | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.28 | 5 (8%)   |
| 23  | CLA  | A     | 406[A] | 41   | 69,73,73     | 1.97 | 18 (26%) | 82,113,113  | 2.71 | 33 (40%) |
| 23  | CLA  | C     | 514    | -    | 69,73,73     | 2.01 | 19 (27%) | 82,113,113  | 2.70 | 31 (37%) |
| 24  | PHO  | a     | 416[B] | -    | 58,69,69     | 2.80 | 14 (24%) | 55,99,99    | 2.99 | 15 (27%) |
| 32  | LMT  | F     | 101    | -    | 36,36,36     | 1.03 | 1 (2%)   | 47,47,47    | 1.05 | 3 (6%)   |
| 33  | LHG  | d     | 412[A] | -    | 48,48,48     | 0.90 | 2 (4%)   | 51,54,54    | 1.14 | 5 (9%)   |
| 35  | HTG  | D     | 710    | -    | 16,16,19     | 0.91 | 1 (6%)   | 20,21,24    | 1.33 | 1 (5%)   |
| 33  | LHG  | D     | 707[B] | -    | 48,48,48     | 0.90 | 2 (4%)   | 51,54,54    | 1.03 | 3 (5%)   |
| 32  | LMT  | a     | 417    | -    | 36,36,36     | 0.98 | 1 (2%)   | 47,47,47    | 1.06 | 2 (4%)   |
| 23  | CLA  | C     | 506    | -    | 69,73,73     | 2.03 | 18 (26%) | 82,113,113  | 2.63 | 30 (36%) |
| 23  | CLA  | a     | 407[A] | 41   | 69,73,73     | 1.94 | 19 (27%) | 82,113,113  | 2.70 | 33 (40%) |
| 23  | CLA  | b     | 603    | -    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.84 | 31 (37%) |
| 23  | CLA  | c     | 508    | 41   | 69,73,73     | 1.96 | 18 (26%) | 82,113,113  | 2.70 | 31 (37%) |
| 23  | CLA  | c     | 511    | -    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.73 | 33 (40%) |
| 25  | BCR  | C     | 515    | -    | 41,41,41     | 1.05 | 1 (2%)   | 56,56,56    | 1.50 | 11 (19%) |
| 23  | CLA  | C     | 508    | 41   | 69,73,73     | 1.97 | 19 (27%) | 82,113,113  | 2.64 | 26 (31%) |
| 23  | CLA  | D     | 702[B] | -    | 69,73,73     | 2.00 | 19 (27%) | 82,113,113  | 2.76 | 32 (39%) |
| 32  | LMT  | M     | 101    | -    | 36,36,36     | 1.11 | 4 (11%)  | 47,47,47    | 1.21 | 3 (6%)   |
| 33  | LHG  | d     | 405[B] | -    | 48,48,48     | 0.90 | 2 (4%)   | 51,54,54    | 1.06 | 4 (7%)   |
| 26  | SQD  | A     | 412    | -    | 52,54,54     | 1.01 | 2 (3%)   | 62,65,65    | 1.19 | 7 (11%)  |
| 23  | CLA  | C     | 502    | -    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.74 | 32 (39%) |
| 25  | BCR  | A     | 409    | -    | 41,41,41     | 1.01 | 1 (2%)   | 56,56,56    | 1.35 | 7 (12%)  |
| 36  | DGD  | h     | 102    | -    | 63,63,67     | 0.86 | 3 (4%)   | 77,77,81    | 1.17 | 9 (11%)  |
| 23  | CLA  | B     | 607    | 41   | 69,73,73     | 1.93 | 20 (28%) | 82,113,113  | 2.68 | 33 (40%) |
| 25  | BCR  | K     | 102    | -    | 41,41,41     | 1.06 | 1 (2%)   | 56,56,56    | 1.43 | 10 (17%) |
| 24  | PHO  | a     | 408[A] | -    | 58,69,69     | 2.73 | 11 (18%) | 55,99,99    | 2.83 | 15 (27%) |
| 32  | LMT  | A     | 418    | -    | 36,36,36     | 0.90 | 0        | 47,47,47    | 1.06 | 2 (4%)   |
| 23  | CLA  | B     | 612    | -    | 69,73,73     | 2.01 | 19 (27%) | 82,113,113  | 2.69 | 29 (35%) |
| 23  | CLA  | c     | 510    | -    | 69,73,73     | 2.05 | 18 (26%) | 82,113,113  | 2.70 | 29 (35%) |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 35  | HTG  | B     | 624    | -      | 19,19,19     | 0.93 | 2 (10%)  | 23,24,24    | 1.19 | 4 (17%)  |
| 23  | CLA  | A     | 405[B] | 41     | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.68 | 33 (40%) |
| 28  | OEX  | a     | 413[A] | 41,3,1 | 0,15,15      | -    | -        | -           |      |          |
| 34  | LMG  | C     | 520    | -      | 51,51,55     | 0.96 | 2 (3%)   | 59,59,63    | 1.12 | 5 (8%)   |
| 32  | LMT  | T     | 101    | -      | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 1.09 | 2 (4%)   |
| 32  | LMT  | B     | 629    | -      | 36,36,36     | 0.98 | 3 (8%)   | 47,47,47    | 1.21 | 5 (10%)  |
| 27  | GOL  | B     | 626    | -      | 5,5,5        | 1.16 | 0        | 5,5,5       | 0.98 | 0        |
| 23  | CLA  | C     | 509    | -      | 69,73,73     | 2.04 | 19 (27%) | 82,113,113  | 2.59 | 30 (36%) |
| 35  | HTG  | d     | 409    | -      | 16,16,19     | 0.89 | 1 (6%)   | 20,21,24    | 1.32 | 1 (5%)   |
| 40  | HEC  | V     | 201    | 16     | 46,50,50     | 1.91 | 5 (10%)  | 58,82,82    | 1.73 | 6 (10%)  |
| 27  | GOL  | v     | 202[A] | -      | 5,5,5        | 1.35 | 1 (20%)  | 5,5,5       | 0.77 | 0        |
| 28  | OEX  | A     | 413[B] | 41,3,1 | 0,15,15      | -    | -        | -           |      |          |
| 25  | BCR  | B     | 619    | -      | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.33 | 7 (12%)  |
| 23  | CLA  | B     | 613    | -      | 69,73,73     | 1.95 | 19 (27%) | 82,113,113  | 2.66 | 32 (39%) |
| 33  | LHG  | A     | 419[B] | -      | 48,48,48     | 0.87 | 2 (4%)   | 51,54,54    | 1.20 | 5 (9%)   |
| 33  | LHG  | d     | 406[B] | -      | 48,48,48     | 0.94 | 2 (4%)   | 51,54,54    | 0.97 | 2 (3%)   |
| 23  | CLA  | c     | 504    | -      | 69,73,73     | 2.04 | 19 (27%) | 82,113,113  | 2.75 | 28 (34%) |
| 34  | LMG  | C     | 521    | -      | 51,51,55     | 1.08 | 3 (5%)   | 59,59,63    | 1.36 | 6 (10%)  |
| 29  | PL9  | D     | 705[B] | -      | 55,55,55     | 0.65 | 2 (3%)   | 68,69,69    | 1.67 | 16 (23%) |
| 24  | PHO  | a     | 416[A] | -      | 58,69,69     | 2.76 | 13 (22%) | 55,99,99    | 3.06 | 17 (30%) |
| 25  | BCR  | B     | 617    | -      | 41,41,41     | 1.05 | 1 (2%)   | 56,56,56    | 1.29 | 5 (8%)   |
| 33  | LHG  | L     | 101[B] | -      | 48,48,48     | 0.95 | 3 (6%)   | 51,54,54    | 1.10 | 3 (5%)   |
| 29  | PL9  | A     | 414[B] | -      | 55,55,55     | 0.67 | 3 (5%)   | 68,69,69    | 2.02 | 25 (36%) |
| 27  | GOL  | o     | 303    | -      | 5,5,5        | 1.18 | 0        | 5,5,5       | 0.94 | 0        |
| 23  | CLA  | B     | 605    | -      | 69,73,73     | 2.02 | 19 (27%) | 82,113,113  | 2.77 | 30 (36%) |
| 33  | LHG  | D     | 707[A] | -      | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.01 | 4 (7%)   |
| 35  | HTG  | b     | 623    | -      | 19,19,19     | 1.01 | 1 (5%)   | 23,24,24    | 1.68 | 1 (4%)   |
| 27  | GOL  | l     | 102[B] | -      | 5,5,5        | 0.94 | 0        | 5,5,5       | 1.10 | 0        |
| 33  | LHG  | E     | 101[B] | -      | 41,41,48     | 1.06 | 2 (4%)   | 44,47,54    | 1.12 | 3 (6%)   |
| 38  | HEM  | f     | 101    | 6,5    | 50,50,50     | 1.51 | 7 (14%)  | 67,82,82    | 1.65 | 15 (22%) |
| 32  | LMT  | b     | 627    | -      | 25,25,36     | 0.88 | 1 (4%)   | 30,30,47    | 1.15 | 2 (6%)   |
| 23  | CLA  | D     | 702[A] | -      | 69,73,73     | 1.96 | 18 (26%) | 82,113,113  | 2.75 | 33 (40%) |
| 32  | LMT  | b     | 621    | -      | 25,25,36     | 0.97 | 2 (8%)   | 30,30,47    | 1.20 | 2 (6%)   |
| 33  | LHG  | d     | 405[A] | -      | 48,48,48     | 0.87 | 2 (4%)   | 51,54,54    | 1.09 | 4 (7%)   |
| 23  | CLA  | A     | 408    | -      | 69,73,73     | 1.94 | 20 (28%) | 82,113,113  | 2.80 | 34 (41%) |
| 26  | SQD  | X     | 101    | -      | 41,43,54     | 1.17 | 3 (7%)   | 51,54,65    | 2.20 | 15 (29%) |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 27  | GOL  | c     | 526[B] | -      | 5,5,5        | 0.90 | 0        | 5,5,5       | 1.06 | 0        |
| 23  | CLA  | d     | 402    | -      | 69,73,73     | 2.03 | 19 (27%) | 82,113,113  | 2.75 | 33 (40%) |
| 25  | BCR  | D     | 704    | -      | 41,41,41     | 1.11 | 1 (2%)   | 56,56,56    | 1.99 | 17 (30%) |
| 23  | CLA  | B     | 606    | -      | 69,73,73     | 1.94 | 20 (28%) | 82,113,113  | 2.81 | 33 (40%) |
| 34  | LMG  | B     | 621    | -      | 51,51,55     | 0.93 | 2 (3%)   | 59,59,63    | 1.28 | 4 (6%)   |
| 23  | CLA  | b     | 606    | -      | 69,73,73     | 1.96 | 19 (27%) | 82,113,113  | 2.79 | 33 (40%) |
| 27  | GOL  | a     | 418    | -      | 5,5,5        | 1.30 | 1 (20%)  | 5,5,5       | 1.07 | 0        |
| 25  | BCR  | B     | 618    | -      | 41,41,41     | 0.99 | 1 (2%)   | 56,56,56    | 1.42 | 8 (14%)  |
| 35  | HTG  | b     | 622    | -      | 19,19,19     | 1.21 | 3 (15%)  | 23,24,24    | 1.89 | 8 (34%)  |
| 23  | CLA  | c     | 513    | -      | 69,73,73     | 2.07 | 19 (27%) | 82,113,113  | 2.68 | 32 (39%) |
| 27  | GOL  | c     | 527    | -      | 5,5,5        | 1.26 | 1 (20%)  | 5,5,5       | 0.98 | 0        |
| 25  | BCR  | k     | 101    | -      | 41,41,41     | 1.07 | 1 (2%)   | 56,56,56    | 1.45 | 12 (21%) |
| 23  | CLA  | A     | 405[A] | 41     | 69,73,73     | 1.91 | 18 (26%) | 82,113,113  | 2.74 | 36 (43%) |
| 23  | CLA  | c     | 505    | 41     | 69,73,73     | 2.06 | 20 (28%) | 82,113,113  | 2.69 | 32 (39%) |
| 23  | CLA  | c     | 506    | -      | 69,73,73     | 2.00 | 19 (27%) | 82,113,113  | 2.71 | 29 (35%) |
| 24  | PHO  | A     | 417[B] | -      | 58,69,69     | 2.78 | 14 (24%) | 55,99,99    | 2.96 | 18 (32%) |
| 32  | LMT  | B     | 630    | -      | 25,25,36     | 0.87 | 1 (4%)   | 30,30,47    | 1.20 | 3 (10%)  |
| 25  | BCR  | c     | 516    | -      | 41,41,41     | 1.04 | 1 (2%)   | 56,56,56    | 1.35 | 8 (14%)  |
| 23  | CLA  | c     | 514    | -      | 69,73,73     | 2.07 | 21 (30%) | 82,113,113  | 2.72 | 30 (36%) |
| 23  | CLA  | b     | 601    | 41     | 69,73,73     | 2.07 | 19 (27%) | 82,113,113  | 2.64 | 31 (37%) |
| 24  | PHO  | A     | 407[A] | -      | 58,69,69     | 2.70 | 13 (22%) | 55,99,99    | 2.89 | 15 (27%) |
| 23  | CLA  | C     | 510    | -      | 69,73,73     | 2.03 | 19 (27%) | 82,113,113  | 2.72 | 30 (36%) |
| 25  | BCR  | b     | 618    | -      | 41,41,41     | 0.98 | 1 (2%)   | 56,56,56    | 1.34 | 11 (19%) |
| 32  | LMT  | B     | 627    | -      | 36,36,36     | 1.14 | 3 (8%)   | 47,47,47    | 1.42 | 6 (12%)  |
| 23  | CLA  | c     | 503    | -      | 69,73,73     | 2.01 | 19 (27%) | 82,113,113  | 2.60 | 28 (34%) |
| 36  | DGD  | H     | 102    | -      | 63,63,67     | 0.86 | 4 (6%)   | 77,77,81    | 1.09 | 7 (9%)   |
| 23  | CLA  | A     | 404[B] | -      | 69,73,73     | 2.03 | 20 (28%) | 82,113,113  | 2.71 | 33 (40%) |
| 25  | BCR  | y     | 101    | -      | 41,41,41     | 1.06 | 1 (2%)   | 56,56,56    | 1.64 | 12 (21%) |
| 27  | GOL  | d     | 411    | -      | 5,5,5        | 1.16 | 1 (20%)  | 5,5,5       | 0.98 | 0        |
| 29  | PL9  | a     | 414[B] | -      | 55,55,55     | 0.65 | 2 (3%)   | 68,69,69    | 1.97 | 21 (30%) |
| 23  | CLA  | B     | 609    | -      | 69,73,73     | 1.99 | 17 (24%) | 82,113,113  | 2.69 | 29 (35%) |
| 26  | SQD  | B     | 620    | -      | 52,54,54     | 1.04 | 3 (5%)   | 62,65,65    | 1.70 | 11 (17%) |
| 28  | OEX  | A     | 413[A] | 41,3,1 | 0,15,15      | -    | -        | -           | -    | -        |
| 25  | BCR  | T     | 102    | -      | 41,41,41     | 1.03 | 1 (2%)   | 56,56,56    | 1.79 | 13 (23%) |
| 23  | CLA  | C     | 503    | -      | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.51 | 30 (36%) |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | CLA  | B     | 604    | -    | 69,73,73     | 1.97 | 22 (31%) | 82,113,113  | 2.63 | 31 (37%) |
| 33  | LHG  | d     | 406[A] | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.00 | 3 (5%)   |
| 35  | HTG  | c     | 522    | -    | 19,19,19     | 0.84 | 1 (5%)   | 23,24,24    | 1.27 | 1 (4%)   |
| 29  | PL9  | D     | 705[A] | -    | 55,55,55     | 0.64 | 2 (3%)   | 68,69,69    | 1.64 | 18 (26%) |
| 33  | LHG  | L     | 101[A] | -    | 48,48,48     | 0.89 | 2 (4%)   | 51,54,54    | 1.16 | 3 (5%)   |
| 35  | HTG  | C     | 522    | -    | 19,19,19     | 0.82 | 1 (5%)   | 23,24,24    | 1.21 | 2 (8%)   |
| 25  | BCR  | H     | 101    | -    | 41,41,41     | 1.04 | 1 (2%)   | 56,56,56    | 1.44 | 7 (12%)  |
| 29  | PL9  | A     | 414[A] | -    | 55,55,55     | 0.70 | 3 (5%)   | 68,69,69    | 2.11 | 27 (39%) |
| 23  | CLA  | b     | 604    | -    | 69,73,73     | 1.96 | 21 (30%) | 82,113,113  | 2.65 | 30 (36%) |
| 33  | LHG  | a     | 420[B] | -    | 41,41,48     | 1.04 | 2 (4%)   | 44,47,54    | 0.95 | 2 (4%)   |
| 26  | SQD  | f     | 102    | -    | 41,43,54     | 1.14 | 2 (4%)   | 51,54,65    | 1.53 | 11 (21%) |
| 29  | PL9  | d     | 404[B] | -    | 55,55,55     | 0.66 | 1 (1%)   | 68,69,69    | 1.62 | 16 (23%) |
| 27  | GOL  | l     | 102[A] | -    | 5,5,5        | 1.01 | 0        | 5,5,5       | 1.04 | 0        |
| 33  | LHG  | E     | 101[A] | -    | 41,41,48     | 1.07 | 2 (4%)   | 44,47,54    | 1.12 | 3 (6%)   |
| 38  | HEM  | F     | 102    | 6,5  | 50,50,50     | 1.56 | 7 (14%)  | 67,82,82    | 1.79 | 18 (26%) |
| 23  | CLA  | a     | 406[B] | 41   | 69,73,73     | 2.04 | 18 (26%) | 82,113,113  | 2.69 | 33 (40%) |
| 31  | BCT  | a     | 404[B] | 21   | 3,3,3        | 0.51 | 0        | 2,3,3       | 1.26 | 0        |
| 23  | CLA  | d     | 401[B] | -    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.66 | 30 (36%) |
| 23  | CLA  | B     | 614    | -    | 69,73,73     | 2.03 | 19 (27%) | 82,113,113  | 2.90 | 33 (40%) |
| 25  | BCR  | C     | 516    | -    | 41,41,41     | 1.09 | 1 (2%)   | 56,56,56    | 1.36 | 7 (12%)  |
| 34  | LMG  | z     | 101    | -    | 39,39,55     | 1.10 | 2 (5%)   | 47,47,63    | 1.04 | 2 (4%)   |
| 27  | GOL  | c     | 526[A] | -    | 5,5,5        | 0.99 | 0        | 5,5,5       | 1.02 | 0        |
| 25  | BCR  | c     | 515    | -    | 41,41,41     | 1.02 | 1 (2%)   | 56,56,56    | 1.62 | 10 (17%) |
| 27  | GOL  | V     | 203[B] | -    | 5,5,5        | 1.17 | 0        | 5,5,5       | 0.96 | 0        |
| 25  | BCR  | h     | 101    | -    | 41,41,41     | 1.07 | 1 (2%)   | 56,56,56    | 1.49 | 13 (23%) |
| 27  | GOL  | b     | 628    | -    | 5,5,5        | 0.51 | 0        | 5,5,5       | 1.44 | 1 (20%)  |
| 25  | BCR  | t     | 102    | -    | 41,41,41     | 1.04 | 1 (2%)   | 56,56,56    | 1.72 | 15 (26%) |
| 34  | LMG  | d     | 410    | 39   | 51,51,55     | 0.90 | 2 (3%)   | 59,59,63    | 1.17 | 5 (8%)   |
| 26  | SQD  | a     | 411[B] | -    | 52,54,54     | 0.91 | 2 (3%)   | 62,65,65    | 1.56 | 12 (19%) |
| 34  | LMG  | m     | 101    | -    | 51,51,55     | 0.87 | 2 (3%)   | 59,59,63    | 1.28 | 8 (13%)  |
| 23  | CLA  | B     | 610    | 41   | 69,73,73     | 2.06 | 20 (28%) | 82,113,113  | 2.81 | 33 (40%) |
| 23  | CLA  | b     | 608    | -    | 69,73,73     | 1.97 | 19 (27%) | 82,113,113  | 2.63 | 32 (39%) |
| 23  | CLA  | b     | 614    | -    | 69,73,73     | 2.02 | 20 (28%) | 82,113,113  | 2.84 | 32 (39%) |
| 32  | LMT  | e     | 101    | -    | 36,36,36     | 1.00 | 2 (5%)   | 47,47,47    | 0.98 | 1 (2%)   |
| 36  | DGD  | C     | 517[B] | -    | 63,63,67     | 0.84 | 2 (3%)   | 77,77,81    | 1.14 | 8 (10%)  |



| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | SQD  | A     | 410[B] | -    | 52,54,54     | 0.85 | 2 (3%)   | 62,65,65    | 1.73 | 10 (16%) |
| 23  | CLA  | b     | 613    | -    | 69,73,73     | 1.93 | 18 (26%) | 82,113,113  | 2.72 | 31 (37%) |
| 35  | HTG  | o     | 301    | -    | 19,19,19     | 1.09 | 2 (10%)  | 23,24,24    | 1.58 | 6 (26%)  |
| 32  | LMT  | t     | 101    | -    | 26,26,36     | 0.89 | 2 (7%)   | 31,31,47    | 1.32 | 2 (6%)   |
| 24  | PHO  | A     | 417[A] | -    | 58,69,69     | 2.74 | 14 (24%) | 55,99,99    | 2.91 | 17 (30%) |
| 27  | GOL  | D     | 701    | -    | 5,5,5        | 1.65 | 2 (40%)  | 5,5,5       | 1.13 | 1 (20%)  |
| 36  | DGD  | c     | 519    | -    | 63,63,67     | 0.88 | 4 (6%)   | 77,77,81    | 1.08 | 6 (7%)   |
| 23  | CLA  | a     | 405[B] | -    | 69,73,73     | 1.96 | 17 (24%) | 82,113,113  | 2.77 | 33 (40%) |
| 32  | LMT  | A     | 420    | -    | 36,36,36     | 1.01 | 2 (5%)   | 47,47,47    | 1.16 | 4 (8%)   |
| 25  | BCR  | b     | 619    | -    | 41,41,41     | 1.10 | 1 (2%)   | 56,56,56    | 1.41 | 10 (17%) |
| 23  | CLA  | b     | 607    | 41   | 69,73,73     | 1.96 | 21 (30%) | 82,113,113  | 2.67 | 30 (36%) |
| 27  | GOL  | A     | 411    | -    | 5,5,5        | 1.27 | 0        | 5,5,5       | 0.72 | 0        |
| 36  | DGD  | c     | 517[B] | -    | 63,63,67     | 0.86 | 2 (3%)   | 77,77,81    | 1.12 | 7 (9%)   |
| 23  | CLA  | B     | 601    | 41   | 69,73,73     | 2.04 | 20 (28%) | 82,113,113  | 2.68 | 31 (37%) |
| 23  | CLA  | b     | 605    | -    | 69,73,73     | 1.91 | 18 (26%) | 82,113,113  | 2.82 | 32 (39%) |
| 23  | CLA  | A     | 404[A] | -    | 69,73,73     | 1.97 | 19 (27%) | 82,113,113  | 2.69 | 33 (40%) |
| 23  | CLA  | C     | 512    | 3    | 69,73,73     | 2.02 | 21 (30%) | 82,113,113  | 2.63 | 29 (35%) |
| 23  | CLA  | b     | 611    | -    | 69,73,73     | 1.96 | 18 (26%) | 82,113,113  | 2.75 | 30 (36%) |
| 29  | PL9  | a     | 414[A] | -    | 55,55,55     | 0.67 | 2 (3%)   | 68,69,69    | 2.01 | 21 (30%) |
| 23  | CLA  | B     | 616    | -    | 69,73,73     | 1.96 | 20 (28%) | 82,113,113  | 2.82 | 30 (36%) |
| 25  | BCR  | Y     | 101    | -    | 41,41,41     | 0.94 | 1 (2%)   | 56,56,56    | 1.71 | 15 (26%) |
| 33  | LHG  | b     | 629[B] | -    | 48,48,48     | 0.89 | 2 (4%)   | 51,54,54    | 1.06 | 5 (9%)   |
| 32  | LMT  | m     | 103    | -    | 36,36,36     | 1.05 | 1 (2%)   | 47,47,47    | 1.17 | 4 (8%)   |
| 23  | CLA  | c     | 512    | 3    | 69,73,73     | 2.07 | 19 (27%) | 82,113,113  | 2.66 | 33 (40%) |
| 23  | CLA  | C     | 505    | 41   | 69,73,73     | 1.99 | 19 (27%) | 82,113,113  | 2.61 | 29 (35%) |
| 26  | SQD  | b     | 620    | -    | 52,54,54     | 1.01 | 2 (3%)   | 62,65,65    | 1.66 | 11 (17%) |
| 27  | GOL  | D     | 712    | -    | 5,5,5        | 1.64 | 2 (40%)  | 5,5,5       | 0.94 | 0        |
| 31  | BCT  | A     | 416[B] | 21   | 3,3,3        | 0.47 | 0        | 2,3,3       | 1.19 | 0        |
| 23  | CLA  | b     | 616    | -    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.84 | 33 (40%) |
| 33  | LHG  | a     | 420[A] | -    | 41,41,48     | 1.04 | 2 (4%)   | 44,47,54    | 0.94 | 2 (4%)   |
| 34  | LMG  | C     | 501    | -    | 51,51,55     | 0.93 | 2 (3%)   | 59,59,63    | 1.51 | 8 (13%)  |
| 35  | HTG  | B     | 622    | -    | 19,19,19     | 0.74 | 1 (5%)   | 23,24,24    | 1.26 | 2 (8%)   |
| 29  | PL9  | d     | 404[A] | -    | 55,55,55     | 0.67 | 1 (1%)   | 68,69,69    | 1.62 | 15 (22%) |
| 33  | LHG  | A     | 419[A] | -    | 48,48,48     | 0.84 | 2 (4%)   | 51,54,54    | 1.33 | 6 (11%)  |
| 36  | DGD  | c     | 518[B] | -    | 63,63,67     | 0.88 | 2 (3%)   | 77,77,81    | 0.92 | 3 (3%)   |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | DGD  | C     | 518[B] | -    | 63,63,67     | 0.89 | 3 (4%)   | 77,77,81    | 1.04 | 6 (7%)   |
| 34  | LMG  | Z     | 101    | -    | 37,37,55     | 1.02 | 2 (5%)   | 45,45,63    | 1.43 | 6 (13%)  |
| 23  | CLA  | a     | 406[A] | 41   | 69,73,73     | 1.98 | 17 (24%) | 82,113,113  | 2.66 | 30 (36%) |
| 40  | HEC  | v     | 201    | 16   | 46,50,50     | 1.92 | 4 (8%)   | 58,82,82    | 1.89 | 7 (12%)  |
| 31  | BCT  | a     | 404[A] | 21   | 3,3,3        | 0.46 | 0        | 2,3,3       | 1.59 | 0        |
| 23  | CLA  | d     | 401[A] | -    | 69,73,73     | 1.92 | 19 (27%) | 82,113,113  | 2.67 | 30 (36%) |
| 36  | DGD  | C     | 519    | -    | 63,63,67     | 0.86 | 3 (4%)   | 77,77,81    | 1.01 | 3 (3%)   |
| 23  | CLA  | B     | 602    | -    | 69,73,73     | 2.00 | 20 (28%) | 82,113,113  | 2.73 | 32 (39%) |
| 23  | CLA  | C     | 507    | -    | 69,73,73     | 2.01 | 21 (30%) | 82,113,113  | 2.69 | 32 (39%) |
| 27  | GOL  | V     | 203[A] | -    | 5,5,5        | 1.29 | 1 (20%)  | 5,5,5       | 0.97 | 0        |
| 33  | LHG  | D     | 706[B] | -    | 48,48,48     | 0.87 | 2 (4%)   | 51,54,54    | 1.00 | 3 (5%)   |
| 35  | HTG  | V     | 202    | -    | 11,11,19     | 0.33 | 0        | 15,15,24    | 1.24 | 1 (6%)   |
| 27  | GOL  | C     | 523[B] | -    | 5,5,5        | 1.25 | 0        | 5,5,5       | 0.85 | 0        |
| 27  | GOL  | o     | 304    | -    | 5,5,5        | 1.15 | 1 (20%)  | 5,5,5       | 1.14 | 0        |
| 34  | LMG  | c     | 501    | -    | 51,51,55     | 0.93 | 2 (3%)   | 59,59,63    | 1.25 | 6 (10%)  |
| 27  | GOL  | B     | 628    | -    | 5,5,5        | 0.93 | 0        | 5,5,5       | 1.22 | 1 (20%)  |
| 23  | CLA  | A     | 406[B] | 41   | 69,73,73     | 2.02 | 19 (27%) | 82,113,113  | 2.76 | 34 (41%) |
| 23  | CLA  | D     | 703    | -    | 69,73,73     | 2.07 | 19 (27%) | 82,113,113  | 2.68 | 33 (40%) |
| 26  | SQD  | a     | 411[A] | -    | 52,54,54     | 0.89 | 2 (3%)   | 62,65,65    | 1.74 | 12 (19%) |
| 26  | SQD  | a     | 412    | -    | 52,54,54     | 1.04 | 2 (3%)   | 62,65,65    | 1.14 | 7 (11%)  |
| 27  | GOL  | O     | 303    | -    | 5,5,5        | 1.06 | 0        | 5,5,5       | 1.10 | 0        |
| 33  | LHG  | d     | 412[B] | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.09 | 4 (7%)   |
| 36  | DGD  | C     | 517[A] | -    | 63,63,67     | 0.82 | 2 (3%)   | 77,77,81    | 1.21 | 9 (11%)  |
| 26  | SQD  | A     | 410[A] | -    | 52,54,54     | 0.86 | 2 (3%)   | 62,65,65    | 1.79 | 9 (14%)  |
| 34  | LMG  | D     | 711    | 39   | 51,51,55     | 0.80 | 3 (5%)   | 59,59,63    | 1.10 | 3 (5%)   |
| 23  | CLA  | C     | 511    | -    | 69,73,73     | 2.01 | 19 (27%) | 82,113,113  | 2.79 | 34 (41%) |
| 23  | CLA  | b     | 602    | -    | 69,73,73     | 2.06 | 18 (26%) | 82,113,113  | 2.86 | 34 (41%) |
| 25  | BCR  | d     | 403    | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 2.01 | 14 (25%) |
| 23  | CLA  | a     | 407[B] | 41   | 69,73,73     | 1.99 | 20 (28%) | 82,113,113  | 2.65 | 31 (37%) |
| 23  | CLA  | a     | 405[A] | -    | 69,73,73     | 1.94 | 19 (27%) | 82,113,113  | 2.76 | 34 (41%) |
| 36  | DGD  | c     | 517[A] | -    | 63,63,67     | 0.85 | 2 (3%)   | 77,77,81    | 1.12 | 6 (7%)   |
| 27  | GOL  | O     | 302    | -    | 5,5,5        | 0.86 | 0        | 5,5,5       | 1.00 | 0        |
| 23  | CLA  | c     | 507    | -    | 69,73,73     | 2.03 | 19 (27%) | 82,113,113  | 2.65 | 34 (41%) |
| 23  | CLA  | c     | 502    | -    | 69,73,73     | 2.00 | 19 (27%) | 82,113,113  | 2.69 | 30 (36%) |
| 23  | CLA  | C     | 513    | -    | 69,73,73     | 2.01 | 19 (27%) | 82,113,113  | 2.71 | 33 (40%) |

| Mol | Type | Chain | Res    | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | BCR  | a     | 410    | -      | 41,41,41     | 1.03 | 1 (2%)   | 56,56,56    | 1.34 | 9 (16%)  |
| 23  | CLA  | B     | 611    | -      | 69,73,73     | 2.47 | 20 (28%) | 82,113,113  | 3.60 | 31 (37%) |
| 23  | CLA  | B     | 603    | -      | 69,73,73     | 2.01 | 21 (30%) | 82,113,113  | 2.79 | 34 (41%) |
| 27  | GOL  | a     | 419    | -      | 5,5,5        | 1.36 | 1 (20%)  | 5,5,5       | 1.00 | 0        |
| 33  | LHG  | b     | 629[A] | -      | 48,48,48     | 0.86 | 3 (6%)   | 51,54,54    | 1.05 | 4 (7%)   |
| 27  | GOL  | b     | 624    | -      | 5,5,5        | 1.26 | 1 (20%)  | 5,5,5       | 0.84 | 0        |
| 23  | CLA  | b     | 612    | -      | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 2.61 | 29 (35%) |
| 24  | PHO  | a     | 408[B] | -      | 58,69,69     | 2.79 | 14 (24%) | 55,99,99    | 2.93 | 17 (30%) |
| 24  | PHO  | A     | 407[B] | -      | 58,69,69     | 2.70 | 13 (22%) | 55,99,99    | 2.89 | 15 (27%) |
| 31  | BCT  | A     | 416[A] | 21     | 3,3,3        | 0.43 | 0        | 2,3,3       | 1.83 | 0        |
| 28  | OEX  | a     | 413[B] | 41,3,1 | 0,15,15      | -    | -        | -           | -    | -        |
| 35  | HTG  | b     | 625    | -      | 19,19,19     | 1.02 | 2 (10%)  | 23,24,24    | 1.50 | 3 (13%)  |
| 23  | CLA  | B     | 615    | -      | 69,73,73     | 2.02 | 20 (28%) | 82,113,113  | 2.71 | 32 (39%) |
| 36  | DGD  | c     | 518[A] | -      | 63,63,67     | 0.84 | 3 (4%)   | 77,77,81    | 0.98 | 5 (6%)   |
| 23  | CLA  | c     | 509    | -      | 69,73,73     | 2.07 | 20 (28%) | 82,113,113  | 2.59 | 28 (34%) |
| 23  | CLA  | B     | 608    | -      | 69,73,73     | 1.91 | 20 (28%) | 82,113,113  | 2.79 | 36 (43%) |
| 27  | GOL  | B     | 623    | -      | 5,5,5        | 0.77 | 0        | 5,5,5       | 1.20 | 1 (20%)  |
| 36  | DGD  | C     | 518[A] | -      | 63,63,67     | 0.89 | 3 (4%)   | 77,77,81    | 1.03 | 5 (6%)   |
| 23  | CLA  | b     | 609    | -      | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.67 | 32 (39%) |
| 23  | CLA  | b     | 610    | 41     | 69,73,73     | 2.03 | 20 (28%) | 82,113,113  | 2.79 | 33 (40%) |
| 23  | CLA  | a     | 409    | -      | 69,73,73     | 1.96 | 18 (26%) | 82,113,113  | 2.81 | 31 (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   |
|-----|------|-------|--------|------|-----------|--------------|---------|
| 27  | GOL  | v     | 202[B] | -    | -         | 2/4/4/4      | -       |
| 23  | CLA  | C     | 504    | -    | 1/1/15/20 | 4/39/115/115 | -       |
| 34  | LMG  | c     | 521    | -    | -         | 12/46/66/70  | 0/1/1/1 |
| 23  | CLA  | b     | 615    | -    | 1/1/15/20 | 8/39/115/115 | -       |
| 34  | LMG  | c     | 520    | -    | -         | 13/46/66/70  | 0/1/1/1 |
| 33  | LHG  | D     | 706[A] | -    | -         | 16/53/53/53  | -       |
| 27  | GOL  | C     | 523[A] | -    | -         | 0/4/4/4      | -       |
| 25  | BCR  | b     | 617    | -    | -         | 2/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 23  | CLA  | C     | 514    | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 23  | CLA  | A     | 406[A] | 41   | -         | 7/39/115/115  | -       |
| 24  | PHO  | a     | 416[B] | -    | -         | 0/37/103/103  | 0/5/6/6 |
| 32  | LMT  | F     | 101    | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 33  | LHG  | d     | 412[A] | -    | -         | 12/53/53/53   | -       |
| 35  | HTG  | D     | 710    | -    | -         | 3/7/27/30     | 0/1/1/1 |
| 33  | LHG  | D     | 707[B] | -    | -         | 14/53/53/53   | -       |
| 32  | LMT  | a     | 417    | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 23  | CLA  | C     | 506    | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 23  | CLA  | a     | 407[A] | 41   | -         | 5/39/115/115  | -       |
| 23  | CLA  | b     | 603    | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 23  | CLA  | c     | 508    | 41   | 1/1/15/20 | 9/39/115/115  | -       |
| 23  | CLA  | c     | 511    | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | BCR  | C     | 515    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 23  | CLA  | C     | 508    | 41   | 1/1/15/20 | 9/39/115/115  | -       |
| 23  | CLA  | D     | 702[B] | -    | 1/1/15/20 | 2/39/115/115  | -       |
| 32  | LMT  | M     | 101    | -    | -         | 5/21/61/61    | 0/2/2/2 |
| 33  | LHG  | d     | 405[B] | -    | -         | 14/53/53/53   | -       |
| 26  | SQD  | A     | 412    | -    | -         | 12/49/69/69   | 0/1/1/1 |
| 23  | CLA  | C     | 502    | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 25  | BCR  | A     | 409    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 36  | DGD  | h     | 102    | -    | -         | 15/51/91/95   | 0/2/2/2 |
| 23  | CLA  | B     | 607    | 41   | 1/1/15/20 | 5/39/115/115  | -       |
| 25  | BCR  | K     | 102    | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 24  | PHO  | a     | 408[A] | -    | -         | 5/37/103/103  | 0/5/6/6 |
| 32  | LMT  | A     | 418    | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 23  | CLA  | B     | 612    | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 23  | CLA  | c     | 510    | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 35  | HTG  | B     | 624    | -    | -         | 3/10/30/30    | 0/1/1/1 |
| 23  | CLA  | A     | 405[B] | 41   | 1/1/15/20 | 2/39/115/115  | -       |
| 34  | LMG  | C     | 520    | -    | -         | 10/46/66/70   | 0/1/1/1 |
| 32  | LMT  | T     | 101    | -    | -         | 9/21/61/61    | 0/2/2/2 |
| 32  | LMT  | B     | 629    | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 27  | GOL  | B     | 626    | -    | -         | 1/4/4/4       | -       |
| 23  | CLA  | C     | 509    | -    | 1/1/15/20 | 4/39/115/115  | -       |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 35  | HTG  | d     | 409    | -    | -         | 1/7/27/30     | 0/1/1/1 |
| 40  | HEC  | V     | 201    | 16   | -         | 6/14/54/54    | -       |
| 27  | GOL  | v     | 202[A] | -    | -         | 1/4/4/4       | -       |
| 25  | BCR  | B     | 619    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 23  | CLA  | B     | 613    | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 33  | LHG  | A     | 419[B] | -    | -         | 12/53/53/53   | -       |
| 33  | LHG  | d     | 406[B] | -    | -         | 12/53/53/53   | -       |
| 23  | CLA  | c     | 504    | -    | 1/1/15/20 | 2/39/115/115  | -       |
| 34  | LMG  | C     | 521    | -    | -         | 15/46/66/70   | 0/1/1/1 |
| 29  | PL9  | D     | 705[B] | -    | -         | 6/53/73/73    | 0/1/1/1 |
| 24  | PHO  | a     | 416[A] | -    | -         | 0/37/103/103  | 0/5/6/6 |
| 25  | BCR  | B     | 617    | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 33  | LHG  | L     | 101[B] | -    | -         | 17/53/53/53   | -       |
| 29  | PL9  | A     | 414[B] | -    | -         | 16/53/73/73   | 0/1/1/1 |
| 27  | GOL  | o     | 303    | -    | -         | 2/4/4/4       | -       |
| 23  | CLA  | B     | 605    | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 33  | LHG  | D     | 707[A] | -    | -         | 13/53/53/53   | -       |
| 35  | HTG  | b     | 623    | -    | -         | 5/10/30/30    | 0/1/1/1 |
| 27  | GOL  | l     | 102[B] | -    | -         | 2/4/4/4       | -       |
| 33  | LHG  | E     | 101[B] | -    | -         | 22/46/46/53   | -       |
| 38  | HEM  | f     | 101    | 6,5  | -         | 6/14/54/54    | -       |
| 32  | LMT  | b     | 627    | -    | -         | 11/17/37/61   | 0/1/1/2 |
| 23  | CLA  | D     | 702[A] | -    | 1/1/15/20 | 0/39/115/115  | -       |
| 32  | LMT  | b     | 621    | -    | -         | 8/17/37/61    | 0/1/1/2 |
| 33  | LHG  | d     | 405[A] | -    | -         | 12/53/53/53   | -       |
| 23  | CLA  | A     | 408    | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 26  | SQD  | X     | 101    | -    | -         | 16/38/58/69   | 0/1/1/1 |
| 27  | GOL  | c     | 526[B] | -    | -         | 0/4/4/4       | -       |
| 23  | CLA  | d     | 402    | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | BCR  | D     | 704    | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 23  | CLA  | B     | 606    | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 34  | LMG  | B     | 621    | -    | -         | 20/46/66/70   | 0/1/1/1 |
| 23  | CLA  | b     | 606    | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 27  | GOL  | a     | 418    | -    | -         | 2/4/4/4       | -       |
| 25  | BCR  | B     | 618    | -    | -         | 0/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 35  | HTG  | b     | 622    | -    | -         | 4/10/30/30    | 0/1/1/1 |
| 23  | CLA  | c     | 513    | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 27  | GOL  | c     | 527    | -    | -         | 2/4/4/4       | -       |
| 25  | BCR  | k     | 101    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 23  | CLA  | A     | 405[A] | 41   | -         | 2/39/115/115  | -       |
| 23  | CLA  | c     | 505    | 41   | 1/1/15/20 | 5/39/115/115  | -       |
| 23  | CLA  | c     | 506    | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 24  | PHO  | A     | 417[B] | -    | -         | 1/37/103/103  | 0/5/6/6 |
| 32  | LMT  | B     | 630    | -    | -         | 10/17/37/61   | 0/1/1/2 |
| 25  | BCR  | c     | 516    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 23  | CLA  | c     | 514    | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 23  | CLA  | b     | 601    | 41   | 1/1/15/20 | 18/39/115/115 | -       |
| 24  | PHO  | A     | 407[A] | -    | -         | 1/37/103/103  | 0/5/6/6 |
| 23  | CLA  | C     | 510    | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 25  | BCR  | b     | 618    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 32  | LMT  | B     | 627    | -    | -         | 12/21/61/61   | 0/2/2/2 |
| 23  | CLA  | c     | 503    | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 36  | DGD  | H     | 102    | -    | -         | 7/51/91/95    | 0/2/2/2 |
| 23  | CLA  | A     | 404[B] | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 25  | BCR  | y     | 101    | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 27  | GOL  | d     | 411    | -    | -         | 4/4/4/4       | -       |
| 29  | PL9  | a     | 414[B] | -    | -         | 14/53/73/73   | 0/1/1/1 |
| 23  | CLA  | B     | 609    | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 26  | SQD  | B     | 620    | -    | -         | 13/49/69/69   | 0/1/1/1 |
| 25  | BCR  | T     | 102    | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 23  | CLA  | C     | 503    | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 23  | CLA  | B     | 604    | -    | 1/1/15/20 | 1/39/115/115  | -       |
| 33  | LHG  | d     | 406[A] | -    | -         | 11/53/53/53   | -       |
| 35  | HTG  | c     | 522    | -    | -         | 1/10/30/30    | 0/1/1/1 |
| 29  | PL9  | D     | 705[A] | -    | -         | 7/53/73/73    | 0/1/1/1 |
| 33  | LHG  | L     | 101[A] | -    | -         | 19/53/53/53   | -       |
| 35  | HTG  | C     | 522    | -    | -         | 0/10/30/30    | 0/1/1/1 |
| 25  | BCR  | H     | 101    | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 29  | PL9  | A     | 414[A] | -    | -         | 15/53/73/73   | 0/1/1/1 |
| 23  | CLA  | b     | 604    | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 33  | LHG  | a     | 420[B] | -    | -         | 16/46/46/53   | -       |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 26  | SQD  | f     | 102    | -    | -         | 9/38/58/69    | 0/1/1/1 |
| 29  | PL9  | d     | 404[B] | -    | -         | 9/53/73/73    | 0/1/1/1 |
| 27  | GOL  | l     | 102[A] | -    | -         | 1/4/4/4       | -       |
| 33  | LHG  | E     | 101[A] | -    | -         | 21/46/46/53   | -       |
| 38  | HEM  | F     | 102    | 6,5  | -         | 6/14/54/54    | -       |
| 23  | CLA  | a     | 406[B] | 41   | 1/1/15/20 | 4/39/115/115  | -       |
| 23  | CLA  | d     | 401[B] | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 23  | CLA  | B     | 614    | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 25  | BCR  | C     | 516    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 34  | LMG  | z     | 101    | -    | -         | 9/34/54/70    | 0/1/1/1 |
| 27  | GOL  | c     | 526[A] | -    | -         | 0/4/4/4       | -       |
| 25  | BCR  | c     | 515    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 27  | GOL  | V     | 203[B] | -    | -         | 2/4/4/4       | -       |
| 25  | BCR  | h     | 101    | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 27  | GOL  | b     | 628    | -    | -         | 0/4/4/4       | -       |
| 25  | BCR  | t     | 102    | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 34  | LMG  | d     | 410    | 39   | -         | 11/46/66/70   | 0/1/1/1 |
| 26  | SQD  | a     | 411[B] | -    | -         | 10/49/69/69   | 0/1/1/1 |
| 34  | LMG  | m     | 101    | -    | -         | 9/46/66/70    | 0/1/1/1 |
| 23  | CLA  | B     | 610    | 41   | 1/1/15/20 | 7/39/115/115  | -       |
| 23  | CLA  | b     | 614    | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 23  | CLA  | b     | 608    | -    | -         | 4/39/115/115  | -       |
| 32  | LMT  | e     | 101    | -    | -         | 14/21/61/61   | 0/2/2/2 |
| 36  | DGD  | C     | 517[B] | -    | -         | 13/51/91/95   | 0/2/2/2 |
| 26  | SQD  | A     | 410[B] | -    | -         | 11/49/69/69   | 0/1/1/1 |
| 23  | CLA  | b     | 613    | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 35  | HTG  | o     | 301    | -    | -         | 4/10/30/30    | 0/1/1/1 |
| 32  | LMT  | t     | 101    | -    | -         | 10/17/38/61   | 0/1/1/2 |
| 24  | PHO  | A     | 417[A] | -    | -         | 1/37/103/103  | 0/5/6/6 |
| 27  | GOL  | D     | 701    | -    | -         | 1/4/4/4       | -       |
| 36  | DGD  | c     | 519    | -    | -         | 8/51/91/95    | 0/2/2/2 |
| 23  | CLA  | a     | 405[B] | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 32  | LMT  | A     | 420    | -    | -         | 15/21/61/61   | 0/2/2/2 |
| 25  | BCR  | b     | 619    | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 23  | CLA  | b     | 607    | 41   | 1/1/15/20 | 3/39/115/115  | -       |
| 27  | GOL  | A     | 411    | -    | -         | 2/4/4/4       | -       |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 36  | DGD  | c     | 517[B] | -    | -         | 18/51/91/95   | 0/2/2/2 |
| 23  | CLA  | B     | 601    | 41   | 1/1/15/20 | 10/39/115/115 | -       |
| 23  | CLA  | b     | 605    | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 23  | CLA  | A     | 404[A] | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 23  | CLA  | C     | 512    | 3    | 1/1/15/20 | 3/39/115/115  | -       |
| 23  | CLA  | b     | 611    | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 29  | PL9  | a     | 414[A] | -    | -         | 14/53/73/73   | 0/1/1/1 |
| 23  | CLA  | B     | 616    | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 25  | BCR  | Y     | 101    | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 33  | LHG  | b     | 629[B] | -    | -         | 16/53/53/53   | -       |
| 32  | LMT  | m     | 103    | -    | -         | 5/21/61/61    | 0/2/2/2 |
| 23  | CLA  | c     | 512    | 3    | 1/1/15/20 | 6/39/115/115  | -       |
| 23  | CLA  | C     | 505    | 41   | 1/1/15/20 | 10/39/115/115 | -       |
| 26  | SQD  | b     | 620    | -    | -         | 18/49/69/69   | 0/1/1/1 |
| 27  | GOL  | D     | 712    | -    | -         | 4/4/4/4       | -       |
| 23  | CLA  | b     | 616    | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 33  | LHG  | a     | 420[A] | -    | -         | 16/46/46/53   | -       |
| 34  | LMG  | C     | 501    | -    | -         | 14/46/66/70   | 0/1/1/1 |
| 35  | HTG  | B     | 622    | -    | -         | 1/10/30/30    | 0/1/1/1 |
| 29  | PL9  | d     | 404[A] | -    | -         | 6/53/73/73    | 0/1/1/1 |
| 33  | LHG  | A     | 419[A] | -    | -         | 10/53/53/53   | -       |
| 36  | DGD  | c     | 518[B] | -    | -         | 15/51/91/95   | 0/2/2/2 |
| 36  | DGD  | C     | 518[B] | -    | -         | 12/51/91/95   | 0/2/2/2 |
| 34  | LMG  | Z     | 101    | -    | -         | 12/31/51/70   | 0/1/1/1 |
| 23  | CLA  | a     | 406[A] | 41   | 1/1/15/20 | 4/39/115/115  | -       |
| 40  | HEC  | v     | 201    | 16   | -         | 6/14/54/54    | -       |
| 23  | CLA  | d     | 401[A] | -    | 1/1/15/20 | 2/39/115/115  | -       |
| 36  | DGD  | C     | 519    | -    | -         | 19/51/91/95   | 0/2/2/2 |
| 23  | CLA  | B     | 602    | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 23  | CLA  | C     | 507    | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 27  | GOL  | V     | 203[A] | -    | -         | 2/4/4/4       | -       |
| 33  | LHG  | D     | 706[B] | -    | -         | 17/53/53/53   | -       |
| 35  | HTG  | V     | 202    | -    | -         | 0/2/19/30     | 0/1/1/1 |
| 27  | GOL  | C     | 523[B] | -    | -         | 0/4/4/4       | -       |
| 27  | GOL  | o     | 304    | -    | -         | 4/4/4/4       | -       |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 34  | LMG  | c     | 501    | -    | -         | 11/46/66/70   | 0/1/1/1 |
| 27  | GOL  | B     | 628    | -    | -         | 4/4/4/4       | -       |
| 23  | CLA  | D     | 703    | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 23  | CLA  | A     | 406[B] | 41   | -         | 7/39/115/115  | -       |
| 26  | SQD  | a     | 411[A] | -    | -         | 9/49/69/69    | 0/1/1/1 |
| 26  | SQD  | a     | 412    | -    | -         | 12/49/69/69   | 0/1/1/1 |
| 27  | GOL  | O     | 303    | -    | -         | 2/4/4/4       | -       |
| 33  | LHG  | d     | 412[B] | -    | -         | 12/53/53/53   | -       |
| 36  | DGD  | C     | 517[A] | -    | -         | 12/51/91/95   | 0/2/2/2 |
| 26  | SQD  | A     | 410[A] | -    | -         | 12/49/69/69   | 0/1/1/1 |
| 34  | LMG  | D     | 711    | 39   | -         | 9/46/66/70    | 0/1/1/1 |
| 23  | CLA  | C     | 511    | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 23  | CLA  | b     | 602    | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 25  | BCR  | d     | 403    | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 23  | CLA  | a     | 407[B] | 41   | -         | 6/39/115/115  | -       |
| 23  | CLA  | a     | 405[A] | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 36  | DGD  | c     | 517[A] | -    | -         | 20/51/91/95   | 0/2/2/2 |
| 27  | GOL  | O     | 302    | -    | -         | 2/4/4/4       | -       |
| 23  | CLA  | c     | 507    | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 23  | CLA  | c     | 502    | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 23  | CLA  | C     | 513    | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | BCR  | a     | 410    | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 23  | CLA  | B     | 611    | -    | 1/1/15/20 | 2/39/115/115  | -       |
| 23  | CLA  | B     | 603    | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 27  | GOL  | a     | 419    | -    | -         | 0/4/4/4       | -       |
| 33  | LHG  | b     | 629[A] | -    | -         | 20/53/53/53   | -       |
| 27  | GOL  | b     | 624    | -    | -         | 2/4/4/4       | -       |
| 23  | CLA  | b     | 612    | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 24  | PHO  | a     | 408[B] | -    | -         | 3/37/103/103  | 0/5/6/6 |
| 24  | PHO  | A     | 407[B] | -    | -         | 1/37/103/103  | 0/5/6/6 |
| 35  | HTG  | b     | 625    | -    | -         | 5/10/30/30    | 0/1/1/1 |
| 36  | DGD  | c     | 518[A] | -    | -         | 17/51/91/95   | 0/2/2/2 |
| 23  | CLA  | B     | 615    | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 23  | CLA  | c     | 509    | -    | 1/1/15/20 | 2/39/115/115  | -       |
| 23  | CLA  | B     | 608    | -    | -         | 3/39/115/115  | -       |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 27  | GOL  | B     | 623    | -    | -         | 4/4/4/4       | -       |
| 36  | DGD  | C     | 518[A] | -    | -         | 14/51/91/95   | 0/2/2/2 |
| 23  | CLA  | b     | 609    | -    | 1/1/15/20 | 1/39/115/115  | -       |
| 23  | CLA  | b     | 610    | 41   | 1/1/15/20 | 6/39/115/115  | -       |
| 23  | CLA  | a     | 409    | -    | -         | 10/39/115/115 | -       |

All (1848) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 24  | a     | 408[B] | PHO  | C1B-C2B | 9.68 | 1.50        | 1.39     |
| 24  | A     | 407[B] | PHO  | C1D-C2D | 9.49 | 1.49        | 1.39     |
| 24  | a     | 416[B] | PHO  | C1B-C2B | 9.44 | 1.49        | 1.39     |
| 24  | A     | 407[A] | PHO  | C1D-C2D | 9.27 | 1.49        | 1.39     |
| 24  | a     | 408[A] | PHO  | C1B-C2B | 9.11 | 1.49        | 1.39     |
| 24  | a     | 416[B] | PHO  | C1D-C2D | 8.93 | 1.49        | 1.39     |
| 24  | a     | 416[A] | PHO  | C1B-C2B | 8.92 | 1.49        | 1.39     |
| 24  | A     | 417[A] | PHO  | C1D-C2D | 8.86 | 1.49        | 1.39     |
| 24  | A     | 417[B] | PHO  | C1B-C2B | 8.75 | 1.49        | 1.39     |
| 24  | a     | 416[A] | PHO  | C1D-C2D | 8.73 | 1.49        | 1.39     |
| 24  | a     | 408[A] | PHO  | C1D-C2D | 8.59 | 1.48        | 1.39     |
| 24  | A     | 417[B] | PHO  | C1D-C2D | 8.55 | 1.48        | 1.39     |
| 24  | A     | 407[A] | PHO  | C1B-C2B | 8.44 | 1.48        | 1.39     |
| 24  | A     | 417[A] | PHO  | C1B-C2B | 8.41 | 1.48        | 1.39     |
| 24  | a     | 408[B] | PHO  | C1D-C2D | 8.40 | 1.48        | 1.39     |
| 24  | A     | 407[B] | PHO  | C1B-C2B | 8.38 | 1.48        | 1.39     |
| 24  | a     | 416[A] | PHO  | C3B-C4B | 8.05 | 1.49        | 1.41     |
| 24  | A     | 417[B] | PHO  | C3B-C4B | 7.80 | 1.49        | 1.41     |
| 24  | a     | 408[B] | PHO  | C3B-C4B | 7.63 | 1.49        | 1.41     |
| 24  | A     | 417[A] | PHO  | C3B-C4B | 7.47 | 1.49        | 1.41     |
| 24  | a     | 408[A] | PHO  | C3B-C4B | 7.36 | 1.49        | 1.41     |
| 24  | a     | 416[B] | PHO  | C3B-C4B | 7.32 | 1.48        | 1.41     |
| 24  | A     | 407[A] | PHO  | C3B-C4B | 7.26 | 1.48        | 1.41     |
| 24  | A     | 407[B] | PHO  | C3B-C4B | 7.22 | 1.48        | 1.41     |
| 40  | V     | 201    | HEC  | CAC-C3C | 7.11 | 1.58        | 1.35     |
| 40  | v     | 201    | HEC  | CAC-C3C | 6.89 | 1.57        | 1.35     |
| 24  | A     | 417[B] | PHO  | C4D-CHA | 6.85 | 1.49        | 1.39     |
| 24  | A     | 417[A] | PHO  | C4D-CHA | 6.82 | 1.49        | 1.39     |
| 23  | B     | 611    | CLA  | CMB-C2B | 6.81 | 1.64        | 1.50     |
| 24  | a     | 408[B] | PHO  | C4D-CHA | 6.81 | 1.49        | 1.39     |
| 24  | A     | 407[A] | PHO  | C4D-CHA | 6.81 | 1.49        | 1.39     |
| 24  | a     | 408[A] | PHO  | C4D-CHA | 6.79 | 1.49        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 40  | v     | 201    | HEC  | CAB-C3B | 6.76 | 1.57        | 1.35     |
| 23  | B     | 611    | CLA  | C1B-C2B | 6.62 | 1.58        | 1.43     |
| 24  | a     | 408[B] | PHO  | C3B-C2B | 6.58 | 1.49        | 1.40     |
| 24  | A     | 407[B] | PHO  | C4D-CHA | 6.55 | 1.49        | 1.39     |
| 24  | a     | 416[B] | PHO  | C3B-C2B | 6.54 | 1.49        | 1.40     |
| 24  | a     | 416[A] | PHO  | C4D-CHA | 6.52 | 1.49        | 1.39     |
| 24  | a     | 408[A] | PHO  | C3B-C2B | 6.52 | 1.49        | 1.40     |
| 24  | A     | 417[B] | PHO  | C3B-C2B | 6.40 | 1.49        | 1.40     |
| 24  | A     | 407[B] | PHO  | C3B-C2B | 6.40 | 1.49        | 1.40     |
| 24  | a     | 416[B] | PHO  | C4D-CHA | 6.35 | 1.49        | 1.39     |
| 24  | A     | 407[A] | PHO  | C3B-C2B | 6.34 | 1.49        | 1.40     |
| 24  | A     | 417[A] | PHO  | C3B-C2B | 6.26 | 1.48        | 1.40     |
| 40  | V     | 201    | HEC  | CAB-C3B | 6.25 | 1.55        | 1.35     |
| 23  | B     | 611    | CLA  | C1D-ND  | 6.09 | 1.45        | 1.37     |
| 24  | a     | 416[A] | PHO  | C3B-C2B | 6.05 | 1.48        | 1.40     |
| 23  | B     | 610    | CLA  | C3C-C2C | 5.72 | 1.49        | 1.36     |
| 24  | a     | 408[B] | PHO  | C3D-C2D | 5.72 | 1.49        | 1.39     |
| 23  | c     | 513    | CLA  | C3C-C2C | 5.58 | 1.48        | 1.36     |
| 23  | B     | 611    | CLA  | CHC-C1C | 5.57 | 1.49        | 1.38     |
| 24  | a     | 408[A] | PHO  | C3D-C2D | 5.56 | 1.49        | 1.39     |
| 23  | b     | 612    | CLA  | C3C-C2C | 5.56 | 1.48        | 1.36     |
| 23  | B     | 611    | CLA  | C3C-C2C | 5.55 | 1.48        | 1.36     |
| 23  | c     | 509    | CLA  | C3C-C2C | 5.53 | 1.48        | 1.36     |
| 40  | v     | 201    | HEC  | C3D-C2D | 5.53 | 1.53        | 1.38     |
| 23  | D     | 703    | CLA  | C3C-C2C | 5.51 | 1.48        | 1.36     |
| 23  | b     | 607    | CLA  | C3C-C2C | 5.51 | 1.48        | 1.36     |
| 24  | a     | 416[B] | PHO  | C3D-C2D | 5.50 | 1.49        | 1.39     |
| 24  | A     | 417[B] | PHO  | C3D-C2D | 5.49 | 1.49        | 1.39     |
| 23  | C     | 513    | CLA  | C3C-C2C | 5.48 | 1.48        | 1.36     |
| 24  | a     | 416[B] | PHO  | OBD-CAD | 5.47 | 1.29        | 1.22     |
| 23  | d     | 402    | CLA  | C3C-C2C | 5.47 | 1.48        | 1.36     |
| 23  | A     | 404[B] | CLA  | C3C-C2C | 5.46 | 1.48        | 1.36     |
| 24  | a     | 416[A] | PHO  | C3D-C2D | 5.42 | 1.48        | 1.39     |
| 23  | b     | 614    | CLA  | C3C-C2C | 5.42 | 1.48        | 1.36     |
| 23  | b     | 606    | CLA  | C3C-C2C | 5.42 | 1.48        | 1.36     |
| 23  | C     | 513    | CLA  | CHC-C1C | 5.41 | 1.49        | 1.38     |
| 24  | A     | 417[A] | PHO  | C3D-C2D | 5.39 | 1.48        | 1.39     |
| 23  | C     | 511    | CLA  | C1D-ND  | 5.38 | 1.44        | 1.37     |
| 23  | b     | 610    | CLA  | C3C-C2C | 5.37 | 1.48        | 1.36     |
| 23  | C     | 509    | CLA  | C3C-C2C | 5.36 | 1.48        | 1.36     |
| 23  | B     | 616    | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |
| 23  | A     | 404[A] | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 505    | CLA  | O2D-CGD | 5.35  | 1.46        | 1.33     |
| 23  | b     | 602    | CLA  | CHC-C1C | 5.35  | 1.49        | 1.38     |
| 23  | a     | 405[B] | CLA  | C3C-C2C | 5.33  | 1.48        | 1.36     |
| 23  | c     | 509    | CLA  | O2D-CGD | 5.33  | 1.46        | 1.33     |
| 23  | a     | 409    | CLA  | C3C-C2C | 5.33  | 1.48        | 1.36     |
| 23  | B     | 601    | CLA  | C3C-C2C | 5.32  | 1.48        | 1.36     |
| 23  | c     | 506    | CLA  | C3C-C2C | 5.31  | 1.48        | 1.36     |
| 23  | c     | 510    | CLA  | C3C-C2C | 5.31  | 1.48        | 1.36     |
| 23  | b     | 611    | CLA  | C3C-C2C | 5.30  | 1.48        | 1.36     |
| 23  | a     | 406[B] | CLA  | C3C-C2C | 5.30  | 1.48        | 1.36     |
| 23  | b     | 605    | CLA  | C3C-C2C | 5.27  | 1.48        | 1.36     |
| 23  | c     | 504    | CLA  | C3C-C2C | 5.27  | 1.48        | 1.36     |
| 23  | A     | 405[B] | CLA  | C3C-C2C | 5.27  | 1.48        | 1.36     |
| 23  | C     | 508    | CLA  | C3C-C2C | 5.26  | 1.48        | 1.36     |
| 23  | a     | 406[A] | CLA  | C3C-C2C | 5.26  | 1.48        | 1.36     |
| 23  | c     | 510    | CLA  | O2D-CGD | 5.25  | 1.46        | 1.33     |
| 24  | A     | 417[B] | PHO  | OBD-CAD | 5.25  | 1.29        | 1.22     |
| 23  | b     | 614    | CLA  | O2D-CGD | 5.25  | 1.46        | 1.33     |
| 23  | A     | 406[B] | CLA  | C3C-C2C | 5.25  | 1.48        | 1.36     |
| 23  | a     | 407[A] | CLA  | C3C-C2C | 5.24  | 1.48        | 1.36     |
| 23  | b     | 603    | CLA  | C3C-C2C | 5.23  | 1.48        | 1.36     |
| 23  | D     | 703    | CLA  | C1D-ND  | 5.23  | 1.44        | 1.37     |
| 23  | c     | 512    | CLA  | C1D-ND  | 5.23  | 1.44        | 1.37     |
| 23  | c     | 511    | CLA  | O2D-CGD | 5.22  | 1.46        | 1.33     |
| 23  | D     | 702[B] | CLA  | C3C-C2C | 5.22  | 1.48        | 1.36     |
| 23  | C     | 504    | CLA  | C3C-C2C | 5.22  | 1.48        | 1.36     |
| 23  | a     | 407[B] | CLA  | C3C-C2C | 5.22  | 1.48        | 1.36     |
| 23  | d     | 401[B] | CLA  | C3C-C2C | 5.21  | 1.48        | 1.36     |
| 23  | b     | 615    | CLA  | C3C-C2C | 5.21  | 1.48        | 1.36     |
| 23  | d     | 402    | CLA  | CHC-C1C | 5.21  | 1.48        | 1.38     |
| 23  | c     | 511    | CLA  | C3C-C2C | 5.20  | 1.48        | 1.36     |
| 40  | V     | 201    | HEC  | C3D-C2D | 5.20  | 1.52        | 1.38     |
| 23  | C     | 505    | CLA  | C3C-C2C | 5.20  | 1.48        | 1.36     |
| 23  | b     | 601    | CLA  | C3C-C2C | 5.19  | 1.48        | 1.36     |
| 23  | c     | 512    | CLA  | C3C-C2C | 5.17  | 1.47        | 1.36     |
| 25  | C     | 516    | BCR  | C23-C22 | -5.17 | 1.34        | 1.46     |
| 23  | B     | 601    | CLA  | O2A-CGA | 5.17  | 1.48        | 1.33     |
| 25  | C     | 515    | BCR  | C23-C22 | -5.16 | 1.34        | 1.46     |
| 24  | a     | 416[A] | PHO  | OBD-CAD | 5.16  | 1.29        | 1.22     |
| 23  | a     | 406[B] | CLA  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 23  | a     | 406[B] | CLA  | C1D-ND  | 5.15  | 1.44        | 1.37     |
| 23  | c     | 505    | CLA  | C1D-ND  | 5.15  | 1.44        | 1.37     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 613    | CLA  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 23  | B     | 602    | CLA  | C3C-C2C | 5.14  | 1.47        | 1.36     |
| 23  | d     | 401[A] | CLA  | C3C-C2C | 5.14  | 1.47        | 1.36     |
| 23  | c     | 505    | CLA  | C3C-C2C | 5.14  | 1.47        | 1.36     |
| 23  | b     | 602    | CLA  | C3C-C2C | 5.13  | 1.47        | 1.36     |
| 23  | D     | 702[A] | CLA  | C3C-C2C | 5.13  | 1.47        | 1.36     |
| 23  | B     | 606    | CLA  | CHC-C1C | 5.12  | 1.48        | 1.38     |
| 23  | a     | 405[A] | CLA  | C3C-C2C | 5.12  | 1.47        | 1.36     |
| 23  | c     | 514    | CLA  | C3C-C2C | 5.12  | 1.47        | 1.36     |
| 23  | C     | 506    | CLA  | CHC-C1C | 5.11  | 1.48        | 1.38     |
| 23  | c     | 513    | CLA  | CHC-C1C | 5.11  | 1.48        | 1.38     |
| 24  | A     | 417[B] | PHO  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 23  | B     | 605    | CLA  | C1D-ND  | 5.10  | 1.44        | 1.37     |
| 23  | b     | 603    | CLA  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 25  | d     | 403    | BCR  | C23-C22 | -5.10 | 1.35        | 1.46     |
| 23  | C     | 511    | CLA  | C3C-C2C | 5.10  | 1.47        | 1.36     |
| 23  | c     | 507    | CLA  | C3C-C2C | 5.10  | 1.47        | 1.36     |
| 23  | C     | 510    | CLA  | C3C-C2C | 5.09  | 1.47        | 1.36     |
| 23  | B     | 616    | CLA  | CHC-C1C | 5.09  | 1.48        | 1.38     |
| 23  | b     | 610    | CLA  | CHC-C1C | 5.09  | 1.48        | 1.38     |
| 23  | B     | 609    | CLA  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 23  | c     | 503    | CLA  | C3C-C2C | 5.08  | 1.47        | 1.36     |
| 23  | B     | 614    | CLA  | C3C-C2C | 5.08  | 1.47        | 1.36     |
| 23  | b     | 609    | CLA  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 23  | b     | 602    | CLA  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 23  | B     | 605    | CLA  | C3C-C2C | 5.08  | 1.47        | 1.36     |
| 23  | b     | 601    | CLA  | C1D-ND  | 5.08  | 1.44        | 1.37     |
| 23  | c     | 504    | CLA  | CHC-C1C | 5.07  | 1.48        | 1.38     |
| 23  | c     | 506    | CLA  | CHC-C1C | 5.07  | 1.48        | 1.38     |
| 23  | C     | 503    | CLA  | O2D-CGD | 5.06  | 1.45        | 1.33     |
| 23  | C     | 503    | CLA  | C3C-C2C | 5.06  | 1.47        | 1.36     |
| 23  | C     | 514    | CLA  | C3C-C2C | 5.05  | 1.47        | 1.36     |
| 23  | B     | 604    | CLA  | C3C-C2C | 5.04  | 1.47        | 1.36     |
| 23  | c     | 514    | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 24  | A     | 407[B] | PHO  | C3D-C2D | 5.04  | 1.48        | 1.39     |
| 23  | c     | 514    | CLA  | C1D-ND  | 5.03  | 1.44        | 1.37     |
| 24  | a     | 408[B] | PHO  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 23  | B     | 608    | CLA  | C3C-C2C | 5.03  | 1.47        | 1.36     |
| 23  | b     | 614    | CLA  | CHC-C1C | 5.01  | 1.48        | 1.38     |
| 25  | k     | 101    | BCR  | C23-C22 | -5.01 | 1.35        | 1.46     |
| 23  | c     | 502    | CLA  | C1D-ND  | 5.01  | 1.44        | 1.37     |
| 23  | A     | 408    | CLA  | C3C-C2C | 5.01  | 1.47        | 1.36     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 24  | A     | 407[A] | PHO  | C3D-C2D | 5.00 | 1.48        | 1.39     |
| 23  | B     | 613    | CLA  | CHC-C1C | 5.00 | 1.48        | 1.38     |
| 23  | C     | 508    | CLA  | CHC-C1C | 5.00 | 1.48        | 1.38     |
| 23  | C     | 502    | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |
| 23  | C     | 504    | CLA  | CHC-C1C | 4.99 | 1.48        | 1.38     |
| 23  | B     | 609    | CLA  | CHC-C1C | 4.99 | 1.48        | 1.38     |
| 23  | C     | 507    | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 23  | B     | 615    | CLA  | C3C-C2C | 4.99 | 1.47        | 1.36     |
| 23  | C     | 509    | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 23  | b     | 616    | CLA  | C3C-C2C | 4.98 | 1.47        | 1.36     |
| 24  | a     | 408[A] | PHO  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 23  | c     | 503    | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 23  | B     | 601    | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 23  | c     | 514    | CLA  | CHC-C1C | 4.97 | 1.48        | 1.38     |
| 23  | A     | 404[B] | CLA  | C1D-ND  | 4.97 | 1.44        | 1.37     |
| 23  | C     | 509    | CLA  | C1D-ND  | 4.97 | 1.44        | 1.37     |
| 23  | C     | 506    | CLA  | C3C-C2C | 4.97 | 1.47        | 1.36     |
| 23  | A     | 406[A] | CLA  | C3C-C2C | 4.96 | 1.47        | 1.36     |
| 23  | d     | 402    | CLA  | C1D-ND  | 4.96 | 1.44        | 1.37     |
| 23  | B     | 609    | CLA  | C3C-C2C | 4.96 | 1.47        | 1.36     |
| 23  | b     | 613    | CLA  | CHC-C1C | 4.95 | 1.48        | 1.38     |
| 23  | b     | 613    | CLA  | C1D-ND  | 4.95 | 1.44        | 1.37     |
| 23  | b     | 605    | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 26  | X     | 101    | SQD  | O47-C7  | 4.95 | 1.48        | 1.34     |
| 23  | c     | 507    | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 23  | B     | 606    | CLA  | C3C-C2C | 4.94 | 1.47        | 1.36     |
| 23  | a     | 406[A] | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 23  | A     | 404[B] | CLA  | CHC-C1C | 4.93 | 1.48        | 1.38     |
| 24  | a     | 416[B] | PHO  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 23  | b     | 615    | CLA  | CHC-C1C | 4.92 | 1.48        | 1.38     |
| 23  | a     | 409    | CLA  | CHC-C1C | 4.92 | 1.48        | 1.38     |
| 23  | b     | 616    | CLA  | CHC-C1C | 4.91 | 1.48        | 1.38     |
| 23  | B     | 612    | CLA  | C3C-C2C | 4.91 | 1.47        | 1.36     |
| 23  | C     | 511    | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 23  | C     | 512    | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 23  | b     | 616    | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 23  | B     | 603    | CLA  | C3C-C2C | 4.90 | 1.47        | 1.36     |
| 24  | a     | 416[A] | PHO  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 23  | b     | 610    | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 23  | b     | 604    | CLA  | C3C-C2C | 4.89 | 1.47        | 1.36     |
| 23  | a     | 407[B] | CLA  | CHC-C1C | 4.89 | 1.48        | 1.38     |
| 23  | B     | 603    | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 511    | CLA  | CHC-C1C | 4.89  | 1.48        | 1.38     |
| 24  | A     | 407[B] | PHO  | O2D-CGD | 4.89  | 1.45        | 1.33     |
| 25  | B     | 619    | BCR  | C23-C22 | -4.88 | 1.35        | 1.46     |
| 23  | a     | 407[B] | CLA  | O2D-CGD | 4.88  | 1.45        | 1.33     |
| 23  | B     | 615    | CLA  | C1D-ND  | 4.88  | 1.44        | 1.37     |
| 25  | T     | 102    | BCR  | C23-C22 | -4.88 | 1.35        | 1.46     |
| 23  | D     | 702[B] | CLA  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 38  | f     | 101    | HEM  | FE-NB   | 4.87  | 2.09        | 1.94     |
| 23  | C     | 505    | CLA  | CHC-C1C | 4.87  | 1.48        | 1.38     |
| 23  | C     | 510    | CLA  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 24  | A     | 417[A] | PHO  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 23  | D     | 703    | CLA  | CHC-C1C | 4.86  | 1.48        | 1.38     |
| 23  | B     | 612    | CLA  | CHC-C1C | 4.85  | 1.48        | 1.38     |
| 23  | c     | 508    | CLA  | CHC-C1C | 4.85  | 1.48        | 1.38     |
| 24  | A     | 407[A] | PHO  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 23  | A     | 406[A] | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 23  | b     | 613    | CLA  | C3C-C2C | 4.85  | 1.47        | 1.36     |
| 23  | c     | 512    | CLA  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 23  | B     | 610    | CLA  | C1D-ND  | 4.85  | 1.44        | 1.37     |
| 23  | B     | 601    | CLA  | CHC-C1C | 4.85  | 1.48        | 1.38     |
| 23  | A     | 406[B] | CLA  | O2D-CGD | 4.84  | 1.45        | 1.33     |
| 23  | b     | 606    | CLA  | CHC-C1C | 4.84  | 1.48        | 1.38     |
| 23  | C     | 502    | CLA  | CHC-C1C | 4.84  | 1.48        | 1.38     |
| 38  | F     | 102    | HEM  | FE-NB   | 4.83  | 2.09        | 1.94     |
| 25  | D     | 704    | BCR  | C23-C22 | -4.83 | 1.35        | 1.46     |
| 23  | b     | 609    | CLA  | CHC-C1C | 4.83  | 1.48        | 1.38     |
| 23  | B     | 614    | CLA  | C1D-ND  | 4.82  | 1.44        | 1.37     |
| 23  | B     | 615    | CLA  | O2D-CGD | 4.81  | 1.45        | 1.33     |
| 23  | C     | 505    | CLA  | O2D-CGD | 4.81  | 1.45        | 1.33     |
| 23  | c     | 502    | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 23  | C     | 512    | CLA  | C3C-C2C | 4.81  | 1.47        | 1.36     |
| 25  | K     | 102    | BCR  | C23-C22 | -4.81 | 1.35        | 1.46     |
| 24  | a     | 408[B] | PHO  | OBD-CAD | 4.81  | 1.28        | 1.22     |
| 23  | b     | 601    | CLA  | O2D-CGD | 4.80  | 1.45        | 1.33     |
| 23  | A     | 406[A] | CLA  | CHC-C1C | 4.80  | 1.48        | 1.38     |
| 23  | A     | 406[B] | CLA  | CHC-C1C | 4.79  | 1.48        | 1.38     |
| 23  | C     | 502    | CLA  | C1D-ND  | 4.78  | 1.44        | 1.37     |
| 23  | c     | 509    | CLA  | CHC-C1C | 4.78  | 1.48        | 1.38     |
| 23  | b     | 601    | CLA  | O2A-CGA | 4.78  | 1.47        | 1.33     |
| 23  | B     | 607    | CLA  | C3C-C2C | 4.78  | 1.47        | 1.36     |
| 23  | A     | 405[A] | CLA  | C3C-C2C | 4.78  | 1.47        | 1.36     |
| 23  | B     | 605    | CLA  | O2D-CGD | 4.77  | 1.45        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | a     | 406[A] | CLA  | C1D-ND  | 4.77  | 1.44        | 1.37     |
| 23  | B     | 603    | CLA  | C1D-ND  | 4.77  | 1.44        | 1.37     |
| 23  | D     | 703    | CLA  | O2D-CGD | 4.77  | 1.44        | 1.33     |
| 23  | c     | 511    | CLA  | C1D-ND  | 4.76  | 1.44        | 1.37     |
| 23  | c     | 504    | CLA  | C1D-ND  | 4.76  | 1.44        | 1.37     |
| 34  | c     | 521    | LMG  | O7-C10  | 4.75  | 1.47        | 1.34     |
| 23  | D     | 702[A] | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 25  | b     | 617    | BCR  | C23-C22 | -4.75 | 1.35        | 1.46     |
| 25  | y     | 101    | BCR  | C23-C22 | -4.74 | 1.35        | 1.46     |
| 25  | c     | 515    | BCR  | C23-C22 | -4.74 | 1.35        | 1.46     |
| 23  | d     | 401[B] | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 23  | b     | 603    | CLA  | CHC-C1C | 4.74  | 1.48        | 1.38     |
| 23  | B     | 605    | CLA  | CHC-C1C | 4.73  | 1.48        | 1.38     |
| 23  | c     | 513    | CLA  | C1D-ND  | 4.73  | 1.44        | 1.37     |
| 23  | c     | 508    | CLA  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 23  | c     | 502    | CLA  | CHC-C1C | 4.72  | 1.47        | 1.38     |
| 23  | b     | 608    | CLA  | C3C-C2C | 4.72  | 1.47        | 1.36     |
| 34  | C     | 521    | LMG  | O7-C10  | 4.72  | 1.47        | 1.34     |
| 23  | b     | 613    | CLA  | O2D-CGD | 4.72  | 1.44        | 1.33     |
| 23  | C     | 507    | CLA  | C3C-C2C | 4.72  | 1.46        | 1.36     |
| 23  | b     | 616    | CLA  | C1D-ND  | 4.71  | 1.44        | 1.37     |
| 23  | A     | 405[B] | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 23  | c     | 506    | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 23  | C     | 514    | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |
| 23  | b     | 609    | CLA  | C3C-C2C | 4.70  | 1.46        | 1.36     |
| 26  | a     | 412    | SQD  | O48-C23 | 4.69  | 1.47        | 1.33     |
| 23  | d     | 402    | CLA  | O2D-CGD | 4.69  | 1.44        | 1.33     |
| 25  | c     | 516    | BCR  | C23-C22 | -4.69 | 1.35        | 1.46     |
| 24  | A     | 407[B] | PHO  | OBD-CAD | 4.68  | 1.28        | 1.22     |
| 23  | A     | 404[A] | CLA  | O2D-CGD | 4.68  | 1.44        | 1.33     |
| 23  | B     | 613    | CLA  | C3C-C2C | 4.68  | 1.46        | 1.36     |
| 23  | B     | 612    | CLA  | CHB-C1B | 4.68  | 1.49        | 1.39     |
| 23  | A     | 408    | CLA  | O2D-CGD | 4.68  | 1.44        | 1.33     |
| 25  | B     | 617    | BCR  | C23-C22 | -4.68 | 1.35        | 1.46     |
| 23  | B     | 601    | CLA  | C1D-ND  | 4.67  | 1.44        | 1.37     |
| 25  | b     | 619    | BCR  | C23-C22 | -4.67 | 1.36        | 1.46     |
| 23  | c     | 509    | CLA  | C1D-ND  | 4.67  | 1.44        | 1.37     |
| 23  | a     | 409    | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 23  | a     | 407[A] | CLA  | CHC-C1C | 4.66  | 1.47        | 1.38     |
| 23  | b     | 607    | CLA  | CHC-C1C | 4.65  | 1.47        | 1.38     |
| 23  | B     | 610    | CLA  | O2D-CGD | 4.65  | 1.44        | 1.33     |
| 23  | A     | 405[B] | CLA  | CHC-C1C | 4.65  | 1.47        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24  | a     | 408[A] | PHO  | OBD-CAD | 4.64  | 1.28        | 1.22     |
| 23  | b     | 615    | CLA  | C1D-ND  | 4.64  | 1.44        | 1.37     |
| 23  | c     | 503    | CLA  | C1D-ND  | 4.64  | 1.44        | 1.37     |
| 23  | b     | 615    | CLA  | O2D-CGD | 4.63  | 1.44        | 1.33     |
| 23  | C     | 508    | CLA  | O2D-CGD | 4.63  | 1.44        | 1.33     |
| 23  | c     | 510    | CLA  | C1D-ND  | 4.63  | 1.43        | 1.37     |
| 23  | c     | 512    | CLA  | CHC-C1C | 4.63  | 1.47        | 1.38     |
| 23  | B     | 611    | CLA  | CHC-C4B | 4.63  | 1.49        | 1.39     |
| 23  | A     | 405[A] | CLA  | CHC-C1C | 4.63  | 1.47        | 1.38     |
| 23  | B     | 611    | CLA  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 23  | A     | 404[B] | CLA  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 23  | C     | 514    | CLA  | C1D-ND  | 4.62  | 1.43        | 1.37     |
| 23  | a     | 405[B] | CLA  | C1D-ND  | 4.62  | 1.43        | 1.37     |
| 23  | d     | 401[A] | CLA  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 23  | C     | 512    | CLA  | CHC-C1C | 4.61  | 1.47        | 1.38     |
| 23  | c     | 508    | CLA  | C3C-C2C | 4.61  | 1.46        | 1.36     |
| 25  | A     | 409    | BCR  | C23-C22 | -4.61 | 1.36        | 1.46     |
| 23  | c     | 507    | CLA  | C1D-ND  | 4.60  | 1.43        | 1.37     |
| 24  | A     | 417[A] | PHO  | OBD-CAD | 4.60  | 1.28        | 1.22     |
| 23  | C     | 503    | CLA  | C1D-ND  | 4.60  | 1.43        | 1.37     |
| 23  | B     | 602    | CLA  | CHC-C1C | 4.59  | 1.47        | 1.38     |
| 23  | B     | 604    | CLA  | O2D-CGD | 4.59  | 1.44        | 1.33     |
| 25  | h     | 101    | BCR  | C23-C22 | -4.59 | 1.36        | 1.46     |
| 23  | a     | 405[B] | CLA  | O2D-CGD | 4.59  | 1.44        | 1.33     |
| 23  | b     | 608    | CLA  | O2D-CGD | 4.59  | 1.44        | 1.33     |
| 23  | C     | 506    | CLA  | CHD-C1D | 4.58  | 1.47        | 1.38     |
| 23  | B     | 611    | CLA  | C4B-NB  | -4.58 | 1.31        | 1.37     |
| 25  | t     | 102    | BCR  | C23-C22 | -4.58 | 1.36        | 1.46     |
| 26  | B     | 620    | SQD  | O47-C7  | 4.58  | 1.47        | 1.34     |
| 23  | c     | 505    | CLA  | CHC-C1C | 4.57  | 1.47        | 1.38     |
| 26  | A     | 412    | SQD  | O48-C23 | 4.57  | 1.46        | 1.33     |
| 23  | B     | 610    | CLA  | CHC-C1C | 4.57  | 1.47        | 1.38     |
| 23  | C     | 506    | CLA  | C1D-ND  | 4.57  | 1.43        | 1.37     |
| 23  | b     | 601    | CLA  | CHC-C1C | 4.57  | 1.47        | 1.38     |
| 23  | D     | 702[B] | CLA  | CHC-C1C | 4.56  | 1.47        | 1.38     |
| 23  | B     | 615    | CLA  | CHC-C1C | 4.56  | 1.47        | 1.38     |
| 23  | B     | 614    | CLA  | O2D-CGD | 4.55  | 1.44        | 1.33     |
| 23  | c     | 513    | CLA  | O2D-CGD | 4.54  | 1.44        | 1.33     |
| 23  | b     | 612    | CLA  | CHC-C1C | 4.54  | 1.47        | 1.38     |
| 23  | B     | 602    | CLA  | C1D-ND  | 4.53  | 1.43        | 1.37     |
| 23  | b     | 612    | CLA  | O2D-CGD | 4.53  | 1.44        | 1.33     |
| 34  | C     | 521    | LMG  | O8-C28  | 4.53  | 1.46        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 604    | CLA  | CHD-C1D | 4.53  | 1.47        | 1.38     |
| 23  | b     | 611    | CLA  | C1D-ND  | 4.53  | 1.43        | 1.37     |
| 23  | b     | 606    | CLA  | O2D-CGD | 4.52  | 1.44        | 1.33     |
| 23  | B     | 606    | CLA  | C1D-ND  | 4.52  | 1.43        | 1.37     |
| 23  | C     | 507    | CLA  | CHD-C1D | 4.51  | 1.47        | 1.38     |
| 23  | A     | 408    | CLA  | O2A-CGA | 4.51  | 1.46        | 1.33     |
| 26  | f     | 102    | SQD  | O47-C7  | 4.51  | 1.47        | 1.34     |
| 23  | b     | 611    | CLA  | O2D-CGD | 4.50  | 1.44        | 1.33     |
| 23  | A     | 405[B] | CLA  | C1D-ND  | 4.50  | 1.43        | 1.37     |
| 34  | z     | 101    | LMG  | O8-C28  | 4.50  | 1.46        | 1.33     |
| 23  | a     | 405[A] | CLA  | O2D-CGD | 4.49  | 1.44        | 1.33     |
| 23  | C     | 513    | CLA  | C1D-ND  | 4.49  | 1.43        | 1.37     |
| 23  | a     | 406[B] | CLA  | CHC-C1C | 4.49  | 1.47        | 1.38     |
| 33  | E     | 101[A] | LHG  | O8-C23  | 4.48  | 1.46        | 1.33     |
| 23  | C     | 510    | CLA  | CHD-C1D | 4.48  | 1.47        | 1.38     |
| 23  | a     | 406[A] | CLA  | CHC-C1C | 4.48  | 1.47        | 1.38     |
| 23  | c     | 514    | CLA  | O2A-CGA | 4.48  | 1.46        | 1.33     |
| 23  | b     | 611    | CLA  | CHC-C1C | 4.48  | 1.47        | 1.38     |
| 23  | c     | 504    | CLA  | O2A-CGA | 4.47  | 1.46        | 1.33     |
| 23  | a     | 407[B] | CLA  | C1D-ND  | 4.47  | 1.43        | 1.37     |
| 23  | A     | 406[B] | CLA  | CHD-C1D | 4.47  | 1.47        | 1.38     |
| 23  | d     | 401[B] | CLA  | CHC-C1C | 4.47  | 1.47        | 1.38     |
| 23  | c     | 507    | CLA  | CHC-C1C | 4.46  | 1.47        | 1.38     |
| 33  | E     | 101[B] | LHG  | O8-C23  | 4.45  | 1.46        | 1.33     |
| 23  | a     | 407[A] | CLA  | O2D-CGD | 4.45  | 1.44        | 1.33     |
| 23  | C     | 502    | CLA  | CHD-C1D | 4.45  | 1.47        | 1.38     |
| 23  | B     | 602    | CLA  | O2D-CGD | 4.44  | 1.44        | 1.33     |
| 23  | a     | 409    | CLA  | O2A-CGA | 4.44  | 1.46        | 1.33     |
| 23  | B     | 614    | CLA  | CHC-C1C | 4.44  | 1.47        | 1.38     |
| 23  | b     | 602    | CLA  | CHD-C1D | 4.44  | 1.47        | 1.38     |
| 23  | a     | 405[A] | CLA  | CHC-C1C | 4.44  | 1.47        | 1.38     |
| 34  | B     | 621    | LMG  | O8-C28  | 4.43  | 1.46        | 1.33     |
| 23  | B     | 604    | CLA  | CHC-C1C | 4.43  | 1.47        | 1.38     |
| 23  | a     | 406[A] | CLA  | C3D-C2D | 4.43  | 1.51        | 1.39     |
| 23  | b     | 609    | CLA  | C1D-ND  | 4.43  | 1.43        | 1.37     |
| 23  | B     | 612    | CLA  | O2D-CGD | 4.43  | 1.44        | 1.33     |
| 23  | b     | 607    | CLA  | O2D-CGD | 4.43  | 1.44        | 1.33     |
| 23  | b     | 614    | CLA  | C1D-ND  | 4.43  | 1.43        | 1.37     |
| 25  | H     | 101    | BCR  | C23-C22 | -4.43 | 1.36        | 1.46     |
| 23  | C     | 510    | CLA  | C1D-ND  | 4.42  | 1.43        | 1.37     |
| 23  | A     | 408    | CLA  | CHC-C1C | 4.42  | 1.47        | 1.38     |
| 24  | A     | 407[A] | PHO  | OBD-CAD | 4.41  | 1.28        | 1.22     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 513    | CLA  | CHD-C1D | 4.41  | 1.47        | 1.38     |
| 23  | B     | 610    | CLA  | OBD-CAD | 4.41  | 1.30        | 1.22     |
| 36  | c     | 519    | DGD  | O1G-C1A | 4.41  | 1.46        | 1.33     |
| 23  | C     | 503    | CLA  | CHC-C1C | 4.41  | 1.47        | 1.38     |
| 33  | a     | 420[B] | LHG  | O8-C23  | 4.41  | 1.46        | 1.33     |
| 23  | C     | 506    | CLA  | O2D-CGD | 4.41  | 1.44        | 1.33     |
| 33  | a     | 420[A] | LHG  | O8-C23  | 4.40  | 1.46        | 1.33     |
| 23  | B     | 614    | CLA  | CHD-C4C | 4.40  | 1.49        | 1.39     |
| 23  | d     | 402    | CLA  | O2A-CGA | 4.40  | 1.46        | 1.33     |
| 23  | A     | 405[B] | CLA  | O2A-CGA | 4.40  | 1.46        | 1.33     |
| 23  | C     | 513    | CLA  | O2D-CGD | 4.39  | 1.44        | 1.33     |
| 23  | C     | 514    | CLA  | CHC-C1C | 4.39  | 1.47        | 1.38     |
| 23  | c     | 511    | CLA  | CHC-C1C | 4.39  | 1.47        | 1.38     |
| 23  | A     | 404[A] | CLA  | CHC-C1C | 4.39  | 1.47        | 1.38     |
| 33  | d     | 406[B] | LHG  | O8-C23  | 4.39  | 1.46        | 1.33     |
| 23  | b     | 602    | CLA  | C1D-ND  | 4.38  | 1.43        | 1.37     |
| 26  | b     | 620    | SQD  | O47-C7  | 4.38  | 1.46        | 1.34     |
| 23  | c     | 504    | CLA  | CHD-C1D | 4.38  | 1.47        | 1.38     |
| 23  | B     | 609    | CLA  | CHD-C1D | 4.37  | 1.46        | 1.38     |
| 23  | B     | 605    | CLA  | CHC-C4B | 4.37  | 1.49        | 1.39     |
| 23  | b     | 613    | CLA  | C3D-C2D | 4.36  | 1.50        | 1.39     |
| 23  | B     | 613    | CLA  | C1D-ND  | 4.36  | 1.43        | 1.37     |
| 23  | c     | 503    | CLA  | C3D-C2D | 4.36  | 1.50        | 1.39     |
| 23  | c     | 513    | CLA  | O2A-CGA | 4.36  | 1.46        | 1.33     |
| 23  | B     | 615    | CLA  | CHD-C1D | 4.35  | 1.46        | 1.38     |
| 23  | B     | 606    | CLA  | O2D-CGD | 4.35  | 1.43        | 1.33     |
| 23  | c     | 502    | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 23  | a     | 406[B] | CLA  | O2A-CGA | 4.34  | 1.46        | 1.33     |
| 23  | c     | 514    | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 23  | a     | 405[B] | CLA  | CHC-C1C | 4.34  | 1.47        | 1.38     |
| 23  | D     | 702[B] | CLA  | C1D-ND  | 4.34  | 1.43        | 1.37     |
| 23  | b     | 601    | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 26  | f     | 102    | SQD  | O48-C23 | 4.34  | 1.46        | 1.33     |
| 23  | b     | 606    | CLA  | C1D-ND  | 4.33  | 1.43        | 1.37     |
| 34  | C     | 520    | LMG  | O8-C28  | 4.33  | 1.46        | 1.33     |
| 23  | D     | 702[A] | CLA  | CHC-C1C | 4.32  | 1.47        | 1.38     |
| 23  | b     | 604    | CLA  | CHC-C1C | 4.32  | 1.47        | 1.38     |
| 23  | B     | 603    | CLA  | CHC-C1C | 4.32  | 1.47        | 1.38     |
| 23  | b     | 604    | CLA  | O2D-CGD | 4.32  | 1.43        | 1.33     |
| 33  | d     | 406[A] | LHG  | O8-C23  | 4.32  | 1.45        | 1.33     |
| 25  | a     | 410    | BCR  | C23-C22 | -4.31 | 1.36        | 1.46     |
| 23  | C     | 504    | CLA  | C1D-ND  | 4.31  | 1.43        | 1.37     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 504    | CLA  | O2D-CGD | 4.30  | 1.43        | 1.33     |
| 23  | A     | 405[A] | CLA  | O2D-CGD | 4.30  | 1.43        | 1.33     |
| 23  | B     | 609    | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 23  | b     | 602    | CLA  | CHC-C4B | 4.29  | 1.49        | 1.39     |
| 23  | D     | 703    | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 26  | b     | 620    | SQD  | O48-C23 | 4.29  | 1.45        | 1.33     |
| 23  | B     | 602    | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 23  | C     | 514    | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 23  | C     | 510    | CLA  | CHC-C1C | 4.28  | 1.47        | 1.38     |
| 23  | b     | 608    | CLA  | CHC-C1C | 4.28  | 1.47        | 1.38     |
| 38  | F     | 102    | HEM  | FE-NC   | 4.28  | 2.09        | 1.95     |
| 34  | c     | 521    | LMG  | O8-C28  | 4.27  | 1.45        | 1.33     |
| 33  | L     | 101[B] | LHG  | O8-C23  | 4.27  | 1.45        | 1.33     |
| 23  | c     | 510    | CLA  | CHC-C1C | 4.27  | 1.47        | 1.38     |
| 23  | C     | 507    | CLA  | C1D-ND  | 4.26  | 1.43        | 1.37     |
| 23  | a     | 405[A] | CLA  | C1D-ND  | 4.26  | 1.43        | 1.37     |
| 23  | a     | 407[B] | CLA  | C3D-C2D | 4.25  | 1.50        | 1.39     |
| 23  | c     | 508    | CLA  | C1D-ND  | 4.25  | 1.43        | 1.37     |
| 23  | b     | 609    | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 23  | c     | 508    | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 23  | B     | 609    | CLA  | C1D-ND  | 4.24  | 1.43        | 1.37     |
| 23  | c     | 512    | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 23  | B     | 613    | CLA  | C3D-C2D | 4.24  | 1.50        | 1.39     |
| 23  | d     | 401[B] | CLA  | C1D-ND  | 4.24  | 1.43        | 1.37     |
| 25  | b     | 618    | BCR  | C23-C22 | -4.24 | 1.36        | 1.46     |
| 23  | B     | 616    | CLA  | O2D-CGD | 4.24  | 1.43        | 1.33     |
| 23  | b     | 612    | CLA  | CHB-C1B | 4.23  | 1.48        | 1.39     |
| 23  | b     | 605    | CLA  | C1D-ND  | 4.23  | 1.43        | 1.37     |
| 23  | C     | 504    | CLA  | CHD-C4C | 4.23  | 1.48        | 1.39     |
| 23  | c     | 509    | CLA  | C3D-C2D | 4.23  | 1.50        | 1.39     |
| 23  | D     | 702[A] | CLA  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 23  | c     | 512    | CLA  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 26  | B     | 620    | SQD  | O48-C23 | 4.22  | 1.45        | 1.33     |
| 23  | b     | 605    | CLA  | CHC-C1C | 4.22  | 1.46        | 1.38     |
| 23  | c     | 505    | CLA  | C3D-C2D | 4.22  | 1.50        | 1.39     |
| 34  | m     | 101    | LMG  | O8-C28  | 4.21  | 1.45        | 1.33     |
| 23  | C     | 513    | CLA  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 23  | B     | 615    | CLA  | OBD-CAD | 4.21  | 1.29        | 1.22     |
| 23  | B     | 607    | CLA  | CHC-C1C | 4.21  | 1.46        | 1.38     |
| 23  | D     | 702[B] | CLA  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 23  | C     | 509    | CLA  | C3D-C2D | 4.21  | 1.50        | 1.39     |
| 23  | d     | 401[A] | CLA  | CHC-C1C | 4.21  | 1.46        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 23  | B     | 608    | CLA  | CHC-C1C | 4.20 | 1.46        | 1.38     |
| 23  | A     | 406[B] | CLA  | O2A-CGA | 4.20 | 1.45        | 1.33     |
| 23  | C     | 507    | CLA  | CHC-C1C | 4.20 | 1.46        | 1.38     |
| 23  | B     | 614    | CLA  | CHB-C1B | 4.20 | 1.48        | 1.39     |
| 36  | C     | 517[B] | DGD  | O2G-C1B | 4.20 | 1.46        | 1.34     |
| 23  | C     | 512    | CLA  | CHD-C1D | 4.20 | 1.46        | 1.38     |
| 23  | b     | 601    | CLA  | C3D-C2D | 4.20 | 1.50        | 1.39     |
| 36  | c     | 518[B] | DGD  | O1G-C1A | 4.20 | 1.45        | 1.33     |
| 33  | E     | 101[B] | LHG  | O7-C7   | 4.19 | 1.46        | 1.34     |
| 23  | c     | 507    | CLA  | CHD-C1D | 4.19 | 1.46        | 1.38     |
| 23  | C     | 512    | CLA  | CHD-C4C | 4.19 | 1.48        | 1.39     |
| 23  | B     | 608    | CLA  | O2D-CGD | 4.19 | 1.43        | 1.33     |
| 33  | E     | 101[A] | LHG  | O7-C7   | 4.19 | 1.46        | 1.34     |
| 23  | b     | 607    | CLA  | CHD-C1D | 4.19 | 1.46        | 1.38     |
| 23  | C     | 509    | CLA  | CHC-C1C | 4.19 | 1.46        | 1.38     |
| 23  | c     | 503    | CLA  | CHC-C1C | 4.18 | 1.46        | 1.38     |
| 23  | b     | 609    | CLA  | CHB-C1B | 4.18 | 1.48        | 1.39     |
| 33  | a     | 420[B] | LHG  | O7-C7   | 4.18 | 1.46        | 1.34     |
| 23  | B     | 603    | CLA  | C3D-C2D | 4.17 | 1.50        | 1.39     |
| 23  | C     | 512    | CLA  | O2A-CGA | 4.17 | 1.45        | 1.33     |
| 34  | Z     | 101    | LMG  | O7-C10  | 4.17 | 1.46        | 1.34     |
| 23  | C     | 503    | CLA  | CHD-C1D | 4.17 | 1.46        | 1.38     |
| 23  | b     | 610    | CLA  | CHD-C4C | 4.17 | 1.48        | 1.39     |
| 36  | C     | 519    | DGD  | O1G-C1A | 4.17 | 1.45        | 1.33     |
| 23  | C     | 514    | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 23  | b     | 604    | CLA  | C1D-ND  | 4.16 | 1.43        | 1.37     |
| 23  | b     | 602    | CLA  | CHD-C4C | 4.16 | 1.48        | 1.39     |
| 23  | C     | 508    | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 23  | c     | 508    | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 23  | b     | 610    | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 23  | c     | 503    | CLA  | CHD-C4C | 4.16 | 1.48        | 1.39     |
| 23  | b     | 608    | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 23  | A     | 406[A] | CLA  | CHD-C1D | 4.15 | 1.46        | 1.38     |
| 26  | A     | 412    | SQD  | O47-C7  | 4.15 | 1.46        | 1.34     |
| 23  | b     | 608    | CLA  | OBD-CAD | 4.15 | 1.29        | 1.22     |
| 23  | c     | 502    | CLA  | O2D-CGD | 4.14 | 1.43        | 1.33     |
| 34  | c     | 501    | LMG  | O7-C10  | 4.14 | 1.46        | 1.34     |
| 23  | a     | 406[B] | CLA  | C3D-C2D | 4.14 | 1.50        | 1.39     |
| 23  | c     | 507    | CLA  | CHD-C4C | 4.14 | 1.48        | 1.39     |
| 23  | C     | 511    | CLA  | CHD-C4C | 4.14 | 1.48        | 1.39     |
| 23  | c     | 509    | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 33  | a     | 420[A] | LHG  | O7-C7   | 4.13 | 1.46        | 1.34     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 34  | c     | 520    | LMG  | O8-C28  | 4.13 | 1.45        | 1.33     |
| 23  | c     | 513    | CLA  | CHC-C4B | 4.13 | 1.48        | 1.39     |
| 23  | a     | 407[A] | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 34  | z     | 101    | LMG  | O7-C10  | 4.13 | 1.45        | 1.34     |
| 23  | C     | 503    | CLA  | C3D-C2D | 4.13 | 1.50        | 1.39     |
| 23  | A     | 404[B] | CLA  | CHD-C1D | 4.13 | 1.46        | 1.38     |
| 23  | c     | 502    | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 23  | A     | 405[B] | CLA  | C3D-C2D | 4.12 | 1.50        | 1.39     |
| 23  | B     | 611    | CLA  | OBD-CAD | 4.12 | 1.29        | 1.22     |
| 23  | A     | 404[B] | CLA  | CHD-C4C | 4.12 | 1.48        | 1.39     |
| 23  | C     | 506    | CLA  | CHD-C4C | 4.12 | 1.48        | 1.39     |
| 23  | c     | 509    | CLA  | OBD-CAD | 4.11 | 1.29        | 1.22     |
| 23  | c     | 507    | CLA  | O2A-CGA | 4.11 | 1.45        | 1.33     |
| 23  | d     | 401[A] | CLA  | CHB-C1B | 4.11 | 1.48        | 1.39     |
| 23  | a     | 406[B] | CLA  | CHD-C1D | 4.11 | 1.46        | 1.38     |
| 23  | c     | 504    | CLA  | CHC-C4B | 4.11 | 1.48        | 1.39     |
| 23  | b     | 604    | CLA  | CHD-C1D | 4.11 | 1.46        | 1.38     |
| 23  | B     | 611    | CLA  | C3B-C2B | 4.11 | 1.55        | 1.41     |
| 23  | c     | 504    | CLA  | CHD-C4C | 4.10 | 1.48        | 1.39     |
| 23  | A     | 405[A] | CLA  | C3D-C2D | 4.10 | 1.50        | 1.39     |
| 26  | a     | 412    | SQD  | O47-C7  | 4.10 | 1.45        | 1.34     |
| 23  | B     | 605    | CLA  | CHB-C1B | 4.10 | 1.48        | 1.39     |
| 23  | B     | 610    | CLA  | CHD-C1D | 4.10 | 1.46        | 1.38     |
| 23  | C     | 514    | CLA  | C3D-C2D | 4.10 | 1.50        | 1.39     |
| 23  | b     | 610    | CLA  | C1D-ND  | 4.10 | 1.43        | 1.37     |
| 26  | a     | 411[B] | SQD  | O47-C7  | 4.09 | 1.45        | 1.34     |
| 23  | c     | 512    | CLA  | CHB-C1B | 4.09 | 1.48        | 1.39     |
| 23  | B     | 608    | CLA  | C1D-ND  | 4.09 | 1.43        | 1.37     |
| 23  | B     | 614    | CLA  | O2A-CGA | 4.09 | 1.45        | 1.33     |
| 23  | b     | 611    | CLA  | CHD-C1D | 4.09 | 1.46        | 1.38     |
| 23  | a     | 406[A] | CLA  | O2A-CGA | 4.09 | 1.45        | 1.33     |
| 36  | c     | 517[A] | DGD  | O2G-C1B | 4.09 | 1.45        | 1.34     |
| 34  | c     | 520    | LMG  | O7-C10  | 4.09 | 1.45        | 1.34     |
| 23  | b     | 611    | CLA  | O2A-CGA | 4.08 | 1.45        | 1.33     |
| 23  | c     | 503    | CLA  | O2A-CGA | 4.08 | 1.45        | 1.33     |
| 23  | b     | 612    | CLA  | CHD-C1D | 4.08 | 1.46        | 1.38     |
| 23  | D     | 703    | CLA  | CHC-C4B | 4.08 | 1.48        | 1.39     |
| 23  | c     | 510    | CLA  | O2A-CGA | 4.08 | 1.45        | 1.33     |
| 23  | c     | 510    | CLA  | CHD-C1D | 4.08 | 1.46        | 1.38     |
| 23  | c     | 514    | CLA  | CHD-C4C | 4.08 | 1.48        | 1.39     |
| 23  | C     | 509    | CLA  | O2A-CGA | 4.08 | 1.45        | 1.33     |
| 23  | b     | 601    | CLA  | CHD-C4C | 4.08 | 1.48        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 512    | CLA  | OBD-CAD | 4.08  | 1.29        | 1.22     |
| 34  | C     | 501    | LMG  | O8-C28  | 4.07  | 1.45        | 1.33     |
| 23  | C     | 509    | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 26  | a     | 411[A] | SQD  | O47-C7  | 4.07  | 1.45        | 1.34     |
| 23  | c     | 502    | CLA  | CHB-C1B | 4.07  | 1.48        | 1.39     |
| 26  | a     | 411[B] | SQD  | O48-C23 | 4.06  | 1.45        | 1.33     |
| 23  | c     | 503    | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 36  | C     | 517[A] | DGD  | O2G-C1B | 4.06  | 1.45        | 1.34     |
| 23  | d     | 401[A] | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 23  | C     | 508    | CLA  | C3D-C2D | 4.06  | 1.50        | 1.39     |
| 34  | c     | 501    | LMG  | O8-C28  | 4.06  | 1.45        | 1.33     |
| 23  | B     | 604    | CLA  | CHB-C1B | 4.05  | 1.48        | 1.39     |
| 23  | D     | 702[A] | CLA  | CHB-C1B | 4.05  | 1.48        | 1.39     |
| 23  | B     | 608    | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 23  | b     | 616    | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 26  | X     | 101    | SQD  | O48-C23 | 4.05  | 1.45        | 1.33     |
| 23  | c     | 506    | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 23  | d     | 402    | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 36  | c     | 517[B] | DGD  | O2G-C1B | 4.05  | 1.45        | 1.34     |
| 25  | Y     | 101    | BCR  | C23-C22 | -4.05 | 1.37        | 1.46     |
| 23  | C     | 512    | CLA  | CHB-C1B | 4.05  | 1.48        | 1.39     |
| 23  | b     | 614    | CLA  | C3D-C2D | 4.04  | 1.50        | 1.39     |
| 23  | C     | 505    | CLA  | C3D-C2D | 4.04  | 1.50        | 1.39     |
| 23  | A     | 408    | CLA  | C1D-ND  | 4.04  | 1.43        | 1.37     |
| 23  | B     | 609    | CLA  | C3D-C2D | 4.04  | 1.50        | 1.39     |
| 23  | B     | 601    | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 23  | a     | 406[B] | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 23  | C     | 513    | CLA  | C3D-C2D | 4.03  | 1.50        | 1.39     |
| 23  | B     | 614    | CLA  | CHC-C4B | 4.03  | 1.48        | 1.39     |
| 23  | d     | 401[B] | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 23  | B     | 615    | CLA  | C3D-C2D | 4.03  | 1.50        | 1.39     |
| 23  | b     | 614    | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 23  | c     | 512    | CLA  | CHD-C4C | 4.02  | 1.48        | 1.39     |
| 36  | C     | 518[B] | DGD  | O1G-C1A | 4.02  | 1.45        | 1.33     |
| 23  | B     | 612    | CLA  | C1B-NB  | -4.02 | 1.32        | 1.37     |
| 23  | C     | 509    | CLA  | CHB-C1B | 4.02  | 1.48        | 1.39     |
| 23  | a     | 405[B] | CLA  | CHD-C4C | 4.02  | 1.48        | 1.39     |
| 23  | B     | 606    | CLA  | O2A-CGA | 4.02  | 1.45        | 1.33     |
| 23  | C     | 506    | CLA  | CHB-C1B | 4.02  | 1.48        | 1.39     |
| 23  | a     | 407[B] | CLA  | O2A-CGA | 4.01  | 1.45        | 1.33     |
| 23  | b     | 605    | CLA  | CHD-C1D | 4.01  | 1.46        | 1.38     |
| 23  | c     | 513    | CLA  | C3D-C2D | 4.01  | 1.49        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 513    | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 23  | C     | 505    | CLA  | C1D-ND  | 4.01  | 1.43        | 1.37     |
| 23  | c     | 507    | CLA  | C3D-C2D | 4.01  | 1.49        | 1.39     |
| 34  | d     | 410    | LMG  | O8-C28  | 4.01  | 1.45        | 1.33     |
| 23  | A     | 406[B] | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 23  | c     | 502    | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 23  | b     | 612    | CLA  | C1D-ND  | 4.01  | 1.43        | 1.37     |
| 38  | f     | 101    | HEM  | FE-NC   | 4.01  | 2.08        | 1.95     |
| 23  | D     | 703    | CLA  | C3D-C2D | 4.01  | 1.49        | 1.39     |
| 23  | A     | 404[A] | CLA  | CHD-C1D | 4.00  | 1.46        | 1.38     |
| 34  | C     | 520    | LMG  | O7-C10  | 4.00  | 1.45        | 1.34     |
| 23  | C     | 513    | CLA  | CHC-C4B | 3.99  | 1.48        | 1.39     |
| 23  | B     | 603    | CLA  | CHB-C1B | 3.99  | 1.48        | 1.39     |
| 33  | d     | 412[B] | LHG  | O8-C23  | 3.99  | 1.45        | 1.33     |
| 36  | h     | 102    | DGD  | O2G-C1B | 3.99  | 1.45        | 1.34     |
| 23  | C     | 504    | CLA  | CHD-C1D | 3.99  | 1.46        | 1.38     |
| 23  | b     | 608    | CLA  | CHD-C1D | 3.99  | 1.46        | 1.38     |
| 23  | B     | 616    | CLA  | C3D-C2D | 3.99  | 1.49        | 1.39     |
| 26  | a     | 411[A] | SQD  | O48-C23 | 3.99  | 1.45        | 1.33     |
| 23  | b     | 616    | CLA  | O2A-CGA | 3.99  | 1.45        | 1.33     |
| 23  | B     | 609    | CLA  | CHC-C4B | 3.98  | 1.48        | 1.39     |
| 33  | L     | 101[B] | LHG  | O7-C7   | 3.98  | 1.45        | 1.34     |
| 33  | D     | 707[A] | LHG  | O7-C7   | 3.98  | 1.45        | 1.34     |
| 23  | c     | 510    | CLA  | CHB-C1B | 3.98  | 1.48        | 1.39     |
| 23  | B     | 616    | CLA  | O2A-CGA | 3.98  | 1.45        | 1.33     |
| 23  | d     | 402    | CLA  | C3D-C2D | 3.98  | 1.49        | 1.39     |
| 23  | a     | 405[A] | CLA  | CHD-C4C | 3.98  | 1.48        | 1.39     |
| 34  | B     | 621    | LMG  | O7-C10  | 3.98  | 1.45        | 1.34     |
| 23  | B     | 610    | CLA  | C3D-C2D | 3.98  | 1.49        | 1.39     |
| 23  | B     | 607    | CLA  | C1B-NB  | -3.97 | 1.32        | 1.37     |
| 23  | b     | 612    | CLA  | C3D-C2D | 3.97  | 1.49        | 1.39     |
| 23  | A     | 408    | CLA  | CHD-C1D | 3.97  | 1.46        | 1.38     |
| 33  | d     | 405[B] | LHG  | O7-C7   | 3.97  | 1.45        | 1.34     |
| 23  | C     | 507    | CLA  | O2A-CGA | 3.97  | 1.44        | 1.33     |
| 23  | b     | 606    | CLA  | CHD-C1D | 3.97  | 1.46        | 1.38     |
| 24  | A     | 417[B] | PHO  | O2A-CGA | 3.97  | 1.44        | 1.33     |
| 23  | C     | 510    | CLA  | O2A-CGA | 3.97  | 1.44        | 1.33     |
| 23  | b     | 615    | CLA  | O2A-CGA | 3.97  | 1.44        | 1.33     |
| 23  | c     | 506    | CLA  | CHC-C4B | 3.97  | 1.48        | 1.39     |
| 23  | c     | 505    | CLA  | CHD-C1D | 3.97  | 1.46        | 1.38     |
| 23  | B     | 601    | CLA  | CHC-C4B | 3.96  | 1.48        | 1.39     |
| 23  | B     | 606    | CLA  | CHB-C1B | 3.96  | 1.48        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | D     | 703    | CLA  | CHD-C4C | 3.96  | 1.48        | 1.39     |
| 23  | c     | 506    | CLA  | C1D-ND  | 3.96  | 1.43        | 1.37     |
| 23  | B     | 615    | CLA  | O2A-CGA | 3.96  | 1.44        | 1.33     |
| 23  | C     | 510    | CLA  | C3D-C2D | 3.96  | 1.49        | 1.39     |
| 23  | a     | 405[A] | CLA  | CHD-C1D | 3.96  | 1.46        | 1.38     |
| 23  | C     | 512    | CLA  | C3D-C2D | 3.95  | 1.49        | 1.39     |
| 23  | C     | 503    | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 23  | B     | 604    | CLA  | OBD-CAD | 3.95  | 1.29        | 1.22     |
| 23  | A     | 406[B] | CLA  | C1D-ND  | 3.95  | 1.43        | 1.37     |
| 23  | b     | 612    | CLA  | CHC-C4B | 3.95  | 1.48        | 1.39     |
| 23  | A     | 405[B] | CLA  | CHD-C1D | 3.95  | 1.46        | 1.38     |
| 33  | D     | 707[B] | LHG  | O8-C23  | 3.95  | 1.44        | 1.33     |
| 23  | c     | 508    | CLA  | OBD-CAD | 3.95  | 1.29        | 1.22     |
| 23  | a     | 407[A] | CLA  | C3D-C2D | 3.95  | 1.49        | 1.39     |
| 23  | C     | 512    | CLA  | C1D-ND  | 3.94  | 1.43        | 1.37     |
| 23  | c     | 510    | CLA  | C1B-NB  | -3.94 | 1.32        | 1.37     |
| 23  | a     | 409    | CLA  | C1D-ND  | 3.94  | 1.43        | 1.37     |
| 23  | c     | 505    | CLA  | O2A-CGA | 3.94  | 1.44        | 1.33     |
| 23  | c     | 510    | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 23  | C     | 504    | CLA  | CHC-C4B | 3.94  | 1.48        | 1.39     |
| 23  | D     | 702[A] | CLA  | C1D-ND  | 3.94  | 1.43        | 1.37     |
| 23  | C     | 502    | CLA  | CHC-C4B | 3.93  | 1.48        | 1.39     |
| 23  | b     | 603    | CLA  | C1D-ND  | 3.93  | 1.43        | 1.37     |
| 23  | c     | 504    | CLA  | O2D-CGD | 3.93  | 1.42        | 1.33     |
| 23  | C     | 506    | CLA  | CHC-C4B | 3.93  | 1.48        | 1.39     |
| 23  | c     | 509    | CLA  | CHD-C1D | 3.93  | 1.46        | 1.38     |
| 23  | B     | 611    | CLA  | CHB-C1B | 3.93  | 1.48        | 1.39     |
| 23  | C     | 509    | CLA  | OBD-CAD | 3.92  | 1.29        | 1.22     |
| 23  | C     | 513    | CLA  | CHD-C1D | 3.92  | 1.46        | 1.38     |
| 23  | D     | 702[A] | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 23  | B     | 613    | CLA  | CHB-C1B | 3.92  | 1.48        | 1.39     |
| 23  | D     | 702[B] | CLA  | CHD-C1D | 3.92  | 1.46        | 1.38     |
| 36  | c     | 518[B] | DGD  | O2G-C1B | 3.92  | 1.45        | 1.34     |
| 23  | b     | 615    | CLA  | CHD-C1D | 3.91  | 1.46        | 1.38     |
| 23  | b     | 608    | CLA  | CHB-C1B | 3.91  | 1.48        | 1.39     |
| 23  | C     | 505    | CLA  | CHD-C1D | 3.91  | 1.46        | 1.38     |
| 33  | D     | 707[A] | LHG  | O8-C23  | 3.91  | 1.44        | 1.33     |
| 23  | b     | 608    | CLA  | C3D-C2D | 3.91  | 1.49        | 1.39     |
| 23  | C     | 505    | CLA  | O2A-CGA | 3.91  | 1.44        | 1.33     |
| 23  | c     | 510    | CLA  | C3D-C2D | 3.91  | 1.49        | 1.39     |
| 23  | c     | 507    | CLA  | CHB-C1B | 3.90  | 1.48        | 1.39     |
| 34  | C     | 501    | LMG  | O7-C10  | 3.90  | 1.45        | 1.34     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 610    | CLA  | CHB-C1B | 3.90  | 1.48        | 1.39     |
| 23  | B     | 607    | CLA  | O2D-CGD | 3.90  | 1.42        | 1.33     |
| 23  | b     | 615    | CLA  | C3D-C2D | 3.90  | 1.49        | 1.39     |
| 23  | B     | 615    | CLA  | CHB-C1B | 3.90  | 1.48        | 1.39     |
| 23  | B     | 612    | CLA  | CHD-C1D | 3.90  | 1.46        | 1.38     |
| 23  | c     | 512    | CLA  | C3D-C2D | 3.90  | 1.49        | 1.39     |
| 23  | C     | 502    | CLA  | O2D-CGD | 3.89  | 1.42        | 1.33     |
| 23  | A     | 404[A] | CLA  | C1D-ND  | 3.89  | 1.43        | 1.37     |
| 23  | C     | 507    | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 23  | b     | 607    | CLA  | C1B-NB  | -3.89 | 1.32        | 1.37     |
| 23  | c     | 508    | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 23  | B     | 612    | CLA  | CHC-C4B | 3.89  | 1.48        | 1.39     |
| 23  | D     | 702[A] | CLA  | CHD-C1D | 3.89  | 1.46        | 1.38     |
| 33  | b     | 629[B] | LHG  | O8-C23  | 3.89  | 1.44        | 1.33     |
| 23  | A     | 406[B] | CLA  | C3D-C2D | 3.89  | 1.49        | 1.39     |
| 23  | A     | 406[A] | CLA  | C3D-C2D | 3.89  | 1.49        | 1.39     |
| 23  | d     | 401[B] | CLA  | CHD-C1D | 3.89  | 1.46        | 1.38     |
| 23  | d     | 401[B] | CLA  | CHB-C1B | 3.89  | 1.48        | 1.39     |
| 24  | a     | 416[B] | PHO  | O2A-CGA | 3.89  | 1.44        | 1.33     |
| 36  | c     | 517[B] | DGD  | O1G-C1A | 3.88  | 1.44        | 1.33     |
| 23  | c     | 514    | CLA  | C3D-C2D | 3.88  | 1.49        | 1.39     |
| 23  | b     | 610    | CLA  | CHB-C1B | 3.88  | 1.48        | 1.39     |
| 23  | b     | 606    | CLA  | OBD-CAD | 3.88  | 1.29        | 1.22     |
| 23  | B     | 611    | CLA  | CHD-C1D | 3.88  | 1.46        | 1.38     |
| 23  | b     | 605    | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 23  | D     | 702[B] | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 23  | B     | 616    | CLA  | CHD-C1D | 3.87  | 1.46        | 1.38     |
| 23  | B     | 614    | CLA  | C4B-NB  | -3.87 | 1.32        | 1.37     |
| 36  | C     | 517[B] | DGD  | O1G-C1A | 3.87  | 1.44        | 1.33     |
| 23  | B     | 602    | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 23  | b     | 610    | CLA  | CHC-C4B | 3.87  | 1.48        | 1.39     |
| 23  | B     | 611    | CLA  | O2A-CGA | 3.87  | 1.44        | 1.33     |
| 24  | A     | 417[A] | PHO  | O2A-CGA | 3.86  | 1.44        | 1.33     |
| 23  | b     | 609    | CLA  | OBD-CAD | 3.86  | 1.29        | 1.22     |
| 23  | d     | 401[B] | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 23  | B     | 610    | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 23  | b     | 604    | CLA  | CHC-C4B | 3.86  | 1.48        | 1.39     |
| 23  | c     | 506    | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 23  | b     | 614    | CLA  | CHC-C4B | 3.85  | 1.48        | 1.39     |
| 23  | c     | 513    | CLA  | CHB-C1B | 3.85  | 1.48        | 1.39     |
| 26  | A     | 410[A] | SQD  | O48-C23 | 3.85  | 1.44        | 1.33     |
| 23  | B     | 605    | CLA  | CHD-C1D | 3.85  | 1.45        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 508    | CLA  | CHD-C1D | 3.85  | 1.45        | 1.38     |
| 36  | C     | 518[A] | DGD  | O2G-C1B | 3.85  | 1.45        | 1.34     |
| 25  | B     | 618    | BCR  | C23-C22 | -3.85 | 1.37        | 1.46     |
| 23  | B     | 608    | CLA  | CHB-C1B | 3.85  | 1.48        | 1.39     |
| 23  | C     | 503    | CLA  | O2A-CGA | 3.85  | 1.44        | 1.33     |
| 33  | L     | 101[A] | LHG  | O8-C23  | 3.85  | 1.44        | 1.33     |
| 33  | b     | 629[B] | LHG  | O7-C7   | 3.84  | 1.45        | 1.34     |
| 36  | c     | 518[A] | DGD  | O1G-C1A | 3.84  | 1.44        | 1.33     |
| 23  | A     | 405[A] | CLA  | O2A-CGA | 3.84  | 1.44        | 1.33     |
| 23  | C     | 505    | CLA  | CHC-C4B | 3.84  | 1.48        | 1.39     |
| 23  | B     | 602    | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 23  | C     | 502    | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 23  | C     | 505    | CLA  | CHB-C1B | 3.84  | 1.48        | 1.39     |
| 24  | a     | 416[A] | PHO  | O2A-CGA | 3.84  | 1.44        | 1.33     |
| 35  | b     | 622    | HTG  | C1'-S1  | -3.83 | 1.76        | 1.81     |
| 23  | A     | 408    | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 23  | b     | 608    | CLA  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 34  | d     | 410    | LMG  | O7-C10  | 3.83  | 1.45        | 1.34     |
| 23  | c     | 502    | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 36  | C     | 518[B] | DGD  | O2G-C1B | 3.83  | 1.45        | 1.34     |
| 33  | d     | 412[B] | LHG  | O7-C7   | 3.83  | 1.45        | 1.34     |
| 26  | A     | 410[B] | SQD  | O48-C23 | 3.83  | 1.44        | 1.33     |
| 23  | a     | 407[A] | CLA  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 23  | B     | 614    | CLA  | CHD-C1D | 3.83  | 1.45        | 1.38     |
| 23  | c     | 509    | CLA  | CHD-C4C | 3.82  | 1.47        | 1.39     |
| 23  | C     | 514    | CLA  | CHB-C1B | 3.82  | 1.48        | 1.39     |
| 23  | b     | 609    | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 33  | L     | 101[A] | LHG  | O7-C7   | 3.82  | 1.45        | 1.34     |
| 23  | D     | 703    | CLA  | CHB-C1B | 3.82  | 1.48        | 1.39     |
| 23  | C     | 514    | CLA  | CHD-C4C | 3.82  | 1.47        | 1.39     |
| 23  | b     | 612    | CLA  | O2A-CGA | 3.82  | 1.44        | 1.33     |
| 23  | b     | 605    | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 23  | C     | 507    | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 23  | c     | 509    | CLA  | CHB-C1B | 3.82  | 1.48        | 1.39     |
| 23  | b     | 602    | CLA  | OBD-CAD | 3.81  | 1.29        | 1.22     |
| 33  | A     | 419[B] | LHG  | O8-C23  | 3.81  | 1.44        | 1.33     |
| 23  | A     | 406[B] | CLA  | CHC-C4B | 3.81  | 1.48        | 1.39     |
| 24  | A     | 407[B] | PHO  | O2A-CGA | 3.81  | 1.44        | 1.33     |
| 23  | C     | 508    | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 23  | A     | 406[A] | CLA  | O2A-CGA | 3.81  | 1.44        | 1.33     |
| 23  | c     | 506    | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 23  | b     | 616    | CLA  | CHC-C4B | 3.80  | 1.47        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 23  | c     | 513    | CLA  | OBD-CAD | 3.80 | 1.29        | 1.22     |
| 23  | A     | 405[B] | CLA  | CHD-C4C | 3.80 | 1.47        | 1.39     |
| 23  | b     | 601    | CLA  | OBD-CAD | 3.80 | 1.29        | 1.22     |
| 23  | c     | 508    | CLA  | CHC-C4B | 3.80 | 1.47        | 1.39     |
| 23  | b     | 610    | CLA  | C3D-C2D | 3.80 | 1.49        | 1.39     |
| 23  | b     | 616    | CLA  | CHD-C4C | 3.80 | 1.47        | 1.39     |
| 23  | b     | 605    | CLA  | OBD-CAD | 3.80 | 1.29        | 1.22     |
| 23  | a     | 409    | CLA  | CHB-C1B | 3.80 | 1.47        | 1.39     |
| 23  | c     | 502    | CLA  | CHC-C4B | 3.80 | 1.47        | 1.39     |
| 23  | B     | 603    | CLA  | CHD-C1D | 3.80 | 1.45        | 1.38     |
| 23  | b     | 609    | CLA  | O2A-CGA | 3.79 | 1.44        | 1.33     |
| 23  | B     | 607    | CLA  | CHD-C4C | 3.79 | 1.47        | 1.39     |
| 23  | a     | 405[B] | CLA  | CHD-C1D | 3.79 | 1.45        | 1.38     |
| 23  | A     | 406[A] | CLA  | CHC-C4B | 3.79 | 1.47        | 1.39     |
| 23  | C     | 511    | CLA  | O2A-CGA | 3.79 | 1.44        | 1.33     |
| 23  | B     | 601    | CLA  | CHD-C4C | 3.79 | 1.47        | 1.39     |
| 23  | B     | 605    | CLA  | C3D-C2D | 3.79 | 1.49        | 1.39     |
| 33  | D     | 706[B] | LHG  | O7-C7   | 3.79 | 1.45        | 1.34     |
| 23  | d     | 402    | CLA  | CHC-C4B | 3.79 | 1.47        | 1.39     |
| 23  | a     | 409    | CLA  | CHD-C1D | 3.79 | 1.45        | 1.38     |
| 23  | C     | 510    | CLA  | OBD-CAD | 3.79 | 1.29        | 1.22     |
| 23  | c     | 511    | CLA  | C3D-C2D | 3.78 | 1.49        | 1.39     |
| 23  | B     | 603    | CLA  | O2A-CGA | 3.78 | 1.44        | 1.33     |
| 23  | D     | 702[B] | CLA  | CHB-C1B | 3.78 | 1.47        | 1.39     |
| 23  | a     | 409    | CLA  | CHC-C4B | 3.78 | 1.47        | 1.39     |
| 23  | A     | 405[A] | CLA  | CHB-C1B | 3.78 | 1.47        | 1.39     |
| 23  | d     | 402    | CLA  | CHB-C1B | 3.78 | 1.47        | 1.39     |
| 23  | d     | 401[A] | CLA  | CHD-C1D | 3.78 | 1.45        | 1.38     |
| 33  | d     | 406[B] | LHG  | O7-C7   | 3.78 | 1.44        | 1.34     |
| 23  | b     | 602    | CLA  | O2A-CGA | 3.78 | 1.44        | 1.33     |
| 23  | C     | 511    | CLA  | CHB-C1B | 3.78 | 1.47        | 1.39     |
| 23  | A     | 408    | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 23  | B     | 612    | CLA  | C1D-ND  | 3.77 | 1.42        | 1.37     |
| 23  | a     | 406[A] | CLA  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 23  | B     | 615    | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 23  | c     | 503    | CLA  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 23  | B     | 606    | CLA  | CHC-C4B | 3.77 | 1.47        | 1.39     |
| 23  | b     | 616    | CLA  | C3D-C2D | 3.77 | 1.49        | 1.39     |
| 23  | a     | 406[A] | CLA  | CHD-C1D | 3.77 | 1.45        | 1.38     |
| 23  | B     | 601    | CLA  | C3D-C2D | 3.76 | 1.49        | 1.39     |
| 23  | c     | 505    | CLA  | CHD-C4C | 3.76 | 1.47        | 1.39     |
| 23  | b     | 612    | CLA  | OBD-CAD | 3.76 | 1.29        | 1.22     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 23  | B     | 602    | CLA  | CHB-C1B | 3.76 | 1.47        | 1.39     |
| 23  | b     | 611    | CLA  | CHD-C4C | 3.76 | 1.47        | 1.39     |
| 23  | b     | 603    | CLA  | CHC-C4B | 3.76 | 1.47        | 1.39     |
| 23  | A     | 404[A] | CLA  | CHD-C4C | 3.76 | 1.47        | 1.39     |
| 23  | b     | 606    | CLA  | C3D-C2D | 3.76 | 1.49        | 1.39     |
| 23  | C     | 503    | CLA  | CHB-C1B | 3.76 | 1.47        | 1.39     |
| 23  | C     | 502    | CLA  | C3D-C2D | 3.75 | 1.49        | 1.39     |
| 23  | c     | 511    | CLA  | CHD-C1D | 3.75 | 1.45        | 1.38     |
| 33  | d     | 412[A] | LHG  | O8-C23  | 3.75 | 1.44        | 1.33     |
| 23  | b     | 604    | CLA  | CHD-C4C | 3.75 | 1.47        | 1.39     |
| 23  | D     | 702[B] | CLA  | C3D-C2D | 3.75 | 1.49        | 1.39     |
| 23  | c     | 511    | CLA  | CHD-C4C | 3.75 | 1.47        | 1.39     |
| 23  | a     | 407[A] | CLA  | CHB-C1B | 3.75 | 1.47        | 1.39     |
| 23  | C     | 508    | CLA  | CHC-C4B | 3.75 | 1.47        | 1.39     |
| 23  | C     | 506    | CLA  | O2A-CGA | 3.75 | 1.44        | 1.33     |
| 23  | B     | 611    | CLA  | C1C-C2C | 3.75 | 1.52        | 1.44     |
| 23  | c     | 503    | CLA  | CHB-C1B | 3.74 | 1.47        | 1.39     |
| 33  | D     | 707[B] | LHG  | O7-C7   | 3.74 | 1.44        | 1.34     |
| 23  | A     | 406[B] | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 23  | B     | 608    | CLA  | C3D-C2D | 3.74 | 1.49        | 1.39     |
| 23  | b     | 603    | CLA  | CHD-C1D | 3.74 | 1.45        | 1.38     |
| 23  | c     | 507    | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 23  | A     | 406[A] | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 23  | c     | 511    | CLA  | O2A-CGA | 3.74 | 1.44        | 1.33     |
| 23  | B     | 602    | CLA  | CHC-C4B | 3.74 | 1.47        | 1.39     |
| 23  | a     | 406[B] | CLA  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 23  | C     | 502    | CLA  | O2A-CGA | 3.74 | 1.44        | 1.33     |
| 23  | b     | 602    | CLA  | C3D-C2D | 3.73 | 1.49        | 1.39     |
| 23  | b     | 613    | CLA  | CHB-C1B | 3.73 | 1.47        | 1.39     |
| 23  | C     | 509    | CLA  | CHD-C4C | 3.73 | 1.47        | 1.39     |
| 23  | B     | 602    | CLA  | O2A-CGA | 3.73 | 1.44        | 1.33     |
| 23  | b     | 604    | CLA  | C3D-C2D | 3.73 | 1.49        | 1.39     |
| 23  | B     | 607    | CLA  | CHD-C1D | 3.73 | 1.45        | 1.38     |
| 23  | C     | 511    | CLA  | CHD-C1D | 3.73 | 1.45        | 1.38     |
| 23  | C     | 510    | CLA  | CHD-C4C | 3.73 | 1.47        | 1.39     |
| 23  | c     | 506    | CLA  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 23  | b     | 615    | CLA  | CHB-C1B | 3.72 | 1.47        | 1.39     |
| 23  | B     | 603    | CLA  | CHD-C4C | 3.72 | 1.47        | 1.39     |
| 33  | d     | 405[A] | LHG  | O7-C7   | 3.72 | 1.44        | 1.34     |
| 23  | C     | 505    | CLA  | CHD-C4C | 3.72 | 1.47        | 1.39     |
| 36  | C     | 518[A] | DGD  | O1G-C1A | 3.72 | 1.44        | 1.33     |
| 23  | c     | 504    | CLA  | CHB-C1B | 3.72 | 1.47        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | A     | 404[B] | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 23  | B     | 606    | CLA  | CHD-C1D | 3.71  | 1.45        | 1.38     |
| 23  | C     | 510    | CLA  | CHB-C1B | 3.71  | 1.47        | 1.39     |
| 23  | a     | 405[A] | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 23  | B     | 603    | CLA  | C1B-NB  | -3.71 | 1.33        | 1.37     |
| 23  | D     | 703    | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 23  | C     | 504    | CLA  | O2A-CGA | 3.71  | 1.44        | 1.33     |
| 23  | b     | 603    | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 23  | D     | 702[B] | CLA  | CHC-C4B | 3.71  | 1.47        | 1.39     |
| 23  | C     | 504    | CLA  | CHB-C1B | 3.71  | 1.47        | 1.39     |
| 23  | A     | 406[A] | CLA  | C1D-ND  | 3.71  | 1.42        | 1.37     |
| 33  | d     | 405[B] | LHG  | O8-C23  | 3.70  | 1.44        | 1.33     |
| 36  | H     | 102    | DGD  | O1G-C1A | 3.70  | 1.44        | 1.33     |
| 23  | a     | 407[B] | CLA  | CHD-C1D | 3.70  | 1.45        | 1.38     |
| 23  | c     | 514    | CLA  | CHB-C1B | 3.70  | 1.47        | 1.39     |
| 23  | b     | 613    | CLA  | O2A-CGA | 3.70  | 1.44        | 1.33     |
| 23  | c     | 511    | CLA  | CHB-C1B | 3.70  | 1.47        | 1.39     |
| 23  | b     | 610    | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 23  | c     | 508    | CLA  | C3D-C2D | 3.70  | 1.49        | 1.39     |
| 23  | a     | 405[B] | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 23  | A     | 406[A] | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 23  | A     | 405[A] | CLA  | CHD-C1D | 3.69  | 1.45        | 1.38     |
| 23  | a     | 405[A] | CLA  | CHB-C1B | 3.69  | 1.47        | 1.39     |
| 23  | B     | 607    | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 23  | c     | 511    | CLA  | CHC-C4B | 3.69  | 1.47        | 1.39     |
| 23  | B     | 609    | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 23  | d     | 401[B] | CLA  | C3D-C2D | 3.69  | 1.49        | 1.39     |
| 23  | b     | 604    | CLA  | CHB-C1B | 3.69  | 1.47        | 1.39     |
| 23  | a     | 405[B] | CLA  | CHB-C1B | 3.68  | 1.47        | 1.39     |
| 26  | A     | 410[A] | SQD  | O47-C7  | 3.68  | 1.44        | 1.34     |
| 23  | A     | 404[A] | CLA  | C3D-C2D | 3.68  | 1.49        | 1.39     |
| 23  | b     | 603    | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 23  | C     | 508    | CLA  | CHB-C1B | 3.68  | 1.47        | 1.39     |
| 23  | a     | 407[B] | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 23  | a     | 407[A] | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 23  | a     | 407[B] | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 23  | d     | 401[A] | CLA  | C1B-NB  | -3.68 | 1.33        | 1.37     |
| 23  | B     | 605    | CLA  | O2A-CGA | 3.68  | 1.44        | 1.33     |
| 23  | b     | 608    | CLA  | C1B-NB  | -3.67 | 1.33        | 1.37     |
| 23  | C     | 510    | CLA  | C4B-NB  | -3.67 | 1.33        | 1.37     |
| 23  | B     | 607    | CLA  | O2A-CGA | 3.67  | 1.44        | 1.33     |
| 23  | b     | 606    | CLA  | O2A-CGA | 3.67  | 1.44        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 26  | A     | 410[B] | SQD  | O47-C7  | 3.66  | 1.44        | 1.34     |
| 33  | d     | 406[A] | LHG  | O7-C7   | 3.66  | 1.44        | 1.34     |
| 23  | a     | 405[B] | CLA  | C3D-C2D | 3.65  | 1.48        | 1.39     |
| 24  | A     | 407[A] | PHO  | O2A-CGA | 3.65  | 1.44        | 1.33     |
| 23  | b     | 611    | CLA  | C3D-C2D | 3.65  | 1.48        | 1.39     |
| 23  | b     | 611    | CLA  | CHB-C1B | 3.64  | 1.47        | 1.39     |
| 23  | b     | 614    | CLA  | CHB-C1B | 3.64  | 1.47        | 1.39     |
| 35  | b     | 623    | HTG  | C1'-S1  | -3.64 | 1.76        | 1.81     |
| 23  | B     | 616    | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 23  | B     | 612    | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 23  | a     | 406[A] | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 23  | C     | 504    | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 23  | C     | 513    | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 23  | C     | 507    | CLA  | CHB-C1B | 3.64  | 1.47        | 1.39     |
| 23  | B     | 612    | CLA  | C4B-NB  | -3.64 | 1.33        | 1.37     |
| 23  | C     | 511    | CLA  | C3D-C2D | 3.64  | 1.48        | 1.39     |
| 23  | B     | 606    | CLA  | C3D-C2D | 3.63  | 1.48        | 1.39     |
| 23  | b     | 616    | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 23  | b     | 607    | CLA  | C1D-ND  | 3.63  | 1.42        | 1.37     |
| 23  | B     | 607    | CLA  | CHC-C4B | 3.63  | 1.47        | 1.39     |
| 33  | D     | 706[B] | LHG  | O8-C23  | 3.63  | 1.43        | 1.33     |
| 36  | c     | 517[A] | DGD  | O1G-C1A | 3.62  | 1.43        | 1.33     |
| 23  | c     | 505    | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 33  | b     | 629[A] | LHG  | O7-C7   | 3.62  | 1.44        | 1.34     |
| 23  | b     | 603    | CLA  | C3D-C2D | 3.62  | 1.48        | 1.39     |
| 23  | a     | 405[A] | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 23  | B     | 604    | CLA  | CHC-C4B | 3.61  | 1.47        | 1.39     |
| 23  | B     | 607    | CLA  | CHB-C1B | 3.61  | 1.47        | 1.39     |
| 23  | B     | 604    | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 23  | b     | 614    | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 23  | C     | 511    | CLA  | C1B-NB  | -3.61 | 1.33        | 1.37     |
| 23  | C     | 512    | CLA  | C4B-NB  | -3.61 | 1.33        | 1.37     |
| 23  | a     | 407[A] | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 23  | B     | 605    | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 23  | b     | 613    | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 23  | d     | 402    | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 23  | b     | 607    | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 33  | D     | 706[A] | LHG  | O7-C7   | 3.60  | 1.44        | 1.34     |
| 23  | b     | 603    | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 23  | d     | 401[A] | CLA  | C3D-C2D | 3.60  | 1.48        | 1.39     |
| 23  | a     | 405[B] | CLA  | O2A-CGA | 3.60  | 1.43        | 1.33     |
| 23  | d     | 401[A] | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 616    | CLA  | CHB-C1B | 3.59  | 1.47        | 1.39     |
| 23  | c     | 509    | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 23  | C     | 514    | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 23  | B     | 607    | CLA  | C3D-C2D | 3.59  | 1.48        | 1.39     |
| 23  | B     | 608    | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 23  | A     | 405[A] | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 23  | A     | 405[A] | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 23  | b     | 615    | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 23  | C     | 513    | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 23  | B     | 610    | CLA  | O2A-CGA | 3.57  | 1.43        | 1.33     |
| 36  | h     | 102    | DGD  | O1G-C1A | 3.57  | 1.43        | 1.33     |
| 23  | A     | 405[B] | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 34  | m     | 101    | LMG  | O7-C10  | 3.57  | 1.44        | 1.34     |
| 23  | a     | 407[B] | CLA  | CHB-C1B | 3.56  | 1.47        | 1.39     |
| 23  | C     | 506    | CLA  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 36  | C     | 517[A] | DGD  | O1G-C1A | 3.56  | 1.43        | 1.33     |
| 23  | A     | 405[A] | CLA  | CHC-C4B | 3.55  | 1.47        | 1.39     |
| 23  | A     | 404[A] | CLA  | CHB-C1B | 3.55  | 1.47        | 1.39     |
| 23  | A     | 404[B] | CLA  | CHB-C1B | 3.55  | 1.47        | 1.39     |
| 23  | C     | 507    | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 23  | A     | 406[B] | CLA  | C1B-NB  | -3.55 | 1.33        | 1.37     |
| 23  | b     | 607    | CLA  | C3D-C2D | 3.55  | 1.48        | 1.39     |
| 23  | B     | 611    | CLA  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 23  | c     | 506    | CLA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 23  | D     | 702[A] | CLA  | C1B-NB  | -3.54 | 1.33        | 1.37     |
| 23  | A     | 405[B] | CLA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 36  | c     | 518[A] | DGD  | O2G-C1B | 3.54  | 1.44        | 1.34     |
| 33  | d     | 405[A] | LHG  | O8-C23  | 3.54  | 1.43        | 1.33     |
| 23  | b     | 604    | CLA  | O2A-CGA | 3.54  | 1.43        | 1.33     |
| 23  | b     | 604    | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 23  | B     | 604    | CLA  | O2A-CGA | 3.53  | 1.43        | 1.33     |
| 23  | B     | 603    | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 23  | b     | 614    | CLA  | O2A-CGA | 3.53  | 1.43        | 1.33     |
| 33  | D     | 706[A] | LHG  | O8-C23  | 3.53  | 1.43        | 1.33     |
| 23  | B     | 616    | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 23  | c     | 514    | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 23  | c     | 506    | CLA  | O2A-CGA | 3.53  | 1.43        | 1.33     |
| 33  | A     | 419[A] | LHG  | O8-C23  | 3.53  | 1.43        | 1.33     |
| 24  | a     | 408[B] | PHO  | O2A-CGA | 3.52  | 1.43        | 1.33     |
| 33  | A     | 419[B] | LHG  | O7-C7   | 3.52  | 1.44        | 1.34     |
| 23  | B     | 613    | CLA  | CHD-C1D | 3.51  | 1.45        | 1.38     |
| 23  | a     | 407[A] | CLA  | CHD-C1D | 3.51  | 1.45        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 610    | CLA  | CHC-C4B | 3.51  | 1.47        | 1.39     |
| 23  | B     | 608    | CLA  | O2A-CGA | 3.51  | 1.43        | 1.33     |
| 23  | B     | 604    | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 23  | b     | 606    | CLA  | CHD-C4C | 3.51  | 1.47        | 1.39     |
| 23  | b     | 607    | CLA  | CHC-C4B | 3.51  | 1.47        | 1.39     |
| 23  | b     | 601    | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 23  | C     | 502    | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 23  | b     | 615    | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 33  | d     | 412[A] | LHG  | O7-C7   | 3.50  | 1.44        | 1.34     |
| 23  | a     | 406[B] | CLA  | CHC-C4B | 3.50  | 1.47        | 1.39     |
| 36  | C     | 519    | DGD  | O2G-C1B | 3.50  | 1.44        | 1.34     |
| 23  | D     | 703    | CLA  | O2A-CGA | 3.50  | 1.43        | 1.33     |
| 23  | A     | 404[A] | CLA  | C4B-NB  | -3.50 | 1.33        | 1.37     |
| 33  | A     | 419[A] | LHG  | O7-C7   | 3.50  | 1.44        | 1.34     |
| 33  | b     | 629[A] | LHG  | O8-C23  | 3.50  | 1.43        | 1.33     |
| 23  | C     | 506    | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 23  | A     | 406[A] | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 23  | B     | 601    | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 23  | b     | 608    | CLA  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 23  | c     | 510    | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 23  | D     | 702[A] | CLA  | C3D-C2D | 3.48  | 1.48        | 1.39     |
| 23  | b     | 605    | CLA  | O2A-CGA | 3.48  | 1.43        | 1.33     |
| 38  | f     | 101    | HEM  | C1B-NB  | -3.48 | 1.34        | 1.40     |
| 23  | A     | 405[A] | CLA  | C1B-NB  | -3.48 | 1.33        | 1.37     |
| 23  | b     | 612    | CLA  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 23  | C     | 504    | CLA  | C3D-C2D | 3.48  | 1.48        | 1.39     |
| 23  | b     | 606    | CLA  | CHC-C4B | 3.48  | 1.47        | 1.39     |
| 23  | a     | 406[A] | CLA  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 23  | c     | 514    | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 23  | c     | 504    | CLA  | C3D-C2D | 3.47  | 1.48        | 1.39     |
| 23  | C     | 508    | CLA  | CHD-C4C | 3.47  | 1.47        | 1.39     |
| 23  | b     | 609    | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 23  | B     | 609    | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 23  | a     | 406[A] | CLA  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 23  | b     | 606    | CLA  | C1B-NB  | -3.46 | 1.33        | 1.37     |
| 23  | A     | 404[B] | CLA  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 23  | a     | 406[B] | CLA  | C1B-NB  | -3.46 | 1.33        | 1.37     |
| 36  | H     | 102    | DGD  | O2G-C1B | 3.46  | 1.44        | 1.34     |
| 23  | B     | 610    | CLA  | C1B-NB  | -3.46 | 1.33        | 1.37     |
| 23  | C     | 502    | CLA  | C1B-NB  | -3.45 | 1.33        | 1.37     |
| 23  | c     | 508    | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 23  | c     | 510    | CLA  | C4B-NB  | -3.45 | 1.33        | 1.37     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 512    | CLA  | CHC-C4B | 3.45  | 1.47        | 1.39     |
| 23  | B     | 612    | CLA  | O2A-CGA | 3.45  | 1.43        | 1.33     |
| 23  | C     | 505    | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 23  | b     | 611    | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 23  | b     | 609    | CLA  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 35  | o     | 301    | HTG  | C1'-S1  | -3.44 | 1.76        | 1.81     |
| 23  | B     | 613    | CLA  | O2A-CGA | 3.43  | 1.43        | 1.33     |
| 23  | a     | 405[B] | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 23  | b     | 615    | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 23  | A     | 406[A] | CLA  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 23  | B     | 603    | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 23  | c     | 507    | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 23  | B     | 601    | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 23  | b     | 613    | CLA  | CHD-C1D | 3.42  | 1.45        | 1.38     |
| 23  | B     | 612    | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 23  | d     | 401[A] | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 23  | d     | 401[B] | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 23  | d     | 401[A] | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 23  | B     | 611    | CLA  | CHD-C4C | 3.41  | 1.47        | 1.39     |
| 23  | c     | 505    | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 23  | C     | 514    | CLA  | C1B-NB  | -3.41 | 1.33        | 1.37     |
| 23  | B     | 606    | CLA  | CHD-C4C | 3.41  | 1.47        | 1.39     |
| 23  | b     | 601    | CLA  | CHC-C4B | 3.40  | 1.47        | 1.39     |
| 23  | B     | 616    | CLA  | CHD-C4C | 3.40  | 1.46        | 1.39     |
| 23  | c     | 512    | CLA  | CHC-C4B | 3.40  | 1.47        | 1.39     |
| 23  | b     | 610    | CLA  | O2A-CGA | 3.40  | 1.43        | 1.33     |
| 24  | a     | 408[A] | PHO  | O2A-CGA | 3.40  | 1.43        | 1.33     |
| 23  | a     | 407[B] | CLA  | CHC-C4B | 3.39  | 1.47        | 1.39     |
| 23  | D     | 702[B] | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 23  | B     | 613    | CLA  | C1B-NB  | -3.39 | 1.33        | 1.37     |
| 36  | c     | 519    | DGD  | O2G-C1B | 3.38  | 1.43        | 1.34     |
| 23  | B     | 612    | CLA  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 38  | f     | 101    | HEM  | C4D-ND  | -3.38 | 1.34        | 1.40     |
| 23  | b     | 607    | CLA  | CHD-C4C | 3.38  | 1.46        | 1.39     |
| 23  | a     | 406[B] | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 38  | F     | 102    | HEM  | C1B-NB  | -3.37 | 1.34        | 1.40     |
| 23  | C     | 506    | CLA  | C1B-C2B | 3.37  | 1.51        | 1.43     |
| 23  | A     | 404[B] | CLA  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 23  | c     | 511    | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 23  | B     | 614    | CLA  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 23  | a     | 405[A] | CLA  | CHC-C4B | 3.36  | 1.46        | 1.39     |
| 34  | D     | 711    | LMG  | O7-C10  | 3.35  | 1.43        | 1.34     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 512    | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 23  | c     | 505    | CLA  | C4B-NB  | -3.35 | 1.33        | 1.37     |
| 23  | c     | 505    | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 23  | a     | 409    | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 23  | b     | 608    | CLA  | CHC-C4B | 3.34  | 1.46        | 1.39     |
| 23  | C     | 509    | CLA  | CHC-C4B | 3.34  | 1.46        | 1.39     |
| 23  | A     | 404[A] | CLA  | OBD-CAD | 3.34  | 1.28        | 1.22     |
| 23  | C     | 503    | CLA  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 23  | b     | 607    | CLA  | O2A-CGA | 3.33  | 1.43        | 1.33     |
| 23  | D     | 702[A] | CLA  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 23  | b     | 606    | CLA  | CHB-C1B | 3.33  | 1.46        | 1.39     |
| 23  | C     | 510    | CLA  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 23  | A     | 404[B] | CLA  | O2A-CGA | 3.33  | 1.43        | 1.33     |
| 23  | B     | 607    | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 23  | b     | 603    | CLA  | O2A-CGA | 3.32  | 1.43        | 1.33     |
| 23  | b     | 613    | CLA  | CHD-C4C | 3.32  | 1.46        | 1.39     |
| 23  | b     | 615    | CLA  | C1B-NB  | -3.31 | 1.33        | 1.37     |
| 23  | a     | 409    | CLA  | CHD-C4C | 3.30  | 1.46        | 1.39     |
| 23  | C     | 503    | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 23  | B     | 613    | CLA  | CHD-C4C | 3.30  | 1.46        | 1.39     |
| 23  | b     | 604    | CLA  | C1B-C2B | 3.29  | 1.50        | 1.43     |
| 23  | d     | 401[B] | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 23  | b     | 614    | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 23  | B     | 604    | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 23  | B     | 613    | CLA  | CHC-C4B | 3.28  | 1.46        | 1.39     |
| 23  | b     | 610    | CLA  | C1B-NB  | -3.27 | 1.33        | 1.37     |
| 23  | B     | 602    | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 23  | b     | 602    | CLA  | C1C-C2C | 3.27  | 1.51        | 1.44     |
| 23  | C     | 506    | CLA  | C1B-NB  | -3.27 | 1.33        | 1.37     |
| 23  | B     | 608    | CLA  | CHC-C4B | 3.27  | 1.46        | 1.39     |
| 23  | C     | 513    | CLA  | CHB-C1B | 3.26  | 1.46        | 1.39     |
| 23  | D     | 702[A] | CLA  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 23  | C     | 507    | CLA  | C1B-NB  | -3.26 | 1.33        | 1.37     |
| 23  | A     | 406[B] | CLA  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 23  | b     | 613    | CLA  | C1B-NB  | -3.25 | 1.33        | 1.37     |
| 23  | b     | 605    | CLA  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 23  | c     | 505    | CLA  | C1B-NB  | -3.25 | 1.33        | 1.37     |
| 23  | C     | 511    | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 23  | C     | 514    | CLA  | CHC-C4B | 3.24  | 1.46        | 1.39     |
| 23  | a     | 407[A] | CLA  | CHC-C4B | 3.23  | 1.46        | 1.39     |
| 23  | A     | 404[B] | CLA  | C4B-NB  | -3.23 | 1.33        | 1.37     |
| 24  | A     | 417[A] | PHO  | CHA-CBD | -3.23 | 1.47        | 1.51     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | A     | 408    | CLA  | CHC-C4B | 3.22  | 1.46        | 1.39     |
| 23  | C     | 507    | CLA  | CHC-C4B | 3.22  | 1.46        | 1.39     |
| 23  | C     | 511    | CLA  | CHC-C4B | 3.22  | 1.46        | 1.39     |
| 23  | b     | 616    | CLA  | CHB-C1B | 3.22  | 1.46        | 1.39     |
| 34  | D     | 711    | LMG  | O8-C28  | 3.22  | 1.42        | 1.33     |
| 23  | c     | 512    | CLA  | C1B-C2B | 3.22  | 1.50        | 1.43     |
| 23  | B     | 613    | CLA  | OBD-CAD | 3.22  | 1.28        | 1.22     |
| 23  | c     | 503    | CLA  | CHC-C4B | 3.22  | 1.46        | 1.39     |
| 23  | a     | 406[A] | CLA  | C1B-NB  | -3.20 | 1.33        | 1.37     |
| 23  | a     | 405[B] | CLA  | C4B-NB  | -3.20 | 1.33        | 1.37     |
| 23  | A     | 405[B] | CLA  | OBD-CAD | 3.20  | 1.28        | 1.22     |
| 38  | F     | 102    | HEM  | C4D-ND  | -3.20 | 1.34        | 1.40     |
| 23  | A     | 404[A] | CLA  | O2A-CGA | 3.20  | 1.42        | 1.33     |
| 23  | C     | 507    | CLA  | C4C-C3C | 3.20  | 1.50        | 1.45     |
| 23  | B     | 616    | CLA  | C4B-NB  | -3.19 | 1.33        | 1.37     |
| 23  | b     | 611    | CLA  | CHC-C4B | 3.19  | 1.46        | 1.39     |
| 23  | B     | 609    | CLA  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 23  | C     | 505    | CLA  | C1B-NB  | -3.17 | 1.33        | 1.37     |
| 23  | c     | 506    | CLA  | C1B-NB  | -3.17 | 1.33        | 1.37     |
| 23  | A     | 408    | CLA  | C1B-NB  | -3.16 | 1.33        | 1.37     |
| 23  | a     | 409    | CLA  | C1B-C2B | 3.15  | 1.50        | 1.43     |
| 23  | A     | 404[A] | CLA  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 23  | C     | 502    | CLA  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 23  | C     | 507    | CLA  | C4B-NB  | -3.15 | 1.33        | 1.37     |
| 23  | a     | 405[A] | CLA  | C1B-NB  | -3.15 | 1.33        | 1.37     |
| 23  | b     | 612    | CLA  | C1B-NB  | -3.14 | 1.33        | 1.37     |
| 35  | b     | 625    | HTG  | C1-S1   | -3.13 | 1.75        | 1.80     |
| 23  | b     | 605    | CLA  | CHC-C4B | 3.12  | 1.46        | 1.39     |
| 23  | B     | 602    | CLA  | C1C-C2C | 3.12  | 1.50        | 1.44     |
| 23  | A     | 405[A] | CLA  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 23  | b     | 602    | CLA  | C1B-NB  | -3.12 | 1.33        | 1.37     |
| 23  | b     | 601    | CLA  | C4B-NB  | -3.11 | 1.33        | 1.37     |
| 23  | b     | 614    | CLA  | C1B-NB  | -3.11 | 1.33        | 1.37     |
| 23  | c     | 503    | CLA  | C4B-NB  | -3.11 | 1.33        | 1.37     |
| 23  | b     | 612    | CLA  | C4B-NB  | -3.11 | 1.33        | 1.37     |
| 23  | c     | 504    | CLA  | C1B-NB  | -3.11 | 1.33        | 1.37     |
| 23  | c     | 508    | CLA  | C1B-NB  | -3.11 | 1.33        | 1.37     |
| 23  | B     | 614    | CLA  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 23  | c     | 502    | CLA  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 23  | c     | 507    | CLA  | C1B-NB  | -3.10 | 1.33        | 1.37     |
| 23  | A     | 405[B] | CLA  | C1B-NB  | -3.10 | 1.33        | 1.37     |
| 23  | c     | 514    | CLA  | C1B-NB  | -3.10 | 1.33        | 1.37     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 615    | CLA  | C1B-C2B | 3.09  | 1.50        | 1.43     |
| 35  | B     | 624    | HTG  | C1'-S1  | -3.09 | 1.77        | 1.81     |
| 23  | b     | 604    | CLA  | C4D-CHA | 3.09  | 1.49        | 1.38     |
| 23  | B     | 612    | CLA  | C1C-C2C | 3.09  | 1.50        | 1.44     |
| 23  | b     | 601    | CLA  | C1B-NB  | -3.08 | 1.33        | 1.37     |
| 23  | C     | 508    | CLA  | OBD-CAD | 3.08  | 1.27        | 1.22     |
| 23  | a     | 405[A] | CLA  | O2A-CGA | 3.08  | 1.42        | 1.33     |
| 23  | d     | 401[B] | CLA  | C4B-NB  | -3.07 | 1.33        | 1.37     |
| 23  | B     | 604    | CLA  | C1B-NB  | -3.07 | 1.33        | 1.37     |
| 23  | c     | 510    | CLA  | C1B-C2B | 3.07  | 1.50        | 1.43     |
| 23  | C     | 514    | CLA  | C1B-C2B | 3.07  | 1.50        | 1.43     |
| 24  | A     | 407[A] | PHO  | CBD-CGD | -3.06 | 1.48        | 1.52     |
| 23  | B     | 608    | CLA  | C1B-NB  | -3.06 | 1.33        | 1.37     |
| 23  | a     | 409    | CLA  | OBD-CAD | 3.05  | 1.27        | 1.22     |
| 23  | b     | 602    | CLA  | CHB-C1B | 3.05  | 1.46        | 1.39     |
| 23  | c     | 511    | CLA  | C1B-NB  | -3.05 | 1.33        | 1.37     |
| 23  | B     | 603    | CLA  | C4B-NB  | -3.05 | 1.33        | 1.37     |
| 23  | c     | 503    | CLA  | C1B-C2B | 3.04  | 1.50        | 1.43     |
| 23  | c     | 507    | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 24  | a     | 416[B] | PHO  | C3A-C2A | -3.04 | 1.52        | 1.54     |
| 23  | C     | 512    | CLA  | C4D-CHA | 3.04  | 1.48        | 1.38     |
| 23  | a     | 407[B] | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 23  | b     | 604    | CLA  | C1B-NB  | -3.03 | 1.33        | 1.37     |
| 23  | B     | 616    | CLA  | C1B-NB  | -3.03 | 1.33        | 1.37     |
| 23  | D     | 702[A] | CLA  | C4B-NB  | -3.03 | 1.33        | 1.37     |
| 23  | a     | 405[A] | CLA  | C4B-NB  | -3.02 | 1.33        | 1.37     |
| 23  | d     | 402    | CLA  | OBD-CAD | 3.02  | 1.27        | 1.22     |
| 23  | c     | 506    | CLA  | C1B-C2B | 3.02  | 1.50        | 1.43     |
| 23  | A     | 408    | CLA  | C4B-NB  | -3.01 | 1.33        | 1.37     |
| 23  | A     | 408    | CLA  | CHB-C1B | 3.01  | 1.46        | 1.39     |
| 23  | d     | 401[A] | CLA  | C1D-ND  | 3.01  | 1.41        | 1.37     |
| 23  | A     | 404[A] | CLA  | C4C-C3C | 3.00  | 1.50        | 1.45     |
| 23  | b     | 614    | CLA  | C1B-C2B | 3.00  | 1.50        | 1.43     |
| 23  | B     | 615    | CLA  | CHC-C4B | 3.00  | 1.46        | 1.39     |
| 23  | b     | 612    | CLA  | C1B-C2B | 2.99  | 1.50        | 1.43     |
| 23  | B     | 614    | CLA  | C1B-C2B | 2.99  | 1.50        | 1.43     |
| 23  | C     | 509    | CLA  | C1B-C2B | 2.98  | 1.50        | 1.43     |
| 23  | c     | 504    | CLA  | C4B-NB  | -2.98 | 1.33        | 1.37     |
| 23  | b     | 614    | CLA  | C4B-NB  | -2.98 | 1.34        | 1.37     |
| 23  | b     | 608    | CLA  | C4B-NB  | -2.97 | 1.34        | 1.37     |
| 23  | d     | 401[B] | CLA  | C1B-NB  | -2.96 | 1.34        | 1.37     |
| 23  | B     | 608    | CLA  | OBD-CAD | 2.96  | 1.27        | 1.22     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 510    | CLA  | C1B-NB  | -2.96 | 1.34        | 1.37     |
| 23  | B     | 604    | CLA  | C1B-C2B | 2.95  | 1.50        | 1.43     |
| 23  | A     | 404[A] | CLA  | C1B-NB  | -2.95 | 1.34        | 1.37     |
| 23  | a     | 407[A] | CLA  | C1B-NB  | -2.95 | 1.34        | 1.37     |
| 23  | a     | 409    | CLA  | C1B-NB  | -2.95 | 1.34        | 1.37     |
| 29  | A     | 414[A] | PL9  | C6-C5   | 2.94  | 1.49        | 1.35     |
| 23  | C     | 508    | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 23  | C     | 508    | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 23  | B     | 608    | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 29  | a     | 414[A] | PL9  | C6-C5   | 2.93  | 1.49        | 1.35     |
| 23  | b     | 611    | CLA  | C1B-NB  | -2.92 | 1.34        | 1.37     |
| 23  | D     | 702[B] | CLA  | C1B-NB  | -2.91 | 1.34        | 1.37     |
| 23  | B     | 606    | CLA  | OBD-CAD | 2.91  | 1.27        | 1.22     |
| 23  | b     | 604    | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 23  | C     | 513    | CLA  | C1C-C2C | 2.91  | 1.50        | 1.44     |
| 23  | B     | 605    | CLA  | C1B-C2B | 2.91  | 1.49        | 1.43     |
| 23  | B     | 613    | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 23  | B     | 615    | CLA  | C1C-C2C | 2.90  | 1.50        | 1.44     |
| 29  | A     | 414[B] | PL9  | C6-C5   | 2.90  | 1.49        | 1.35     |
| 23  | D     | 702[B] | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 23  | D     | 702[A] | CLA  | C1B-C2B | 2.90  | 1.49        | 1.43     |
| 29  | a     | 414[B] | PL9  | C6-C5   | 2.89  | 1.49        | 1.35     |
| 23  | B     | 607    | CLA  | C1B-C2B | 2.89  | 1.49        | 1.43     |
| 23  | c     | 502    | CLA  | C1B-C2B | 2.89  | 1.49        | 1.43     |
| 23  | b     | 605    | CLA  | C1B-NB  | -2.89 | 1.34        | 1.37     |
| 23  | C     | 510    | CLA  | C1B-C2B | 2.89  | 1.49        | 1.43     |
| 35  | d     | 409    | HTG  | C1'-S1  | -2.88 | 1.77        | 1.81     |
| 23  | B     | 609    | CLA  | C1B-NB  | -2.88 | 1.34        | 1.37     |
| 23  | C     | 508    | CLA  | C1B-C2B | 2.88  | 1.49        | 1.43     |
| 23  | B     | 612    | CLA  | C4D-CHA | 2.88  | 1.48        | 1.38     |
| 23  | D     | 703    | CLA  | C1C-C2C | 2.88  | 1.50        | 1.44     |
| 23  | A     | 408    | CLA  | OBD-CAD | 2.88  | 1.27        | 1.22     |
| 24  | A     | 417[B] | PHO  | C3A-C2A | -2.88 | 1.52        | 1.54     |
| 23  | c     | 504    | CLA  | OBD-CAD | 2.87  | 1.27        | 1.22     |
| 23  | c     | 510    | CLA  | CHC-C4B | 2.87  | 1.45        | 1.39     |
| 23  | b     | 603    | CLA  | C1B-C2B | 2.87  | 1.49        | 1.43     |
| 23  | B     | 616    | CLA  | OBD-CAD | 2.87  | 1.27        | 1.22     |
| 23  | b     | 603    | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 23  | C     | 508    | CLA  | C1B-NB  | -2.86 | 1.34        | 1.37     |
| 23  | B     | 602    | CLA  | C1B-NB  | -2.86 | 1.34        | 1.37     |
| 23  | b     | 607    | CLA  | C1B-C2B | 2.86  | 1.49        | 1.43     |
| 23  | c     | 512    | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | d     | 401[A] | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 23  | c     | 511    | CLA  | C1B-C2B | 2.86  | 1.49        | 1.43     |
| 34  | Z     | 101    | LMG  | O8-C28  | 2.85  | 1.47        | 1.33     |
| 23  | B     | 613    | CLA  | C1B-C2B | 2.85  | 1.49        | 1.43     |
| 23  | C     | 514    | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 23  | d     | 401[B] | CLA  | C1B-C2B | 2.85  | 1.49        | 1.43     |
| 23  | b     | 611    | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 23  | B     | 604    | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 23  | c     | 514    | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 23  | B     | 614    | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 23  | c     | 510    | CLA  | C4C-C3C | 2.84  | 1.49        | 1.45     |
| 23  | C     | 506    | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 23  | D     | 703    | CLA  | C1B-NB  | -2.84 | 1.34        | 1.37     |
| 23  | b     | 602    | CLA  | C3B-C4B | 2.83  | 1.51        | 1.42     |
| 23  | c     | 512    | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 23  | B     | 616    | CLA  | C1B-C2B | 2.83  | 1.49        | 1.43     |
| 23  | A     | 408    | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 23  | b     | 603    | CLA  | C1B-NB  | -2.83 | 1.34        | 1.37     |
| 23  | c     | 509    | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 23  | B     | 610    | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 23  | C     | 503    | CLA  | C1B-NB  | -2.83 | 1.34        | 1.37     |
| 23  | a     | 405[B] | CLA  | C1B-NB  | -2.83 | 1.34        | 1.37     |
| 23  | C     | 502    | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 23  | A     | 406[A] | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 23  | c     | 513    | CLA  | C1B-NB  | -2.82 | 1.34        | 1.37     |
| 23  | b     | 612    | CLA  | C1C-C2C | 2.82  | 1.50        | 1.44     |
| 23  | C     | 512    | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 23  | D     | 703    | CLA  | C3B-C4B | 2.82  | 1.50        | 1.42     |
| 35  | b     | 625    | HTG  | C1'-S1  | -2.82 | 1.77        | 1.81     |
| 23  | b     | 611    | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 23  | A     | 404[A] | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 23  | B     | 607    | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 23  | D     | 702[A] | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 23  | c     | 513    | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 23  | C     | 505    | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 23  | C     | 505    | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 23  | a     | 409    | CLA  | C1C-C2C | 2.80  | 1.50        | 1.44     |
| 23  | B     | 616    | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 23  | B     | 601    | CLA  | C1B-NB  | -2.79 | 1.34        | 1.37     |
| 23  | d     | 401[B] | CLA  | C4C-C3C | 2.79  | 1.49        | 1.45     |
| 23  | a     | 406[A] | CLA  | C1B-C2B | 2.79  | 1.49        | 1.43     |
| 23  | A     | 405[A] | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 502    | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 23  | B     | 609    | CLA  | C3B-C4B | 2.78  | 1.50        | 1.42     |
| 23  | B     | 610    | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 23  | C     | 505    | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 23  | c     | 509    | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 23  | C     | 503    | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 23  | b     | 605    | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 23  | A     | 404[B] | CLA  | C1B-NB  | -2.76 | 1.34        | 1.37     |
| 23  | a     | 406[B] | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 23  | b     | 613    | CLA  | C1B-C2B | 2.76  | 1.49        | 1.43     |
| 23  | C     | 503    | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 23  | B     | 605    | CLA  | OBD-CAD | 2.75  | 1.27        | 1.22     |
| 23  | c     | 506    | CLA  | C3B-C4B | 2.75  | 1.50        | 1.42     |
| 23  | c     | 510    | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 23  | A     | 406[A] | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 23  | b     | 607    | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 23  | C     | 502    | CLA  | C1C-C2C | 2.74  | 1.50        | 1.44     |
| 23  | C     | 509    | CLA  | C4C-C3C | 2.74  | 1.49        | 1.45     |
| 23  | a     | 407[A] | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 23  | B     | 605    | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 23  | C     | 504    | CLA  | C1B-NB  | -2.74 | 1.34        | 1.37     |
| 23  | B     | 608    | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 35  | D     | 710    | HTG  | C1'-S1  | -2.74 | 1.77        | 1.81     |
| 23  | d     | 401[B] | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 23  | b     | 616    | CLA  | C1C-C2C | 2.73  | 1.50        | 1.44     |
| 23  | B     | 605    | CLA  | C3D-C4D | -2.73 | 1.38        | 1.44     |
| 23  | C     | 511    | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 23  | B     | 612    | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 23  | c     | 508    | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 23  | c     | 506    | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 23  | c     | 505    | CLA  | C1C-C2C | 2.73  | 1.50        | 1.44     |
| 23  | B     | 602    | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 23  | A     | 404[B] | CLA  | C4C-C3C | 2.72  | 1.49        | 1.45     |
| 23  | B     | 609    | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 23  | a     | 405[A] | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 23  | d     | 402    | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 23  | C     | 510    | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 23  | B     | 602    | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 23  | b     | 610    | CLA  | C4C-C3C | 2.72  | 1.49        | 1.45     |
| 23  | a     | 407[A] | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 23  | B     | 605    | CLA  | C3B-C4B | 2.72  | 1.50        | 1.42     |
| 23  | d     | 401[A] | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 613    | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 23  | B     | 610    | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 23  | C     | 507    | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 23  | B     | 603    | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 24  | a     | 416[A] | PHO  | C3A-C2A | -2.70 | 1.52        | 1.54     |
| 23  | b     | 609    | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 23  | b     | 613    | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 23  | c     | 511    | CLA  | C1C-C2C | 2.70  | 1.50        | 1.44     |
| 23  | c     | 511    | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 23  | B     | 614    | CLA  | C1B-NB  | -2.69 | 1.34        | 1.37     |
| 23  | D     | 702[B] | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 23  | B     | 606    | CLA  | C1C-C2C | 2.69  | 1.50        | 1.44     |
| 23  | d     | 402    | CLA  | C1B-NB  | -2.69 | 1.34        | 1.37     |
| 23  | c     | 504    | CLA  | C1C-C2C | 2.69  | 1.50        | 1.44     |
| 23  | b     | 612    | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 23  | C     | 509    | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 23  | a     | 407[B] | CLA  | C1C-C2C | 2.69  | 1.50        | 1.44     |
| 23  | a     | 407[B] | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 35  | c     | 522    | HTG  | C1'-S1  | -2.69 | 1.77        | 1.81     |
| 23  | c     | 512    | CLA  | C1B-NB  | -2.69 | 1.34        | 1.37     |
| 24  | A     | 417[B] | PHO  | CHA-CBD | -2.68 | 1.48        | 1.51     |
| 23  | B     | 608    | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 23  | c     | 507    | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 23  | B     | 611    | CLA  | C3B-C4B | 2.68  | 1.50        | 1.42     |
| 23  | C     | 513    | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 23  | A     | 405[A] | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 29  | D     | 705[B] | PL9  | C6-C5   | 2.68  | 1.48        | 1.35     |
| 23  | B     | 606    | CLA  | C3D-C4D | -2.68 | 1.38        | 1.44     |
| 23  | c     | 509    | CLA  | C4C-C3C | 2.68  | 1.49        | 1.45     |
| 23  | b     | 609    | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 23  | b     | 601    | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 23  | C     | 502    | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 23  | c     | 504    | CLA  | C3B-C4B | 2.67  | 1.50        | 1.42     |
| 23  | B     | 602    | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 23  | C     | 513    | CLA  | C1B-NB  | -2.67 | 1.34        | 1.37     |
| 23  | b     | 615    | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 23  | b     | 610    | CLA  | C1C-C2C | 2.67  | 1.49        | 1.44     |
| 23  | A     | 404[B] | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 23  | A     | 404[A] | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 23  | A     | 405[B] | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 23  | c     | 505    | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 23  | b     | 616    | CLA  | C1B-NB  | -2.66 | 1.34        | 1.37     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | b     | 614    | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 23  | A     | 406[B] | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 23  | a     | 405[B] | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 23  | A     | 404[B] | CLA  | C1C-C2C | 2.66  | 1.49        | 1.44     |
| 23  | c     | 504    | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 23  | c     | 514    | CLA  | C1C-C2C | 2.66  | 1.49        | 1.44     |
| 36  | c     | 519    | DGD  | O2G-C2G | -2.65 | 1.40        | 1.46     |
| 23  | A     | 406[B] | CLA  | C3B-C4B | 2.65  | 1.50        | 1.42     |
| 23  | C     | 514    | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 23  | b     | 610    | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 35  | C     | 522    | HTG  | C1'-S1  | -2.64 | 1.77        | 1.81     |
| 23  | B     | 615    | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 23  | b     | 615    | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 23  | b     | 607    | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 23  | c     | 508    | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 23  | B     | 605    | CLA  | C1C-C2C | 2.64  | 1.49        | 1.44     |
| 23  | b     | 616    | CLA  | C3D-C4D | -2.63 | 1.38        | 1.44     |
| 23  | c     | 504    | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 23  | a     | 409    | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 23  | b     | 611    | CLA  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 23  | a     | 407[B] | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 23  | b     | 608    | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 23  | a     | 406[B] | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 23  | C     | 513    | CLA  | C3B-C4B | 2.63  | 1.50        | 1.42     |
| 23  | c     | 505    | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 23  | D     | 703    | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 23  | C     | 509    | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 38  | F     | 102    | HEM  | C1C-C2C | -2.62 | 1.40        | 1.45     |
| 23  | c     | 502    | CLA  | C4C-C3C | 2.62  | 1.49        | 1.45     |
| 23  | a     | 407[A] | CLA  | C1C-C2C | 2.62  | 1.49        | 1.44     |
| 23  | C     | 511    | CLA  | C4C-C3C | 2.62  | 1.49        | 1.45     |
| 23  | A     | 405[A] | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 23  | d     | 402    | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 23  | c     | 513    | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 23  | B     | 601    | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 23  | c     | 514    | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 23  | B     | 607    | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 23  | A     | 408    | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 23  | C     | 504    | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 23  | c     | 504    | CLA  | C3D-C4D | -2.60 | 1.38        | 1.44     |
| 23  | C     | 510    | CLA  | C3B-C2B | 2.60  | 1.49        | 1.41     |
| 23  | A     | 404[B] | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | d     | 401[A] | CLA  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 23  | b     | 602    | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 23  | C     | 505    | CLA  | C1C-C2C | 2.59  | 1.49        | 1.44     |
| 25  | d     | 403    | BCR  | C30-C25 | -2.59 | 1.50        | 1.53     |
| 36  | C     | 519    | DGD  | O2G-C2G | -2.59 | 1.40        | 1.46     |
| 23  | B     | 606    | CLA  | C1B-NB  | -2.59 | 1.34        | 1.37     |
| 23  | C     | 504    | CLA  | C3B-C4B | 2.59  | 1.50        | 1.42     |
| 23  | C     | 508    | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 23  | b     | 606    | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 23  | A     | 406[B] | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 23  | b     | 615    | CLA  | C3D-C4D | -2.58 | 1.38        | 1.44     |
| 23  | b     | 613    | CLA  | C4B-NB  | -2.58 | 1.34        | 1.37     |
| 23  | b     | 603    | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 23  | B     | 606    | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 27  | D     | 701    | GOL  | C3-C2   | 2.58  | 1.61        | 1.51     |
| 23  | C     | 510    | CLA  | C4C-C3C | 2.58  | 1.49        | 1.45     |
| 23  | A     | 405[A] | CLA  | C3B-C4B | 2.58  | 1.50        | 1.42     |
| 23  | C     | 511    | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 23  | C     | 510    | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 35  | o     | 301    | HTG  | O5-C1   | 2.58  | 1.46        | 1.42     |
| 23  | B     | 612    | CLA  | C4C-C3C | 2.58  | 1.49        | 1.45     |
| 23  | B     | 605    | CLA  | C1B-NB  | -2.57 | 1.34        | 1.37     |
| 23  | B     | 601    | CLA  | C4B-NB  | -2.57 | 1.34        | 1.37     |
| 23  | D     | 703    | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 23  | C     | 507    | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 23  | D     | 702[B] | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 23  | a     | 405[A] | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 23  | b     | 609    | CLA  | C3B-C4B | 2.57  | 1.50        | 1.42     |
| 23  | a     | 406[A] | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 23  | c     | 509    | CLA  | C1B-NB  | -2.56 | 1.34        | 1.37     |
| 23  | b     | 616    | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 23  | b     | 616    | CLA  | C3B-C4B | 2.56  | 1.50        | 1.42     |
| 34  | C     | 521    | LMG  | O1-C1   | 2.56  | 1.44        | 1.40     |
| 23  | C     | 504    | CLA  | C3D-C4D | -2.56 | 1.38        | 1.44     |
| 24  | a     | 416[B] | PHO  | C4B-NB  | -2.55 | 1.34        | 1.38     |
| 23  | C     | 512    | CLA  | C3B-C2B | 2.55  | 1.49        | 1.41     |
| 23  | c     | 503    | CLA  | C4D-CHA | 2.55  | 1.47        | 1.38     |
| 23  | c     | 508    | CLA  | C1C-C2C | 2.55  | 1.49        | 1.44     |
| 23  | C     | 509    | CLA  | C3B-C2B | 2.55  | 1.49        | 1.41     |
| 23  | b     | 608    | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 23  | b     | 616    | CLA  | C4D-CHA | 2.55  | 1.47        | 1.38     |
| 23  | B     | 603    | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 507    | CLA  | C4D-CHA | 2.54  | 1.47        | 1.38     |
| 23  | B     | 609    | CLA  | C4D-CHA | 2.54  | 1.47        | 1.38     |
| 23  | C     | 502    | CLA  | C4C-C3C | 2.54  | 1.49        | 1.45     |
| 23  | C     | 502    | CLA  | C3B-C4B | 2.54  | 1.50        | 1.42     |
| 24  | a     | 416[B] | PHO  | C1B-NB  | -2.54 | 1.34        | 1.38     |
| 23  | c     | 506    | CLA  | C1C-C2C | 2.53  | 1.49        | 1.44     |
| 23  | C     | 506    | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 23  | b     | 607    | CLA  | C1C-C2C | 2.53  | 1.49        | 1.44     |
| 23  | a     | 405[A] | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 23  | D     | 702[B] | CLA  | C1C-C2C | 2.53  | 1.49        | 1.44     |
| 23  | b     | 606    | CLA  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 23  | C     | 512    | CLA  | C1C-C2C | 2.53  | 1.49        | 1.44     |
| 23  | c     | 507    | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 23  | c     | 506    | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 35  | b     | 622    | HTG  | O5-C1   | 2.53  | 1.46        | 1.42     |
| 24  | a     | 408[A] | PHO  | CBD-CGD | -2.52 | 1.49        | 1.52     |
| 23  | b     | 615    | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 23  | B     | 607    | CLA  | C1C-C2C | 2.52  | 1.49        | 1.44     |
| 23  | A     | 405[B] | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 23  | c     | 502    | CLA  | C1C-C2C | 2.52  | 1.49        | 1.44     |
| 23  | A     | 406[A] | CLA  | C3B-C4B | 2.52  | 1.50        | 1.42     |
| 27  | a     | 419    | GOL  | C1-C2   | 2.52  | 1.61        | 1.51     |
| 23  | d     | 402    | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 23  | B     | 616    | CLA  | C3B-C2B | 2.52  | 1.49        | 1.41     |
| 23  | a     | 407[A] | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 23  | C     | 507    | CLA  | C1C-C2C | 2.51  | 1.49        | 1.44     |
| 23  | b     | 603    | CLA  | C3B-C2B | 2.51  | 1.49        | 1.41     |
| 29  | d     | 404[A] | PL9  | C6-C5   | 2.51  | 1.47        | 1.35     |
| 23  | C     | 506    | CLA  | C1C-C2C | 2.51  | 1.49        | 1.44     |
| 23  | b     | 605    | CLA  | C4D-CHA | 2.51  | 1.47        | 1.38     |
| 23  | c     | 514    | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 23  | A     | 406[A] | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 23  | c     | 505    | CLA  | C3B-C2B | 2.50  | 1.49        | 1.41     |
| 29  | d     | 404[B] | PL9  | C6-C5   | 2.50  | 1.47        | 1.35     |
| 23  | c     | 509    | CLA  | C4B-NB  | -2.50 | 1.34        | 1.37     |
| 23  | C     | 514    | CLA  | C1C-C2C | 2.50  | 1.49        | 1.44     |
| 23  | A     | 405[B] | CLA  | C3B-C4B | 2.50  | 1.50        | 1.42     |
| 23  | b     | 609    | CLA  | C1C-C2C | 2.49  | 1.49        | 1.44     |
| 23  | B     | 607    | CLA  | C3D-C4D | -2.49 | 1.38        | 1.44     |
| 23  | C     | 511    | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 23  | A     | 408    | CLA  | C3B-C2B | 2.49  | 1.49        | 1.41     |
| 23  | A     | 405[B] | CLA  | C3D-C4D | -2.49 | 1.38        | 1.44     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 29  | D     | 705[A] | PL9  | C6-C5   | 2.49  | 1.47        | 1.35     |
| 24  | A     | 417[B] | PHO  | C4B-NB  | -2.49 | 1.34        | 1.38     |
| 23  | A     | 404[B] | CLA  | C3B-C2B | 2.49  | 1.49        | 1.41     |
| 24  | A     | 417[A] | PHO  | C3A-C2A | -2.49 | 1.52        | 1.54     |
| 23  | c     | 513    | CLA  | C3B-C4B | 2.49  | 1.50        | 1.42     |
| 23  | A     | 406[B] | CLA  | C4D-CHA | 2.49  | 1.46        | 1.38     |
| 23  | B     | 602    | CLA  | C4C-C3C | 2.48  | 1.49        | 1.45     |
| 23  | B     | 615    | CLA  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 23  | B     | 616    | CLA  | C3B-C4B | 2.48  | 1.50        | 1.42     |
| 23  | C     | 509    | CLA  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 23  | a     | 405[B] | CLA  | C4D-CHA | 2.48  | 1.46        | 1.38     |
| 23  | b     | 611    | CLA  | C4D-CHA | 2.48  | 1.46        | 1.38     |
| 32  | B     | 627    | LMT  | C3'-C2' | 2.48  | 1.58        | 1.52     |
| 23  | b     | 613    | CLA  | OBD-CAD | 2.48  | 1.26        | 1.22     |
| 23  | C     | 511    | CLA  | C4D-CHA | 2.48  | 1.46        | 1.38     |
| 27  | D     | 701    | GOL  | O2-C2   | -2.47 | 1.36        | 1.43     |
| 23  | b     | 606    | CLA  | C1C-C2C | 2.47  | 1.49        | 1.44     |
| 23  | c     | 503    | CLA  | C3B-C2B | 2.47  | 1.49        | 1.41     |
| 23  | a     | 405[B] | CLA  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 23  | C     | 504    | CLA  | C4B-NB  | -2.47 | 1.34        | 1.37     |
| 23  | b     | 609    | CLA  | C1B-NB  | -2.47 | 1.34        | 1.37     |
| 23  | B     | 601    | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 23  | a     | 409    | CLA  | C4D-CHA | 2.47  | 1.46        | 1.38     |
| 23  | B     | 605    | CLA  | C4D-CHA | 2.47  | 1.46        | 1.38     |
| 32  | t     | 101    | LMT  | O3'-C3' | -2.47 | 1.36        | 1.43     |
| 23  | B     | 608    | CLA  | C3B-C2B | 2.47  | 1.49        | 1.41     |
| 23  | d     | 401[A] | CLA  | C4D-CHA | 2.47  | 1.46        | 1.38     |
| 38  | f     | 101    | HEM  | C1D-ND  | -2.46 | 1.34        | 1.38     |
| 23  | C     | 505    | CLA  | C3D-C4D | -2.46 | 1.38        | 1.44     |
| 23  | B     | 604    | CLA  | C4B-NB  | -2.46 | 1.34        | 1.37     |
| 23  | c     | 502    | CLA  | C1B-NB  | -2.46 | 1.34        | 1.37     |
| 24  | A     | 417[A] | PHO  | C3D-C4D | -2.46 | 1.37        | 1.41     |
| 23  | C     | 512    | CLA  | C1B-NB  | -2.46 | 1.34        | 1.37     |
| 23  | B     | 606    | CLA  | C4B-NB  | -2.46 | 1.34        | 1.37     |
| 23  | b     | 607    | CLA  | OBD-CAD | 2.46  | 1.26        | 1.22     |
| 23  | B     | 608    | CLA  | C3D-C4D | -2.46 | 1.38        | 1.44     |
| 23  | c     | 505    | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 32  | m     | 103    | LMT  | C3'-C2' | 2.46  | 1.58        | 1.52     |
| 23  | B     | 610    | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 23  | B     | 601    | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 36  | H     | 102    | DGD  | O5D-C1E | 2.46  | 1.44        | 1.40     |
| 23  | a     | 407[A] | CLA  | C3B-C4B | 2.46  | 1.49        | 1.42     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | a     | 407[A] | CLA  | C3D-C4D | -2.46 | 1.38        | 1.44     |
| 23  | d     | 402    | CLA  | C3B-C4B | 2.46  | 1.49        | 1.42     |
| 23  | A     | 406[B] | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 23  | D     | 702[B] | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 24  | A     | 407[B] | PHO  | C4B-NB  | -2.45 | 1.34        | 1.38     |
| 23  | A     | 405[B] | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 23  | C     | 507    | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 25  | B     | 619    | BCR  | C30-C25 | -2.45 | 1.50        | 1.53     |
| 23  | C     | 503    | CLA  | C3B-C2B | 2.45  | 1.49        | 1.41     |
| 23  | b     | 601    | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 23  | D     | 703    | CLA  | C4D-CHA | 2.44  | 1.46        | 1.38     |
| 23  | B     | 608    | CLA  | C4C-C3C | 2.44  | 1.49        | 1.45     |
| 23  | b     | 610    | CLA  | C4B-NB  | -2.44 | 1.34        | 1.37     |
| 23  | B     | 603    | CLA  | C3B-C2B | 2.44  | 1.49        | 1.41     |
| 23  | c     | 502    | CLA  | C4B-NB  | -2.43 | 1.34        | 1.37     |
| 23  | B     | 607    | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 23  | C     | 513    | CLA  | C4B-NB  | -2.43 | 1.34        | 1.37     |
| 23  | B     | 609    | CLA  | C1C-C2C | 2.43  | 1.49        | 1.44     |
| 23  | D     | 703    | CLA  | C4B-NB  | -2.43 | 1.34        | 1.37     |
| 23  | C     | 514    | CLA  | C3B-C2B | 2.43  | 1.49        | 1.41     |
| 23  | c     | 512    | CLA  | C1C-C2C | 2.43  | 1.49        | 1.44     |
| 23  | C     | 503    | CLA  | C3D-C4D | -2.43 | 1.38        | 1.44     |
| 23  | b     | 603    | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 23  | b     | 609    | CLA  | C4B-NB  | -2.42 | 1.34        | 1.37     |
| 23  | C     | 506    | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 23  | c     | 502    | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 23  | b     | 614    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 23  | d     | 402    | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 32  | A     | 420    | LMT  | O3'-C3' | -2.41 | 1.37        | 1.43     |
| 23  | b     | 602    | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 23  | D     | 702[A] | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 24  | a     | 408[B] | PHO  | CHA-CBD | -2.41 | 1.48        | 1.51     |
| 23  | B     | 614    | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 23  | b     | 602    | CLA  | C4B-NB  | -2.41 | 1.34        | 1.37     |
| 23  | b     | 608    | CLA  | C1C-C2C | 2.40  | 1.49        | 1.44     |
| 23  | A     | 404[A] | CLA  | C1C-C2C | 2.40  | 1.49        | 1.44     |
| 27  | o     | 304    | GOL  | C1-C2   | 2.40  | 1.60        | 1.51     |
| 23  | c     | 508    | CLA  | C4B-NB  | -2.40 | 1.34        | 1.37     |
| 23  | B     | 610    | CLA  | C1C-C2C | 2.39  | 1.49        | 1.44     |
| 23  | b     | 613    | CLA  | C3B-C2B | 2.39  | 1.49        | 1.41     |
| 32  | b     | 621    | LMT  | C3'-C2' | 2.39  | 1.58        | 1.52     |
| 23  | B     | 616    | CLA  | C1C-C2C | 2.39  | 1.49        | 1.44     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | a     | 407[B] | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 23  | D     | 702[B] | CLA  | C4D-CHA | 2.39  | 1.46        | 1.38     |
| 27  | D     | 712    | GOL  | C3-C2   | 2.39  | 1.60        | 1.51     |
| 23  | B     | 606    | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 23  | c     | 512    | CLA  | C3B-C2B | 2.39  | 1.49        | 1.41     |
| 23  | c     | 511    | CLA  | C4B-NB  | -2.39 | 1.34        | 1.37     |
| 23  | b     | 610    | CLA  | C3D-C4D | -2.39 | 1.38        | 1.44     |
| 23  | B     | 604    | CLA  | C3D-C4D | -2.39 | 1.38        | 1.44     |
| 32  | M     | 101    | LMT  | O1'-C1' | -2.39 | 1.36        | 1.40     |
| 23  | b     | 605    | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 23  | b     | 608    | CLA  | C3D-C4D | -2.38 | 1.38        | 1.44     |
| 23  | b     | 611    | CLA  | C3D-C4D | -2.38 | 1.38        | 1.44     |
| 23  | a     | 406[A] | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 23  | A     | 406[B] | CLA  | C1C-C2C | 2.38  | 1.49        | 1.44     |
| 23  | B     | 615    | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 23  | B     | 605    | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 23  | C     | 503    | CLA  | C4D-CHA | 2.38  | 1.46        | 1.38     |
| 23  | a     | 405[B] | CLA  | C3B-C2B | 2.37  | 1.49        | 1.41     |
| 23  | b     | 601    | CLA  | C3B-C2B | 2.37  | 1.49        | 1.41     |
| 23  | c     | 512    | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 23  | C     | 502    | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 23  | a     | 409    | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 23  | c     | 511    | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 23  | b     | 613    | CLA  | C1C-C2C | 2.36  | 1.49        | 1.44     |
| 23  | B     | 602    | CLA  | C3D-C4D | -2.36 | 1.38        | 1.44     |
| 23  | B     | 601    | CLA  | C1C-C2C | 2.36  | 1.49        | 1.44     |
| 23  | C     | 503    | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 23  | c     | 514    | CLA  | C3B-C2B | 2.36  | 1.49        | 1.41     |
| 23  | C     | 504    | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 24  | a     | 408[B] | PHO  | C4B-NB  | -2.36 | 1.34        | 1.38     |
| 23  | A     | 405[A] | CLA  | C3D-C4D | -2.36 | 1.38        | 1.44     |
| 23  | C     | 513    | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 23  | c     | 513    | CLA  | C4B-NB  | -2.36 | 1.34        | 1.37     |
| 23  | b     | 610    | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 23  | C     | 504    | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 32  | T     | 101    | LMT  | O3'-C3' | -2.35 | 1.37        | 1.43     |
| 23  | d     | 401[B] | CLA  | C3D-C4D | -2.35 | 1.38        | 1.44     |
| 27  | b     | 624    | GOL  | C3-C2   | 2.35  | 1.60        | 1.51     |
| 23  | D     | 702[B] | CLA  | C3B-C2B | 2.35  | 1.49        | 1.41     |
| 24  | A     | 417[A] | PHO  | C4B-NB  | -2.35 | 1.34        | 1.38     |
| 23  | C     | 511    | CLA  | C3D-C4D | -2.35 | 1.38        | 1.44     |
| 23  | B     | 611    | CLA  | MG-NB   | 2.35  | 2.10        | 2.05     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 612    | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 26  | X     | 101    | SQD  | O6-C1   | 2.34  | 1.44        | 1.40     |
| 23  | A     | 404[B] | CLA  | C3D-C4D | -2.34 | 1.38        | 1.44     |
| 23  | a     | 405[A] | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 23  | A     | 404[A] | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 23  | C     | 512    | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 23  | c     | 510    | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 23  | B     | 611    | CLA  | C4D-CHA | 2.33  | 1.46        | 1.38     |
| 23  | B     | 606    | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 23  | b     | 601    | CLA  | C1C-C2C | 2.33  | 1.49        | 1.44     |
| 23  | c     | 514    | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 23  | b     | 606    | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 23  | a     | 407[B] | CLA  | C1B-NB  | -2.32 | 1.34        | 1.37     |
| 23  | B     | 612    | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 23  | b     | 604    | CLA  | C3B-C2B | 2.32  | 1.49        | 1.41     |
| 23  | A     | 405[A] | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 23  | A     | 406[A] | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 36  | h     | 102    | DGD  | O5D-C1E | 2.32  | 1.44        | 1.40     |
| 23  | d     | 401[B] | CLA  | C3B-C2B | 2.32  | 1.49        | 1.41     |
| 23  | b     | 614    | CLA  | C3B-C2B | 2.32  | 1.49        | 1.41     |
| 23  | b     | 612    | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 23  | b     | 609    | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 23  | d     | 401[A] | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 24  | A     | 417[B] | PHO  | C1D-ND  | -2.32 | 1.34        | 1.38     |
| 23  | A     | 408    | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 23  | c     | 503    | CLA  | C1B-NB  | -2.32 | 1.34        | 1.37     |
| 23  | c     | 513    | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 23  | c     | 511    | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 23  | B     | 615    | CLA  | C4B-NB  | -2.31 | 1.34        | 1.37     |
| 35  | B     | 624    | HTG  | C1-S1   | -2.31 | 1.76        | 1.80     |
| 23  | b     | 603    | CLA  | C4D-CHA | 2.31  | 1.46        | 1.38     |
| 38  | f     | 101    | HEM  | C1C-C2C | -2.31 | 1.40        | 1.45     |
| 23  | B     | 610    | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 23  | b     | 606    | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 23  | b     | 612    | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 23  | c     | 509    | CLA  | C1C-C2C | 2.30  | 1.49        | 1.44     |
| 23  | a     | 407[B] | CLA  | C3D-C4D | -2.30 | 1.39        | 1.44     |
| 29  | a     | 414[A] | PL9  | C2-C3   | 2.30  | 1.40        | 1.34     |
| 23  | c     | 503    | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 23  | c     | 509    | CLA  | C3B-C2B | 2.30  | 1.48        | 1.41     |
| 23  | b     | 610    | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 32  | M     | 101    | LMT  | O2'-C2' | -2.29 | 1.37        | 1.43     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 513    | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 23  | a     | 406[B] | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 23  | a     | 406[B] | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 23  | a     | 407[B] | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 23  | b     | 612    | CLA  | C3B-C2B | 2.29  | 1.48        | 1.41     |
| 24  | A     | 417[B] | PHO  | C3D-C4D | -2.28 | 1.38        | 1.41     |
| 23  | C     | 505    | CLA  | C3B-C2B | 2.28  | 1.48        | 1.41     |
| 24  | A     | 417[A] | PHO  | C1D-ND  | -2.28 | 1.34        | 1.38     |
| 23  | b     | 601    | CLA  | C4C-C3C | 2.28  | 1.48        | 1.45     |
| 23  | b     | 603    | CLA  | C4C-C3C | 2.28  | 1.48        | 1.45     |
| 23  | b     | 614    | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 23  | B     | 613    | CLA  | C1C-C2C | 2.27  | 1.49        | 1.44     |
| 23  | c     | 514    | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 29  | D     | 705[B] | PL9  | C2-C3   | 2.27  | 1.40        | 1.34     |
| 23  | c     | 513    | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 23  | B     | 616    | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 23  | b     | 603    | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 23  | B     | 604    | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 23  | d     | 402    | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 35  | B     | 622    | HTG  | C1'-S1  | -2.27 | 1.78        | 1.81     |
| 23  | B     | 602    | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 23  | b     | 611    | CLA  | C3B-C2B | 2.26  | 1.48        | 1.41     |
| 32  | e     | 101    | LMT  | O3'-C3' | -2.26 | 1.37        | 1.43     |
| 23  | b     | 607    | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 23  | c     | 514    | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 23  | C     | 509    | CLA  | C1C-C2C | 2.26  | 1.49        | 1.44     |
| 32  | F     | 101    | LMT  | O3'-C3' | -2.26 | 1.37        | 1.43     |
| 23  | A     | 406[A] | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 36  | C     | 518[A] | DGD  | O5D-C1E | 2.26  | 1.44        | 1.40     |
| 23  | B     | 615    | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 23  | C     | 512    | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 23  | A     | 408    | CLA  | C1C-NC  | -2.25 | 1.34        | 1.37     |
| 23  | A     | 405[B] | CLA  | C1C-C2C | 2.25  | 1.49        | 1.44     |
| 23  | B     | 609    | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 40  | v     | 201    | HEC  | CMC-C2C | 2.25  | 1.55        | 1.50     |
| 23  | c     | 511    | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 23  | c     | 507    | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 32  | A     | 420    | LMT  | O2'-C2' | -2.24 | 1.37        | 1.43     |
| 23  | D     | 702[A] | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 23  | a     | 409    | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 40  | V     | 201    | HEC  | CMB-C2B | 2.24  | 1.55        | 1.50     |
| 23  | C     | 512    | CLA  | C1C-NC  | -2.24 | 1.34        | 1.37     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | d     | 401[B] | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 23  | B     | 608    | CLA  | C1C-NC  | -2.24 | 1.34        | 1.37     |
| 23  | C     | 503    | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 26  | B     | 620    | SQD  | O6-C1   | 2.23  | 1.43        | 1.40     |
| 23  | B     | 603    | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 23  | b     | 606    | CLA  | C4B-NB  | -2.23 | 1.34        | 1.37     |
| 32  | B     | 627    | LMT  | O3'-C3' | -2.23 | 1.37        | 1.43     |
| 23  | b     | 604    | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 23  | a     | 406[B] | CLA  | C4B-NB  | -2.23 | 1.34        | 1.37     |
| 23  | b     | 607    | CLA  | C3B-C2B | 2.23  | 1.48        | 1.41     |
| 24  | a     | 408[A] | PHO  | C4B-NB  | -2.22 | 1.34        | 1.38     |
| 32  | T     | 101    | LMT  | O2'-C2' | -2.22 | 1.37        | 1.43     |
| 23  | B     | 601    | CLA  | C3B-C2B | 2.22  | 1.48        | 1.41     |
| 23  | b     | 608    | CLA  | C3B-C2B | 2.22  | 1.48        | 1.41     |
| 27  | D     | 712    | GOL  | O2-C2   | -2.22 | 1.36        | 1.43     |
| 23  | d     | 401[A] | CLA  | C1C-C2C | 2.22  | 1.49        | 1.44     |
| 32  | B     | 630    | LMT  | O3'-C3' | -2.22 | 1.37        | 1.43     |
| 23  | C     | 508    | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 23  | c     | 505    | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 23  | c     | 509    | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 24  | a     | 416[A] | PHO  | C4B-NB  | -2.21 | 1.34        | 1.38     |
| 23  | b     | 610    | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 23  | D     | 702[A] | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 23  | B     | 608    | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 24  | A     | 407[A] | PHO  | C4B-NB  | -2.21 | 1.34        | 1.38     |
| 29  | A     | 414[A] | PL9  | C2-C1   | -2.21 | 1.39        | 1.44     |
| 23  | C     | 506    | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 23  | A     | 405[B] | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 24  | a     | 408[B] | PHO  | C1B-NB  | -2.20 | 1.34        | 1.38     |
| 23  | b     | 604    | CLA  | C1C-C2C | 2.20  | 1.49        | 1.44     |
| 23  | C     | 502    | CLA  | C4B-NB  | -2.20 | 1.35        | 1.37     |
| 23  | B     | 613    | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 23  | B     | 603    | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 38  | F     | 102    | HEM  | C3C-C4C | -2.19 | 1.42        | 1.46     |
| 38  | F     | 102    | HEM  | C3B-C4B | 2.19  | 1.49        | 1.44     |
| 23  | b     | 616    | CLA  | C4B-NB  | -2.19 | 1.35        | 1.37     |
| 23  | b     | 605    | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 23  | b     | 605    | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 23  | c     | 506    | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 32  | M     | 101    | LMT  | O3'-C3' | -2.18 | 1.37        | 1.43     |
| 23  | B     | 603    | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 32  | B     | 629    | LMT  | O2'-C2' | -2.18 | 1.37        | 1.43     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | B     | 614    | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 23  | C     | 508    | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 32  | M     | 101    | LMT  | O2B-C2B | -2.18 | 1.37        | 1.43     |
| 23  | c     | 502    | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 24  | A     | 407[A] | PHO  | C1B-NB  | -2.18 | 1.34        | 1.38     |
| 23  | B     | 610    | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 23  | D     | 703    | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 24  | a     | 416[A] | PHO  | CBD-CGD | -2.17 | 1.49        | 1.52     |
| 23  | B     | 604    | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 23  | c     | 507    | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 23  | a     | 405[A] | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 23  | C     | 507    | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 23  | b     | 614    | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 23  | C     | 514    | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 23  | A     | 406[B] | CLA  | C4C-C3C | 2.16  | 1.48        | 1.45     |
| 23  | B     | 603    | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 33  | b     | 629[A] | LHG  | O7-C5   | -2.16 | 1.41        | 1.46     |
| 23  | B     | 604    | CLA  | C1A-CHA | 2.15  | 1.52        | 1.43     |
| 23  | C     | 510    | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 40  | V     | 201    | HEC  | CMA-C3A | 2.15  | 1.55        | 1.50     |
| 23  | B     | 614    | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 23  | B     | 607    | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 24  | A     | 407[A] | PHO  | C1D-ND  | -2.14 | 1.34        | 1.38     |
| 23  | c     | 503    | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 23  | b     | 604    | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 27  | V     | 203[A] | GOL  | C1-C2   | 2.14  | 1.59        | 1.51     |
| 23  | c     | 509    | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 23  | c     | 511    | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 29  | D     | 705[A] | PL9  | C2-C3   | 2.14  | 1.40        | 1.34     |
| 23  | b     | 601    | CLA  | C1B-C2B | 2.14  | 1.48        | 1.43     |
| 23  | C     | 511    | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 29  | a     | 414[B] | PL9  | C2-C3   | 2.13  | 1.40        | 1.34     |
| 23  | B     | 613    | CLA  | C4C-C3C | 2.13  | 1.48        | 1.45     |
| 23  | C     | 513    | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 23  | b     | 616    | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 32  | a     | 417    | LMT  | O3'-C3' | -2.13 | 1.37        | 1.43     |
| 32  | T     | 101    | LMT  | O3B-C3B | -2.13 | 1.37        | 1.43     |
| 36  | C     | 518[B] | DGD  | O5D-C1E | 2.13  | 1.43        | 1.40     |
| 24  | A     | 407[B] | PHO  | CBD-CGD | -2.12 | 1.49        | 1.52     |
| 29  | A     | 414[B] | PL9  | C2-C1   | -2.12 | 1.39        | 1.44     |
| 23  | B     | 602    | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 23  | C     | 513    | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | b     | 607    | CLA  | CBD-CAD | -2.12 | 1.47        | 1.56     |
| 23  | a     | 406[A] | CLA  | C4B-NB  | -2.12 | 1.35        | 1.37     |
| 23  | C     | 504    | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 23  | b     | 604    | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 23  | B     | 606    | CLA  | C3B-C2B | 2.12  | 1.48        | 1.41     |
| 23  | a     | 407[A] | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 24  | a     | 416[A] | PHO  | C1B-NB  | -2.11 | 1.34        | 1.38     |
| 23  | B     | 616    | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 23  | c     | 508    | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 23  | A     | 408    | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 23  | a     | 406[B] | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 23  | B     | 604    | CLA  | MG-NA   | 2.10  | 2.11        | 2.06     |
| 23  | a     | 407[B] | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 23  | B     | 607    | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 23  | C     | 514    | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 36  | c     | 518[A] | DGD  | O2G-C2G | -2.10 | 1.41        | 1.46     |
| 23  | c     | 508    | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 23  | c     | 507    | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 32  | B     | 629    | LMT  | O2B-C2B | -2.09 | 1.37        | 1.43     |
| 23  | B     | 603    | CLA  | C1C-NC  | -2.09 | 1.34        | 1.37     |
| 23  | b     | 606    | CLA  | C3B-C2B | 2.09  | 1.48        | 1.41     |
| 27  | v     | 202[A] | GOL  | C3-C2   | 2.09  | 1.59        | 1.51     |
| 36  | c     | 519    | DGD  | O5D-C1E | 2.09  | 1.43        | 1.40     |
| 23  | d     | 401[A] | CLA  | C3B-C2B | 2.09  | 1.48        | 1.41     |
| 32  | B     | 627    | LMT  | O5'-C5' | -2.08 | 1.39        | 1.44     |
| 23  | B     | 601    | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 29  | A     | 414[B] | PL9  | C2-C3   | 2.08  | 1.39        | 1.34     |
| 23  | c     | 514    | CLA  | C1D-C2D | 2.08  | 1.49        | 1.45     |
| 27  | a     | 418    | GOL  | C3-C2   | 2.08  | 1.59        | 1.51     |
| 23  | B     | 614    | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 23  | a     | 405[A] | CLA  | C3B-C4B | 2.07  | 1.48        | 1.42     |
| 33  | L     | 101[B] | LHG  | O7-C5   | -2.07 | 1.41        | 1.46     |
| 23  | B     | 601    | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 24  | a     | 416[B] | PHO  | C1D-ND  | -2.07 | 1.34        | 1.38     |
| 23  | b     | 607    | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 32  | t     | 101    | LMT  | O2'-C2' | -2.07 | 1.37        | 1.43     |
| 23  | c     | 503    | CLA  | C3B-C4B | 2.07  | 1.48        | 1.42     |
| 23  | C     | 507    | CLA  | C3B-C4B | 2.07  | 1.48        | 1.42     |
| 34  | D     | 711    | LMG  | O7-C8   | -2.07 | 1.41        | 1.46     |
| 23  | b     | 607    | CLA  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 23  | b     | 612    | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 23  | b     | 605    | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | C     | 507    | CLA  | C1D-C2D | 2.07  | 1.49        | 1.45     |
| 23  | d     | 402    | CLA  | C3B-C2B | 2.06  | 1.48        | 1.41     |
| 27  | c     | 527    | GOL  | C3-C2   | 2.06  | 1.59        | 1.51     |
| 23  | C     | 509    | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 23  | b     | 604    | CLA  | MG-NA   | 2.06  | 2.11        | 2.06     |
| 25  | b     | 617    | BCR  | C1-C6   | -2.06 | 1.51        | 1.53     |
| 23  | b     | 615    | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 32  | B     | 629    | LMT  | O3'-C3' | -2.06 | 1.37        | 1.43     |
| 23  | b     | 615    | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 24  | a     | 408[B] | PHO  | C3A-C2A | -2.05 | 1.52        | 1.54     |
| 32  | e     | 101    | LMT  | O2B-C2B | -2.05 | 1.37        | 1.43     |
| 24  | A     | 407[B] | PHO  | CHA-CBD | -2.05 | 1.49        | 1.51     |
| 23  | b     | 609    | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 23  | c     | 505    | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 23  | B     | 615    | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 24  | a     | 416[B] | PHO  | CHA-CBD | -2.04 | 1.49        | 1.51     |
| 23  | a     | 406[A] | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 23  | c     | 510    | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 32  | T     | 101    | LMT  | O1'-C1' | -2.04 | 1.36        | 1.40     |
| 23  | c     | 506    | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 23  | b     | 613    | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 27  | d     | 411    | GOL  | O2-C2   | -2.04 | 1.37        | 1.43     |
| 32  | b     | 627    | LMT  | O3'-C3' | -2.04 | 1.37        | 1.43     |
| 23  | A     | 408    | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 24  | a     | 408[B] | PHO  | C3D-C4D | -2.03 | 1.38        | 1.41     |
| 23  | C     | 512    | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 23  | C     | 508    | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 23  | b     | 609    | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 23  | b     | 608    | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |
| 23  | A     | 404[A] | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 35  | b     | 622    | HTG  | C1-C2   | 2.03  | 1.56        | 1.53     |
| 33  | D     | 706[A] | LHG  | O7-C5   | -2.03 | 1.41        | 1.46     |
| 23  | B     | 606    | CLA  | MG-NA   | 2.03  | 2.11        | 2.06     |
| 23  | b     | 614    | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 38  | f     | 101    | HEM  | C3B-C4B | 2.02  | 1.48        | 1.44     |
| 23  | B     | 613    | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 23  | c     | 504    | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 29  | A     | 414[A] | PL9  | C2-C3   | 2.02  | 1.39        | 1.34     |
| 23  | B     | 604    | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 23  | B     | 615    | CLA  | MG-NA   | 2.02  | 2.11        | 2.06     |
| 23  | A     | 404[B] | CLA  | C3B-C4B | 2.02  | 1.48        | 1.42     |
| 32  | b     | 621    | LMT  | O3'-C3' | -2.02 | 1.38        | 1.43     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23  | c     | 512    | CLA  | C3B-C4B | 2.01  | 1.48        | 1.42     |
| 23  | C     | 505    | CLA  | C3B-C4B | 2.01  | 1.48        | 1.42     |
| 24  | A     | 407[B] | PHO  | C1D-ND  | -2.01 | 1.35        | 1.38     |
| 23  | B     | 610    | CLA  | C1C-NC  | -2.00 | 1.34        | 1.37     |
| 23  | b     | 615    | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 23  | B     | 611    | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 23  | B     | 604    | CLA  | C3B-C4B | 2.00  | 1.48        | 1.42     |
| 34  | c     | 521    | LMG  | O1-C1   | 2.00  | 1.43        | 1.40     |
| 36  | H     | 102    | DGD  | O2G-C2G | -2.00 | 1.41        | 1.46     |
| 23  | b     | 602    | CLA  | C4C-C3C | 2.00  | 1.48        | 1.45     |

All (3412) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|--------|-------------|----------|
| 23  | B     | 611    | CLA  | C3B-C2B-C1B | -13.58 | 91.17       | 107.17   |
| 23  | B     | 611    | CLA  | C1D-ND-C4D  | -11.95 | 97.93       | 106.31   |
| 24  | a     | 416[A] | PHO  | C2D-C1D-ND  | 11.51  | 117.75      | 109.43   |
| 24  | a     | 416[B] | PHO  | C2D-C1D-ND  | 11.12  | 117.47      | 109.43   |
| 24  | A     | 407[A] | PHO  | C2D-C1D-ND  | 11.05  | 117.42      | 109.43   |
| 24  | A     | 417[B] | PHO  | C2D-C1D-ND  | 11.05  | 117.41      | 109.43   |
| 24  | a     | 408[A] | PHO  | C2D-C1D-ND  | 10.84  | 117.26      | 109.43   |
| 23  | a     | 409    | CLA  | C1D-ND-C4D  | -10.70 | 98.80       | 106.31   |
| 24  | a     | 408[B] | PHO  | C2D-C1D-ND  | 10.65  | 117.12      | 109.43   |
| 24  | A     | 407[B] | PHO  | C2D-C1D-ND  | 10.64  | 117.12      | 109.43   |
| 23  | B     | 614    | CLA  | C1D-ND-C4D  | -10.41 | 99.00       | 106.31   |
| 23  | B     | 612    | CLA  | C1D-ND-C4D  | -10.40 | 99.01       | 106.31   |
| 23  | C     | 504    | CLA  | C1D-ND-C4D  | -10.39 | 99.02       | 106.31   |
| 24  | A     | 417[A] | PHO  | C2D-C1D-ND  | 10.38  | 116.93      | 109.43   |
| 23  | B     | 611    | CLA  | C2B-C1B-NB  | 10.27  | 120.98      | 110.33   |
| 23  | b     | 605    | CLA  | C1D-ND-C4D  | -10.21 | 99.15       | 106.31   |
| 23  | b     | 603    | CLA  | C1D-ND-C4D  | -10.14 | 99.20       | 106.31   |
| 40  | v     | 201    | HEC  | CBB-CAB-C3B | -9.96  | 107.53      | 127.43   |
| 23  | B     | 615    | CLA  | C1D-ND-C4D  | -9.85  | 99.40       | 106.31   |
| 23  | c     | 504    | CLA  | C1D-ND-C4D  | -9.83  | 99.41       | 106.31   |
| 23  | c     | 502    | CLA  | C1D-ND-C4D  | -9.81  | 99.43       | 106.31   |
| 23  | d     | 402    | CLA  | C1D-ND-C4D  | -9.80  | 99.44       | 106.31   |
| 23  | a     | 407[A] | CLA  | C1D-ND-C4D  | -9.78  | 99.45       | 106.31   |
| 23  | b     | 614    | CLA  | C1D-ND-C4D  | -9.77  | 99.46       | 106.31   |
| 23  | A     | 406[B] | CLA  | C1D-ND-C4D  | -9.74  | 99.48       | 106.31   |
| 23  | a     | 405[B] | CLA  | C1D-ND-C4D  | -9.73  | 99.49       | 106.31   |
| 23  | A     | 408    | CLA  | C1D-ND-C4D  | -9.71  | 99.50       | 106.31   |
| 23  | B     | 601    | CLA  | C1D-ND-C4D  | -9.65  | 99.54       | 106.31   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 514    | CLA  | C1D-ND-C4D  | -9.65 | 99.54       | 106.31   |
| 23  | b     | 610    | CLA  | C1D-ND-C4D  | -9.64 | 99.55       | 106.31   |
| 23  | a     | 407[B] | CLA  | C1D-ND-C4D  | -9.61 | 99.57       | 106.31   |
| 23  | C     | 511    | CLA  | C1D-ND-C4D  | -9.59 | 99.58       | 106.31   |
| 23  | b     | 602    | CLA  | C1D-ND-C4D  | -9.59 | 99.58       | 106.31   |
| 23  | c     | 512    | CLA  | C1D-ND-C4D  | -9.57 | 99.59       | 106.31   |
| 23  | b     | 611    | CLA  | C1D-ND-C4D  | -9.55 | 99.61       | 106.31   |
| 23  | B     | 606    | CLA  | C1D-ND-C4D  | -9.55 | 99.61       | 106.31   |
| 23  | b     | 607    | CLA  | C1D-ND-C4D  | -9.53 | 99.63       | 106.31   |
| 23  | A     | 406[A] | CLA  | C1D-ND-C4D  | -9.49 | 99.65       | 106.31   |
| 23  | C     | 514    | CLA  | C1D-ND-C4D  | -9.48 | 99.66       | 106.31   |
| 23  | C     | 510    | CLA  | C1D-ND-C4D  | -9.44 | 99.69       | 106.31   |
| 23  | B     | 610    | CLA  | C1D-ND-C4D  | -9.43 | 99.69       | 106.31   |
| 23  | b     | 606    | CLA  | C1D-ND-C4D  | -9.43 | 99.70       | 106.31   |
| 23  | B     | 608    | CLA  | C1D-ND-C4D  | -9.38 | 99.73       | 106.31   |
| 23  | c     | 506    | CLA  | C1D-ND-C4D  | -9.37 | 99.74       | 106.31   |
| 23  | C     | 502    | CLA  | C1D-ND-C4D  | -9.33 | 99.76       | 106.31   |
| 23  | B     | 605    | CLA  | C1D-ND-C4D  | -9.29 | 99.79       | 106.31   |
| 23  | D     | 702[A] | CLA  | C1D-ND-C4D  | -9.22 | 99.84       | 106.31   |
| 23  | D     | 702[B] | CLA  | C1D-ND-C4D  | -9.20 | 99.85       | 106.31   |
| 23  | A     | 405[A] | CLA  | C1D-ND-C4D  | -9.14 | 99.90       | 106.31   |
| 23  | B     | 609    | CLA  | C1D-ND-C4D  | -9.12 | 99.91       | 106.31   |
| 23  | A     | 405[B] | CLA  | C1D-ND-C4D  | -9.12 | 99.91       | 106.31   |
| 23  | b     | 615    | CLA  | C1D-ND-C4D  | -9.12 | 99.91       | 106.31   |
| 23  | b     | 608    | CLA  | C1D-ND-C4D  | -9.11 | 99.92       | 106.31   |
| 23  | d     | 401[A] | CLA  | C1D-ND-C4D  | -9.11 | 99.92       | 106.31   |
| 23  | B     | 602    | CLA  | C1D-ND-C4D  | -9.10 | 99.93       | 106.31   |
| 24  | a     | 408[B] | PHO  | O2D-CGD-CBD | 9.09  | 120.93      | 110.95   |
| 23  | b     | 609    | CLA  | C1D-ND-C4D  | -9.07 | 99.95       | 106.31   |
| 23  | a     | 405[A] | CLA  | C1D-ND-C4D  | -9.05 | 99.96       | 106.31   |
| 23  | D     | 703    | CLA  | C1D-ND-C4D  | -9.02 | 99.98       | 106.31   |
| 23  | B     | 613    | CLA  | C1D-ND-C4D  | -9.00 | 100.00      | 106.31   |
| 23  | a     | 406[B] | CLA  | C1D-ND-C4D  | -8.97 | 100.02      | 106.31   |
| 23  | c     | 507    | CLA  | C1D-ND-C4D  | -8.97 | 100.02      | 106.31   |
| 23  | C     | 513    | CLA  | C1D-ND-C4D  | -8.94 | 100.04      | 106.31   |
| 23  | C     | 505    | CLA  | C1D-ND-C4D  | -8.89 | 100.08      | 106.31   |
| 23  | B     | 607    | CLA  | C1D-ND-C4D  | -8.87 | 100.08      | 106.31   |
| 24  | A     | 407[B] | PHO  | O2D-CGD-CBD | 8.87  | 120.69      | 110.95   |
| 40  | V     | 201    | HEC  | CBB-CAB-C3B | -8.87 | 109.71      | 127.43   |
| 23  | c     | 508    | CLA  | C1D-ND-C4D  | -8.86 | 100.09      | 106.31   |
| 23  | B     | 616    | CLA  | C1D-ND-C4D  | -8.84 | 100.11      | 106.31   |
| 23  | c     | 505    | CLA  | C1D-ND-C4D  | -8.81 | 100.13      | 106.31   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | A     | 417[B] | PHO  | O2D-CGD-CBD | 8.80  | 120.62      | 110.95   |
| 23  | b     | 601    | CLA  | C1D-ND-C4D  | -8.80 | 100.14      | 106.31   |
| 23  | c     | 513    | CLA  | C1D-ND-C4D  | -8.78 | 100.15      | 106.31   |
| 23  | c     | 510    | CLA  | C1D-ND-C4D  | -8.78 | 100.15      | 106.31   |
| 23  | c     | 511    | CLA  | C1D-ND-C4D  | -8.77 | 100.16      | 106.31   |
| 23  | b     | 616    | CLA  | C1D-ND-C4D  | -8.77 | 100.16      | 106.31   |
| 23  | B     | 603    | CLA  | C1D-ND-C4D  | -8.77 | 100.16      | 106.31   |
| 23  | A     | 404[B] | CLA  | C1D-ND-C4D  | -8.76 | 100.17      | 106.31   |
| 23  | C     | 506    | CLA  | C1D-ND-C4D  | -8.75 | 100.17      | 106.31   |
| 23  | a     | 406[A] | CLA  | C1D-ND-C4D  | -8.74 | 100.18      | 106.31   |
| 23  | d     | 401[B] | CLA  | C1D-ND-C4D  | -8.72 | 100.19      | 106.31   |
| 23  | b     | 613    | CLA  | C1D-ND-C4D  | -8.67 | 100.23      | 106.31   |
| 23  | b     | 612    | CLA  | C1D-ND-C4D  | -8.66 | 100.23      | 106.31   |
| 23  | C     | 512    | CLA  | C1D-ND-C4D  | -8.59 | 100.28      | 106.31   |
| 24  | A     | 417[A] | PHO  | O2D-CGD-CBD | 8.55  | 120.34      | 110.95   |
| 23  | C     | 507    | CLA  | C1D-ND-C4D  | -8.45 | 100.38      | 106.31   |
| 23  | c     | 503    | CLA  | C1D-ND-C4D  | -8.43 | 100.40      | 106.31   |
| 23  | C     | 508    | CLA  | C1D-ND-C4D  | -8.41 | 100.41      | 106.31   |
| 24  | a     | 416[A] | PHO  | O2D-CGD-CBD | 8.36  | 120.13      | 110.95   |
| 24  | a     | 408[A] | PHO  | O2D-CGD-CBD | 8.30  | 120.07      | 110.95   |
| 23  | c     | 509    | CLA  | C1D-ND-C4D  | -8.26 | 100.52      | 106.31   |
| 24  | A     | 407[A] | PHO  | C3B-C4B-NB  | 8.22  | 112.82      | 107.46   |
| 23  | C     | 503    | CLA  | C1D-ND-C4D  | -8.21 | 100.56      | 106.31   |
| 24  | a     | 408[B] | PHO  | C3B-C4B-NB  | 8.18  | 112.80      | 107.46   |
| 24  | a     | 416[B] | PHO  | O2D-CGD-CBD | 8.13  | 119.88      | 110.95   |
| 23  | C     | 509    | CLA  | C1D-ND-C4D  | -8.07 | 100.65      | 106.31   |
| 24  | A     | 407[A] | PHO  | O2D-CGD-CBD | 8.01  | 119.75      | 110.95   |
| 24  | a     | 408[A] | PHO  | C3B-C4B-NB  | 8.00  | 112.68      | 107.46   |
| 23  | B     | 616    | CLA  | O2D-CGD-CBD | 7.99  | 125.20      | 111.23   |
| 26  | X     | 101    | SQD  | O6-C1-C2    | 7.97  | 120.37      | 108.27   |
| 23  | B     | 604    | CLA  | C1D-ND-C4D  | -7.94 | 100.74      | 106.31   |
| 23  | B     | 611    | CLA  | CHD-C4C-C3C | -7.91 | 113.24      | 124.77   |
| 23  | b     | 602    | CLA  | C4A-NA-C1A  | -7.87 | 103.09      | 106.68   |
| 24  | a     | 416[B] | PHO  | C3B-C4B-NB  | 7.77  | 112.53      | 107.46   |
| 23  | A     | 404[A] | CLA  | C1D-ND-C4D  | -7.76 | 100.87      | 106.31   |
| 23  | c     | 504    | CLA  | C4A-NA-C1A  | -7.75 | 103.14      | 106.68   |
| 23  | C     | 511    | CLA  | CMD-C2D-C1D | 7.75  | 138.38      | 124.73   |
| 24  | a     | 416[A] | PHO  | C3B-C4B-NB  | 7.69  | 112.47      | 107.46   |
| 23  | B     | 611    | CLA  | C2D-C1D-ND  | 7.64  | 117.68      | 110.13   |
| 24  | A     | 407[B] | PHO  | C3B-C4B-NB  | 7.63  | 112.44      | 107.46   |
| 23  | b     | 604    | CLA  | C1D-ND-C4D  | -7.56 | 101.01      | 106.31   |
| 23  | b     | 616    | CLA  | O2D-CGD-CBD | 7.34  | 124.06      | 111.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 606    | CLA  | CMD-C2D-C1D | 7.31  | 137.60      | 124.73   |
| 23  | C     | 504    | CLA  | C4A-NA-C1A  | -7.27 | 103.36      | 106.68   |
| 23  | b     | 613    | CLA  | C2D-C1D-ND  | 7.22  | 117.27      | 110.13   |
| 23  | B     | 611    | CLA  | CMB-C2B-C1B | 7.16  | 136.33      | 125.42   |
| 23  | B     | 614    | CLA  | CMD-C2D-C1D | 7.13  | 137.28      | 124.73   |
| 23  | B     | 605    | CLA  | CHD-C4C-C3C | -7.12 | 114.39      | 124.77   |
| 24  | A     | 417[B] | PHO  | C3B-C4B-NB  | 7.07  | 112.07      | 107.46   |
| 23  | a     | 409    | CLA  | C2D-C1D-ND  | 7.07  | 117.12      | 110.13   |
| 23  | B     | 603    | CLA  | O2D-CGD-CBD | 7.05  | 123.56      | 111.23   |
| 23  | B     | 611    | CLA  | CHB-C1B-NB  | -7.04 | 113.48      | 124.05   |
| 24  | A     | 417[B] | PHO  | C2B-C1B-NB  | 7.04  | 114.52      | 109.43   |
| 23  | c     | 508    | CLA  | O2D-CGD-CBD | 7.02  | 123.50      | 111.23   |
| 23  | A     | 408    | CLA  | C2D-C1D-ND  | 7.01  | 117.06      | 110.13   |
| 24  | A     | 417[A] | PHO  | C2B-C1B-NB  | 6.94  | 114.44      | 109.43   |
| 23  | b     | 616    | CLA  | CHD-C4C-C3C | -6.94 | 114.66      | 124.77   |
| 24  | a     | 416[A] | PHO  | C2B-C1B-NB  | 6.93  | 114.44      | 109.43   |
| 23  | b     | 614    | CLA  | C2D-C1D-ND  | 6.92  | 116.97      | 110.13   |
| 23  | c     | 502    | CLA  | CMD-C2D-C1D | 6.91  | 136.90      | 124.73   |
| 23  | c     | 504    | CLA  | CMD-C2D-C1D | 6.90  | 136.88      | 124.73   |
| 23  | C     | 513    | CLA  | CHD-C4C-C3C | -6.86 | 114.78      | 124.77   |
| 23  | b     | 606    | CLA  | CHD-C4C-C3C | -6.86 | 114.78      | 124.77   |
| 23  | B     | 616    | CLA  | CHD-C4C-C3C | -6.85 | 114.78      | 124.77   |
| 23  | B     | 613    | CLA  | C2D-C1D-ND  | 6.85  | 116.90      | 110.13   |
| 23  | B     | 614    | CLA  | C2D-C1D-ND  | 6.81  | 116.87      | 110.13   |
| 23  | B     | 610    | CLA  | O2D-CGD-CBD | 6.79  | 123.10      | 111.23   |
| 24  | A     | 417[A] | PHO  | C3B-C4B-NB  | 6.78  | 111.89      | 107.46   |
| 23  | c     | 514    | CLA  | CMD-C2D-C1D | 6.77  | 136.65      | 124.73   |
| 23  | B     | 606    | CLA  | CHD-C4C-C3C | -6.74 | 114.94      | 124.77   |
| 23  | A     | 405[A] | CLA  | C2D-C1D-ND  | 6.74  | 116.79      | 110.13   |
| 23  | B     | 606    | CLA  | C2D-C1D-ND  | 6.74  | 116.79      | 110.13   |
| 23  | b     | 613    | CLA  | CHD-C4C-C3C | -6.72 | 114.97      | 124.77   |
| 23  | b     | 615    | CLA  | C4A-NA-C1A  | -6.72 | 103.61      | 106.68   |
| 23  | B     | 609    | CLA  | C4A-NA-C1A  | -6.71 | 103.62      | 106.68   |
| 23  | a     | 409    | CLA  | CHD-C4C-C3C | -6.69 | 115.02      | 124.77   |
| 23  | b     | 607    | CLA  | C2D-C1D-ND  | 6.69  | 116.74      | 110.13   |
| 23  | b     | 612    | CLA  | CHD-C4C-C3C | -6.68 | 115.03      | 124.77   |
| 23  | d     | 402    | CLA  | CMD-C2D-C1D | 6.68  | 136.49      | 124.73   |
| 23  | C     | 504    | CLA  | CMD-C2D-C1D | 6.64  | 136.43      | 124.73   |
| 35  | b     | 623    | HTG  | C1'-S1-C1   | 6.63  | 114.76      | 100.45   |
| 23  | c     | 508    | CLA  | CMD-C2D-C1D | 6.63  | 136.40      | 124.73   |
| 23  | A     | 404[A] | CLA  | CMD-C2D-C1D | 6.62  | 136.38      | 124.73   |
| 23  | A     | 404[B] | CLA  | CMD-C2D-C1D | 6.62  | 136.38      | 124.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 605    | CLA  | CHD-C4C-C3C | -6.62 | 115.12      | 124.77   |
| 23  | b     | 605    | CLA  | CMD-C2D-C1D | 6.61  | 136.38      | 124.73   |
| 26  | B     | 620    | SQD  | O6-C1-C2    | 6.60  | 118.29      | 108.27   |
| 23  | b     | 614    | CLA  | CHD-C4C-C3C | -6.59 | 115.16      | 124.77   |
| 23  | B     | 616    | CLA  | C2D-C1D-ND  | 6.59  | 116.65      | 110.13   |
| 23  | B     | 615    | CLA  | C2D-C1D-ND  | 6.59  | 116.65      | 110.13   |
| 23  | b     | 601    | CLA  | O2D-CGD-CBD | 6.58  | 122.74      | 111.23   |
| 23  | C     | 502    | CLA  | O2D-CGD-CBD | 6.57  | 122.72      | 111.23   |
| 23  | B     | 611    | CLA  | CMD-C2D-C1D | 6.57  | 136.30      | 124.73   |
| 23  | D     | 703    | CLA  | C4A-NA-C1A  | -6.57 | 103.68      | 106.68   |
| 23  | D     | 702[B] | CLA  | C4A-NA-C1A  | -6.56 | 103.69      | 106.68   |
| 23  | d     | 402    | CLA  | C2D-C1D-ND  | 6.55  | 116.61      | 110.13   |
| 23  | b     | 607    | CLA  | CMD-C2D-C1D | 6.55  | 136.26      | 124.73   |
| 23  | a     | 407[A] | CLA  | C2D-C1D-ND  | 6.54  | 116.60      | 110.13   |
| 23  | c     | 507    | CLA  | CMD-C2D-C1D | 6.54  | 136.25      | 124.73   |
| 24  | a     | 408[B] | PHO  | C2B-C1B-NB  | 6.54  | 114.16      | 109.43   |
| 23  | b     | 605    | CLA  | C2D-C1D-ND  | 6.53  | 116.59      | 110.13   |
| 23  | b     | 616    | CLA  | C4A-NA-C1A  | -6.52 | 103.70      | 106.68   |
| 23  | B     | 605    | CLA  | CMD-C2D-C1D | 6.51  | 136.19      | 124.73   |
| 23  | C     | 507    | CLA  | CMD-C2D-C1D | 6.50  | 136.18      | 124.73   |
| 26  | X     | 101    | SQD  | O47-C7-C8   | 6.50  | 125.53      | 111.48   |
| 23  | b     | 610    | CLA  | CHD-C4C-C3C | -6.49 | 115.30      | 124.77   |
| 23  | C     | 504    | CLA  | C2D-C1D-ND  | 6.48  | 116.54      | 110.13   |
| 23  | b     | 616    | CLA  | CMD-C2D-C1D | 6.48  | 136.14      | 124.73   |
| 23  | C     | 505    | CLA  | C2D-C1D-ND  | 6.47  | 116.53      | 110.13   |
| 23  | D     | 702[A] | CLA  | CMD-C2D-C1D | 6.46  | 136.10      | 124.73   |
| 23  | b     | 606    | CLA  | CMD-C2D-C1D | 6.45  | 136.08      | 124.73   |
| 23  | b     | 602    | CLA  | CMD-C2D-C1D | 6.45  | 136.08      | 124.73   |
| 23  | b     | 603    | CLA  | C2D-C1D-ND  | 6.40  | 116.46      | 110.13   |
| 23  | b     | 615    | CLA  | CMD-C2D-C1D | 6.40  | 135.99      | 124.73   |
| 23  | A     | 406[A] | CLA  | C2D-C1D-ND  | 6.39  | 116.45      | 110.13   |
| 23  | B     | 608    | CLA  | C2D-C1D-ND  | 6.39  | 116.45      | 110.13   |
| 23  | b     | 602    | CLA  | CHD-C4C-C3C | -6.38 | 115.47      | 124.77   |
| 23  | d     | 401[B] | CLA  | CMD-C2D-C1D | 6.38  | 135.97      | 124.73   |
| 23  | C     | 502    | CLA  | C4A-NA-C1A  | -6.38 | 103.77      | 106.68   |
| 23  | D     | 702[A] | CLA  | C4A-NA-C1A  | -6.37 | 103.77      | 106.68   |
| 23  | C     | 513    | CLA  | C4A-NA-C1A  | -6.36 | 103.78      | 106.68   |
| 23  | b     | 606    | CLA  | C4A-NA-C1A  | -6.35 | 103.78      | 106.68   |
| 23  | B     | 610    | CLA  | C2D-C1D-ND  | 6.35  | 116.41      | 110.13   |
| 23  | a     | 407[A] | CLA  | CHD-C4C-C3C | -6.34 | 115.52      | 124.77   |
| 23  | a     | 406[B] | CLA  | CHD-C4C-C3C | -6.34 | 115.53      | 124.77   |
| 23  | a     | 406[A] | CLA  | C2D-C1D-ND  | 6.33  | 116.39      | 110.13   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 606    | CLA  | C2D-C1D-ND  | 6.31  | 116.37      | 110.13   |
| 23  | d     | 402    | CLA  | CHD-C4C-C3C | -6.31 | 115.58      | 124.77   |
| 23  | C     | 508    | CLA  | O2D-CGD-CBD | 6.30  | 122.25      | 111.23   |
| 23  | a     | 407[B] | CLA  | C2D-C1D-ND  | 6.30  | 116.36      | 110.13   |
| 23  | c     | 502    | CLA  | C2D-C1D-ND  | 6.30  | 116.36      | 110.13   |
| 23  | D     | 702[A] | CLA  | C2D-C1D-ND  | 6.29  | 116.35      | 110.13   |
| 23  | C     | 508    | CLA  | CHD-C4C-C3C | -6.29 | 115.61      | 124.77   |
| 23  | c     | 511    | CLA  | CMD-C2D-C1D | 6.28  | 135.79      | 124.73   |
| 23  | b     | 610    | CLA  | CMD-C2D-C1D | 6.28  | 135.79      | 124.73   |
| 23  | A     | 408    | CLA  | CHD-C4C-C3C | -6.28 | 115.62      | 124.77   |
| 24  | a     | 416[B] | PHO  | C1-C2-C3    | -6.27 | 115.93      | 126.20   |
| 23  | c     | 506    | CLA  | CHD-C4C-C3C | -6.27 | 115.63      | 124.77   |
| 23  | b     | 609    | CLA  | CHD-C4C-C3C | -6.26 | 115.64      | 124.77   |
| 23  | a     | 405[B] | CLA  | CMD-C2D-C1D | 6.26  | 135.76      | 124.73   |
| 23  | C     | 504    | CLA  | CHD-C4C-C3C | -6.26 | 115.65      | 124.77   |
| 24  | a     | 408[A] | PHO  | C2B-C1B-NB  | 6.26  | 113.95      | 109.43   |
| 23  | B     | 601    | CLA  | CMD-C2D-C1D | 6.26  | 135.75      | 124.73   |
| 23  | c     | 505    | CLA  | CMD-C2D-C1D | 6.25  | 135.74      | 124.73   |
| 23  | b     | 603    | CLA  | CHD-C4C-C3C | -6.25 | 115.66      | 124.77   |
| 23  | C     | 514    | CLA  | C2D-C1D-ND  | 6.25  | 116.31      | 110.13   |
| 23  | C     | 506    | CLA  | CMD-C2D-C1D | 6.25  | 135.73      | 124.73   |
| 23  | B     | 607    | CLA  | C2D-C1D-ND  | 6.25  | 116.31      | 110.13   |
| 23  | c     | 503    | CLA  | C2C-C1C-NC  | 6.24  | 116.54      | 109.98   |
| 23  | c     | 512    | CLA  | CHD-C4C-C3C | -6.24 | 115.67      | 124.77   |
| 23  | c     | 512    | CLA  | C2D-C1D-ND  | 6.24  | 116.30      | 110.13   |
| 23  | B     | 610    | CLA  | CMD-C2D-C1D | 6.24  | 135.71      | 124.73   |
| 23  | b     | 611    | CLA  | C2D-C1D-ND  | 6.23  | 116.29      | 110.13   |
| 23  | D     | 702[B] | CLA  | CMD-C2D-C1D | 6.23  | 135.70      | 124.73   |
| 26  | A     | 410[A] | SQD  | O6-C1-C2    | 6.22  | 117.72      | 108.27   |
| 23  | c     | 509    | CLA  | C2D-C1D-ND  | 6.22  | 116.28      | 110.13   |
| 23  | a     | 406[A] | CLA  | CHD-C4C-C3C | -6.22 | 115.70      | 124.77   |
| 23  | b     | 610    | CLA  | C2D-C1D-ND  | 6.22  | 116.28      | 110.13   |
| 24  | a     | 416[B] | PHO  | C2B-C1B-NB  | 6.22  | 113.92      | 109.43   |
| 23  | C     | 513    | CLA  | C2D-C1D-ND  | 6.21  | 116.28      | 110.13   |
| 23  | B     | 609    | CLA  | CHD-C4C-C3C | -6.21 | 115.72      | 124.77   |
| 23  | B     | 616    | CLA  | C4A-NA-C1A  | -6.21 | 103.85      | 106.68   |
| 24  | A     | 407[B] | PHO  | C2B-C1B-NB  | 6.21  | 113.92      | 109.43   |
| 23  | B     | 612    | CLA  | CHD-C4C-C3C | -6.21 | 115.72      | 124.77   |
| 23  | c     | 504    | CLA  | CHD-C4C-C3C | -6.20 | 115.73      | 124.77   |
| 23  | B     | 612    | CLA  | C2D-C1D-ND  | 6.19  | 116.26      | 110.13   |
| 23  | B     | 603    | CLA  | C2D-C1D-ND  | 6.19  | 116.25      | 110.13   |
| 23  | A     | 406[B] | CLA  | C2D-C1D-ND  | 6.18  | 116.25      | 110.13   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 405[B] | CLA  | C2D-C1D-ND  | 6.18  | 116.24      | 110.13   |
| 23  | B     | 601    | CLA  | C2D-C1D-ND  | 6.17  | 116.24      | 110.13   |
| 23  | c     | 511    | CLA  | CHD-C4C-C3C | -6.17 | 115.78      | 124.77   |
| 23  | B     | 615    | CLA  | CHD-C4C-C3C | -6.16 | 115.79      | 124.77   |
| 23  | b     | 611    | CLA  | CMD-C2D-C1D | 6.16  | 135.58      | 124.73   |
| 23  | b     | 609    | CLA  | C4A-NA-C1A  | -6.16 | 103.87      | 106.68   |
| 25  | D     | 704    | BCR  | C7-C8-C9    | -6.16 | 117.13      | 126.23   |
| 23  | A     | 406[B] | CLA  | CMD-C2D-C1D | 6.15  | 135.56      | 124.73   |
| 23  | C     | 510    | CLA  | C2D-C1D-ND  | 6.15  | 116.21      | 110.13   |
| 23  | c     | 504    | CLA  | C2D-C1D-ND  | 6.15  | 116.21      | 110.13   |
| 23  | B     | 601    | CLA  | CHD-C4C-C3C | -6.13 | 115.83      | 124.77   |
| 23  | b     | 614    | CLA  | O2D-CGD-CBD | 6.13  | 121.95      | 111.23   |
| 23  | B     | 602    | CLA  | CHD-C4C-C3C | -6.13 | 115.83      | 124.77   |
| 23  | a     | 406[B] | CLA  | CMD-C2D-C1D | 6.13  | 135.52      | 124.73   |
| 23  | B     | 602    | CLA  | C2D-C1D-ND  | 6.12  | 116.18      | 110.13   |
| 23  | c     | 506    | CLA  | O2D-CGD-CBD | 6.12  | 121.92      | 111.23   |
| 23  | c     | 513    | CLA  | C4A-NA-C1A  | -6.11 | 103.89      | 106.68   |
| 23  | B     | 606    | CLA  | C4A-NA-C1A  | -6.10 | 103.89      | 106.68   |
| 24  | A     | 407[A] | PHO  | C2B-C1B-NB  | 6.10  | 113.84      | 109.43   |
| 23  | C     | 506    | CLA  | CHD-C4C-C3C | -6.09 | 115.89      | 124.77   |
| 23  | b     | 616    | CLA  | C2D-C1D-ND  | 6.08  | 116.15      | 110.13   |
| 23  | C     | 502    | CLA  | CMD-C2D-C1D | 6.08  | 135.44      | 124.73   |
| 23  | C     | 511    | CLA  | C2D-C1D-ND  | 6.07  | 116.13      | 110.13   |
| 23  | d     | 401[B] | CLA  | C2C-C1C-NC  | 6.07  | 116.36      | 109.98   |
| 23  | A     | 405[B] | CLA  | C2D-C1D-ND  | 6.06  | 116.12      | 110.13   |
| 23  | D     | 703    | CLA  | CMD-C2D-C1D | 6.05  | 135.39      | 124.73   |
| 26  | A     | 410[B] | SQD  | O6-C1-C2    | 6.05  | 117.46      | 108.27   |
| 23  | C     | 511    | CLA  | CHD-C4C-C3C | -6.05 | 115.95      | 124.77   |
| 23  | B     | 605    | CLA  | C2D-C1D-ND  | 6.05  | 116.11      | 110.13   |
| 24  | a     | 416[A] | PHO  | C4D-ND-C1D  | -6.05 | 101.62      | 108.87   |
| 23  | c     | 505    | CLA  | C2D-C1D-ND  | 6.04  | 116.11      | 110.13   |
| 23  | a     | 405[A] | CLA  | C4A-NA-C1A  | -6.04 | 103.92      | 106.68   |
| 23  | B     | 609    | CLA  | C2D-C1D-ND  | 6.04  | 116.11      | 110.13   |
| 24  | a     | 416[B] | PHO  | C4D-ND-C1D  | -6.03 | 101.64      | 108.87   |
| 23  | B     | 603    | CLA  | CHD-C4C-C3C | -6.03 | 115.98      | 124.77   |
| 23  | C     | 503    | CLA  | CMD-C2D-C1D | 6.03  | 135.35      | 124.73   |
| 23  | b     | 601    | CLA  | CMD-C2D-C1D | 6.03  | 135.35      | 124.73   |
| 23  | A     | 405[B] | CLA  | CHD-C4C-C3C | -6.02 | 116.00      | 124.77   |
| 23  | C     | 508    | CLA  | C2D-C1D-ND  | 6.01  | 116.07      | 110.13   |
| 23  | C     | 512    | CLA  | CHD-C4C-C3C | -6.01 | 116.01      | 124.77   |
| 23  | C     | 507    | CLA  | C2C-C1C-NC  | 6.01  | 116.29      | 109.98   |
| 23  | A     | 405[B] | CLA  | CMD-C2D-C1D | 6.01  | 135.31      | 124.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 602    | CLA  | O2D-CGD-CBD | 6.00  | 121.71      | 111.23   |
| 23  | b     | 615    | CLA  | CHD-C4C-C3C | -6.00 | 116.03      | 124.77   |
| 23  | A     | 404[B] | CLA  | C4A-NA-C1A  | -5.99 | 103.94      | 106.68   |
| 23  | A     | 406[B] | CLA  | C4A-NA-C1A  | -5.99 | 103.94      | 106.68   |
| 23  | C     | 512    | CLA  | C2D-C1D-ND  | 5.99  | 116.06      | 110.13   |
| 23  | B     | 602    | CLA  | O2D-CGD-CBD | 5.99  | 121.70      | 111.23   |
| 23  | B     | 614    | CLA  | CHD-C4C-C3C | -5.99 | 116.04      | 124.77   |
| 23  | c     | 510    | CLA  | CMD-C2D-C1D | 5.99  | 135.27      | 124.73   |
| 23  | A     | 406[A] | CLA  | CHD-C4C-C3C | -5.99 | 116.05      | 124.77   |
| 23  | B     | 608    | CLA  | CHD-C4C-C3C | -5.98 | 116.06      | 124.77   |
| 23  | b     | 604    | CLA  | C2C-C1C-NC  | 5.96  | 116.25      | 109.98   |
| 23  | b     | 615    | CLA  | C2D-C1D-ND  | 5.96  | 116.02      | 110.13   |
| 23  | a     | 405[A] | CLA  | C2D-C1D-ND  | 5.96  | 116.02      | 110.13   |
| 23  | C     | 509    | CLA  | C2C-C1C-NC  | 5.96  | 116.24      | 109.98   |
| 23  | c     | 514    | CLA  | C4A-NA-C1A  | -5.94 | 103.97      | 106.68   |
| 23  | B     | 601    | CLA  | O2D-CGD-CBD | 5.94  | 121.61      | 111.23   |
| 23  | c     | 510    | CLA  | C1-C2-C3    | -5.93 | 116.48      | 126.20   |
| 23  | C     | 514    | CLA  | CHD-C4C-C3C | -5.93 | 116.12      | 124.77   |
| 23  | B     | 608    | CLA  | CMD-C2D-C1D | 5.93  | 135.16      | 124.73   |
| 23  | b     | 603    | CLA  | CMD-C2D-C1D | 5.92  | 135.15      | 124.73   |
| 23  | b     | 609    | CLA  | C2D-C1D-ND  | 5.92  | 115.98      | 110.13   |
| 23  | B     | 615    | CLA  | CMD-C2D-C1D | 5.91  | 135.13      | 124.73   |
| 23  | B     | 611    | CLA  | O2D-CGD-CBD | 5.91  | 121.55      | 111.23   |
| 23  | a     | 407[B] | CLA  | CHD-C4C-C3C | -5.90 | 116.17      | 124.77   |
| 23  | c     | 506    | CLA  | C4A-NA-C1A  | -5.90 | 103.99      | 106.68   |
| 23  | c     | 514    | CLA  | C2D-C1D-ND  | 5.89  | 115.96      | 110.13   |
| 23  | A     | 405[A] | CLA  | CHD-C4C-C3C | -5.89 | 116.18      | 124.77   |
| 23  | b     | 601    | CLA  | C4A-NA-C1A  | -5.89 | 103.99      | 106.68   |
| 23  | b     | 607    | CLA  | CHD-C4C-C3C | -5.89 | 116.18      | 124.77   |
| 23  | b     | 604    | CLA  | O2D-CGD-CBD | 5.89  | 121.53      | 111.23   |
| 23  | d     | 401[A] | CLA  | C4A-NA-C1A  | -5.88 | 104.00      | 106.68   |
| 23  | d     | 401[A] | CLA  | C2D-C1D-ND  | 5.88  | 115.94      | 110.13   |
| 23  | c     | 506    | CLA  | C2D-C1D-ND  | 5.88  | 115.94      | 110.13   |
| 23  | a     | 406[B] | CLA  | C2D-C1D-ND  | 5.87  | 115.94      | 110.13   |
| 23  | c     | 513    | CLA  | CMD-C2D-C1D | 5.87  | 135.07      | 124.73   |
| 23  | B     | 609    | CLA  | CMD-C2D-C1D | 5.87  | 135.06      | 124.73   |
| 23  | a     | 405[B] | CLA  | C2C-C1C-NC  | 5.86  | 116.13      | 109.98   |
| 23  | c     | 512    | CLA  | CMD-C2D-C1D | 5.85  | 135.03      | 124.73   |
| 24  | A     | 407[A] | PHO  | C4D-ND-C1D  | -5.85 | 101.86      | 108.87   |
| 23  | c     | 508    | CLA  | C2D-C1D-ND  | 5.85  | 115.91      | 110.13   |
| 23  | c     | 505    | CLA  | CHD-C4C-C3C | -5.84 | 116.25      | 124.77   |
| 23  | B     | 604    | CLA  | CMD-C2D-C1D | 5.84  | 135.01      | 124.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 613    | CLA  | CHD-C4C-C3C | -5.83 | 116.27      | 124.77   |
| 23  | b     | 601    | CLA  | CHD-C4C-C3C | -5.82 | 116.28      | 124.77   |
| 23  | B     | 611    | CLA  | C3D-C2D-C1D | -5.82 | 97.89       | 105.83   |
| 24  | a     | 416[B] | PHO  | C3D-C4D-ND  | 5.82  | 115.17      | 107.71   |
| 23  | d     | 402    | CLA  | O2D-CGD-CBD | 5.82  | 121.40      | 111.23   |
| 23  | B     | 604    | CLA  | C2C-C1C-NC  | 5.82  | 116.09      | 109.98   |
| 23  | b     | 608    | CLA  | CHD-C4C-C3C | -5.81 | 116.30      | 124.77   |
| 23  | b     | 605    | CLA  | O2D-CGD-CBD | 5.81  | 121.39      | 111.23   |
| 23  | b     | 611    | CLA  | O2D-CGD-CBD | 5.81  | 121.38      | 111.23   |
| 23  | D     | 702[B] | CLA  | C2D-C1D-ND  | 5.81  | 115.87      | 110.13   |
| 23  | d     | 401[A] | CLA  | C2C-C1C-NC  | 5.80  | 116.07      | 109.98   |
| 23  | b     | 601    | CLA  | C2D-C1D-ND  | 5.79  | 115.86      | 110.13   |
| 23  | C     | 508    | CLA  | CMD-C2D-C1D | 5.78  | 134.91      | 124.73   |
| 23  | c     | 507    | CLA  | C2D-C1D-ND  | 5.77  | 115.83      | 110.13   |
| 26  | b     | 620    | SQD  | O6-C1-C2    | 5.77  | 117.03      | 108.27   |
| 23  | C     | 502    | CLA  | CHD-C4C-C3C | -5.77 | 116.37      | 124.77   |
| 25  | Y     | 101    | BCR  | C33-C5-C6   | -5.76 | 118.20      | 124.48   |
| 24  | a     | 416[A] | PHO  | C1-C2-C3    | -5.76 | 116.76      | 126.20   |
| 26  | a     | 411[A] | SQD  | O6-C1-C2    | 5.76  | 117.02      | 108.27   |
| 23  | b     | 603    | CLA  | C4A-NA-C1A  | -5.75 | 104.06      | 106.68   |
| 23  | A     | 404[B] | CLA  | CHD-C4C-C3C | -5.75 | 116.39      | 124.77   |
| 23  | C     | 509    | CLA  | C2D-C1D-ND  | 5.74  | 115.81      | 110.13   |
| 23  | a     | 405[A] | CLA  | CMD-C2D-C1D | 5.74  | 134.84      | 124.73   |
| 23  | B     | 602    | CLA  | CMD-C2D-C1D | 5.74  | 134.84      | 124.73   |
| 23  | c     | 513    | CLA  | CHD-C4C-C3C | -5.74 | 116.40      | 124.77   |
| 23  | A     | 404[A] | CLA  | C4A-NA-C1A  | -5.74 | 104.06      | 106.68   |
| 23  | C     | 502    | CLA  | C2D-C1D-ND  | 5.73  | 115.79      | 110.13   |
| 23  | c     | 514    | CLA  | CHD-C4C-C3C | -5.72 | 116.43      | 124.77   |
| 23  | B     | 606    | CLA  | O2D-CGD-CBD | 5.72  | 121.23      | 111.23   |
| 23  | c     | 508    | CLA  | C4A-NA-C1A  | -5.72 | 104.07      | 106.68   |
| 29  | A     | 414[A] | PL9  | C7-C8-C9    | -5.71 | 116.99      | 126.83   |
| 23  | B     | 612    | CLA  | O2D-CGD-CBD | 5.70  | 121.20      | 111.23   |
| 23  | c     | 508    | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.77   |
| 23  | c     | 510    | CLA  | C2D-C1D-ND  | 5.68  | 115.74      | 110.13   |
| 23  | B     | 607    | CLA  | C2C-C1C-NC  | 5.67  | 115.93      | 109.98   |
| 23  | b     | 610    | CLA  | C1-C2-C3    | -5.66 | 116.92      | 126.20   |
| 23  | b     | 613    | CLA  | C3D-C2D-C1D | -5.66 | 98.10       | 105.83   |
| 24  | A     | 407[B] | PHO  | C4D-ND-C1D  | -5.66 | 102.09      | 108.87   |
| 23  | B     | 615    | CLA  | C4A-NA-C1A  | -5.66 | 104.10      | 106.68   |
| 23  | D     | 703    | CLA  | CHD-C4C-C3C | -5.65 | 116.53      | 124.77   |
| 23  | c     | 503    | CLA  | O2D-CGD-CBD | 5.65  | 121.11      | 111.23   |
| 40  | v     | 201    | HEC  | CBC-CAC-C3C | -5.65 | 116.14      | 127.43   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | D     | 702[B] | CLA  | CHD-C4C-C3C | -5.65 | 116.54      | 124.77   |
| 23  | c     | 503    | CLA  | C2D-C1D-ND  | 5.65  | 115.72      | 110.13   |
| 23  | C     | 509    | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 23  | b     | 604    | CLA  | CMD-C2D-C1D | 5.64  | 134.66      | 124.73   |
| 23  | b     | 611    | CLA  | CHD-C4C-C3C | -5.64 | 116.56      | 124.77   |
| 23  | b     | 609    | CLA  | CMD-C2D-C1D | 5.63  | 134.65      | 124.73   |
| 23  | d     | 401[A] | CLA  | CMD-C2D-C1D | 5.63  | 134.65      | 124.73   |
| 23  | c     | 511    | CLA  | C4A-NA-C1A  | -5.63 | 104.11      | 106.68   |
| 23  | B     | 614    | CLA  | O2D-CGD-CBD | 5.63  | 121.07      | 111.23   |
| 23  | c     | 513    | CLA  | C2D-C1D-ND  | 5.62  | 115.69      | 110.13   |
| 23  | C     | 510    | CLA  | CMD-C2D-C1D | 5.62  | 134.63      | 124.73   |
| 23  | A     | 408    | CLA  | CMD-C2D-C1D | 5.62  | 134.62      | 124.73   |
| 23  | c     | 506    | CLA  | CMD-C2D-C1D | 5.61  | 134.60      | 124.73   |
| 26  | A     | 410[A] | SQD  | C1-O5-C5    | -5.61 | 102.77      | 113.72   |
| 23  | B     | 610    | CLA  | CHD-C4C-C3C | -5.61 | 116.60      | 124.77   |
| 23  | c     | 509    | CLA  | CHD-C4C-C3C | -5.60 | 116.60      | 124.77   |
| 23  | a     | 406[A] | CLA  | C4A-NA-C1A  | -5.60 | 104.12      | 106.68   |
| 23  | B     | 607    | CLA  | CMD-C2D-C1D | 5.60  | 134.59      | 124.73   |
| 23  | C     | 510    | CLA  | CHD-C4C-C3C | -5.60 | 116.61      | 124.77   |
| 23  | b     | 602    | CLA  | C2D-C1D-ND  | 5.60  | 115.67      | 110.13   |
| 23  | A     | 404[A] | CLA  | C2D-C1D-ND  | 5.59  | 115.66      | 110.13   |
| 23  | b     | 608    | CLA  | C2D-C1D-ND  | 5.59  | 115.65      | 110.13   |
| 23  | A     | 406[A] | CLA  | C4A-NA-C1A  | -5.58 | 104.13      | 106.68   |
| 23  | C     | 503    | CLA  | CHD-C4C-C3C | -5.58 | 116.64      | 124.77   |
| 23  | c     | 511    | CLA  | C2D-C1D-ND  | 5.58  | 115.64      | 110.13   |
| 23  | D     | 702[A] | CLA  | C2C-C1C-NC  | 5.57  | 115.84      | 109.98   |
| 23  | C     | 512    | CLA  | O2D-CGD-CBD | 5.57  | 120.97      | 111.23   |
| 23  | C     | 505    | CLA  | CHD-C4C-C3C | -5.57 | 116.65      | 124.77   |
| 23  | a     | 405[A] | CLA  | C2C-C1C-NC  | 5.57  | 115.83      | 109.98   |
| 23  | c     | 502    | CLA  | CHD-C4C-C3C | -5.57 | 116.66      | 124.77   |
| 23  | d     | 401[B] | CLA  | C2D-C1D-ND  | 5.57  | 115.64      | 110.13   |
| 24  | A     | 417[B] | PHO  | C4D-ND-C1D  | -5.56 | 102.21      | 108.87   |
| 23  | D     | 702[B] | CLA  | C2C-C1C-NC  | 5.56  | 115.82      | 109.98   |
| 23  | B     | 606    | CLA  | C3D-C2D-C1D | -5.55 | 98.25       | 105.83   |
| 23  | b     | 613    | CLA  | C2C-C1C-NC  | 5.55  | 115.81      | 109.98   |
| 23  | b     | 612    | CLA  | C2D-C1D-ND  | 5.55  | 115.62      | 110.13   |
| 23  | d     | 401[A] | CLA  | CHD-C4C-C3C | -5.55 | 116.69      | 124.77   |
| 23  | B     | 607    | CLA  | C4A-NA-C1A  | -5.54 | 104.15      | 106.68   |
| 23  | b     | 603    | CLA  | O2D-CGD-CBD | 5.54  | 120.91      | 111.23   |
| 23  | D     | 702[A] | CLA  | CHD-C4C-C3C | -5.53 | 116.71      | 124.77   |
| 23  | A     | 408    | CLA  | C3D-C2D-C1D | -5.53 | 98.29       | 105.83   |
| 24  | A     | 407[A] | PHO  | C3D-C4D-ND  | 5.51  | 114.77      | 107.71   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 603    | CLA  | CMD-C2D-C1D | 5.50  | 134.42      | 124.73   |
| 23  | b     | 604    | CLA  | C1-C2-C3    | -5.50 | 117.19      | 126.20   |
| 23  | C     | 512    | CLA  | C3B-C2B-C1B | -5.49 | 100.70      | 107.17   |
| 24  | A     | 417[A] | PHO  | C4D-ND-C1D  | -5.48 | 102.30      | 108.87   |
| 23  | C     | 513    | CLA  | CMD-C2D-C1D | 5.47  | 134.37      | 124.73   |
| 23  | c     | 510    | CLA  | C2C-C1C-NC  | 5.47  | 115.72      | 109.98   |
| 23  | A     | 405[A] | CLA  | O2D-CGD-CBD | 5.46  | 120.78      | 111.23   |
| 23  | c     | 505    | CLA  | C3B-C2B-C1B | -5.46 | 100.73      | 107.17   |
| 23  | b     | 610    | CLA  | O2D-CGD-CBD | 5.45  | 120.76      | 111.23   |
| 23  | c     | 503    | CLA  | CHD-C4C-C3C | -5.45 | 116.83      | 124.77   |
| 23  | B     | 614    | CLA  | C3B-C2B-C1B | -5.44 | 100.75      | 107.17   |
| 26  | b     | 620    | SQD  | O47-C7-C8   | 5.44  | 123.25      | 111.48   |
| 23  | A     | 406[B] | CLA  | CHD-C4C-C3C | -5.44 | 116.85      | 124.77   |
| 23  | B     | 602    | CLA  | C4A-NA-C1A  | -5.43 | 104.20      | 106.68   |
| 23  | D     | 703    | CLA  | O2D-CGD-CBD | 5.43  | 120.72      | 111.23   |
| 24  | a     | 408[A] | PHO  | C4D-ND-C1D  | -5.42 | 102.38      | 108.87   |
| 23  | c     | 509    | CLA  | C2C-C1C-NC  | 5.42  | 115.67      | 109.98   |
| 23  | b     | 607    | CLA  | C3D-C2D-C1D | -5.42 | 98.43       | 105.83   |
| 23  | c     | 505    | CLA  | O2D-CGD-CBD | 5.42  | 120.70      | 111.23   |
| 24  | a     | 416[A] | PHO  | C3D-C4D-ND  | 5.42  | 114.66      | 107.71   |
| 23  | b     | 611    | CLA  | C4A-NA-C1A  | -5.42 | 104.21      | 106.68   |
| 23  | B     | 604    | CLA  | CHD-C4C-C3C | -5.42 | 116.87      | 124.77   |
| 23  | A     | 404[A] | CLA  | C2C-C1C-NC  | 5.41  | 115.67      | 109.98   |
| 23  | a     | 407[A] | CLA  | C4A-NA-C1A  | -5.41 | 104.21      | 106.68   |
| 24  | a     | 408[B] | PHO  | C4D-ND-C1D  | -5.41 | 102.39      | 108.87   |
| 23  | C     | 503    | CLA  | C2C-C1C-NC  | 5.41  | 115.66      | 109.98   |
| 23  | c     | 503    | CLA  | C1C-C2C-C3C | -5.40 | 101.30      | 106.98   |
| 24  | A     | 407[B] | PHO  | C3D-C4D-ND  | 5.40  | 114.63      | 107.71   |
| 25  | d     | 403    | BCR  | C7-C8-C9    | -5.40 | 118.25      | 126.23   |
| 23  | B     | 614    | CLA  | C3D-C2D-C1D | -5.40 | 98.47       | 105.83   |
| 23  | b     | 602    | CLA  | C2B-C1B-NB  | 5.39  | 115.92      | 110.33   |
| 23  | a     | 405[A] | CLA  | CHD-C4C-C3C | -5.38 | 116.92      | 124.77   |
| 23  | a     | 405[B] | CLA  | CHD-C4C-C3C | -5.38 | 116.93      | 124.77   |
| 23  | C     | 511    | CLA  | O2D-CGD-CBD | 5.38  | 120.63      | 111.23   |
| 23  | C     | 507    | CLA  | C2D-C1D-ND  | 5.37  | 115.44      | 110.13   |
| 23  | b     | 614    | CLA  | C3B-C2B-C1B | -5.37 | 100.84      | 107.17   |
| 23  | C     | 508    | CLA  | C4A-NA-C1A  | -5.37 | 104.23      | 106.68   |
| 23  | B     | 608    | CLA  | O2D-CGD-CBD | 5.37  | 120.61      | 111.23   |
| 23  | a     | 407[B] | CLA  | C4A-NA-C1A  | -5.37 | 104.23      | 106.68   |
| 23  | d     | 401[B] | CLA  | CHD-C4C-C3C | -5.36 | 116.95      | 124.77   |
| 23  | C     | 513    | CLA  | O2D-CGD-CBD | 5.36  | 120.60      | 111.23   |
| 23  | C     | 505    | CLA  | CMD-C2D-C1D | 5.36  | 134.17      | 124.73   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 514    | CLA  | CMD-C2D-C1D | 5.35  | 134.16      | 124.73   |
| 23  | B     | 604    | CLA  | C1-C2-C3    | -5.35 | 117.42      | 126.20   |
| 23  | B     | 604    | CLA  | O2D-CGD-CBD | 5.35  | 120.59      | 111.23   |
| 23  | B     | 603    | CLA  | C4A-NA-C1A  | -5.35 | 104.24      | 106.68   |
| 23  | B     | 612    | CLA  | CMD-C2D-C1D | 5.35  | 134.15      | 124.73   |
| 23  | c     | 513    | CLA  | O2D-CGD-CBD | 5.34  | 120.57      | 111.23   |
| 23  | b     | 614    | CLA  | CMD-C2D-C1D | 5.34  | 134.14      | 124.73   |
| 23  | C     | 505    | CLA  | O2D-CGD-CBD | 5.34  | 120.57      | 111.23   |
| 23  | D     | 703    | CLA  | C2D-C1D-ND  | 5.34  | 115.41      | 110.13   |
| 23  | B     | 605    | CLA  | C4A-NA-C1A  | -5.34 | 104.24      | 106.68   |
| 23  | a     | 407[A] | CLA  | CMD-C2D-C1D | 5.33  | 134.12      | 124.73   |
| 23  | a     | 409    | CLA  | O2D-CGD-CBD | 5.32  | 120.53      | 111.23   |
| 23  | A     | 404[B] | CLA  | C2D-C1D-ND  | 5.31  | 115.39      | 110.13   |
| 23  | C     | 506    | CLA  | O2D-CGD-CBD | 5.31  | 120.51      | 111.23   |
| 23  | B     | 605    | CLA  | O2D-CGD-CBD | 5.31  | 120.51      | 111.23   |
| 23  | C     | 503    | CLA  | C2D-C1D-ND  | 5.30  | 115.37      | 110.13   |
| 23  | c     | 507    | CLA  | C2C-C1C-NC  | 5.30  | 115.55      | 109.98   |
| 23  | b     | 604    | CLA  | C2D-C1D-ND  | 5.30  | 115.37      | 110.13   |
| 23  | C     | 512    | CLA  | CMD-C2D-C1D | 5.29  | 134.04      | 124.73   |
| 23  | b     | 604    | CLA  | CHD-C4C-C3C | -5.29 | 117.06      | 124.77   |
| 23  | C     | 509    | CLA  | CMD-C2D-C1D | 5.28  | 134.03      | 124.73   |
| 35  | D     | 710    | HTG  | C1'-S1-C1   | 5.28  | 111.85      | 100.45   |
| 23  | c     | 513    | CLA  | C2B-C1B-NB  | 5.26  | 115.78      | 110.33   |
| 23  | B     | 604    | CLA  | C2D-C1D-ND  | 5.26  | 115.33      | 110.13   |
| 23  | c     | 507    | CLA  | CHD-C4C-C3C | -5.25 | 117.12      | 124.77   |
| 23  | b     | 606    | CLA  | O2D-CGD-CBD | 5.24  | 120.40      | 111.23   |
| 23  | b     | 613    | CLA  | CMD-C2D-C1D | 5.24  | 133.96      | 124.73   |
| 23  | b     | 614    | CLA  | C3D-C2D-C1D | -5.24 | 98.68       | 105.83   |
| 23  | c     | 509    | CLA  | CMD-C2D-C1D | 5.24  | 133.95      | 124.73   |
| 23  | D     | 702[B] | CLA  | C1-C2-C3    | -5.23 | 117.62      | 126.20   |
| 24  | A     | 417[A] | PHO  | C3D-C4D-ND  | 5.23  | 114.42      | 107.71   |
| 23  | B     | 605    | CLA  | C3D-C2D-C1D | -5.23 | 98.69       | 105.83   |
| 23  | B     | 607    | CLA  | CHD-C4C-C3C | -5.23 | 117.14      | 124.77   |
| 23  | C     | 510    | CLA  | C2C-C1C-NC  | 5.23  | 115.47      | 109.98   |
| 23  | B     | 613    | CLA  | C3D-C2D-C1D | -5.23 | 98.70       | 105.83   |
| 23  | b     | 613    | CLA  | C1-C2-C3    | -5.22 | 117.64      | 126.20   |
| 23  | c     | 510    | CLA  | CHD-C4C-C3C | -5.22 | 117.16      | 124.77   |
| 23  | b     | 616    | CLA  | C3D-C2D-C1D | -5.22 | 98.70       | 105.83   |
| 23  | c     | 513    | CLA  | C3B-C2B-C1B | -5.22 | 101.02      | 107.17   |
| 23  | A     | 406[B] | CLA  | C2B-C1B-NB  | 5.22  | 115.74      | 110.33   |
| 23  | A     | 404[B] | CLA  | C2C-C1C-NC  | 5.21  | 115.46      | 109.98   |
| 23  | B     | 613    | CLA  | C1-C2-C3    | -5.20 | 117.67      | 126.20   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26  | a     | 411[A] | SQD  | O47-C7-C8   | 5.20  | 122.73      | 111.48   |
| 26  | A     | 410[A] | SQD  | C1-C2-C3    | -5.20 | 99.07       | 110.01   |
| 23  | A     | 408    | CLA  | C3B-C2B-C1B | -5.20 | 101.04      | 107.17   |
| 23  | A     | 405[A] | CLA  | C3D-C2D-C1D | -5.19 | 98.75       | 105.83   |
| 23  | a     | 406[A] | CLA  | CMD-C2D-C1D | 5.18  | 133.85      | 124.73   |
| 23  | C     | 510    | CLA  | C3B-C2B-C1B | -5.18 | 101.07      | 107.17   |
| 23  | B     | 616    | CLA  | C3D-C2D-C1D | -5.17 | 98.78       | 105.83   |
| 23  | C     | 511    | CLA  | C1-C2-C3    | -5.16 | 117.74      | 126.20   |
| 23  | C     | 505    | CLA  | C2C-C1C-NC  | 5.16  | 115.40      | 109.98   |
| 23  | d     | 402    | CLA  | C3B-C2B-C1B | -5.16 | 101.09      | 107.17   |
| 23  | C     | 508    | CLA  | C3B-C2B-C1B | -5.15 | 101.09      | 107.17   |
| 25  | H     | 101    | BCR  | C38-C26-C25 | -5.15 | 118.86      | 124.48   |
| 23  | C     | 506    | CLA  | C2D-C1D-ND  | 5.15  | 115.22      | 110.13   |
| 23  | C     | 511    | CLA  | C3D-C2D-C1D | -5.14 | 98.82       | 105.83   |
| 23  | c     | 503    | CLA  | C3B-C2B-C1B | -5.13 | 101.13      | 107.17   |
| 23  | d     | 402    | CLA  | C2B-C1B-NB  | 5.12  | 115.64      | 110.33   |
| 23  | D     | 702[A] | CLA  | C3D-C2D-C1D | -5.12 | 98.84       | 105.83   |
| 23  | A     | 406[A] | CLA  | CMD-C2D-C1D | 5.12  | 133.74      | 124.73   |
| 23  | d     | 402    | CLA  | C3D-C2D-C1D | -5.11 | 98.86       | 105.83   |
| 34  | B     | 621    | LMG  | O7-C10-C11  | 5.11  | 122.53      | 111.48   |
| 23  | C     | 507    | CLA  | C4A-NA-C1A  | -5.11 | 104.35      | 106.68   |
| 23  | C     | 505    | CLA  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 23  | c     | 505    | CLA  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 23  | B     | 616    | CLA  | C3B-C2B-C1B | -5.09 | 101.17      | 107.17   |
| 23  | a     | 406[B] | CLA  | C2C-C1C-NC  | 5.09  | 115.33      | 109.98   |
| 23  | c     | 509    | CLA  | C3D-C2D-C1D | -5.08 | 98.90       | 105.83   |
| 23  | C     | 514    | CLA  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 23  | b     | 612    | CLA  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 23  | b     | 605    | CLA  | C4A-NA-C1A  | -5.08 | 104.36      | 106.68   |
| 24  | a     | 408[B] | PHO  | C3D-C4D-ND  | 5.07  | 114.20      | 107.71   |
| 23  | a     | 406[B] | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 23  | c     | 512    | CLA  | O2D-CGD-CBD | 5.06  | 120.08      | 111.23   |
| 23  | B     | 602    | CLA  | C2C-C1C-NC  | 5.06  | 115.30      | 109.98   |
| 23  | B     | 608    | CLA  | C3D-C2D-C1D | -5.06 | 98.93       | 105.83   |
| 23  | A     | 408    | CLA  | C2C-C1C-NC  | 5.06  | 115.29      | 109.98   |
| 23  | B     | 613    | CLA  | CMD-C2D-C1D | 5.06  | 133.63      | 124.73   |
| 23  | b     | 612    | CLA  | C2C-C1C-NC  | 5.05  | 115.28      | 109.98   |
| 23  | c     | 510    | CLA  | O2D-CGD-CBD | 5.05  | 120.05      | 111.23   |
| 23  | B     | 610    | CLA  | C3D-C2D-C1D | -5.04 | 98.95       | 105.83   |
| 23  | c     | 505    | CLA  | C4A-NA-C1A  | -5.04 | 104.38      | 106.68   |
| 23  | a     | 407[B] | CLA  | CMD-C2D-C1D | 5.04  | 133.60      | 124.73   |
| 23  | A     | 408    | CLA  | C2B-C1B-NB  | 5.04  | 115.55      | 110.33   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 502    | CLA  | O2D-CGD-CBD | 5.03  | 120.02      | 111.23   |
| 23  | C     | 509    | CLA  | C1-C2-C3    | -5.03 | 117.96      | 126.20   |
| 23  | B     | 607    | CLA  | O2D-CGD-CBD | 5.03  | 120.02      | 111.23   |
| 23  | B     | 616    | CLA  | C2B-C1B-NB  | 5.03  | 115.54      | 110.33   |
| 24  | A     | 417[B] | PHO  | C3D-C4D-ND  | 5.03  | 114.15      | 107.71   |
| 23  | C     | 512    | CLA  | C2C-C1C-NC  | 5.02  | 115.26      | 109.98   |
| 24  | A     | 417[B] | PHO  | C1-C2-C3    | -5.02 | 117.97      | 126.20   |
| 23  | A     | 405[B] | CLA  | C2C-C1C-NC  | 5.02  | 115.25      | 109.98   |
| 23  | B     | 616    | CLA  | CMD-C2D-C1D | 5.01  | 133.55      | 124.73   |
| 23  | A     | 404[B] | CLA  | C3B-C2B-C1B | -5.01 | 101.26      | 107.17   |
| 23  | A     | 404[A] | CLA  | C3B-C2B-C1B | -5.01 | 101.27      | 107.17   |
| 34  | C     | 501    | LMG  | C7-O1-C1    | -5.00 | 103.07      | 113.80   |
| 23  | b     | 606    | CLA  | C2B-C1B-NB  | 5.00  | 115.51      | 110.33   |
| 23  | c     | 504    | CLA  | C3D-C2D-C1D | -5.00 | 99.01       | 105.83   |
| 23  | b     | 611    | CLA  | C3D-C2D-C1D | -5.00 | 99.01       | 105.83   |
| 23  | B     | 608    | CLA  | C4A-NA-C1A  | -5.00 | 104.40      | 106.68   |
| 23  | a     | 406[A] | CLA  | C2C-C1C-NC  | 4.99  | 115.22      | 109.98   |
| 26  | a     | 411[B] | SQD  | O6-C1-C2    | 4.99  | 115.85      | 108.27   |
| 26  | B     | 620    | SQD  | O47-C7-C8   | 4.99  | 122.27      | 111.48   |
| 23  | a     | 407[B] | CLA  | C3B-C2B-C1B | -4.98 | 101.30      | 107.17   |
| 23  | a     | 409    | CLA  | CMD-C2D-C1D | 4.98  | 133.50      | 124.73   |
| 23  | C     | 514    | CLA  | C2C-C1C-NC  | 4.98  | 115.21      | 109.98   |
| 23  | c     | 509    | CLA  | O2D-CGD-CBD | 4.98  | 119.93      | 111.23   |
| 23  | B     | 615    | CLA  | C3D-C2D-C1D | -4.98 | 99.04       | 105.83   |
| 24  | a     | 408[A] | PHO  | C3D-C4D-ND  | 4.97  | 114.08      | 107.71   |
| 35  | c     | 522    | HTG  | C1'-S1-C1   | 4.97  | 111.19      | 100.45   |
| 23  | B     | 616    | CLA  | O2D-CGD-O1D | -4.97 | 114.18      | 123.85   |
| 23  | B     | 616    | CLA  | C3C-C4C-NC  | 4.97  | 116.79      | 110.43   |
| 23  | A     | 405[A] | CLA  | C2C-C1C-NC  | 4.96  | 115.19      | 109.98   |
| 23  | b     | 615    | CLA  | C2C-C1C-NC  | 4.96  | 115.19      | 109.98   |
| 23  | C     | 513    | CLA  | C2B-C1B-NB  | 4.96  | 115.47      | 110.33   |
| 23  | C     | 507    | CLA  | CHD-C4C-C3C | -4.96 | 117.54      | 124.77   |
| 23  | A     | 405[B] | CLA  | C3D-C2D-C1D | -4.96 | 99.07       | 105.83   |
| 23  | c     | 502    | CLA  | C3D-C2D-C1D | -4.96 | 99.07       | 105.83   |
| 23  | b     | 603    | CLA  | C2C-C1C-NC  | 4.95  | 115.19      | 109.98   |
| 23  | D     | 703    | CLA  | C2B-C1B-NB  | 4.95  | 115.46      | 110.33   |
| 23  | B     | 615    | CLA  | CMB-C2B-C1B | 4.95  | 132.96      | 125.42   |
| 23  | B     | 614    | CLA  | C2C-C1C-NC  | 4.95  | 115.18      | 109.98   |
| 23  | b     | 611    | CLA  | C2C-C1C-NC  | 4.95  | 115.18      | 109.98   |
| 23  | B     | 604    | CLA  | C4A-NA-C1A  | -4.94 | 104.42      | 106.68   |
| 23  | B     | 603    | CLA  | C3D-C2D-C1D | -4.94 | 99.09       | 105.83   |
| 23  | C     | 504    | CLA  | C3D-C2D-C1D | -4.94 | 99.09       | 105.83   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 614    | CLA  | C2B-C1B-NB  | 4.94  | 115.45      | 110.33   |
| 23  | a     | 409    | CLA  | C3D-C2D-C1D | -4.94 | 99.09       | 105.83   |
| 23  | b     | 608    | CLA  | CMD-C2D-C1D | 4.93  | 133.41      | 124.73   |
| 23  | B     | 615    | CLA  | C2C-C1C-NC  | 4.92  | 115.15      | 109.98   |
| 25  | t     | 102    | BCR  | C33-C5-C6   | -4.92 | 119.12      | 124.48   |
| 23  | C     | 507    | CLA  | O2D-CGD-CBD | 4.92  | 119.83      | 111.23   |
| 23  | B     | 601    | CLA  | C2B-C1B-NB  | 4.91  | 115.42      | 110.33   |
| 23  | a     | 407[A] | CLA  | C3D-C2D-C1D | -4.91 | 99.12       | 105.83   |
| 23  | d     | 402    | CLA  | C4A-NA-C1A  | -4.91 | 104.44      | 106.68   |
| 23  | a     | 406[B] | CLA  | C3D-C2D-C1D | -4.91 | 99.14       | 105.83   |
| 23  | C     | 513    | CLA  | C3B-C2B-C1B | -4.90 | 101.39      | 107.17   |
| 23  | b     | 611    | CLA  | C3B-C2B-C1B | -4.89 | 101.40      | 107.17   |
| 26  | A     | 410[B] | SQD  | C1-O5-C5    | -4.89 | 104.17      | 113.72   |
| 23  | b     | 608    | CLA  | O2D-CGD-CBD | 4.89  | 119.78      | 111.23   |
| 23  | c     | 512    | CLA  | C2C-C1C-NC  | 4.89  | 115.12      | 109.98   |
| 23  | a     | 406[A] | CLA  | C3D-C2D-C1D | -4.89 | 99.16       | 105.83   |
| 23  | c     | 511    | CLA  | C3B-C2B-C1B | -4.89 | 101.41      | 107.17   |
| 23  | A     | 406[B] | CLA  | C3D-C4D-ND  | 4.88  | 117.92      | 109.99   |
| 23  | b     | 614    | CLA  | C2B-C1B-NB  | 4.88  | 115.39      | 110.33   |
| 26  | f     | 102    | SQD  | O47-C7-C8   | 4.88  | 122.03      | 111.48   |
| 23  | B     | 608    | CLA  | C2C-C1C-NC  | 4.88  | 115.10      | 109.98   |
| 24  | A     | 417[A] | PHO  | C1-C2-C3    | -4.87 | 118.22      | 126.20   |
| 23  | D     | 702[B] | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 23  | B     | 608    | CLA  | C3B-C2B-C1B | -4.86 | 101.44      | 107.17   |
| 23  | B     | 601    | CLA  | C4A-NA-C1A  | -4.86 | 104.46      | 106.68   |
| 23  | b     | 602    | CLA  | C3B-C2B-C1B | -4.86 | 101.45      | 107.17   |
| 23  | A     | 406[B] | CLA  | O2D-CGD-CBD | 4.86  | 119.72      | 111.23   |
| 23  | B     | 603    | CLA  | C2C-C1C-NC  | 4.85  | 115.08      | 109.98   |
| 23  | B     | 601    | CLA  | C3B-C2B-C1B | -4.85 | 101.45      | 107.17   |
| 25  | y     | 101    | BCR  | C33-C5-C6   | -4.85 | 119.19      | 124.48   |
| 23  | b     | 605    | CLA  | C3D-C4D-ND  | 4.85  | 117.88      | 109.99   |
| 23  | b     | 602    | CLA  | C3D-C4D-ND  | 4.85  | 117.87      | 109.99   |
| 23  | B     | 610    | CLA  | C4A-NA-C1A  | -4.85 | 104.47      | 106.68   |
| 23  | c     | 512    | CLA  | C3B-C2B-C1B | -4.85 | 101.46      | 107.17   |
| 23  | c     | 507    | CLA  | C4A-NA-C1A  | -4.84 | 104.47      | 106.68   |
| 23  | A     | 406[A] | CLA  | O2D-CGD-CBD | 4.84  | 119.69      | 111.23   |
| 23  | a     | 405[B] | CLA  | C3B-C2B-C1B | -4.84 | 101.47      | 107.17   |
| 23  | b     | 603    | CLA  | C3D-C4D-ND  | 4.84  | 117.85      | 109.99   |
| 23  | B     | 607    | CLA  | C3D-C2D-C1D | -4.84 | 99.23       | 105.83   |
| 23  | b     | 605    | CLA  | C3D-C2D-C1D | -4.84 | 99.23       | 105.83   |
| 23  | b     | 605    | CLA  | C3B-C2B-C1B | -4.83 | 101.47      | 107.17   |
| 23  | A     | 404[A] | CLA  | CHD-C4C-C3C | -4.83 | 117.73      | 124.77   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 511    | CLA  | C2B-C1B-NB  | 4.83  | 115.33      | 110.33   |
| 23  | a     | 407[B] | CLA  | O2D-CGD-CBD | 4.83  | 119.67      | 111.23   |
| 23  | b     | 606    | CLA  | C3D-C2D-C1D | -4.83 | 99.24       | 105.83   |
| 23  | C     | 514    | CLA  | C3B-C2B-C1B | -4.82 | 101.48      | 107.17   |
| 23  | A     | 405[B] | CLA  | C1C-C2C-C3C | -4.82 | 101.91      | 106.98   |
| 23  | C     | 511    | CLA  | C2C-C1C-NC  | 4.82  | 115.05      | 109.98   |
| 23  | B     | 604    | CLA  | C3C-C4C-NC  | 4.82  | 116.60      | 110.43   |
| 23  | c     | 505    | CLA  | C2B-C1B-NB  | 4.81  | 115.32      | 110.33   |
| 23  | a     | 407[A] | CLA  | C3D-C4D-ND  | 4.81  | 117.81      | 109.99   |
| 38  | F     | 102    | HEM  | CAD-CBD-CGD | 4.81  | 126.43      | 113.67   |
| 23  | c     | 511    | CLA  | C1-C2-C3    | -4.81 | 118.31      | 126.20   |
| 23  | a     | 409    | CLA  | C3B-C2B-C1B | -4.81 | 101.50      | 107.17   |
| 23  | C     | 506    | CLA  | C2C-C1C-NC  | 4.81  | 115.04      | 109.98   |
| 23  | C     | 506    | CLA  | C4A-NA-C1A  | -4.81 | 104.48      | 106.68   |
| 23  | c     | 506    | CLA  | C2C-C1C-NC  | 4.81  | 115.03      | 109.98   |
| 23  | c     | 506    | CLA  | C2B-C1B-NB  | 4.81  | 115.31      | 110.33   |
| 26  | X     | 101    | SQD  | C1-O5-C5    | -4.81 | 104.33      | 113.72   |
| 23  | B     | 612    | CLA  | C3B-C2B-C1B | -4.81 | 101.50      | 107.17   |
| 23  | B     | 602    | CLA  | C3D-C2D-C1D | -4.81 | 99.27       | 105.83   |
| 23  | b     | 608    | CLA  | C4A-NA-C1A  | -4.80 | 104.49      | 106.68   |
| 23  | b     | 615    | CLA  | C3D-C2D-C1D | -4.80 | 99.27       | 105.83   |
| 23  | c     | 510    | CLA  | C3B-C4B-NB  | 4.80  | 114.82      | 110.53   |
| 23  | B     | 607    | CLA  | C1C-C2C-C3C | -4.79 | 101.94      | 106.98   |
| 23  | c     | 504    | CLA  | C2B-C1B-NB  | 4.79  | 115.29      | 110.33   |
| 23  | b     | 614    | CLA  | C2C-C1C-NC  | 4.78  | 115.01      | 109.98   |
| 23  | c     | 505    | CLA  | C1-O2A-CGA  | 4.78  | 128.22      | 116.65   |
| 23  | B     | 611    | CLA  | C3D-C4D-ND  | 4.78  | 117.76      | 109.99   |
| 23  | a     | 407[B] | CLA  | C3D-C4D-ND  | 4.78  | 117.75      | 109.99   |
| 23  | B     | 602    | CLA  | C3B-C2B-C1B | -4.77 | 101.54      | 107.17   |
| 23  | C     | 513    | CLA  | C3D-C2D-C1D | -4.77 | 99.32       | 105.83   |
| 23  | C     | 509    | CLA  | O2D-CGD-CBD | 4.77  | 119.57      | 111.23   |
| 23  | b     | 607    | CLA  | C2C-C1C-NC  | 4.77  | 114.99      | 109.98   |
| 23  | c     | 509    | CLA  | C4A-NA-C1A  | -4.77 | 104.50      | 106.68   |
| 23  | b     | 616    | CLA  | C2B-C1B-NB  | 4.76  | 115.26      | 110.33   |
| 23  | b     | 604    | CLA  | C1C-C2C-C3C | -4.76 | 101.98      | 106.98   |
| 23  | C     | 504    | CLA  | C2B-C1B-NB  | 4.76  | 115.26      | 110.33   |
| 23  | c     | 512    | CLA  | C3D-C2D-C1D | -4.75 | 99.34       | 105.83   |
| 23  | b     | 611    | CLA  | C2B-C1B-NB  | 4.75  | 115.25      | 110.33   |
| 23  | b     | 609    | CLA  | C3D-C2D-C1D | -4.75 | 99.35       | 105.83   |
| 25  | d     | 403    | BCR  | C15-C14-C13 | -4.75 | 120.62      | 127.28   |
| 23  | d     | 401[B] | CLA  | C1C-C2C-C3C | -4.75 | 101.99      | 106.98   |
| 23  | c     | 514    | CLA  | O2D-CGD-CBD | 4.75  | 119.53      | 111.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 406[A] | CLA  | C2C-C1C-NC  | 4.74  | 114.97      | 109.98   |
| 23  | b     | 603    | CLA  | C3B-C2B-C1B | -4.74 | 101.58      | 107.17   |
| 23  | c     | 508    | CLA  | C2C-C1C-NC  | 4.74  | 114.96      | 109.98   |
| 23  | d     | 401[B] | CLA  | O2D-CGD-CBD | 4.74  | 119.51      | 111.23   |
| 23  | B     | 605    | CLA  | C2C-C1C-NC  | 4.73  | 114.95      | 109.98   |
| 23  | A     | 405[A] | CLA  | C1C-C2C-C3C | -4.73 | 102.00      | 106.98   |
| 23  | c     | 504    | CLA  | C3B-C2B-C1B | -4.73 | 101.60      | 107.17   |
| 23  | B     | 612    | CLA  | C3D-C4D-ND  | 4.73  | 117.67      | 109.99   |
| 23  | b     | 612    | CLA  | C3C-C4C-NC  | 4.72  | 116.48      | 110.43   |
| 23  | A     | 405[A] | CLA  | C4A-NA-C1A  | -4.72 | 104.53      | 106.68   |
| 23  | C     | 504    | CLA  | C3B-C2B-C1B | -4.72 | 101.61      | 107.17   |
| 23  | a     | 405[B] | CLA  | C1C-C2C-C3C | -4.71 | 102.02      | 106.98   |
| 23  | b     | 601    | CLA  | C2B-C1B-NB  | 4.71  | 115.21      | 110.33   |
| 23  | A     | 404[A] | CLA  | C3D-C2D-C1D | -4.71 | 99.41       | 105.83   |
| 23  | C     | 509    | CLA  | C3B-C4B-NB  | 4.71  | 114.73      | 110.53   |
| 23  | b     | 613    | CLA  | C1C-C2C-C3C | -4.70 | 102.03      | 106.98   |
| 23  | C     | 504    | CLA  | C3D-C4D-ND  | 4.70  | 117.63      | 109.99   |
| 23  | b     | 610    | CLA  | C3D-C2D-C1D | -4.70 | 99.42       | 105.83   |
| 23  | b     | 604    | CLA  | C3B-C4B-NB  | 4.69  | 114.72      | 110.53   |
| 23  | B     | 609    | CLA  | C2C-C1C-NC  | 4.69  | 114.91      | 109.98   |
| 23  | A     | 406[A] | CLA  | C3D-C4D-ND  | 4.69  | 117.61      | 109.99   |
| 23  | A     | 406[B] | CLA  | CHD-C1D-ND  | -4.69 | 118.21      | 124.80   |
| 23  | B     | 603    | CLA  | C2B-C1B-NB  | 4.69  | 115.19      | 110.33   |
| 23  | C     | 508    | CLA  | C3D-C2D-C1D | -4.68 | 99.44       | 105.83   |
| 23  | C     | 505    | CLA  | C4A-NA-C1A  | -4.68 | 104.54      | 106.68   |
| 23  | b     | 608    | CLA  | C2C-C1C-NC  | 4.68  | 114.90      | 109.98   |
| 23  | b     | 603    | CLA  | C3D-C2D-C1D | -4.68 | 99.44       | 105.83   |
| 23  | b     | 608    | CLA  | C3D-C4D-ND  | 4.68  | 117.59      | 109.99   |
| 23  | d     | 401[B] | CLA  | C3B-C2B-C1B | -4.67 | 101.66      | 107.17   |
| 23  | C     | 510    | CLA  | C1-C2-C3    | -4.67 | 118.54      | 126.20   |
| 23  | a     | 407[A] | CLA  | O2D-CGD-CBD | 4.67  | 119.40      | 111.23   |
| 23  | a     | 407[B] | CLA  | C3D-C2D-C1D | -4.67 | 99.46       | 105.83   |
| 23  | b     | 606    | CLA  | C3B-C2B-C1B | -4.67 | 101.67      | 107.17   |
| 38  | F     | 102    | HEM  | CHC-C4B-NB  | 4.67  | 129.45      | 124.42   |
| 23  | C     | 507    | CLA  | C3D-C2D-C1D | -4.67 | 99.46       | 105.83   |
| 29  | A     | 414[A] | PL9  | C7-C3-C2    | -4.67 | 117.89      | 123.39   |
| 23  | C     | 506    | CLA  | CMB-C2B-C1B | 4.66  | 132.52      | 125.42   |
| 23  | c     | 509    | CLA  | C3B-C2B-C1B | -4.66 | 101.67      | 107.17   |
| 23  | D     | 703    | CLA  | C3B-C2B-C1B | -4.66 | 101.68      | 107.17   |
| 23  | C     | 502    | CLA  | C2B-C1B-NB  | 4.66  | 115.16      | 110.33   |
| 23  | C     | 507    | CLA  | C1C-C2C-C3C | -4.65 | 102.08      | 106.98   |
| 23  | b     | 605    | CLA  | CHD-C1D-ND  | -4.65 | 118.25      | 124.80   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 506    | CLA  | C3D-C4D-ND  | 4.65  | 117.55      | 109.99   |
| 23  | D     | 702[A] | CLA  | O2D-CGD-CBD | 4.65  | 119.36      | 111.23   |
| 23  | B     | 609    | CLA  | C3D-C2D-C1D | -4.65 | 99.48       | 105.83   |
| 23  | c     | 514    | CLA  | C3D-C2D-C1D | -4.65 | 99.49       | 105.83   |
| 23  | b     | 605    | CLA  | C2B-C1B-NB  | 4.64  | 115.14      | 110.33   |
| 23  | C     | 514    | CLA  | C3D-C2D-C1D | -4.64 | 99.49       | 105.83   |
| 23  | C     | 503    | CLA  | C4A-NA-C1A  | -4.64 | 104.56      | 106.68   |
| 23  | D     | 702[B] | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 23  | A     | 406[B] | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 23  | a     | 409    | CLA  | C4A-NA-C1A  | -4.63 | 104.56      | 106.68   |
| 23  | C     | 508    | CLA  | C2C-C1C-NC  | 4.63  | 114.85      | 109.98   |
| 23  | B     | 606    | CLA  | CHD-C1D-ND  | -4.63 | 118.28      | 124.80   |
| 23  | A     | 405[B] | CLA  | C4A-NA-C1A  | -4.63 | 104.57      | 106.68   |
| 23  | C     | 509    | CLA  | C3D-C2D-C1D | -4.63 | 99.52       | 105.83   |
| 23  | b     | 607    | CLA  | CHD-C1D-ND  | -4.63 | 118.29      | 124.80   |
| 23  | b     | 610    | CLA  | C2C-C1C-NC  | 4.63  | 114.84      | 109.98   |
| 23  | a     | 409    | CLA  | C3D-C4D-ND  | 4.63  | 117.51      | 109.99   |
| 23  | a     | 405[B] | CLA  | C4A-NA-C1A  | -4.62 | 104.57      | 106.68   |
| 23  | A     | 406[A] | CLA  | C3D-C2D-C1D | -4.62 | 99.52       | 105.83   |
| 23  | b     | 616    | CLA  | C3B-C2B-C1B | -4.62 | 101.72      | 107.17   |
| 23  | c     | 514    | CLA  | C3B-C2B-C1B | -4.62 | 101.72      | 107.17   |
| 23  | C     | 510    | CLA  | C2B-C1B-NB  | 4.62  | 115.12      | 110.33   |
| 23  | B     | 601    | CLA  | C3D-C2D-C1D | -4.62 | 99.52       | 105.83   |
| 23  | c     | 508    | CLA  | C3B-C2B-C1B | -4.62 | 101.72      | 107.17   |
| 23  | c     | 502    | CLA  | CHD-C1D-ND  | -4.62 | 118.30      | 124.80   |
| 23  | A     | 406[B] | CLA  | C3B-C2B-C1B | -4.62 | 101.72      | 107.17   |
| 23  | B     | 611    | CLA  | CMC-C2C-C1C | 4.62  | 132.25      | 125.03   |
| 23  | b     | 610    | CLA  | C3D-C4D-ND  | 4.62  | 117.49      | 109.99   |
| 23  | B     | 613    | CLA  | C3B-C2B-C1B | -4.62 | 101.73      | 107.17   |
| 23  | c     | 508    | CLA  | CHD-C1D-ND  | -4.62 | 118.30      | 124.80   |
| 23  | C     | 505    | CLA  | C1C-C2C-C3C | -4.62 | 102.12      | 106.98   |
| 23  | c     | 504    | CLA  | O2D-CGD-CBD | 4.61  | 119.30      | 111.23   |
| 23  | b     | 601    | CLA  | C2C-C1C-NC  | 4.61  | 114.83      | 109.98   |
| 23  | c     | 507    | CLA  | C3D-C2D-C1D | -4.61 | 99.54       | 105.83   |
| 23  | a     | 405[B] | CLA  | C3D-C2D-C1D | -4.61 | 99.54       | 105.83   |
| 35  | d     | 409    | HTG  | C1'-S1-C1   | 4.61  | 110.41      | 100.45   |
| 23  | C     | 510    | CLA  | C4A-NA-C1A  | -4.61 | 104.58      | 106.68   |
| 23  | b     | 609    | CLA  | O2D-CGD-CBD | 4.60  | 119.28      | 111.23   |
| 23  | c     | 511    | CLA  | C2C-C1C-NC  | 4.60  | 114.81      | 109.98   |
| 23  | a     | 405[A] | CLA  | C3B-C2B-C1B | -4.60 | 101.75      | 107.17   |
| 23  | C     | 505    | CLA  | C3B-C2B-C1B | -4.59 | 101.76      | 107.17   |
| 23  | C     | 510    | CLA  | C3D-C4D-ND  | 4.59  | 117.44      | 109.99   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 612    | CLA  | C3C-C4C-NC  | 4.59  | 116.31      | 110.43   |
| 23  | c     | 510    | CLA  | C3B-C2B-C1B | -4.58 | 101.77      | 107.17   |
| 32  | t     | 101    | LMT  | C3'-C4'-C5' | -4.58 | 100.78      | 110.93   |
| 23  | a     | 405[A] | CLA  | C3D-C2D-C1D | -4.58 | 99.58       | 105.83   |
| 23  | d     | 402    | CLA  | CHD-C1D-ND  | -4.58 | 118.36      | 124.80   |
| 23  | b     | 601    | CLA  | C3D-C2D-C1D | -4.57 | 99.59       | 105.83   |
| 23  | d     | 401[A] | CLA  | C3D-C4D-ND  | 4.57  | 117.42      | 109.99   |
| 23  | a     | 405[B] | CLA  | C3D-C4D-ND  | 4.57  | 117.41      | 109.99   |
| 23  | C     | 514    | CLA  | C4A-NA-C1A  | -4.57 | 104.59      | 106.68   |
| 23  | c     | 508    | CLA  | C3D-C2D-C1D | -4.57 | 99.60       | 105.83   |
| 23  | B     | 603    | CLA  | C3B-C2B-C1B | -4.57 | 101.79      | 107.17   |
| 23  | A     | 404[A] | CLA  | C2B-C1B-NB  | 4.56  | 115.06      | 110.33   |
| 23  | b     | 613    | CLA  | C3C-C4C-NC  | 4.56  | 116.27      | 110.43   |
| 23  | B     | 614    | CLA  | CHD-C1D-ND  | -4.56 | 118.39      | 124.80   |
| 23  | d     | 401[B] | CLA  | C4A-NA-C1A  | -4.55 | 104.60      | 106.68   |
| 23  | a     | 407[B] | CLA  | C2B-C1B-NB  | 4.55  | 115.05      | 110.33   |
| 23  | A     | 406[B] | CLA  | C2C-C1C-NC  | 4.55  | 114.76      | 109.98   |
| 23  | c     | 514    | CLA  | C3D-C4D-ND  | 4.55  | 117.38      | 109.99   |
| 23  | B     | 610    | CLA  | O2A-CGA-CBA | 4.55  | 125.70      | 111.83   |
| 23  | A     | 404[B] | CLA  | C2B-C1B-NB  | 4.55  | 115.04      | 110.33   |
| 23  | c     | 514    | CLA  | C2B-C1B-NB  | 4.55  | 115.04      | 110.33   |
| 23  | B     | 613    | CLA  | C2C-C1C-NC  | 4.55  | 114.76      | 109.98   |
| 23  | A     | 405[A] | CLA  | CMD-C2D-C1D | 4.54  | 132.73      | 124.73   |
| 23  | b     | 601    | CLA  | C3B-C2B-C1B | -4.54 | 101.82      | 107.17   |
| 23  | b     | 607    | CLA  | C4A-NA-C1A  | -4.54 | 104.61      | 106.68   |
| 23  | c     | 511    | CLA  | O2D-CGD-CBD | 4.53  | 119.15      | 111.23   |
| 23  | c     | 514    | CLA  | CHD-C1D-ND  | -4.53 | 118.43      | 124.80   |
| 23  | c     | 507    | CLA  | C3D-C4D-ND  | 4.53  | 117.35      | 109.99   |
| 26  | a     | 411[B] | SQD  | O47-C7-C8   | 4.53  | 121.28      | 111.48   |
| 23  | b     | 605    | CLA  | C2C-C1C-NC  | 4.53  | 114.74      | 109.98   |
| 23  | c     | 513    | CLA  | C3D-C2D-C1D | -4.53 | 99.66       | 105.83   |
| 23  | B     | 609    | CLA  | C3D-C4D-ND  | 4.52  | 117.34      | 109.99   |
| 23  | C     | 510    | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 23  | C     | 512    | CLA  | C4A-NA-C1A  | -4.52 | 104.62      | 106.68   |
| 23  | C     | 512    | CLA  | C3D-C2D-C1D | -4.52 | 99.67       | 105.83   |
| 38  | f     | 101    | HEM  | CHC-C4B-NB  | 4.52  | 129.28      | 124.42   |
| 23  | c     | 506    | CLA  | C3C-C4C-NC  | 4.51  | 116.21      | 110.43   |
| 23  | D     | 703    | CLA  | C3D-C4D-ND  | 4.51  | 117.32      | 109.99   |
| 23  | C     | 514    | CLA  | C3D-C4D-ND  | 4.51  | 117.32      | 109.99   |
| 23  | D     | 702[B] | CLA  | C3D-C4D-ND  | 4.51  | 117.32      | 109.99   |
| 23  | a     | 406[A] | CLA  | C1C-C2C-C3C | -4.51 | 102.24      | 106.98   |
| 23  | c     | 502    | CLA  | C2C-C1C-NC  | 4.51  | 114.72      | 109.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | D     | 702[A] | CLA  | C3B-C2B-C1B | -4.51 | 101.86      | 107.17   |
| 29  | A     | 414[A] | PL9  | C32-C33-C34 | -4.50 | 117.31      | 127.62   |
| 23  | C     | 512    | CLA  | C2B-C1B-NB  | 4.50  | 115.00      | 110.33   |
| 23  | A     | 406[A] | CLA  | C2B-C1B-NB  | 4.50  | 114.99      | 110.33   |
| 23  | c     | 502    | CLA  | C3D-C4D-ND  | 4.50  | 117.30      | 109.99   |
| 23  | B     | 615    | CLA  | C3D-C4D-ND  | 4.50  | 117.30      | 109.99   |
| 29  | D     | 705[B] | PL9  | C42-C43-C44 | -4.49 | 117.34      | 127.62   |
| 23  | C     | 508    | CLA  | C3C-C4C-NC  | 4.49  | 116.18      | 110.43   |
| 23  | C     | 503    | CLA  | C3B-C2B-C1B | -4.49 | 101.88      | 107.17   |
| 23  | b     | 607    | CLA  | C3B-C2B-C1B | -4.49 | 101.88      | 107.17   |
| 23  | b     | 615    | CLA  | C3B-C2B-C1B | -4.49 | 101.88      | 107.17   |
| 23  | b     | 610    | CLA  | C4A-NA-C1A  | -4.48 | 104.63      | 106.68   |
| 23  | a     | 406[A] | CLA  | O2D-CGD-CBD | 4.48  | 119.07      | 111.23   |
| 23  | a     | 409    | CLA  | C2C-C1C-NC  | 4.48  | 114.69      | 109.98   |
| 29  | A     | 414[B] | PL9  | C32-C33-C34 | -4.48 | 117.37      | 127.62   |
| 23  | B     | 605    | CLA  | C3C-C4C-NC  | 4.48  | 116.17      | 110.43   |
| 23  | C     | 502    | CLA  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 23  | A     | 405[B] | CLA  | C3D-C4D-ND  | 4.48  | 117.26      | 109.99   |
| 23  | b     | 616    | CLA  | C1D-CHD-C4C | -4.47 | 116.51      | 126.02   |
| 29  | a     | 414[A] | PL9  | C7-C8-C9    | -4.47 | 119.13      | 126.83   |
| 23  | B     | 601    | CLA  | C3D-C4D-ND  | 4.47  | 117.25      | 109.99   |
| 23  | A     | 404[A] | CLA  | C3B-C4B-NB  | 4.47  | 114.52      | 110.53   |
| 23  | d     | 401[A] | CLA  | C1C-C2C-C3C | -4.47 | 102.28      | 106.98   |
| 23  | B     | 610    | CLA  | CAA-C2A-C3A | -4.46 | 100.94      | 113.00   |
| 23  | C     | 510    | CLA  | O2D-CGD-CBD | 4.46  | 119.03      | 111.23   |
| 23  | c     | 506    | CLA  | C3B-C2B-C1B | -4.45 | 101.92      | 107.17   |
| 23  | C     | 504    | CLA  | O2D-CGD-CBD | 4.45  | 119.02      | 111.23   |
| 23  | b     | 609    | CLA  | C1-C2-C3    | -4.45 | 118.90      | 126.20   |
| 23  | B     | 610    | CLA  | C2C-C1C-NC  | 4.45  | 114.66      | 109.98   |
| 23  | b     | 603    | CLA  | C2B-C1B-NB  | 4.45  | 114.94      | 110.33   |
| 23  | a     | 409    | CLA  | C3C-C4C-NC  | 4.45  | 116.13      | 110.43   |
| 23  | b     | 610    | CLA  | C3B-C2B-C1B | -4.44 | 101.93      | 107.17   |
| 23  | A     | 404[B] | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 23  | c     | 502    | CLA  | C3B-C2B-C1B | -4.44 | 101.93      | 107.17   |
| 23  | C     | 502    | CLA  | C2C-C1C-NC  | 4.44  | 114.65      | 109.98   |
| 26  | A     | 410[B] | SQD  | C1-C2-C3    | -4.44 | 100.67      | 110.01   |
| 23  | b     | 606    | CLA  | CHD-C1D-ND  | -4.44 | 118.56      | 124.80   |
| 23  | C     | 502    | CLA  | C3D-C4D-ND  | 4.44  | 117.20      | 109.99   |
| 23  | c     | 503    | CLA  | C3D-C4D-ND  | 4.43  | 117.19      | 109.99   |
| 23  | c     | 503    | CLA  | C2B-C1B-NB  | 4.43  | 114.92      | 110.33   |
| 23  | b     | 602    | CLA  | CHD-C1D-ND  | -4.43 | 118.56      | 124.80   |
| 34  | c     | 521    | LMG  | O6-C5-C4    | 4.43  | 117.69      | 109.70   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 612    | CLA  | CMD-C2D-C1D | 4.43  | 132.53      | 124.73   |
| 23  | B     | 610    | CLA  | C3D-C4D-ND  | 4.43  | 117.19      | 109.99   |
| 23  | a     | 405[A] | CLA  | C2B-C1B-NB  | 4.43  | 114.92      | 110.33   |
| 23  | b     | 607    | CLA  | C3D-C4D-ND  | 4.43  | 117.19      | 109.99   |
| 23  | b     | 614    | CLA  | C3D-C4D-ND  | 4.43  | 117.19      | 109.99   |
| 23  | d     | 402    | CLA  | C3D-C4D-ND  | 4.43  | 117.19      | 109.99   |
| 23  | b     | 611    | CLA  | C3D-C4D-ND  | 4.43  | 117.18      | 109.99   |
| 23  | C     | 504    | CLA  | CHD-C1D-ND  | -4.42 | 118.58      | 124.80   |
| 23  | b     | 605    | CLA  | O2D-CGD-O1D | -4.42 | 115.25      | 123.85   |
| 23  | b     | 609    | CLA  | C3D-C4D-ND  | 4.41  | 117.16      | 109.99   |
| 23  | b     | 615    | CLA  | C2B-C1B-NB  | 4.41  | 114.90      | 110.33   |
| 34  | C     | 501    | LMG  | O1-C1-C2    | 4.41  | 114.97      | 108.27   |
| 23  | c     | 504    | CLA  | C3D-C4D-ND  | 4.41  | 117.15      | 109.99   |
| 23  | C     | 511    | CLA  | CHD-C1D-ND  | -4.41 | 118.60      | 124.80   |
| 23  | b     | 606    | CLA  | C4-C3-C5    | 4.41  | 122.88      | 115.23   |
| 23  | b     | 603    | CLA  | C1D-CHD-C4C | -4.41 | 116.65      | 126.02   |
| 25  | d     | 403    | BCR  | C29-C30-C25 | 4.40  | 116.84      | 110.44   |
| 23  | A     | 404[B] | CLA  | C1D-CHD-C4C | -4.40 | 116.66      | 126.02   |
| 23  | C     | 503    | CLA  | O2D-CGD-CBD | 4.40  | 118.93      | 111.23   |
| 23  | b     | 607    | CLA  | C3C-C4C-NC  | 4.40  | 116.07      | 110.43   |
| 23  | c     | 504    | CLA  | C2C-C1C-NC  | 4.40  | 114.61      | 109.98   |
| 23  | c     | 511    | CLA  | C3D-C2D-C1D | -4.40 | 99.83       | 105.83   |
| 23  | a     | 407[A] | CLA  | C2C-C1C-NC  | 4.39  | 114.60      | 109.98   |
| 23  | C     | 513    | CLA  | C3C-C4C-NC  | 4.39  | 116.06      | 110.43   |
| 23  | A     | 404[B] | CLA  | CAA-C2A-C3A | -4.39 | 101.13      | 113.00   |
| 23  | c     | 512    | CLA  | C1D-CHD-C4C | -4.39 | 116.69      | 126.02   |
| 23  | c     | 507    | CLA  | C3B-C2B-C1B | -4.39 | 101.99      | 107.17   |
| 23  | c     | 507    | CLA  | CHD-C1D-ND  | -4.39 | 118.63      | 124.80   |
| 23  | a     | 406[B] | CLA  | C2B-C1B-NB  | 4.39  | 114.88      | 110.33   |
| 34  | d     | 410    | LMG  | O7-C10-C11  | 4.39  | 120.97      | 111.48   |
| 23  | C     | 502    | CLA  | O2D-CGD-O1D | -4.39 | 115.31      | 123.85   |
| 23  | c     | 505    | CLA  | C2C-C1C-NC  | 4.38  | 114.59      | 109.98   |
| 23  | A     | 405[B] | CLA  | C2B-C1B-NB  | 4.38  | 114.87      | 110.33   |
| 29  | a     | 414[B] | PL9  | C7-C8-C9    | -4.38 | 119.28      | 126.83   |
| 23  | C     | 506    | CLA  | C3C-C4C-NC  | 4.38  | 116.04      | 110.43   |
| 23  | d     | 401[B] | CLA  | C3D-C2D-C1D | -4.38 | 99.85       | 105.83   |
| 23  | c     | 514    | CLA  | C2C-C1C-NC  | 4.37  | 114.58      | 109.98   |
| 23  | B     | 611    | CLA  | C3C-C4C-NC  | 4.37  | 116.03      | 110.43   |
| 23  | a     | 405[B] | CLA  | C3B-C4B-NB  | 4.37  | 114.43      | 110.53   |
| 23  | D     | 702[B] | CLA  | O2D-CGD-CBD | 4.37  | 118.87      | 111.23   |
| 23  | a     | 407[A] | CLA  | CHD-C1D-ND  | -4.37 | 118.66      | 124.80   |
| 23  | A     | 405[B] | CLA  | CHD-C1D-ND  | -4.36 | 118.66      | 124.80   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 409    | CLA  | C2B-C1B-NB  | 4.36  | 114.85      | 110.33   |
| 29  | a     | 414[A] | PL9  | C7-C3-C2    | -4.36 | 118.25      | 123.39   |
| 23  | a     | 405[B] | CLA  | C2B-C1B-NB  | 4.35  | 114.84      | 110.33   |
| 23  | C     | 507    | CLA  | C3D-C4D-ND  | 4.35  | 117.06      | 109.99   |
| 23  | a     | 405[A] | CLA  | C3D-C4D-ND  | 4.35  | 117.06      | 109.99   |
| 35  | B     | 622    | HTG  | C1'-S1-C1   | 4.35  | 109.85      | 100.45   |
| 23  | a     | 406[B] | CLA  | C3D-C4D-ND  | 4.35  | 117.06      | 109.99   |
| 33  | E     | 101[B] | LHG  | O7-C7-C8    | 4.35  | 120.88      | 111.48   |
| 23  | A     | 404[A] | CLA  | C1C-C2C-C3C | -4.34 | 102.41      | 106.98   |
| 23  | c     | 510    | CLA  | C3D-C2D-C1D | -4.34 | 99.90       | 105.83   |
| 23  | a     | 407[A] | CLA  | C2B-C1B-NB  | 4.34  | 114.83      | 110.33   |
| 23  | B     | 610    | CLA  | C2B-C1B-NB  | 4.34  | 114.83      | 110.33   |
| 23  | b     | 610    | CLA  | C2B-C1B-NB  | 4.34  | 114.83      | 110.33   |
| 23  | b     | 611    | CLA  | C3B-C4B-NB  | 4.34  | 114.40      | 110.53   |
| 23  | B     | 605    | CLA  | C3B-C2B-C1B | -4.34 | 102.05      | 107.17   |
| 23  | b     | 601    | CLA  | C3D-C4D-ND  | 4.34  | 117.04      | 109.99   |
| 23  | A     | 408    | CLA  | C1-C2-C3    | -4.34 | 119.09      | 126.20   |
| 23  | c     | 510    | CLA  | C4A-NA-C1A  | -4.34 | 104.70      | 106.68   |
| 23  | b     | 613    | CLA  | O2D-CGD-CBD | 4.34  | 118.81      | 111.23   |
| 23  | B     | 614    | CLA  | C3D-C4D-ND  | 4.33  | 117.03      | 109.99   |
| 23  | b     | 604    | CLA  | C3B-C2B-C1B | -4.33 | 102.06      | 107.17   |
| 23  | B     | 613    | CLA  | C2B-C1B-NB  | 4.33  | 114.82      | 110.33   |
| 23  | B     | 613    | CLA  | C3B-C4B-NB  | 4.33  | 114.40      | 110.53   |
| 23  | C     | 506    | CLA  | C3B-C2B-C1B | -4.33 | 102.07      | 107.17   |
| 23  | B     | 613    | CLA  | C3C-C4C-NC  | 4.33  | 115.98      | 110.43   |
| 23  | b     | 609    | CLA  | C2C-C1C-NC  | 4.33  | 114.53      | 109.98   |
| 23  | c     | 502    | CLA  | CMB-C2B-C1B | 4.33  | 132.01      | 125.42   |
| 34  | C     | 501    | LMG  | O7-C10-C11  | 4.33  | 120.84      | 111.48   |
| 23  | a     | 407[A] | CLA  | C3B-C2B-C1B | -4.32 | 102.07      | 107.17   |
| 23  | A     | 408    | CLA  | C3D-C4D-ND  | 4.32  | 117.01      | 109.99   |
| 23  | C     | 507    | CLA  | C3B-C2B-C1B | -4.32 | 102.08      | 107.17   |
| 23  | b     | 613    | CLA  | C3B-C2B-C1B | -4.32 | 102.08      | 107.17   |
| 33  | E     | 101[A] | LHG  | O7-C7-C8    | 4.32  | 120.82      | 111.48   |
| 23  | b     | 606    | CLA  | C3D-C4D-ND  | 4.32  | 117.00      | 109.99   |
| 23  | B     | 611    | CLA  | C1D-CHD-C4C | -4.31 | 116.85      | 126.02   |
| 23  | a     | 406[B] | CLA  | C1C-C2C-C3C | -4.31 | 102.44      | 106.98   |
| 23  | a     | 405[A] | CLA  | CAA-C2A-C3A | -4.31 | 101.34      | 113.00   |
| 23  | C     | 511    | CLA  | C3D-C4D-ND  | 4.31  | 117.00      | 109.99   |
| 23  | B     | 605    | CLA  | C1D-CHD-C4C | -4.31 | 116.86      | 126.02   |
| 23  | a     | 405[A] | CLA  | C1C-C2C-C3C | -4.31 | 102.45      | 106.98   |
| 23  | C     | 502    | CLA  | C3B-C2B-C1B | -4.31 | 102.09      | 107.17   |
| 23  | B     | 608    | CLA  | C3D-C4D-ND  | 4.31  | 116.98      | 109.99   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 514    | CLA  | C2B-C1B-NB  | 4.30  | 114.79      | 110.33   |
| 23  | c     | 507    | CLA  | O2D-CGD-CBD | 4.30  | 118.75      | 111.23   |
| 23  | a     | 406[B] | CLA  | C1D-CHD-C4C | -4.30 | 116.87      | 126.02   |
| 23  | c     | 503    | CLA  | C3D-C2D-C1D | -4.30 | 99.96       | 105.83   |
| 23  | b     | 616    | CLA  | O2D-CGD-O1D | -4.30 | 115.47      | 123.85   |
| 23  | b     | 606    | CLA  | C2C-C1C-NC  | 4.30  | 114.50      | 109.98   |
| 23  | C     | 503    | CLA  | C3D-C2D-C1D | -4.30 | 99.96       | 105.83   |
| 29  | A     | 414[B] | PL9  | C7-C8-C9    | -4.30 | 119.43      | 126.83   |
| 23  | D     | 702[B] | CLA  | C1C-C2C-C3C | -4.30 | 102.46      | 106.98   |
| 23  | c     | 508    | CLA  | C1C-C2C-C3C | -4.30 | 102.46      | 106.98   |
| 25  | b     | 617    | BCR  | C7-C8-C9    | -4.30 | 119.88      | 126.23   |
| 23  | C     | 507    | CLA  | CHD-C1D-ND  | -4.30 | 118.76      | 124.80   |
| 23  | c     | 513    | CLA  | C3D-C4D-ND  | 4.29  | 116.97      | 109.99   |
| 35  | b     | 622    | HTG  | C1-O5-C5    | 4.29  | 120.26      | 112.56   |
| 23  | A     | 404[B] | CLA  | C3D-C4D-ND  | 4.29  | 116.96      | 109.99   |
| 23  | c     | 502    | CLA  | C2B-C1B-NB  | 4.29  | 114.78      | 110.33   |
| 23  | c     | 509    | CLA  | C2B-C1B-NB  | 4.29  | 114.77      | 110.33   |
| 23  | b     | 614    | CLA  | C4A-NA-C1A  | -4.29 | 104.72      | 106.68   |
| 29  | a     | 414[A] | PL9  | C7-C3-C4    | 4.28  | 120.44      | 116.91   |
| 23  | B     | 616    | CLA  | C2C-C1C-NC  | 4.28  | 114.48      | 109.98   |
| 23  | B     | 602    | CLA  | C2B-C1B-NB  | 4.28  | 114.76      | 110.33   |
| 23  | B     | 602    | CLA  | C3D-C4D-ND  | 4.28  | 116.94      | 109.99   |
| 23  | B     | 604    | CLA  | C3B-C2B-C1B | -4.27 | 102.13      | 107.17   |
| 23  | D     | 702[A] | CLA  | CHD-C1D-ND  | -4.27 | 118.79      | 124.80   |
| 23  | c     | 512    | CLA  | C3D-C4D-ND  | 4.27  | 116.93      | 109.99   |
| 23  | b     | 615    | CLA  | C3D-C4D-ND  | 4.27  | 116.93      | 109.99   |
| 23  | b     | 615    | CLA  | C1D-CHD-C4C | -4.27 | 116.95      | 126.02   |
| 23  | A     | 408    | CLA  | C4A-NA-C1A  | -4.27 | 104.73      | 106.68   |
| 23  | B     | 608    | CLA  | C2B-C1B-NB  | 4.26  | 114.75      | 110.33   |
| 29  | a     | 414[B] | PL9  | C32-C33-C34 | -4.26 | 117.87      | 127.62   |
| 23  | C     | 506    | CLA  | C3D-C4D-ND  | 4.26  | 116.91      | 109.99   |
| 23  | a     | 407[B] | CLA  | C2C-C1C-NC  | 4.26  | 114.45      | 109.98   |
| 34  | C     | 521    | LMG  | O6-C5-C4    | 4.26  | 117.37      | 109.70   |
| 23  | a     | 406[A] | CLA  | C3D-C4D-ND  | 4.25  | 116.90      | 109.99   |
| 23  | d     | 401[B] | CLA  | C3D-C4D-ND  | 4.25  | 116.90      | 109.99   |
| 23  | b     | 606    | CLA  | C3C-C4C-NC  | 4.25  | 115.88      | 110.43   |
| 23  | C     | 511    | CLA  | C3B-C2B-C1B | -4.25 | 102.16      | 107.17   |
| 23  | C     | 511    | CLA  | C4A-NA-C1A  | -4.25 | 104.74      | 106.68   |
| 23  | a     | 405[A] | CLA  | C1D-CHD-C4C | -4.25 | 116.98      | 126.02   |
| 23  | b     | 602    | CLA  | C3D-C2D-C1D | -4.25 | 100.03      | 105.83   |
| 23  | b     | 604    | CLA  | C4A-NA-C1A  | -4.25 | 104.74      | 106.68   |
| 23  | B     | 609    | CLA  | C3C-C4C-NC  | 4.25  | 115.87      | 110.43   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 509    | CLA  | C3C-C4C-NC  | 4.25  | 115.87      | 110.43   |
| 23  | c     | 504    | CLA  | C1D-CHD-C4C | -4.25 | 116.99      | 126.02   |
| 26  | f     | 102    | SQD  | C1-O5-C5    | 4.25  | 122.01      | 113.72   |
| 23  | c     | 510    | CLA  | C3D-C4D-ND  | 4.24  | 116.88      | 109.99   |
| 23  | D     | 702[A] | CLA  | C1-C2-C3    | -4.24 | 119.25      | 126.20   |
| 23  | A     | 405[A] | CLA  | C2B-C1B-NB  | 4.24  | 114.72      | 110.33   |
| 23  | C     | 511    | CLA  | C2B-C1B-NB  | 4.24  | 114.72      | 110.33   |
| 23  | A     | 408    | CLA  | CHD-C1D-ND  | -4.24 | 118.84      | 124.80   |
| 23  | a     | 405[A] | CLA  | C3B-C4B-NB  | 4.24  | 114.31      | 110.53   |
| 23  | B     | 608    | CLA  | CHD-C1D-ND  | -4.24 | 118.84      | 124.80   |
| 23  | b     | 604    | CLA  | C3D-C2D-C1D | -4.24 | 100.05      | 105.83   |
| 23  | C     | 503    | CLA  | C3D-C4D-ND  | 4.23  | 116.87      | 109.99   |
| 23  | A     | 405[A] | CLA  | C3D-C4D-ND  | 4.23  | 116.87      | 109.99   |
| 34  | c     | 501    | LMG  | O7-C10-C11  | 4.23  | 120.64      | 111.48   |
| 23  | b     | 612    | CLA  | C3D-C4D-ND  | 4.23  | 116.86      | 109.99   |
| 23  | D     | 703    | CLA  | C3D-C2D-C1D | -4.23 | 100.06      | 105.83   |
| 23  | a     | 406[B] | CLA  | C3B-C2B-C1B | -4.23 | 102.19      | 107.17   |
| 23  | B     | 607    | CLA  | C3D-C4D-ND  | 4.22  | 116.85      | 109.99   |
| 23  | a     | 406[A] | CLA  | C2B-C1B-NB  | 4.22  | 114.71      | 110.33   |
| 23  | c     | 509    | CLA  | C1C-C2C-C3C | -4.22 | 102.54      | 106.98   |
| 23  | c     | 504    | CLA  | CHD-C1D-ND  | -4.22 | 118.86      | 124.80   |
| 23  | b     | 614    | CLA  | C1-C2-C3    | -4.22 | 119.28      | 126.20   |
| 23  | A     | 406[B] | CLA  | C1C-C2C-C3C | -4.22 | 102.54      | 106.98   |
| 23  | C     | 508    | CLA  | CMB-C2B-C1B | 4.22  | 131.85      | 125.42   |
| 23  | B     | 605    | CLA  | C3D-C4D-ND  | 4.22  | 116.85      | 109.99   |
| 23  | b     | 610    | CLA  | O2A-CGA-CBA | 4.22  | 124.70      | 111.83   |
| 23  | b     | 612    | CLA  | C1-C2-C3    | -4.22 | 119.29      | 126.20   |
| 23  | B     | 609    | CLA  | CMB-C2B-C1B | 4.22  | 131.84      | 125.42   |
| 23  | b     | 610    | CLA  | C3C-C4C-NC  | 4.22  | 115.83      | 110.43   |
| 23  | c     | 508    | CLA  | CMC-C2C-C1C | 4.22  | 131.62      | 125.03   |
| 23  | B     | 612    | CLA  | C2C-C1C-NC  | 4.21  | 114.41      | 109.98   |
| 23  | A     | 404[A] | CLA  | CAA-C2A-C3A | -4.21 | 101.61      | 113.00   |
| 23  | A     | 405[A] | CLA  | CAA-C2A-C3A | -4.21 | 101.61      | 113.00   |
| 23  | b     | 612    | CLA  | C3B-C2B-C1B | -4.21 | 102.20      | 107.17   |
| 23  | A     | 408    | CLA  | O2D-CGD-CBD | 4.21  | 118.59      | 111.23   |
| 23  | D     | 703    | CLA  | C2C-C1C-NC  | 4.21  | 114.41      | 109.98   |
| 23  | c     | 505    | CLA  | C3D-C4D-ND  | 4.21  | 116.83      | 109.99   |
| 23  | B     | 609    | CLA  | O2D-CGD-CBD | 4.21  | 118.59      | 111.23   |
| 23  | a     | 405[B] | CLA  | CAA-C2A-C3A | -4.21 | 101.62      | 113.00   |
| 23  | D     | 702[B] | CLA  | CHD-C1D-ND  | -4.21 | 118.88      | 124.80   |
| 23  | b     | 614    | CLA  | C3C-C4C-NC  | 4.21  | 115.82      | 110.43   |
| 23  | c     | 502    | CLA  | O2D-CGD-O1D | -4.21 | 115.66      | 123.85   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 616    | CLA  | O2A-CGA-CBA | 4.21  | 124.66      | 111.83   |
| 23  | d     | 401[A] | CLA  | O2D-CGD-CBD | 4.20  | 118.58      | 111.23   |
| 25  | T     | 102    | BCR  | C15-C16-C17 | -4.20 | 114.92      | 123.52   |
| 23  | D     | 702[A] | CLA  | C3D-C4D-ND  | 4.20  | 116.82      | 109.99   |
| 23  | c     | 507    | CLA  | C2B-C1B-NB  | 4.20  | 114.68      | 110.33   |
| 23  | d     | 401[A] | CLA  | C3C-C4C-NC  | 4.19  | 115.80      | 110.43   |
| 23  | b     | 608    | CLA  | C3B-C4B-NB  | 4.19  | 114.27      | 110.53   |
| 23  | b     | 608    | CLA  | C1C-C2C-C3C | -4.19 | 102.57      | 106.98   |
| 23  | C     | 514    | CLA  | C3B-C4B-NB  | 4.19  | 114.27      | 110.53   |
| 23  | c     | 505    | CLA  | CHD-C1D-ND  | -4.19 | 118.91      | 124.80   |
| 23  | B     | 606    | CLA  | C3B-C2B-C1B | -4.19 | 102.23      | 107.17   |
| 23  | B     | 614    | CLA  | C1-C2-C3    | -4.19 | 119.34      | 126.20   |
| 23  | B     | 606    | CLA  | C2C-C1C-NC  | 4.18  | 114.38      | 109.98   |
| 23  | B     | 611    | CLA  | CHD-C4C-NC  | 4.18  | 130.72      | 124.23   |
| 23  | c     | 506    | CLA  | C3D-C2D-C1D | -4.18 | 100.13      | 105.83   |
| 23  | a     | 406[B] | CLA  | CAA-C2A-C3A | -4.18 | 101.71      | 113.00   |
| 23  | C     | 505    | CLA  | CHD-C1D-ND  | -4.18 | 118.92      | 124.80   |
| 23  | A     | 406[A] | CLA  | C1C-C2C-C3C | -4.18 | 102.59      | 106.98   |
| 23  | C     | 510    | CLA  | C3B-C4B-NB  | 4.18  | 114.26      | 110.53   |
| 23  | a     | 406[B] | CLA  | C4A-NA-C1A  | -4.17 | 104.78      | 106.68   |
| 25  | B     | 618    | BCR  | C29-C30-C25 | 4.17  | 116.50      | 110.44   |
| 23  | B     | 615    | CLA  | C3B-C2B-C1B | -4.17 | 102.25      | 107.17   |
| 23  | B     | 609    | CLA  | C2B-C1B-NB  | 4.17  | 114.65      | 110.33   |
| 23  | c     | 512    | CLA  | C3B-C4B-NB  | 4.17  | 114.25      | 110.53   |
| 23  | b     | 612    | CLA  | C4A-NA-C1A  | -4.17 | 104.78      | 106.68   |
| 23  | c     | 503    | CLA  | CMD-C2D-C1D | 4.17  | 132.07      | 124.73   |
| 23  | c     | 511    | CLA  | C1C-C2C-C3C | -4.17 | 102.60      | 106.98   |
| 26  | b     | 620    | SQD  | C1-O5-C5    | -4.16 | 105.59      | 113.72   |
| 23  | B     | 601    | CLA  | CHD-C1D-ND  | -4.16 | 118.94      | 124.80   |
| 23  | D     | 702[A] | CLA  | C1C-C2C-C3C | -4.16 | 102.60      | 106.98   |
| 23  | C     | 513    | CLA  | C3D-C4D-ND  | 4.16  | 116.75      | 109.99   |
| 23  | b     | 607    | CLA  | O2D-CGD-CBD | 4.16  | 118.50      | 111.23   |
| 23  | c     | 512    | CLA  | C2B-C1B-NB  | 4.16  | 114.64      | 110.33   |
| 23  | C     | 514    | CLA  | CHD-C1D-ND  | -4.16 | 118.95      | 124.80   |
| 23  | B     | 616    | CLA  | C3D-C4D-ND  | 4.15  | 116.74      | 109.99   |
| 26  | a     | 411[A] | SQD  | C1-C2-C3    | -4.15 | 101.27      | 110.01   |
| 35  | b     | 625    | HTG  | C1-O5-C5    | 4.15  | 120.01      | 112.56   |
| 23  | c     | 502    | CLA  | C4A-NA-C1A  | -4.15 | 104.78      | 106.68   |
| 23  | b     | 603    | CLA  | CAA-C2A-C3A | -4.15 | 101.79      | 113.00   |
| 23  | a     | 409    | CLA  | C1D-CHD-C4C | -4.15 | 117.20      | 126.02   |
| 23  | A     | 405[B] | CLA  | C3B-C2B-C1B | -4.14 | 102.28      | 107.17   |
| 23  | c     | 503    | CLA  | C1D-CHD-C4C | -4.14 | 117.22      | 126.02   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 610    | CLA  | CHD-C1D-ND  | -4.14 | 118.97      | 124.80   |
| 23  | a     | 407[B] | CLA  | CHD-C1D-ND  | -4.14 | 118.98      | 124.80   |
| 23  | B     | 603    | CLA  | C3D-C4D-ND  | 4.14  | 116.71      | 109.99   |
| 23  | B     | 613    | CLA  | O2D-CGD-CBD | 4.13  | 118.46      | 111.23   |
| 23  | B     | 608    | CLA  | O2D-CGD-O1D | -4.13 | 115.80      | 123.85   |
| 23  | B     | 610    | CLA  | C3B-C2B-C1B | -4.13 | 102.30      | 107.17   |
| 23  | c     | 504    | CLA  | C3C-C4C-NC  | 4.13  | 115.72      | 110.43   |
| 23  | B     | 601    | CLA  | C2C-C1C-NC  | 4.13  | 114.32      | 109.98   |
| 23  | B     | 607    | CLA  | O2D-CGD-O1D | -4.13 | 115.81      | 123.85   |
| 23  | c     | 514    | CLA  | C1D-CHD-C4C | -4.13 | 117.25      | 126.02   |
| 23  | C     | 505    | CLA  | C3D-C4D-ND  | 4.13  | 116.69      | 109.99   |
| 23  | a     | 405[B] | CLA  | C1D-CHD-C4C | -4.12 | 117.25      | 126.02   |
| 29  | d     | 404[A] | PL9  | C42-C43-C44 | -4.12 | 118.19      | 127.62   |
| 23  | C     | 509    | CLA  | C1C-C2C-C3C | -4.12 | 102.64      | 106.98   |
| 23  | C     | 507    | CLA  | C1-C2-C3    | -4.12 | 119.44      | 126.20   |
| 23  | C     | 505    | CLA  | C3C-C4C-NC  | 4.12  | 115.71      | 110.43   |
| 23  | B     | 606    | CLA  | C1D-CHD-C4C | -4.12 | 117.26      | 126.02   |
| 24  | A     | 407[B] | PHO  | C1A-C2A-C3A | -4.12 | 98.92       | 102.84   |
| 23  | B     | 602    | CLA  | C1C-C2C-C3C | -4.12 | 102.65      | 106.98   |
| 23  | B     | 613    | CLA  | C4A-NA-C1A  | -4.12 | 104.80      | 106.68   |
| 23  | C     | 513    | CLA  | C1D-CHD-C4C | -4.12 | 117.27      | 126.02   |
| 23  | C     | 502    | CLA  | C1D-CHD-C4C | -4.12 | 117.27      | 126.02   |
| 23  | b     | 608    | CLA  | C2B-C1B-NB  | 4.12  | 114.59      | 110.33   |
| 23  | C     | 512    | CLA  | C3D-C4D-ND  | 4.11  | 116.67      | 109.99   |
| 23  | d     | 401[A] | CLA  | C3D-C2D-C1D | -4.11 | 100.22      | 105.83   |
| 23  | B     | 615    | CLA  | CHD-C1D-ND  | -4.11 | 119.02      | 124.80   |
| 26  | a     | 411[A] | SQD  | C1-O5-C5    | -4.11 | 105.69      | 113.72   |
| 23  | A     | 408    | CLA  | C3C-C4C-NC  | 4.11  | 115.69      | 110.43   |
| 23  | C     | 513    | CLA  | C1-C2-C3    | -4.11 | 119.47      | 126.20   |
| 23  | b     | 603    | CLA  | C3C-C4C-NC  | 4.11  | 115.69      | 110.43   |
| 34  | c     | 521    | LMG  | O7-C10-C11  | 4.11  | 120.36      | 111.48   |
| 23  | c     | 508    | CLA  | C3D-C4D-ND  | 4.11  | 116.66      | 109.99   |
| 23  | B     | 604    | CLA  | C3D-C2D-C1D | -4.10 | 100.23      | 105.83   |
| 23  | d     | 401[B] | CLA  | C2B-C1B-NB  | 4.10  | 114.58      | 110.33   |
| 23  | D     | 703    | CLA  | CMB-C2B-C1B | 4.10  | 131.66      | 125.42   |
| 23  | d     | 401[A] | CLA  | C3B-C2B-C1B | -4.10 | 102.34      | 107.17   |
| 23  | b     | 608    | CLA  | C3B-C2B-C1B | -4.10 | 102.34      | 107.17   |
| 23  | c     | 513    | CLA  | C1-C2-C3    | -4.10 | 119.49      | 126.20   |
| 25  | D     | 704    | BCR  | C10-C11-C12 | -4.10 | 111.33      | 123.20   |
| 23  | b     | 616    | CLA  | C3C-C4C-NC  | 4.10  | 115.68      | 110.43   |
| 38  | F     | 102    | HEM  | CHD-C4C-NC  | 4.10  | 128.91      | 124.45   |
| 23  | a     | 406[A] | CLA  | C3B-C2B-C1B | -4.09 | 102.34      | 107.17   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 511    | CLA  | C3D-C4D-ND  | 4.09  | 116.64      | 109.99   |
| 23  | b     | 601    | CLA  | CHD-C1D-ND  | -4.09 | 119.04      | 124.80   |
| 23  | A     | 405[B] | CLA  | O2D-CGD-CBD | 4.09  | 118.38      | 111.23   |
| 23  | C     | 506    | CLA  | C2B-C1B-NB  | 4.09  | 114.57      | 110.33   |
| 34  | Z     | 101    | LMG  | O7-C10-C11  | 4.09  | 120.33      | 111.48   |
| 23  | A     | 406[A] | CLA  | CHD-C1D-ND  | -4.09 | 119.05      | 124.80   |
| 23  | c     | 503    | CLA  | O2D-CGD-O1D | -4.09 | 115.89      | 123.85   |
| 23  | B     | 608    | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 23  | a     | 405[B] | CLA  | O2D-CGD-CBD | 4.08  | 118.36      | 111.23   |
| 29  | a     | 414[A] | PL9  | C32-C33-C34 | -4.08 | 118.28      | 127.62   |
| 23  | b     | 609    | CLA  | C3C-C4C-NC  | 4.08  | 115.66      | 110.43   |
| 23  | C     | 510    | CLA  | C1C-C2C-C3C | -4.08 | 102.69      | 106.98   |
| 25  | c     | 515    | BCR  | C11-C10-C9  | -4.08 | 121.56      | 127.28   |
| 23  | b     | 608    | CLA  | C3D-C2D-C1D | -4.07 | 100.27      | 105.83   |
| 36  | C     | 517[A] | DGD  | O2G-C1B-C2B | 4.07  | 120.29      | 111.48   |
| 23  | A     | 404[B] | CLA  | C1C-C2C-C3C | -4.07 | 102.70      | 106.98   |
| 23  | B     | 615    | CLA  | C1C-C2C-C3C | -4.07 | 102.70      | 106.98   |
| 23  | c     | 507    | CLA  | C3B-C4B-NB  | 4.07  | 114.16      | 110.53   |
| 23  | B     | 602    | CLA  | C3C-C4C-NC  | 4.07  | 115.64      | 110.43   |
| 23  | A     | 404[B] | CLA  | CHD-C1D-ND  | -4.07 | 119.08      | 124.80   |
| 34  | C     | 521    | LMG  | O7-C10-C11  | 4.07  | 120.28      | 111.48   |
| 40  | V     | 201    | HEC  | CBC-CAC-C3C | -4.06 | 119.31      | 127.43   |
| 23  | a     | 405[B] | CLA  | CHD-C1D-ND  | -4.06 | 119.09      | 124.80   |
| 35  | C     | 522    | HTG  | C1'-S1-C1   | 4.06  | 109.21      | 100.45   |
| 23  | a     | 406[A] | CLA  | C1D-CHD-C4C | -4.05 | 117.41      | 126.02   |
| 23  | b     | 608    | CLA  | CMC-C2C-C1C | 4.05  | 131.37      | 125.03   |
| 23  | B     | 603    | CLA  | C3C-C4C-NC  | 4.05  | 115.62      | 110.43   |
| 23  | A     | 406[A] | CLA  | C3B-C2B-C1B | -4.05 | 102.39      | 107.17   |
| 34  | C     | 520    | LMG  | O7-C10-C11  | 4.05  | 120.24      | 111.48   |
| 23  | B     | 614    | CLA  | C3B-C4B-NB  | 4.05  | 114.14      | 110.53   |
| 23  | b     | 611    | CLA  | CHD-C1D-ND  | -4.04 | 119.11      | 124.80   |
| 23  | B     | 603    | CLA  | C3B-C4B-NB  | 4.04  | 114.14      | 110.53   |
| 23  | A     | 404[A] | CLA  | CHD-C1D-ND  | -4.04 | 119.11      | 124.80   |
| 23  | b     | 603    | CLA  | C1C-C2C-C3C | -4.04 | 102.73      | 106.98   |
| 23  | C     | 503    | CLA  | C1C-C2C-C3C | -4.04 | 102.73      | 106.98   |
| 23  | c     | 507    | CLA  | C1C-C2C-C3C | -4.04 | 102.73      | 106.98   |
| 23  | b     | 609    | CLA  | C1D-CHD-C4C | -4.04 | 117.44      | 126.02   |
| 23  | b     | 612    | CLA  | C1D-CHD-C4C | -4.04 | 117.44      | 126.02   |
| 29  | A     | 414[B] | PL9  | C7-C3-C2    | -4.03 | 118.64      | 123.39   |
| 23  | C     | 512    | CLA  | C1D-CHD-C4C | -4.03 | 117.45      | 126.02   |
| 23  | b     | 601    | CLA  | C1D-CHD-C4C | -4.03 | 117.45      | 126.02   |
| 34  | m     | 101    | LMG  | O7-C10-C11  | 4.02  | 120.19      | 111.48   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 514    | CLA  | C3C-C4C-NC  | 4.02  | 115.58      | 110.43   |
| 23  | c     | 510    | CLA  | C2B-C1B-NB  | 4.02  | 114.50      | 110.33   |
| 23  | B     | 609    | CLA  | CHD-C1D-ND  | -4.02 | 119.15      | 124.80   |
| 23  | B     | 615    | CLA  | C1D-CHD-C4C | -4.02 | 117.48      | 126.02   |
| 23  | D     | 702[B] | CLA  | C3C-C4C-NC  | 4.02  | 115.58      | 110.43   |
| 25  | C     | 515    | BCR  | C7-C8-C9    | -4.01 | 120.30      | 126.23   |
| 23  | b     | 603    | CLA  | O2D-CGD-O1D | -4.01 | 116.04      | 123.85   |
| 23  | d     | 401[B] | CLA  | C3B-C4B-NB  | 4.01  | 114.11      | 110.53   |
| 23  | C     | 505    | CLA  | C2B-C1B-NB  | 4.01  | 114.49      | 110.33   |
| 23  | A     | 405[A] | CLA  | C3B-C2B-C1B | -4.01 | 102.44      | 107.17   |
| 23  | C     | 506    | CLA  | C1D-CHD-C4C | -4.00 | 117.51      | 126.02   |
| 23  | a     | 406[A] | CLA  | CAA-C2A-C3A | -4.00 | 102.19      | 113.00   |
| 23  | C     | 511    | CLA  | C3B-C4B-NB  | 4.00  | 114.10      | 110.53   |
| 23  | D     | 702[B] | CLA  | C2B-C1B-NB  | 4.00  | 114.47      | 110.33   |
| 23  | B     | 605    | CLA  | CMB-C2B-C1B | 4.00  | 131.51      | 125.42   |
| 23  | B     | 612    | CLA  | C3D-C2D-C1D | -4.00 | 100.37      | 105.83   |
| 23  | C     | 509    | CLA  | C3B-C2B-C1B | -4.00 | 102.46      | 107.17   |
| 23  | B     | 606    | CLA  | C3D-C4D-ND  | 4.00  | 116.48      | 109.99   |
| 23  | c     | 511    | CLA  | CHD-C1D-ND  | -4.00 | 119.18      | 124.80   |
| 23  | B     | 603    | CLA  | C1D-CHD-C4C | -4.00 | 117.53      | 126.02   |
| 23  | B     | 614    | CLA  | C4A-NA-C1A  | -3.99 | 104.86      | 106.68   |
| 23  | C     | 507    | CLA  | C2B-C1B-NB  | 3.99  | 114.47      | 110.33   |
| 23  | c     | 503    | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 23  | D     | 703    | CLA  | CHD-C1D-ND  | -3.99 | 119.19      | 124.80   |
| 23  | B     | 602    | CLA  | CMC-C2C-C1C | 3.99  | 131.26      | 125.03   |
| 23  | B     | 614    | CLA  | C1D-CHD-C4C | -3.99 | 117.55      | 126.02   |
| 23  | B     | 613    | CLA  | C3D-C4D-ND  | 3.99  | 116.47      | 109.99   |
| 23  | C     | 512    | CLA  | C3C-C4C-NC  | 3.98  | 115.53      | 110.43   |
| 23  | b     | 606    | CLA  | C1D-CHD-C4C | -3.97 | 117.58      | 126.02   |
| 29  | A     | 414[B] | PL9  | C37-C38-C39 | -3.97 | 118.54      | 127.62   |
| 23  | B     | 611    | CLA  | CHD-C1D-ND  | -3.97 | 119.22      | 124.80   |
| 23  | C     | 508    | CLA  | O2D-CGD-O1D | -3.97 | 116.13      | 123.85   |
| 23  | C     | 504    | CLA  | C1D-CHD-C4C | -3.96 | 117.60      | 126.02   |
| 23  | C     | 511    | CLA  | C1C-C2C-C3C | -3.96 | 102.81      | 106.98   |
| 23  | C     | 513    | CLA  | C2C-C1C-NC  | 3.96  | 114.14      | 109.98   |
| 23  | b     | 614    | CLA  | O2D-CGD-O1D | -3.96 | 116.14      | 123.85   |
| 23  | C     | 508    | CLA  | C1D-CHD-C4C | -3.96 | 117.61      | 126.02   |
| 23  | c     | 507    | CLA  | C1-C2-C3    | -3.95 | 119.72      | 126.20   |
| 23  | B     | 607    | CLA  | C3B-C2B-C1B | -3.95 | 102.51      | 107.17   |
| 23  | B     | 606    | CLA  | C3C-C4C-NC  | 3.95  | 115.50      | 110.43   |
| 25  | t     | 102    | BCR  | C11-C10-C9  | -3.95 | 121.73      | 127.28   |
| 23  | C     | 508    | CLA  | C3D-C4D-ND  | 3.95  | 116.41      | 109.99   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 407[A] | CLA  | C1C-C2C-C3C | -3.95 | 102.83      | 106.98   |
| 23  | B     | 612    | CLA  | CAC-C3C-C4C | 3.95  | 129.93      | 124.79   |
| 23  | C     | 510    | CLA  | CHD-C1D-ND  | -3.95 | 119.25      | 124.80   |
| 23  | B     | 616    | CLA  | C4C-C3C-C2C | -3.94 | 101.15      | 106.89   |
| 23  | c     | 513    | CLA  | C2C-C1C-NC  | 3.94  | 114.12      | 109.98   |
| 23  | B     | 615    | CLA  | C3C-C4C-NC  | 3.94  | 115.48      | 110.43   |
| 29  | a     | 414[B] | PL9  | C7-C3-C2    | -3.94 | 118.74      | 123.39   |
| 23  | D     | 703    | CLA  | O2D-CGD-O1D | -3.94 | 116.18      | 123.85   |
| 23  | B     | 603    | CLA  | CHD-C1D-ND  | -3.93 | 119.27      | 124.80   |
| 23  | B     | 601    | CLA  | C1D-CHD-C4C | -3.93 | 117.66      | 126.02   |
| 33  | A     | 419[A] | LHG  | O8-C23-O10  | -3.93 | 113.79      | 123.63   |
| 23  | b     | 616    | CLA  | C3D-C4D-ND  | 3.93  | 116.38      | 109.99   |
| 25  | T     | 102    | BCR  | C11-C10-C9  | -3.93 | 121.77      | 127.28   |
| 23  | c     | 509    | CLA  | C1-C2-C3    | -3.93 | 119.76      | 126.20   |
| 23  | b     | 614    | CLA  | CHD-C1D-ND  | -3.92 | 119.28      | 124.80   |
| 23  | B     | 603    | CLA  | O2D-CGD-O1D | -3.92 | 116.21      | 123.85   |
| 25  | c     | 515    | BCR  | C15-C14-C13 | -3.92 | 121.78      | 127.28   |
| 34  | c     | 520    | LMG  | O7-C10-C11  | 3.92  | 119.97      | 111.48   |
| 23  | A     | 408    | CLA  | C3B-C4B-NB  | 3.92  | 114.03      | 110.53   |
| 23  | B     | 614    | CLA  | C1C-C2C-C3C | -3.92 | 102.86      | 106.98   |
| 25  | k     | 101    | BCR  | C29-C30-C25 | 3.92  | 116.13      | 110.44   |
| 23  | a     | 407[B] | CLA  | C1C-C2C-C3C | -3.91 | 102.86      | 106.98   |
| 23  | C     | 509    | CLA  | C3D-C4D-ND  | 3.91  | 116.35      | 109.99   |
| 23  | B     | 610    | CLA  | C3B-C4B-NB  | 3.91  | 114.02      | 110.53   |
| 23  | b     | 606    | CLA  | C1C-C2C-C3C | -3.91 | 102.87      | 106.98   |
| 23  | A     | 404[B] | CLA  | C3B-C4B-NB  | 3.91  | 114.02      | 110.53   |
| 23  | c     | 509    | CLA  | C3D-C4D-ND  | 3.90  | 116.33      | 109.99   |
| 23  | B     | 606    | CLA  | C2B-C1B-NB  | 3.90  | 114.37      | 110.33   |
| 23  | C     | 503    | CLA  | CHD-C1D-ND  | -3.90 | 119.32      | 124.80   |
| 23  | B     | 607    | CLA  | C3B-C4B-NB  | 3.89  | 114.01      | 110.53   |
| 23  | b     | 608    | CLA  | C1D-CHD-C4C | -3.89 | 117.74      | 126.02   |
| 23  | B     | 603    | CLA  | CAA-C2A-C3A | -3.89 | 102.48      | 113.00   |
| 23  | C     | 507    | CLA  | CAC-C3C-C4C | 3.89  | 129.85      | 124.79   |
| 23  | C     | 506    | CLA  | C3D-C2D-C1D | -3.89 | 100.52      | 105.83   |
| 23  | b     | 609    | CLA  | C3B-C2B-C1B | -3.89 | 102.58      | 107.17   |
| 23  | b     | 604    | CLA  | C2B-C1B-NB  | 3.89  | 114.36      | 110.33   |
| 23  | D     | 702[A] | CLA  | C3C-C4C-NC  | 3.89  | 115.41      | 110.43   |
| 23  | c     | 510    | CLA  | C1C-C2C-C3C | -3.89 | 102.89      | 106.98   |
| 23  | b     | 615    | CLA  | C3C-C4C-NC  | 3.88  | 115.41      | 110.43   |
| 23  | c     | 510    | CLA  | C1D-CHD-C4C | -3.88 | 117.78      | 126.02   |
| 36  | c     | 517[A] | DGD  | O2G-C1B-C2B | 3.88  | 119.87      | 111.48   |
| 23  | d     | 401[A] | CLA  | CHD-C1D-ND  | -3.88 | 119.35      | 124.80   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 32  | B     | 627    | LMT  | C1'-O5'-C5' | -3.88 | 106.15      | 113.72   |
| 23  | B     | 607    | CLA  | C3C-C4C-NC  | 3.88  | 115.40      | 110.43   |
| 23  | A     | 405[B] | CLA  | C1D-CHD-C4C | -3.88 | 117.78      | 126.02   |
| 23  | b     | 612    | CLA  | C3B-C4B-NB  | 3.87  | 113.99      | 110.53   |
| 23  | B     | 604    | CLA  | C1D-CHD-C4C | -3.87 | 117.79      | 126.02   |
| 23  | a     | 409    | CLA  | O2D-CGD-O1D | -3.87 | 116.32      | 123.85   |
| 24  | A     | 407[A] | PHO  | C1A-C2A-C3A | -3.87 | 99.16       | 102.84   |
| 23  | B     | 607    | CLA  | CHD-C1D-ND  | -3.87 | 119.36      | 124.80   |
| 23  | B     | 610    | CLA  | CMB-C2B-C1B | 3.87  | 131.31      | 125.42   |
| 23  | B     | 604    | CLA  | C1C-C2C-C3C | -3.87 | 102.91      | 106.98   |
| 23  | b     | 610    | CLA  | C1D-CHD-C4C | -3.87 | 117.80      | 126.02   |
| 23  | D     | 703    | CLA  | C1D-CHD-C4C | -3.86 | 117.81      | 126.02   |
| 23  | c     | 513    | CLA  | C1D-CHD-C4C | -3.86 | 117.81      | 126.02   |
| 23  | b     | 614    | CLA  | C1C-C2C-C3C | -3.86 | 102.92      | 106.98   |
| 23  | A     | 405[A] | CLA  | CHD-C1D-ND  | -3.86 | 119.37      | 124.80   |
| 23  | b     | 615    | CLA  | C1C-C2C-C3C | -3.86 | 102.92      | 106.98   |
| 23  | A     | 404[A] | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 23  | C     | 502    | CLA  | CHD-C1D-ND  | -3.85 | 119.38      | 124.80   |
| 23  | C     | 512    | CLA  | O2D-CGD-O1D | -3.85 | 116.35      | 123.85   |
| 23  | C     | 514    | CLA  | C1C-C2C-C3C | -3.85 | 102.93      | 106.98   |
| 23  | d     | 401[A] | CLA  | C1-C2-C3    | -3.85 | 119.89      | 126.20   |
| 23  | B     | 615    | CLA  | C2B-C1B-NB  | 3.85  | 114.32      | 110.33   |
| 23  | c     | 503    | CLA  | C4A-NA-C1A  | -3.85 | 104.92      | 106.68   |
| 35  | V     | 202    | HTG  | C1-O5-C5    | 3.84  | 117.34      | 112.19   |
| 29  | A     | 414[A] | PL9  | C37-C38-C39 | -3.84 | 118.82      | 127.62   |
| 23  | b     | 614    | CLA  | C1D-CHD-C4C | -3.84 | 117.85      | 126.02   |
| 23  | B     | 604    | CLA  | C3B-C4B-NB  | 3.84  | 113.96      | 110.53   |
| 23  | c     | 509    | CLA  | C3C-C4C-NC  | 3.84  | 115.35      | 110.43   |
| 23  | b     | 612    | CLA  | C1C-C2C-C3C | -3.84 | 102.95      | 106.98   |
| 23  | c     | 512    | CLA  | C1C-C2C-C3C | -3.84 | 102.95      | 106.98   |
| 23  | c     | 513    | CLA  | CHD-C1D-ND  | -3.84 | 119.41      | 124.80   |
| 23  | d     | 402    | CLA  | C2C-C1C-NC  | 3.84  | 114.01      | 109.98   |
| 23  | b     | 603    | CLA  | CHD-C1D-ND  | -3.83 | 119.41      | 124.80   |
| 23  | a     | 407[A] | CLA  | C3C-C4C-NC  | 3.83  | 115.34      | 110.43   |
| 23  | C     | 511    | CLA  | C1D-CHD-C4C | -3.83 | 117.88      | 126.02   |
| 23  | b     | 612    | CLA  | C3D-C2D-C1D | -3.83 | 100.60      | 105.83   |
| 23  | A     | 405[A] | CLA  | CBC-CAC-C3C | -3.83 | 102.04      | 112.42   |
| 23  | C     | 504    | CLA  | C2C-C1C-NC  | 3.83  | 114.00      | 109.98   |
| 23  | A     | 408    | CLA  | C1D-CHD-C4C | -3.83 | 117.89      | 126.02   |
| 23  | A     | 405[B] | CLA  | CBC-CAC-C3C | -3.83 | 102.05      | 112.42   |
| 23  | B     | 602    | CLA  | CHD-C1D-ND  | -3.82 | 119.42      | 124.80   |
| 23  | b     | 610    | CLA  | CHD-C1D-ND  | -3.82 | 119.43      | 124.80   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 611    | CLA  | O2D-CGD-O1D | -3.82 | 116.41      | 123.85   |
| 25  | D     | 704    | BCR  | C38-C26-C25 | -3.82 | 120.32      | 124.48   |
| 23  | b     | 605    | CLA  | C3C-C4C-NC  | 3.82  | 115.32      | 110.43   |
| 29  | A     | 414[B] | PL9  | C22-C23-C24 | -3.82 | 118.88      | 127.62   |
| 29  | A     | 414[A] | PL9  | C7-C3-C4    | 3.82  | 120.05      | 116.91   |
| 23  | b     | 604    | CLA  | C3C-C4C-NC  | 3.82  | 115.32      | 110.43   |
| 23  | b     | 609    | CLA  | C2B-C1B-NB  | 3.82  | 114.28      | 110.33   |
| 23  | a     | 406[B] | CLA  | CHD-C1D-ND  | -3.82 | 119.43      | 124.80   |
| 23  | B     | 612    | CLA  | O2D-CGD-O1D | -3.81 | 116.42      | 123.85   |
| 23  | B     | 604    | CLA  | C2B-C1B-NB  | 3.81  | 114.28      | 110.33   |
| 23  | B     | 605    | CLA  | C4-C3-C5    | 3.81  | 121.84      | 115.23   |
| 36  | C     | 518[B] | DGD  | O2G-C1B-C2B | 3.81  | 119.72      | 111.48   |
| 23  | b     | 602    | CLA  | CMC-C2C-C1C | 3.81  | 130.99      | 125.03   |
| 23  | B     | 604    | CLA  | C3D-C4D-ND  | 3.81  | 116.18      | 109.99   |
| 25  | b     | 617    | BCR  | C33-C5-C6   | -3.81 | 120.33      | 124.48   |
| 23  | b     | 602    | CLA  | C1D-CHD-C4C | -3.80 | 117.93      | 126.02   |
| 36  | C     | 517[B] | DGD  | O2G-C1B-C2B | 3.80  | 119.71      | 111.48   |
| 23  | B     | 616    | CLA  | C3B-C4B-NB  | 3.80  | 113.92      | 110.53   |
| 23  | b     | 605    | CLA  | C1D-CHD-C4C | -3.80 | 117.94      | 126.02   |
| 24  | A     | 417[A] | PHO  | C1A-C2A-C3A | -3.80 | 99.22       | 102.84   |
| 23  | a     | 406[A] | CLA  | CHD-C1D-ND  | -3.80 | 119.46      | 124.80   |
| 25  | D     | 704    | BCR  | C16-C17-C18 | -3.80 | 121.95      | 127.28   |
| 33  | A     | 419[A] | LHG  | O7-C7-C8    | 3.80  | 119.69      | 111.48   |
| 23  | B     | 606    | CLA  | C1C-C2C-C3C | -3.79 | 102.99      | 106.98   |
| 23  | C     | 508    | CLA  | C2B-C1B-NB  | 3.79  | 114.26      | 110.33   |
| 23  | C     | 508    | CLA  | CHD-C1D-ND  | -3.79 | 119.47      | 124.80   |
| 23  | B     | 609    | CLA  | C1C-C2C-C3C | -3.79 | 103.00      | 106.98   |
| 23  | A     | 404[B] | CLA  | C3C-C4C-NC  | 3.79  | 115.28      | 110.43   |
| 23  | A     | 405[A] | CLA  | CMC-C2C-C1C | 3.79  | 130.95      | 125.03   |
| 23  | d     | 401[B] | CLA  | C1D-CHD-C4C | -3.79 | 117.97      | 126.02   |
| 23  | c     | 506    | CLA  | CHD-C1D-ND  | -3.78 | 119.48      | 124.80   |
| 34  | Z     | 101    | LMG  | C1-C2-C3    | 3.78  | 117.97      | 110.01   |
| 23  | C     | 510    | CLA  | C3C-C4C-NC  | 3.78  | 115.27      | 110.43   |
| 29  | A     | 414[B] | PL9  | C7-C3-C4    | 3.78  | 120.02      | 116.91   |
| 23  | C     | 510    | CLA  | CAC-C3C-C4C | 3.77  | 129.70      | 124.79   |
| 23  | b     | 613    | CLA  | C2B-C1B-NB  | 3.77  | 114.24      | 110.33   |
| 23  | a     | 406[A] | CLA  | CMB-C2B-C1B | 3.77  | 131.16      | 125.42   |
| 23  | A     | 406[A] | CLA  | C1D-CHD-C4C | -3.77 | 118.01      | 126.02   |
| 23  | A     | 404[B] | CLA  | O2D-CGD-CBD | 3.77  | 117.81      | 111.23   |
| 23  | B     | 605    | CLA  | C2B-C1B-NB  | 3.76  | 114.23      | 110.33   |
| 23  | D     | 702[A] | CLA  | C3B-C4B-NB  | 3.76  | 113.89      | 110.53   |
| 23  | b     | 604    | CLA  | CMC-C2C-C1C | 3.76  | 130.91      | 125.03   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 612    | CLA  | C2B-C1B-NB  | 3.76  | 114.22      | 110.33   |
| 23  | A     | 408    | CLA  | C1C-C2C-C3C | -3.76 | 103.03      | 106.98   |
| 23  | C     | 503    | CLA  | C2B-C1B-NB  | 3.76  | 114.22      | 110.33   |
| 23  | B     | 610    | CLA  | CAA-CBA-CGA | -3.76 | 102.54      | 113.21   |
| 23  | C     | 505    | CLA  | O2D-CGD-O1D | -3.75 | 116.55      | 123.85   |
| 26  | X     | 101    | SQD  | C1-C2-C3    | -3.75 | 102.12      | 110.01   |
| 23  | D     | 703    | CLA  | C3C-C4C-NC  | 3.75  | 115.23      | 110.43   |
| 23  | C     | 506    | CLA  | C1-C2-C3    | -3.75 | 120.06      | 126.20   |
| 33  | L     | 101[B] | LHG  | O7-C7-C8    | 3.75  | 119.58      | 111.48   |
| 23  | d     | 401[B] | CLA  | CHD-C1D-ND  | -3.74 | 119.53      | 124.80   |
| 25  | d     | 403    | BCR  | C40-C30-C25 | -3.74 | 104.37      | 110.24   |
| 25  | C     | 515    | BCR  | C33-C5-C6   | -3.74 | 120.40      | 124.48   |
| 26  | A     | 410[A] | SQD  | O47-C7-C8   | 3.74  | 119.56      | 111.48   |
| 23  | C     | 503    | CLA  | C3C-C4C-NC  | 3.73  | 115.21      | 110.43   |
| 35  | b     | 622    | HTG  | O2-C2-C1    | 3.73  | 116.93      | 110.30   |
| 23  | B     | 602    | CLA  | O2D-CGD-O1D | -3.73 | 116.58      | 123.85   |
| 26  | A     | 412    | SQD  | O47-C7-C8   | 3.73  | 119.55      | 111.48   |
| 26  | A     | 410[B] | SQD  | C44-O6-C1   | -3.73 | 105.80      | 113.80   |
| 25  | d     | 403    | BCR  | C38-C26-C25 | -3.73 | 120.42      | 124.48   |
| 23  | B     | 601    | CLA  | C3C-C4C-NC  | 3.72  | 115.20      | 110.43   |
| 23  | d     | 402    | CLA  | C3C-C4C-NC  | 3.72  | 115.20      | 110.43   |
| 23  | b     | 604    | CLA  | O2D-CGD-O1D | -3.72 | 116.61      | 123.85   |
| 34  | c     | 521    | LMG  | C3-C4-C5    | 3.72  | 116.97      | 110.23   |
| 23  | b     | 602    | CLA  | C3C-C4C-NC  | 3.72  | 115.19      | 110.43   |
| 23  | B     | 611    | CLA  | O2D-CGD-O1D | -3.71 | 116.62      | 123.85   |
| 23  | a     | 405[A] | CLA  | O2A-CGA-O1A | -3.71 | 114.34      | 123.63   |
| 29  | a     | 414[A] | PL9  | C27-C28-C29 | -3.71 | 119.13      | 127.62   |
| 23  | a     | 409    | CLA  | C1C-C2C-C3C | -3.71 | 103.08      | 106.98   |
| 25  | B     | 617    | BCR  | C33-C5-C6   | -3.71 | 120.44      | 124.48   |
| 25  | B     | 619    | BCR  | C24-C23-C22 | -3.71 | 120.75      | 126.23   |
| 23  | d     | 401[A] | CLA  | C3B-C4B-NB  | 3.71  | 113.84      | 110.53   |
| 23  | b     | 609    | CLA  | CHD-C1D-ND  | -3.71 | 119.59      | 124.80   |
| 23  | B     | 616    | CLA  | C1D-CHD-C4C | -3.70 | 118.14      | 126.02   |
| 25  | C     | 516    | BCR  | C7-C8-C9    | -3.70 | 120.75      | 126.23   |
| 23  | C     | 511    | CLA  | C4-C3-C5    | 3.70  | 121.66      | 115.23   |
| 23  | a     | 405[A] | CLA  | CHD-C1D-ND  | -3.70 | 119.59      | 124.80   |
| 23  | D     | 702[A] | CLA  | C2B-C1B-NB  | 3.70  | 114.17      | 110.33   |
| 23  | C     | 509    | CLA  | C4A-NA-C1A  | -3.70 | 104.99      | 106.68   |
| 23  | C     | 509    | CLA  | O2D-CGD-O1D | -3.70 | 116.65      | 123.85   |
| 33  | b     | 629[B] | LHG  | O7-C7-C8    | 3.70  | 119.48      | 111.48   |
| 36  | C     | 518[A] | DGD  | O2G-C1B-C2B | 3.69  | 119.46      | 111.48   |
| 23  | b     | 608    | CLA  | C4B-C3B-C2B | -3.69 | 102.71      | 107.30   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26  | X     | 101    | SQD  | O8-S-C6     | 3.69  | 113.09      | 105.97   |
| 23  | C     | 513    | CLA  | CHD-C1D-ND  | -3.69 | 119.61      | 124.80   |
| 23  | d     | 401[B] | CLA  | C3C-C4C-NC  | 3.69  | 115.15      | 110.43   |
| 23  | B     | 602    | CLA  | C1D-CHD-C4C | -3.69 | 118.19      | 126.02   |
| 23  | b     | 607    | CLA  | C1C-C2C-C3C | -3.68 | 103.11      | 106.98   |
| 29  | A     | 414[A] | PL9  | C22-C23-C24 | -3.68 | 119.19      | 127.62   |
| 23  | c     | 512    | CLA  | CHD-C1D-ND  | -3.68 | 119.62      | 124.80   |
| 23  | b     | 615    | CLA  | O2D-CGD-CBD | 3.68  | 117.67      | 111.23   |
| 33  | L     | 101[A] | LHG  | O7-C7-C8    | 3.68  | 119.43      | 111.48   |
| 23  | C     | 503    | CLA  | C1D-CHD-C4C | -3.67 | 118.21      | 126.02   |
| 23  | b     | 612    | CLA  | O2D-CGD-O1D | -3.67 | 116.70      | 123.85   |
| 23  | C     | 509    | CLA  | C1D-CHD-C4C | -3.67 | 118.21      | 126.02   |
| 23  | c     | 514    | CLA  | C3C-C4C-NC  | 3.67  | 115.13      | 110.43   |
| 23  | C     | 504    | CLA  | C4-C3-C5    | 3.67  | 121.59      | 115.23   |
| 24  | a     | 416[A] | PHO  | C4-C3-C5    | 3.67  | 121.59      | 115.23   |
| 23  | c     | 508    | CLA  | C2B-C1B-NB  | 3.67  | 114.13      | 110.33   |
| 36  | c     | 517[B] | DGD  | O2G-C1B-C2B | 3.67  | 119.41      | 111.48   |
| 23  | a     | 409    | CLA  | CMC-C2C-C1C | 3.67  | 130.76      | 125.03   |
| 23  | A     | 406[A] | CLA  | C3C-C4C-NC  | 3.67  | 115.13      | 110.43   |
| 25  | K     | 102    | BCR  | C7-C8-C9    | -3.67 | 120.81      | 126.23   |
| 23  | C     | 507    | CLA  | C3B-C4B-NB  | 3.67  | 113.80      | 110.53   |
| 23  | B     | 612    | CLA  | CHD-C1D-ND  | -3.66 | 119.65      | 124.80   |
| 23  | a     | 406[A] | CLA  | C3C-C4C-NC  | 3.66  | 115.12      | 110.43   |
| 23  | A     | 406[B] | CLA  | O2D-CGD-O1D | -3.66 | 116.72      | 123.85   |
| 23  | c     | 508    | CLA  | O2D-CGD-O1D | -3.66 | 116.72      | 123.85   |
| 23  | b     | 602    | CLA  | O2D-CGD-O1D | -3.66 | 116.73      | 123.85   |
| 23  | b     | 611    | CLA  | C3C-C4C-NC  | 3.66  | 115.11      | 110.43   |
| 23  | A     | 405[A] | CLA  | C1D-CHD-C4C | -3.65 | 118.25      | 126.02   |
| 23  | b     | 609    | CLA  | CAC-C3C-C4C | 3.65  | 129.54      | 124.79   |
| 25  | h     | 101    | BCR  | C38-C26-C25 | -3.65 | 120.50      | 124.48   |
| 23  | c     | 505    | CLA  | C1C-C2C-C3C | -3.65 | 103.14      | 106.98   |
| 26  | A     | 410[B] | SQD  | O47-C7-C8   | 3.65  | 119.38      | 111.48   |
| 23  | C     | 503    | CLA  | C3B-C4B-NB  | 3.65  | 113.79      | 110.53   |
| 23  | c     | 512    | CLA  | C4A-NA-C1A  | -3.65 | 105.01      | 106.68   |
| 23  | b     | 613    | CLA  | C1D-CHD-C4C | -3.65 | 118.26      | 126.02   |
| 23  | b     | 602    | CLA  | C1-C2-C3    | -3.65 | 120.22      | 126.20   |
| 23  | c     | 505    | CLA  | C3C-C4C-NC  | 3.65  | 115.10      | 110.43   |
| 29  | a     | 414[A] | PL9  | C15-C14-C16 | 3.65  | 121.56      | 115.23   |
| 23  | b     | 612    | CLA  | C4-C3-C5    | 3.65  | 121.56      | 115.23   |
| 33  | d     | 412[B] | LHG  | O8-C23-C24  | 3.65  | 122.95      | 111.83   |
| 23  | A     | 406[A] | CLA  | CMB-C2B-C1B | 3.64  | 130.97      | 125.42   |
| 23  | c     | 512    | CLA  | O2D-CGD-O1D | -3.64 | 116.76      | 123.85   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 608    | CLA  | CAC-C3C-C4C | 3.64  | 129.53      | 124.79   |
| 23  | B     | 611    | CLA  | C1-C2-C3    | -3.64 | 120.23      | 126.20   |
| 23  | c     | 510    | CLA  | C4B-C3B-C2B | -3.64 | 102.77      | 107.30   |
| 23  | B     | 609    | CLA  | CBC-CAC-C3C | -3.64 | 102.55      | 112.42   |
| 23  | C     | 509    | CLA  | C4B-C3B-C2B | -3.64 | 102.78      | 107.30   |
| 23  | c     | 506    | CLA  | C1-C2-C3    | -3.64 | 120.23      | 126.20   |
| 29  | D     | 705[A] | PL9  | C42-C43-C44 | -3.64 | 119.29      | 127.62   |
| 23  | B     | 610    | CLA  | C1C-C2C-C3C | -3.64 | 103.16      | 106.98   |
| 38  | F     | 102    | HEM  | C1B-NB-C4B  | 3.64  | 109.51      | 105.21   |
| 23  | b     | 601    | CLA  | C1C-C2C-C3C | -3.63 | 103.16      | 106.98   |
| 23  | b     | 616    | CLA  | C2C-C1C-NC  | 3.63  | 113.80      | 109.98   |
| 23  | c     | 505    | CLA  | C1D-CHD-C4C | -3.63 | 118.31      | 126.02   |
| 23  | B     | 613    | CLA  | CAC-C3C-C4C | 3.63  | 129.51      | 124.79   |
| 32  | B     | 627    | LMT  | C4B-C3B-C2B | 3.63  | 117.20      | 110.83   |
| 26  | B     | 620    | SQD  | C3-C4-C5    | 3.63  | 116.81      | 110.23   |
| 23  | b     | 615    | CLA  | CHD-C1D-ND  | -3.62 | 119.70      | 124.80   |
| 23  | C     | 512    | CLA  | C1C-C2C-C3C | -3.62 | 103.17      | 106.98   |
| 26  | X     | 101    | SQD  | C44-O6-C1   | -3.62 | 106.03      | 113.80   |
| 23  | b     | 616    | CLA  | CMB-C2B-C1B | 3.62  | 130.93      | 125.42   |
| 23  | C     | 512    | CLA  | C3B-C4B-NB  | 3.62  | 113.76      | 110.53   |
| 23  | b     | 613    | CLA  | C3D-C4D-ND  | 3.61  | 115.86      | 109.99   |
| 23  | B     | 609    | CLA  | C3B-C2B-C1B | -3.61 | 102.91      | 107.17   |
| 23  | c     | 510    | CLA  | CHD-C1D-ND  | -3.61 | 119.72      | 124.80   |
| 23  | c     | 511    | CLA  | C1D-CHD-C4C | -3.61 | 118.34      | 126.02   |
| 23  | A     | 404[A] | CLA  | O2D-CGD-CBD | 3.61  | 117.54      | 111.23   |
| 23  | C     | 504    | CLA  | C1-C2-C3    | -3.61 | 120.28      | 126.20   |
| 29  | a     | 414[B] | PL9  | C15-C14-C16 | 3.61  | 121.49      | 115.23   |
| 23  | A     | 404[A] | CLA  | O2A-CGA-CBA | 3.61  | 122.83      | 111.83   |
| 23  | A     | 405[A] | CLA  | O2D-CGD-O1D | -3.61 | 116.83      | 123.85   |
| 29  | a     | 414[B] | PL9  | C27-C28-C29 | -3.60 | 119.38      | 127.62   |
| 25  | D     | 704    | BCR  | C29-C30-C25 | 3.60  | 115.67      | 110.44   |
| 25  | T     | 102    | BCR  | C12-C13-C14 | -3.60 | 113.34      | 119.01   |
| 23  | a     | 406[B] | CLA  | C3B-C4B-NB  | 3.60  | 113.74      | 110.53   |
| 23  | B     | 612    | CLA  | C4C-C3C-C2C | -3.59 | 101.66      | 106.89   |
| 23  | c     | 502    | CLA  | C1C-C2C-C3C | -3.59 | 103.20      | 106.98   |
| 23  | C     | 504    | CLA  | C3C-C4C-NC  | 3.59  | 115.03      | 110.43   |
| 23  | B     | 608    | CLA  | C3B-C4B-NB  | 3.59  | 113.74      | 110.53   |
| 26  | a     | 411[A] | SQD  | C44-O6-C1   | -3.59 | 106.09      | 113.80   |
| 25  | c     | 516    | BCR  | C7-C8-C9    | -3.59 | 120.92      | 126.23   |
| 23  | d     | 401[A] | CLA  | O2A-CGA-CBA | 3.59  | 122.77      | 111.83   |
| 23  | c     | 508    | CLA  | C3C-C4C-NC  | 3.59  | 115.02      | 110.43   |
| 23  | B     | 613    | CLA  | CHD-C1D-ND  | -3.58 | 119.77      | 124.80   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 404[B] | CLA  | O2A-CGA-CBA | 3.58  | 122.75      | 111.83   |
| 23  | B     | 610    | CLA  | C3C-C4C-NC  | 3.58  | 115.01      | 110.43   |
| 23  | B     | 606    | CLA  | O2D-CGD-O1D | -3.57 | 116.89      | 123.85   |
| 23  | B     | 610    | CLA  | O2D-CGD-O1D | -3.57 | 116.89      | 123.85   |
| 23  | c     | 510    | CLA  | CAC-C3C-C4C | 3.57  | 129.44      | 124.79   |
| 23  | d     | 401[A] | CLA  | C2B-C1B-NB  | 3.57  | 114.03      | 110.33   |
| 23  | B     | 603    | CLA  | C4B-C3B-C2B | -3.57 | 102.86      | 107.30   |
| 23  | a     | 405[A] | CLA  | C3C-C4C-NC  | 3.57  | 115.00      | 110.43   |
| 23  | b     | 604    | CLA  | C1D-CHD-C4C | -3.57 | 118.43      | 126.02   |
| 29  | D     | 705[B] | PL9  | C10-C9-C11  | 3.57  | 121.42      | 115.23   |
| 23  | A     | 404[A] | CLA  | C3C-C4C-NC  | 3.57  | 115.00      | 110.43   |
| 23  | B     | 611    | CLA  | CHB-C4A-NA  | 3.56  | 129.54      | 124.40   |
| 23  | C     | 502    | CLA  | C3C-C4C-NC  | 3.56  | 115.00      | 110.43   |
| 23  | B     | 615    | CLA  | C3B-C4B-NB  | 3.56  | 113.71      | 110.53   |
| 23  | A     | 405[B] | CLA  | CAA-C2A-C3A | -3.56 | 103.38      | 113.00   |
| 23  | A     | 406[B] | CLA  | CBC-CAC-C3C | -3.56 | 102.77      | 112.42   |
| 23  | c     | 511    | CLA  | C3C-C4C-NC  | 3.56  | 114.99      | 110.43   |
| 23  | C     | 512    | CLA  | CHD-C1D-ND  | -3.56 | 119.80      | 124.80   |
| 23  | B     | 608    | CLA  | C1C-C2C-C3C | -3.56 | 103.24      | 106.98   |
| 23  | c     | 506    | CLA  | C4C-C3C-C2C | -3.56 | 101.72      | 106.89   |
| 23  | C     | 514    | CLA  | C1D-CHD-C4C | -3.55 | 118.47      | 126.02   |
| 23  | b     | 616    | CLA  | O2A-CGA-O1A | -3.55 | 114.75      | 123.63   |
| 23  | a     | 405[A] | CLA  | O2D-CGD-CBD | 3.55  | 117.43      | 111.23   |
| 23  | b     | 608    | CLA  | CHD-C1D-ND  | -3.54 | 119.81      | 124.80   |
| 23  | b     | 604    | CLA  | C4B-C3B-C2B | -3.54 | 102.89      | 107.30   |
| 23  | A     | 404[A] | CLA  | C1D-CHD-C4C | -3.54 | 118.49      | 126.02   |
| 23  | B     | 612    | CLA  | C1D-CHD-C4C | -3.54 | 118.49      | 126.02   |
| 23  | c     | 512    | CLA  | C3C-C4C-NC  | 3.54  | 114.97      | 110.43   |
| 23  | b     | 608    | CLA  | CAC-C3C-C4C | 3.54  | 129.40      | 124.79   |
| 23  | a     | 405[A] | CLA  | O2A-CGA-CBA | 3.54  | 122.61      | 111.83   |
| 33  | A     | 419[B] | LHG  | O7-C7-C8    | 3.53  | 119.12      | 111.48   |
| 23  | b     | 603    | CLA  | C3B-C4B-NB  | 3.53  | 113.68      | 110.53   |
| 29  | a     | 414[B] | PL9  | C7-C3-C4    | 3.53  | 119.81      | 116.91   |
| 23  | a     | 407[A] | CLA  | C1D-CHD-C4C | -3.53 | 118.53      | 126.02   |
| 23  | C     | 502    | CLA  | CAC-C3C-C4C | 3.52  | 129.37      | 124.79   |
| 23  | c     | 513    | CLA  | CMB-C2B-C1B | 3.52  | 130.78      | 125.42   |
| 23  | a     | 407[B] | CLA  | C1D-CHD-C4C | -3.52 | 118.53      | 126.02   |
| 24  | A     | 417[A] | PHO  | C4D-CHA-CBD | 3.52  | 110.14      | 108.45   |
| 23  | b     | 610    | CLA  | O2A-CGA-O1A | -3.52 | 114.83      | 123.63   |
| 23  | C     | 506    | CLA  | C4C-C3C-C2C | -3.51 | 101.78      | 106.89   |
| 23  | C     | 508    | CLA  | C4C-C3C-C2C | -3.51 | 101.78      | 106.89   |
| 29  | a     | 414[B] | PL9  | C37-C38-C39 | -3.51 | 119.58      | 127.62   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 407[B] | CLA  | C3C-C4C-NC  | 3.51  | 114.93      | 110.43   |
| 23  | c     | 514    | CLA  | C1C-C2C-C3C | -3.51 | 103.29      | 106.98   |
| 24  | a     | 408[B] | PHO  | C1A-C2A-C3A | -3.51 | 99.50       | 102.84   |
| 25  | d     | 403    | BCR  | C16-C17-C18 | -3.51 | 122.35      | 127.28   |
| 23  | B     | 613    | CLA  | O2A-CGA-O1A | -3.51 | 114.85      | 123.63   |
| 23  | b     | 604    | CLA  | CHD-C1D-ND  | -3.51 | 119.86      | 124.80   |
| 23  | B     | 614    | CLA  | CMC-C2C-C1C | 3.51  | 130.52      | 125.03   |
| 23  | A     | 405[B] | CLA  | CHD-C4C-NC  | 3.51  | 129.67      | 124.23   |
| 23  | A     | 406[A] | CLA  | O2A-CGA-O1A | -3.51 | 114.85      | 123.63   |
| 23  | c     | 509    | CLA  | C1D-CHD-C4C | -3.51 | 118.57      | 126.02   |
| 23  | b     | 613    | CLA  | C3B-C4B-NB  | 3.50  | 113.66      | 110.53   |
| 23  | b     | 616    | CLA  | CHD-C4C-NC  | 3.50  | 129.66      | 124.23   |
| 23  | b     | 604    | CLA  | C3D-C4D-ND  | 3.50  | 115.68      | 109.99   |
| 23  | B     | 611    | CLA  | C4C-C3C-C2C | -3.50 | 101.80      | 106.89   |
| 24  | a     | 408[B] | PHO  | CMA-C3A-C4A | -3.50 | 107.07      | 114.61   |
| 23  | B     | 605    | CLA  | CHD-C1D-ND  | -3.50 | 119.88      | 124.80   |
| 23  | a     | 409    | CLA  | CHD-C1D-ND  | -3.49 | 119.89      | 124.80   |
| 23  | b     | 611    | CLA  | C1-C2-C3    | -3.49 | 120.47      | 126.20   |
| 23  | B     | 603    | CLA  | C1C-C2C-C3C | -3.49 | 103.31      | 106.98   |
| 23  | B     | 612    | CLA  | C1-C2-C3    | -3.49 | 120.47      | 126.20   |
| 23  | C     | 512    | CLA  | C4-C3-C5    | 3.49  | 121.29      | 115.23   |
| 23  | B     | 612    | CLA  | C4A-NA-C1A  | -3.49 | 105.09      | 106.68   |
| 23  | B     | 605    | CLA  | C1-C2-C3    | -3.49 | 120.48      | 126.20   |
| 23  | d     | 401[B] | CLA  | C1-C2-C3    | -3.49 | 120.48      | 126.20   |
| 23  | C     | 506    | CLA  | CAC-C3C-C4C | 3.49  | 129.33      | 124.79   |
| 23  | B     | 605    | CLA  | O2D-CGD-O1D | -3.49 | 117.06      | 123.85   |
| 25  | H     | 101    | BCR  | C16-C17-C18 | -3.49 | 122.39      | 127.28   |
| 23  | b     | 605    | CLA  | C1C-C2C-C3C | -3.48 | 103.31      | 106.98   |
| 23  | A     | 405[A] | CLA  | C3C-C4C-NC  | 3.48  | 114.89      | 110.43   |
| 23  | C     | 507    | CLA  | O2D-CGD-O1D | -3.48 | 117.07      | 123.85   |
| 24  | A     | 407[A] | PHO  | CMA-C3A-C4A | -3.48 | 107.11      | 114.61   |
| 33  | A     | 419[B] | LHG  | C5-O7-C7    | -3.48 | 109.47      | 117.80   |
| 23  | d     | 402    | CLA  | C1C-C2C-C3C | -3.48 | 103.32      | 106.98   |
| 23  | B     | 616    | CLA  | CHD-C1D-ND  | -3.48 | 119.91      | 124.80   |
| 23  | c     | 508    | CLA  | CMB-C2B-C1B | 3.47  | 130.71      | 125.42   |
| 23  | B     | 615    | CLA  | CMC-C2C-C1C | 3.47  | 130.46      | 125.03   |
| 26  | A     | 410[A] | SQD  | C44-O6-C1   | -3.47 | 106.36      | 113.80   |
| 23  | b     | 602    | CLA  | CAA-C2A-C3A | -3.47 | 103.62      | 113.00   |
| 23  | a     | 406[B] | CLA  | CHD-C4C-NC  | 3.47  | 129.61      | 124.23   |
| 23  | b     | 607    | CLA  | C4C-C3C-C2C | -3.47 | 101.84      | 106.89   |
| 26  | a     | 412    | SQD  | O47-C7-C8   | 3.47  | 118.98      | 111.48   |
| 29  | d     | 404[B] | PL9  | C7-C8-C9    | -3.47 | 120.86      | 126.83   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 610    | CLA  | C4C-C3C-C2C | -3.47 | 101.84      | 106.89   |
| 29  | A     | 414[B] | PL9  | C15-C14-C16 | 3.47  | 121.24      | 115.23   |
| 23  | b     | 614    | CLA  | C3B-C4B-NB  | 3.46  | 113.62      | 110.53   |
| 40  | V     | 201    | HEC  | C4D-ND-C1D  | 3.46  | 111.47      | 105.82   |
| 23  | c     | 502    | CLA  | C3C-C4C-NC  | 3.46  | 114.86      | 110.43   |
| 29  | d     | 404[A] | PL9  | C40-C39-C41 | 3.46  | 121.23      | 115.23   |
| 23  | b     | 611    | CLA  | C1D-CHD-C4C | -3.46 | 118.67      | 126.02   |
| 23  | c     | 510    | CLA  | CHC-C1C-C2C | -3.46 | 117.12      | 126.95   |
| 23  | B     | 607    | CLA  | C4B-C3B-C2B | -3.46 | 103.00      | 107.30   |
| 23  | C     | 502    | CLA  | C1C-C2C-C3C | -3.46 | 103.34      | 106.98   |
| 23  | B     | 607    | CLA  | O2A-CGA-O1A | -3.46 | 114.98      | 123.63   |
| 23  | a     | 406[B] | CLA  | C3C-C4C-NC  | 3.46  | 114.86      | 110.43   |
| 23  | B     | 610    | CLA  | C1D-CHD-C4C | -3.45 | 118.68      | 126.02   |
| 23  | c     | 511    | CLA  | CMC-C2C-C1C | 3.45  | 130.43      | 125.03   |
| 23  | B     | 604    | CLA  | C4C-C3C-C2C | -3.45 | 101.87      | 106.89   |
| 29  | d     | 404[B] | PL9  | C42-C43-C44 | -3.45 | 119.73      | 127.62   |
| 40  | V     | 201    | HEC  | CBD-CAD-C3D | -3.45 | 103.00      | 112.53   |
| 23  | C     | 507    | CLA  | C3C-C4C-NC  | 3.44  | 114.84      | 110.43   |
| 23  | d     | 402    | CLA  | C1D-CHD-C4C | -3.44 | 118.70      | 126.02   |
| 23  | D     | 702[B] | CLA  | CAA-C2A-C3A | -3.44 | 103.70      | 113.00   |
| 23  | C     | 509    | CLA  | C2B-C1B-NB  | 3.44  | 113.89      | 110.33   |
| 23  | c     | 514    | CLA  | C3B-C4B-NB  | 3.44  | 113.60      | 110.53   |
| 23  | B     | 612    | CLA  | C2B-C1B-NB  | 3.44  | 113.89      | 110.33   |
| 23  | C     | 508    | CLA  | C1C-C2C-C3C | -3.44 | 103.36      | 106.98   |
| 23  | B     | 606    | CLA  | CHD-C4C-NC  | 3.44  | 129.56      | 124.23   |
| 23  | c     | 509    | CLA  | CHD-C1D-ND  | -3.44 | 119.96      | 124.80   |
| 23  | B     | 613    | CLA  | O2A-CGA-CBA | 3.44  | 122.32      | 111.83   |
| 34  | B     | 621    | LMG  | O8-C28-C29  | 3.44  | 122.31      | 111.83   |
| 26  | a     | 411[B] | SQD  | C1-O5-C5    | -3.44 | 107.01      | 113.72   |
| 23  | b     | 616    | CLA  | CHD-C1D-ND  | -3.44 | 119.97      | 124.80   |
| 23  | b     | 612    | CLA  | C4B-C3B-C2B | -3.44 | 103.03      | 107.30   |
| 23  | C     | 510    | CLA  | C1D-CHD-C4C | -3.44 | 118.72      | 126.02   |
| 23  | B     | 609    | CLA  | C1D-CHD-C4C | -3.43 | 118.72      | 126.02   |
| 23  | B     | 608    | CLA  | C4C-C3C-C2C | -3.43 | 101.90      | 106.89   |
| 23  | A     | 406[A] | CLA  | C3B-C4B-NB  | 3.43  | 113.59      | 110.53   |
| 23  | a     | 406[B] | CLA  | CMB-C2B-C1B | 3.43  | 130.64      | 125.42   |
| 23  | c     | 507    | CLA  | C1D-CHD-C4C | -3.43 | 118.74      | 126.02   |
| 29  | A     | 414[A] | PL9  | C15-C14-C16 | 3.43  | 121.18      | 115.23   |
| 23  | b     | 605    | CLA  | CHD-C4C-NC  | 3.43  | 129.54      | 124.23   |
| 23  | b     | 607    | CLA  | C2B-C1B-NB  | 3.43  | 113.88      | 110.33   |
| 32  | A     | 418    | LMT  | O5B-C5B-C4B | 3.43  | 115.87      | 109.70   |
| 23  | D     | 703    | CLA  | C1C-C2C-C3C | -3.42 | 103.38      | 106.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 607    | CLA  | C3B-C4B-NB  | 3.42  | 113.59      | 110.53   |
| 23  | A     | 406[B] | CLA  | CAA-C2A-C3A | -3.42 | 103.75      | 113.00   |
| 23  | b     | 610    | CLA  | C1C-C2C-C3C | -3.42 | 103.38      | 106.98   |
| 23  | b     | 616    | CLA  | C4C-C3C-C2C | -3.42 | 101.91      | 106.89   |
| 23  | c     | 506    | CLA  | C1D-CHD-C4C | -3.42 | 118.75      | 126.02   |
| 23  | B     | 614    | CLA  | O2A-CGA-O1A | -3.42 | 115.08      | 123.63   |
| 23  | B     | 605    | CLA  | C4C-C3C-C2C | -3.42 | 101.92      | 106.89   |
| 23  | B     | 615    | CLA  | O2D-CGD-CBD | 3.41  | 117.20      | 111.23   |
| 36  | h     | 102    | DGD  | O2G-C1B-C2B | 3.41  | 118.86      | 111.48   |
| 23  | C     | 510    | CLA  | CMC-C2C-C1C | 3.41  | 130.37      | 125.03   |
| 34  | Z     | 101    | LMG  | O6-C1-C2    | 3.41  | 117.38      | 110.37   |
| 23  | B     | 602    | CLA  | CAA-C2A-C3A | -3.41 | 103.78      | 113.00   |
| 23  | b     | 603    | CLA  | C2A-C1A-CHA | -3.41 | 117.95      | 123.87   |
| 23  | B     | 614    | CLA  | CAC-C3C-C4C | 3.41  | 129.22      | 124.79   |
| 23  | b     | 611    | CLA  | C1C-C2C-C3C | -3.41 | 103.40      | 106.98   |
| 23  | b     | 606    | CLA  | O2D-CGD-O1D | -3.40 | 117.22      | 123.85   |
| 23  | b     | 601    | CLA  | C3C-C4C-NC  | 3.40  | 114.79      | 110.43   |
| 23  | b     | 608    | CLA  | C3C-C4C-NC  | 3.40  | 114.79      | 110.43   |
| 23  | c     | 502    | CLA  | CAC-C3C-C4C | 3.40  | 129.22      | 124.79   |
| 34  | C     | 521    | LMG  | C3-C4-C5    | 3.40  | 116.40      | 110.23   |
| 34  | c     | 521    | LMG  | C9-C8-C7    | -3.40 | 103.86      | 111.78   |
| 29  | a     | 414[A] | PL9  | C30-C29-C31 | 3.40  | 121.13      | 115.23   |
| 25  | D     | 704    | BCR  | C28-C27-C26 | -3.40 | 108.00      | 114.06   |
| 29  | A     | 414[B] | PL9  | C27-C28-C29 | -3.40 | 119.85      | 127.62   |
| 23  | a     | 407[A] | CLA  | C1-C2-C3    | -3.39 | 120.64      | 126.20   |
| 23  | b     | 604    | CLA  | CAC-C3C-C4C | 3.39  | 129.20      | 124.79   |
| 23  | b     | 614    | CLA  | O2A-CGA-O1A | -3.39 | 115.14      | 123.63   |
| 23  | b     | 601    | CLA  | O2D-CGD-O1D | -3.39 | 117.25      | 123.85   |
| 23  | B     | 609    | CLA  | CMC-C2C-C1C | 3.39  | 130.32      | 125.03   |
| 23  | B     | 610    | CLA  | C4B-C3B-C2B | -3.39 | 103.09      | 107.30   |
| 23  | C     | 511    | CLA  | C4B-C3B-C2B | -3.38 | 103.09      | 107.30   |
| 35  | o     | 301    | HTG  | O5-C1-C2    | 3.38  | 114.98      | 110.32   |
| 23  | b     | 612    | CLA  | C4C-C3C-C2C | -3.38 | 101.97      | 106.89   |
| 23  | c     | 511    | CLA  | C3B-C4B-NB  | 3.38  | 113.55      | 110.53   |
| 23  | c     | 503    | CLA  | CHC-C1C-C2C | -3.38 | 117.34      | 126.95   |
| 25  | K     | 102    | BCR  | C38-C26-C25 | -3.38 | 120.80      | 124.48   |
| 23  | A     | 405[A] | CLA  | C4B-C3B-C2B | -3.38 | 103.10      | 107.30   |
| 33  | d     | 412[B] | LHG  | O7-C7-C8    | 3.38  | 118.78      | 111.48   |
| 23  | A     | 408    | CLA  | CAA-C2A-C3A | -3.37 | 103.88      | 113.00   |
| 23  | a     | 409    | CLA  | C3B-C4B-NB  | 3.37  | 113.54      | 110.53   |
| 23  | b     | 602    | CLA  | C2C-C1C-NC  | 3.37  | 113.52      | 109.98   |
| 38  | f     | 101    | HEM  | CHA-C4D-ND  | 3.37  | 128.53      | 124.37   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 36  | c     | 518[A] | DGD  | O2G-C1B-C2B | 3.37  | 118.77      | 111.48   |
| 23  | a     | 405[A] | CLA  | C4B-C3B-C2B | -3.37 | 103.11      | 107.30   |
| 26  | a     | 412    | SQD  | O48-C23-C24 | 3.37  | 122.10      | 111.83   |
| 23  | b     | 615    | CLA  | C3B-C4B-NB  | 3.36  | 113.53      | 110.53   |
| 23  | B     | 613    | CLA  | C4-C3-C5    | 3.36  | 121.07      | 115.23   |
| 23  | c     | 506    | CLA  | CMB-C2B-C1B | 3.36  | 130.54      | 125.42   |
| 23  | B     | 613    | CLA  | C1D-CHD-C4C | -3.36 | 118.87      | 126.02   |
| 23  | C     | 511    | CLA  | C3C-C4C-NC  | 3.36  | 114.74      | 110.43   |
| 23  | d     | 401[A] | CLA  | C1D-CHD-C4C | -3.36 | 118.87      | 126.02   |
| 23  | C     | 505    | CLA  | C3B-C4B-NB  | 3.36  | 113.53      | 110.53   |
| 35  | B     | 624    | HTG  | C1'-S1-C1   | 3.36  | 107.70      | 100.45   |
| 23  | B     | 605    | CLA  | CHD-C4C-NC  | 3.36  | 129.44      | 124.23   |
| 23  | C     | 506    | CLA  | CHD-C1D-ND  | -3.36 | 120.08      | 124.80   |
| 32  | b     | 627    | LMT  | C3'-C4'-C5' | -3.36 | 103.49      | 110.93   |
| 29  | D     | 705[A] | PL9  | C53-C6-C1   | 3.35  | 122.15      | 115.28   |
| 23  | B     | 611    | CLA  | C2A-C1A-CHA | -3.34 | 118.07      | 123.87   |
| 23  | B     | 613    | CLA  | C4C-C3C-C2C | -3.34 | 102.03      | 106.89   |
| 36  | c     | 518[B] | DGD  | O2G-C1B-C2B | 3.34  | 118.71      | 111.48   |
| 33  | d     | 412[A] | LHG  | O8-C23-O10  | -3.34 | 115.27      | 123.63   |
| 23  | c     | 510    | CLA  | O2A-CGA-CBA | 3.34  | 122.02      | 111.83   |
| 23  | A     | 406[B] | CLA  | C3B-C4B-NB  | 3.34  | 113.51      | 110.53   |
| 25  | A     | 409    | BCR  | C11-C10-C9  | -3.34 | 122.59      | 127.28   |
| 23  | c     | 504    | CLA  | CMB-C2B-C1B | 3.34  | 130.50      | 125.42   |
| 23  | c     | 507    | CLA  | C4B-C3B-C2B | -3.34 | 103.15      | 107.30   |
| 23  | A     | 405[A] | CLA  | C3B-C4B-NB  | 3.34  | 113.51      | 110.53   |
| 25  | T     | 102    | BCR  | C16-C17-C18 | -3.34 | 122.60      | 127.28   |
| 23  | a     | 405[A] | CLA  | C1-C2-C3    | -3.34 | 120.73      | 126.20   |
| 23  | c     | 510    | CLA  | C3C-C4C-NC  | 3.34  | 114.70      | 110.43   |
| 23  | c     | 506    | CLA  | C1C-C2C-C3C | -3.34 | 103.47      | 106.98   |
| 23  | C     | 506    | CLA  | C3B-C4B-NB  | 3.34  | 113.51      | 110.53   |
| 23  | B     | 604    | CLA  | O2A-CGA-O1A | -3.34 | 115.28      | 123.63   |
| 29  | a     | 414[A] | PL9  | C17-C18-C19 | -3.34 | 119.99      | 127.62   |
| 33  | d     | 412[A] | LHG  | O8-C23-C24  | 3.33  | 122.00      | 111.83   |
| 38  | F     | 102    | HEM  | CBD-CAD-C3D | -3.33 | 103.31      | 112.53   |
| 23  | A     | 406[A] | CLA  | C4B-C3B-C2B | -3.33 | 103.16      | 107.30   |
| 23  | b     | 604    | CLA  | CMB-C2B-C1B | 3.33  | 130.49      | 125.42   |
| 29  | a     | 414[A] | PL9  | C35-C34-C36 | 3.33  | 121.01      | 115.23   |
| 29  | A     | 414[A] | PL9  | C27-C28-C29 | -3.33 | 120.01      | 127.62   |
| 23  | c     | 514    | CLA  | CAC-C3C-C4C | 3.33  | 129.12      | 124.79   |
| 23  | B     | 605    | CLA  | O2A-CGA-O1A | -3.33 | 115.31      | 123.63   |
| 23  | A     | 405[B] | CLA  | C4B-C3B-C2B | -3.33 | 103.17      | 107.30   |
| 23  | C     | 513    | CLA  | C4C-C3C-C2C | -3.33 | 102.05      | 106.89   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 613    | CLA  | CHD-C1D-ND  | -3.32 | 120.13      | 124.80   |
| 23  | b     | 615    | CLA  | CMB-C2B-C1B | 3.32  | 130.47      | 125.42   |
| 33  | D     | 707[B] | LHG  | O7-C7-C8    | 3.32  | 118.66      | 111.48   |
| 33  | A     | 419[B] | LHG  | O8-C23-O10  | -3.32 | 115.32      | 123.63   |
| 23  | c     | 502    | CLA  | C1D-CHD-C4C | -3.32 | 118.97      | 126.02   |
| 23  | B     | 601    | CLA  | C1C-C2C-C3C | -3.32 | 103.49      | 106.98   |
| 23  | A     | 406[B] | CLA  | CMB-C2B-C1B | 3.31  | 130.47      | 125.42   |
| 23  | c     | 513    | CLA  | O2A-CGA-CBA | 3.31  | 121.94      | 111.83   |
| 29  | D     | 705[A] | PL9  | C25-C24-C26 | 3.31  | 120.97      | 115.23   |
| 29  | A     | 414[B] | PL9  | C17-C18-C19 | -3.31 | 120.06      | 127.62   |
| 23  | b     | 609    | CLA  | CMC-C2C-C1C | 3.31  | 130.20      | 125.03   |
| 23  | a     | 405[B] | CLA  | O2A-CGA-CBA | 3.31  | 121.91      | 111.83   |
| 23  | c     | 506    | CLA  | O2D-CGD-O1D | -3.31 | 117.41      | 123.85   |
| 23  | b     | 613    | CLA  | O2A-CGA-O1A | -3.31 | 115.36      | 123.63   |
| 23  | C     | 514    | CLA  | C1-C2-C3    | -3.30 | 120.78      | 126.20   |
| 23  | B     | 603    | CLA  | C4C-C3C-C2C | -3.30 | 102.08      | 106.89   |
| 23  | c     | 512    | CLA  | CHD-C4C-NC  | 3.30  | 129.35      | 124.23   |
| 23  | A     | 406[B] | CLA  | C1D-CHD-C4C | -3.30 | 119.00      | 126.02   |
| 34  | z     | 101    | LMG  | O7-C10-C11  | 3.30  | 118.62      | 111.48   |
| 25  | t     | 102    | BCR  | C28-C27-C26 | -3.30 | 108.17      | 114.06   |
| 23  | c     | 508    | CLA  | C4-C3-C5    | 3.30  | 120.95      | 115.23   |
| 23  | c     | 504    | CLA  | C1C-C2C-C3C | -3.30 | 103.51      | 106.98   |
| 23  | B     | 609    | CLA  | O2A-CGA-CBA | 3.30  | 121.89      | 111.83   |
| 23  | c     | 513    | CLA  | C3C-C4C-NC  | 3.30  | 114.65      | 110.43   |
| 23  | B     | 607    | CLA  | C4-C3-C5    | 3.30  | 120.95      | 115.23   |
| 23  | b     | 606    | CLA  | CHD-C4C-NC  | 3.30  | 129.34      | 124.23   |
| 23  | B     | 614    | CLA  | C3C-C4C-NC  | 3.30  | 114.65      | 110.43   |
| 29  | D     | 705[A] | PL9  | C17-C18-C19 | -3.30 | 120.08      | 127.62   |
| 38  | f     | 101    | HEM  | CHD-C1D-ND  | 3.29  | 127.97      | 124.42   |
| 23  | b     | 602    | CLA  | CHD-C4C-NC  | 3.29  | 129.34      | 124.23   |
| 23  | b     | 614    | CLA  | CMB-C2B-C1B | 3.29  | 130.43      | 125.42   |
| 23  | A     | 404[A] | CLA  | C1-C2-C3    | -3.29 | 120.81      | 126.20   |
| 33  | d     | 406[A] | LHG  | O7-C7-C8    | 3.29  | 118.59      | 111.48   |
| 25  | Y     | 101    | BCR  | C15-C14-C13 | -3.29 | 122.67      | 127.28   |
| 23  | C     | 507    | CLA  | CBC-CAC-C3C | -3.29 | 103.51      | 112.42   |
| 29  | a     | 414[B] | PL9  | C25-C24-C26 | 3.29  | 120.93      | 115.23   |
| 25  | T     | 102    | BCR  | C33-C5-C6   | -3.29 | 120.90      | 124.48   |
| 23  | c     | 513    | CLA  | C1C-C2C-C3C | -3.28 | 103.53      | 106.98   |
| 23  | c     | 503    | CLA  | C1-C2-C3    | -3.28 | 120.82      | 126.20   |
| 23  | C     | 504    | CLA  | CHD-C4C-NC  | 3.28  | 129.32      | 124.23   |
| 23  | c     | 507    | CLA  | CHC-C1C-C2C | -3.28 | 117.63      | 126.95   |
| 23  | B     | 603    | CLA  | CAC-C3C-C4C | 3.28  | 129.05      | 124.79   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | a     | 406[B] | CLA  | C4B-C3B-C2B | -3.27 | 103.23      | 107.30   |
| 23  | d     | 401[A] | CLA  | C4B-C3B-C2B | -3.27 | 103.23      | 107.30   |
| 23  | B     | 615    | CLA  | CED-O2D-CGD | 3.27  | 123.34      | 115.92   |
| 23  | B     | 614    | CLA  | O2A-CGA-CBA | 3.27  | 121.81      | 111.83   |
| 23  | d     | 402    | CLA  | CAA-C2A-C3A | -3.27 | 104.16      | 113.00   |
| 25  | Y     | 101    | BCR  | C16-C17-C18 | -3.27 | 122.69      | 127.28   |
| 23  | C     | 507    | CLA  | CHC-C1C-C2C | -3.27 | 117.66      | 126.95   |
| 23  | d     | 401[B] | CLA  | O2A-CGA-CBA | 3.27  | 121.80      | 111.83   |
| 23  | C     | 511    | CLA  | CHD-C4C-NC  | 3.27  | 129.30      | 124.23   |
| 23  | B     | 607    | CLA  | C2B-C1B-NB  | 3.27  | 113.71      | 110.33   |
| 23  | b     | 609    | CLA  | CBC-CAC-C3C | -3.27 | 103.57      | 112.42   |
| 23  | A     | 405[B] | CLA  | C3B-C4B-NB  | 3.27  | 113.44      | 110.53   |
| 33  | A     | 419[A] | LHG  | O8-C23-C24  | 3.26  | 121.79      | 111.83   |
| 23  | A     | 408    | CLA  | C4C-C3C-C2C | -3.26 | 102.14      | 106.89   |
| 23  | C     | 513    | CLA  | C1C-C2C-C3C | -3.26 | 103.55      | 106.98   |
| 34  | c     | 520    | LMG  | O1-C7-C8    | -3.26 | 102.88      | 110.82   |
| 23  | B     | 609    | CLA  | C4B-C3B-C2B | -3.26 | 103.25      | 107.30   |
| 23  | B     | 612    | CLA  | CMC-C2C-C1C | 3.26  | 130.13      | 125.03   |
| 23  | B     | 614    | CLA  | CHD-C4C-NC  | 3.26  | 129.28      | 124.23   |
| 23  | B     | 608    | CLA  | C1D-CHD-C4C | -3.26 | 119.09      | 126.02   |
| 23  | A     | 406[B] | CLA  | C3C-C4C-NC  | 3.26  | 114.60      | 110.43   |
| 23  | b     | 606    | CLA  | C3B-C4B-NB  | 3.26  | 113.44      | 110.53   |
| 23  | a     | 405[B] | CLA  | CAA-C2A-C1A | -3.26 | 101.30      | 111.97   |
| 23  | b     | 611    | CLA  | C4C-C3C-C2C | -3.26 | 102.15      | 106.89   |
| 23  | c     | 507    | CLA  | C3C-C4C-NC  | 3.26  | 114.60      | 110.43   |
| 23  | B     | 616    | CLA  | C1-O2A-CGA  | 3.26  | 124.53      | 116.65   |
| 23  | D     | 702[B] | CLA  | O2A-CGA-CBA | 3.25  | 121.76      | 111.83   |
| 23  | b     | 616    | CLA  | CBC-CAC-C3C | -3.25 | 103.60      | 112.42   |
| 34  | C     | 521    | LMG  | O8-C28-C29  | 3.25  | 121.74      | 111.83   |
| 34  | m     | 101    | LMG  | O8-C28-C29  | 3.25  | 121.74      | 111.83   |
| 23  | c     | 513    | CLA  | C4-C3-C5    | 3.25  | 120.86      | 115.23   |
| 23  | a     | 405[B] | CLA  | C3C-C4C-NC  | 3.25  | 114.59      | 110.43   |
| 23  | B     | 604    | CLA  | CAC-C3C-C4C | 3.25  | 129.01      | 124.79   |
| 33  | d     | 412[A] | LHG  | O7-C7-C8    | 3.24  | 118.50      | 111.48   |
| 23  | c     | 507    | CLA  | O2D-CGD-O1D | -3.24 | 117.53      | 123.85   |
| 33  | A     | 419[A] | LHG  | C5-O7-C7    | -3.24 | 110.03      | 117.80   |
| 23  | c     | 509    | CLA  | C3B-C4B-NB  | 3.24  | 113.42      | 110.53   |
| 23  | a     | 405[B] | CLA  | CHC-C1C-C2C | -3.24 | 117.73      | 126.95   |
| 23  | C     | 510    | CLA  | O2A-CGA-CBA | 3.24  | 121.71      | 111.83   |
| 25  | d     | 403    | BCR  | C21-C20-C19 | -3.24 | 113.82      | 123.20   |
| 23  | C     | 509    | CLA  | C4C-C3C-C2C | -3.24 | 102.18      | 106.89   |
| 23  | b     | 613    | CLA  | C4A-NA-C1A  | -3.24 | 105.20      | 106.68   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 613    | CLA  | C1C-C2C-C3C | -3.24 | 103.58      | 106.98   |
| 24  | A     | 407[A] | PHO  | O1D-CGD-CBD | -3.24 | 119.81      | 124.72   |
| 23  | a     | 406[A] | CLA  | C3B-C4B-NB  | 3.24  | 113.42      | 110.53   |
| 23  | D     | 702[B] | CLA  | C1D-CHD-C4C | -3.23 | 119.15      | 126.02   |
| 23  | c     | 511    | CLA  | C4-C3-C5    | 3.23  | 120.84      | 115.23   |
| 23  | C     | 507    | CLA  | C4B-C3B-C2B | -3.23 | 103.28      | 107.30   |
| 23  | d     | 402    | CLA  | CMB-C2B-C1B | 3.23  | 130.34      | 125.42   |
| 26  | B     | 620    | SQD  | O7-S-C6     | 3.23  | 111.58      | 106.76   |
| 25  | c     | 515    | BCR  | C16-C17-C18 | -3.23 | 122.75      | 127.28   |
| 25  | T     | 102    | BCR  | C15-C14-C13 | 3.23  | 131.81      | 127.28   |
| 23  | b     | 605    | CLA  | C1-C2-C3    | -3.23 | 120.90      | 126.20   |
| 23  | d     | 401[B] | CLA  | O2D-CGD-O1D | -3.23 | 117.56      | 123.85   |
| 23  | C     | 507    | CLA  | CMC-C2C-C1C | 3.23  | 130.08      | 125.03   |
| 34  | C     | 520    | LMG  | O8-C28-C29  | 3.23  | 121.68      | 111.83   |
| 23  | B     | 612    | CLA  | O2A-CGA-CBA | 3.23  | 121.67      | 111.83   |
| 23  | c     | 511    | CLA  | CHD-C4C-NC  | 3.22  | 129.23      | 124.23   |
| 24  | a     | 416[A] | PHO  | C4A-C3A-C2A | -3.22 | 99.77       | 102.84   |
| 23  | B     | 613    | CLA  | C4B-C3B-C2B | -3.22 | 103.30      | 107.30   |
| 23  | b     | 603    | CLA  | CMA-C3A-C2A | -3.22 | 101.54      | 113.98   |
| 23  | B     | 610    | CLA  | C4C-C3C-C2C | -3.22 | 102.21      | 106.89   |
| 23  | C     | 505    | CLA  | C1D-CHD-C4C | -3.22 | 119.18      | 126.02   |
| 29  | a     | 414[B] | PL9  | C30-C29-C31 | 3.22  | 120.81      | 115.23   |
| 23  | B     | 605    | CLA  | C1C-C2C-C3C | -3.22 | 103.60      | 106.98   |
| 38  | f     | 101    | HEM  | CHB-C1B-NB  | 3.21  | 128.34      | 124.37   |
| 23  | d     | 402    | CLA  | CHD-C4C-NC  | 3.21  | 129.22      | 124.23   |
| 23  | A     | 404[A] | CLA  | O2A-CGA-O1A | -3.21 | 115.59      | 123.63   |
| 29  | D     | 705[B] | PL9  | C25-C24-C26 | 3.21  | 120.80      | 115.23   |
| 23  | b     | 602    | CLA  | C1C-C2C-C3C | -3.21 | 103.61      | 106.98   |
| 23  | B     | 606    | CLA  | O2A-CGA-CBA | 3.21  | 121.61      | 111.83   |
| 23  | c     | 504    | CLA  | O2D-CGD-O1D | -3.20 | 117.61      | 123.85   |
| 25  | A     | 409    | BCR  | C24-C23-C22 | -3.20 | 121.50      | 126.23   |
| 25  | T     | 102    | BCR  | C7-C8-C9    | -3.20 | 121.50      | 126.23   |
| 23  | b     | 608    | CLA  | C1-C2-C3    | -3.20 | 120.95      | 126.20   |
| 23  | c     | 504    | CLA  | C1-C2-C3    | -3.20 | 120.95      | 126.20   |
| 23  | C     | 514    | CLA  | CMC-C2C-C1C | 3.20  | 130.04      | 125.03   |
| 23  | c     | 514    | CLA  | CMC-C2C-C1C | 3.20  | 130.04      | 125.03   |
| 23  | A     | 408    | CLA  | O2D-CGD-O1D | -3.20 | 117.62      | 123.85   |
| 23  | b     | 608    | CLA  | CBC-CAC-C3C | -3.20 | 103.75      | 112.42   |
| 33  | d     | 412[B] | LHG  | O8-C23-O10  | -3.20 | 115.62      | 123.63   |
| 23  | D     | 702[A] | CLA  | C1D-CHD-C4C | -3.20 | 119.22      | 126.02   |
| 23  | A     | 406[A] | CLA  | O2D-CGD-O1D | -3.20 | 117.62      | 123.85   |
| 23  | a     | 405[A] | CLA  | CHC-C1C-C2C | -3.20 | 117.86      | 126.95   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 615    | CLA  | C4-C3-C5    | 3.19  | 120.77      | 115.23   |
| 25  | C     | 516    | BCR  | C24-C23-C22 | -3.19 | 121.51      | 126.23   |
| 23  | a     | 405[A] | CLA  | CAA-C2A-C1A | -3.19 | 101.52      | 111.97   |
| 23  | C     | 507    | CLA  | C1D-CHD-C4C | -3.19 | 119.24      | 126.02   |
| 23  | b     | 605    | CLA  | C4C-C3C-C2C | -3.19 | 102.25      | 106.89   |
| 29  | d     | 404[B] | PL9  | C10-C9-C11  | 3.19  | 120.77      | 115.23   |
| 23  | b     | 614    | CLA  | C4C-C3C-C2C | -3.19 | 102.25      | 106.89   |
| 23  | C     | 502    | CLA  | C1-C2-C3    | -3.19 | 120.97      | 126.20   |
| 25  | T     | 102    | BCR  | C2-C1-C6    | 3.19  | 115.07      | 110.44   |
| 29  | a     | 414[B] | PL9  | C42-C43-C44 | -3.19 | 120.33      | 127.62   |
| 23  | b     | 609    | CLA  | C1C-C2C-C3C | -3.19 | 103.63      | 106.98   |
| 23  | B     | 608    | CLA  | C1-C2-C3    | -3.19 | 120.98      | 126.20   |
| 34  | c     | 501    | LMG  | C7-O1-C1    | -3.18 | 106.97      | 113.80   |
| 23  | a     | 406[A] | CLA  | CHD-C4C-NC  | 3.18  | 129.17      | 124.23   |
| 23  | c     | 514    | CLA  | O2A-CGA-CBA | 3.18  | 121.54      | 111.83   |
| 25  | a     | 410    | BCR  | C38-C26-C25 | -3.18 | 121.01      | 124.48   |
| 23  | c     | 503    | CLA  | C3C-C4C-NC  | 3.18  | 114.51      | 110.43   |
| 23  | C     | 513    | CLA  | CHD-C4C-NC  | 3.18  | 129.16      | 124.23   |
| 25  | k     | 101    | BCR  | C7-C8-C9    | -3.18 | 121.53      | 126.23   |
| 23  | B     | 604    | CLA  | C4B-C3B-C2B | -3.18 | 103.35      | 107.30   |
| 23  | b     | 601    | CLA  | C4B-C3B-C2B | -3.18 | 103.35      | 107.30   |
| 23  | c     | 504    | CLA  | C4C-C3C-C2C | -3.18 | 102.27      | 106.89   |
| 23  | b     | 611    | CLA  | CHC-C1C-C2C | -3.18 | 117.92      | 126.95   |
| 32  | m     | 103    | LMT  | C1'-O5'-C5' | -3.18 | 107.52      | 113.72   |
| 23  | B     | 606    | CLA  | CMC-C2C-C1C | 3.17  | 130.00      | 125.03   |
| 23  | c     | 502    | CLA  | C3B-C4B-NB  | 3.17  | 113.36      | 110.53   |
| 23  | B     | 601    | CLA  | C4C-C3C-C2C | -3.17 | 102.27      | 106.89   |
| 25  | D     | 704    | BCR  | C37-C22-C23 | 3.17  | 122.93      | 118.09   |
| 23  | A     | 404[B] | CLA  | O2A-CGA-O1A | -3.17 | 115.70      | 123.63   |
| 23  | B     | 607    | CLA  | CAA-C2A-C3A | -3.17 | 104.44      | 113.00   |
| 23  | a     | 409    | CLA  | C4-C3-C5    | 3.17  | 120.73      | 115.23   |
| 35  | b     | 625    | HTG  | O5-C5-C4    | 3.17  | 115.41      | 109.70   |
| 23  | C     | 514    | CLA  | O2D-CGD-O1D | -3.17 | 117.69      | 123.85   |
| 23  | D     | 702[A] | CLA  | O2A-CGA-CBA | 3.16  | 121.48      | 111.83   |
| 29  | d     | 404[A] | PL9  | C37-C38-C39 | -3.16 | 120.38      | 127.62   |
| 34  | D     | 711    | LMG  | O8-C28-O10  | -3.16 | 115.72      | 123.63   |
| 23  | a     | 407[A] | CLA  | CHD-C4C-NC  | 3.16  | 129.13      | 124.23   |
| 23  | C     | 512    | CLA  | C4C-C3C-C2C | -3.16 | 102.29      | 106.89   |
| 23  | b     | 613    | CLA  | C4B-C3B-C2B | -3.16 | 103.37      | 107.30   |
| 23  | b     | 609    | CLA  | C4C-C3C-C2C | -3.16 | 102.30      | 106.89   |
| 38  | f     | 101    | HEM  | CAD-CBD-CGD | 3.15  | 122.03      | 113.67   |
| 23  | a     | 407[A] | CLA  | C3B-C4B-NB  | 3.15  | 113.34      | 110.53   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 29  | a     | 414[A] | PL9  | C42-C43-C44 | -3.15 | 120.41      | 127.62   |
| 25  | d     | 403    | BCR  | C39-C30-C25 | -3.15 | 105.30      | 110.24   |
| 23  | b     | 610    | CLA  | CMB-C2B-C1B | 3.15  | 130.22      | 125.42   |
| 26  | a     | 411[B] | SQD  | C1-C2-C3    | -3.15 | 103.38      | 110.01   |
| 23  | C     | 503    | CLA  | CHC-C1C-C2C | -3.15 | 118.00      | 126.95   |
| 29  | D     | 705[B] | PL9  | C17-C18-C19 | -3.15 | 120.42      | 127.62   |
| 23  | C     | 514    | CLA  | C4B-C3B-C2B | -3.15 | 103.39      | 107.30   |
| 23  | C     | 506    | CLA  | O2D-CGD-O1D | -3.15 | 117.73      | 123.85   |
| 23  | d     | 401[A] | CLA  | O2D-CGD-O1D | -3.15 | 117.73      | 123.85   |
| 23  | A     | 406[A] | CLA  | O2A-CGA-CBA | 3.14  | 121.42      | 111.83   |
| 23  | a     | 409    | CLA  | C4C-C3C-C2C | -3.14 | 102.32      | 106.89   |
| 23  | B     | 602    | CLA  | CAC-C3C-C4C | 3.14  | 128.88      | 124.79   |
| 25  | h     | 101    | BCR  | C16-C17-C18 | -3.14 | 122.87      | 127.28   |
| 25  | b     | 619    | BCR  | C15-C14-C13 | -3.14 | 122.88      | 127.28   |
| 23  | A     | 404[A] | CLA  | C4B-C3B-C2B | -3.13 | 103.41      | 107.30   |
| 23  | C     | 506    | CLA  | C1C-C2C-C3C | -3.13 | 103.69      | 106.98   |
| 23  | b     | 611    | CLA  | O2A-CGA-CBA | 3.12  | 121.36      | 111.83   |
| 23  | b     | 613    | CLA  | O2A-CGA-CBA | 3.12  | 121.36      | 111.83   |
| 23  | C     | 510    | CLA  | C4B-C3B-C2B | -3.12 | 103.42      | 107.30   |
| 23  | b     | 603    | CLA  | C4-C3-C5    | 3.12  | 120.65      | 115.23   |
| 23  | C     | 509    | CLA  | CHC-C1C-C2C | -3.12 | 118.08      | 126.95   |
| 33  | d     | 406[B] | LHG  | O7-C7-C8    | 3.12  | 118.23      | 111.48   |
| 29  | a     | 414[B] | PL9  | C17-C18-C19 | -3.12 | 120.48      | 127.62   |
| 23  | A     | 405[A] | CLA  | CMB-C2B-C1B | 3.12  | 130.17      | 125.42   |
| 23  | D     | 702[B] | CLA  | C3B-C4B-NB  | 3.12  | 113.31      | 110.53   |
| 24  | A     | 417[B] | PHO  | C4-C3-C5    | 3.12  | 120.64      | 115.23   |
| 23  | c     | 503    | CLA  | CMB-C2B-C1B | 3.12  | 130.17      | 125.42   |
| 29  | d     | 404[B] | PL9  | C40-C39-C41 | 3.12  | 120.64      | 115.23   |
| 25  | t     | 102    | BCR  | C15-C16-C17 | -3.12 | 117.14      | 123.52   |
| 23  | c     | 514    | CLA  | C4B-C3B-C2B | -3.12 | 103.43      | 107.30   |
| 38  | f     | 101    | HEM  | C1B-NB-C4B  | 3.12  | 108.90      | 105.21   |
| 23  | A     | 406[B] | CLA  | C4B-C3B-C2B | -3.11 | 103.43      | 107.30   |
| 23  | B     | 616    | CLA  | C4B-C3B-C2B | -3.11 | 103.43      | 107.30   |
| 23  | c     | 508    | CLA  | C1D-CHD-C4C | -3.11 | 119.41      | 126.02   |
| 24  | a     | 416[B] | PHO  | C4-C3-C5    | 3.11  | 120.63      | 115.23   |
| 24  | a     | 408[A] | PHO  | O1D-CGD-CBD | -3.11 | 120.01      | 124.72   |
| 34  | c     | 501    | LMG  | C8-O7-C10   | -3.11 | 110.36      | 117.80   |
| 23  | C     | 507    | CLA  | C4-C3-C5    | 3.11  | 120.62      | 115.23   |
| 23  | b     | 611    | CLA  | O2A-CGA-O1A | -3.11 | 115.86      | 123.63   |
| 23  | B     | 602    | CLA  | C3B-C4B-NB  | 3.11  | 113.30      | 110.53   |
| 23  | A     | 406[B] | CLA  | O2A-CGA-CBA | 3.11  | 121.30      | 111.83   |
| 23  | b     | 613    | CLA  | CHC-C1C-C2C | -3.11 | 118.12      | 126.95   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 603    | CLA  | CHC-C1C-C2C | -3.10 | 118.13      | 126.95   |
| 23  | C     | 505    | CLA  | C1-O2A-CGA  | 3.10  | 124.16      | 116.65   |
| 23  | B     | 603    | CLA  | O2A-CGA-O1A | -3.10 | 115.87      | 123.63   |
| 25  | K     | 102    | BCR  | C24-C23-C22 | -3.10 | 121.65      | 126.23   |
| 29  | a     | 414[A] | PL9  | C25-C24-C26 | 3.10  | 120.61      | 115.23   |
| 23  | C     | 513    | CLA  | O2A-CGA-CBA | 3.10  | 121.28      | 111.83   |
| 23  | c     | 514    | CLA  | CAA-C2A-C3A | -3.10 | 104.63      | 113.00   |
| 23  | a     | 409    | CLA  | O2A-CGA-CBA | 3.09  | 121.27      | 111.83   |
| 33  | D     | 707[A] | LHG  | O8-C23-C24  | 3.09  | 121.27      | 111.83   |
| 38  | f     | 101    | HEM  | CHD-C4C-NC  | 3.09  | 127.82      | 124.45   |
| 23  | c     | 506    | CLA  | C3B-C4B-NB  | 3.09  | 113.29      | 110.53   |
| 23  | B     | 605    | CLA  | CMC-C2C-C1C | 3.09  | 129.87      | 125.03   |
| 23  | B     | 607    | CLA  | C1D-CHD-C4C | -3.09 | 119.45      | 126.02   |
| 33  | b     | 629[A] | LHG  | O7-C7-C8    | 3.09  | 118.16      | 111.48   |
| 23  | b     | 614    | CLA  | CHD-C4C-NC  | 3.09  | 129.02      | 124.23   |
| 23  | b     | 603    | CLA  | C4B-C3B-C2B | -3.09 | 103.46      | 107.30   |
| 23  | b     | 609    | CLA  | C4B-C3B-C2B | -3.09 | 103.47      | 107.30   |
| 23  | c     | 503    | CLA  | CBC-CAC-C3C | -3.08 | 104.06      | 112.42   |
| 26  | a     | 411[A] | SQD  | C45-O47-C7  | -3.08 | 110.42      | 117.80   |
| 33  | E     | 101[A] | LHG  | O8-C23-C24  | 3.08  | 121.23      | 111.83   |
| 24  | A     | 417[A] | PHO  | C4-C3-C5    | 3.08  | 120.58      | 115.23   |
| 23  | C     | 509    | CLA  | CHD-C1D-ND  | -3.08 | 120.47      | 124.80   |
| 23  | C     | 510    | CLA  | C16-C15-C13 | -3.08 | 105.74      | 115.97   |
| 23  | d     | 401[A] | CLA  | C2A-C1A-CHA | -3.07 | 118.53      | 123.87   |
| 23  | d     | 401[A] | CLA  | O2A-CGA-O1A | -3.07 | 115.94      | 123.63   |
| 29  | A     | 414[A] | PL9  | C17-C18-C19 | -3.07 | 120.59      | 127.62   |
| 23  | b     | 612    | CLA  | O2A-CGA-O1A | -3.07 | 115.95      | 123.63   |
| 23  | b     | 609    | CLA  | C3B-C4B-NB  | 3.07  | 113.27      | 110.53   |
| 23  | C     | 502    | CLA  | CMC-C2C-C1C | 3.07  | 129.83      | 125.03   |
| 38  | F     | 102    | HEM  | CHB-C1B-NB  | 3.07  | 128.16      | 124.37   |
| 29  | d     | 404[A] | PL9  | C22-C23-C24 | -3.07 | 120.60      | 127.62   |
| 23  | d     | 401[B] | CLA  | CHC-C1C-C2C | -3.07 | 118.23      | 126.95   |
| 36  | h     | 102    | DGD  | O1G-C1A-C2A | 3.07  | 121.19      | 111.83   |
| 23  | B     | 601    | CLA  | O2D-CGD-O1D | -3.07 | 117.88      | 123.85   |
| 25  | C     | 515    | BCR  | C15-C14-C13 | -3.06 | 122.98      | 127.28   |
| 23  | b     | 601    | CLA  | C3B-C4B-NB  | 3.06  | 113.27      | 110.53   |
| 23  | a     | 406[A] | CLA  | CMA-C3A-C2A | -3.06 | 102.14      | 113.98   |
| 29  | d     | 404[A] | PL9  | C27-C28-C29 | -3.06 | 120.61      | 127.62   |
| 23  | b     | 612    | CLA  | O2A-CGA-CBA | 3.06  | 121.17      | 111.83   |
| 23  | c     | 505    | CLA  | C3B-C4B-NB  | 3.06  | 113.26      | 110.53   |
| 33  | D     | 706[B] | LHG  | O8-C23-O10  | -3.06 | 115.97      | 123.63   |
| 23  | b     | 607    | CLA  | C1D-CHD-C4C | -3.06 | 119.52      | 126.02   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 405[B] | CLA  | CHC-C1C-C2C | -3.06 | 118.25      | 126.95   |
| 23  | b     | 609    | CLA  | O2D-CGD-O1D | -3.06 | 117.90      | 123.85   |
| 23  | a     | 407[B] | CLA  | CMC-C2C-C1C | 3.06  | 129.81      | 125.03   |
| 23  | d     | 401[B] | CLA  | C4-C3-C5    | 3.06  | 120.53      | 115.23   |
| 23  | B     | 601    | CLA  | CHD-C4C-NC  | 3.05  | 128.97      | 124.23   |
| 23  | a     | 405[B] | CLA  | C4B-C3B-C2B | -3.05 | 103.51      | 107.30   |
| 36  | C     | 519    | DGD  | O1G-C1A-C2A | 3.05  | 121.14      | 111.83   |
| 23  | b     | 605    | CLA  | CHC-C1C-C2C | -3.05 | 118.27      | 126.95   |
| 29  | a     | 414[A] | PL9  | C22-C23-C24 | -3.05 | 120.64      | 127.62   |
| 25  | d     | 403    | BCR  | C10-C11-C12 | -3.05 | 114.36      | 123.20   |
| 23  | C     | 504    | CLA  | C4C-C3C-C2C | -3.05 | 102.45      | 106.89   |
| 23  | C     | 502    | CLA  | C3B-C4B-NB  | 3.05  | 113.25      | 110.53   |
| 23  | c     | 510    | CLA  | C4C-C3C-C2C | -3.05 | 102.46      | 106.89   |
| 23  | b     | 616    | CLA  | CMC-C2C-C1C | 3.05  | 129.79      | 125.03   |
| 23  | D     | 703    | CLA  | C4C-C3C-C2C | -3.04 | 102.46      | 106.89   |
| 23  | b     | 610    | CLA  | CAA-C2A-C3A | -3.04 | 104.77      | 113.00   |
| 23  | d     | 401[A] | CLA  | C4C-C3C-C2C | -3.04 | 102.46      | 106.89   |
| 23  | A     | 405[B] | CLA  | C3C-C4C-NC  | 3.04  | 114.33      | 110.43   |
| 25  | D     | 704    | BCR  | C15-C14-C13 | -3.04 | 123.01      | 127.28   |
| 23  | A     | 406[A] | CLA  | CAA-C2A-C3A | -3.04 | 104.78      | 113.00   |
| 29  | A     | 414[B] | PL9  | C20-C19-C21 | 3.04  | 120.50      | 115.23   |
| 23  | c     | 513    | CLA  | CHD-C4C-NC  | 3.04  | 128.94      | 124.23   |
| 23  | d     | 401[B] | CLA  | C4B-C3B-C2B | -3.04 | 103.52      | 107.30   |
| 23  | D     | 702[A] | CLA  | C4B-C3B-C2B | -3.04 | 103.52      | 107.30   |
| 32  | B     | 629    | LMT  | O1'-C1'-C2' | 3.04  | 112.89      | 108.27   |
| 23  | b     | 615    | CLA  | C11-C10-C8  | -3.04 | 105.87      | 115.97   |
| 29  | D     | 705[A] | PL9  | C10-C9-C11  | 3.03  | 120.50      | 115.23   |
| 24  | a     | 408[B] | PHO  | O1D-CGD-CBD | -3.03 | 120.12      | 124.72   |
| 38  | F     | 102    | HEM  | CHD-C1D-ND  | 3.03  | 127.69      | 124.42   |
| 23  | C     | 502    | CLA  | C4B-C3B-C2B | -3.03 | 103.53      | 107.30   |
| 23  | b     | 607    | CLA  | CAA-C2A-C3A | -3.03 | 104.81      | 113.00   |
| 26  | b     | 620    | SQD  | C3-C4-C5    | 3.03  | 115.73      | 110.23   |
| 32  | A     | 420    | LMT  | O5B-C5B-C4B | 3.03  | 115.16      | 109.70   |
| 33  | A     | 419[B] | LHG  | O8-C23-C24  | 3.03  | 121.08      | 111.83   |
| 23  | a     | 407[B] | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 23  | A     | 405[A] | CLA  | CHD-C4C-NC  | 3.03  | 128.93      | 124.23   |
| 29  | A     | 414[A] | PL9  | C10-C9-C11  | 3.03  | 120.48      | 115.23   |
| 26  | B     | 620    | SQD  | O48-C23-C24 | 3.03  | 121.06      | 111.83   |
| 23  | b     | 601    | CLA  | CHD-C4C-NC  | 3.02  | 128.92      | 124.23   |
| 23  | C     | 512    | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.79   |
| 35  | b     | 622    | HTG  | O5-C5-C4    | 3.02  | 115.15      | 109.70   |
| 36  | h     | 102    | DGD  | O1G-C1A-O1A | -3.02 | 116.07      | 123.63   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 33  | D     | 707[B] | LHG  | O8-C23-C24  | 3.02  | 121.05      | 111.83   |
| 23  | C     | 511    | CLA  | CHC-C1C-C2C | -3.02 | 118.36      | 126.95   |
| 24  | A     | 407[B] | PHO  | C1-C2-C3    | -3.02 | 121.25      | 126.20   |
| 23  | b     | 608    | CLA  | CHD-C4C-NC  | 3.02  | 128.91      | 124.23   |
| 23  | C     | 503    | CLA  | C4-C3-C5    | 3.02  | 120.47      | 115.23   |
| 23  | C     | 504    | CLA  | O2A-CGA-O1A | -3.02 | 116.08      | 123.63   |
| 26  | A     | 410[A] | SQD  | O48-C23-C24 | 3.02  | 121.04      | 111.83   |
| 23  | D     | 703    | CLA  | O2A-CGA-O1A | -3.02 | 116.08      | 123.63   |
| 23  | B     | 612    | CLA  | C1C-C2C-C3C | -3.02 | 103.81      | 106.98   |
| 23  | b     | 611    | CLA  | C4B-C3B-C2B | -3.02 | 103.55      | 107.30   |
| 23  | D     | 702[A] | CLA  | CAC-C3C-C4C | 3.02  | 128.71      | 124.79   |
| 23  | A     | 404[A] | CLA  | CAA-C2A-C1A | -3.01 | 102.09      | 111.97   |
| 23  | B     | 612    | CLA  | O2A-CGA-O1A | -3.01 | 116.09      | 123.63   |
| 24  | a     | 408[B] | PHO  | O2A-CGA-CBA | 3.01  | 121.02      | 111.83   |
| 34  | z     | 101    | LMG  | O8-C28-C29  | 3.01  | 121.02      | 111.83   |
| 29  | a     | 414[B] | PL9  | C22-C23-C24 | -3.01 | 120.73      | 127.62   |
| 26  | a     | 411[A] | SQD  | O9-S-C6     | 3.01  | 111.25      | 106.76   |
| 23  | d     | 402    | CLA  | C4C-C3C-C2C | -3.01 | 102.51      | 106.89   |
| 33  | a     | 420[B] | LHG  | O7-C7-C8    | 3.01  | 118.00      | 111.48   |
| 23  | b     | 604    | CLA  | CHC-C1C-C2C | -3.01 | 118.39      | 126.95   |
| 29  | a     | 414[A] | PL9  | C10-C9-C11  | 3.01  | 120.45      | 115.23   |
| 23  | c     | 505    | CLA  | C4C-C3C-C2C | -3.01 | 102.51      | 106.89   |
| 23  | b     | 603    | CLA  | C4C-C3C-C2C | -3.01 | 102.51      | 106.89   |
| 23  | b     | 614    | CLA  | CBC-CAC-C3C | -3.01 | 104.26      | 112.42   |
| 23  | a     | 407[B] | CLA  | CHD-C4C-NC  | 3.01  | 128.90      | 124.23   |
| 23  | a     | 406[B] | CLA  | CHC-C1C-C2C | -3.01 | 118.40      | 126.95   |
| 33  | d     | 405[A] | LHG  | O7-C7-C8    | 3.01  | 117.99      | 111.48   |
| 23  | b     | 601    | CLA  | C4-C3-C5    | 3.01  | 120.45      | 115.23   |
| 23  | a     | 406[A] | CLA  | C4B-C3B-C2B | -3.01 | 103.56      | 107.30   |
| 34  | D     | 711    | LMG  | O7-C10-C11  | 3.00  | 117.98      | 111.48   |
| 23  | c     | 509    | CLA  | C4C-C3C-C2C | -3.00 | 102.52      | 106.89   |
| 33  | d     | 405[B] | LHG  | O7-C7-C8    | 3.00  | 117.97      | 111.48   |
| 23  | b     | 609    | CLA  | CMB-C2B-C1B | 3.00  | 129.99      | 125.42   |
| 23  | b     | 612    | CLA  | CMC-C2C-C1C | 3.00  | 129.72      | 125.03   |
| 26  | A     | 412    | SQD  | O48-C23-C24 | 3.00  | 120.98      | 111.83   |
| 23  | c     | 511    | CLA  | O2A-CGA-CBA | 3.00  | 120.98      | 111.83   |
| 23  | A     | 404[A] | CLA  | CHC-C1C-C2C | -3.00 | 118.43      | 126.95   |
| 29  | D     | 705[A] | PL9  | C51-C49-C50 | 3.00  | 121.49      | 114.59   |
| 29  | a     | 414[A] | PL9  | C37-C38-C39 | -3.00 | 120.77      | 127.62   |
| 23  | b     | 611    | CLA  | C2A-C1A-CHA | -2.99 | 118.67      | 123.87   |
| 23  | C     | 504    | CLA  | C1C-C2C-C3C | -2.99 | 103.83      | 106.98   |
| 23  | C     | 503    | CLA  | C4B-C3B-C2B | -2.99 | 103.58      | 107.30   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 608    | CLA  | CHC-C1C-C2C | -2.99 | 118.45      | 126.95   |
| 23  | b     | 602    | CLA  | C2A-C1A-CHA | -2.99 | 118.68      | 123.87   |
| 23  | B     | 616    | CLA  | C1C-C2C-C3C | -2.99 | 103.84      | 106.98   |
| 23  | c     | 507    | CLA  | CAC-C3C-C4C | 2.99  | 128.68      | 124.79   |
| 23  | B     | 609    | CLA  | C3B-C4B-NB  | 2.99  | 113.20      | 110.53   |
| 23  | b     | 610    | CLA  | CHD-C4C-NC  | 2.99  | 128.86      | 124.23   |
| 29  | d     | 404[A] | PL9  | C10-C9-C11  | 2.98  | 120.41      | 115.23   |
| 23  | C     | 514    | CLA  | C4C-C3C-C2C | -2.98 | 102.55      | 106.89   |
| 29  | a     | 414[B] | PL9  | C35-C34-C36 | 2.98  | 120.41      | 115.23   |
| 23  | c     | 514    | CLA  | C4C-C3C-C2C | -2.98 | 102.55      | 106.89   |
| 23  | b     | 614    | CLA  | O2A-CGA-CBA | 2.98  | 120.93      | 111.83   |
| 23  | a     | 405[A] | CLA  | C4-C3-C5    | 2.98  | 120.41      | 115.23   |
| 23  | C     | 503    | CLA  | CMB-C2B-C1B | 2.98  | 129.96      | 125.42   |
| 24  | a     | 408[A] | PHO  | O2A-CGA-CBA | 2.98  | 120.92      | 111.83   |
| 23  | c     | 503    | CLA  | CHD-C1D-ND  | -2.98 | 120.61      | 124.80   |
| 23  | c     | 510    | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 23  | C     | 510    | CLA  | O2A-CGA-O1A | -2.98 | 116.18      | 123.63   |
| 23  | a     | 407[A] | CLA  | CMC-C2C-C1C | 2.98  | 129.68      | 125.03   |
| 33  | D     | 706[A] | LHG  | O8-C23-O10  | -2.97 | 116.19      | 123.63   |
| 23  | a     | 409    | CLA  | CHD-C4C-NC  | 2.97  | 128.84      | 124.23   |
| 23  | b     | 605    | CLA  | CMB-C2B-C1B | 2.97  | 129.94      | 125.42   |
| 23  | b     | 616    | CLA  | CAC-C3C-C4C | 2.97  | 128.66      | 124.79   |
| 23  | A     | 404[B] | CLA  | C4C-C3C-C2C | -2.97 | 102.57      | 106.89   |
| 23  | B     | 608    | CLA  | CMA-C3A-C4A | -2.97 | 103.79      | 111.77   |
| 23  | D     | 703    | CLA  | CAC-C3C-C4C | 2.97  | 128.65      | 124.79   |
| 29  | A     | 414[A] | PL9  | C20-C19-C21 | 2.97  | 120.38      | 115.23   |
| 23  | b     | 605    | CLA  | C2A-C1A-CHA | -2.97 | 118.72      | 123.87   |
| 23  | a     | 406[A] | CLA  | CBC-CAC-C3C | -2.97 | 104.38      | 112.42   |
| 23  | c     | 509    | CLA  | CHC-C1C-C2C | -2.97 | 118.52      | 126.95   |
| 23  | c     | 513    | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 23  | A     | 406[A] | CLA  | CHD-C4C-NC  | 2.96  | 128.83      | 124.23   |
| 23  | a     | 406[A] | CLA  | CHC-C1C-C2C | -2.96 | 118.53      | 126.95   |
| 26  | A     | 410[B] | SQD  | O48-C23-C24 | 2.96  | 120.86      | 111.83   |
| 34  | c     | 520    | LMG  | O8-C28-C29  | 2.96  | 120.86      | 111.83   |
| 29  | d     | 404[B] | PL9  | C37-C38-C39 | -2.96 | 120.85      | 127.62   |
| 23  | d     | 402    | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 23  | b     | 607    | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 23  | A     | 404[B] | CLA  | C4B-C3B-C2B | -2.96 | 103.62      | 107.30   |
| 23  | b     | 615    | CLA  | CHC-C1C-C2C | -2.96 | 118.55      | 126.95   |
| 33  | b     | 629[A] | LHG  | O8-C23-C24  | 2.96  | 120.84      | 111.83   |
| 23  | d     | 401[A] | CLA  | C4-C3-C5    | 2.95  | 120.36      | 115.23   |
| 23  | a     | 409    | CLA  | CAA-C2A-C3A | -2.95 | 105.03      | 113.00   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 33  | D     | 707[A] | LHG  | O8-C23-O10  | -2.95 | 116.25      | 123.63   |
| 23  | B     | 614    | CLA  | CHC-C1C-C2C | -2.95 | 118.57      | 126.95   |
| 25  | c     | 516    | BCR  | C37-C22-C23 | 2.95  | 122.59      | 118.09   |
| 23  | C     | 512    | CLA  | C1-C2-C3    | -2.95 | 121.37      | 126.20   |
| 23  | b     | 603    | CLA  | O2A-CGA-O1A | -2.94 | 116.27      | 123.63   |
| 33  | D     | 706[B] | LHG  | O7-C7-C8    | 2.94  | 117.85      | 111.48   |
| 23  | b     | 613    | CLA  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 34  | D     | 711    | LMG  | O8-C28-C29  | 2.94  | 120.79      | 111.83   |
| 23  | c     | 506    | CLA  | C4B-C3B-C2B | -2.94 | 103.65      | 107.30   |
| 23  | C     | 510    | CLA  | C4C-C3C-C2C | -2.94 | 102.62      | 106.89   |
| 23  | A     | 408    | CLA  | C4B-C3B-C2B | -2.94 | 103.65      | 107.30   |
| 33  | a     | 420[A] | LHG  | O7-C7-C8    | 2.93  | 117.83      | 111.48   |
| 25  | D     | 704    | BCR  | C40-C30-C25 | -2.93 | 105.64      | 110.24   |
| 25  | c     | 516    | BCR  | C21-C20-C19 | -2.93 | 114.70      | 123.20   |
| 34  | C     | 501    | LMG  | O6-C1-O1    | -2.93 | 103.12      | 110.04   |
| 23  | A     | 406[B] | CLA  | O2A-CGA-O1A | -2.93 | 116.30      | 123.63   |
| 23  | c     | 512    | CLA  | CHC-C1C-C2C | -2.93 | 118.63      | 126.95   |
| 23  | B     | 606    | CLA  | O2A-CGA-O1A | -2.93 | 116.31      | 123.63   |
| 23  | c     | 509    | CLA  | CMB-C2B-C1B | 2.93  | 129.87      | 125.42   |
| 25  | y     | 101    | BCR  | C38-C26-C25 | -2.93 | 121.29      | 124.48   |
| 23  | A     | 404[A] | CLA  | C4C-C3C-C2C | -2.92 | 102.63      | 106.89   |
| 23  | C     | 512    | CLA  | CHC-C1C-C2C | -2.92 | 118.64      | 126.95   |
| 23  | A     | 405[B] | CLA  | CMC-C2C-C1C | 2.92  | 129.60      | 125.03   |
| 23  | c     | 511    | CLA  | O2A-CGA-O1A | -2.92 | 116.32      | 123.63   |
| 38  | f     | 101    | HEM  | CBD-CAD-C3D | -2.92 | 104.45      | 112.53   |
| 25  | T     | 102    | BCR  | C35-C13-C12 | 2.92  | 122.55      | 118.09   |
| 23  | a     | 405[A] | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 32  | T     | 101    | LMT  | C1'-O5'-C5' | -2.92 | 108.01      | 113.72   |
| 23  | B     | 609    | CLA  | O2A-CGA-O1A | -2.92 | 116.32      | 123.63   |
| 23  | b     | 606    | CLA  | C4B-C3B-C2B | -2.92 | 103.67      | 107.30   |
| 23  | c     | 512    | CLA  | C4B-C3B-C2B | -2.92 | 103.67      | 107.30   |
| 23  | b     | 612    | CLA  | CHD-C1D-ND  | -2.92 | 120.69      | 124.80   |
| 23  | c     | 505    | CLA  | CMC-C2C-C1C | 2.92  | 129.60      | 125.03   |
| 23  | B     | 608    | CLA  | CMA-C3A-C2A | -2.92 | 102.71      | 113.98   |
| 23  | A     | 405[B] | CLA  | CMB-C2B-C1B | 2.92  | 129.86      | 125.42   |
| 23  | a     | 405[B] | CLA  | CMA-C3A-C4A | -2.92 | 103.94      | 111.77   |
| 23  | A     | 406[A] | CLA  | C1-C2-C3    | -2.92 | 121.42      | 126.20   |
| 24  | A     | 417[B] | PHO  | C1A-C2A-C3A | -2.92 | 100.06      | 102.84   |
| 23  | b     | 606    | CLA  | C4C-C3C-C2C | -2.91 | 102.65      | 106.89   |
| 23  | B     | 601    | CLA  | C1-O2A-CGA  | 2.91  | 123.70      | 116.65   |
| 23  | b     | 613    | CLA  | CHD-C4C-NC  | 2.91  | 128.75      | 124.23   |
| 25  | h     | 101    | BCR  | C7-C8-C9    | -2.91 | 121.93      | 126.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 612    | CLA  | C11-C12-C13 | -2.91 | 106.29      | 115.97   |
| 23  | D     | 702[A] | CLA  | O2A-CGA-O1A | -2.91 | 116.35      | 123.63   |
| 23  | B     | 615    | CLA  | C4-C3-C5    | 2.91  | 120.28      | 115.23   |
| 26  | A     | 412    | SQD  | O8-S-C6     | 2.91  | 111.59      | 105.97   |
| 23  | B     | 608    | CLA  | CAA-C2A-C3A | -2.91 | 105.14      | 113.00   |
| 23  | B     | 604    | CLA  | O2A-CGA-CBA | 2.91  | 120.70      | 111.83   |
| 23  | C     | 508    | CLA  | C1-C2-C3    | -2.91 | 121.44      | 126.20   |
| 23  | C     | 502    | CLA  | CMB-C2B-C1B | 2.91  | 129.84      | 125.42   |
| 23  | B     | 604    | CLA  | CHC-C1C-C2C | -2.91 | 118.69      | 126.95   |
| 23  | b     | 607    | CLA  | C4B-C3B-C2B | -2.90 | 103.69      | 107.30   |
| 33  | E     | 101[B] | LHG  | O8-C23-C24  | 2.90  | 120.69      | 111.83   |
| 29  | d     | 404[B] | PL9  | C17-C18-C19 | -2.90 | 120.98      | 127.62   |
| 23  | a     | 407[A] | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.89   |
| 23  | C     | 505    | CLA  | C4B-C3B-C2B | -2.90 | 103.70      | 107.30   |
| 23  | B     | 609    | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.89   |
| 23  | A     | 408    | CLA  | CBC-CAC-C3C | -2.90 | 104.57      | 112.42   |
| 33  | b     | 629[B] | LHG  | O8-C23-C24  | 2.90  | 120.66      | 111.83   |
| 23  | A     | 405[A] | CLA  | CHC-C1C-C2C | -2.89 | 118.72      | 126.95   |
| 23  | D     | 702[A] | CLA  | CHC-C1C-C2C | -2.89 | 118.72      | 126.95   |
| 23  | a     | 407[B] | CLA  | C1-C2-C3    | -2.89 | 121.46      | 126.20   |
| 23  | a     | 405[B] | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 23  | C     | 514    | CLA  | CAC-C3C-C4C | 2.89  | 128.55      | 124.79   |
| 23  | b     | 608    | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 23  | b     | 603    | CLA  | CMB-C2B-C1B | 2.89  | 129.82      | 125.42   |
| 25  | a     | 410    | BCR  | C29-C30-C25 | 2.89  | 114.63      | 110.44   |
| 23  | B     | 615    | CLA  | CHD-C4C-NC  | 2.89  | 128.71      | 124.23   |
| 23  | D     | 702[A] | CLA  | C4C-C3C-C2C | -2.89 | 102.69      | 106.89   |
| 23  | c     | 502    | CLA  | CHC-C1C-C2C | -2.89 | 118.75      | 126.95   |
| 23  | c     | 510    | CLA  | C1-O2A-CGA  | 2.89  | 123.64      | 116.65   |
| 25  | h     | 101    | BCR  | C33-C5-C6   | -2.88 | 121.34      | 124.48   |
| 23  | c     | 512    | CLA  | C4-C3-C5    | 2.88  | 120.23      | 115.23   |
| 23  | a     | 407[A] | CLA  | C4B-C3B-C2B | -2.88 | 103.72      | 107.30   |
| 23  | B     | 614    | CLA  | CMB-C2B-C1B | 2.88  | 129.81      | 125.42   |
| 24  | a     | 416[A] | PHO  | CMB-C2B-C3B | 2.88  | 130.44      | 124.68   |
| 40  | v     | 201    | HEC  | C4D-ND-C1D  | 2.88  | 110.52      | 105.82   |
| 23  | b     | 614    | CLA  | CHC-C1C-C2C | -2.88 | 118.76      | 126.95   |
| 23  | C     | 514    | CLA  | C2A-C1A-CHA | -2.88 | 118.87      | 123.87   |
| 23  | b     | 613    | CLA  | C4-C3-C5    | 2.88  | 120.22      | 115.23   |
| 29  | D     | 705[B] | PL9  | C20-C19-C21 | 2.88  | 120.22      | 115.23   |
| 26  | a     | 411[A] | SQD  | O47-C7-O49  | -2.88 | 116.98      | 123.70   |
| 25  | b     | 618    | BCR  | C29-C30-C25 | 2.88  | 114.62      | 110.44   |
| 23  | b     | 601    | CLA  | C4C-C3C-C2C | -2.88 | 102.70      | 106.89   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 29  | A     | 414[A] | PL9  | C30-C29-C31 | 2.88  | 120.22      | 115.23   |
| 25  | d     | 403    | BCR  | C33-C5-C6   | -2.87 | 121.35      | 124.48   |
| 23  | A     | 408    | CLA  | CHD-C4C-NC  | 2.87  | 128.69      | 124.23   |
| 23  | c     | 502    | CLA  | C1-C2-C3    | -2.87 | 121.49      | 126.20   |
| 26  | a     | 411[B] | SQD  | C44-O6-C1   | -2.87 | 107.64      | 113.80   |
| 23  | C     | 502    | CLA  | O2A-CGA-O1A | -2.87 | 116.44      | 123.63   |
| 23  | b     | 615    | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 25  | y     | 101    | BCR  | C21-C20-C19 | -2.87 | 114.88      | 123.20   |
| 29  | D     | 705[B] | PL9  | C27-C28-C29 | -2.87 | 121.05      | 127.62   |
| 23  | B     | 610    | CLA  | CHC-C1C-C2C | -2.87 | 118.79      | 126.95   |
| 23  | B     | 608    | CLA  | C4B-C3B-C2B | -2.87 | 103.73      | 107.30   |
| 23  | c     | 513    | CLA  | CHC-C1C-C2C | -2.87 | 118.79      | 126.95   |
| 26  | f     | 102    | SQD  | O48-C23-C24 | 2.87  | 120.58      | 111.83   |
| 23  | b     | 601    | CLA  | CHC-C1C-C2C | -2.87 | 118.80      | 126.95   |
| 26  | f     | 102    | SQD  | O5-C1-C2    | 2.87  | 116.26      | 110.37   |
| 23  | b     | 609    | CLA  | CHD-C4C-NC  | 2.87  | 128.68      | 124.23   |
| 23  | C     | 512    | CLA  | C1-O2A-CGA  | 2.87  | 123.59      | 116.65   |
| 23  | a     | 407[A] | CLA  | CMB-C2B-C1B | 2.86  | 129.78      | 125.42   |
| 23  | B     | 608    | CLA  | O2A-CGA-CBA | 2.86  | 120.56      | 111.83   |
| 23  | D     | 702[B] | CLA  | C4C-C3C-C2C | -2.86 | 102.73      | 106.89   |
| 25  | Y     | 101    | BCR  | C10-C11-C12 | -2.86 | 114.91      | 123.20   |
| 25  | t     | 102    | BCR  | C21-C20-C19 | -2.86 | 114.91      | 123.20   |
| 24  | a     | 408[A] | PHO  | CMA-C3A-C4A | -2.86 | 108.45      | 114.61   |
| 23  | c     | 503    | CLA  | CHD-C4C-NC  | 2.86  | 128.66      | 124.23   |
| 23  | b     | 606    | CLA  | CAA-C2A-C3A | -2.86 | 105.28      | 113.00   |
| 23  | D     | 702[B] | CLA  | CHC-C1C-C2C | -2.86 | 118.83      | 126.95   |
| 23  | b     | 603    | CLA  | O2A-CGA-CBA | 2.86  | 120.55      | 111.83   |
| 23  | c     | 508    | CLA  | O2A-CGA-CBA | 2.86  | 120.54      | 111.83   |
| 23  | b     | 603    | CLA  | CHD-C4C-NC  | 2.85  | 128.65      | 124.23   |
| 24  | a     | 408[A] | PHO  | C1A-C2A-C3A | -2.85 | 100.13      | 102.84   |
| 23  | B     | 614    | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 23  | C     | 510    | CLA  | CHC-C1C-C2C | -2.85 | 118.85      | 126.95   |
| 23  | c     | 505    | CLA  | CAC-C3C-C4C | 2.85  | 128.50      | 124.79   |
| 26  | X     | 101    | SQD  | O48-C23-C24 | 2.85  | 120.52      | 111.83   |
| 23  | A     | 406[B] | CLA  | CHC-C1C-C2C | -2.85 | 118.85      | 126.95   |
| 23  | c     | 511    | CLA  | CHC-C1C-C2C | -2.85 | 118.85      | 126.95   |
| 25  | C     | 516    | BCR  | C33-C5-C6   | -2.85 | 121.38      | 124.48   |
| 23  | C     | 513    | CLA  | CMC-C2C-C1C | 2.85  | 129.48      | 125.03   |
| 32  | B     | 627    | LMT  | C2'-C3'-C4' | 2.85  | 116.14      | 109.68   |
| 23  | c     | 505    | CLA  | CHD-C4C-NC  | 2.85  | 128.64      | 124.23   |
| 23  | b     | 613    | CLA  | CMC-C2C-C1C | 2.85  | 129.48      | 125.03   |
| 23  | A     | 404[A] | CLA  | CAA-CBA-CGA | -2.84 | 105.14      | 113.21   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 405[A] | CLA  | C4-C3-C5    | 2.84  | 120.16      | 115.23   |
| 23  | C     | 502    | CLA  | CHD-C4C-NC  | 2.84  | 128.64      | 124.23   |
| 35  | o     | 301    | HTG  | C1'-S1-C1   | 2.84  | 106.58      | 100.45   |
| 23  | c     | 513    | CLA  | C4C-C3C-C2C | -2.84 | 102.76      | 106.89   |
| 23  | b     | 602    | CLA  | C4C-C3C-C2C | -2.84 | 102.76      | 106.89   |
| 29  | A     | 414[B] | PL9  | C12-C13-C14 | -2.84 | 121.13      | 127.62   |
| 23  | D     | 702[A] | CLA  | CAA-C2A-C3A | -2.84 | 105.33      | 113.00   |
| 23  | C     | 506    | CLA  | C4B-C3B-C2B | -2.84 | 103.77      | 107.30   |
| 23  | c     | 502    | CLA  | C4C-C3C-C2C | -2.84 | 102.76      | 106.89   |
| 25  | y     | 101    | BCR  | C15-C14-C13 | -2.84 | 123.30      | 127.28   |
| 23  | a     | 409    | CLA  | C2A-C1A-CHA | -2.83 | 118.95      | 123.87   |
| 23  | a     | 405[B] | CLA  | O2A-CGA-O1A | -2.83 | 116.54      | 123.63   |
| 23  | C     | 506    | CLA  | CHC-C1C-C2C | -2.83 | 118.90      | 126.95   |
| 25  | B     | 618    | BCR  | C37-C22-C21 | -2.83 | 118.23      | 122.82   |
| 23  | B     | 603    | CLA  | O2A-CGA-CBA | 2.83  | 120.46      | 111.83   |
| 33  | d     | 406[A] | LHG  | O8-C23-C24  | 2.83  | 120.46      | 111.83   |
| 23  | b     | 607    | CLA  | C4-C3-C5    | 2.83  | 120.14      | 115.23   |
| 23  | a     | 407[B] | CLA  | CBC-CAC-C3C | -2.83 | 104.75      | 112.42   |
| 23  | C     | 504    | CLA  | CMB-C2B-C1B | 2.83  | 129.72      | 125.42   |
| 23  | C     | 509    | CLA  | C4-C3-C5    | 2.83  | 120.13      | 115.23   |
| 23  | c     | 502    | CLA  | CMC-C2C-C1C | 2.82  | 129.45      | 125.03   |
| 23  | B     | 610    | CLA  | O2A-CGA-O1A | -2.82 | 116.57      | 123.63   |
| 25  | h     | 101    | BCR  | C16-C15-C14 | -2.82 | 117.74      | 123.52   |
| 23  | B     | 611    | CLA  | C4B-C3B-C2B | 2.82  | 110.81      | 107.30   |
| 23  | B     | 608    | CLA  | O2A-CGA-O1A | -2.82 | 116.58      | 123.63   |
| 23  | D     | 702[B] | CLA  | C2A-C1A-CHA | -2.82 | 118.98      | 123.87   |
| 25  | y     | 101    | BCR  | C34-C9-C8   | 2.82  | 122.39      | 118.09   |
| 23  | b     | 615    | CLA  | C1-C2-C3    | -2.81 | 121.58      | 126.20   |
| 23  | C     | 514    | CLA  | CBC-CAC-C3C | -2.81 | 104.79      | 112.42   |
| 29  | A     | 414[B] | PL9  | C30-C29-C31 | 2.81  | 120.11      | 115.23   |
| 23  | C     | 513    | CLA  | C4-C3-C5    | 2.81  | 120.11      | 115.23   |
| 23  | b     | 615    | CLA  | O2A-CGA-CBA | 2.81  | 120.41      | 111.83   |
| 25  | A     | 409    | BCR  | C33-C5-C6   | -2.81 | 121.42      | 124.48   |
| 23  | C     | 505    | CLA  | CMC-C2C-C1C | 2.81  | 129.43      | 125.03   |
| 33  | A     | 419[A] | LHG  | O7-C7-O9    | -2.81 | 117.13      | 123.70   |
| 23  | C     | 511    | CLA  | O2A-CGA-O1A | -2.81 | 116.60      | 123.63   |
| 23  | A     | 408    | CLA  | CHC-C1C-C2C | -2.81 | 118.96      | 126.95   |
| 23  | C     | 506    | CLA  | C4-C3-C5    | 2.81  | 120.10      | 115.23   |
| 23  | d     | 401[A] | CLA  | CHC-C1C-C2C | -2.81 | 118.97      | 126.95   |
| 24  | a     | 408[B] | PHO  | O2A-CGA-O1A | -2.81 | 116.60      | 123.63   |
| 36  | C     | 517[A] | DGD  | C2G-O2G-C1B | -2.81 | 111.07      | 117.80   |
| 25  | B     | 619    | BCR  | C21-C20-C19 | -2.81 | 115.06      | 123.20   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25  | B     | 618    | BCR  | C37-C22-C23 | 2.81  | 122.38      | 118.09   |
| 23  | B     | 603    | CLA  | CBC-CAC-C3C | -2.81 | 104.81      | 112.42   |
| 23  | a     | 406[B] | CLA  | O2D-CGD-O1D | -2.81 | 118.39      | 123.85   |
| 23  | b     | 615    | CLA  | O2A-CGA-O1A | -2.80 | 116.62      | 123.63   |
| 23  | B     | 606    | CLA  | C1-C2-C3    | -2.80 | 121.61      | 126.20   |
| 25  | k     | 101    | BCR  | C24-C23-C22 | -2.80 | 122.09      | 126.23   |
| 23  | A     | 406[A] | CLA  | CHC-C1C-C2C | -2.80 | 118.99      | 126.95   |
| 25  | B     | 618    | BCR  | C2-C1-C6    | 2.80  | 114.51      | 110.44   |
| 32  | b     | 621    | LMT  | C1'-O5'-C5' | -2.80 | 108.25      | 113.72   |
| 23  | b     | 615    | CLA  | C4B-C3B-C2B | -2.80 | 103.82      | 107.30   |
| 25  | B     | 617    | BCR  | C7-C8-C9    | -2.80 | 122.09      | 126.23   |
| 32  | M     | 101    | LMT  | C1'-O5'-C5' | -2.80 | 108.25      | 113.72   |
| 29  | D     | 705[A] | PL9  | C37-C38-C39 | -2.80 | 121.22      | 127.62   |
| 34  | Z     | 101    | LMG  | C4-C3-C2    | 2.80  | 115.74      | 110.83   |
| 23  | D     | 702[B] | CLA  | CMB-C2B-C1B | 2.80  | 129.68      | 125.42   |
| 23  | b     | 610    | CLA  | C4B-C3B-C2B | -2.80 | 103.83      | 107.30   |
| 23  | a     | 409    | CLA  | CMA-C3A-C2A | -2.80 | 103.17      | 113.98   |
| 34  | c     | 521    | LMG  | O8-C28-C29  | 2.79  | 120.36      | 111.83   |
| 23  | b     | 615    | CLA  | CHD-C4C-NC  | 2.79  | 128.56      | 124.23   |
| 23  | c     | 506    | CLA  | CHC-C1C-C2C | -2.79 | 119.01      | 126.95   |
| 23  | B     | 613    | CLA  | CMC-C2C-C1C | 2.79  | 129.40      | 125.03   |
| 23  | c     | 512    | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.89   |
| 23  | C     | 502    | CLA  | CHC-C1C-C2C | -2.79 | 119.01      | 126.95   |
| 23  | C     | 502    | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.89   |
| 23  | C     | 505    | CLA  | CHC-C1C-C2C | -2.79 | 119.02      | 126.95   |
| 23  | B     | 614    | CLA  | CBC-CAC-C3C | -2.79 | 104.86      | 112.42   |
| 23  | D     | 703    | CLA  | O2A-CGA-CBA | 2.79  | 120.34      | 111.83   |
| 23  | d     | 402    | CLA  | O2A-CGA-CBA | 2.79  | 120.33      | 111.83   |
| 26  | f     | 102    | SQD  | C4-C3-C2    | -2.79 | 105.94      | 110.83   |
| 23  | C     | 503    | CLA  | C4C-C3C-C2C | -2.79 | 102.84      | 106.89   |
| 23  | C     | 513    | CLA  | CMB-C2B-C1B | 2.79  | 129.66      | 125.42   |
| 23  | A     | 404[B] | CLA  | C1-C2-C3    | -2.79 | 121.63      | 126.20   |
| 33  | D     | 707[A] | LHG  | O7-C7-C8    | 2.78  | 117.50      | 111.48   |
| 23  | A     | 406[B] | CLA  | CHD-C4C-NC  | 2.78  | 128.55      | 124.23   |
| 26  | A     | 412    | SQD  | C4-C3-C2    | -2.78 | 105.94      | 110.83   |
| 23  | b     | 608    | CLA  | CHC-C1C-C2C | -2.78 | 119.04      | 126.95   |
| 23  | C     | 509    | CLA  | CAC-C3C-C4C | 2.78  | 128.41      | 124.79   |
| 23  | c     | 508    | CLA  | CAC-C3C-C4C | 2.78  | 128.41      | 124.79   |
| 23  | B     | 611    | CLA  | C3B-C4B-NB  | 2.78  | 113.01      | 110.53   |
| 23  | b     | 602    | CLA  | C11-C12-C13 | -2.78 | 106.72      | 115.97   |
| 23  | B     | 602    | CLA  | C4C-C3C-C2C | -2.78 | 102.84      | 106.89   |
| 23  | B     | 615    | CLA  | C4C-C3C-C2C | -2.78 | 102.85      | 106.89   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 504    | CLA  | CHD-C4C-NC  | 2.78  | 128.54      | 124.23   |
| 33  | a     | 420[A] | LHG  | O8-C23-C24  | 2.78  | 120.30      | 111.83   |
| 24  | a     | 416[A] | PHO  | O1D-CGD-CBD | -2.78 | 120.51      | 124.72   |
| 23  | c     | 505    | CLA  | CBC-CAC-C3C | -2.78 | 104.89      | 112.42   |
| 23  | a     | 407[B] | CLA  | CMB-C2B-C1B | 2.78  | 129.65      | 125.42   |
| 23  | B     | 608    | CLA  | CMC-C2C-C1C | 2.78  | 129.37      | 125.03   |
| 23  | a     | 407[A] | CLA  | CAA-C2A-C3A | -2.78 | 105.50      | 113.00   |
| 23  | b     | 613    | CLA  | C4C-C3C-C2C | -2.77 | 102.85      | 106.89   |
| 23  | A     | 406[A] | CLA  | CBC-CAC-C3C | -2.77 | 104.90      | 112.42   |
| 25  | c     | 516    | BCR  | C32-C1-C6   | -2.77 | 105.89      | 110.24   |
| 23  | B     | 607    | CLA  | CMC-C2C-C1C | 2.77  | 129.37      | 125.03   |
| 23  | c     | 511    | CLA  | C4B-C3B-C2B | -2.77 | 103.85      | 107.30   |
| 25  | b     | 618    | BCR  | C15-C14-C13 | -2.77 | 123.39      | 127.28   |
| 23  | B     | 602    | CLA  | CHD-C4C-NC  | 2.77  | 128.53      | 124.23   |
| 23  | D     | 702[B] | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 29  | d     | 404[A] | PL9  | C53-C6-C1   | 2.77  | 120.95      | 115.28   |
| 23  | B     | 606    | CLA  | CBC-CAC-C3C | -2.77 | 104.91      | 112.42   |
| 26  | a     | 411[B] | SQD  | C45-O47-C7  | -2.77 | 111.17      | 117.80   |
| 34  | C     | 501    | LMG  | C8-O7-C10   | -2.77 | 111.18      | 117.80   |
| 23  | c     | 509    | CLA  | O2A-CGA-CBA | 2.77  | 120.27      | 111.83   |
| 26  | B     | 620    | SQD  | C4-C3-C2    | 2.77  | 115.68      | 110.83   |
| 33  | d     | 405[B] | LHG  | O8-C23-O10  | -2.76 | 116.71      | 123.63   |
| 25  | A     | 409    | BCR  | C8-C7-C6    | -2.76 | 119.61      | 127.00   |
| 29  | D     | 705[A] | PL9  | C42-C41-C39 | -2.76 | 104.03      | 113.19   |
| 23  | a     | 409    | CLA  | C4B-C3B-C2B | -2.76 | 103.87      | 107.30   |
| 23  | c     | 512    | CLA  | O2A-CGA-CBA | 2.76  | 120.26      | 111.83   |
| 23  | B     | 615    | CLA  | C4B-C3B-C2B | -2.76 | 103.87      | 107.30   |
| 23  | C     | 511    | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.89   |
| 23  | A     | 404[B] | CLA  | CHC-C1C-C2C | -2.76 | 119.11      | 126.95   |
| 36  | c     | 517[A] | DGD  | O3G-C3G-C2G | -2.76 | 104.11      | 110.82   |
| 23  | B     | 611    | CLA  | C4A-NA-C1A  | -2.76 | 105.42      | 106.68   |
| 23  | c     | 509    | CLA  | CAA-C2A-C3A | -2.76 | 105.54      | 113.00   |
| 29  | D     | 705[B] | PL9  | C37-C38-C39 | -2.76 | 121.31      | 127.62   |
| 23  | C     | 504    | CLA  | O2D-CGD-O1D | -2.76 | 118.48      | 123.85   |
| 23  | b     | 605    | CLA  | C4-C3-C5    | 2.76  | 120.01      | 115.23   |
| 23  | c     | 511    | CLA  | CAC-C3C-C4C | 2.75  | 128.37      | 124.79   |
| 23  | c     | 508    | CLA  | CHD-C4C-NC  | 2.75  | 128.50      | 124.23   |
| 36  | H     | 102    | DGD  | O1G-C1A-C2A | 2.75  | 120.21      | 111.83   |
| 25  | b     | 619    | BCR  | C24-C23-C22 | -2.75 | 122.17      | 126.23   |
| 23  | B     | 601    | CLA  | C3B-C4B-NB  | 2.75  | 112.98      | 110.53   |
| 23  | a     | 406[B] | CLA  | C1-C2-C3    | -2.75 | 121.70      | 126.20   |
| 23  | c     | 506    | CLA  | O2A-CGA-CBA | 2.74  | 120.20      | 111.83   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 36  | c     | 517[B] | DGD  | C2G-O2G-C1B | -2.74 | 111.23      | 117.80   |
| 33  | D     | 707[B] | LHG  | O8-C23-O10  | -2.74 | 116.77      | 123.63   |
| 23  | A     | 404[A] | CLA  | CAC-C3C-C4C | 2.74  | 128.36      | 124.79   |
| 24  | A     | 417[B] | PHO  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 23  | b     | 606    | CLA  | CHC-C1C-C2C | -2.74 | 119.16      | 126.95   |
| 25  | H     | 101    | BCR  | C10-C11-C12 | -2.74 | 115.26      | 123.20   |
| 23  | c     | 514    | CLA  | C2A-C1A-CHA | -2.74 | 119.11      | 123.87   |
| 33  | d     | 406[B] | LHG  | O8-C23-C24  | 2.74  | 120.19      | 111.83   |
| 23  | c     | 502    | CLA  | CHD-C4C-NC  | 2.74  | 128.48      | 124.23   |
| 23  | a     | 406[A] | CLA  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 36  | C     | 517[A] | DGD  | O3G-C3G-C2G | -2.74 | 104.16      | 110.82   |
| 36  | C     | 518[A] | DGD  | O1G-C1A-O1A | -2.74 | 116.78      | 123.63   |
| 23  | d     | 401[A] | CLA  | CAA-C2A-C3A | -2.74 | 105.61      | 113.00   |
| 23  | b     | 612    | CLA  | CHD-C4C-NC  | 2.73  | 128.47      | 124.23   |
| 23  | d     | 402    | CLA  | C2A-C1A-CHA | -2.73 | 119.12      | 123.87   |
| 23  | a     | 407[B] | CLA  | C3B-C4B-NB  | 2.73  | 112.97      | 110.53   |
| 23  | a     | 407[B] | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 23  | B     | 606    | CLA  | C4B-C3B-C2B | -2.73 | 103.91      | 107.30   |
| 23  | a     | 405[B] | CLA  | CHD-C4C-NC  | 2.73  | 128.47      | 124.23   |
| 23  | b     | 602    | CLA  | C4-C3-C5    | 2.73  | 119.97      | 115.23   |
| 23  | A     | 406[A] | CLA  | C2A-C1A-CHA | -2.73 | 119.13      | 123.87   |
| 23  | C     | 512    | CLA  | CMB-C2B-C1B | 2.73  | 129.58      | 125.42   |
| 23  | A     | 404[A] | CLA  | C2A-C1A-CHA | -2.73 | 119.13      | 123.87   |
| 34  | C     | 501    | LMG  | C6-C5-C4    | 2.73  | 119.72      | 113.02   |
| 23  | b     | 605    | CLA  | C3B-C4B-NB  | 2.73  | 112.97      | 110.53   |
| 35  | b     | 622    | HTG  | C1'-S1-C1   | 2.73  | 106.34      | 100.45   |
| 23  | b     | 610    | CLA  | O2D-CGD-O1D | -2.73 | 118.54      | 123.85   |
| 25  | b     | 618    | BCR  | C37-C22-C21 | -2.73 | 118.40      | 122.82   |
| 25  | t     | 102    | BCR  | C35-C13-C12 | 2.73  | 122.25      | 118.09   |
| 35  | b     | 622    | HTG  | O2-C2-C3    | -2.73 | 103.95      | 110.38   |
| 23  | a     | 407[A] | CLA  | O2D-CGD-O1D | -2.73 | 118.54      | 123.85   |
| 23  | D     | 703    | CLA  | CAA-C2A-C3A | -2.73 | 105.64      | 113.00   |
| 23  | A     | 406[B] | CLA  | C2A-C1A-CHA | -2.72 | 119.14      | 123.87   |
| 23  | a     | 407[B] | CLA  | CAA-C2A-C3A | -2.72 | 105.64      | 113.00   |
| 23  | A     | 408    | CLA  | O2A-CGA-CBA | 2.72  | 120.14      | 111.83   |
| 33  | a     | 420[B] | LHG  | O8-C23-C24  | 2.72  | 120.14      | 111.83   |
| 23  | C     | 512    | CLA  | CHD-C4C-NC  | 2.72  | 128.45      | 124.23   |
| 23  | c     | 509    | CLA  | C4B-C3B-C2B | -2.72 | 103.92      | 107.30   |
| 29  | D     | 705[B] | PL9  | C45-C44-C46 | 2.72  | 119.95      | 115.23   |
| 25  | b     | 617    | BCR  | C24-C23-C22 | -2.72 | 122.21      | 126.23   |
| 25  | B     | 617    | BCR  | C31-C1-C6   | -2.72 | 105.98      | 110.24   |
| 23  | B     | 615    | CLA  | CHC-C1C-C2C | -2.72 | 119.23      | 126.95   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25  | H     | 101    | BCR  | C31-C1-C6   | -2.72 | 105.98      | 110.24   |
| 29  | A     | 414[A] | PL9  | C10-C9-C8   | -2.71 | 116.66      | 123.63   |
| 23  | c     | 503    | CLA  | C4B-C3B-C2B | -2.71 | 103.93      | 107.30   |
| 36  | c     | 517[A] | DGD  | C3G-C2G-C1G | -2.71 | 105.46      | 111.78   |
| 32  | a     | 417    | LMT  | C3'-C4'-C5' | -2.71 | 104.92      | 110.93   |
| 23  | c     | 502    | CLA  | CBC-CAC-C3C | -2.71 | 105.07      | 112.42   |
| 23  | b     | 602    | CLA  | CMB-C2B-C1B | 2.71  | 129.55      | 125.42   |
| 23  | c     | 514    | CLA  | CHD-C4C-NC  | 2.71  | 128.43      | 124.23   |
| 23  | D     | 702[B] | CLA  | O2A-CGA-O1A | -2.71 | 116.85      | 123.63   |
| 23  | c     | 507    | CLA  | C4C-C3C-C2C | -2.71 | 102.95      | 106.89   |
| 33  | D     | 706[A] | LHG  | O8-C23-C24  | 2.71  | 120.09      | 111.83   |
| 24  | a     | 416[B] | PHO  | O2D-CGD-O1D | -2.71 | 118.58      | 123.85   |
| 23  | c     | 506    | CLA  | CAC-C3C-C4C | 2.71  | 128.31      | 124.79   |
| 25  | B     | 619    | BCR  | C38-C26-C25 | -2.71 | 121.53      | 124.48   |
| 38  | F     | 102    | HEM  | CBA-CAA-C2A | -2.71 | 105.05      | 112.53   |
| 23  | D     | 703    | CLA  | C4-C3-C5    | 2.71  | 119.92      | 115.23   |
| 32  | m     | 103    | LMT  | C3'-C4'-C5' | -2.70 | 104.94      | 110.93   |
| 23  | B     | 616    | CLA  | CHD-C4C-NC  | 2.70  | 128.42      | 124.23   |
| 29  | A     | 414[B] | PL9  | C40-C39-C41 | 2.70  | 119.92      | 115.23   |
| 24  | A     | 407[B] | PHO  | O2A-CGA-CBA | 2.70  | 120.08      | 111.83   |
| 23  | B     | 607    | CLA  | CHC-C1C-C2C | -2.70 | 119.27      | 126.95   |
| 29  | D     | 705[A] | PL9  | C2-C1-C6    | 2.70  | 122.21      | 119.00   |
| 23  | C     | 508    | CLA  | O2A-CGA-CBA | 2.70  | 120.07      | 111.83   |
| 33  | L     | 101[A] | LHG  | O8-C23-C24  | 2.70  | 120.06      | 111.83   |
| 29  | A     | 414[B] | PL9  | C42-C43-C44 | -2.70 | 121.45      | 127.62   |
| 35  | o     | 301    | HTG  | O2-C2-C3    | -2.70 | 104.02      | 110.38   |
| 23  | c     | 504    | CLA  | C3B-C4B-NB  | 2.70  | 112.94      | 110.53   |
| 23  | D     | 703    | CLA  | C2A-C1A-CHA | -2.70 | 119.19      | 123.87   |
| 23  | b     | 601    | CLA  | C1-O2A-CGA  | 2.69  | 123.17      | 116.65   |
| 23  | a     | 407[A] | CLA  | CHC-C1C-C2C | -2.69 | 119.29      | 126.95   |
| 23  | a     | 406[A] | CLA  | O2A-CGA-CBA | 2.69  | 120.05      | 111.83   |
| 23  | b     | 609    | CLA  | CHC-C1C-C2C | -2.69 | 119.30      | 126.95   |
| 23  | a     | 409    | CLA  | CMB-C2B-C1B | 2.69  | 129.52      | 125.42   |
| 26  | A     | 410[A] | SQD  | O48-C23-O10 | -2.69 | 116.89      | 123.63   |
| 25  | k     | 101    | BCR  | C15-C14-C13 | -2.69 | 123.50      | 127.28   |
| 23  | B     | 609    | CLA  | CHD-C4C-NC  | 2.69  | 128.41      | 124.23   |
| 23  | B     | 615    | CLA  | C11-C10-C8  | -2.69 | 107.02      | 115.97   |
| 23  | C     | 506    | CLA  | CMC-C2C-C1C | 2.69  | 129.24      | 125.03   |
| 23  | A     | 405[A] | CLA  | CMA-C3A-C2A | -2.69 | 103.58      | 113.98   |
| 24  | A     | 407[B] | PHO  | O2D-CGD-O1D | -2.69 | 118.61      | 123.85   |
| 32  | B     | 627    | LMT  | O1'-C1'-C2' | 2.69  | 112.36      | 108.27   |
| 23  | b     | 610    | CLA  | C4-C3-C5    | 2.69  | 119.90      | 115.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 36  | H     | 102    | DGD  | O1G-C1A-O1A | -2.69 | 116.90      | 123.63   |
| 23  | a     | 407[B] | CLA  | C4-C3-C5    | 2.69  | 119.90      | 115.23   |
| 29  | A     | 414[A] | PL9  | C40-C39-C41 | 2.69  | 119.90      | 115.23   |
| 23  | A     | 405[A] | CLA  | CAC-C3C-C4C | 2.69  | 128.29      | 124.79   |
| 23  | B     | 603    | CLA  | CHD-C4C-NC  | 2.69  | 128.40      | 124.23   |
| 23  | a     | 405[A] | CLA  | C4C-C3C-C2C | -2.69 | 102.98      | 106.89   |
| 23  | b     | 603    | CLA  | CHC-C1C-C2C | -2.69 | 119.32      | 126.95   |
| 23  | B     | 612    | CLA  | C4B-C3B-C2B | -2.69 | 103.96      | 107.30   |
| 40  | v     | 201    | HEC  | CHA-C1A-NA  | 2.68  | 127.38      | 124.45   |
| 23  | d     | 401[B] | CLA  | CAA-C2A-C3A | -2.68 | 105.75      | 113.00   |
| 23  | B     | 610    | CLA  | CHD-C4C-NC  | 2.68  | 128.39      | 124.23   |
| 23  | B     | 609    | CLA  | CHC-C1C-C2C | -2.68 | 119.33      | 126.95   |
| 23  | b     | 616    | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 23  | B     | 601    | CLA  | O2A-CGA-CBA | 2.68  | 120.01      | 111.83   |
| 23  | B     | 601    | CLA  | CHC-C1C-C2C | -2.68 | 119.33      | 126.95   |
| 23  | C     | 514    | CLA  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 23  | C     | 503    | CLA  | O2D-CGD-O1D | -2.68 | 118.64      | 123.85   |
| 24  | A     | 407[B] | PHO  | CMB-C2B-C3B | 2.68  | 130.03      | 124.68   |
| 25  | C     | 516    | BCR  | C11-C10-C9  | -2.68 | 123.53      | 127.28   |
| 23  | B     | 607    | CLA  | CBC-CAC-C3C | -2.67 | 105.17      | 112.42   |
| 25  | Y     | 101    | BCR  | C37-C22-C23 | 2.67  | 122.17      | 118.09   |
| 25  | b     | 619    | BCR  | C38-C26-C25 | -2.67 | 121.57      | 124.48   |
| 25  | k     | 101    | BCR  | C39-C30-C25 | -2.67 | 106.05      | 110.24   |
| 29  | d     | 404[B] | PL9  | C27-C28-C29 | -2.67 | 121.51      | 127.62   |
| 23  | C     | 502    | CLA  | O2A-CGA-CBA | 2.67  | 119.98      | 111.83   |
| 36  | c     | 519    | DGD  | O1G-C1A-C2A | 2.67  | 119.98      | 111.83   |
| 36  | C     | 519    | DGD  | O3G-C3G-C2G | -2.67 | 104.32      | 110.82   |
| 32  | B     | 630    | LMT  | O5'-C5'-C4' | 2.67  | 115.24      | 109.72   |
| 23  | A     | 406[A] | CLA  | CMA-C3A-C2A | -2.67 | 103.66      | 113.98   |
| 23  | b     | 616    | CLA  | OBD-CAD-C3D | -2.67 | 122.18      | 128.42   |
| 32  | M     | 101    | LMT  | C3'-C4'-C5' | -2.67 | 105.02      | 110.93   |
| 23  | c     | 504    | CLA  | CMC-C2C-C1C | 2.67  | 129.20      | 125.03   |
| 33  | D     | 706[B] | LHG  | O8-C23-C24  | 2.67  | 119.97      | 111.83   |
| 23  | B     | 608    | CLA  | CHB-C4A-NA  | 2.66  | 128.25      | 124.40   |
| 23  | C     | 506    | CLA  | O2A-CGA-CBA | 2.66  | 119.95      | 111.83   |
| 33  | d     | 405[B] | LHG  | O8-C23-C24  | 2.66  | 119.95      | 111.83   |
| 26  | a     | 412    | SQD  | C3-C4-C5    | 2.66  | 115.06      | 110.23   |
| 26  | X     | 101    | SQD  | O47-C7-O49  | -2.66 | 117.48      | 123.70   |
| 23  | b     | 612    | CLA  | CHC-C1C-C2C | -2.66 | 119.38      | 126.95   |
| 23  | b     | 616    | CLA  | C3B-C4B-NB  | 2.66  | 112.91      | 110.53   |
| 23  | a     | 405[A] | CLA  | CAC-C3C-C4C | 2.66  | 128.25      | 124.79   |
| 25  | K     | 102    | BCR  | C29-C30-C25 | 2.66  | 114.30      | 110.44   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 514    | CLA  | CHC-C1C-C2C | -2.66 | 119.39      | 126.95   |
| 23  | d     | 402    | CLA  | CBC-CAC-C3C | -2.66 | 105.21      | 112.42   |
| 25  | d     | 403    | BCR  | C37-C22-C23 | 2.66  | 122.15      | 118.09   |
| 23  | a     | 406[B] | CLA  | CBC-CAC-C3C | -2.66 | 105.22      | 112.42   |
| 24  | A     | 407[B] | PHO  | O1D-CGD-CBD | -2.65 | 120.70      | 124.72   |
| 23  | B     | 616    | CLA  | CHC-C1C-C2C | -2.65 | 119.41      | 126.95   |
| 23  | B     | 607    | CLA  | C4C-C3C-C2C | -2.65 | 103.03      | 106.89   |
| 24  | A     | 417[A] | PHO  | O2D-CGD-O1D | -2.65 | 118.69      | 123.85   |
| 23  | a     | 409    | CLA  | O2A-CGA-O1A | -2.65 | 117.00      | 123.63   |
| 24  | a     | 416[B] | PHO  | CMB-C2B-C3B | 2.65  | 129.98      | 124.68   |
| 23  | B     | 606    | CLA  | C4C-C3C-C2C | -2.65 | 103.04      | 106.89   |
| 23  | b     | 604    | CLA  | O2A-CGA-CBA | 2.65  | 119.91      | 111.83   |
| 23  | B     | 603    | CLA  | C7-C6-C5    | -2.65 | 106.20      | 113.26   |
| 23  | A     | 408    | CLA  | CMA-C3A-C2A | -2.65 | 103.75      | 113.98   |
| 23  | C     | 505    | CLA  | C4C-C3C-C2C | -2.65 | 103.04      | 106.89   |
| 23  | B     | 602    | CLA  | C4B-C3B-C2B | -2.65 | 104.01      | 107.30   |
| 27  | b     | 628    | GOL  | C3-C2-C1    | -2.65 | 102.09      | 111.80   |
| 25  | h     | 101    | BCR  | C24-C23-C22 | -2.65 | 122.32      | 126.23   |
| 23  | b     | 611    | CLA  | CHD-C4C-NC  | 2.64  | 128.33      | 124.23   |
| 23  | c     | 504    | CLA  | C4B-C3B-C2B | -2.64 | 104.02      | 107.30   |
| 23  | b     | 603    | CLA  | CBC-CAC-C3C | -2.64 | 105.25      | 112.42   |
| 24  | a     | 416[A] | PHO  | CBA-CAA-C2A | -2.64 | 105.99      | 113.78   |
| 23  | A     | 404[B] | CLA  | CHD-C4C-NC  | 2.64  | 128.32      | 124.23   |
| 23  | a     | 406[B] | CLA  | C4C-C3C-C2C | -2.64 | 103.05      | 106.89   |
| 23  | B     | 606    | CLA  | CHC-C1C-C2C | -2.64 | 119.45      | 126.95   |
| 33  | A     | 419[B] | LHG  | O7-C7-O9    | -2.64 | 117.54      | 123.70   |
| 38  | F     | 102    | HEM  | C3B-C4B-NB  | -2.64 | 107.57      | 109.47   |
| 23  | b     | 605    | CLA  | O2A-CGA-O1A | -2.64 | 117.03      | 123.63   |
| 23  | C     | 504    | CLA  | CMC-C2C-C1C | 2.64  | 129.16      | 125.03   |
| 23  | c     | 505    | CLA  | CHC-C1C-C2C | -2.64 | 119.45      | 126.95   |
| 23  | A     | 406[A] | CLA  | C4C-C3C-C2C | -2.64 | 103.05      | 106.89   |
| 23  | a     | 405[B] | CLA  | C1-C2-C3    | -2.64 | 121.88      | 126.20   |
| 23  | D     | 703    | CLA  | CMC-C2C-C1C | 2.63  | 129.15      | 125.03   |
| 23  | b     | 607    | CLA  | CHC-C1C-C2C | -2.63 | 119.47      | 126.95   |
| 26  | b     | 620    | SQD  | O8-S-C6     | 2.63  | 111.05      | 105.97   |
| 23  | d     | 401[B] | CLA  | C4C-C3C-C2C | -2.63 | 103.06      | 106.89   |
| 23  | b     | 610    | CLA  | CHC-C1C-C2C | -2.63 | 119.47      | 126.95   |
| 25  | D     | 704    | BCR  | C3-C4-C5    | -2.63 | 109.36      | 114.06   |
| 23  | D     | 702[A] | CLA  | CMC-C2C-C1C | 2.63  | 129.15      | 125.03   |
| 23  | a     | 407[B] | CLA  | O2A-CGA-O1A | -2.63 | 117.05      | 123.63   |
| 23  | B     | 603    | CLA  | C4-C3-C5    | 2.63  | 119.79      | 115.23   |
| 32  | B     | 630    | LMT  | O1'-C1'-C2' | 2.63  | 112.27      | 108.27   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 507    | CLA  | O2A-CGA-CBA | 2.63  | 119.85      | 111.83   |
| 36  | C     | 517[B] | DGD  | C2G-O2G-C1B | -2.63 | 111.51      | 117.80   |
| 25  | T     | 102    | BCR  | C21-C20-C19 | -2.63 | 115.58      | 123.20   |
| 23  | b     | 606    | CLA  | CMB-C2B-C1B | 2.63  | 129.42      | 125.42   |
| 23  | c     | 503    | CLA  | O2A-CGA-CBA | 2.63  | 119.84      | 111.83   |
| 23  | D     | 702[B] | CLA  | C4-C3-C5    | 2.63  | 119.79      | 115.23   |
| 32  | A     | 420    | LMT  | O5'-C5'-C6' | 2.63  | 112.95      | 106.44   |
| 23  | C     | 508    | CLA  | CBC-CAC-C3C | -2.63 | 105.30      | 112.42   |
| 25  | t     | 102    | BCR  | C12-C13-C14 | -2.63 | 114.88      | 119.01   |
| 23  | A     | 405[A] | CLA  | OBD-CAD-C3D | -2.63 | 122.28      | 128.42   |
| 36  | H     | 102    | DGD  | C3G-C2G-C1G | -2.63 | 105.66      | 111.78   |
| 23  | a     | 407[B] | CLA  | CHC-C1C-C2C | -2.62 | 119.49      | 126.95   |
| 36  | c     | 517[B] | DGD  | O3G-C3G-C2G | -2.62 | 104.44      | 110.82   |
| 23  | d     | 401[B] | CLA  | CBC-CAC-C3C | -2.62 | 105.31      | 112.42   |
| 23  | B     | 604    | CLA  | CMB-C2B-C1B | 2.62  | 129.41      | 125.42   |
| 23  | b     | 612    | CLA  | CAC-C3C-C4C | 2.62  | 128.20      | 124.79   |
| 23  | A     | 404[B] | CLA  | CMC-C2C-C1C | 2.62  | 129.13      | 125.03   |
| 23  | b     | 608    | CLA  | C11-C12-C13 | -2.62 | 107.25      | 115.97   |
| 23  | A     | 404[A] | CLA  | CMA-C3A-C2A | -2.62 | 103.85      | 113.98   |
| 23  | a     | 406[B] | CLA  | O2A-CGA-CBA | 2.62  | 119.82      | 111.83   |
| 23  | b     | 602    | CLA  | O2A-CGA-O1A | -2.62 | 117.08      | 123.63   |
| 23  | C     | 502    | CLA  | CBC-CAC-C3C | -2.62 | 105.33      | 112.42   |
| 23  | C     | 514    | CLA  | CHD-C4C-NC  | 2.62  | 128.29      | 124.23   |
| 25  | H     | 101    | BCR  | C7-C8-C9    | -2.62 | 122.36      | 126.23   |
| 23  | A     | 406[A] | CLA  | CMC-C2C-C1C | 2.62  | 129.12      | 125.03   |
| 23  | C     | 507    | CLA  | CAA-C2A-C3A | -2.62 | 105.93      | 113.00   |
| 23  | B     | 606    | CLA  | C1-O2A-CGA  | 2.62  | 122.98      | 116.65   |
| 23  | a     | 405[B] | CLA  | C2A-C1A-CHA | -2.62 | 119.33      | 123.87   |
| 29  | a     | 414[A] | PL9  | C53-C6-C1   | 2.62  | 120.64      | 115.28   |
| 29  | d     | 404[B] | PL9  | C51-C49-C50 | 2.62  | 120.61      | 114.59   |
| 23  | b     | 607    | CLA  | CBC-CAC-C3C | -2.61 | 105.33      | 112.42   |
| 23  | C     | 507    | CLA  | C2A-C1A-CHA | -2.61 | 119.33      | 123.87   |
| 23  | b     | 602    | CLA  | CMA-C3A-C4A | -2.61 | 104.75      | 111.77   |
| 23  | a     | 405[A] | CLA  | C2A-C1A-CHA | -2.61 | 119.34      | 123.87   |
| 23  | B     | 601    | CLA  | C4B-C3B-C2B | -2.61 | 104.06      | 107.30   |
| 23  | b     | 616    | CLA  | C4B-C3B-C2B | -2.61 | 104.06      | 107.30   |
| 23  | B     | 608    | CLA  | CHD-C4C-NC  | 2.61  | 128.28      | 124.23   |
| 23  | B     | 602    | CLA  | CMA-C3A-C4A | -2.61 | 104.76      | 111.77   |
| 36  | C     | 518[B] | DGD  | C2G-O2G-C1B | -2.61 | 111.55      | 117.80   |
| 23  | c     | 507    | CLA  | CHD-C4C-NC  | 2.61  | 128.28      | 124.23   |
| 23  | c     | 512    | CLA  | CMC-C2C-C1C | 2.61  | 129.11      | 125.03   |
| 36  | C     | 517[B] | DGD  | O6D-C1D-O3G | -2.61 | 103.88      | 110.04   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | A     | 407[A] | PHO  | O2A-CGA-CBA | 2.61  | 119.78      | 111.83   |
| 33  | D     | 706[A] | LHG  | O7-C7-C8    | 2.61  | 117.12      | 111.48   |
| 23  | A     | 408    | CLA  | CMC-C2C-C1C | 2.61  | 129.10      | 125.03   |
| 23  | b     | 614    | CLA  | CMC-C2C-C1C | 2.61  | 129.10      | 125.03   |
| 23  | C     | 504    | CLA  | CHC-C1C-C2C | -2.60 | 119.55      | 126.95   |
| 25  | a     | 410    | BCR  | C33-C5-C6   | -2.60 | 121.64      | 124.48   |
| 23  | B     | 607    | CLA  | CMB-C2B-C1B | 2.60  | 129.38      | 125.42   |
| 23  | c     | 502    | CLA  | C4B-C3B-C2B | -2.60 | 104.07      | 107.30   |
| 23  | a     | 406[B] | CLA  | CMA-C3A-C2A | -2.60 | 103.92      | 113.98   |
| 23  | C     | 503    | CLA  | C2A-C1A-CHA | -2.60 | 119.35      | 123.87   |
| 23  | a     | 407[B] | CLA  | CAC-C3C-C4C | 2.60  | 128.17      | 124.79   |
| 23  | C     | 510    | CLA  | C11-C12-C13 | -2.60 | 107.32      | 115.97   |
| 23  | c     | 514    | CLA  | C1-C2-C3    | -2.60 | 121.94      | 126.20   |
| 23  | b     | 602    | CLA  | CHB-C1B-C2B | -2.60 | 119.88      | 127.43   |
| 36  | c     | 517[A] | DGD  | O1G-C1A-O1A | -2.60 | 117.13      | 123.63   |
| 32  | B     | 627    | LMT  | C1B-C2B-C3B | 2.60  | 115.47      | 110.01   |
| 23  | c     | 506    | CLA  | O2A-CGA-O1A | -2.60 | 117.13      | 123.63   |
| 23  | B     | 604    | CLA  | C6-C7-C8    | -2.60 | 107.33      | 115.97   |
| 23  | c     | 507    | CLA  | CAA-C2A-C3A | -2.59 | 105.99      | 113.00   |
| 23  | b     | 614    | CLA  | C2A-C1A-CHA | -2.59 | 119.36      | 123.87   |
| 23  | d     | 402    | CLA  | CHC-C1C-C2C | -2.59 | 119.58      | 126.95   |
| 23  | a     | 407[B] | CLA  | C2A-C1A-CHA | -2.59 | 119.36      | 123.87   |
| 23  | C     | 503    | CLA  | CAC-C3C-C4C | 2.59  | 128.16      | 124.79   |
| 23  | b     | 607    | CLA  | C2A-C1A-CHA | -2.59 | 119.37      | 123.87   |
| 29  | d     | 404[A] | PL9  | C17-C18-C19 | -2.59 | 121.69      | 127.62   |
| 25  | d     | 403    | BCR  | C40-C30-C39 | 2.59  | 116.06      | 108.63   |
| 23  | C     | 509    | CLA  | O2A-CGA-O1A | -2.59 | 117.14      | 123.63   |
| 23  | B     | 616    | CLA  | CAC-C3C-C4C | 2.59  | 128.16      | 124.79   |
| 29  | D     | 705[A] | PL9  | C40-C39-C41 | 2.59  | 119.72      | 115.23   |
| 34  | C     | 520    | LMG  | O8-C28-O10  | -2.59 | 117.15      | 123.63   |
| 23  | c     | 512    | CLA  | CBC-CAC-C3C | -2.59 | 105.40      | 112.42   |
| 23  | C     | 505    | CLA  | CAC-C3C-C4C | 2.59  | 128.16      | 124.79   |
| 25  | a     | 410    | BCR  | C24-C23-C22 | -2.59 | 122.41      | 126.23   |
| 23  | D     | 702[A] | CLA  | C2A-C1A-CHA | -2.59 | 119.38      | 123.87   |
| 23  | a     | 407[A] | CLA  | O2A-CGA-CBA | 2.59  | 119.72      | 111.83   |
| 23  | b     | 612    | CLA  | C2A-C1A-CHA | -2.58 | 119.38      | 123.87   |
| 36  | c     | 517[B] | DGD  | O6D-C1D-O3G | -2.58 | 103.94      | 110.04   |
| 23  | D     | 703    | CLA  | CHD-C4C-NC  | 2.58  | 128.24      | 124.23   |
| 23  | B     | 613    | CLA  | CHC-C1C-C2C | -2.58 | 119.61      | 126.95   |
| 23  | C     | 511    | CLA  | O2D-CGD-O1D | -2.58 | 118.82      | 123.85   |
| 24  | A     | 407[B] | PHO  | CMA-C3A-C4A | -2.58 | 109.05      | 114.61   |
| 26  | A     | 410[B] | SQD  | O48-C23-O10 | -2.58 | 117.17      | 123.63   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 505    | CLA  | CBC-CAC-C3C | -2.58 | 105.42      | 112.42   |
| 25  | t     | 102    | BCR  | C37-C22-C23 | 2.58  | 122.03      | 118.09   |
| 29  | A     | 414[B] | PL9  | C47-C48-C49 | -2.58 | 119.04      | 127.64   |
| 23  | c     | 513    | CLA  | O2A-CGA-O1A | -2.58 | 117.17      | 123.63   |
| 23  | B     | 605    | CLA  | C2A-C1A-CHA | -2.58 | 119.39      | 123.87   |
| 23  | D     | 702[A] | CLA  | O2D-CGD-O1D | -2.58 | 118.83      | 123.85   |
| 29  | D     | 705[B] | PL9  | C42-C41-C39 | -2.58 | 104.64      | 113.19   |
| 23  | A     | 406[A] | CLA  | C4-C3-C5    | 2.58  | 119.70      | 115.23   |
| 23  | b     | 604    | CLA  | C4-C3-C5    | 2.58  | 119.70      | 115.23   |
| 26  | B     | 620    | SQD  | C1-O5-C5    | -2.58 | 108.69      | 113.72   |
| 32  | T     | 101    | LMT  | C3'-C4'-C5' | -2.58 | 105.22      | 110.93   |
| 36  | H     | 102    | DGD  | C3E-C4E-C5E | -2.58 | 105.56      | 110.23   |
| 23  | C     | 511    | CLA  | O2A-CGA-CBA | 2.58  | 119.69      | 111.83   |
| 23  | C     | 508    | CLA  | CHC-C1C-C2C | -2.57 | 119.63      | 126.95   |
| 40  | v     | 201    | HEC  | CBD-CAD-C3D | -2.57 | 105.42      | 112.53   |
| 23  | a     | 405[A] | CLA  | CMA-C3A-C4A | -2.57 | 104.87      | 111.77   |
| 29  | a     | 414[B] | PL9  | C40-C39-C41 | 2.57  | 119.69      | 115.23   |
| 23  | D     | 703    | CLA  | CHC-C1C-C2C | -2.57 | 119.65      | 126.95   |
| 23  | b     | 614    | CLA  | C4-C3-C5    | 2.57  | 119.68      | 115.23   |
| 23  | C     | 508    | CLA  | CHD-C4C-NC  | 2.57  | 128.21      | 124.23   |
| 23  | B     | 604    | CLA  | CMC-C2C-C1C | 2.57  | 129.04      | 125.03   |
| 29  | a     | 414[B] | PL9  | C53-C6-C1   | 2.56  | 120.53      | 115.28   |
| 23  | c     | 512    | CLA  | C1-O2A-CGA  | 2.56  | 122.85      | 116.65   |
| 34  | c     | 520    | LMG  | C8-O7-C10   | -2.56 | 111.67      | 117.80   |
| 32  | B     | 630    | LMT  | C3'-C4'-C5' | -2.56 | 105.25      | 110.93   |
| 23  | B     | 604    | CLA  | C4-C3-C5    | 2.56  | 119.67      | 115.23   |
| 25  | C     | 515    | BCR  | C20-C21-C22 | -2.56 | 123.69      | 127.28   |
| 23  | B     | 601    | CLA  | CAC-C3C-C4C | 2.56  | 128.12      | 124.79   |
| 35  | o     | 301    | HTG  | C1-O5-C5    | 2.56  | 117.15      | 112.56   |
| 29  | D     | 705[A] | PL9  | C27-C28-C29 | -2.56 | 121.77      | 127.62   |
| 23  | d     | 401[B] | CLA  | O2A-CGA-O1A | -2.56 | 117.23      | 123.63   |
| 23  | C     | 504    | CLA  | CBC-CAC-C3C | -2.55 | 105.50      | 112.42   |
| 23  | B     | 604    | CLA  | C6-C5-C3    | -2.55 | 107.25      | 113.47   |
| 23  | c     | 510    | CLA  | C4-C3-C5    | 2.55  | 119.66      | 115.23   |
| 23  | A     | 405[A] | CLA  | C2A-C1A-CHA | -2.55 | 119.44      | 123.87   |
| 26  | X     | 101    | SQD  | O5-C1-O6    | 2.55  | 116.08      | 110.04   |
| 23  | B     | 616    | CLA  | O2A-CGA-CBA | 2.55  | 119.62      | 111.83   |
| 32  | B     | 629    | LMT  | O5B-C5B-C4B | 2.55  | 114.30      | 109.70   |
| 23  | c     | 506    | CLA  | C4-C3-C5    | 2.55  | 119.66      | 115.23   |
| 23  | C     | 514    | CLA  | CAA-C2A-C3A | -2.55 | 106.10      | 113.00   |
| 23  | c     | 514    | CLA  | O2A-CGA-O1A | -2.55 | 117.25      | 123.63   |
| 23  | a     | 407[A] | CLA  | C2A-C1A-CHA | -2.55 | 119.45      | 123.87   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 613    | CLA  | O2D-CGD-O1D | -2.55 | 118.89      | 123.85   |
| 23  | a     | 407[A] | CLA  | O2A-CGA-O1A | -2.54 | 117.26      | 123.63   |
| 29  | a     | 414[A] | PL9  | C47-C48-C49 | -2.54 | 119.16      | 127.64   |
| 23  | a     | 407[B] | CLA  | O2A-CGA-CBA | 2.54  | 119.59      | 111.83   |
| 24  | A     | 417[B] | PHO  | O1D-CGD-CBD | -2.54 | 120.87      | 124.72   |
| 23  | A     | 408    | CLA  | C4-C3-C5    | 2.54  | 119.64      | 115.23   |
| 23  | C     | 505    | CLA  | CMB-C2B-C1B | 2.54  | 129.29      | 125.42   |
| 23  | c     | 511    | CLA  | C2A-C1A-CHA | -2.54 | 119.46      | 123.87   |
| 23  | B     | 607    | CLA  | C2A-C1A-CHA | -2.54 | 119.46      | 123.87   |
| 23  | b     | 606    | CLA  | C1-C2-C3    | -2.54 | 122.04      | 126.20   |
| 23  | b     | 604    | CLA  | C6-C5-C3    | -2.54 | 107.29      | 113.47   |
| 23  | D     | 702[B] | CLA  | C4B-C3B-C2B | -2.54 | 104.15      | 107.30   |
| 23  | B     | 612    | CLA  | C3B-C4B-NB  | 2.54  | 112.79      | 110.53   |
| 23  | C     | 511    | CLA  | CAC-C3C-C4C | 2.53  | 128.09      | 124.79   |
| 23  | a     | 406[A] | CLA  | C2A-C1A-CHA | -2.53 | 119.47      | 123.87   |
| 23  | b     | 614    | CLA  | C4B-C3B-C2B | -2.53 | 104.15      | 107.30   |
| 26  | a     | 412    | SQD  | C1-O5-C5    | 2.53  | 118.66      | 113.72   |
| 23  | A     | 406[B] | CLA  | CMC-C2C-C1C | 2.53  | 128.99      | 125.03   |
| 23  | c     | 503    | CLA  | CMC-C2C-C1C | 2.53  | 128.99      | 125.03   |
| 23  | c     | 513    | CLA  | CAC-C3C-C4C | 2.53  | 128.08      | 124.79   |
| 23  | c     | 506    | CLA  | CHD-C4C-NC  | 2.53  | 128.15      | 124.23   |
| 32  | F     | 101    | LMT  | C1'-O5'-C5' | -2.53 | 108.78      | 113.72   |
| 23  | C     | 508    | CLA  | O2A-CGA-O1A | -2.53 | 117.31      | 123.63   |
| 26  | f     | 102    | SQD  | O47-C7-O49  | -2.53 | 117.80      | 123.70   |
| 24  | a     | 408[B] | PHO  | O2D-CGD-O1D | -2.53 | 118.93      | 123.85   |
| 23  | C     | 503    | CLA  | CHD-C4C-NC  | 2.52  | 128.15      | 124.23   |
| 23  | D     | 703    | CLA  | C4B-C3B-C2B | -2.52 | 104.17      | 107.30   |
| 23  | C     | 507    | CLA  | O2A-CGA-O1A | -2.52 | 117.32      | 123.63   |
| 25  | b     | 618    | BCR  | C28-C27-C26 | -2.52 | 109.56      | 114.06   |
| 23  | B     | 604    | CLA  | C11-C12-C13 | -2.52 | 107.59      | 115.97   |
| 23  | c     | 510    | CLA  | CHD-C4C-NC  | 2.52  | 128.14      | 124.23   |
| 25  | Y     | 101    | BCR  | C15-C16-C17 | -2.52 | 118.36      | 123.52   |
| 23  | b     | 602    | CLA  | CAA-CBA-CGA | -2.52 | 106.06      | 113.21   |
| 25  | B     | 618    | BCR  | C28-C27-C26 | -2.52 | 109.56      | 114.06   |
| 23  | A     | 408    | CLA  | CAC-C3C-C4C | 2.52  | 128.07      | 124.79   |
| 23  | B     | 606    | CLA  | C3B-C4B-NB  | 2.52  | 112.78      | 110.53   |
| 23  | B     | 605    | CLA  | CED-O2D-CGD | 2.52  | 121.63      | 115.92   |
| 23  | B     | 602    | CLA  | CHC-C1C-C2C | -2.52 | 119.79      | 126.95   |
| 23  | b     | 612    | CLA  | CMB-C2B-C1B | 2.52  | 129.25      | 125.42   |
| 23  | C     | 509    | CLA  | O2A-CGA-CBA | 2.52  | 119.50      | 111.83   |
| 29  | A     | 414[A] | PL9  | C42-C43-C44 | -2.51 | 121.87      | 127.62   |
| 23  | B     | 615    | CLA  | C6-C7-C8    | -2.51 | 107.61      | 115.97   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 614    | CLA  | C4C-C3C-C2C | -2.51 | 103.23      | 106.89   |
| 24  | A     | 407[A] | PHO  | O2A-CGA-O1A | -2.51 | 117.34      | 123.63   |
| 23  | b     | 616    | CLA  | C4-C3-C5    | 2.51  | 119.59      | 115.23   |
| 36  | c     | 519    | DGD  | O2G-C1B-C2B | 2.51  | 116.91      | 111.48   |
| 23  | a     | 405[B] | CLA  | C4-C3-C5    | 2.51  | 119.58      | 115.23   |
| 23  | d     | 402    | CLA  | C3B-C4B-NB  | 2.51  | 112.77      | 110.53   |
| 29  | a     | 414[B] | PL9  | C20-C19-C21 | 2.51  | 119.58      | 115.23   |
| 23  | B     | 611    | CLA  | CMB-C2B-C3B | 2.51  | 132.45      | 126.55   |
| 24  | a     | 416[B] | PHO  | CBA-CAA-C2A | -2.51 | 106.39      | 113.78   |
| 23  | C     | 510    | CLA  | CHD-C4C-NC  | 2.51  | 128.12      | 124.23   |
| 25  | b     | 619    | BCR  | C16-C17-C18 | -2.51 | 123.76      | 127.28   |
| 23  | b     | 610    | CLA  | C3B-C4B-NB  | 2.51  | 112.77      | 110.53   |
| 23  | A     | 406[B] | CLA  | C4C-C3C-C2C | -2.51 | 103.24      | 106.89   |
| 23  | B     | 615    | CLA  | CAC-C3C-C4C | 2.51  | 128.05      | 124.79   |
| 23  | B     | 614    | CLA  | C4B-C3B-C2B | -2.51 | 104.19      | 107.30   |
| 23  | B     | 609    | CLA  | CAC-C3C-C4C | 2.50  | 128.05      | 124.79   |
| 23  | B     | 610    | CLA  | CAC-C3C-C4C | 2.50  | 128.05      | 124.79   |
| 23  | c     | 505    | CLA  | C4B-C3B-C2B | -2.50 | 104.19      | 107.30   |
| 29  | D     | 705[B] | PL9  | C12-C13-C14 | -2.50 | 121.89      | 127.62   |
| 23  | a     | 406[B] | CLA  | C1-O2A-CGA  | 2.50  | 122.71      | 116.65   |
| 23  | b     | 607    | CLA  | O2A-CGA-O1A | -2.50 | 117.37      | 123.63   |
| 23  | c     | 505    | CLA  | O2A-CGA-CBA | 2.50  | 119.46      | 111.83   |
| 24  | A     | 417[A] | PHO  | CMA-C3A-C4A | -2.50 | 109.23      | 114.61   |
| 38  | F     | 102    | HEM  | O2D-CGD-CBD | 2.50  | 121.89      | 114.00   |
| 33  | d     | 405[A] | LHG  | O8-C23-O10  | -2.50 | 117.38      | 123.63   |
| 35  | o     | 301    | HTG  | C2'-C1'-S1  | -2.50 | 103.95      | 112.36   |
| 23  | c     | 507    | CLA  | O2A-CGA-O1A | -2.50 | 117.38      | 123.63   |
| 23  | C     | 503    | CLA  | O2A-CGA-CBA | 2.50  | 119.45      | 111.83   |
| 25  | y     | 101    | BCR  | C16-C17-C18 | -2.50 | 123.78      | 127.28   |
| 23  | C     | 505    | CLA  | C4-C3-C5    | 2.50  | 119.56      | 115.23   |
| 25  | b     | 618    | BCR  | C20-C21-C22 | -2.50 | 123.78      | 127.28   |
| 23  | B     | 614    | CLA  | C2A-C1A-CHA | -2.50 | 119.54      | 123.87   |
| 23  | c     | 514    | CLA  | CHC-C1C-C2C | -2.49 | 119.86      | 126.95   |
| 25  | D     | 704    | BCR  | C21-C20-C19 | -2.49 | 115.97      | 123.20   |
| 26  | a     | 411[B] | SQD  | O48-C23-C24 | 2.49  | 119.43      | 111.83   |
| 23  | c     | 508    | CLA  | CHC-C1C-C2C | -2.49 | 119.87      | 126.95   |
| 38  | f     | 101    | HEM  | C4C-NC-C1C  | 2.49  | 109.88      | 105.82   |
| 25  | K     | 102    | BCR  | C2-C1-C6    | 2.49  | 114.05      | 110.44   |
| 23  | b     | 616    | CLA  | CHC-C1C-C2C | -2.49 | 119.88      | 126.95   |
| 25  | c     | 515    | BCR  | C20-C21-C22 | -2.48 | 123.79      | 127.28   |
| 34  | d     | 410    | LMG  | O8-C28-C29  | 2.48  | 119.41      | 111.83   |
| 23  | A     | 404[B] | CLA  | C2A-C1A-CHA | -2.48 | 119.56      | 123.87   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 405[B] | CLA  | C2A-C1A-CHA | -2.48 | 119.56      | 123.87   |
| 23  | B     | 612    | CLA  | C2A-C1A-CHA | -2.48 | 119.56      | 123.87   |
| 26  | f     | 102    | SQD  | O5-C5-C4    | 2.48  | 114.17      | 109.70   |
| 23  | c     | 508    | CLA  | C1-C2-C3    | -2.48 | 122.13      | 126.20   |
| 25  | b     | 619    | BCR  | C11-C10-C9  | -2.48 | 123.80      | 127.28   |
| 23  | B     | 601    | CLA  | CMB-C2B-C1B | 2.48  | 129.20      | 125.42   |
| 23  | c     | 504    | CLA  | C2A-C1A-CHA | -2.48 | 119.56      | 123.87   |
| 24  | A     | 417[A] | PHO  | O1D-CGD-CBD | -2.48 | 120.96      | 124.72   |
| 29  | a     | 414[B] | PL9  | C10-C9-C11  | 2.48  | 119.53      | 115.23   |
| 29  | A     | 414[A] | PL9  | C35-C34-C36 | 2.48  | 119.53      | 115.23   |
| 23  | A     | 408    | CLA  | C1-O2A-CGA  | 2.48  | 122.64      | 116.65   |
| 23  | A     | 405[A] | CLA  | O2A-CGA-O1A | -2.48 | 117.44      | 123.63   |
| 23  | c     | 509    | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 23  | c     | 511    | CLA  | CBC-CAC-C3C | -2.47 | 105.71      | 112.42   |
| 23  | c     | 502    | CLA  | O2A-CGA-CBA | 2.47  | 119.38      | 111.83   |
| 23  | b     | 615    | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 23  | B     | 608    | CLA  | C11-C12-C13 | -2.47 | 107.75      | 115.97   |
| 23  | B     | 616    | CLA  | CBC-CAC-C3C | -2.47 | 105.72      | 112.42   |
| 23  | C     | 503    | CLA  | O2A-CGA-O1A | -2.47 | 117.45      | 123.63   |
| 26  | B     | 620    | SQD  | O9-S-C6     | 2.47  | 110.45      | 106.76   |
| 26  | a     | 412    | SQD  | O7-S-C6     | 2.47  | 110.44      | 106.76   |
| 23  | C     | 506    | CLA  | CHD-C4C-NC  | 2.47  | 128.06      | 124.23   |
| 23  | b     | 608    | CLA  | O2A-CGA-CBA | 2.47  | 119.36      | 111.83   |
| 29  | A     | 414[A] | PL9  | C53-C6-C1   | 2.47  | 120.33      | 115.28   |
| 23  | b     | 601    | CLA  | CBC-CAC-C3C | -2.47 | 105.73      | 112.42   |
| 26  | A     | 410[A] | SQD  | O9-S-C6     | 2.47  | 110.44      | 106.76   |
| 23  | C     | 513    | CLA  | O2D-CGD-O1D | -2.47 | 119.05      | 123.85   |
| 29  | d     | 404[A] | PL9  | C36-C34-C33 | -2.47 | 115.63      | 121.17   |
| 24  | a     | 408[A] | PHO  | O2A-CGA-O1A | -2.47 | 117.46      | 123.63   |
| 23  | c     | 509    | CLA  | O2A-CGA-O1A | -2.47 | 117.46      | 123.63   |
| 29  | D     | 705[A] | PL9  | C22-C23-C24 | -2.47 | 121.98      | 127.62   |
| 26  | B     | 620    | SQD  | O48-C23-O10 | -2.46 | 117.46      | 123.63   |
| 23  | c     | 504    | CLA  | C4-C3-C5    | 2.46  | 119.50      | 115.23   |
| 23  | c     | 509    | CLA  | C4-C3-C5    | 2.46  | 119.50      | 115.23   |
| 23  | c     | 509    | CLA  | CHD-C4C-NC  | 2.46  | 128.05      | 124.23   |
| 25  | T     | 102    | BCR  | C7-C6-C5    | -2.46 | 115.88      | 121.56   |
| 25  | k     | 101    | BCR  | C2-C1-C6    | 2.46  | 114.02      | 110.44   |
| 23  | D     | 702[B] | CLA  | CMC-C2C-C1C | 2.46  | 128.88      | 125.03   |
| 23  | c     | 513    | CLA  | CMA-C3A-C4A | -2.46 | 105.16      | 111.77   |
| 23  | C     | 506    | CLA  | O2A-CGA-O1A | -2.46 | 117.47      | 123.63   |
| 23  | b     | 611    | CLA  | CMB-C2B-C1B | 2.46  | 129.17      | 125.42   |
| 23  | a     | 405[A] | CLA  | CHD-C4C-NC  | 2.46  | 128.05      | 124.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 505    | CLA  | CED-O2D-CGD | 2.46  | 121.49      | 115.92   |
| 23  | c     | 511    | CLA  | C11-C10-C8  | -2.46 | 107.79      | 115.97   |
| 29  | A     | 414[B] | PL9  | C10-C9-C11  | 2.46  | 119.50      | 115.23   |
| 23  | D     | 703    | CLA  | C3B-C4B-NB  | 2.46  | 112.72      | 110.53   |
| 23  | B     | 602    | CLA  | CMB-C2B-C1B | 2.45  | 129.16      | 125.42   |
| 23  | a     | 405[B] | CLA  | C4C-C3C-C2C | -2.45 | 103.32      | 106.89   |
| 29  | A     | 414[B] | PL9  | C35-C34-C36 | 2.45  | 119.49      | 115.23   |
| 25  | c     | 515    | BCR  | C36-C18-C19 | 2.45  | 121.83      | 118.09   |
| 35  | b     | 625    | HTG  | C1-C2-C3    | -2.45 | 105.75      | 110.55   |
| 29  | D     | 705[B] | PL9  | C7-C8-C9    | -2.45 | 122.61      | 126.83   |
| 29  | d     | 404[A] | PL9  | C47-C48-C49 | -2.45 | 119.47      | 127.64   |
| 23  | a     | 406[A] | CLA  | C4C-C3C-C2C | -2.45 | 103.32      | 106.89   |
| 23  | C     | 514    | CLA  | C4-C3-C5    | 2.45  | 119.48      | 115.23   |
| 23  | c     | 511    | CLA  | C4C-C3C-C2C | -2.45 | 103.32      | 106.89   |
| 29  | d     | 404[B] | PL9  | C22-C23-C24 | -2.45 | 122.01      | 127.62   |
| 23  | b     | 605    | CLA  | C4B-C3B-C2B | -2.45 | 104.25      | 107.30   |
| 23  | c     | 505    | CLA  | C2A-C1A-CHA | -2.45 | 119.61      | 123.87   |
| 23  | A     | 405[A] | CLA  | CMA-C3A-C4A | -2.45 | 105.19      | 111.77   |
| 26  | X     | 101    | SQD  | C46-C45-C44 | -2.45 | 106.08      | 111.78   |
| 23  | b     | 606    | CLA  | C1-O2A-CGA  | 2.45  | 122.58      | 116.65   |
| 26  | b     | 620    | SQD  | O47-C7-O49  | -2.45 | 117.98      | 123.70   |
| 29  | d     | 404[B] | PL9  | C53-C6-C1   | 2.45  | 120.29      | 115.28   |
| 23  | C     | 502    | CLA  | C4-C3-C5    | 2.45  | 119.48      | 115.23   |
| 23  | C     | 511    | CLA  | C2A-C1A-CHA | -2.45 | 119.62      | 123.87   |
| 23  | C     | 512    | CLA  | C4B-C3B-C2B | -2.44 | 104.26      | 107.30   |
| 25  | T     | 102    | BCR  | C1-C6-C7    | 2.44  | 122.28      | 115.65   |
| 23  | c     | 507    | CLA  | O2A-CGA-CBA | 2.44  | 119.29      | 111.83   |
| 36  | c     | 518[B] | DGD  | O1G-C1A-C2A | 2.44  | 119.29      | 111.83   |
| 23  | B     | 604    | CLA  | CHD-C1D-ND  | -2.44 | 121.37      | 124.80   |
| 23  | b     | 604    | CLA  | O2A-CGA-O1A | -2.44 | 117.52      | 123.63   |
| 23  | C     | 504    | CLA  | O2A-CGA-CBA | 2.44  | 119.28      | 111.83   |
| 23  | a     | 406[A] | CLA  | C1-O2A-CGA  | 2.44  | 122.56      | 116.65   |
| 23  | C     | 513    | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 23  | B     | 602    | CLA  | C2A-C1A-CHA | -2.44 | 119.63      | 123.87   |
| 32  | B     | 629    | LMT  | O5'-C5'-C6' | 2.44  | 112.48      | 106.44   |
| 36  | c     | 517[B] | DGD  | C3G-C2G-C1G | -2.44 | 106.10      | 111.78   |
| 25  | t     | 102    | BCR  | C7-C8-C9    | -2.44 | 122.63      | 126.23   |
| 23  | A     | 405[B] | CLA  | C4-C3-C5    | 2.44  | 119.46      | 115.23   |
| 25  | C     | 515    | BCR  | C38-C26-C25 | -2.44 | 121.83      | 124.48   |
| 23  | a     | 405[A] | CLA  | CMC-C2C-C1C | 2.44  | 128.84      | 125.03   |
| 23  | b     | 613    | CLA  | CMA-C3A-C4A | -2.44 | 105.23      | 111.77   |
| 23  | c     | 507    | CLA  | C2A-C1A-CHA | -2.43 | 119.64      | 123.87   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 38  | f     | 101    | HEM  | C4D-ND-C1D  | 2.43  | 108.09      | 105.21   |
| 32  | A     | 420    | LMT  | O1'-C1'-C2' | 2.43  | 111.97      | 108.27   |
| 26  | a     | 411[B] | SQD  | O9-S-C6     | 2.43  | 110.39      | 106.76   |
| 23  | d     | 401[B] | CLA  | C2A-C1A-CHA | -2.43 | 119.65      | 123.87   |
| 23  | B     | 605    | CLA  | CHC-C1C-C2C | -2.43 | 120.04      | 126.95   |
| 25  | c     | 516    | BCR  | C15-C14-C13 | -2.43 | 123.87      | 127.28   |
| 23  | a     | 409    | CLA  | CAC-C3C-C4C | 2.43  | 127.95      | 124.79   |
| 23  | D     | 702[B] | CLA  | CBC-CAC-C3C | -2.43 | 105.84      | 112.42   |
| 23  | B     | 612    | CLA  | CHC-C1C-C2C | -2.43 | 120.05      | 126.95   |
| 33  | L     | 101[B] | LHG  | O8-C23-C24  | 2.43  | 119.23      | 111.83   |
| 23  | c     | 505    | CLA  | O2D-CGD-O1D | -2.43 | 119.13      | 123.85   |
| 32  | e     | 101    | LMT  | O1'-C1'-C2' | 2.43  | 111.96      | 108.27   |
| 23  | c     | 508    | CLA  | O1D-CGD-CBD | -2.42 | 119.74      | 124.52   |
| 29  | A     | 414[B] | PL9  | C53-C6-C1   | 2.42  | 120.24      | 115.28   |
| 23  | C     | 507    | CLA  | C4C-C3C-C2C | -2.42 | 103.36      | 106.89   |
| 25  | A     | 409    | BCR  | C37-C22-C23 | 2.42  | 121.79      | 118.09   |
| 23  | B     | 612    | CLA  | C4-C3-C5    | 2.42  | 119.43      | 115.23   |
| 36  | C     | 518[A] | DGD  | O1G-C1A-C2A | 2.42  | 119.21      | 111.83   |
| 36  | c     | 518[A] | DGD  | O1G-C1A-C2A | 2.42  | 119.21      | 111.83   |
| 23  | B     | 601    | CLA  | CBC-CAC-C3C | -2.42 | 105.86      | 112.42   |
| 25  | c     | 515    | BCR  | C28-C27-C26 | -2.42 | 109.74      | 114.06   |
| 33  | d     | 405[A] | LHG  | O8-C23-C24  | 2.42  | 119.21      | 111.83   |
| 26  | X     | 101    | SQD  | O8-S-O7     | -2.42 | 105.35      | 111.40   |
| 24  | A     | 407[A] | PHO  | C1-C2-C3    | -2.42 | 122.24      | 126.20   |
| 23  | B     | 614    | CLA  | CED-O2D-CGD | 2.42  | 121.39      | 115.92   |
| 33  | L     | 101[A] | LHG  | O8-C23-O10  | -2.42 | 117.59      | 123.63   |
| 25  | y     | 101    | BCR  | C24-C23-C22 | -2.41 | 122.66      | 126.23   |
| 23  | C     | 507    | CLA  | CGD-CBD-CAD | -2.41 | 103.03      | 110.85   |
| 23  | b     | 609    | CLA  | O2A-CGA-CBA | 2.41  | 119.19      | 111.83   |
| 23  | a     | 405[A] | CLA  | CMA-C3A-C2A | -2.41 | 104.66      | 113.98   |
| 26  | f     | 102    | SQD  | O6-C1-C2    | 2.41  | 111.93      | 108.27   |
| 26  | X     | 101    | SQD  | O7-S-C6     | 2.41  | 110.36      | 106.76   |
| 23  | B     | 611    | CLA  | O2A-CGA-O1A | -2.41 | 117.60      | 123.63   |
| 23  | b     | 601    | CLA  | CMC-C2C-C1C | 2.41  | 128.80      | 125.03   |
| 23  | B     | 612    | CLA  | CHD-C4C-NC  | 2.41  | 127.97      | 124.23   |
| 26  | a     | 411[A] | SQD  | O48-C23-C24 | 2.41  | 119.17      | 111.83   |
| 23  | D     | 702[B] | CLA  | CAC-C3C-C4C | 2.41  | 127.92      | 124.79   |
| 23  | b     | 602    | CLA  | O2A-CGA-CBA | 2.40  | 119.17      | 111.83   |
| 23  | c     | 507    | CLA  | C4-C3-C5    | 2.40  | 119.40      | 115.23   |
| 26  | b     | 620    | SQD  | C44-O6-C1   | -2.40 | 108.64      | 113.80   |
| 26  | b     | 620    | SQD  | O7-S-C6     | 2.40  | 110.34      | 106.76   |
| 23  | B     | 604    | CLA  | O1D-CGD-CBD | -2.40 | 119.78      | 124.52   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25  | y     | 101    | BCR  | C10-C11-C12 | -2.40 | 116.25      | 123.20   |
| 23  | c     | 512    | CLA  | CMB-C2B-C1B | 2.40  | 129.07      | 125.42   |
| 23  | C     | 511    | CLA  | CMC-C2C-C1C | 2.40  | 128.78      | 125.03   |
| 23  | A     | 404[B] | CLA  | C4-C3-C5    | 2.40  | 119.39      | 115.23   |
| 23  | B     | 603    | CLA  | CMA-C3A-C2A | -2.40 | 104.71      | 113.98   |
| 25  | y     | 101    | BCR  | C16-C15-C14 | -2.40 | 118.61      | 123.52   |
| 23  | B     | 608    | CLA  | C2A-C1A-CHA | -2.40 | 119.70      | 123.87   |
| 34  | m     | 101    | LMG  | C8-O7-C10   | -2.40 | 112.06      | 117.80   |
| 29  | a     | 414[A] | PL9  | C40-C39-C41 | 2.40  | 119.39      | 115.23   |
| 23  | c     | 502    | CLA  | O2A-CGA-O1A | -2.40 | 117.64      | 123.63   |
| 23  | C     | 512    | CLA  | CMC-C2C-C1C | 2.40  | 128.78      | 125.03   |
| 25  | B     | 619    | BCR  | C34-C9-C8   | 2.40  | 121.75      | 118.09   |
| 23  | c     | 505    | CLA  | O2A-CGA-O1A | -2.40 | 117.64      | 123.63   |
| 23  | b     | 606    | CLA  | O2A-CGA-O1A | -2.39 | 117.64      | 123.63   |
| 29  | a     | 414[A] | PL9  | C20-C19-C21 | 2.39  | 119.38      | 115.23   |
| 26  | X     | 101    | SQD  | O48-C23-O10 | -2.39 | 117.64      | 123.63   |
| 26  | b     | 620    | SQD  | C1-C2-C3    | -2.39 | 104.98      | 110.01   |
| 36  | c     | 517[A] | DGD  | C2G-O2G-C1B | -2.39 | 112.07      | 117.80   |
| 23  | b     | 608    | CLA  | CAA-C2A-C3A | -2.39 | 106.54      | 113.00   |
| 24  | A     | 417[B] | PHO  | OBD-CAD-C3D | -2.39 | 124.16      | 127.89   |
| 23  | B     | 609    | CLA  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 29  | A     | 414[A] | PL9  | C35-C34-C33 | -2.39 | 117.49      | 123.63   |
| 38  | f     | 101    | HEM  | CMD-C2D-C1D | 2.39  | 128.77      | 125.03   |
| 25  | K     | 102    | BCR  | C36-C18-C19 | 2.39  | 121.74      | 118.09   |
| 23  | c     | 503    | CLA  | O2A-CGA-O1A | -2.39 | 117.65      | 123.63   |
| 23  | b     | 610    | CLA  | CAA-CBA-CGA | -2.39 | 106.42      | 113.21   |
| 23  | d     | 402    | CLA  | CMC-C2C-C1C | 2.39  | 128.76      | 125.03   |
| 29  | a     | 414[B] | PL9  | C47-C48-C49 | -2.38 | 119.69      | 127.64   |
| 23  | a     | 406[A] | CLA  | O2A-CGA-O1A | -2.38 | 117.67      | 123.63   |
| 23  | A     | 406[B] | CLA  | CAC-C3C-C4C | 2.38  | 127.89      | 124.79   |
| 23  | B     | 606    | CLA  | CHB-C1B-C2B | -2.38 | 120.52      | 127.43   |
| 38  | F     | 102    | HEM  | CMD-C2D-C1D | 2.38  | 128.75      | 125.03   |
| 29  | D     | 705[B] | PL9  | C40-C39-C41 | 2.38  | 119.35      | 115.23   |
| 29  | A     | 414[A] | PL9  | C2-C3-C4    | 2.38  | 121.97      | 118.78   |
| 29  | D     | 705[B] | PL9  | C51-C49-C50 | 2.37  | 120.05      | 114.59   |
| 23  | C     | 511    | CLA  | CBC-CAC-C3C | -2.37 | 105.99      | 112.42   |
| 34  | C     | 521    | LMG  | C9-C8-C7    | -2.37 | 106.25      | 111.78   |
| 23  | b     | 609    | CLA  | O2A-CGA-O1A | -2.37 | 117.69      | 123.63   |
| 23  | B     | 611    | CLA  | C1C-C2C-C3C | -2.37 | 104.49      | 106.98   |
| 25  | t     | 102    | BCR  | C1-C6-C7    | 2.37  | 122.08      | 115.65   |
| 23  | C     | 502    | CLA  | C2A-C1A-CHA | -2.37 | 119.75      | 123.87   |
| 23  | B     | 616    | CLA  | CMB-C2B-C3B | 2.37  | 132.12      | 126.55   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | B     | 607    | CLA  | O2A-CGA-CBA | 2.37  | 119.06      | 111.83   |
| 23  | c     | 510    | CLA  | CMB-C2B-C1B | 2.37  | 129.03      | 125.42   |
| 38  | F     | 102    | HEM  | O2A-CGA-CBA | 2.37  | 121.48      | 114.00   |
| 23  | C     | 505    | CLA  | C2A-C1A-CHA | -2.37 | 119.76      | 123.87   |
| 23  | b     | 604    | CLA  | C4C-C3C-C2C | -2.37 | 103.45      | 106.89   |
| 25  | k     | 101    | BCR  | C38-C26-C25 | -2.37 | 121.90      | 124.48   |
| 23  | B     | 613    | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 25  | h     | 101    | BCR  | C36-C18-C17 | -2.37 | 118.98      | 122.82   |
| 23  | c     | 504    | CLA  | CAC-C3C-C4C | 2.37  | 127.87      | 124.79   |
| 25  | C     | 515    | BCR  | C29-C30-C25 | 2.36  | 113.87      | 110.44   |
| 25  | B     | 618    | BCR  | C7-C8-C9    | -2.36 | 122.74      | 126.23   |
| 23  | c     | 513    | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 23  | d     | 401[B] | CLA  | CHD-C4C-NC  | 2.36  | 127.89      | 124.23   |
| 25  | C     | 515    | BCR  | C40-C30-C25 | -2.36 | 106.54      | 110.24   |
| 23  | A     | 406[B] | CLA  | C1-C2-C3    | -2.36 | 122.33      | 126.20   |
| 23  | b     | 608    | CLA  | C4C-C3C-C2C | -2.36 | 103.46      | 106.89   |
| 25  | D     | 704    | BCR  | C15-C16-C17 | -2.36 | 118.70      | 123.52   |
| 34  | c     | 501    | LMG  | O8-C28-C29  | 2.36  | 119.02      | 111.83   |
| 23  | b     | 603    | CLA  | C7-C6-C5    | -2.36 | 106.98      | 113.26   |
| 36  | C     | 518[A] | DGD  | O6E-C5E-C6E | 2.36  | 112.28      | 106.44   |
| 29  | A     | 414[A] | PL9  | C37-C36-C34 | -2.36 | 105.38      | 113.19   |
| 23  | D     | 702[B] | CLA  | CHD-C4C-NC  | 2.36  | 127.88      | 124.23   |
| 23  | A     | 405[B] | CLA  | CMA-C3A-C2A | -2.35 | 104.88      | 113.98   |
| 29  | a     | 414[A] | PL9  | C10-C9-C8   | -2.35 | 117.58      | 123.63   |
| 23  | b     | 608    | CLA  | O2A-CGA-O1A | -2.35 | 117.74      | 123.63   |
| 25  | K     | 102    | BCR  | C39-C30-C25 | -2.35 | 106.55      | 110.24   |
| 23  | A     | 404[B] | CLA  | CAA-CBA-CGA | -2.35 | 106.53      | 113.21   |
| 23  | b     | 608    | CLA  | C11-C10-C8  | -2.35 | 108.15      | 115.97   |
| 25  | h     | 101    | BCR  | C36-C18-C19 | 2.35  | 121.68      | 118.09   |
| 32  | B     | 629    | LMT  | O5'-C5'-C4' | 2.35  | 114.59      | 109.72   |
| 23  | D     | 702[A] | CLA  | CHD-C4C-NC  | 2.35  | 127.88      | 124.23   |
| 25  | y     | 101    | BCR  | C11-C10-C9  | -2.35 | 123.98      | 127.28   |
| 23  | B     | 605    | CLA  | CAC-C3C-C4C | 2.35  | 127.85      | 124.79   |
| 27  | D     | 701    | GOL  | C3-C2-C1    | -2.35 | 103.18      | 111.80   |
| 23  | D     | 703    | CLA  | C1-C2-C3    | -2.35 | 122.35      | 126.20   |
| 26  | B     | 620    | SQD  | C44-O6-C1   | -2.35 | 108.76      | 113.80   |
| 24  | A     | 407[A] | PHO  | CMB-C2B-C3B | 2.35  | 129.37      | 124.68   |
| 26  | a     | 412    | SQD  | O48-C23-O10 | -2.35 | 117.76      | 123.63   |
| 25  | c     | 515    | BCR  | C38-C26-C25 | -2.35 | 121.92      | 124.48   |
| 24  | A     | 417[B] | PHO  | C4D-CHA-CBD | 2.35  | 109.58      | 108.45   |
| 23  | b     | 614    | CLA  | CAC-C3C-C4C | 2.34  | 127.84      | 124.79   |
| 24  | a     | 408[B] | PHO  | C1-C2-C3    | -2.34 | 122.36      | 126.20   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | A     | 408    | CLA  | C2A-C1A-CHA | -2.34 | 119.80      | 123.87   |
| 29  | A     | 414[B] | PL9  | C45-C44-C46 | 2.34  | 119.29      | 115.23   |
| 23  | A     | 408    | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 24  | A     | 407[B] | PHO  | C4-C3-C5    | 2.34  | 119.29      | 115.23   |
| 23  | C     | 504    | CLA  | CAC-C3C-C4C | 2.34  | 127.83      | 124.79   |
| 33  | d     | 412[A] | LHG  | O7-C7-O9    | -2.34 | 118.24      | 123.70   |
| 23  | c     | 508    | CLA  | CBC-CAC-C3C | -2.34 | 106.08      | 112.42   |
| 24  | a     | 416[B] | PHO  | C4-C3-C2    | -2.34 | 117.63      | 123.63   |
| 23  | B     | 609    | CLA  | C2A-C1A-CHA | -2.34 | 119.81      | 123.87   |
| 23  | C     | 513    | CLA  | CHC-C1C-C2C | -2.33 | 120.32      | 126.95   |
| 23  | c     | 506    | CLA  | CMC-C2C-C1C | 2.33  | 128.68      | 125.03   |
| 25  | y     | 101    | BCR  | C1-C6-C7    | 2.33  | 121.97      | 115.65   |
| 24  | a     | 416[B] | PHO  | C1A-C2A-C3A | -2.33 | 100.62      | 102.84   |
| 23  | d     | 402    | CLA  | C6-C7-C8    | -2.33 | 108.23      | 115.97   |
| 29  | D     | 705[A] | PL9  | C45-C44-C46 | 2.33  | 119.27      | 115.23   |
| 24  | a     | 408[A] | PHO  | CMB-C2B-C3B | 2.32  | 129.33      | 124.68   |
| 23  | B     | 616    | CLA  | C2A-C1A-CHA | -2.32 | 119.83      | 123.87   |
| 25  | t     | 102    | BCR  | C36-C18-C19 | 2.32  | 121.64      | 118.09   |
| 33  | d     | 406[A] | LHG  | O8-C23-O10  | -2.32 | 117.82      | 123.63   |
| 23  | a     | 407[A] | CLA  | CBC-CAC-C3C | -2.32 | 106.12      | 112.42   |
| 23  | b     | 605    | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 36  | c     | 519    | DGD  | O3G-C3G-C2G | -2.32 | 105.17      | 110.82   |
| 29  | A     | 414[A] | PL9  | C2-C1-C6    | 2.32  | 121.76      | 119.00   |
| 23  | c     | 507    | CLA  | CBC-CAC-C3C | -2.32 | 106.13      | 112.42   |
| 23  | a     | 405[B] | CLA  | CMA-C3A-C2A | -2.32 | 105.01      | 113.98   |
| 23  | C     | 513    | CLA  | C4B-C3B-C2B | -2.32 | 104.42      | 107.30   |
| 29  | d     | 404[A] | PL9  | C7-C8-C9    | -2.32 | 122.84      | 126.83   |
| 25  | a     | 410    | BCR  | C2-C1-C6    | 2.32  | 113.81      | 110.44   |
| 35  | b     | 622    | HTG  | O5-C1-C2    | 2.32  | 113.51      | 110.32   |
| 23  | A     | 404[A] | CLA  | CMA-C3A-C4A | -2.32 | 105.54      | 111.77   |
| 23  | C     | 504    | CLA  | C2A-C1A-CHA | -2.32 | 119.84      | 123.87   |
| 23  | b     | 601    | CLA  | O2A-CGA-CBA | 2.32  | 118.90      | 111.83   |
| 29  | A     | 414[A] | PL9  | C47-C48-C49 | -2.32 | 119.92      | 127.64   |
| 25  | a     | 410    | BCR  | C40-C30-C25 | -2.32 | 106.61      | 110.24   |
| 23  | c     | 511    | CLA  | CED-O2D-CGD | 2.32  | 121.17      | 115.92   |
| 23  | b     | 603    | CLA  | CMC-C2C-C1C | 2.32  | 128.65      | 125.03   |
| 36  | h     | 102    | DGD  | C6D-C5D-C4D | 2.32  | 116.93      | 112.07   |
| 29  | a     | 414[B] | PL9  | C45-C44-C46 | 2.32  | 119.25      | 115.23   |
| 23  | b     | 601    | CLA  | CAC-C3C-C4C | 2.32  | 127.80      | 124.79   |
| 26  | B     | 620    | SQD  | O5-C1-C2    | -2.31 | 105.62      | 110.37   |
| 34  | B     | 621    | LMG  | C12-C11-C10 | -2.31 | 105.22      | 113.69   |
| 25  | B     | 618    | BCR  | C3-C4-C5    | -2.31 | 109.93      | 114.06   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | d     | 402    | CLA  | C4-C3-C5    | 2.31  | 119.24      | 115.23   |
| 36  | C     | 518[B] | DGD  | O1G-C1A-C2A | 2.31  | 118.88      | 111.83   |
| 29  | D     | 705[B] | PL9  | C22-C23-C24 | -2.31 | 122.34      | 127.62   |
| 25  | h     | 101    | BCR  | C34-C9-C8   | 2.31  | 121.61      | 118.09   |
| 23  | A     | 404[B] | CLA  | CAC-C3C-C4C | 2.31  | 127.79      | 124.79   |
| 23  | c     | 514    | CLA  | CBC-CAC-C3C | -2.31 | 106.17      | 112.42   |
| 23  | A     | 405[B] | CLA  | CMA-C3A-C4A | -2.31 | 105.57      | 111.77   |
| 24  | a     | 416[A] | PHO  | O2D-CGD-O1D | -2.31 | 119.36      | 123.85   |
| 23  | b     | 605    | CLA  | C1-O2A-CGA  | 2.31  | 122.23      | 116.65   |
| 29  | a     | 414[A] | PL9  | C35-C34-C33 | -2.31 | 117.70      | 123.63   |
| 38  | F     | 102    | HEM  | C4C-NC-C1C  | 2.31  | 109.58      | 105.82   |
| 33  | E     | 101[B] | LHG  | O7-C7-O9    | -2.30 | 118.32      | 123.70   |
| 23  | C     | 510    | CLA  | C2A-C1A-CHA | -2.30 | 119.87      | 123.87   |
| 23  | b     | 605    | CLA  | CAC-C3C-C4C | 2.30  | 127.79      | 124.79   |
| 36  | H     | 102    | DGD  | O6E-C5E-C6E | 2.30  | 112.15      | 106.44   |
| 25  | Y     | 101    | BCR  | C29-C30-C25 | 2.30  | 113.78      | 110.44   |
| 26  | f     | 102    | SQD  | O48-C23-O10 | -2.30 | 117.87      | 123.63   |
| 29  | A     | 414[A] | PL9  | C45-C44-C46 | 2.30  | 119.22      | 115.23   |
| 29  | a     | 414[A] | PL9  | C45-C44-C46 | 2.30  | 119.22      | 115.23   |
| 25  | b     | 618    | BCR  | C37-C22-C23 | 2.30  | 121.60      | 118.09   |
| 23  | B     | 601    | CLA  | C2A-C1A-CHA | -2.30 | 119.88      | 123.87   |
| 23  | a     | 407[B] | CLA  | C4B-C3B-C2B | -2.30 | 104.44      | 107.30   |
| 23  | C     | 508    | CLA  | C4-C3-C5    | 2.30  | 119.22      | 115.23   |
| 23  | C     | 507    | CLA  | CMB-C2B-C1B | 2.30  | 128.92      | 125.42   |
| 23  | a     | 405[B] | CLA  | CHB-C4A-NA  | 2.30  | 127.71      | 124.40   |
| 23  | B     | 608    | CLA  | CBC-CAC-C3C | -2.30 | 106.19      | 112.42   |
| 25  | b     | 619    | BCR  | C37-C22-C23 | 2.30  | 121.59      | 118.09   |
| 29  | d     | 404[B] | PL9  | C12-C13-C14 | -2.29 | 122.38      | 127.62   |
| 23  | B     | 605    | CLA  | O2A-CGA-CBA | 2.29  | 118.83      | 111.83   |
| 33  | b     | 629[B] | LHG  | O8-C23-O10  | -2.29 | 117.89      | 123.63   |
| 33  | b     | 629[A] | LHG  | O8-C23-O10  | -2.29 | 117.90      | 123.63   |
| 33  | d     | 405[A] | LHG  | C6-C5-C4    | -2.29 | 106.44      | 111.78   |
| 23  | a     | 406[B] | CLA  | C2A-C1A-CHA | -2.29 | 119.89      | 123.87   |
| 23  | c     | 504    | CLA  | O2A-CGA-CBA | 2.29  | 118.82      | 111.83   |
| 23  | C     | 512    | CLA  | O2A-CGA-O1A | -2.29 | 117.90      | 123.63   |
| 23  | B     | 606    | CLA  | C4-C3-C5    | 2.29  | 119.20      | 115.23   |
| 23  | b     | 602    | CLA  | CMA-C3A-C2A | -2.29 | 105.13      | 113.98   |
| 26  | a     | 411[B] | SQD  | O47-C7-O49  | -2.29 | 118.35      | 123.70   |
| 33  | b     | 629[B] | LHG  | C5-O7-C7    | -2.29 | 112.32      | 117.80   |
| 25  | B     | 617    | BCR  | C34-C9-C8   | 2.29  | 121.58      | 118.09   |
| 23  | B     | 610    | CLA  | O1D-CGD-CBD | -2.29 | 120.01      | 124.52   |
| 23  | c     | 513    | CLA  | C3B-C4B-NB  | 2.29  | 112.57      | 110.53   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 601    | CLA  | O1D-CGD-CBD | -2.29 | 120.01      | 124.52   |
| 26  | a     | 411[A] | SQD  | O9-S-O7     | -2.29 | 106.39      | 113.82   |
| 23  | d     | 402    | CLA  | CMA-C3A-C2A | -2.28 | 105.15      | 113.98   |
| 24  | A     | 417[A] | PHO  | O2A-CGA-CBA | 2.28  | 118.80      | 111.83   |
| 23  | c     | 513    | CLA  | CBA-CAA-C2A | -2.28 | 107.00      | 113.79   |
| 23  | c     | 512    | CLA  | CAC-C3C-C4C | 2.28  | 127.76      | 124.79   |
| 36  | C     | 517[B] | DGD  | O1G-C1A-C2A | 2.28  | 118.79      | 111.83   |
| 29  | d     | 404[B] | PL9  | C20-C19-C21 | 2.28  | 119.19      | 115.23   |
| 23  | A     | 404[B] | CLA  | CAA-C2A-C1A | -2.28 | 104.50      | 111.97   |
| 23  | C     | 503    | CLA  | CBC-CAC-C3C | -2.28 | 106.24      | 112.42   |
| 24  | A     | 407[B] | PHO  | O2A-CGA-O1A | -2.28 | 117.93      | 123.63   |
| 36  | C     | 517[B] | DGD  | O3G-C3G-C2G | -2.28 | 105.28      | 110.82   |
| 23  | b     | 615    | CLA  | C6-C7-C8    | -2.28 | 108.40      | 115.97   |
| 26  | A     | 410[B] | SQD  | O9-S-O7     | -2.28 | 106.42      | 113.82   |
| 25  | C     | 515    | BCR  | C16-C17-C18 | -2.28 | 124.09      | 127.28   |
| 23  | c     | 504    | CLA  | CHC-C1C-C2C | -2.27 | 120.48      | 126.95   |
| 23  | C     | 511    | CLA  | CMB-C2B-C1B | 2.27  | 128.88      | 125.42   |
| 34  | d     | 410    | LMG  | O8-C28-O10  | -2.27 | 117.94      | 123.63   |
| 23  | a     | 407[A] | CLA  | C4-C3-C5    | 2.27  | 119.17      | 115.23   |
| 23  | B     | 606    | CLA  | C2A-C1A-CHA | -2.27 | 119.92      | 123.87   |
| 26  | X     | 101    | SQD  | O5-C1-C2    | -2.27 | 105.70      | 110.37   |
| 24  | A     | 417[A] | PHO  | C6-C5-C3    | -2.27 | 107.94      | 113.47   |
| 23  | a     | 409    | CLA  | OBD-CAD-C3D | -2.27 | 123.11      | 128.42   |
| 25  | c     | 515    | BCR  | C34-C9-C10  | -2.27 | 119.14      | 122.82   |
| 23  | b     | 602    | CLA  | CAC-C3C-C4C | 2.27  | 127.74      | 124.79   |
| 23  | b     | 607    | CLA  | CHD-C4C-NC  | 2.27  | 127.75      | 124.23   |
| 34  | C     | 520    | LMG  | C8-O7-C10   | -2.27 | 112.37      | 117.80   |
| 23  | B     | 613    | CLA  | CHD-C4C-NC  | 2.27  | 127.75      | 124.23   |
| 29  | A     | 414[B] | PL9  | C37-C36-C34 | -2.27 | 105.67      | 113.19   |
| 23  | b     | 606    | CLA  | O2A-CGA-CBA | 2.27  | 118.75      | 111.83   |
| 23  | b     | 608    | CLA  | C2A-C1A-CHA | -2.27 | 119.93      | 123.87   |
| 23  | c     | 513    | CLA  | CMC-C2C-C1C | 2.27  | 128.57      | 125.03   |
| 23  | B     | 608    | CLA  | CMB-C2B-C1B | 2.26  | 128.87      | 125.42   |
| 25  | k     | 101    | BCR  | C3-C4-C5    | -2.26 | 110.02      | 114.06   |
| 24  | A     | 417[B] | PHO  | CMB-C2B-C3B | 2.26  | 129.20      | 124.68   |
| 23  | d     | 401[B] | CLA  | CAC-C3C-C4C | 2.26  | 127.73      | 124.79   |
| 23  | b     | 607    | CLA  | C1-O2A-CGA  | 2.26  | 122.12      | 116.65   |
| 33  | A     | 419[A] | LHG  | O4-P-O5     | 2.26  | 122.95      | 112.44   |
| 23  | B     | 601    | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 23  | B     | 606    | CLA  | CMB-C2B-C1B | 2.26  | 128.86      | 125.42   |
| 23  | b     | 605    | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 26  | A     | 410[A] | SQD  | O9-S-O7     | -2.26 | 106.48      | 113.82   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | c     | 508    | CLA  | C4C-C3C-C2C | -2.26 | 103.61      | 106.89   |
| 23  | b     | 615    | CLA  | CHA-C1A-NA  | -2.26 | 121.28      | 126.39   |
| 25  | b     | 617    | BCR  | C29-C30-C25 | 2.26  | 113.72      | 110.44   |
| 23  | C     | 502    | CLA  | C1-O2A-CGA  | 2.26  | 122.11      | 116.65   |
| 23  | a     | 406[B] | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 34  | C     | 501    | LMG  | O8-C28-C29  | 2.26  | 118.71      | 111.83   |
| 29  | D     | 705[B] | PL9  | C53-C6-C1   | 2.25  | 119.90      | 115.28   |
| 25  | b     | 617    | BCR  | C21-C20-C19 | -2.25 | 116.67      | 123.20   |
| 23  | c     | 508    | CLA  | O2A-CGA-O1A | -2.25 | 117.99      | 123.63   |
| 23  | A     | 404[B] | CLA  | CMB-C2B-C3B | 2.25  | 131.85      | 126.55   |
| 25  | Y     | 101    | BCR  | C28-C27-C26 | -2.25 | 110.04      | 114.06   |
| 25  | b     | 619    | BCR  | C39-C30-C25 | -2.25 | 106.72      | 110.24   |
| 34  | c     | 501    | LMG  | O6-C5-C4    | 2.25  | 113.75      | 109.70   |
| 23  | d     | 401[A] | CLA  | CMC-C2C-C1C | 2.25  | 128.55      | 125.03   |
| 25  | b     | 618    | BCR  | C2-C1-C6    | 2.25  | 113.70      | 110.44   |
| 25  | C     | 516    | BCR  | C21-C20-C19 | -2.25 | 116.69      | 123.20   |
| 24  | a     | 408[B] | PHO  | CMB-C2B-C3B | 2.25  | 129.17      | 124.68   |
| 36  | C     | 517[A] | DGD  | C3G-C2G-C1G | -2.25 | 106.55      | 111.78   |
| 26  | a     | 412    | SQD  | O5-C5-C4    | 2.25  | 113.75      | 109.70   |
| 34  | C     | 521    | LMG  | O1-C1-C2    | 2.25  | 111.68      | 108.27   |
| 35  | C     | 522    | HTG  | C1-O5-C5    | 2.25  | 116.59      | 112.56   |
| 34  | c     | 521    | LMG  | O8-C28-O10  | -2.24 | 118.02      | 123.63   |
| 24  | a     | 416[A] | PHO  | CED-O2D-CGD | 2.24  | 121.00      | 115.92   |
| 23  | A     | 404[A] | CLA  | CMC-C2C-C1C | 2.24  | 128.54      | 125.03   |
| 34  | c     | 520    | LMG  | O8-C28-O10  | -2.24 | 118.02      | 123.63   |
| 23  | B     | 610    | CLA  | CMA-C3A-C2A | -2.24 | 105.31      | 113.98   |
| 36  | c     | 518[A] | DGD  | C2G-O2G-C1B | -2.24 | 112.43      | 117.80   |
| 23  | b     | 615    | CLA  | C6-C5-C3    | -2.24 | 108.01      | 113.47   |
| 23  | C     | 513    | CLA  | O2A-CGA-O1A | -2.24 | 118.03      | 123.63   |
| 29  | D     | 705[B] | PL9  | C30-C29-C31 | 2.24  | 119.11      | 115.23   |
| 23  | a     | 406[B] | CLA  | C4-C3-C5    | 2.24  | 119.11      | 115.23   |
| 23  | b     | 608    | CLA  | CMA-C3A-C4A | -2.24 | 105.76      | 111.77   |
| 23  | A     | 405[B] | CLA  | O2A-CGA-CBA | 2.24  | 118.65      | 111.83   |
| 23  | c     | 507    | CLA  | CGD-CBD-CAD | -2.24 | 103.61      | 110.85   |
| 32  | B     | 627    | LMT  | O1B-C4'-C5' | -2.23 | 103.61      | 109.48   |
| 23  | C     | 512    | CLA  | O2A-CGA-CBA | 2.23  | 118.65      | 111.83   |
| 23  | a     | 409    | CLA  | CHC-C1C-C2C | -2.23 | 120.60      | 126.95   |
| 24  | a     | 416[A] | PHO  | C4-C3-C2    | -2.23 | 117.89      | 123.63   |
| 23  | B     | 615    | CLA  | O2D-CGD-O1D | -2.23 | 119.50      | 123.85   |
| 23  | b     | 607    | CLA  | CAC-C3C-C4C | 2.23  | 127.69      | 124.79   |
| 23  | B     | 611    | CLA  | OBD-CAD-C3D | -2.23 | 123.20      | 128.42   |
| 27  | B     | 623    | GOL  | C3-C2-C1    | -2.23 | 103.61      | 111.80   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 504    | CLA  | C4B-C3B-C2B | -2.23 | 104.53      | 107.30   |
| 23  | b     | 615    | CLA  | CBC-CAC-C3C | -2.23 | 106.37      | 112.42   |
| 23  | b     | 602    | CLA  | C11-C10-C8  | -2.23 | 108.55      | 115.97   |
| 23  | a     | 405[A] | CLA  | C7-C6-C5    | -2.23 | 107.32      | 113.26   |
| 24  | A     | 417[B] | PHO  | O2A-CGA-CBA | 2.23  | 118.63      | 111.83   |
| 23  | A     | 406[B] | CLA  | CMA-C3A-C2A | -2.23 | 105.37      | 113.98   |
| 26  | X     | 101    | SQD  | O6-C44-C45  | 2.23  | 116.23      | 110.82   |
| 26  | A     | 412    | SQD  | O48-C23-O10 | -2.23 | 118.06      | 123.63   |
| 23  | b     | 614    | CLA  | CAA-C2A-C3A | -2.23 | 106.98      | 113.00   |
| 25  | Y     | 101    | BCR  | C1-C6-C7    | 2.23  | 121.69      | 115.65   |
| 29  | A     | 414[B] | PL9  | C51-C49-C50 | 2.22  | 119.71      | 114.59   |
| 25  | b     | 619    | BCR  | C7-C6-C5    | 2.22  | 126.68      | 121.56   |
| 25  | t     | 102    | BCR  | C7-C6-C5    | -2.22 | 116.43      | 121.56   |
| 26  | A     | 412    | SQD  | C1-C2-C3    | -2.22 | 105.33      | 110.01   |
| 23  | B     | 615    | CLA  | C2A-C1A-CHA | -2.22 | 120.01      | 123.87   |
| 32  | A     | 420    | LMT  | O5'-C5'-C4' | 2.22  | 114.31      | 109.72   |
| 23  | C     | 506    | CLA  | CHA-C1A-NA  | -2.22 | 121.36      | 126.39   |
| 23  | a     | 406[B] | CLA  | OBD-CAD-C3D | -2.22 | 123.23      | 128.42   |
| 36  | C     | 517[B] | DGD  | O5D-C6D-C5D | -2.22 | 104.42      | 109.42   |
| 23  | C     | 505    | CLA  | O2A-CGA-O1A | -2.22 | 118.08      | 123.63   |
| 34  | d     | 410    | LMG  | O7-C10-O9   | -2.22 | 118.52      | 123.70   |
| 23  | b     | 613    | CLA  | CED-O2D-CGD | 2.22  | 120.95      | 115.92   |
| 36  | C     | 518[B] | DGD  | O2G-C1B-O1B | -2.22 | 118.52      | 123.70   |
| 23  | C     | 504    | CLA  | CHB-C1B-C2B | -2.22 | 120.99      | 127.43   |
| 25  | b     | 618    | BCR  | C33-C5-C6   | -2.22 | 122.06      | 124.48   |
| 23  | b     | 611    | CLA  | OBD-CAD-C3D | -2.22 | 123.24      | 128.42   |
| 23  | c     | 510    | CLA  | C2A-C1A-CHA | -2.22 | 120.02      | 123.87   |
| 23  | D     | 702[A] | CLA  | C4-C3-C5    | 2.22  | 119.07      | 115.23   |
| 23  | B     | 611    | CLA  | CBC-CAC-C3C | -2.21 | 106.42      | 112.42   |
| 25  | D     | 704    | BCR  | C11-C10-C9  | -2.21 | 124.17      | 127.28   |
| 36  | C     | 518[A] | DGD  | C2G-O2G-C1B | -2.21 | 112.50      | 117.80   |
| 26  | a     | 411[B] | SQD  | O8-S-C6     | 2.21  | 110.25      | 105.97   |
| 23  | C     | 508    | CLA  | C3B-C4B-NB  | 2.21  | 112.50      | 110.53   |
| 29  | A     | 414[A] | PL9  | C12-C13-C14 | -2.21 | 122.56      | 127.62   |
| 25  | Y     | 101    | BCR  | C40-C30-C25 | -2.21 | 106.77      | 110.24   |
| 23  | c     | 514    | CLA  | O2D-CGD-O1D | -2.21 | 119.54      | 123.85   |
| 23  | b     | 606    | CLA  | CAC-C3C-C2C | 2.21  | 131.62      | 127.56   |
| 36  | C     | 519    | DGD  | O2G-C1B-C2B | 2.21  | 116.27      | 111.48   |
| 23  | c     | 502    | CLA  | C4-C3-C5    | 2.21  | 119.07      | 115.23   |
| 23  | B     | 605    | CLA  | OBD-CAD-C3D | -2.21 | 123.25      | 128.42   |
| 23  | C     | 513    | CLA  | CBA-CAA-C2A | -2.21 | 107.22      | 113.79   |
| 23  | a     | 407[A] | CLA  | CAC-C3C-C4C | 2.21  | 127.67      | 124.79   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25  | c     | 515    | BCR  | C36-C18-C17 | -2.21 | 119.24      | 122.82   |
| 25  | A     | 409    | BCR  | C40-C30-C25 | -2.21 | 106.78      | 110.24   |
| 23  | B     | 606    | CLA  | OBD-CAD-C3D | -2.21 | 123.25      | 128.42   |
| 23  | b     | 606    | CLA  | CMC-C2C-C1C | 2.21  | 128.49      | 125.03   |
| 25  | K     | 102    | BCR  | C15-C14-C13 | -2.21 | 124.18      | 127.28   |
| 23  | c     | 505    | CLA  | O1D-CGD-CBD | -2.21 | 120.17      | 124.52   |
| 23  | d     | 402    | CLA  | C4B-C3B-C2B | -2.21 | 104.56      | 107.30   |
| 23  | A     | 405[A] | CLA  | O2A-CGA-CBA | 2.21  | 118.56      | 111.83   |
| 23  | C     | 511    | CLA  | C4-C3-C2    | -2.21 | 117.96      | 123.63   |
| 25  | h     | 101    | BCR  | C2-C1-C6    | 2.21  | 113.64      | 110.44   |
| 32  | b     | 627    | LMT  | O1'-C1'-C2' | 2.21  | 111.62      | 108.27   |
| 23  | b     | 609    | CLA  | CAA-C2A-C3A | -2.20 | 107.04      | 113.00   |
| 23  | A     | 405[B] | CLA  | O2D-CGD-O1D | -2.20 | 119.56      | 123.85   |
| 23  | B     | 605    | CLA  | C4B-C3B-C2B | -2.20 | 104.56      | 107.30   |
| 29  | D     | 705[A] | PL9  | C20-C19-C21 | 2.20  | 119.05      | 115.23   |
| 23  | A     | 405[A] | CLA  | CHB-C4A-NA  | 2.20  | 127.58      | 124.40   |
| 26  | f     | 102    | SQD  | C44-O6-C1   | -2.20 | 109.07      | 113.80   |
| 29  | d     | 404[A] | PL9  | C2-C1-C6    | 2.20  | 121.62      | 119.00   |
| 36  | C     | 517[A] | DGD  | O5D-C6D-C5D | -2.20 | 104.46      | 109.42   |
| 23  | A     | 405[B] | CLA  | CED-O2D-CGD | 2.20  | 120.91      | 115.92   |
| 23  | B     | 615    | CLA  | O2A-CGA-CBA | 2.20  | 118.55      | 111.83   |
| 23  | B     | 603    | CLA  | O1D-CGD-CBD | -2.20 | 120.18      | 124.52   |
| 23  | B     | 610    | CLA  | C2A-C1A-CHA | -2.20 | 120.05      | 123.87   |
| 34  | Z     | 101    | LMG  | C1-O6-C5    | 2.20  | 118.02      | 113.72   |
| 23  | C     | 503    | CLA  | C1-C2-C3    | -2.20 | 122.59      | 126.20   |
| 23  | b     | 601    | CLA  | CAA-C2A-C3A | -2.20 | 107.06      | 113.00   |
| 26  | b     | 620    | SQD  | O5-C1-C2    | -2.20 | 105.85      | 110.37   |
| 23  | b     | 606    | CLA  | C2A-C1A-CHA | -2.20 | 120.05      | 123.87   |
| 36  | c     | 519    | DGD  | O3G-C1D-C2D | -2.20 | 104.93      | 108.27   |
| 29  | A     | 414[B] | PL9  | C25-C24-C26 | 2.20  | 119.04      | 115.23   |
| 23  | B     | 603    | CLA  | CMB-C2B-C3B | 2.20  | 131.72      | 126.55   |
| 25  | T     | 102    | BCR  | C29-C30-C25 | 2.20  | 113.63      | 110.44   |
| 25  | D     | 704    | BCR  | C29-C28-C27 | -2.20 | 106.45      | 111.28   |
| 34  | C     | 520    | LMG  | O7-C10-O9   | -2.20 | 118.57      | 123.70   |
| 23  | B     | 603    | CLA  | CMC-C2C-C1C | 2.20  | 128.47      | 125.03   |
| 25  | B     | 619    | BCR  | C31-C1-C6   | -2.19 | 106.80      | 110.24   |
| 33  | b     | 629[B] | LHG  | O7-C7-O9    | -2.19 | 118.57      | 123.70   |
| 29  | d     | 404[A] | PL9  | C12-C13-C14 | -2.19 | 122.60      | 127.62   |
| 29  | d     | 404[B] | PL9  | C36-C34-C33 | -2.19 | 116.24      | 121.17   |
| 23  | A     | 406[B] | CLA  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 36  | c     | 519    | DGD  | O2E-C2E-C3E | -2.19 | 105.21      | 110.38   |
| 23  | B     | 614    | CLA  | CMA-C3A-C2A | -2.19 | 105.51      | 113.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 601    | CLA  | CHB-C1B-C2B | -2.19 | 121.07      | 127.43   |
| 23  | C     | 505    | CLA  | CHD-C4C-NC  | 2.19  | 127.63      | 124.23   |
| 38  | F     | 102    | HEM  | CAD-C3D-C4D | 2.19  | 128.51      | 124.70   |
| 23  | D     | 702[A] | CLA  | CED-O2D-CGD | 2.19  | 120.88      | 115.92   |
| 23  | B     | 607    | CLA  | OBD-CAD-C3D | -2.19 | 123.30      | 128.42   |
| 23  | d     | 401[A] | CLA  | CAC-C3C-C4C | 2.19  | 127.64      | 124.79   |
| 23  | B     | 615    | CLA  | O2A-CGA-O1A | -2.19 | 118.16      | 123.63   |
| 23  | c     | 505    | CLA  | CAA-C2A-C3A | -2.19 | 107.09      | 113.00   |
| 23  | B     | 604    | CLA  | O2D-CGD-O1D | -2.19 | 119.59      | 123.85   |
| 23  | b     | 609    | CLA  | C7-C6-C5    | -2.19 | 107.44      | 113.26   |
| 23  | A     | 408    | CLA  | C11-C12-C13 | -2.19 | 108.70      | 115.97   |
| 36  | h     | 102    | DGD  | O3G-C1D-C2D | 2.18  | 111.59      | 108.27   |
| 23  | b     | 604    | CLA  | CHD-C4C-NC  | 2.18  | 127.62      | 124.23   |
| 25  | b     | 619    | BCR  | C21-C20-C19 | -2.18 | 116.87      | 123.20   |
| 36  | C     | 518[B] | DGD  | O1G-C1A-O1A | -2.18 | 118.17      | 123.63   |
| 32  | B     | 629    | LMT  | O5B-C5B-C6B | 2.18  | 111.85      | 106.44   |
| 36  | c     | 518[A] | DGD  | O4E-C4E-C3E | -2.18 | 105.23      | 110.38   |
| 32  | m     | 103    | LMT  | C3B-C4B-C5B | -2.18 | 106.27      | 110.23   |
| 23  | B     | 606    | CLA  | C7-C6-C5    | -2.18 | 107.45      | 113.26   |
| 23  | C     | 507    | CLA  | CHD-C4C-NC  | 2.18  | 127.61      | 124.23   |
| 36  | c     | 517[A] | DGD  | O6D-C1D-O3G | -2.18 | 104.89      | 110.04   |
| 23  | b     | 606    | CLA  | C4-C3-C2    | -2.18 | 118.03      | 123.63   |
| 23  | c     | 512    | CLA  | O2A-CGA-O1A | -2.18 | 118.17      | 123.63   |
| 23  | B     | 602    | CLA  | CHB-C4A-NA  | 2.18  | 127.55      | 124.40   |
| 23  | c     | 508    | CLA  | C3B-C4B-NB  | 2.18  | 112.48      | 110.53   |
| 25  | D     | 704    | BCR  | C30-C25-C24 | 2.18  | 121.56      | 115.65   |
| 23  | C     | 513    | CLA  | CHB-C1B-C2B | -2.18 | 121.10      | 127.43   |
| 32  | b     | 621    | LMT  | C2'-C3'-C4' | 2.18  | 114.62      | 109.68   |
| 25  | k     | 101    | BCR  | C36-C18-C19 | 2.18  | 121.41      | 118.09   |
| 23  | c     | 507    | CLA  | CMB-C2B-C1B | 2.18  | 128.73      | 125.42   |
| 23  | c     | 511    | CLA  | C4-C3-C2    | -2.18 | 118.04      | 123.63   |
| 25  | Y     | 101    | BCR  | C7-C6-C5    | -2.18 | 116.55      | 121.56   |
| 23  | c     | 502    | CLA  | C2A-C1A-CHA | -2.17 | 120.09      | 123.87   |
| 25  | b     | 618    | BCR  | C3-C4-C5    | -2.17 | 110.18      | 114.06   |
| 38  | F     | 102    | HEM  | CHA-C4D-ND  | 2.17  | 127.05      | 124.37   |
| 33  | b     | 629[A] | LHG  | O7-C7-O9    | -2.17 | 118.63      | 123.70   |
| 23  | c     | 506    | CLA  | CHA-C1A-NA  | -2.17 | 121.48      | 126.39   |
| 25  | t     | 102    | BCR  | C10-C11-C12 | -2.17 | 116.92      | 123.20   |
| 29  | d     | 404[B] | PL9  | C15-C14-C16 | 2.17  | 118.99      | 115.23   |
| 25  | d     | 403    | BCR  | C28-C27-C26 | -2.17 | 110.19      | 114.06   |
| 40  | V     | 201    | HEC  | CAD-CBD-CGD | -2.17 | 107.92      | 113.67   |
| 33  | E     | 101[A] | LHG  | O7-C7-O9    | -2.17 | 118.64      | 123.70   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | b     | 613    | CLA  | CAC-C3C-C4C | 2.16  | 127.61      | 124.79   |
| 35  | B     | 622    | HTG  | C1-C2-C3    | 2.16  | 114.78      | 110.55   |
| 36  | H     | 102    | DGD  | O2G-C1B-C2B | 2.16  | 116.16      | 111.48   |
| 23  | C     | 510    | CLA  | O2D-CGD-O1D | -2.16 | 119.64      | 123.85   |
| 25  | k     | 101    | BCR  | C34-C9-C8   | 2.16  | 121.39      | 118.09   |
| 23  | B     | 607    | CLA  | CAA-CBA-CGA | 2.16  | 119.35      | 113.21   |
| 23  | A     | 405[A] | CLA  | C4C-C3C-C2C | -2.16 | 103.75      | 106.89   |
| 29  | D     | 705[A] | PL9  | C12-C13-C14 | -2.16 | 122.68      | 127.62   |
| 25  | C     | 515    | BCR  | C11-C10-C9  | -2.16 | 124.25      | 127.28   |
| 36  | C     | 517[A] | DGD  | O1G-C1A-O1A | -2.16 | 118.22      | 123.63   |
| 36  | c     | 518[A] | DGD  | O1G-C1A-O1A | -2.16 | 118.23      | 123.63   |
| 25  | Y     | 101    | BCR  | C38-C26-C25 | -2.16 | 122.13      | 124.48   |
| 23  | C     | 509    | CLA  | CHD-C4C-NC  | 2.16  | 127.58      | 124.23   |
| 36  | C     | 517[A] | DGD  | O6D-C1D-O3G | -2.16 | 104.95      | 110.04   |
| 26  | a     | 411[B] | SQD  | C3-C4-C5    | 2.16  | 114.14      | 110.23   |
| 35  | b     | 622    | HTG  | C3-C4-C5    | 2.15  | 114.14      | 110.23   |
| 26  | A     | 410[B] | SQD  | O9-S-C6     | 2.15  | 109.97      | 106.76   |
| 24  | A     | 417[B] | PHO  | CED-O2D-CGD | 2.15  | 120.80      | 115.92   |
| 24  | A     | 417[B] | PHO  | C6-C5-C3    | -2.15 | 108.23      | 113.47   |
| 23  | C     | 514    | CLA  | O2A-CGA-O1A | -2.15 | 118.25      | 123.63   |
| 32  | A     | 418    | LMT  | O1'-C1'-C2' | 2.15  | 111.53      | 108.27   |
| 23  | b     | 613    | CLA  | CBC-CAC-C3C | -2.15 | 106.60      | 112.42   |
| 36  | C     | 518[B] | DGD  | O3G-C1D-C2D | 2.15  | 111.53      | 108.27   |
| 25  | y     | 101    | BCR  | C37-C22-C23 | 2.15  | 121.37      | 118.09   |
| 23  | b     | 606    | CLA  | CHB-C1B-C2B | -2.15 | 121.20      | 127.43   |
| 23  | B     | 611    | CLA  | C2C-C1C-NC  | 2.15  | 112.24      | 109.98   |
| 25  | d     | 403    | BCR  | C3-C4-C5    | -2.15 | 110.23      | 114.06   |
| 36  | C     | 517[B] | DGD  | C3G-C2G-C1G | -2.15 | 106.78      | 111.78   |
| 23  | c     | 507    | CLA  | C1-O2A-CGA  | 2.15  | 121.84      | 116.65   |
| 23  | B     | 610    | CLA  | CHB-C4A-NA  | 2.14  | 127.50      | 124.40   |
| 25  | a     | 410    | BCR  | C8-C7-C6    | -2.14 | 121.27      | 127.00   |
| 36  | c     | 517[B] | DGD  | C4E-C3E-C2E | -2.14 | 107.07      | 110.83   |
| 36  | c     | 519    | DGD  | O2G-C1B-O1B | -2.14 | 118.70      | 123.70   |
| 23  | b     | 609    | CLA  | CHA-C1A-NA  | -2.14 | 121.54      | 126.39   |
| 23  | c     | 514    | CLA  | C4-C3-C5    | 2.14  | 118.95      | 115.23   |
| 38  | f     | 101    | HEM  | CHC-C1C-NC  | 2.14  | 126.78      | 124.45   |
| 23  | B     | 602    | CLA  | C11-C10-C8  | -2.14 | 108.85      | 115.97   |
| 23  | b     | 607    | CLA  | CMB-C2B-C1B | 2.14  | 128.68      | 125.42   |
| 23  | D     | 703    | CLA  | CMA-C3A-C2A | -2.14 | 105.71      | 113.98   |
| 24  | a     | 408[A] | PHO  | CBA-CAA-C2A | -2.14 | 107.47      | 113.78   |
| 23  | b     | 610    | CLA  | C11-C12-C13 | -2.14 | 108.86      | 115.97   |
| 25  | D     | 704    | BCR  | C39-C30-C25 | -2.14 | 106.89      | 110.24   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 511    | CLA  | CMD-C2D-C3D | -2.13 | 122.80      | 127.69   |
| 38  | F     | 102    | HEM  | CHA-C1A-NA  | 2.13  | 127.73      | 123.86   |
| 25  | A     | 409    | BCR  | C15-C14-C13 | -2.13 | 124.29      | 127.28   |
| 23  | D     | 703    | CLA  | CMA-C3A-C4A | -2.13 | 106.04      | 111.77   |
| 23  | b     | 607    | CLA  | CAA-CBA-CGA | 2.13  | 119.27      | 113.21   |
| 23  | c     | 512    | CLA  | C1-C2-C3    | -2.13 | 122.70      | 126.20   |
| 23  | B     | 613    | CLA  | C2A-C1A-CHA | -2.13 | 120.17      | 123.87   |
| 23  | C     | 509    | CLA  | C2A-C1A-CHA | -2.13 | 120.17      | 123.87   |
| 32  | m     | 103    | LMT  | O1'-C1'-C2' | 2.13  | 111.51      | 108.27   |
| 23  | B     | 601    | CLA  | CMC-C2C-C1C | 2.13  | 128.36      | 125.03   |
| 23  | B     | 613    | CLA  | CMA-C3A-C4A | -2.13 | 106.05      | 111.77   |
| 34  | m     | 101    | LMG  | C3-C4-C5    | 2.13  | 114.09      | 110.23   |
| 29  | d     | 404[B] | PL9  | C2-C1-C6    | 2.13  | 121.53      | 119.00   |
| 33  | D     | 707[A] | LHG  | O4-P-O5     | 2.13  | 122.34      | 112.44   |
| 36  | h     | 102    | DGD  | O4D-C4D-C3D | -2.13 | 105.36      | 110.38   |
| 25  | c     | 516    | BCR  | C33-C5-C6   | -2.12 | 122.17      | 124.48   |
| 25  | K     | 102    | BCR  | C20-C21-C22 | -2.12 | 124.30      | 127.28   |
| 24  | a     | 416[A] | PHO  | C1A-C2A-C3A | -2.12 | 100.82      | 102.84   |
| 23  | B     | 607    | CLA  | CAC-C3C-C4C | 2.12  | 127.55      | 124.79   |
| 23  | C     | 513    | CLA  | C2A-C1A-CHA | -2.12 | 120.19      | 123.87   |
| 25  | C     | 516    | BCR  | C3-C4-C5    | -2.12 | 110.28      | 114.06   |
| 38  | F     | 102    | HEM  | C4C-CHD-C1D | -2.12 | 121.52      | 126.02   |
| 23  | B     | 614    | CLA  | CAA-C2A-C3A | -2.12 | 107.28      | 113.00   |
| 25  | b     | 618    | BCR  | C7-C8-C9    | -2.12 | 123.10      | 126.23   |
| 23  | D     | 702[B] | CLA  | CMA-C3A-C2A | -2.12 | 105.80      | 113.98   |
| 29  | D     | 705[A] | PL9  | O2-C1-C6    | -2.12 | 117.11      | 120.48   |
| 23  | b     | 610    | CLA  | CMC-C2C-C1C | 2.12  | 128.34      | 125.03   |
| 23  | C     | 509    | CLA  | C7-C6-C5    | -2.12 | 107.62      | 113.26   |
| 23  | b     | 614    | CLA  | CMA-C3A-C2A | -2.12 | 105.80      | 113.98   |
| 23  | c     | 508    | CLA  | C4B-C3B-C2B | -2.11 | 104.67      | 107.30   |
| 29  | A     | 414[A] | PL9  | C51-C49-C50 | 2.11  | 119.46      | 114.59   |
| 32  | M     | 101    | LMT  | O1B-C1B-C2B | 2.11  | 113.29      | 108.09   |
| 23  | C     | 513    | CLA  | O1D-CGD-CBD | -2.11 | 120.35      | 124.52   |
| 36  | H     | 102    | DGD  | O3G-C3G-C2G | -2.11 | 105.68      | 110.82   |
| 25  | H     | 101    | BCR  | C24-C23-C22 | -2.11 | 123.11      | 126.23   |
| 23  | B     | 610    | CLA  | C4-C3-C5    | 2.11  | 118.89      | 115.23   |
| 23  | B     | 608    | CLA  | C11-C10-C8  | -2.11 | 108.95      | 115.97   |
| 25  | B     | 618    | BCR  | C15-C14-C13 | -2.11 | 124.32      | 127.28   |
| 24  | a     | 408[B] | PHO  | CMC-C2C-C1C | 2.11  | 128.53      | 124.73   |
| 23  | a     | 405[A] | CLA  | CMB-C2B-C3B | 2.11  | 131.51      | 126.55   |
| 24  | a     | 416[B] | PHO  | C4A-C3A-C2A | -2.11 | 100.83      | 102.84   |
| 25  | h     | 101    | BCR  | C37-C22-C21 | -2.11 | 119.40      | 122.82   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 34  | m     | 101    | LMG  | C7-O1-C1    | -2.11 | 109.28      | 113.80   |
| 24  | A     | 407[A] | PHO  | CBA-CAA-C2A | -2.11 | 107.57      | 113.78   |
| 29  | d     | 404[A] | PL9  | C35-C34-C36 | 2.11  | 118.88      | 115.23   |
| 26  | f     | 102    | SQD  | O7-S-C6     | 2.11  | 109.90      | 106.76   |
| 23  | B     | 616    | CLA  | OBD-CAD-C3D | -2.10 | 123.50      | 128.42   |
| 25  | k     | 101    | BCR  | C20-C21-C22 | -2.10 | 124.33      | 127.28   |
| 25  | h     | 101    | BCR  | C10-C11-C12 | -2.10 | 117.10      | 123.20   |
| 40  | v     | 201    | HEC  | CBA-CAA-C2A | -2.10 | 106.71      | 112.53   |
| 24  | a     | 416[A] | PHO  | O2A-CGA-CBA | 2.10  | 118.25      | 111.83   |
| 23  | A     | 405[B] | CLA  | CAA-CBA-CGA | 2.10  | 119.18      | 113.21   |
| 29  | a     | 414[B] | PL9  | C35-C34-C33 | -2.10 | 118.23      | 123.63   |
| 24  | A     | 417[A] | PHO  | CMB-C2B-C3B | 2.10  | 128.88      | 124.68   |
| 34  | m     | 101    | LMG  | O8-C28-O10  | -2.10 | 118.37      | 123.63   |
| 32  | a     | 417    | LMT  | O5B-C5B-C4B | 2.10  | 113.48      | 109.70   |
| 23  | d     | 401[A] | CLA  | CHD-C4C-NC  | 2.10  | 127.49      | 124.23   |
| 23  | B     | 601    | CLA  | CAA-C2A-C3A | -2.10 | 107.32      | 113.00   |
| 23  | c     | 503    | CLA  | C2A-C1A-CHA | -2.10 | 120.22      | 123.87   |
| 23  | B     | 616    | CLA  | C4-C3-C2    | -2.10 | 118.24      | 123.63   |
| 29  | A     | 414[A] | PL9  | C25-C24-C26 | 2.10  | 118.87      | 115.23   |
| 25  | k     | 101    | BCR  | C10-C11-C12 | -2.10 | 117.12      | 123.20   |
| 23  | b     | 611    | CLA  | CBC-CAC-C3C | -2.10 | 106.73      | 112.42   |
| 29  | d     | 404[A] | PL9  | C51-C49-C50 | 2.10  | 119.42      | 114.59   |
| 25  | C     | 515    | BCR  | C37-C22-C23 | 2.10  | 121.29      | 118.09   |
| 24  | a     | 416[B] | PHO  | O1D-CGD-CBD | -2.10 | 121.54      | 124.72   |
| 25  | C     | 516    | BCR  | C32-C1-C6   | -2.10 | 106.95      | 110.24   |
| 35  | B     | 624    | HTG  | O5-C5-C4    | 2.10  | 113.48      | 109.70   |
| 25  | c     | 515    | BCR  | C37-C22-C21 | -2.10 | 119.42      | 122.82   |
| 23  | b     | 604    | CLA  | C11-C12-C13 | -2.10 | 109.00      | 115.97   |
| 23  | c     | 512    | CLA  | C2A-C1A-CHA | -2.09 | 120.23      | 123.87   |
| 23  | d     | 402    | CLA  | OBD-CAD-C3D | -2.09 | 123.52      | 128.42   |
| 29  | A     | 414[A] | PL9  | O1-C4-C3    | -2.09 | 118.52      | 120.73   |
| 40  | V     | 201    | HEC  | CBA-CAA-C2A | -2.09 | 106.75      | 112.53   |
| 25  | c     | 516    | BCR  | C15-C16-C17 | -2.09 | 119.24      | 123.52   |
| 23  | C     | 510    | CLA  | C4-C3-C5    | 2.09  | 118.86      | 115.23   |
| 23  | A     | 404[A] | CLA  | C7-C6-C5    | -2.09 | 107.69      | 113.26   |
| 23  | A     | 405[A] | CLA  | C1-C2-C3    | -2.09 | 122.77      | 126.20   |
| 34  | m     | 101    | LMG  | C12-C11-C10 | -2.09 | 106.04      | 113.69   |
| 23  | B     | 602    | CLA  | CAA-CBA-CGA | -2.09 | 107.28      | 113.21   |
| 25  | Y     | 101    | BCR  | C3-C4-C5    | -2.09 | 110.33      | 114.06   |
| 29  | A     | 414[B] | PL9  | C10-C9-C8   | -2.09 | 118.27      | 123.63   |
| 23  | d     | 402    | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.40   |
| 25  | b     | 619    | BCR  | C7-C8-C9    | -2.09 | 123.15      | 126.23   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 514    | CLA  | CMB-C2B-C1B | 2.09  | 128.59      | 125.42   |
| 34  | c     | 521    | LMG  | C1-C2-C3    | -2.08 | 105.62      | 110.01   |
| 23  | C     | 513    | CLA  | C3B-C4B-NB  | 2.08  | 112.39      | 110.53   |
| 34  | d     | 410    | LMG  | C7-O1-C1    | -2.08 | 109.33      | 113.80   |
| 23  | b     | 615    | CLA  | C2A-C1A-CHA | -2.08 | 120.25      | 123.87   |
| 23  | B     | 607    | CLA  | CHD-C4C-NC  | 2.08  | 127.46      | 124.23   |
| 23  | b     | 616    | CLA  | CHA-C1A-NA  | -2.08 | 121.68      | 126.39   |
| 25  | B     | 619    | BCR  | C10-C11-C12 | -2.08 | 117.17      | 123.20   |
| 29  | A     | 414[B] | PL9  | C2-C1-C6    | 2.08  | 121.47      | 119.00   |
| 26  | a     | 411[A] | SQD  | O7-S-C6     | 2.08  | 109.86      | 106.76   |
| 23  | a     | 405[B] | CLA  | CAA-CBA-CGA | -2.08 | 107.30      | 113.21   |
| 25  | a     | 410    | BCR  | C11-C10-C9  | -2.08 | 124.36      | 127.28   |
| 36  | C     | 517[B] | DGD  | O1G-C1A-O1A | -2.08 | 118.43      | 123.63   |
| 23  | a     | 405[B] | CLA  | C7-C6-C5    | -2.08 | 107.72      | 113.26   |
| 32  | F     | 101    | LMT  | O1'-C1'-C2' | 2.08  | 111.43      | 108.27   |
| 29  | a     | 414[B] | PL9  | C51-C49-C50 | 2.08  | 119.37      | 114.59   |
| 23  | B     | 608    | CLA  | OBD-CAD-C3D | -2.08 | 123.56      | 128.42   |
| 23  | A     | 405[B] | CLA  | C4C-C3C-C2C | -2.08 | 103.87      | 106.89   |
| 23  | b     | 611    | CLA  | C4-C3-C5    | 2.07  | 118.83      | 115.23   |
| 23  | A     | 405[B] | CLA  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 33  | d     | 405[B] | LHG  | C5-O7-C7    | -2.07 | 112.84      | 117.80   |
| 23  | B     | 615    | CLA  | CHA-C1A-NA  | -2.07 | 121.70      | 126.39   |
| 24  | a     | 408[B] | PHO  | CAC-C3C-C4C | 2.07  | 129.35      | 124.03   |
| 24  | a     | 408[A] | PHO  | CBC-CAC-C3C | -2.07 | 109.91      | 112.87   |
| 23  | C     | 511    | CLA  | OBD-CAD-C3D | -2.07 | 123.58      | 128.42   |
| 23  | c     | 507    | CLA  | CAA-CBA-CGA | 2.07  | 119.08      | 113.21   |
| 34  | c     | 501    | LMG  | C30-C29-C28 | -2.07 | 106.12      | 113.69   |
| 25  | h     | 101    | BCR  | C32-C1-C6   | -2.07 | 107.00      | 110.24   |
| 25  | c     | 516    | BCR  | C37-C22-C21 | -2.07 | 119.47      | 122.82   |
| 23  | d     | 401[B] | CLA  | CMC-C2C-C1C | 2.07  | 128.26      | 125.03   |
| 23  | c     | 509    | CLA  | CAC-C3C-C4C | 2.07  | 127.48      | 124.79   |
| 23  | B     | 613    | CLA  | C4-C3-C2    | -2.07 | 118.32      | 123.63   |
| 25  | Y     | 101    | BCR  | C36-C18-C19 | 2.06  | 121.24      | 118.09   |
| 23  | C     | 502    | CLA  | CAA-C2A-C3A | -2.06 | 107.42      | 113.00   |
| 23  | c     | 510    | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 36  | C     | 517[A] | DGD  | O1G-C1A-C2A | 2.06  | 118.13      | 111.83   |
| 23  | b     | 611    | CLA  | CAC-C3C-C4C | 2.06  | 127.47      | 124.79   |
| 23  | b     | 616    | CLA  | C11-C12-C13 | -2.06 | 109.11      | 115.97   |
| 26  | a     | 411[A] | SQD  | O48-C23-O10 | -2.06 | 118.47      | 123.63   |
| 36  | h     | 102    | DGD  | C3E-C4E-C5E | -2.06 | 106.49      | 110.23   |
| 23  | B     | 611    | CLA  | CAC-C3C-C4C | 2.06  | 127.47      | 124.79   |
| 23  | C     | 513    | CLA  | CAC-C3C-C4C | 2.06  | 127.47      | 124.79   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | C     | 503    | CLA  | CMC-C2C-C1C | 2.06  | 128.25      | 125.03   |
| 23  | b     | 601    | CLA  | C2A-C1A-CHA | -2.06 | 120.29      | 123.87   |
| 23  | b     | 610    | CLA  | CAC-C3C-C2C | 2.06  | 131.34      | 127.56   |
| 23  | D     | 702[A] | CLA  | CMB-C2B-C1B | 2.06  | 128.56      | 125.42   |
| 25  | D     | 704    | BCR  | C24-C23-C22 | -2.06 | 123.19      | 126.23   |
| 26  | a     | 411[B] | SQD  | O9-S-O7     | -2.06 | 107.13      | 113.82   |
| 33  | d     | 412[B] | LHG  | O7-C7-O9    | -2.06 | 118.89      | 123.70   |
| 23  | b     | 616    | CLA  | O1D-CGD-CBD | -2.06 | 120.46      | 124.52   |
| 23  | C     | 509    | CLA  | CMC-C2C-C1C | 2.06  | 128.25      | 125.03   |
| 23  | b     | 605    | CLA  | C6-C7-C8    | -2.06 | 109.13      | 115.97   |
| 23  | b     | 610    | CLA  | C4-C3-C2    | -2.06 | 118.34      | 123.63   |
| 23  | b     | 610    | CLA  | CMA-C3A-C2A | -2.06 | 106.04      | 113.98   |
| 34  | Z     | 101    | LMG  | C9-C8-C7    | -2.05 | 107.00      | 111.78   |
| 23  | A     | 406[B] | CLA  | C4-C3-C5    | 2.05  | 118.79      | 115.23   |
| 23  | B     | 613    | CLA  | CBC-CAC-C3C | -2.05 | 106.85      | 112.42   |
| 25  | H     | 101    | BCR  | C33-C5-C6   | -2.05 | 122.24      | 124.48   |
| 36  | h     | 102    | DGD  | C4D-C3D-C2D | -2.05 | 107.23      | 110.83   |
| 29  | d     | 404[B] | PL9  | C45-C44-C46 | 2.05  | 118.79      | 115.23   |
| 23  | A     | 406[A] | CLA  | CMA-C3A-C4A | -2.05 | 106.26      | 111.77   |
| 32  | F     | 101    | LMT  | C3B-C4B-C5B | -2.05 | 106.52      | 110.23   |
| 25  | C     | 515    | BCR  | C10-C11-C12 | -2.05 | 117.27      | 123.20   |
| 23  | D     | 702[A] | CLA  | CMA-C3A-C2A | -2.05 | 106.06      | 113.98   |
| 23  | A     | 404[B] | CLA  | CHB-C1B-C2B | -2.05 | 121.48      | 127.43   |
| 23  | C     | 506    | CLA  | CBC-CAC-C3C | -2.05 | 106.87      | 112.42   |
| 25  | Y     | 101    | BCR  | C21-C20-C19 | -2.05 | 117.27      | 123.20   |
| 23  | B     | 607    | CLA  | C1-C2-C3    | -2.05 | 122.84      | 126.20   |
| 23  | C     | 509    | CLA  | CHB-C4A-NA  | 2.04  | 127.35      | 124.40   |
| 23  | a     | 406[A] | CLA  | CAA-CBA-CGA | 2.04  | 119.01      | 113.21   |
| 23  | B     | 602    | CLA  | C11-C12-C13 | -2.04 | 109.17      | 115.97   |
| 34  | B     | 621    | LMG  | O8-C28-O10  | -2.04 | 118.52      | 123.63   |
| 23  | d     | 401[A] | CLA  | CBC-CAC-C3C | -2.04 | 106.88      | 112.42   |
| 23  | B     | 603    | CLA  | C2A-C3A-C4A | -2.04 | 98.57       | 101.87   |
| 23  | B     | 610    | CLA  | C1-C2-C3    | -2.04 | 122.85      | 126.20   |
| 23  | B     | 603    | CLA  | C2A-C1A-CHA | -2.04 | 120.32      | 123.87   |
| 23  | B     | 609    | CLA  | CHA-C1A-NA  | -2.04 | 121.77      | 126.39   |
| 33  | D     | 706[A] | LHG  | O4-P-O5     | 2.04  | 121.95      | 112.44   |
| 25  | a     | 410    | BCR  | C7-C8-C9    | -2.04 | 123.21      | 126.23   |
| 29  | D     | 705[A] | PL9  | C25-C24-C23 | -2.04 | 118.38      | 123.63   |
| 23  | B     | 602    | CLA  | CMA-C3A-C2A | -2.04 | 106.09      | 113.98   |
| 24  | A     | 417[B] | PHO  | CMA-C3A-C4A | -2.04 | 110.21      | 114.61   |
| 23  | A     | 404[A] | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.40   |
| 23  | c     | 511    | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.40   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23  | D     | 702[A] | CLA  | CBC-CAC-C3C | -2.04 | 106.89      | 112.42   |
| 23  | c     | 512    | CLA  | CMA-C3A-C4A | 2.04  | 117.26      | 111.77   |
| 35  | B     | 624    | HTG  | C3-C4-C5    | 2.04  | 113.93      | 110.23   |
| 23  | c     | 512    | CLA  | OBD-CAD-C3D | -2.04 | 123.65      | 128.42   |
| 40  | v     | 201    | HEC  | CMC-C2C-C1C | -2.04 | 122.31      | 125.42   |
| 25  | B     | 617    | BCR  | C16-C17-C18 | -2.04 | 124.42      | 127.28   |
| 33  | d     | 412[A] | LHG  | C5-O7-C7    | -2.04 | 112.92      | 117.80   |
| 34  | m     | 101    | LMG  | O7-C10-O9   | -2.04 | 118.94      | 123.70   |
| 23  | A     | 408    | CLA  | OBD-CAD-C3D | -2.04 | 123.66      | 128.42   |
| 25  | b     | 618    | BCR  | C38-C26-C25 | -2.04 | 122.26      | 124.48   |
| 23  | b     | 605    | CLA  | CED-O2D-CGD | 2.03  | 120.53      | 115.92   |
| 23  | c     | 513    | CLA  | CHA-C1A-NA  | -2.03 | 121.78      | 126.39   |
| 24  | a     | 408[B] | PHO  | OBD-CAD-C3D | -2.03 | 124.72      | 127.89   |
| 23  | d     | 402    | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 23  | A     | 406[B] | CLA  | CHB-C1B-C2B | -2.03 | 121.52      | 127.43   |
| 27  | B     | 628    | GOL  | C3-C2-C1    | -2.03 | 104.34      | 111.80   |
| 34  | C     | 501    | LMG  | O7-C10-O9   | -2.03 | 118.95      | 123.70   |
| 36  | c     | 517[B] | DGD  | O1G-C1A-C2A | 2.03  | 118.03      | 111.83   |
| 23  | c     | 511    | CLA  | C7-C6-C5    | -2.03 | 107.85      | 113.26   |
| 23  | A     | 404[A] | CLA  | C4-C3-C5    | 2.03  | 118.75      | 115.23   |
| 38  | f     | 101    | HEM  | O2D-CGD-CBD | 2.03  | 120.42      | 114.00   |
| 23  | B     | 601    | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 32  | t     | 101    | LMT  | C1-O1'-C1'  | 2.03  | 117.15      | 113.68   |
| 35  | B     | 624    | HTG  | C1-O5-C5    | 2.03  | 116.20      | 112.56   |
| 36  | h     | 102    | DGD  | O2G-C1B-O1B | -2.03 | 118.96      | 123.70   |
| 29  | D     | 705[A] | PL9  | C30-C29-C31 | 2.03  | 118.75      | 115.23   |
| 24  | a     | 408[A] | PHO  | O2D-CGD-O1D | -2.03 | 119.90      | 123.85   |
| 33  | L     | 101[B] | LHG  | O4-P-O5     | 2.03  | 121.87      | 112.44   |
| 25  | K     | 102    | BCR  | C3-C4-C5    | -2.03 | 110.44      | 114.06   |
| 25  | B     | 619    | BCR  | C2-C1-C6    | 2.03  | 113.38      | 110.44   |
| 35  | b     | 622    | HTG  | C6-C5-C4    | -2.02 | 108.05      | 113.02   |
| 23  | a     | 407[A] | CLA  | CAA-CBA-CGA | 2.02  | 118.96      | 113.21   |
| 35  | o     | 301    | HTG  | C1-C2-C3    | 2.02  | 114.51      | 110.55   |
| 23  | a     | 407[A] | CLA  | CMA-C3A-C2A | -2.02 | 106.16      | 113.98   |
| 36  | C     | 517[A] | DGD  | C3E-C4E-C5E | 2.02  | 113.90      | 110.23   |
| 23  | B     | 614    | CLA  | O1D-CGD-CBD | -2.02 | 120.53      | 124.52   |
| 25  | t     | 102    | BCR  | C2-C1-C6    | 2.02  | 113.38      | 110.44   |
| 23  | c     | 507    | CLA  | CMC-C2C-C1C | 2.02  | 128.19      | 125.03   |
| 26  | A     | 410[B] | SQD  | O7-S-C6     | 2.02  | 109.77      | 106.76   |
| 23  | A     | 404[B] | CLA  | CED-O2D-CGD | 2.02  | 120.50      | 115.92   |
| 38  | f     | 101    | HEM  | O2A-CGA-CBA | 2.02  | 120.38      | 114.00   |
| 36  | c     | 518[B] | DGD  | O1G-C1A-O1A | -2.02 | 118.58      | 123.63   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | A     | 417[A] | PHO  | CED-O2D-CGD | 2.02  | 120.49      | 115.92   |
| 25  | t     | 102    | BCR  | C29-C28-C27 | -2.02 | 106.84      | 111.28   |
| 23  | b     | 609    | CLA  | C4-C3-C5    | 2.02  | 118.73      | 115.23   |
| 23  | b     | 613    | CLA  | C16-C15-C13 | -2.02 | 109.27      | 115.97   |
| 38  | f     | 101    | HEM  | CHB-C1B-C2B | -2.02 | 121.22      | 126.95   |
| 29  | A     | 414[B] | PL9  | C35-C34-C33 | -2.01 | 118.45      | 123.63   |
| 23  | C     | 511    | CLA  | O1D-CGD-CBD | -2.01 | 120.55      | 124.52   |
| 23  | b     | 602    | CLA  | CHC-C1C-C2C | -2.01 | 121.22      | 126.95   |
| 23  | A     | 405[A] | CLA  | C4D-C3D-CAD | -2.01 | 105.92      | 108.11   |
| 23  | A     | 406[A] | CLA  | CHB-C4A-NA  | 2.01  | 127.30      | 124.40   |
| 34  | c     | 520    | LMG  | O7-C10-O9   | -2.01 | 119.00      | 123.70   |
| 38  | F     | 102    | HEM  | O2D-CGD-O1D | -2.01 | 118.16      | 123.33   |
| 23  | D     | 703    | CLA  | CBC-CAC-C3C | -2.01 | 106.97      | 112.42   |
| 23  | c     | 513    | CLA  | CHB-C1B-C2B | -2.01 | 121.60      | 127.43   |
| 23  | a     | 406[B] | CLA  | CMC-C2C-C1C | 2.01  | 128.17      | 125.03   |
| 23  | c     | 508    | CLA  | CHA-C1A-NA  | -2.01 | 121.84      | 126.39   |
| 23  | b     | 616    | CLA  | C2A-C1A-CHA | -2.01 | 120.38      | 123.87   |
| 23  | c     | 505    | CLA  | CMB-C2B-C3B | 2.00  | 131.27      | 126.55   |
| 23  | b     | 615    | CLA  | CAC-C3C-C4C | 2.00  | 127.40      | 124.79   |
| 23  | B     | 616    | CLA  | CHA-C1A-NA  | -2.00 | 121.85      | 126.39   |
| 24  | A     | 407[A] | PHO  | C4-C3-C5    | 2.00  | 118.70      | 115.23   |
| 23  | c     | 503    | CLA  | C4C-C3C-C2C | -2.00 | 103.98      | 106.89   |
| 26  | b     | 620    | SQD  | C4-C3-C2    | 2.00  | 114.34      | 110.83   |
| 26  | A     | 412    | SQD  | O6-C1-C2    | 2.00  | 111.31      | 108.27   |

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[B] | CLA  | ND   |
| 23  | A     | 408    | 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   |

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| Mol | Chain | Res    | Type | Atom |
|-----|-------|--------|------|------|
| 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   |
| 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     | 702[A] | CLA  | ND   |
| 23  | D     | 702[B] | CLA  | ND   |
| 23  | D     | 703    | CLA  | ND   |
| 23  | a     | 405[A] | CLA  | ND   |
| 23  | a     | 405[B] | CLA  | ND   |
| 23  | a     | 406[A] | CLA  | ND   |
| 23  | a     | 406[B] | 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   |

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| Mol | Chain | Res    | Type | Atom |
|-----|-------|--------|------|------|
| 23  | c     | 504    | 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     | 401[A] | CLA  | ND   |
| 23  | d     | 401[B] | CLA  | ND   |
| 23  | d     | 402    | CLA  | ND   |

All (1593) 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     | 508    | CLA  | C2B-C3B-CAB-CBB |
| 23  | C     | 508    | CLA  | C4B-C3B-CAB-CBB |
| 23  | C     | 508    | CLA  | CHA-CBD-CGD-O1D |
| 23  | C     | 508    | CLA  | CHA-CBD-CGD-O2D |
| 23  | C     | 510    | CLA  | CHA-CBD-CGD-O1D |
| 23  | C     | 510    | CLA  | CHA-CBD-CGD-O2D |
| 23  | b     | 614    | CLA  | CAD-CBD-CGD-O1D |
| 23  | b     | 614    | CLA  | CAD-CBD-CGD-O2D |
| 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  | CHA-CBD-CGD-O2D |
| 23  | c     | 510    | CLA  | C11-C10-C8-C9   |
| 23  | c     | 514    | CLA  | C2B-C3B-CAB-CBB |
| 23  | c     | 514    | CLA  | C4B-C3B-CAB-CBB |
| 25  | T     | 102    | BCR  | C13-C14-C15-C16 |
| 25  | Y     | 101    | BCR  | C1-C6-C7-C8     |
| 25  | Y     | 101    | BCR  | C5-C6-C7-C8     |
| 25  | y     | 101    | BCR  | C1-C6-C7-C8     |
| 25  | y     | 101    | BCR  | C5-C6-C7-C8     |
| 26  | A     | 410[A] | SQD  | O49-C7-O47-C45  |
| 26  | A     | 412    | SQD  | O6-C44-C45-O47  |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | B     | 620    | SQD  | O5-C1-O6-C44    |
| 26  | B     | 620    | SQD  | O49-C7-O47-C45  |
| 26  | B     | 620    | SQD  | C8-C7-O47-C45   |
| 26  | X     | 101    | SQD  | C2-C1-O6-C44    |
| 26  | X     | 101    | SQD  | O49-C7-O47-C45  |
| 26  | X     | 101    | SQD  | C8-C7-O47-C45   |
| 26  | a     | 412    | SQD  | O6-C44-C45-O47  |
| 26  | a     | 412    | SQD  | C5-C6-S-O7      |
| 26  | a     | 412    | SQD  | C5-C6-S-O8      |
| 26  | a     | 412    | SQD  | C5-C6-S-O9      |
| 26  | b     | 620    | SQD  | C8-C7-O47-C45   |
| 26  | f     | 102    | SQD  | O6-C44-C45-O47  |
| 26  | f     | 102    | SQD  | O49-C7-O47-C45  |
| 26  | f     | 102    | SQD  | C8-C7-O47-C45   |
| 27  | A     | 411    | GOL  | O1-C1-C2-C3     |
| 27  | B     | 623    | GOL  | C1-C2-C3-O3     |
| 27  | B     | 628    | GOL  | O1-C1-C2-C3     |
| 27  | D     | 712    | GOL  | C1-C2-C3-O3     |
| 27  | V     | 203[A] | GOL  | C1-C2-C3-O3     |
| 27  | V     | 203[B] | GOL  | C1-C2-C3-O3     |
| 27  | b     | 624    | GOL  | C1-C2-C3-O3     |
| 27  | c     | 527    | GOL  | C1-C2-C3-O3     |
| 27  | o     | 303    | GOL  | C1-C2-C3-O3     |
| 27  | o     | 304    | GOL  | C1-C2-C3-O3     |
| 29  | a     | 414[A] | PL9  | C25-C24-C26-C27 |
| 29  | a     | 414[B] | PL9  | C23-C24-C26-C27 |
| 29  | a     | 414[B] | PL9  | C25-C24-C26-C27 |
| 32  | A     | 420    | LMT  | C2'-C1'-O1'-C1  |
| 32  | A     | 420    | LMT  | O5'-C1'-O1'-C1  |
| 32  | B     | 630    | LMT  | O5'-C1'-O1'-C1  |
| 32  | B     | 630    | LMT  | C2-C1-O1'-C1'   |
| 32  | F     | 101    | LMT  | C2'-C1'-O1'-C1  |
| 32  | F     | 101    | LMT  | O5'-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  |
| 33  | A     | 419[B] | LHG  | C4-O6-P-O3      |
| 33  | A     | 419[B] | LHG  | C4-O6-P-O5      |
| 33  | D     | 706[A] | LHG  | O2-C2-C3-O3     |
| 33  | D     | 706[A] | LHG  | C3-O3-P-O4      |
| 33  | D     | 706[A] | LHG  | C3-O3-P-O5      |
| 33  | D     | 706[A] | LHG  | C3-O3-P-O6      |

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| Mol | Chain | Res    | Type | Atoms         |
|-----|-------|--------|------|---------------|
| 33  | D     | 706[A] | LHG  | C4-O6-P-O4    |
| 33  | D     | 706[B] | LHG  | O2-C2-C3-O3   |
| 33  | D     | 706[B] | LHG  | C3-O3-P-O4    |
| 33  | D     | 706[B] | LHG  | C3-O3-P-O6    |
| 33  | D     | 706[B] | LHG  | C4-O6-P-O3    |
| 33  | D     | 706[B] | LHG  | C4-O6-P-O4    |
| 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  | a     | 420[A] | LHG  | C3-O3-P-O4    |
| 33  | a     | 420[A] | LHG  | C3-O3-P-O6    |
| 33  | a     | 420[A] | LHG  | C4-O6-P-O3    |
| 33  | a     | 420[A] | LHG  | C4-O6-P-O5    |
| 33  | a     | 420[A] | LHG  | O10-C23-O8-C6 |
| 33  | a     | 420[A] | LHG  | C24-C23-O8-C6 |
| 33  | a     | 420[B] | LHG  | C3-O3-P-O4    |
| 33  | a     | 420[B] | LHG  | C3-O3-P-O6    |
| 33  | a     | 420[B] | LHG  | C4-O6-P-O3    |
| 33  | a     | 420[B] | LHG  | C4-O6-P-O5    |
| 33  | a     | 420[B] | LHG  | O10-C23-O8-C6 |
| 33  | a     | 420[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    |
| 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     | 405[A] | LHG  | C3-O3-P-O5    |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | d     | 405[A] | LHG  | C3-O3-P-O6      |
| 33  | d     | 405[A] | LHG  | C4-O6-P-O4      |
| 33  | d     | 405[B] | LHG  | C3-O3-P-O4      |
| 33  | d     | 405[B] | LHG  | C3-O3-P-O6      |
| 33  | d     | 405[B] | LHG  | C4-O6-P-O4      |
| 33  | d     | 412[A] | LHG  | C3-O3-P-O5      |
| 34  | C     | 521    | LMG  | C11-C10-O7-C8   |
| 34  | c     | 521    | LMG  | O9-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     |
| 35  | b     | 623    | HTG  | O5-C1-S1-C1'    |
| 38  | F     | 102    | HEM  | C2C-C3C-CAC-CBC |
| 38  | F     | 102    | HEM  | C4C-C3C-CAC-CBC |
| 40  | V     | 201    | HEC  | C2B-C3B-CAB-CBB |
| 40  | V     | 201    | HEC  | C4B-C3B-CAB-CBB |
| 40  | V     | 201    | HEC  | C2C-C3C-CAC-CBC |
| 40  | V     | 201    | HEC  | C4C-C3C-CAC-CBC |
| 40  | v     | 201    | HEC  | C2B-C3B-CAB-CBB |
| 40  | v     | 201    | HEC  | C4B-C3B-CAB-CBB |
| 40  | v     | 201    | HEC  | C2C-C3C-CAC-CBC |
| 40  | v     | 201    | HEC  | C4C-C3C-CAC-CBC |
| 32  | A     | 420    | LMT  | O5B-C1B-O1B-C4' |
| 32  | B     | 629    | LMT  | C4'-C5'-C6'-O6' |
| 32  | m     | 103    | LMT  | C4B-C5B-C6B-O6B |
| 26  | A     | 410[B] | SQD  | O49-C7-O47-C45  |
| 26  | b     | 620    | SQD  | O49-C7-O47-C45  |
| 32  | T     | 101    | LMT  | C4B-C5B-C6B-O6B |
| 23  | D     | 703    | CLA  | C3-C5-C6-C7     |
| 23  | b     | 616    | CLA  | C3-C5-C6-C7     |
| 23  | c     | 513    | CLA  | C3-C5-C6-C7     |
| 23  | d     | 402    | CLA  | C3-C5-C6-C7     |
| 32  | T     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 26  | A     | 410[A] | SQD  | C8-C7-O47-C45   |
| 26  | A     | 410[B] | SQD  | C8-C7-O47-C45   |
| 34  | c     | 521    | LMG  | C11-C10-O7-C8   |
| 32  | a     | 417    | LMT  | O5B-C5B-C6B-O6B |
| 23  | A     | 408    | CLA  | C4-C3-C5-C6     |
| 23  | C     | 505    | CLA  | C4-C3-C5-C6     |
| 23  | C     | 508    | CLA  | C4-C3-C5-C6     |
| 23  | a     | 409    | CLA  | C4-C3-C5-C6     |
| 23  | c     | 508    | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | d     | 402    | CLA  | C4-C3-C5-C6     |
| 29  | A     | 414[A] | PL9  | C15-C14-C16-C17 |
| 29  | A     | 414[B] | PL9  | C15-C14-C16-C17 |
| 23  | A     | 408    | CLA  | C2-C3-C5-C6     |
| 23  | d     | 402    | CLA  | C2-C3-C5-C6     |
| 32  | B     | 629    | LMT  | O5B-C5B-C6B-O6B |
| 32  | m     | 103    | LMT  | O5B-C5B-C6B-O6B |
| 23  | B     | 614    | CLA  | C3-C5-C6-C7     |
| 35  | D     | 710    | HTG  | O5-C5-C6-O6     |
| 32  | B     | 627    | LMT  | C4'-C5'-C6'-O6' |
| 32  | F     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 34  | C     | 521    | LMG  | O9-C10-O7-C8    |
| 32  | B     | 627    | LMT  | O5'-C5'-C6'-O6' |
| 23  | A     | 408    | CLA  | C3-C5-C6-C7     |
| 23  | B     | 616    | CLA  | C3-C5-C6-C7     |
| 33  | E     | 101[A] | LHG  | O2-C2-C3-O3     |
| 33  | d     | 405[A] | LHG  | O2-C2-C3-O3     |
| 33  | d     | 405[B] | LHG  | O2-C2-C3-O3     |
| 32  | B     | 627    | LMT  | O5B-C5B-C6B-O6B |
| 32  | T     | 101    | LMT  | C4'-C5'-C6'-O6' |
| 34  | c     | 521    | LMG  | C4-C5-C6-O5     |
| 34  | z     | 101    | LMG  | C11-C10-O7-C8   |
| 23  | D     | 703    | CLA  | CBD-CGD-O2D-CED |
| 23  | c     | 512    | CLA  | CBD-CGD-O2D-CED |
| 32  | a     | 417    | LMT  | C4B-C5B-C6B-O6B |
| 35  | b     | 625    | HTG  | S1-C1'-C2'-C3'  |
| 23  | b     | 603    | CLA  | C4-C3-C5-C6     |
| 23  | b     | 614    | CLA  | C4-C3-C5-C6     |
| 29  | A     | 414[B] | PL9  | C30-C29-C31-C32 |
| 29  | a     | 414[A] | PL9  | C30-C29-C31-C32 |
| 29  | a     | 414[B] | PL9  | C30-C29-C31-C32 |
| 23  | C     | 505    | CLA  | C2-C3-C5-C6     |
| 23  | C     | 508    | CLA  | C2-C3-C5-C6     |
| 23  | b     | 603    | CLA  | C2-C3-C5-C6     |
| 23  | b     | 614    | CLA  | C2-C3-C5-C6     |
| 23  | c     | 508    | CLA  | C2-C3-C5-C6     |
| 29  | A     | 414[A] | PL9  | C13-C14-C16-C17 |
| 29  | A     | 414[A] | PL9  | C18-C19-C21-C22 |
| 29  | A     | 414[B] | PL9  | C13-C14-C16-C17 |
| 29  | A     | 414[B] | PL9  | C18-C19-C21-C22 |
| 29  | a     | 414[A] | PL9  | C13-C14-C16-C17 |
| 29  | a     | 414[A] | PL9  | C28-C29-C31-C32 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 29  | a     | 414[B] | PL9  | C13-C14-C16-C17 |
| 29  | a     | 414[B] | PL9  | C28-C29-C31-C32 |
| 34  | C     | 521    | LMG  | O6-C5-C6-O5     |
| 35  | b     | 625    | HTG  | O5-C5-C6-O6     |
| 29  | A     | 414[A] | PL9  | C9-C11-C12-C13  |
| 29  | A     | 414[A] | PL9  | C14-C16-C17-C18 |
| 29  | A     | 414[B] | PL9  | C9-C11-C12-C13  |
| 29  | A     | 414[B] | PL9  | C14-C16-C17-C18 |
| 29  | A     | 414[B] | PL9  | C44-C46-C47-C48 |
| 29  | D     | 705[A] | PL9  | C39-C41-C42-C43 |
| 29  | a     | 414[A] | PL9  | C9-C11-C12-C13  |
| 29  | a     | 414[A] | PL9  | C14-C16-C17-C18 |
| 29  | a     | 414[B] | PL9  | C9-C11-C12-C13  |
| 29  | a     | 414[B] | PL9  | C14-C16-C17-C18 |
| 29  | d     | 404[B] | PL9  | C39-C41-C42-C43 |
| 32  | B     | 629    | LMT  | C4B-C5B-C6B-O6B |
| 32  | F     | 101    | LMT  | C4'-C5'-C6'-O6' |
| 32  | e     | 101    | LMT  | C4'-C5'-C6'-O6' |
| 32  | A     | 418    | LMT  | O5'-C1'-O1'-C1  |
| 32  | B     | 629    | LMT  | O5'-C1'-O1'-C1  |
| 32  | b     | 621    | LMT  | O5'-C1'-O1'-C1  |
| 23  | c     | 514    | CLA  | CBD-CGD-O2D-CED |
| 32  | B     | 629    | LMT  | O5'-C5'-C6'-O6' |
| 32  | T     | 101    | LMT  | O5B-C5B-C6B-O6B |
| 32  | b     | 621    | LMT  | O5'-C5'-C6'-O6' |
| 32  | b     | 627    | LMT  | O5'-C5'-C6'-O6' |
| 35  | D     | 710    | HTG  | C4-C5-C6-O6     |
| 32  | A     | 420    | LMT  | O5B-C5B-C6B-O6B |
| 32  | A     | 420    | LMT  | O5'-C5'-C6'-O6' |
| 32  | B     | 630    | LMT  | O5'-C5'-C6'-O6' |
| 34  | c     | 521    | LMG  | O6-C5-C6-O5     |
| 34  | z     | 101    | LMG  | O9-C10-O7-C8    |
| 33  | D     | 706[B] | LHG  | C1-C2-C3-O3     |
| 33  | d     | 405[A] | LHG  | C1-C2-C3-O3     |
| 23  | a     | 409    | CLA  | CBA-CGA-O2A-C1  |
| 23  | c     | 510    | CLA  | CBA-CGA-O2A-C1  |
| 23  | C     | 510    | CLA  | CBD-CGD-O2D-CED |
| 32  | A     | 420    | LMT  | C4B-C5B-C6B-O6B |
| 23  | B     | 605    | CLA  | C4-C3-C5-C6     |
| 23  | b     | 605    | CLA  | C4-C3-C5-C6     |
| 29  | A     | 414[A] | PL9  | C20-C19-C21-C22 |
| 29  | A     | 414[B] | PL9  | C20-C19-C21-C22 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 29  | a     | 414[A] | PL9  | C15-C14-C16-C17 |
| 29  | a     | 414[B] | PL9  | C15-C14-C16-C17 |
| 23  | B     | 605    | CLA  | C2-C3-C5-C6     |
| 23  | a     | 409    | CLA  | C2-C3-C5-C6     |
| 23  | b     | 605    | CLA  | C2-C3-C5-C6     |
| 29  | a     | 414[A] | PL9  | C23-C24-C26-C27 |
| 23  | B     | 602    | CLA  | C6-C7-C8-C9     |
| 23  | B     | 613    | CLA  | C11-C12-C13-C14 |
| 23  | C     | 503    | CLA  | C14-C13-C15-C16 |
| 23  | C     | 507    | CLA  | C14-C13-C15-C16 |
| 23  | b     | 601    | CLA  | C11-C10-C8-C9   |
| 23  | b     | 604    | CLA  | C6-C7-C8-C9     |
| 23  | b     | 616    | CLA  | C6-C7-C8-C9     |
| 23  | c     | 505    | CLA  | C11-C12-C13-C14 |
| 32  | t     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 32  | B     | 630    | LMT  | C4'-C5'-C6'-O6' |
| 32  | b     | 627    | LMT  | C4'-C5'-C6'-O6' |
| 32  | A     | 418    | LMT  | C2'-C1'-O1'-C1  |
| 32  | B     | 629    | LMT  | C2'-C1'-O1'-C1  |
| 32  | b     | 621    | LMT  | C2'-C1'-O1'-C1  |
| 33  | E     | 101[B] | LHG  | O2-C2-C3-O3     |
| 34  | B     | 621    | LMG  | C39-C40-C41-C42 |
| 35  | D     | 710    | HTG  | S1-C1'-C2'-C3'  |
| 35  | b     | 622    | HTG  | S1-C1'-C2'-C3'  |
| 32  | e     | 101    | LMT  | O5B-C5B-C6B-O6B |
| 23  | b     | 606    | CLA  | C10-C11-C12-C13 |
| 32  | B     | 627    | LMT  | C6-C7-C8-C9     |
| 23  | B     | 601    | CLA  | C10-C11-C12-C13 |
| 23  | C     | 509    | CLA  | C10-C11-C12-C13 |
| 27  | A     | 411    | GOL  | O1-C1-C2-O2     |
| 27  | B     | 628    | GOL  | O1-C1-C2-O2     |
| 27  | V     | 203[A] | GOL  | O2-C2-C3-O3     |
| 27  | V     | 203[B] | GOL  | O2-C2-C3-O3     |
| 27  | v     | 202[B] | GOL  | O1-C1-C2-O2     |
| 23  | C     | 512    | CLA  | C3-C5-C6-C7     |
| 23  | B     | 602    | CLA  | C13-C15-C16-C17 |
| 32  | e     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 23  | A     | 408    | CLA  | C12-C13-C15-C16 |
| 23  | C     | 511    | CLA  | C11-C12-C13-C15 |
| 23  | b     | 606    | CLA  | C12-C13-C15-C16 |
| 32  | a     | 417    | LMT  | O1'-C1-C2-C3    |
| 32  | A     | 420    | LMT  | C5'-C4'-O1B-C1B |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 29  | A     | 414[A] | PL9  | C44-C46-C47-C48 |
| 29  | D     | 705[B] | PL9  | C39-C41-C42-C43 |
| 29  | d     | 404[A] | PL9  | C39-C41-C42-C43 |
| 34  | c     | 520    | LMG  | C4-C5-C6-O5     |
| 32  | A     | 418    | LMT  | O5B-C5B-C6B-O6B |
| 33  | D     | 707[A] | LHG  | C33-C34-C35-C36 |
| 23  | C     | 502    | CLA  | CBD-CGD-O2D-CED |
| 23  | C     | 514    | CLA  | CBD-CGD-O2D-CED |
| 23  | b     | 601    | CLA  | C10-C11-C12-C13 |
| 23  | b     | 606    | CLA  | C13-C15-C16-C17 |
| 23  | c     | 513    | CLA  | C15-C16-C17-C18 |
| 32  | A     | 420    | LMT  | O1'-C1-C2-C3    |
| 23  | B     | 606    | CLA  | C2A-CAA-CBA-CGA |
| 23  | b     | 606    | CLA  | C2A-CAA-CBA-CGA |
| 23  | B     | 601    | CLA  | C5-C6-C7-C8     |
| 23  | B     | 614    | CLA  | C8-C10-C11-C12  |
| 23  | b     | 611    | CLA  | C15-C16-C17-C18 |
| 23  | b     | 614    | CLA  | C8-C10-C11-C12  |
| 26  | X     | 101    | SQD  | C23-C24-C25-C26 |
| 34  | Z     | 101    | LMG  | C10-C11-C12-C13 |
| 36  | c     | 518[A] | DGD  | C1B-C2B-C3B-C4B |
| 36  | c     | 518[B] | DGD  | C1B-C2B-C3B-C4B |
| 23  | c     | 510    | CLA  | C3-C5-C6-C7     |
| 32  | e     | 101    | LMT  | O5'-C1'-O1'-C1  |
| 32  | B     | 627    | LMT  | C4B-C5B-C6B-O6B |
| 23  | A     | 408    | CLA  | C5-C6-C7-C8     |
| 23  | B     | 603    | CLA  | C13-C15-C16-C17 |
| 23  | B     | 606    | CLA  | C10-C11-C12-C13 |
| 23  | b     | 604    | CLA  | C5-C6-C7-C8     |
| 23  | b     | 604    | CLA  | C8-C10-C11-C12  |
| 23  | a     | 409    | CLA  | O1A-CGA-O2A-C1  |
| 23  | c     | 510    | CLA  | O1A-CGA-O2A-C1  |
| 32  | A     | 420    | LMT  | C4'-C5'-C6'-O6' |
| 32  | A     | 418    | LMT  | O1'-C1-C2-C3    |
| 23  | D     | 703    | CLA  | C10-C11-C12-C13 |
| 23  | c     | 514    | CLA  | C10-C11-C12-C13 |
| 33  | E     | 101[A] | LHG  | C23-C24-C25-C26 |
| 32  | B     | 627    | LMT  | C5'-C4'-O1B-C1B |
| 33  | D     | 707[B] | LHG  | C33-C34-C35-C36 |
| 33  | D     | 706[A] | LHG  | C1-C2-C3-O3     |
| 33  | d     | 405[B] | LHG  | C1-C2-C3-O3     |
| 23  | C     | 508    | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | c     | 517[B] | DGD  | O6D-C5D-C6D-O5D |
| 33  | E     | 101[B] | LHG  | C23-C24-C25-C26 |
| 34  | B     | 621    | LMG  | O6-C5-C6-O5     |
| 35  | B     | 624    | HTG  | O5-C5-C6-O6     |
| 36  | h     | 102    | DGD  | C6B-C7B-C8B-C9B |
| 35  | B     | 624    | HTG  | S1-C1'-C2'-C3'  |
| 23  | C     | 503    | CLA  | C13-C15-C16-C17 |
| 23  | a     | 405[A] | CLA  | C15-C16-C17-C18 |
| 23  | b     | 606    | CLA  | C15-C16-C17-C18 |
| 23  | D     | 703    | CLA  | C4-C3-C5-C6     |
| 23  | b     | 605    | CLA  | C8-C10-C11-C12  |
| 34  | B     | 621    | LMG  | C11-C10-O7-C8   |
| 34  | B     | 621    | LMG  | O9-C10-O7-C8    |
| 26  | A     | 412    | SQD  | C2-C1-O6-C44    |
| 32  | B     | 630    | LMT  | C2'-C1'-O1'-C1  |
| 32  | e     | 101    | LMT  | C2'-C1'-O1'-C1  |
| 32  | t     | 101    | LMT  | C2'-C1'-O1'-C1  |
| 34  | B     | 621    | LMG  | C2-C1-O1-C7     |
| 36  | C     | 518[A] | DGD  | C2E-C1E-O5D-C6D |
| 36  | C     | 518[B] | DGD  | C2E-C1E-O5D-C6D |
| 23  | B     | 614    | CLA  | C10-C11-C12-C13 |
| 23  | a     | 405[B] | CLA  | C15-C16-C17-C18 |
| 23  | B     | 608    | CLA  | C16-C17-C18-C20 |
| 23  | c     | 509    | CLA  | C16-C17-C18-C19 |
| 25  | b     | 619    | BCR  | C7-C8-C9-C34    |
| 25  | d     | 403    | BCR  | C7-C8-C9-C34    |
| 34  | Z     | 101    | LMG  | C11-C12-C13-C14 |
| 32  | M     | 101    | LMT  | O5'-C5'-C6'-O6' |
| 25  | D     | 704    | BCR  | C21-C22-C23-C24 |
| 25  | b     | 619    | BCR  | C7-C8-C9-C10    |
| 36  | h     | 102    | DGD  | C3B-C4B-C5B-C6B |
| 23  | b     | 610    | CLA  | C2A-CAA-CBA-CGA |
| 36  | c     | 517[B] | DGD  | C4D-C5D-C6D-O5D |
| 27  | B     | 623    | GOL  | O1-C1-C2-C3     |
| 27  | B     | 628    | GOL  | C1-C2-C3-O3     |
| 27  | D     | 712    | GOL  | O1-C1-C2-C3     |
| 27  | O     | 302    | GOL  | O1-C1-C2-C3     |
| 27  | a     | 418    | GOL  | O1-C1-C2-C3     |
| 27  | d     | 411    | GOL  | O1-C1-C2-C3     |
| 27  | l     | 102[B] | GOL  | O1-C1-C2-C3     |
| 27  | o     | 304    | GOL  | O1-C1-C2-C3     |
| 27  | v     | 202[B] | GOL  | O1-C1-C2-C3     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | A     | 410[A] | SQD  | C7-C8-C9-C10    |
| 23  | B     | 603    | CLA  | C16-C17-C18-C19 |
| 23  | B     | 603    | CLA  | C16-C17-C18-C20 |
| 23  | a     | 409    | CLA  | C16-C17-C18-C19 |
| 23  | b     | 614    | CLA  | C16-C17-C18-C20 |
| 23  | c     | 510    | CLA  | C16-C17-C18-C20 |
| 26  | X     | 101    | SQD  | O5-C1-O6-C44    |
| 36  | C     | 518[B] | DGD  | O6E-C1E-O5D-C6D |
| 34  | d     | 410    | LMG  | C10-C11-C12-C13 |
| 26  | b     | 620    | SQD  | C18-C19-C20-C21 |
| 23  | B     | 615    | CLA  | C5-C6-C7-C8     |
| 23  | c     | 507    | CLA  | C15-C16-C17-C18 |
| 23  | c     | 513    | CLA  | CBD-CGD-O2D-CED |
| 34  | Z     | 101    | LMG  | O6-C5-C6-O5     |
| 23  | B     | 602    | CLA  | C3-C5-C6-C7     |
| 23  | B     | 616    | CLA  | C2-C1-O2A-CGA   |
| 23  | B     | 615    | CLA  | C16-C17-C18-C19 |
| 23  | a     | 409    | CLA  | C16-C17-C18-C20 |
| 23  | b     | 615    | CLA  | C16-C17-C18-C19 |
| 23  | c     | 510    | CLA  | C16-C17-C18-C19 |
| 23  | d     | 402    | CLA  | C16-C17-C18-C20 |
| 32  | A     | 420    | LMT  | C1-C2-C3-C4     |
| 32  | A     | 420    | LMT  | C3-C4-C5-C6     |
| 32  | a     | 417    | LMT  | C1-C2-C3-C4     |
| 26  | A     | 410[A] | SQD  | C15-C16-C17-C18 |
| 26  | A     | 412    | SQD  | C17-C18-C19-C20 |
| 26  | X     | 101    | SQD  | C30-C31-C32-C33 |
| 33  | L     | 101[A] | LHG  | C12-C13-C14-C15 |
| 33  | d     | 405[B] | LHG  | C34-C35-C36-C37 |
| 33  | d     | 412[A] | LHG  | C16-C17-C18-C19 |
| 34  | C     | 501    | LMG  | C17-C18-C19-C20 |
| 34  | D     | 711    | LMG  | C19-C20-C21-C22 |
| 34  | c     | 501    | LMG  | C34-C35-C36-C37 |
| 35  | b     | 622    | HTG  | C2'-C3'-C4'-C5' |
| 36  | c     | 518[A] | DGD  | CAA-CBA-CCA-CDA |
| 23  | c     | 512    | CLA  | O1D-CGD-O2D-CED |
| 23  | B     | 605    | CLA  | C5-C6-C7-C8     |
| 26  | A     | 410[B] | SQD  | C15-C16-C17-C18 |
| 34  | C     | 521    | LMG  | C18-C19-C20-C21 |
| 34  | c     | 520    | LMG  | C33-C34-C35-C36 |
| 36  | c     | 518[B] | DGD  | C9A-CAA-CBA-CCA |
| 36  | c     | 517[A] | DGD  | C2A-C1A-O1G-C1G |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | c     | 517[A] | DGD  | O6D-C5D-C6D-O5D |
| 32  | B     | 627    | LMT  | C5-C6-C7-C8     |
| 33  | L     | 101[A] | LHG  | C17-C18-C19-C20 |
| 33  | b     | 629[B] | LHG  | C14-C15-C16-C17 |
| 33  | d     | 412[B] | LHG  | C16-C17-C18-C19 |
| 34  | B     | 621    | LMG  | C17-C18-C19-C20 |
| 35  | B     | 622    | HTG  | C3'-C4'-C5'-C6' |
| 36  | C     | 517[B] | DGD  | C5B-C6B-C7B-C8B |
| 36  | c     | 518[B] | DGD  | CAA-CBA-CCA-CDA |
| 36  | h     | 102    | DGD  | C7B-C8B-C9B-CAB |
| 27  | B     | 623    | GOL  | O2-C2-C3-O3     |
| 27  | D     | 712    | GOL  | O1-C1-C2-O2     |
| 27  | O     | 302    | GOL  | O1-C1-C2-O2     |
| 27  | b     | 624    | GOL  | O2-C2-C3-O3     |
| 27  | c     | 527    | GOL  | O2-C2-C3-O3     |
| 27  | o     | 303    | GOL  | O2-C2-C3-O3     |
| 32  | T     | 101    | LMT  | C2-C1-O1'-C1'   |
| 32  | t     | 101    | LMT  | C2-C1-O1'-C1'   |
| 34  | m     | 101    | LMG  | C35-C36-C37-C38 |
| 23  | C     | 513    | CLA  | C10-C11-C12-C13 |
| 23  | b     | 614    | CLA  | C10-C11-C12-C13 |
| 23  | D     | 702[B] | CLA  | C4B-C3B-CAB-CBB |
| 34  | c     | 501    | LMG  | C10-C11-C12-C13 |
| 35  | o     | 301    | HTG  | C1'-C2'-C3'-C4' |
| 33  | D     | 707[B] | LHG  | C32-C33-C34-C35 |
| 36  | c     | 518[A] | DGD  | C9A-CAA-CBA-CCA |
| 23  | b     | 602    | CLA  | C16-C17-C18-C19 |
| 23  | b     | 602    | CLA  | C16-C17-C18-C20 |
| 23  | b     | 615    | CLA  | C16-C17-C18-C20 |
| 32  | b     | 621    | LMT  | C4'-C5'-C6'-O6' |
| 23  | B     | 614    | CLA  | C5-C6-C7-C8     |
| 23  | b     | 611    | CLA  | C8-C10-C11-C12  |
| 34  | m     | 101    | LMG  | C11-C10-O7-C8   |
| 33  | L     | 101[B] | LHG  | C25-C26-C27-C28 |
| 23  | B     | 614    | CLA  | C11-C10-C8-C7   |
| 35  | d     | 409    | HTG  | S1-C1'-C2'-C3'  |
| 33  | d     | 405[B] | LHG  | C11-C10-C9-C8   |
| 32  | e     | 101    | LMT  | C4-C5-C6-C7     |
| 36  | C     | 518[A] | DGD  | CCB-CDB-CEB-CFB |
| 36  | c     | 518[B] | DGD  | CBA-CCA-CDA-CEA |
| 36  | C     | 518[B] | DGD  | CCB-CDB-CEB-CFB |
| 32  | t     | 101    | LMT  | O1'-C1-C2-C3    |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | c     | 517[A] | DGD  | C2B-C3B-C4B-C5B |
| 23  | C     | 503    | CLA  | C15-C16-C17-C18 |
| 33  | D     | 707[A] | LHG  | C32-C33-C34-C35 |
| 23  | B     | 610    | CLA  | C16-C17-C18-C19 |
| 32  | e     | 101    | LMT  | C1-C2-C3-C4     |
| 32  | B     | 630    | LMT  | C3-C4-C5-C6     |
| 33  | L     | 101[A] | LHG  | C25-C26-C27-C28 |
| 33  | L     | 101[B] | LHG  | C15-C16-C17-C18 |
| 33  | d     | 412[A] | LHG  | C32-C33-C34-C35 |
| 36  | c     | 517[B] | DGD  | C2B-C3B-C4B-C5B |
| 32  | b     | 627    | LMT  | C3-C4-C5-C6     |
| 32  | b     | 627    | LMT  | C7-C8-C9-C10    |
| 35  | b     | 623    | HTG  | C1'-C2'-C3'-C4' |
| 26  | a     | 412    | SQD  | C31-C32-C33-C34 |
| 26  | f     | 102    | SQD  | C32-C33-C34-C35 |
| 33  | L     | 101[B] | LHG  | C12-C13-C14-C15 |
| 33  | a     | 420[A] | LHG  | C26-C27-C28-C29 |
| 33  | d     | 405[A] | LHG  | C11-C10-C9-C8   |
| 36  | C     | 517[A] | DGD  | C4B-C5B-C6B-C7B |
| 36  | C     | 517[A] | DGD  | C5B-C6B-C7B-C8B |
| 36  | c     | 517[A] | DGD  | C9A-CAA-CBA-CCA |
| 33  | a     | 420[B] | LHG  | C26-C27-C28-C29 |
| 23  | D     | 703    | CLA  | O1D-CGD-O2D-CED |
| 33  | b     | 629[A] | LHG  | C14-C15-C16-C17 |
| 34  | C     | 521    | LMG  | C17-C18-C19-C20 |
| 34  | c     | 520    | LMG  | C34-C35-C36-C37 |
| 23  | B     | 615    | CLA  | C16-C17-C18-C20 |
| 23  | d     | 402    | CLA  | C16-C17-C18-C19 |
| 23  | a     | 407[A] | CLA  | C2B-C3B-CAB-CBB |
| 23  | c     | 508    | CLA  | C2B-C3B-CAB-CBB |
| 25  | b     | 619    | BCR  | C1-C6-C7-C8     |
| 25  | b     | 619    | BCR  | C5-C6-C7-C8     |
| 36  | h     | 102    | DGD  | CAA-CBA-CCA-CDA |
| 26  | b     | 620    | SQD  | C24-C23-O48-C46 |
| 26  | A     | 410[A] | SQD  | C12-C13-C14-C15 |
| 26  | X     | 101    | SQD  | C24-C25-C26-C27 |
| 33  | D     | 706[B] | LHG  | C16-C17-C18-C19 |
| 33  | b     | 629[A] | LHG  | C16-C17-C18-C19 |
| 34  | D     | 711    | LMG  | C35-C36-C37-C38 |
| 36  | C     | 517[B] | DGD  | C8A-C9A-CAA-CBA |
| 32  | b     | 621    | LMT  | C3'-C4'-O1B-C1B |
| 33  | A     | 419[A] | LHG  | C12-C13-C14-C15 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | L     | 101[A] | LHG  | C15-C16-C17-C18 |
| 34  | C     | 521    | LMG  | C19-C20-C21-C22 |
| 34  | c     | 501    | LMG  | C30-C31-C32-C33 |
| 36  | c     | 517[B] | DGD  | C9A-CAA-CBA-CCA |
| 26  | B     | 620    | SQD  | C7-C8-C9-C10    |
| 32  | B     | 630    | LMT  | C4-C5-C6-C7     |
| 32  | T     | 101    | LMT  | C7-C8-C9-C10    |
| 32  | e     | 101    | LMT  | C5-C6-C7-C8     |
| 29  | A     | 414[A] | PL9  | C30-C29-C31-C32 |
| 33  | A     | 419[B] | LHG  | C34-C35-C36-C37 |
| 33  | D     | 706[A] | LHG  | C16-C17-C18-C19 |
| 33  | E     | 101[A] | LHG  | C24-C25-C26-C27 |
| 34  | C     | 501    | LMG  | C12-C13-C14-C15 |
| 23  | D     | 703    | CLA  | C2-C3-C5-C6     |
| 23  | B     | 610    | CLA  | C16-C17-C18-C20 |
| 36  | c     | 518[A] | DGD  | CBA-CCA-CDA-CEA |
| 23  | d     | 402    | CLA  | CBA-CGA-O2A-C1  |
| 23  | b     | 610    | CLA  | C11-C12-C13-C14 |
| 32  | A     | 420    | LMT  | C3'-C4'-O1B-C1B |
| 33  | A     | 419[A] | LHG  | C34-C35-C36-C37 |
| 34  | C     | 520    | LMG  | C16-C17-C18-C19 |
| 26  | b     | 620    | SQD  | C27-C28-C29-C30 |
| 33  | D     | 707[A] | LHG  | C15-C16-C17-C18 |
| 34  | D     | 711    | LMG  | C12-C13-C14-C15 |
| 36  | c     | 517[A] | DGD  | C5A-C6A-C7A-C8A |
| 26  | A     | 412    | SQD  | O5-C1-O6-C44    |
| 34  | B     | 621    | LMG  | O6-C1-O1-C7     |
| 36  | C     | 518[A] | DGD  | O6E-C1E-O5D-C6D |
| 36  | c     | 517[B] | DGD  | O6E-C1E-O5D-C6D |
| 33  | L     | 101[B] | LHG  | C17-C18-C19-C20 |
| 36  | H     | 102    | DGD  | C5B-C6B-C7B-C8B |
| 36  | c     | 517[A] | DGD  | O1A-C1A-O1G-C1G |
| 33  | L     | 101[B] | LHG  | C13-C14-C15-C16 |
| 36  | c     | 518[A] | DGD  | CBB-CCB-CDB-CEB |
| 32  | B     | 629    | LMT  | C2-C3-C4-C5     |
| 32  | t     | 101    | LMT  | C4-C5-C6-C7     |
| 34  | c     | 501    | LMG  | C21-C22-C23-C24 |
| 32  | B     | 629    | LMT  | C5-C6-C7-C8     |
| 33  | E     | 101[B] | LHG  | C24-C25-C26-C27 |
| 32  | b     | 627    | LMT  | C1-C2-C3-C4     |
| 34  | m     | 101    | LMG  | O9-C10-O7-C8    |
| 33  | D     | 707[B] | LHG  | C29-C30-C31-C32 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | d     | 412[A] | LHG  | C29-C30-C31-C32 |
| 33  | d     | 412[B] | LHG  | C32-C33-C34-C35 |
| 36  | c     | 517[A] | DGD  | C7A-C8A-C9A-CAA |
| 36  | C     | 517[B] | DGD  | O6D-C5D-C6D-O5D |
| 25  | D     | 704    | BCR  | C37-C22-C23-C24 |
| 33  | b     | 629[B] | LHG  | C16-C17-C18-C19 |
| 26  | A     | 410[B] | SQD  | C7-C8-C9-C10    |
| 34  | C     | 501    | LMG  | C10-C11-C12-C13 |
| 23  | C     | 513    | CLA  | CBA-CGA-O2A-C1  |
| 23  | B     | 608    | CLA  | C16-C17-C18-C19 |
| 23  | c     | 509    | CLA  | C16-C17-C18-C20 |
| 34  | d     | 410    | LMG  | C29-C30-C31-C32 |
| 29  | A     | 414[A] | PL9  | C45-C44-C46-C47 |
| 29  | d     | 404[A] | PL9  | C13-C14-C16-C17 |
| 33  | L     | 101[A] | LHG  | C13-C14-C15-C16 |
| 33  | d     | 405[A] | LHG  | C34-C35-C36-C37 |
| 23  | c     | 514    | CLA  | O1D-CGD-O2D-CED |
| 23  | b     | 604    | CLA  | C15-C16-C17-C18 |
| 34  | m     | 101    | LMG  | C39-C40-C41-C42 |
| 23  | d     | 402    | CLA  | O1A-CGA-O2A-C1  |
| 23  | B     | 601    | CLA  | C13-C15-C16-C17 |
| 23  | b     | 601    | CLA  | C13-C15-C16-C17 |
| 23  | b     | 605    | CLA  | C5-C6-C7-C8     |
| 33  | D     | 707[A] | LHG  | C29-C30-C31-C32 |
| 35  | b     | 623    | HTG  | O5-C5-C6-O6     |
| 26  | B     | 620    | SQD  | C30-C31-C32-C33 |
| 33  | d     | 406[A] | LHG  | C27-C28-C29-C30 |
| 34  | B     | 621    | LMG  | C34-C35-C36-C37 |
| 34  | C     | 501    | LMG  | C36-C37-C38-C39 |
| 23  | B     | 615    | CLA  | C10-C11-C12-C13 |
| 36  | C     | 517[A] | DGD  | O6E-C5E-C6E-O5E |
| 26  | a     | 412    | SQD  | C25-C26-C27-C28 |
| 34  | C     | 501    | LMG  | C19-C20-C21-C22 |
| 36  | c     | 517[B] | DGD  | C5A-C6A-C7A-C8A |
| 36  | C     | 517[B] | DGD  | O6E-C5E-C6E-O5E |
| 26  | A     | 410[A] | SQD  | O6-C44-C45-O47  |
| 26  | A     | 410[B] | SQD  | O6-C44-C45-O47  |
| 33  | A     | 419[B] | LHG  | C12-C13-C14-C15 |
| 33  | d     | 412[B] | LHG  | C24-C25-C26-C27 |
| 36  | C     | 517[B] | DGD  | C4B-C5B-C6B-C7B |
| 23  | B     | 601    | CLA  | CBA-CGA-O2A-C1  |
| 26  | X     | 101    | SQD  | C29-C30-C31-C32 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | d     | 406[B] | LHG  | C29-C30-C31-C32 |
| 34  | D     | 711    | LMG  | C30-C31-C32-C33 |
| 36  | c     | 517[B] | DGD  | O6E-C5E-C6E-O5E |
| 33  | D     | 707[B] | LHG  | C15-C16-C17-C18 |
| 36  | C     | 519    | DGD  | C6B-C7B-C8B-C9B |
| 36  | H     | 102    | DGD  | C9B-CAB-CBB-CCB |
| 36  | H     | 102    | DGD  | CCB-CDB-CEB-CFB |
| 36  | c     | 519    | DGD  | CBA-CCA-CDA-CEA |
| 23  | b     | 601    | CLA  | C2-C1-O2A-CGA   |
| 23  | b     | 614    | CLA  | C16-C17-C18-C19 |
| 23  | d     | 401[B] | CLA  | C16-C17-C18-C20 |
| 23  | A     | 406[B] | CLA  | C13-C15-C16-C17 |
| 23  | B     | 601    | CLA  | C15-C16-C17-C18 |
| 32  | b     | 627    | LMT  | C5-C6-C7-C8     |
| 34  | d     | 410    | LMG  | O6-C5-C6-O5     |
| 26  | f     | 102    | SQD  | C25-C26-C27-C28 |
| 23  | C     | 507    | CLA  | C4-C3-C5-C6     |
| 29  | A     | 414[B] | PL9  | C45-C44-C46-C47 |
| 29  | d     | 404[B] | PL9  | C15-C14-C16-C17 |
| 23  | b     | 607    | CLA  | C3-C5-C6-C7     |
| 29  | A     | 414[A] | PL9  | C12-C11-C9-C8   |
| 29  | D     | 705[A] | PL9  | C13-C14-C16-C17 |
| 23  | B     | 602    | CLA  | C15-C16-C17-C18 |
| 33  | D     | 706[B] | LHG  | C26-C27-C28-C29 |
| 36  | C     | 517[B] | DGD  | C9A-CAA-CBA-CCA |
| 36  | c     | 517[A] | DGD  | CAA-CBA-CCA-CDA |
| 23  | B     | 610    | CLA  | C2A-CAA-CBA-CGA |
| 23  | c     | 502    | CLA  | CBD-CGD-O2D-CED |
| 23  | c     | 513    | CLA  | CBA-CGA-O2A-C1  |
| 26  | b     | 620    | SQD  | C26-C27-C28-C29 |
| 32  | t     | 101    | LMT  | C7-C8-C9-C10    |
| 36  | h     | 102    | DGD  | C9A-CAA-CBA-CCA |
| 23  | c     | 513    | CLA  | C10-C11-C12-C13 |
| 32  | B     | 627    | LMT  | C3'-C4'-O1B-C1B |
| 26  | A     | 412    | SQD  | C26-C27-C28-C29 |
| 32  | B     | 630    | LMT  | O1'-C1-C2-C3    |
| 23  | d     | 401[A] | CLA  | C16-C17-C18-C20 |
| 27  | B     | 628    | GOL  | O2-C2-C3-O3     |
| 27  | D     | 712    | GOL  | O2-C2-C3-O3     |
| 27  | o     | 304    | GOL  | O2-C2-C3-O3     |
| 26  | b     | 620    | SQD  | O10-C23-O48-C46 |
| 36  | h     | 102    | DGD  | C2B-C3B-C4B-C5B |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | c     | 517[A] | DGD  | C4D-C5D-C6D-O5D |
| 23  | A     | 405[A] | CLA  | C1A-C2A-CAA-CBA |
| 23  | a     | 406[B] | CLA  | C1A-C2A-CAA-CBA |
| 23  | c     | 514    | CLA  | C1A-C2A-CAA-CBA |
| 23  | A     | 404[B] | CLA  | C13-C15-C16-C17 |
| 36  | C     | 517[A] | DGD  | C8A-C9A-CAA-CBA |
| 36  | h     | 102    | DGD  | C9B-CAB-CBB-CCB |
| 36  | c     | 518[A] | DGD  | C6A-C7A-C8A-C9A |
| 26  | B     | 620    | SQD  | C11-C10-C9-C8   |
| 32  | B     | 630    | LMT  | C11-C10-C9-C8   |
| 33  | D     | 707[B] | LHG  | C17-C18-C19-C20 |
| 23  | C     | 513    | CLA  | C3-C5-C6-C7     |
| 23  | B     | 602    | CLA  | C11-C12-C13-C15 |
| 23  | C     | 505    | CLA  | C12-C13-C15-C16 |
| 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  | c     | 506    | CLA  | C11-C12-C13-C15 |
| 23  | c     | 511    | CLA  | C11-C10-C8-C7   |
| 23  | c     | 513    | CLA  | C12-C13-C15-C16 |
| 35  | b     | 623    | HTG  | S1-C1'-C2'-C3'  |
| 23  | B     | 613    | CLA  | C13-C15-C16-C17 |
| 34  | C     | 521    | LMG  | C13-C14-C15-C16 |
| 23  | A     | 406[A] | CLA  | C13-C15-C16-C17 |
| 34  | c     | 520    | LMG  | C28-C29-C30-C31 |
| 26  | A     | 412    | SQD  | C27-C28-C29-C30 |
| 23  | C     | 511    | CLA  | C2-C3-C5-C6     |
| 29  | A     | 414[B] | PL9  | C12-C11-C9-C8   |
| 29  | D     | 705[B] | PL9  | C13-C14-C16-C17 |
| 23  | B     | 601    | CLA  | O1A-CGA-O2A-C1  |
| 23  | C     | 513    | CLA  | O1A-CGA-O2A-C1  |
| 32  | m     | 103    | LMT  | O5'-C5'-C6'-O6' |
| 33  | D     | 706[A] | LHG  | C13-C14-C15-C16 |
| 23  | c     | 513    | CLA  | C13-C15-C16-C17 |
| 23  | B     | 602    | CLA  | C11-C12-C13-C14 |
| 23  | C     | 506    | CLA  | C11-C12-C13-C14 |
| 23  | b     | 601    | CLA  | C6-C7-C8-C9     |
| 23  | c     | 511    | CLA  | C11-C10-C8-C9   |
| 32  | B     | 629    | LMT  | C6-C7-C8-C9     |
| 36  | c     | 517[B] | DGD  | C2A-C1A-O1G-C1G |
| 23  | A     | 404[A] | CLA  | C13-C15-C16-C17 |
| 34  | m     | 101    | LMG  | C38-C39-C40-C41 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | d     | 406[A] | LHG  | C25-C26-C27-C28 |
| 34  | d     | 410    | LMG  | C35-C36-C37-C38 |
| 33  | L     | 101[B] | LHG  | C23-C24-C25-C26 |
| 26  | A     | 410[A] | SQD  | O6-C44-C45-C46  |
| 26  | A     | 412    | SQD  | O6-C44-C45-C46  |
| 26  | a     | 411[A] | SQD  | O6-C44-C45-C46  |
| 26  | f     | 102    | SQD  | O6-C44-C45-C46  |
| 26  | f     | 102    | SQD  | C44-C45-C46-O48 |
| 32  | t     | 101    | LMT  | C4'-C5'-C6'-O6' |
| 34  | C     | 520    | LMG  | C34-C35-C36-C37 |
| 36  | c     | 519    | DGD  | CBB-CCB-CDB-CEB |
| 34  | D     | 711    | LMG  | O6-C5-C6-O5     |
| 36  | c     | 517[A] | DGD  | O6E-C5E-C6E-O5E |
| 23  | d     | 401[B] | CLA  | C16-C17-C18-C19 |
| 26  | a     | 411[A] | SQD  | C9-C10-C11-C12  |
| 34  | C     | 501    | LMG  | C11-C12-C13-C14 |
| 33  | E     | 101[A] | LHG  | C25-C26-C27-C28 |
| 23  | C     | 510    | CLA  | O1D-CGD-O2D-CED |
| 36  | H     | 102    | DGD  | C7A-C8A-C9A-CAA |
| 34  | c     | 520    | LMG  | C10-C11-C12-C13 |
| 33  | d     | 406[B] | LHG  | C27-C28-C29-C30 |
| 23  | C     | 511    | CLA  | C4-C3-C5-C6     |
| 23  | C     | 506    | CLA  | C2-C3-C5-C6     |
| 34  | D     | 711    | LMG  | C36-C37-C38-C39 |
| 23  | A     | 405[A] | CLA  | C15-C16-C17-C18 |
| 26  | B     | 620    | SQD  | C34-C35-C36-C37 |
| 23  | d     | 401[A] | CLA  | C16-C17-C18-C19 |
| 36  | C     | 517[A] | DGD  | C9A-CAA-CBA-CCA |
| 23  | C     | 507    | CLA  | C5-C6-C7-C8     |
| 36  | C     | 517[A] | DGD  | C3B-C4B-C5B-C6B |
| 26  | A     | 410[B] | SQD  | C12-C13-C14-C15 |
| 36  | c     | 518[A] | DGD  | C2B-C3B-C4B-C5B |
| 32  | a     | 417    | LMT  | C2-C3-C4-C5     |
| 33  | b     | 629[A] | LHG  | C13-C14-C15-C16 |
| 27  | O     | 303    | GOL  | O1-C1-C2-C3     |
| 26  | B     | 620    | SQD  | C46-C45-O47-C7  |
| 26  | b     | 620    | SQD  | C46-C45-O47-C7  |
| 23  | a     | 406[A] | CLA  | C2C-C3C-CAC-CBC |
| 33  | D     | 707[A] | LHG  | C17-C18-C19-C20 |
| 34  | d     | 410    | LMG  | C11-C12-C13-C14 |
| 36  | c     | 517[B] | DGD  | CAA-CBA-CCA-CDA |
| 36  | C     | 517[A] | DGD  | O6D-C5D-C6D-O5D |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | a     | 411[B] | SQD  | C9-C10-C11-C12  |
| 32  | M     | 101    | LMT  | C3-C4-C5-C6     |
| 33  | D     | 706[B] | LHG  | C13-C14-C15-C16 |
| 33  | d     | 412[B] | LHG  | C25-C26-C27-C28 |
| 36  | h     | 102    | DGD  | CAB-CBB-CCB-CDB |
| 26  | A     | 410[B] | SQD  | C11-C10-C9-C8   |
| 33  | d     | 406[B] | LHG  | C28-C29-C30-C31 |
| 36  | h     | 102    | DGD  | CBA-CCA-CDA-CEA |
| 36  | c     | 518[B] | DGD  | CBB-CCB-CDB-CEB |
| 23  | b     | 601    | CLA  | CBA-CGA-O2A-C1  |
| 36  | c     | 519    | DGD  | C2A-C1A-O1G-C1G |
| 35  | b     | 622    | HTG  | C1'-C2'-C3'-C4' |
| 32  | e     | 101    | LMT  | C4B-C5B-C6B-O6B |
| 29  | a     | 414[B] | PL9  | C12-C11-C9-C10  |
| 23  | c     | 506    | CLA  | C2-C3-C5-C6     |
| 36  | C     | 518[B] | DGD  | CDA-CEA-CFA-CGA |
| 23  | b     | 606    | CLA  | C16-C17-C18-C20 |
| 26  | a     | 411[A] | SQD  | C12-C13-C14-C15 |
| 32  | b     | 621    | LMT  | C11-C10-C9-C8   |
| 34  | c     | 520    | LMG  | C31-C32-C33-C34 |
| 32  | a     | 417    | LMT  | C9-C10-C11-C12  |
| 34  | c     | 520    | LMG  | O6-C5-C6-O5     |
| 33  | d     | 406[A] | LHG  | C34-C35-C36-C37 |
| 33  | d     | 406[B] | LHG  | C9-C10-C11-C12  |
| 36  | c     | 518[A] | DGD  | C4A-C5A-C6A-C7A |
| 36  | C     | 518[A] | DGD  | CDA-CEA-CFA-CGA |
| 36  | C     | 517[B] | DGD  | CCA-CDA-CEA-CFA |
| 36  | c     | 518[B] | DGD  | C2B-C3B-C4B-C5B |
| 32  | e     | 101    | LMT  | C9-C10-C11-C12  |
| 34  | C     | 501    | LMG  | C13-C14-C15-C16 |
| 36  | c     | 518[B] | DGD  | C6A-C7A-C8A-C9A |
| 26  | b     | 620    | SQD  | C11-C10-C9-C8   |
| 32  | A     | 420    | LMT  | C4-C5-C6-C7     |
| 34  | C     | 520    | LMG  | C17-C18-C19-C20 |
| 26  | a     | 412    | SQD  | C16-C17-C18-C19 |
| 26  | b     | 620    | SQD  | C14-C15-C16-C17 |
| 23  | C     | 511    | CLA  | CBA-CGA-O2A-C1  |
| 36  | c     | 517[B] | DGD  | O1A-C1A-O1G-C1G |
| 33  | d     | 406[A] | LHG  | C29-C30-C31-C32 |
| 35  | B     | 624    | HTG  | C4'-C5'-C6'-C7' |
| 34  | z     | 101    | LMG  | C10-C11-C12-C13 |
| 23  | C     | 511    | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | c     | 511    | CLA  | CBD-CGD-O2D-CED |
| 23  | B     | 603    | CLA  | C4-C3-C5-C6     |
| 29  | d     | 404[A] | PL9  | C45-C44-C46-C47 |
| 34  | B     | 621    | LMG  | C37-C38-C39-C40 |
| 33  | D     | 707[B] | LHG  | C24-C23-O8-C6   |
| 36  | C     | 519    | DGD  | CAB-CBB-CCB-CDB |
| 33  | d     | 412[A] | LHG  | C33-C34-C35-C36 |
| 36  | H     | 102    | DGD  | CCA-CDA-CEA-CFA |
| 32  | b     | 627    | 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     | 513    | CLA  | C6-C7-C8-C9     |
| 23  | C     | 514    | CLA  | C11-C10-C8-C9   |
| 23  | D     | 703    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 506    | CLA  | C11-C12-C13-C14 |
| 32  | e     | 101    | LMT  | C3-C4-C5-C6     |
| 33  | b     | 629[B] | LHG  | C12-C13-C14-C15 |
| 33  | b     | 629[B] | LHG  | C13-C14-C15-C16 |
| 23  | C     | 507    | CLA  | C15-C16-C17-C18 |
| 23  | A     | 406[A] | CLA  | C4B-C3B-CAB-CBB |
| 23  | B     | 602    | CLA  | C4B-C3B-CAB-CBB |
| 23  | C     | 505    | CLA  | C4B-C3B-CAB-CBB |
| 23  | a     | 407[A] | CLA  | C4B-C3B-CAB-CBB |
| 23  | c     | 508    | CLA  | C4B-C3B-CAB-CBB |
| 33  | D     | 706[A] | LHG  | C12-C13-C14-C15 |
| 33  | E     | 101[B] | LHG  | C25-C26-C27-C28 |
| 34  | C     | 520    | LMG  | C31-C32-C33-C34 |
| 36  | c     | 517[B] | DGD  | C2E-C1E-O5D-C6D |
| 36  | h     | 102    | DGD  | CDB-CEB-CFB-CGB |
| 33  | b     | 629[A] | LHG  | O6-C4-C5-C6     |
| 23  | A     | 406[A] | CLA  | C12-C13-C15-C16 |
| 23  | A     | 406[B] | CLA  | C12-C13-C15-C16 |
| 23  | B     | 610    | CLA  | C12-C13-C15-C16 |
| 23  | B     | 614    | CLA  | C12-C13-C15-C16 |
| 23  | C     | 507    | CLA  | C6-C7-C8-C10    |
| 23  | C     | 511    | CLA  | C12-C13-C15-C16 |
| 23  | D     | 703    | CLA  | C12-C13-C15-C16 |
| 23  | a     | 409    | CLA  | C11-C10-C8-C7   |
| 23  | b     | 601    | CLA  | C6-C7-C8-C10    |
| 23  | b     | 601    | CLA  | C11-C10-C8-C7   |
| 23  | b     | 601    | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | c     | 510    | CLA  | C11-C10-C8-C7   |
| 23  | b     | 602    | CLA  | C10-C11-C12-C13 |
| 36  | c     | 518[B] | DGD  | C4A-C5A-C6A-C7A |
| 23  | C     | 503    | CLA  | C3-C5-C6-C7     |
| 23  | C     | 506    | CLA  | C4-C3-C5-C6     |
| 29  | a     | 414[A] | PL9  | C12-C11-C9-C10  |
| 23  | c     | 513    | CLA  | O1A-CGA-O2A-C1  |
| 36  | C     | 517[B] | DGD  | C4D-C5D-C6D-O5D |
| 34  | c     | 521    | LMG  | C29-C28-O8-C9   |
| 26  | b     | 620    | SQD  | C31-C32-C33-C34 |
| 33  | d     | 406[A] | LHG  | C28-C29-C30-C31 |
| 34  | c     | 501    | LMG  | C35-C36-C37-C38 |
| 25  | t     | 102    | BCR  | C13-C14-C15-C16 |
| 25  | K     | 102    | BCR  | C7-C8-C9-C34    |
| 32  | t     | 101    | LMT  | C11-C10-C9-C8   |
| 32  | M     | 101    | LMT  | O1'-C1-C2-C3    |
| 33  | D     | 707[B] | LHG  | C13-C14-C15-C16 |
| 35  | b     | 625    | HTG  | C4-C5-C6-O6     |
| 35  | c     | 522    | HTG  | C4'-C5'-C6'-C7' |
| 23  | C     | 514    | CLA  | O1D-CGD-O2D-CED |
| 36  | c     | 518[A] | DGD  | CDA-CEA-CFA-CGA |
| 33  | b     | 629[A] | LHG  | C27-C28-C29-C30 |
| 23  | c     | 512    | CLA  | CBA-CGA-O2A-C1  |
| 34  | z     | 101    | LMG  | C14-C15-C16-C17 |
| 26  | A     | 410[B] | SQD  | O6-C44-C45-C46  |
| 26  | B     | 620    | SQD  | C44-C45-C46-O48 |
| 26  | b     | 620    | SQD  | C44-C45-C46-O48 |
| 33  | a     | 420[A] | LHG  | C4-C5-C6-O8     |
| 33  | a     | 420[B] | LHG  | C4-C5-C6-O8     |
| 34  | c     | 501    | LMG  | C7-C8-C9-O8     |
| 34  | C     | 520    | LMG  | C37-C38-C39-C40 |
| 35  | o     | 301    | HTG  | C2'-C3'-C4'-C5' |
| 34  | c     | 520    | LMG  | C29-C30-C31-C32 |
| 36  | C     | 518[A] | DGD  | C5B-C6B-C7B-C8B |
| 23  | b     | 606    | CLA  | C16-C17-C18-C19 |
| 33  | D     | 707[A] | LHG  | C13-C14-C15-C16 |
| 33  | d     | 406[A] | LHG  | C9-C10-C11-C12  |
| 32  | A     | 420    | LMT  | C5-C6-C7-C8     |
| 33  | D     | 706[A] | LHG  | C10-C11-C12-C13 |
| 33  | d     | 405[A] | LHG  | C13-C14-C15-C16 |
| 34  | c     | 501    | LMG  | C29-C30-C31-C32 |
| 23  | c     | 506    | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 29  | D     | 705[B] | PL9  | C15-C14-C16-C17 |
| 33  | L     | 101[B] | LHG  | C11-C12-C13-C14 |
| 29  | D     | 705[A] | PL9  | C43-C44-C46-C47 |
| 23  | b     | 601    | CLA  | O1A-CGA-O2A-C1  |
| 33  | E     | 101[B] | LHG  | C17-C18-C19-C20 |
| 33  | b     | 629[B] | LHG  | C27-C28-C29-C30 |
| 32  | B     | 627    | LMT  | C1-C2-C3-C4     |
| 33  | A     | 419[A] | LHG  | C26-C27-C28-C29 |
| 33  | E     | 101[A] | LHG  | O6-C4-C5-O7     |
| 36  | C     | 517[A] | DGD  | C7A-C8A-C9A-CAA |
| 25  | D     | 704    | BCR  | C23-C24-C25-C30 |
| 25  | b     | 617    | BCR  | C1-C6-C7-C8     |
| 36  | c     | 517[B] | DGD  | C7A-C8A-C9A-CAA |
| 23  | b     | 610    | CLA  | C15-C16-C17-C18 |
| 23  | c     | 510    | CLA  | C8-C10-C11-C12  |
| 33  | L     | 101[B] | LHG  | C24-C25-C26-C27 |
| 33  | d     | 406[B] | LHG  | C34-C35-C36-C37 |
| 36  | c     | 517[B] | DGD  | C4B-C5B-C6B-C7B |
| 23  | B     | 610    | CLA  | C13-C15-C16-C17 |
| 36  | C     | 519    | DGD  | CDB-CEB-CFB-CGB |
| 23  | C     | 502    | CLA  | O1D-CGD-O2D-CED |
| 26  | X     | 101    | SQD  | C32-C33-C34-C35 |
| 33  | D     | 706[B] | LHG  | C12-C13-C14-C15 |
| 36  | C     | 517[B] | DGD  | C7A-C8A-C9A-CAA |
| 32  | F     | 101    | LMT  | C4-C5-C6-C7     |
| 26  | B     | 620    | SQD  | O47-C45-C46-O48 |
| 26  | a     | 411[A] | SQD  | O6-C44-C45-O47  |
| 26  | X     | 101    | SQD  | C34-C35-C36-C37 |
| 36  | c     | 518[B] | DGD  | C5A-C6A-C7A-C8A |
| 35  | b     | 622    | HTG  | C3'-C4'-C5'-C6' |
| 34  | m     | 101    | LMG  | C37-C38-C39-C40 |
| 29  | d     | 404[A] | PL9  | C15-C14-C16-C17 |
| 32  | b     | 621    | LMT  | C3-C4-C5-C6     |
| 33  | a     | 420[A] | LHG  | C10-C11-C12-C13 |
| 33  | b     | 629[A] | LHG  | C12-C13-C14-C15 |
| 23  | c     | 507    | CLA  | C13-C15-C16-C17 |
| 29  | A     | 414[A] | PL9  | C43-C44-C46-C47 |
| 29  | d     | 404[B] | PL9  | C13-C14-C16-C17 |
| 32  | a     | 417    | LMT  | C3-C4-C5-C6     |
| 33  | L     | 101[A] | LHG  | C24-C25-C26-C27 |
| 23  | C     | 503    | CLA  | C16-C17-C18-C19 |
| 33  | L     | 101[A] | LHG  | C11-C12-C13-C14 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | H     | 102    | DGD  | CAB-CBB-CCB-CDB |
| 36  | c     | 518[A] | DGD  | C5A-C6A-C7A-C8A |
| 23  | C     | 511    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 513    | CLA  | C6-C7-C8-C9     |
| 33  | b     | 629[B] | LHG  | C25-C26-C27-C28 |
| 34  | C     | 520    | LMG  | C30-C31-C32-C33 |
| 34  | C     | 521    | LMG  | C35-C36-C37-C38 |
| 23  | C     | 503    | CLA  | C16-C17-C18-C20 |
| 23  | c     | 513    | CLA  | O1D-CGD-O2D-CED |
| 26  | a     | 411[A] | SQD  | C34-C35-C36-C37 |
| 33  | b     | 629[A] | LHG  | C31-C32-C33-C34 |
| 29  | a     | 414[A] | PL9  | C24-C26-C27-C28 |
| 29  | a     | 414[B] | PL9  | C24-C26-C27-C28 |
| 26  | a     | 411[B] | SQD  | C35-C36-C37-C38 |
| 33  | E     | 101[A] | LHG  | C17-C18-C19-C20 |
| 33  | A     | 419[B] | LHG  | C18-C19-C20-C21 |
| 23  | B     | 612    | CLA  | C10-C11-C12-C13 |
| 23  | c     | 510    | CLA  | C13-C15-C16-C17 |
| 24  | a     | 408[B] | PHO  | C2-C3-C5-C6     |
| 23  | A     | 406[A] | CLA  | C16-C17-C18-C20 |
| 33  | a     | 420[B] | LHG  | C10-C11-C12-C13 |
| 34  | C     | 520    | LMG  | C36-C37-C38-C39 |
| 36  | C     | 518[A] | DGD  | C8B-C9B-CAB-CBB |
| 33  | d     | 406[B] | LHG  | C25-C26-C27-C28 |
| 23  | b     | 612    | CLA  | C10-C11-C12-C13 |
| 33  | D     | 707[A] | LHG  | C10-C11-C12-C13 |
| 23  | C     | 512    | CLA  | C8-C10-C11-C12  |
| 36  | C     | 518[A] | DGD  | C8A-C9A-CAA-CBA |
| 33  | E     | 101[A] | LHG  | O6-C4-C5-C6     |
| 33  | b     | 629[B] | LHG  | O6-C4-C5-C6     |
| 23  | b     | 616    | CLA  | C5-C6-C7-C8     |
| 32  | b     | 621    | LMT  | C7-C8-C9-C10    |
| 23  | B     | 602    | CLA  | C6-C7-C8-C10    |
| 23  | C     | 503    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 604    | CLA  | C6-C7-C8-C10    |
| 23  | b     | 615    | CLA  | C12-C13-C15-C16 |
| 23  | c     | 506    | CLA  | C12-C13-C15-C16 |
| 23  | c     | 507    | CLA  | C11-C10-C8-C7   |
| 23  | c     | 510    | CLA  | C6-C7-C8-C10    |
| 23  | d     | 401[B] | CLA  | C11-C12-C13-C15 |
| 33  | a     | 420[A] | LHG  | C7-C8-C9-C10    |
| 32  | m     | 103    | LMT  | C7-C8-C9-C10    |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 25  | K     | 102    | BCR  | C7-C8-C9-C10    |
| 25  | d     | 403    | BCR  | C7-C8-C9-C10    |
| 23  | C     | 511    | CLA  | O1A-CGA-O2A-C1  |
| 23  | c     | 512    | CLA  | O1A-CGA-O2A-C1  |
| 36  | c     | 519    | DGD  | O1A-C1A-O1G-C1G |
| 36  | C     | 518[A] | DGD  | C2G-C3G-O3G-C1D |
| 36  | c     | 518[A] | DGD  | C2G-C3G-O3G-C1D |
| 36  | c     | 518[A] | DGD  | C5D-C6D-O5D-C1E |
| 36  | c     | 518[B] | DGD  | C5D-C6D-O5D-C1E |
| 33  | d     | 412[A] | LHG  | C25-C26-C27-C28 |
| 23  | c     | 514    | CLA  | C4-C3-C5-C6     |
| 29  | D     | 705[A] | PL9  | C15-C14-C16-C17 |
| 29  | D     | 705[A] | PL9  | C45-C44-C46-C47 |
| 33  | D     | 707[B] | LHG  | O10-C23-O8-C6   |
| 29  | A     | 414[B] | PL9  | C43-C44-C46-C47 |
| 29  | a     | 414[B] | PL9  | C12-C11-C9-C8   |
| 29  | d     | 404[B] | PL9  | C28-C29-C31-C32 |
| 38  | f     | 101    | HEM  | C2B-C3B-CAB-CBB |
| 33  | D     | 706[B] | LHG  | C11-C10-C9-C8   |
| 24  | a     | 408[A] | PHO  | O2A-C1-C2-C3    |
| 34  | c     | 521    | LMG  | O10-C28-O8-C9   |
| 34  | B     | 621    | LMG  | C32-C33-C34-C35 |
| 23  | B     | 606    | CLA  | C15-C16-C17-C18 |
| 33  | D     | 706[B] | LHG  | C34-C35-C36-C37 |
| 23  | A     | 406[B] | CLA  | C16-C17-C18-C20 |
| 36  | C     | 519    | DGD  | C6A-C7A-C8A-C9A |
| 34  | B     | 621    | LMG  | C18-C19-C20-C21 |
| 33  | E     | 101[B] | LHG  | O6-C4-C5-O7     |
| 33  | b     | 629[A] | LHG  | O6-C4-C5-O7     |
| 33  | b     | 629[B] | LHG  | O6-C4-C5-O7     |
| 33  | L     | 101[A] | LHG  | C11-C10-C9-C8   |
| 33  | d     | 412[A] | LHG  | C24-C25-C26-C27 |
| 36  | c     | 518[B] | DGD  | O6E-C1E-O5D-C6D |
| 26  | a     | 412    | SQD  | O6-C44-C45-C46  |
| 33  | E     | 101[A] | LHG  | C4-C5-C6-O8     |
| 33  | E     | 101[B] | LHG  | C4-C5-C6-O8     |
| 33  | b     | 629[A] | LHG  | C34-C35-C36-C37 |
| 23  | D     | 703    | CLA  | O1A-CGA-O2A-C1  |
| 36  | C     | 517[A] | DGD  | C4D-C5D-C6D-O5D |
| 23  | b     | 601    | CLA  | C4-C3-C5-C6     |
| 24  | a     | 408[B] | PHO  | C4-C3-C5-C6     |
| 36  | C     | 517[A] | DGD  | CCA-CDA-CEA-CFA |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | a     | 406[B] | CLA  | C2C-C3C-CAC-CBC |
| 33  | b     | 629[A] | LHG  | C9-C10-C11-C12  |
| 26  | b     | 620    | SQD  | O47-C45-C46-O48 |
| 26  | f     | 102    | SQD  | O47-C45-C46-O48 |
| 33  | a     | 420[A] | LHG  | O7-C5-C6-O8     |
| 33  | a     | 420[B] | LHG  | O7-C5-C6-O8     |
| 34  | B     | 621    | LMG  | O1-C7-C8-O7     |
| 23  | B     | 610    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 506    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 514    | CLA  | C6-C7-C8-C9     |
| 23  | d     | 401[B] | CLA  | C11-C12-C13-C14 |
| 32  | B     | 629    | LMT  | C3-C4-C5-C6     |
| 33  | E     | 101[A] | LHG  | C13-C14-C15-C16 |
| 33  | d     | 412[B] | LHG  | C33-C34-C35-C36 |
| 26  | A     | 412    | SQD  | C24-C23-O48-C46 |
| 26  | a     | 411[A] | SQD  | C27-C28-C29-C30 |
| 33  | L     | 101[B] | LHG  | C11-C10-C9-C8   |
| 26  | b     | 620    | SQD  | C13-C14-C15-C16 |
| 34  | m     | 101    | LMG  | C32-C33-C34-C35 |
| 23  | B     | 615    | CLA  | C13-C15-C16-C17 |
| 33  | D     | 707[B] | LHG  | C10-C11-C12-C13 |
| 33  | E     | 101[B] | LHG  | C13-C14-C15-C16 |
| 36  | C     | 518[A] | DGD  | C7A-C8A-C9A-CAA |
| 33  | D     | 706[A] | LHG  | C34-C35-C36-C37 |
| 33  | d     | 405[B] | LHG  | C24-C23-O8-C6   |
| 26  | a     | 411[B] | SQD  | C12-C13-C14-C15 |
| 32  | b     | 627    | LMT  | C6-C7-C8-C9     |
| 36  | C     | 519    | DGD  | CBA-CCA-CDA-CEA |
| 23  | b     | 601    | CLA  | C8-C10-C11-C12  |
| 33  | d     | 406[A] | LHG  | C24-C23-O8-C6   |
| 32  | M     | 101    | LMT  | C2-C3-C4-C5     |
| 36  | c     | 517[B] | DGD  | C8B-C9B-CAB-CBB |
| 33  | d     | 405[B] | LHG  | O10-C23-O8-C6   |
| 34  | d     | 410    | LMG  | C16-C17-C18-C19 |
| 23  | b     | 601    | CLA  | C3-C5-C6-C7     |
| 33  | d     | 406[B] | LHG  | O10-C23-O8-C6   |
| 34  | C     | 501    | LMG  | C29-C30-C31-C32 |
| 34  | C     | 501    | LMG  | C20-C21-C22-C23 |
| 27  | D     | 701    | GOL  | O1-C1-C2-O2     |
| 27  | o     | 304    | GOL  | O1-C1-C2-O2     |
| 32  | A     | 420    | LMT  | C2-C1-O1'-C1'   |
| 23  | A     | 406[B] | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | B     | 611    | CLA  | C1A-C2A-CAA-CBA |
| 23  | C     | 512    | CLA  | C1A-C2A-CAA-CBA |
| 23  | a     | 406[A] | CLA  | C1A-C2A-CAA-CBA |
| 23  | a     | 407[B] | CLA  | C4B-C3B-CAB-CBB |
| 23  | b     | 606    | CLA  | C4B-C3B-CAB-CBB |
| 23  | D     | 703    | CLA  | CBA-CGA-O2A-C1  |
| 33  | d     | 406[B] | LHG  | C24-C23-O8-C6   |
| 26  | a     | 411[A] | SQD  | C35-C36-C37-C38 |
| 36  | h     | 102    | DGD  | CDA-CEA-CFA-CGA |
| 23  | a     | 405[A] | CLA  | C2C-C3C-CAC-CBC |
| 23  | B     | 601    | CLA  | C2A-CAA-CBA-CGA |
| 34  | C     | 521    | LMG  | C20-C21-C22-C23 |
| 36  | C     | 518[B] | DGD  | C3B-C4B-C5B-C6B |
| 33  | A     | 419[A] | LHG  | C32-C33-C34-C35 |
| 23  | B     | 607    | CLA  | C12-C13-C15-C16 |
| 23  | B     | 616    | CLA  | C12-C13-C15-C16 |
| 23  | C     | 506    | CLA  | C12-C13-C15-C16 |
| 23  | C     | 507    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 616    | CLA  | C6-C7-C8-C10    |
| 23  | c     | 505    | CLA  | C11-C12-C13-C15 |
| 36  | C     | 519    | DGD  | CAA-CBA-CCA-CDA |
| 34  | C     | 521    | LMG  | C38-C39-C40-C41 |
| 26  | A     | 412    | SQD  | O10-C23-O48-C46 |
| 33  | d     | 406[A] | LHG  | O10-C23-O8-C6   |
| 33  | D     | 707[A] | LHG  | C24-C23-O8-C6   |
| 32  | B     | 627    | LMT  | C7-C8-C9-C10    |
| 34  | m     | 101    | LMG  | C14-C15-C16-C17 |
| 36  | C     | 519    | DGD  | C7B-C8B-C9B-CAB |
| 33  | D     | 707[A] | LHG  | O10-C23-O8-C6   |
| 36  | c     | 518[A] | DGD  | C1A-C2A-C3A-C4A |
| 33  | D     | 707[B] | LHG  | C2-C3-O3-P      |
| 33  | D     | 706[B] | LHG  | C28-C29-C30-C31 |
| 23  | c     | 511    | CLA  | C4-C3-C5-C6     |
| 23  | B     | 603    | CLA  | C2-C3-C5-C6     |
| 34  | C     | 501    | LMG  | C39-C40-C41-C42 |
| 26  | A     | 410[A] | SQD  | C18-C19-C20-C21 |
| 23  | A     | 406[A] | CLA  | C14-C13-C15-C16 |
| 23  | B     | 607    | CLA  | C14-C13-C15-C16 |
| 23  | a     | 409    | CLA  | C11-C10-C8-C9   |
| 23  | b     | 615    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 510    | CLA  | C6-C7-C8-C9     |
| 23  | b     | 612    | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | B     | 620    | SQD  | C33-C34-C35-C36 |
| 33  | d     | 412[A] | LHG  | C27-C28-C29-C30 |
| 36  | c     | 517[A] | DGD  | CCB-CDB-CEB-CFB |
| 26  | X     | 101    | SQD  | C7-C8-C9-C10    |
| 33  | d     | 412[B] | LHG  | C7-C8-C9-C10    |
| 23  | C     | 510    | CLA  | C3-C5-C6-C7     |
| 32  | T     | 101    | LMT  | C1-C2-C3-C4     |
| 23  | D     | 703    | CLA  | C8-C10-C11-C12  |
| 32  | B     | 630    | LMT  | C6-C7-C8-C9     |
| 33  | E     | 101[A] | LHG  | O7-C5-C6-O8     |
| 34  | c     | 501    | LMG  | O7-C8-C9-O8     |
| 23  | b     | 604    | CLA  | C10-C11-C12-C13 |
| 23  | c     | 510    | CLA  | C15-C16-C17-C18 |
| 26  | A     | 412    | SQD  | C30-C31-C32-C33 |
| 29  | D     | 705[B] | PL9  | C45-C44-C46-C47 |
| 23  | A     | 405[B] | CLA  | C15-C16-C17-C18 |
| 36  | C     | 519    | DGD  | O1A-C1A-O1G-C1G |
| 29  | a     | 414[A] | PL9  | C12-C11-C9-C8   |
| 33  | a     | 420[A] | LHG  | C23-C24-C25-C26 |
| 33  | b     | 629[B] | LHG  | C9-C10-C11-C12  |
| 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  | c     | 503    | CLA  | CAD-CBD-CGD-O2D |
| 36  | h     | 102    | DGD  | CCB-CDB-CEB-CFB |
| 34  | C     | 520    | LMG  | C12-C13-C14-C15 |
| 26  | A     | 410[A] | SQD  | C34-C35-C36-C37 |
| 34  | C     | 501    | LMG  | C18-C19-C20-C21 |
| 36  | c     | 517[A] | DGD  | C8B-C9B-CAB-CBB |
| 23  | B     | 601    | CLA  | CAD-CBD-CGD-O1D |
| 23  | B     | 607    | CLA  | CAD-CBD-CGD-O1D |
| 23  | B     | 609    | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 503    | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 505    | CLA  | CAD-CBD-CGD-O1D |
| 23  | C     | 507    | CLA  | CAD-CBD-CGD-O1D |
| 23  | b     | 601    | CLA  | CAD-CBD-CGD-O1D |
| 23  | c     | 503    | CLA  | CAD-CBD-CGD-O1D |
| 23  | c     | 510    | CLA  | CHA-CBD-CGD-O1D |
| 33  | A     | 419[B] | LHG  | C3-O3-P-O6      |
| 33  | A     | 419[B] | LHG  | C4-O6-P-O4      |
| 33  | D     | 706[A] | LHG  | C4-O6-P-O3      |
| 33  | D     | 706[A] | LHG  | C4-O6-P-O5      |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | D     | 706[B] | LHG  | C4-O6-P-O5      |
| 33  | D     | 707[B] | LHG  | C4-O6-P-O4      |
| 33  | E     | 101[A] | LHG  | C4-O6-P-O5      |
| 33  | E     | 101[B] | LHG  | C4-O6-P-O5      |
| 33  | L     | 101[B] | LHG  | C4-O6-P-O5      |
| 33  | a     | 420[A] | LHG  | C4-O6-P-O4      |
| 33  | a     | 420[B] | LHG  | C4-O6-P-O4      |
| 33  | d     | 405[A] | LHG  | C3-O3-P-O4      |
| 33  | d     | 405[B] | LHG  | C4-O6-P-O3      |
| 33  | d     | 405[B] | LHG  | C4-O6-P-O5      |
| 33  | d     | 412[B] | LHG  | C3-O3-P-O5      |
| 24  | a     | 408[A] | PHO  | C8-C10-C11-C12  |
| 23  | A     | 406[A] | CLA  | C2B-C3B-CAB-CBB |
| 23  | A     | 406[B] | CLA  | C2B-C3B-CAB-CBB |
| 23  | D     | 702[B] | CLA  | C2B-C3B-CAB-CBB |
| 36  | C     | 517[B] | DGD  | C6A-C7A-C8A-C9A |
| 23  | b     | 601    | CLA  | C2-C3-C5-C6     |
| 29  | A     | 414[A] | PL9  | C28-C29-C31-C32 |
| 29  | A     | 414[B] | PL9  | C28-C29-C31-C32 |
| 29  | a     | 414[B] | PL9  | C43-C44-C46-C47 |
| 23  | c     | 504    | CLA  | C8-C10-C11-C12  |
| 33  | D     | 707[A] | LHG  | C2-C3-O3-P      |
| 33  | d     | 406[A] | LHG  | C2-C3-O3-P      |
| 33  | d     | 406[B] | LHG  | C2-C3-O3-P      |
| 33  | d     | 406[B] | LHG  | C33-C34-C35-C36 |
| 26  | B     | 620    | SQD  | C29-C30-C31-C32 |
| 32  | F     | 101    | LMT  | C2-C3-C4-C5     |
| 33  | b     | 629[B] | LHG  | C34-C35-C36-C37 |
| 34  | d     | 410    | LMG  | C18-C19-C20-C21 |
| 26  | a     | 411[A] | SQD  | C11-C12-C13-C14 |
| 34  | z     | 101    | LMG  | C19-C20-C21-C22 |
| 34  | z     | 101    | LMG  | C20-C21-C22-C23 |
| 29  | A     | 414[B] | PL9  | C4-C3-C7-C8     |
| 29  | a     | 414[A] | PL9  | C4-C3-C7-C8     |
| 29  | a     | 414[B] | PL9  | C4-C3-C7-C8     |
| 36  | C     | 518[A] | DGD  | C1A-C2A-C3A-C4A |
| 23  | C     | 507    | CLA  | C2-C3-C5-C6     |
| 34  | B     | 621    | LMG  | C14-C15-C16-C17 |
| 34  | Z     | 101    | LMG  | C29-C28-O8-C9   |
| 33  | E     | 101[B] | LHG  | O6-C4-C5-C6     |
| 33  | L     | 101[A] | LHG  | O6-C4-C5-C6     |
| 34  | m     | 101    | LMG  | C11-C12-C13-C14 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | b     | 601    | CLA  | CAA-CBA-CGA-O2A |
| 23  | A     | 406[B] | CLA  | C14-C13-C15-C16 |
| 23  | B     | 614    | CLA  | C11-C10-C8-C9   |
| 23  | C     | 511    | CLA  | C11-C12-C13-C14 |
| 23  | b     | 601    | CLA  | C11-C12-C13-C14 |
| 23  | d     | 402    | CLA  | C11-C12-C13-C14 |
| 23  | B     | 613    | CLA  | C11-C10-C8-C7   |
| 23  | c     | 512    | CLA  | C8-C10-C11-C12  |
| 33  | a     | 420[B] | LHG  | C23-C24-C25-C26 |
| 23  | b     | 616    | CLA  | O1A-CGA-O2A-C1  |
| 33  | E     | 101[A] | LHG  | C1-C2-C3-O3     |
| 33  | L     | 101[A] | LHG  | O6-C4-C5-O7     |
| 32  | A     | 418    | LMT  | C7-C8-C9-C10    |
| 36  | c     | 517[A] | DGD  | O6E-C1E-O5D-C6D |
| 33  | D     | 707[B] | LHG  | C27-C28-C29-C30 |
| 36  | c     | 518[A] | DGD  | C2E-C1E-O5D-C6D |
| 36  | c     | 518[B] | DGD  | C2E-C1E-O5D-C6D |
| 24  | a     | 408[A] | PHO  | C4-C3-C5-C6     |
| 26  | A     | 410[A] | SQD  | C16-C17-C18-C19 |
| 32  | F     | 101    | LMT  | C6-C7-C8-C9     |
| 23  | a     | 406[B] | CLA  | C15-C16-C17-C18 |
| 33  | d     | 405[A] | LHG  | O10-C23-O8-C6   |
| 26  | b     | 620    | SQD  | C10-C11-C12-C13 |
| 33  | D     | 706[B] | LHG  | C10-C11-C12-C13 |
| 33  | d     | 412[A] | LHG  | C34-C35-C36-C37 |
| 36  | c     | 518[B] | DGD  | C9B-CAB-CBB-CCB |
| 26  | A     | 410[B] | SQD  | C16-C17-C18-C19 |
| 33  | E     | 101[B] | LHG  | O7-C5-C6-O8     |
| 23  | B     | 601    | CLA  | CAA-CBA-CGA-O2A |
| 36  | C     | 518[B] | DGD  | C8A-C9A-CAA-CBA |
| 36  | c     | 517[B] | DGD  | CCB-CDB-CEB-CFB |
| 33  | d     | 406[A] | LHG  | C32-C33-C34-C35 |
| 33  | d     | 405[A] | LHG  | C24-C23-O8-C6   |
| 36  | C     | 519    | DGD  | C2A-C1A-O1G-C1G |
| 25  | a     | 410    | BCR  | C19-C20-C21-C22 |
| 36  | H     | 102    | DGD  | O2G-C1B-C2B-C3B |
| 33  | b     | 629[B] | LHG  | C17-C18-C19-C20 |
| 23  | b     | 608    | CLA  | C13-C15-C16-C17 |
| 23  | B     | 607    | CLA  | C3-C5-C6-C7     |
| 26  | f     | 102    | SQD  | C26-C27-C28-C29 |
| 29  | a     | 414[B] | PL9  | C45-C44-C46-C47 |
| 29  | d     | 404[B] | PL9  | C45-C44-C46-C47 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | C     | 518[B] | DGD  | C7A-C8A-C9A-CAA |
| 34  | c     | 501    | LMG  | O8-C28-C29-C30  |
| 26  | a     | 411[B] | SQD  | C34-C35-C36-C37 |
| 32  | B     | 629    | LMT  | C7-C8-C9-C10    |
| 36  | C     | 518[B] | DGD  | C5B-C6B-C7B-C8B |
| 34  | B     | 621    | LMG  | O1-C7-C8-C9     |
| 33  | A     | 419[B] | LHG  | C26-C27-C28-C29 |
| 36  | C     | 517[A] | DGD  | C6A-C7A-C8A-C9A |
| 34  | B     | 621    | LMG  | O8-C28-C29-C30  |
| 25  | t     | 102    | BCR  | C7-C8-C9-C34    |
| 33  | a     | 420[B] | LHG  | C7-C8-C9-C10    |
| 36  | c     | 517[B] | DGD  | C5D-C6D-O5D-C1E |
| 34  | d     | 410    | LMG  | C19-C20-C21-C22 |
| 35  | o     | 301    | HTG  | C4'-C5'-C6'-C7' |
| 24  | a     | 408[A] | PHO  | C2-C3-C5-C6     |
| 23  | b     | 616    | CLA  | CBA-CGA-O2A-C1  |
| 33  | L     | 101[B] | LHG  | C27-C28-C29-C30 |
| 36  | c     | 519    | DGD  | C2B-C3B-C4B-C5B |
| 23  | c     | 511    | CLA  | O1A-CGA-O2A-C1  |
| 23  | a     | 406[A] | CLA  | C4C-C3C-CAC-CBC |
| 23  | A     | 404[B] | CLA  | C2C-C3C-CAC-CBC |
| 33  | L     | 101[A] | LHG  | C26-C27-C28-C29 |
| 33  | E     | 101[B] | LHG  | C1-C2-C3-O3     |
| 33  | d     | 412[A] | LHG  | C1-C2-C3-O3     |
| 23  | C     | 514    | CLA  | C6-C7-C8-C9     |
| 23  | b     | 606    | CLA  | C11-C10-C8-C9   |
| 23  | c     | 502    | CLA  | O1D-CGD-O2D-CED |
| 23  | C     | 513    | CLA  | C4B-C3B-CAB-CBB |
| 23  | b     | 614    | CLA  | CBD-CGD-O2D-CED |
| 33  | L     | 101[A] | LHG  | C27-C28-C29-C30 |
| 26  | a     | 412    | SQD  | C24-C23-O48-C46 |
| 29  | D     | 705[B] | PL9  | C35-C34-C36-C37 |
| 29  | d     | 404[A] | PL9  | C43-C44-C46-C47 |
| 35  | b     | 623    | HTG  | C4'-C5'-C6'-C7' |
| 26  | a     | 411[B] | SQD  | C11-C12-C13-C14 |
| 26  | a     | 412    | SQD  | O10-C23-O48-C46 |
| 36  | C     | 517[B] | DGD  | CDB-CEB-CFB-CGB |
| 34  | D     | 711    | LMG  | C18-C19-C20-C21 |
| 23  | C     | 504    | CLA  | C6-C7-C8-C10    |
| 23  | b     | 614    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 605    | CLA  | C3-C5-C6-C7     |
| 24  | A     | 417[B] | PHO  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | c     | 511    | CLA  | CBA-CGA-O2A-C1  |
| 23  | a     | 405[A] | CLA  | C4C-C3C-CAC-CBC |
| 32  | T     | 101    | LMT  | C3-C4-C5-C6     |
| 33  | D     | 707[A] | LHG  | C27-C28-C29-C30 |
| 33  | d     | 406[A] | LHG  | C33-C34-C35-C36 |
| 26  | X     | 101    | SQD  | O47-C45-C46-O48 |
| 36  | C     | 518[B] | DGD  | C8B-C9B-CAB-CBB |
| 29  | a     | 414[A] | PL9  | C45-C44-C46-C47 |
| 23  | c     | 511    | CLA  | C2-C3-C5-C6     |
| 33  | d     | 405[B] | LHG  | C25-C26-C27-C28 |
| 36  | c     | 517[A] | DGD  | C4B-C5B-C6B-C7B |
| 23  | B     | 608    | CLA  | C13-C15-C16-C17 |
| 23  | a     | 406[A] | CLA  | C15-C16-C17-C18 |
| 33  | a     | 420[B] | LHG  | C24-C25-C26-C27 |
| 23  | C     | 510    | CLA  | C2-C1-O2A-CGA   |
| 26  | A     | 410[A] | SQD  | C11-C10-C9-C8   |
| 32  | a     | 417    | LMT  | C4-C5-C6-C7     |
| 23  | B     | 606    | CLA  | C8-C10-C11-C12  |
| 25  | Y     | 101    | BCR  | C21-C22-C23-C24 |
| 25  | d     | 403    | BCR  | C21-C22-C23-C24 |
| 23  | b     | 616    | CLA  | C4-C3-C5-C6     |
| 29  | D     | 705[A] | PL9  | C35-C34-C36-C37 |
| 34  | z     | 101    | LMG  | O7-C10-C11-C12  |
| 29  | a     | 414[A] | PL9  | C43-C44-C46-C47 |
| 33  | a     | 420[A] | LHG  | C24-C25-C26-C27 |
| 40  | V     | 201    | HEC  | CAD-CBD-CGD-O1D |
| 23  | B     | 606    | CLA  | C11-C10-C8-C9   |
| 23  | B     | 614    | CLA  | C6-C7-C8-C9     |
| 23  | B     | 616    | CLA  | C14-C13-C15-C16 |
| 23  | C     | 506    | CLA  | C14-C13-C15-C16 |
| 23  | C     | 510    | CLA  | C6-C7-C8-C9     |
| 23  | D     | 703    | CLA  | C11-C10-C8-C9   |
| 23  | a     | 407[A] | CLA  | C11-C12-C13-C14 |
| 27  | d     | 411    | GOL  | C1-C2-C3-O3     |
| 27  | l     | 102[A] | GOL  | O1-C1-C2-C3     |
| 27  | v     | 202[A] | GOL  | O1-C1-C2-C3     |
| 33  | b     | 629[A] | LHG  | C25-C26-C27-C28 |
| 34  | d     | 410    | LMG  | C36-C37-C38-C39 |
| 23  | B     | 613    | CLA  | C15-C16-C17-C18 |
| 33  | D     | 706[A] | LHG  | C11-C10-C9-C8   |
| 36  | C     | 519    | DGD  | CDA-CEA-CFA-CGA |
| 36  | c     | 518[B] | DGD  | C1A-C2A-C3A-C4A |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | C     | 507    | CLA  | C16-C17-C18-C20 |
| 36  | h     | 102    | DGD  | O2G-C1B-C2B-C3B |
| 29  | D     | 705[B] | PL9  | C43-C44-C46-C47 |
| 29  | d     | 404[B] | PL9  | C43-C44-C46-C47 |
| 34  | d     | 410    | LMG  | C40-C41-C42-C43 |
| 27  | a     | 418    | GOL  | O1-C1-C2-O2     |
| 27  | d     | 411    | GOL  | O2-C2-C3-O3     |
| 27  | l     | 102[B] | GOL  | O1-C1-C2-O2     |
| 23  | B     | 604    | CLA  | C1A-C2A-CAA-CBA |
| 23  | C     | 502    | CLA  | C1A-C2A-CAA-CBA |
| 23  | a     | 407[B] | CLA  | C1A-C2A-CAA-CBA |
| 23  | A     | 404[A] | CLA  | C2C-C3C-CAC-CBC |
| 23  | a     | 409    | CLA  | C15-C16-C17-C18 |
| 23  | a     | 405[B] | CLA  | C2C-C3C-CAC-CBC |
| 23  | B     | 602    | CLA  | C2B-C3B-CAB-CBB |
| 23  | C     | 505    | CLA  | C2B-C3B-CAB-CBB |
| 23  | C     | 513    | CLA  | C2B-C3B-CAB-CBB |
| 23  | a     | 407[B] | CLA  | C2B-C3B-CAB-CBB |
| 23  | b     | 604    | CLA  | C2B-C3B-CAB-CBB |
| 23  | b     | 606    | CLA  | C2B-C3B-CAB-CBB |
| 25  | D     | 704    | BCR  | C23-C24-C25-C26 |
| 25  | H     | 101    | BCR  | C23-C24-C25-C30 |
| 25  | b     | 617    | BCR  | C5-C6-C7-C8     |
| 23  | C     | 504    | CLA  | CBD-CGD-O2D-CED |
| 40  | V     | 201    | HEC  | CAD-CBD-CGD-O2D |
| 26  | A     | 410[A] | SQD  | C13-C14-C15-C16 |
| 33  | A     | 419[A] | LHG  | C18-C19-C20-C21 |
| 33  | d     | 412[B] | LHG  | C17-C18-C19-C20 |
| 36  | C     | 519    | DGD  | C7A-C8A-C9A-CAA |
| 23  | A     | 406[A] | CLA  | C16-C17-C18-C19 |
| 23  | c     | 505    | CLA  | C4-C3-C5-C6     |
| 32  | e     | 101    | LMT  | O1'-C1-C2-C3    |
| 36  | c     | 518[A] | DGD  | C7B-C8B-C9B-CAB |
| 34  | d     | 410    | LMG  | C28-C29-C30-C31 |
| 33  | b     | 629[A] | LHG  | C17-C18-C19-C20 |
| 23  | B     | 606    | CLA  | C11-C10-C8-C7   |
| 23  | B     | 613    | CLA  | C12-C13-C15-C16 |
| 23  | B     | 615    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 603    | CLA  | C11-C10-C8-C7   |
| 23  | b     | 606    | CLA  | C11-C10-C8-C7   |
| 23  | b     | 608    | CLA  | C12-C13-C15-C16 |
| 23  | b     | 613    | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | b     | 615    | CLA  | C11-C12-C13-C15 |
| 29  | A     | 414[B] | PL9  | C39-C41-C42-C43 |
| 23  | A     | 404[B] | CLA  | C2A-CAA-CBA-CGA |
| 23  | C     | 502    | CLA  | C2A-CAA-CBA-CGA |
| 26  | a     | 411[B] | SQD  | O6-C44-C45-O47  |
| 29  | A     | 414[A] | PL9  | C4-C3-C7-C8     |
| 34  | z     | 101    | LMG  | C13-C14-C15-C16 |
| 36  | c     | 519    | DGD  | C9B-CAB-CBB-CCB |
| 38  | F     | 102    | HEM  | CAD-CBD-CGD-O1D |
| 36  | C     | 519    | DGD  | C9A-CAA-CBA-CCA |
| 32  | B     | 627    | LMT  | C9-C10-C11-C12  |
| 33  | D     | 706[A] | LHG  | C26-C27-C28-C29 |
| 36  | C     | 517[B] | DGD  | C3B-C4B-C5B-C6B |
| 23  | B     | 606    | CLA  | C4-C3-C5-C6     |
| 33  | d     | 405[A] | LHG  | C16-C17-C18-C19 |
| 29  | d     | 404[B] | PL9  | C18-C19-C21-C22 |
| 33  | d     | 406[B] | LHG  | C32-C33-C34-C35 |
| 32  | a     | 417    | LMT  | O5'-C5'-C6'-O6' |
| 38  | f     | 101    | HEM  | CAD-CBD-CGD-O1D |
| 36  | C     | 519    | DGD  | C4A-C5A-C6A-C7A |
| 26  | b     | 620    | SQD  | C28-C29-C30-C31 |
| 33  | d     | 412[B] | LHG  | C13-C14-C15-C16 |
| 36  | c     | 517[B] | DGD  | CAB-CBB-CCB-CDB |
| 36  | c     | 518[A] | DGD  | O6E-C1E-O5D-C6D |
| 38  | f     | 101    | HEM  | CAD-CBD-CGD-O2D |
| 23  | b     | 616    | CLA  | C2-C3-C5-C6     |
| 23  | c     | 514    | CLA  | C2-C3-C5-C6     |
| 23  | c     | 510    | CLA  | C10-C11-C12-C13 |
| 34  | Z     | 101    | LMG  | C2-C1-O1-C7     |
| 36  | c     | 517[A] | DGD  | C2E-C1E-O5D-C6D |
| 36  | c     | 519    | DGD  | O6D-C5D-C6D-O5D |
| 26  | a     | 411[B] | SQD  | O6-C44-C45-C46  |
| 33  | A     | 419[B] | LHG  | C11-C12-C13-C14 |
| 34  | C     | 521    | LMG  | C12-C13-C14-C15 |
| 33  | L     | 101[A] | LHG  | C23-C24-C25-C26 |
| 23  | B     | 614    | CLA  | C2A-CAA-CBA-CGA |
| 23  | a     | 405[B] | CLA  | C2A-CAA-CBA-CGA |
| 23  | b     | 602    | CLA  | C2A-CAA-CBA-CGA |
| 26  | a     | 412    | SQD  | C26-C27-C28-C29 |
| 27  | B     | 623    | GOL  | O1-C1-C2-O2     |
| 27  | O     | 303    | GOL  | O1-C1-C2-O2     |
| 27  | d     | 411    | GOL  | O1-C1-C2-O2     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 32  | B     | 627    | LMT  | C2-C1-O1'-C1'   |
| 33  | A     | 419[A] | LHG  | C29-C30-C31-C32 |
| 23  | B     | 614    | CLA  | C4-C3-C5-C6     |
| 23  | A     | 405[B] | CLA  | C2C-C3C-CAC-CBC |
| 23  | A     | 404[B] | CLA  | C4C-C3C-CAC-CBC |
| 34  | Z     | 101    | LMG  | C21-C22-C23-C24 |
| 23  | b     | 604    | CLA  | C4B-C3B-CAB-CBB |
| 38  | f     | 101    | HEM  | CAA-CBA-CGA-O2A |
| 32  | e     | 101    | LMT  | C2-C3-C4-C5     |
| 23  | A     | 404[A] | CLA  | C16-C17-C18-C19 |
| 23  | c     | 512    | CLA  | C3-C5-C6-C7     |
| 38  | F     | 102    | HEM  | CAD-CBD-CGD-O2D |
| 29  | A     | 414[A] | PL9  | C25-C24-C26-C27 |
| 34  | c     | 521    | LMG  | O1-C7-C8-O7     |
| 36  | c     | 517[A] | DGD  | CAB-CBB-CCB-CDB |
| 23  | c     | 508    | CLA  | C5-C6-C7-C8     |
| 26  | A     | 412    | SQD  | C15-C16-C17-C18 |
| 23  | D     | 703    | CLA  | C11-C10-C8-C7   |
| 23  | c     | 514    | CLA  | C12-C13-C15-C16 |
| 26  | a     | 411[B] | SQD  | C18-C19-C20-C21 |
| 23  | C     | 509    | CLA  | C13-C15-C16-C17 |
| 33  | E     | 101[B] | LHG  | C11-C10-C9-C8   |
| 23  | B     | 610    | CLA  | C11-C12-C13-C14 |
| 23  | B     | 615    | CLA  | C14-C13-C15-C16 |
| 23  | a     | 407[B] | CLA  | C11-C12-C13-C14 |
| 23  | c     | 505    | CLA  | C14-C13-C15-C16 |
| 34  | B     | 621    | LMG  | C29-C30-C31-C32 |
| 36  | C     | 519    | DGD  | C2B-C3B-C4B-C5B |
| 34  | C     | 521    | LMG  | C8-C7-O1-C1     |
| 36  | C     | 518[A] | DGD  | C5D-C6D-O5D-C1E |
| 36  | c     | 517[A] | DGD  | C5D-C6D-O5D-C1E |
| 26  | a     | 411[B] | SQD  | C27-C28-C29-C30 |
| 40  | v     | 201    | HEC  | CAD-CBD-CGD-O2D |
| 35  | b     | 625    | HTG  | C1'-C2'-C3'-C4' |
| 23  | b     | 608    | CLA  | C2-C1-O2A-CGA   |
| 23  | b     | 613    | CLA  | C2-C1-O2A-CGA   |
| 23  | b     | 614    | CLA  | C2-C1-O2A-CGA   |
| 33  | A     | 419[A] | LHG  | C35-C36-C37-C38 |
| 23  | C     | 507    | CLA  | C3A-C2A-CAA-CBA |
| 23  | c     | 507    | CLA  | C3A-C2A-CAA-CBA |
| 33  | b     | 629[A] | LHG  | C10-C11-C12-C13 |
| 23  | C     | 504    | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 36  | h     | 102    | DGD  | C6A-C7A-C8A-C9A |
| 34  | c     | 521    | LMG  | C31-C32-C33-C34 |
| 36  | c     | 519    | DGD  | C1A-C2A-C3A-C4A |
| 33  | L     | 101[A] | LHG  | C16-C17-C18-C19 |
| 34  | B     | 621    | LMG  | C20-C21-C22-C23 |
| 32  | M     | 101    | LMT  | C9-C10-C11-C12  |
| 23  | b     | 615    | CLA  | C10-C11-C12-C13 |
| 26  | b     | 620    | SQD  | C30-C31-C32-C33 |
| 38  | f     | 101    | HEM  | CAA-CBA-CGA-O1A |
| 23  | b     | 604    | CLA  | C13-C15-C16-C17 |
| 33  | d     | 406[B] | LHG  | C11-C10-C9-C8   |
| 36  | h     | 102    | DGD  | CCA-CDA-CEA-CFA |
| 23  | A     | 404[A] | CLA  | C15-C16-C17-C18 |
| 40  | v     | 201    | HEC  | CAD-CBD-CGD-O1D |
| 36  | c     | 518[A] | DGD  | C9B-CAB-CBB-CCB |
| 29  | A     | 414[A] | PL9  | C39-C41-C42-C43 |
| 38  | f     | 101    | HEM  | C4B-C3B-CAB-CBB |
| 34  | c     | 521    | LMG  | C32-C33-C34-C35 |
| 36  | C     | 519    | DGD  | C8A-C9A-CAA-CBA |
| 27  | B     | 626    | GOL  | O1-C1-C2-O2     |
| 29  | A     | 414[B] | PL9  | C25-C24-C26-C27 |
| 33  | D     | 707[A] | LHG  | C28-C29-C30-C31 |
| 33  | b     | 629[A] | LHG  | C30-C31-C32-C33 |
| 33  | d     | 412[B] | LHG  | C29-C30-C31-C32 |
| 23  | B     | 612    | CLA  | CBA-CGA-O2A-C1  |
| 36  | C     | 518[B] | DGD  | C1A-C2A-C3A-C4A |
| 36  | c     | 518[B] | DGD  | CDA-CEA-CFA-CGA |
| 36  | c     | 517[B] | DGD  | CBA-CCA-CDA-CEA |
| 36  | C     | 518[B] | DGD  | C7B-C8B-C9B-CAB |
| 23  | C     | 505    | CLA  | C11-C12-C13-C14 |
| 23  | a     | 407[A] | CLA  | C14-C13-C15-C16 |
| 23  | b     | 603    | CLA  | C11-C10-C8-C9   |
| 23  | c     | 510    | CLA  | C11-C12-C13-C14 |
| 34  | c     | 520    | LMG  | C14-C15-C16-C17 |
| 33  | b     | 629[B] | LHG  | O7-C7-C8-C9     |
| 34  | B     | 621    | LMG  | C15-C16-C17-C18 |
| 23  | C     | 505    | CLA  | C3-C5-C6-C7     |
| 26  | B     | 620    | SQD  | C24-C25-C26-C27 |
| 26  | b     | 620    | SQD  | C16-C17-C18-C19 |
| 23  | C     | 513    | CLA  | CAA-CBA-CGA-O2A |
| 33  | A     | 419[A] | LHG  | O8-C23-C24-C25  |
| 33  | A     | 419[B] | LHG  | O8-C23-C24-C25  |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | C     | 502    | CLA  | C16-C17-C18-C20 |
| 35  | b     | 625    | HTG  | C3'-C4'-C5'-C6' |
| 23  | C     | 509    | CLA  | C12-C13-C15-C16 |
| 23  | a     | 407[A] | CLA  | C11-C12-C13-C15 |
| 23  | c     | 511    | CLA  | C12-C13-C15-C16 |
| 25  | B     | 617    | BCR  | C1-C6-C7-C8     |
| 25  | B     | 617    | BCR  | C5-C6-C7-C8     |
| 25  | H     | 101    | BCR  | C23-C24-C25-C26 |
| 25  | t     | 102    | BCR  | C1-C6-C7-C8     |
| 25  | t     | 102    | BCR  | C5-C6-C7-C8     |
| 34  | C     | 501    | LMG  | C31-C32-C33-C34 |
| 23  | a     | 406[B] | CLA  | C4C-C3C-CAC-CBC |
| 23  | C     | 507    | CLA  | C2-C1-O2A-CGA   |
| 23  | c     | 514    | CLA  | C2-C1-O2A-CGA   |
| 33  | d     | 405[B] | LHG  | C12-C13-C14-C15 |
| 23  | C     | 511    | CLA  | CAA-CBA-CGA-O2A |
| 33  | E     | 101[B] | LHG  | O7-C7-C8-C9     |
| 33  | a     | 420[B] | LHG  | O8-C23-C24-C25  |
| 34  | Z     | 101    | LMG  | O7-C10-C11-C12  |
| 33  | L     | 101[B] | LHG  | O7-C7-C8-C9     |
| 23  | B     | 609    | CLA  | C2-C3-C5-C6     |
| 23  | b     | 615    | CLA  | C5-C6-C7-C8     |
| 35  | o     | 301    | HTG  | C2'-C1'-S1-C1   |
| 23  | A     | 404[A] | CLA  | C4C-C3C-CAC-CBC |
| 33  | d     | 412[A] | LHG  | C13-C14-C15-C16 |
| 33  | L     | 101[A] | LHG  | O7-C7-C8-C9     |
| 33  | A     | 419[A] | LHG  | C17-C18-C19-C20 |
| 36  | C     | 518[A] | DGD  | CAB-CBB-CCB-CDB |
| 23  | B     | 613    | CLA  | CAA-CBA-CGA-O2A |
| 33  | a     | 420[A] | LHG  | O8-C23-C24-C25  |
| 33  | b     | 629[A] | LHG  | O7-C7-C8-C9     |
| 26  | X     | 101    | SQD  | C33-C34-C35-C36 |
| 32  | T     | 101    | LMT  | O1'-C1-C2-C3    |
| 32  | b     | 627    | LMT  | O1'-C1-C2-C3    |
| 26  | A     | 412    | SQD  | C19-C20-C21-C22 |
| 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  | A     | 408    | CLA  | C11-C12-C13-C14 |
| 23  | a     | 407[B] | CLA  | C14-C13-C15-C16 |
| 23  | b     | 608    | CLA  | C14-C13-C15-C16 |
| 23  | c     | 507    | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 25  | Y     | 101    | BCR  | C37-C22-C23-C24 |
| 34  | B     | 621    | LMG  | C4-C5-C6-O5     |
| 23  | c     | 513    | CLA  | CAA-CBA-CGA-O2A |
| 26  | A     | 410[B] | SQD  | C13-C14-C15-C16 |
| 26  | X     | 101    | SQD  | C44-C45-C46-O48 |
| 23  | c     | 502    | CLA  | C4B-C3B-CAB-CBB |
| 33  | d     | 412[A] | LHG  | C18-C19-C20-C21 |
| 33  | b     | 629[A] | LHG  | C24-C25-C26-C27 |
| 23  | B     | 609    | CLA  | C4-C3-C5-C6     |
| 29  | A     | 414[B] | PL9  | C12-C11-C9-C10  |
| 29  | D     | 705[A] | PL9  | C40-C39-C41-C42 |
| 32  | a     | 417    | LMT  | O5'-C1'-O1'-C1  |
| 23  | c     | 511    | CLA  | CAA-CBA-CGA-O2A |
| 34  | D     | 711    | LMG  | O7-C10-C11-C12  |
| 36  | C     | 519    | DGD  | O1G-C1A-C2A-C3A |
| 25  | t     | 102    | BCR  | C7-C8-C9-C10    |
| 25  | y     | 101    | BCR  | C21-C22-C23-C24 |
| 26  | X     | 101    | SQD  | C24-C23-O48-C46 |
| 33  | d     | 405[B] | LHG  | C13-C14-C15-C16 |
| 34  | c     | 501    | LMG  | C18-C19-C20-C21 |
| 23  | B     | 612    | CLA  | O1A-CGA-O2A-C1  |
| 23  | c     | 508    | CLA  | C2A-CAA-CBA-CGA |
| 23  | b     | 615    | CLA  | C13-C15-C16-C17 |
| 34  | C     | 521    | LMG  | C4-C5-C6-O5     |
| 33  | D     | 707[B] | LHG  | O8-C23-C24-C25  |
| 34  | c     | 520    | LMG  | O7-C10-C11-C12  |
| 36  | C     | 519    | DGD  | C3B-C4B-C5B-C6B |
| 23  | a     | 405[B] | CLA  | C4C-C3C-CAC-CBC |
| 33  | d     | 412[B] | LHG  | C1-C2-C3-O3     |
| 23  | b     | 610    | CLA  | C13-C15-C16-C17 |
| 23  | A     | 408    | CLA  | C2-C1-O2A-CGA   |
| 32  | a     | 417    | LMT  | C7-C8-C9-C10    |
| 23  | B     | 603    | CLA  | C11-C12-C13-C15 |
| 23  | B     | 613    | CLA  | C11-C12-C13-C15 |
| 23  | C     | 505    | CLA  | C6-C7-C8-C10    |
| 23  | a     | 407[B] | CLA  | C11-C12-C13-C15 |
| 23  | b     | 604    | CLA  | C11-C12-C13-C15 |
| 23  | b     | 607    | CLA  | C12-C13-C15-C16 |
| 23  | c     | 505    | CLA  | C12-C13-C15-C16 |
| 24  | A     | 407[B] | PHO  | C6-C7-C8-C10    |
| 23  | C     | 509    | CLA  | C5-C6-C7-C8     |
| 23  | b     | 611    | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 23  | c     | 508    | CLA  | C8-C10-C11-C12  |
| 33  | A     | 419[B] | LHG  | C17-C18-C19-C20 |
| 24  | a     | 408[B] | PHO  | O2A-C1-C2-C3    |
| 34  | c     | 501    | LMG  | C13-C14-C15-C16 |
| 33  | d     | 412[B] | LHG  | O8-C23-C24-C25  |
| 23  | B     | 603    | CLA  | C2A-CAA-CBA-CGA |
| 23  | c     | 504    | CLA  | C5-C6-C7-C8     |
| 23  | A     | 408    | CLA  | C16-C17-C18-C19 |
| 23  | b     | 610    | CLA  | C16-C17-C18-C19 |
| 34  | Z     | 101    | LMG  | C19-C20-C21-C22 |
| 34  | c     | 521    | LMG  | C39-C40-C41-C42 |
| 23  | C     | 504    | CLA  | C5-C6-C7-C8     |
| 23  | a     | 409    | CLA  | C8-C10-C11-C12  |
| 33  | D     | 706[B] | LHG  | C23-C24-C25-C26 |
| 33  | b     | 629[B] | LHG  | O9-C7-C8-C9     |
| 23  | B     | 611    | CLA  | C8-C10-C11-C12  |
| 23  | c     | 503    | CLA  | C16-C17-C18-C19 |
| 33  | E     | 101[A] | LHG  | O7-C7-C8-C9     |
| 36  | c     | 517[A] | DGD  | O2G-C1B-C2B-C3B |
| 26  | a     | 411[A] | SQD  | C10-C11-C12-C13 |
| 34  | Z     | 101    | LMG  | O9-C10-C11-C12  |
| 26  | X     | 101    | SQD  | O10-C23-O48-C46 |
| 34  | c     | 520    | LMG  | O10-C28-O8-C9   |
| 26  | A     | 410[B] | SQD  | C18-C19-C20-C21 |
| 32  | A     | 418    | LMT  | C9-C10-C11-C12  |
| 29  | d     | 404[B] | PL9  | C11-C12-C13-C14 |
| 33  | b     | 629[A] | LHG  | O9-C7-C8-C9     |
| 33  | D     | 706[B] | LHG  | C32-C33-C34-C35 |
| 23  | B     | 603    | CLA  | C11-C12-C13-C14 |
| 23  | b     | 606    | CLA  | C14-C13-C15-C16 |
| 23  | b     | 607    | CLA  | C14-C13-C15-C16 |
| 34  | c     | 521    | LMG  | C28-C29-C30-C31 |
| 23  | c     | 511    | CLA  | O1D-CGD-O2D-CED |
| 29  | d     | 404[B] | PL9  | C30-C29-C31-C32 |
| 23  | C     | 513    | CLA  | CAA-CBA-CGA-O1A |
| 33  | L     | 101[B] | LHG  | O9-C7-C8-C9     |
| 24  | A     | 417[A] | PHO  | C2C-C3C-CAC-CBC |
| 34  | C     | 521    | LMG  | C33-C34-C35-C36 |
| 36  | C     | 518[A] | DGD  | C3A-C4A-C5A-C6A |
| 38  | F     | 102    | HEM  | CAA-CBA-CGA-O2A |
| 33  | A     | 419[A] | LHG  | O10-C23-C24-C25 |
| 33  | a     | 420[A] | LHG  | O10-C23-C24-C25 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 33  | a     | 420[B] | LHG  | O10-C23-C24-C25 |
| 33  | D     | 706[A] | LHG  | C28-C29-C30-C31 |
| 23  | c     | 513    | CLA  | CAA-CBA-CGA-O1A |
| 33  | A     | 419[B] | LHG  | O10-C23-C24-C25 |
| 34  | c     | 520    | LMG  | C40-C41-C42-C43 |
| 23  | B     | 612    | CLA  | C8-C10-C11-C12  |
| 36  | C     | 517[A] | DGD  | C5D-C6D-O5D-C1E |
| 36  | C     | 517[B] | DGD  | C5D-C6D-O5D-C1E |
| 36  | C     | 518[B] | DGD  | C5D-C6D-O5D-C1E |
| 23  | C     | 508    | CLA  | C2A-CAA-CBA-CGA |
| 34  | Z     | 101    | LMG  | O10-C28-O8-C9   |
| 23  | b     | 610    | CLA  | C16-C17-C18-C20 |
| 33  | E     | 101[A] | LHG  | C11-C10-C9-C8   |
| 34  | C     | 501    | LMG  | C7-C8-C9-O8     |
| 23  | B     | 613    | CLA  | CAA-CBA-CGA-O1A |
| 23  | C     | 511    | CLA  | CAA-CBA-CGA-O1A |
| 34  | D     | 711    | LMG  | O9-C10-C11-C12  |
| 36  | C     | 519    | DGD  | O1A-C1A-C2A-C3A |
| 29  | d     | 404[A] | PL9  | C11-C12-C13-C14 |
| 33  | L     | 101[B] | LHG  | C7-C8-C9-C10    |
| 23  | C     | 508    | CLA  | C13-C15-C16-C17 |
| 33  | E     | 101[B] | LHG  | O9-C7-C8-C9     |
| 33  | L     | 101[A] | LHG  | O9-C7-C8-C9     |
| 23  | A     | 406[B] | CLA  | C16-C17-C18-C19 |
| 23  | C     | 507    | CLA  | CAD-CBD-CGD-O2D |
| 23  | b     | 601    | CLA  | CAD-CBD-CGD-O2D |
| 23  | b     | 609    | CLA  | CAD-CBD-CGD-O2D |
| 23  | b     | 616    | CLA  | CAD-CBD-CGD-O2D |
| 23  | c     | 507    | CLA  | CAD-CBD-CGD-O2D |
| 24  | A     | 407[A] | PHO  | CAD-CBD-CGD-O2D |
| 24  | a     | 408[A] | PHO  | CAD-CBD-CGD-O2D |
| 34  | B     | 621    | LMG  | C36-C37-C38-C39 |
| 32  | t     | 101    | LMT  | C2-C3-C4-C5     |
| 33  | L     | 101[B] | LHG  | O6-C4-C5-C6     |
| 23  | B     | 613    | CLA  | C2-C1-O2A-CGA   |
| 38  | F     | 102    | HEM  | CAA-CBA-CGA-O1A |
| 34  | C     | 521    | LMG  | C11-C12-C13-C14 |
| 36  | C     | 519    | DGD  | C2A-C3A-C4A-C5A |
| 23  | b     | 612    | CLA  | CAA-CBA-CGA-O2A |
| 23  | b     | 613    | CLA  | CAA-CBA-CGA-O2A |
| 34  | C     | 520    | LMG  | C10-C11-C12-C13 |
| 36  | c     | 517[A] | DGD  | C1A-C2A-C3A-C4A |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 34  | C     | 520    | LMG  | C29-C30-C31-C32 |
| 36  | c     | 517[A] | DGD  | CBA-CCA-CDA-CEA |
| 34  | c     | 520    | LMG  | O9-C10-C11-C12  |
| 26  | a     | 411[B] | SQD  | C7-C8-C9-C10    |
| 23  | b     | 602    | CLA  | CAA-CBA-CGA-O2A |
| 33  | D     | 707[A] | LHG  | O8-C23-C24-C25  |
| 33  | E     | 101[B] | LHG  | O8-C23-C24-C25  |
| 34  | C     | 501    | LMG  | O8-C28-C29-C30  |
| 33  | D     | 707[B] | LHG  | O10-C23-C24-C25 |
| 23  | c     | 502    | CLA  | CAA-CBA-CGA-O2A |
| 26  | a     | 412    | SQD  | O48-C23-C24-C25 |
| 33  | E     | 101[A] | LHG  | O8-C23-C24-C25  |
| 34  | c     | 521    | LMG  | O7-C10-C11-C12  |
| 36  | C     | 518[A] | DGD  | O2G-C1B-C2B-C3B |
| 23  | c     | 511    | CLA  | CAA-CBA-CGA-O1A |

There are no ring outliers.

182 monomers are involved in 378 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 27  | v     | 202[B] | GOL  | 1       | 0            |
| 23  | C     | 504    | CLA  | 4       | 0            |
| 34  | c     | 521    | LMG  | 1       | 0            |
| 23  | b     | 615    | CLA  | 3       | 0            |
| 34  | c     | 520    | LMG  | 1       | 0            |
| 33  | D     | 706[A] | LHG  | 2       | 0            |
| 25  | b     | 617    | BCR  | 1       | 0            |
| 23  | A     | 406[A] | CLA  | 1       | 0            |
| 23  | C     | 514    | CLA  | 2       | 0            |
| 24  | a     | 416[B] | PHO  | 1       | 0            |
| 33  | D     | 707[B] | LHG  | 4       | 0            |
| 32  | a     | 417    | LMT  | 1       | 0            |
| 23  | C     | 506    | CLA  | 6       | 0            |
| 23  | a     | 407[A] | CLA  | 2       | 0            |
| 23  | b     | 603    | CLA  | 1       | 0            |
| 23  | c     | 508    | CLA  | 2       | 0            |
| 25  | C     | 515    | BCR  | 1       | 0            |
| 23  | C     | 508    | CLA  | 4       | 0            |
| 23  | D     | 702[B] | CLA  | 3       | 0            |
| 32  | M     | 101    | LMT  | 1       | 0            |
| 33  | d     | 405[B] | LHG  | 3       | 0            |
| 26  | A     | 412    | SQD  | 1       | 0            |

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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 23  | C     | 502    | CLA  | 6       | 0            |
| 25  | A     | 409    | BCR  | 1       | 0            |
| 36  | h     | 102    | DGD  | 2       | 0            |
| 25  | K     | 102    | BCR  | 1       | 0            |
| 32  | A     | 418    | LMT  | 1       | 0            |
| 23  | B     | 612    | CLA  | 1       | 0            |
| 23  | c     | 510    | CLA  | 1       | 0            |
| 35  | B     | 624    | HTG  | 1       | 0            |
| 23  | A     | 405[B] | CLA  | 3       | 0            |
| 32  | T     | 101    | LMT  | 1       | 0            |
| 32  | B     | 629    | LMT  | 2       | 0            |
| 23  | C     | 509    | CLA  | 6       | 0            |
| 35  | d     | 409    | HTG  | 1       | 0            |
| 40  | V     | 201    | HEC  | 1       | 0            |
| 27  | v     | 202[A] | GOL  | 1       | 0            |
| 25  | B     | 619    | BCR  | 1       | 0            |
| 23  | B     | 613    | CLA  | 4       | 0            |
| 33  | A     | 419[B] | LHG  | 1       | 0            |
| 33  | d     | 406[B] | LHG  | 8       | 0            |
| 23  | c     | 504    | CLA  | 3       | 0            |
| 34  | C     | 521    | LMG  | 2       | 0            |
| 24  | a     | 416[A] | PHO  | 2       | 0            |
| 25  | B     | 617    | BCR  | 1       | 0            |
| 29  | A     | 414[B] | PL9  | 8       | 0            |
| 23  | B     | 605    | CLA  | 4       | 0            |
| 33  | D     | 707[A] | LHG  | 6       | 0            |
| 27  | l     | 102[B] | GOL  | 1       | 0            |
| 33  | E     | 101[B] | LHG  | 2       | 0            |
| 23  | D     | 702[A] | CLA  | 3       | 0            |
| 32  | b     | 621    | LMT  | 1       | 0            |
| 33  | d     | 405[A] | LHG  | 3       | 0            |
| 23  | A     | 408    | CLA  | 4       | 0            |
| 26  | X     | 101    | SQD  | 2       | 0            |
| 27  | c     | 526[B] | GOL  | 1       | 0            |
| 23  | d     | 402    | CLA  | 2       | 0            |
| 25  | D     | 704    | BCR  | 1       | 0            |
| 23  | B     | 606    | CLA  | 3       | 0            |
| 34  | B     | 621    | LMG  | 1       | 0            |
| 23  | b     | 606    | CLA  | 3       | 0            |
| 27  | a     | 418    | GOL  | 2       | 0            |
| 25  | B     | 618    | BCR  | 4       | 0            |
| 35  | b     | 622    | HTG  | 2       | 0            |

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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 23  | c     | 513    | CLA  | 7       | 0            |
| 25  | k     | 101    | BCR  | 1       | 0            |
| 23  | A     | 405[A] | CLA  | 4       | 0            |
| 23  | c     | 505    | CLA  | 3       | 0            |
| 23  | c     | 506    | CLA  | 5       | 0            |
| 24  | A     | 417[B] | PHO  | 2       | 0            |
| 32  | B     | 630    | LMT  | 1       | 0            |
| 25  | c     | 516    | BCR  | 1       | 0            |
| 23  | c     | 514    | CLA  | 3       | 0            |
| 23  | b     | 601    | CLA  | 1       | 0            |
| 24  | A     | 407[A] | PHO  | 2       | 0            |
| 23  | C     | 510    | CLA  | 2       | 0            |
| 25  | b     | 618    | BCR  | 3       | 0            |
| 23  | c     | 503    | CLA  | 2       | 0            |
| 36  | H     | 102    | DGD  | 1       | 0            |
| 23  | A     | 404[B] | CLA  | 4       | 0            |
| 25  | y     | 101    | BCR  | 2       | 0            |
| 29  | a     | 414[B] | PL9  | 4       | 0            |
| 23  | B     | 609    | CLA  | 2       | 0            |
| 26  | B     | 620    | SQD  | 2       | 0            |
| 25  | T     | 102    | BCR  | 6       | 0            |
| 23  | C     | 503    | CLA  | 5       | 0            |
| 23  | B     | 604    | CLA  | 1       | 0            |
| 33  | d     | 406[A] | LHG  | 10      | 0            |
| 35  | c     | 522    | HTG  | 1       | 0            |
| 25  | H     | 101    | BCR  | 1       | 0            |
| 29  | A     | 414[A] | PL9  | 10      | 0            |
| 23  | b     | 604    | CLA  | 2       | 0            |
| 33  | a     | 420[B] | LHG  | 4       | 0            |
| 26  | f     | 102    | SQD  | 1       | 0            |
| 29  | d     | 404[B] | PL9  | 1       | 0            |
| 27  | l     | 102[A] | GOL  | 1       | 0            |
| 33  | E     | 101[A] | LHG  | 5       | 0            |
| 23  | a     | 406[B] | CLA  | 3       | 0            |
| 23  | d     | 401[B] | CLA  | 2       | 0            |
| 23  | B     | 614    | CLA  | 1       | 0            |
| 25  | C     | 516    | BCR  | 2       | 0            |
| 34  | z     | 101    | LMG  | 2       | 0            |
| 25  | c     | 515    | BCR  | 3       | 0            |
| 25  | h     | 101    | BCR  | 4       | 0            |
| 27  | b     | 628    | GOL  | 2       | 0            |
| 25  | t     | 102    | BCR  | 5       | 0            |

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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 34  | d     | 410    | LMG  | 3       | 0            |
| 26  | a     | 411[B] | SQD  | 4       | 0            |
| 34  | m     | 101    | LMG  | 2       | 0            |
| 23  | B     | 610    | CLA  | 1       | 0            |
| 23  | b     | 614    | CLA  | 1       | 0            |
| 32  | e     | 101    | LMT  | 1       | 0            |
| 36  | C     | 517[B] | DGD  | 3       | 0            |
| 26  | A     | 410[B] | SQD  | 2       | 0            |
| 23  | b     | 613    | CLA  | 3       | 0            |
| 35  | o     | 301    | HTG  | 2       | 0            |
| 32  | t     | 101    | LMT  | 2       | 0            |
| 24  | A     | 417[A] | PHO  | 2       | 0            |
| 27  | D     | 701    | GOL  | 4       | 0            |
| 36  | c     | 519    | DGD  | 3       | 0            |
| 23  | a     | 405[B] | CLA  | 5       | 0            |
| 32  | A     | 420    | LMT  | 1       | 0            |
| 25  | b     | 619    | BCR  | 4       | 0            |
| 23  | b     | 607    | CLA  | 1       | 0            |
| 36  | c     | 517[B] | DGD  | 2       | 0            |
| 23  | B     | 601    | CLA  | 2       | 0            |
| 23  | b     | 605    | CLA  | 4       | 0            |
| 23  | A     | 404[A] | CLA  | 5       | 0            |
| 23  | C     | 512    | CLA  | 2       | 0            |
| 23  | b     | 611    | CLA  | 1       | 0            |
| 29  | a     | 414[A] | PL9  | 5       | 0            |
| 23  | B     | 616    | CLA  | 6       | 0            |
| 25  | Y     | 101    | BCR  | 1       | 0            |
| 33  | b     | 629[B] | LHG  | 1       | 0            |
| 32  | m     | 103    | LMT  | 2       | 0            |
| 23  | c     | 512    | CLA  | 5       | 0            |
| 23  | C     | 505    | CLA  | 1       | 0            |
| 26  | b     | 620    | SQD  | 2       | 0            |
| 27  | D     | 712    | GOL  | 2       | 0            |
| 23  | b     | 616    | CLA  | 1       | 0            |
| 33  | a     | 420[A] | LHG  | 4       | 0            |
| 35  | B     | 622    | HTG  | 2       | 0            |
| 33  | A     | 419[A] | LHG  | 2       | 0            |
| 36  | c     | 518[B] | DGD  | 1       | 0            |
| 36  | C     | 518[B] | DGD  | 1       | 0            |
| 34  | Z     | 101    | LMG  | 2       | 0            |
| 23  | a     | 406[A] | CLA  | 2       | 0            |
| 23  | d     | 401[A] | CLA  | 3       | 0            |

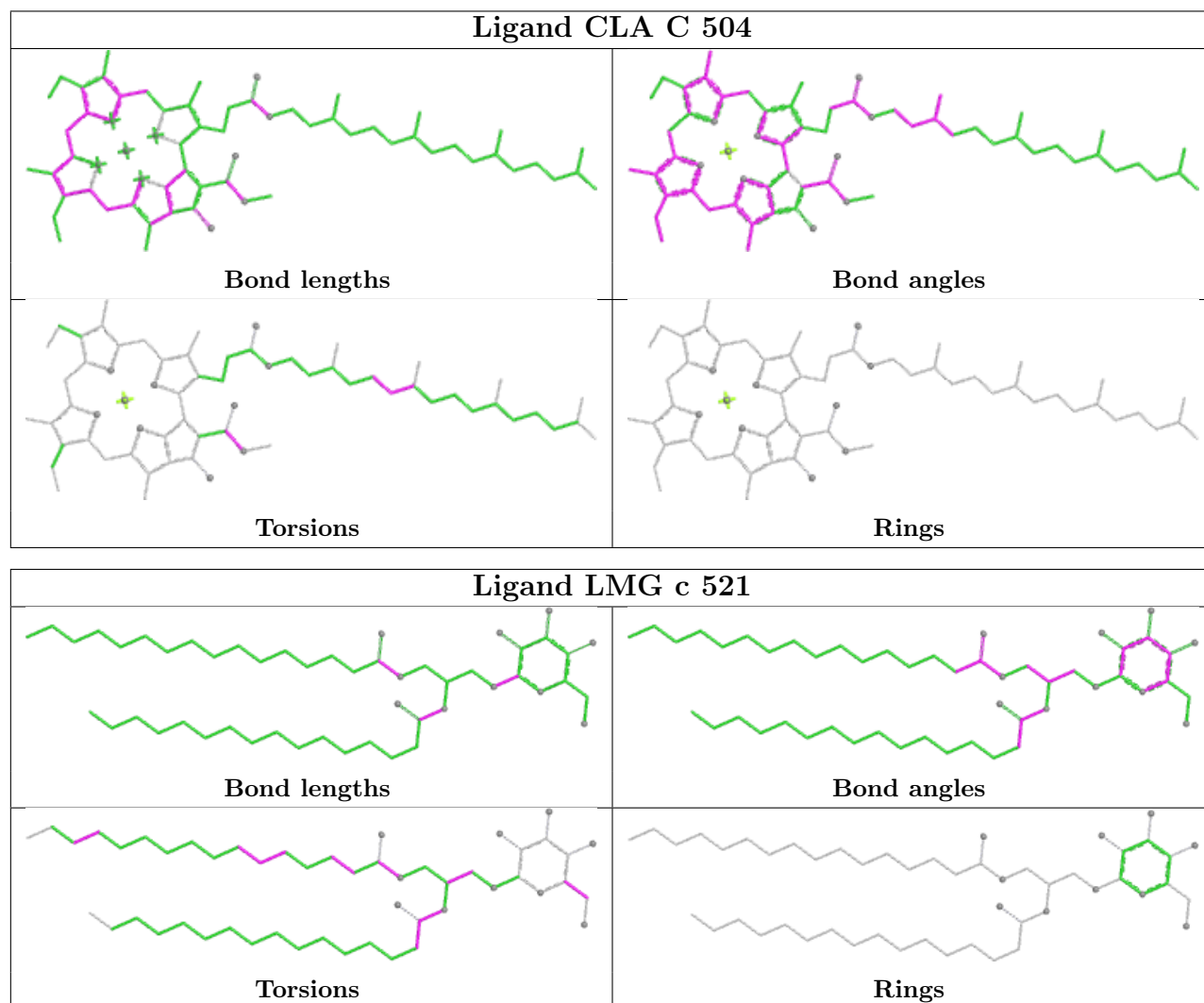
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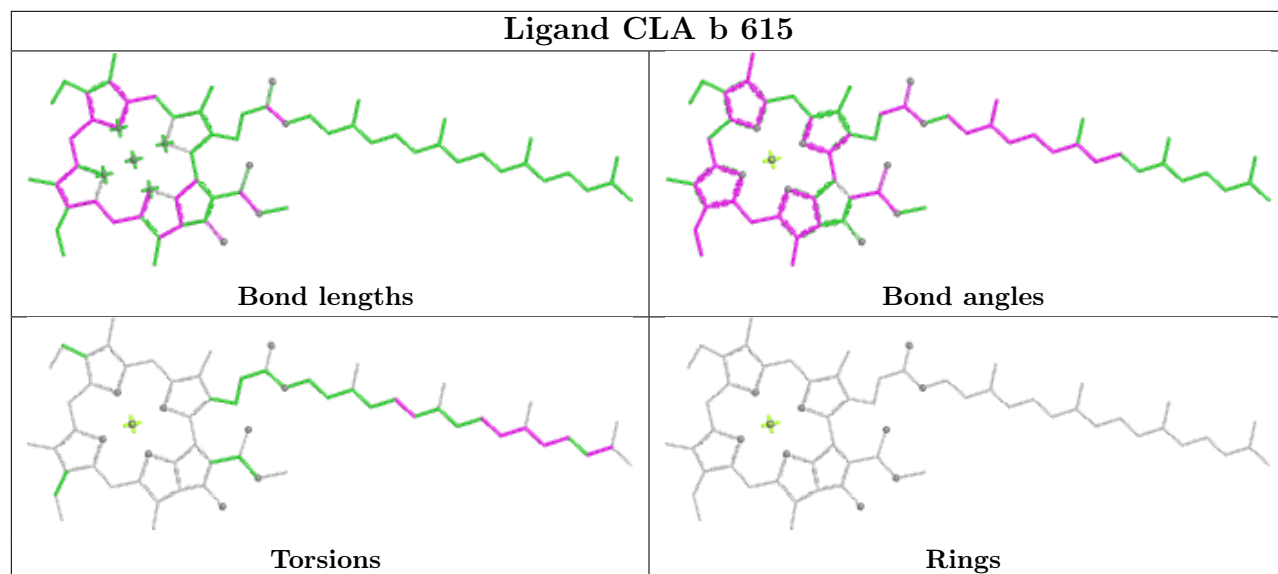
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 36  | C     | 519    | DGD  | 2       | 0            |
| 23  | B     | 602    | CLA  | 3       | 0            |
| 23  | C     | 507    | CLA  | 5       | 0            |
| 33  | D     | 706[B] | LHG  | 1       | 0            |
| 23  | A     | 406[B] | CLA  | 1       | 0            |
| 26  | a     | 411[A] | SQD  | 4       | 0            |
| 26  | a     | 412    | SQD  | 2       | 0            |
| 27  | O     | 303    | GOL  | 3       | 0            |
| 33  | d     | 412[B] | LHG  | 2       | 0            |
| 36  | C     | 517[A] | DGD  | 2       | 0            |
| 26  | A     | 410[A] | SQD  | 2       | 0            |
| 23  | C     | 511    | CLA  | 5       | 0            |
| 23  | b     | 602    | CLA  | 1       | 0            |
| 25  | d     | 403    | BCR  | 3       | 0            |
| 23  | a     | 407[B] | CLA  | 3       | 0            |
| 23  | a     | 405[A] | CLA  | 3       | 0            |
| 36  | c     | 517[A] | DGD  | 2       | 0            |
| 27  | O     | 302    | GOL  | 1       | 0            |
| 23  | c     | 507    | CLA  | 3       | 0            |
| 23  | c     | 502    | CLA  | 2       | 0            |
| 23  | C     | 513    | CLA  | 2       | 0            |
| 25  | a     | 410    | BCR  | 1       | 0            |
| 27  | a     | 419    | GOL  | 3       | 0            |
| 23  | b     | 612    | CLA  | 3       | 0            |
| 24  | a     | 408[B] | PHO  | 1       | 0            |
| 24  | A     | 407[B] | PHO  | 1       | 0            |
| 35  | b     | 625    | HTG  | 1       | 0            |
| 23  | B     | 615    | CLA  | 7       | 0            |
| 36  | c     | 518[A] | DGD  | 2       | 0            |
| 23  | c     | 509    | CLA  | 9       | 0            |
| 27  | B     | 623    | GOL  | 2       | 0            |
| 36  | C     | 518[A] | DGD  | 2       | 0            |
| 23  | b     | 609    | CLA  | 5       | 0            |
| 23  | a     | 409    | CLA  | 4       | 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

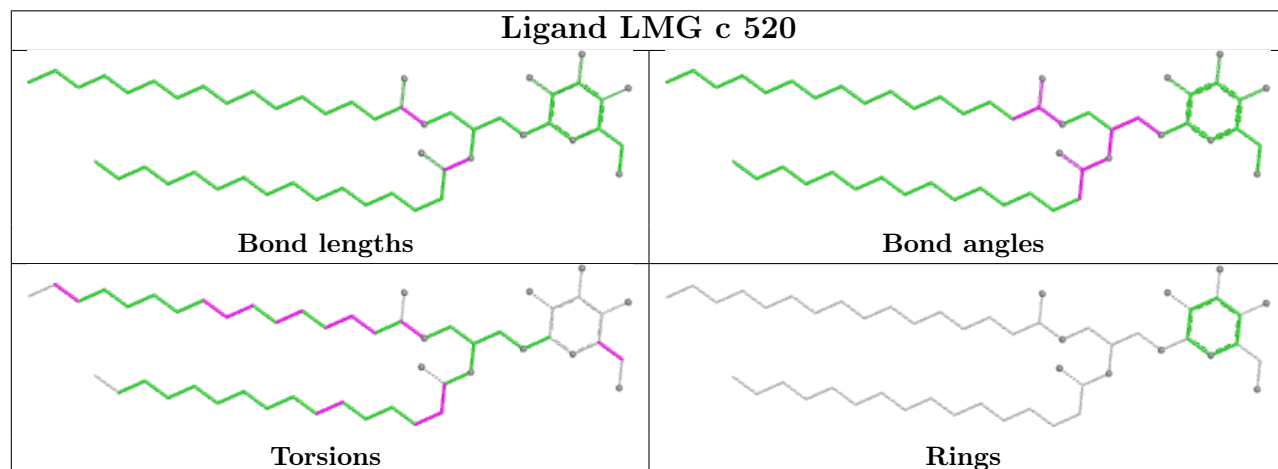
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

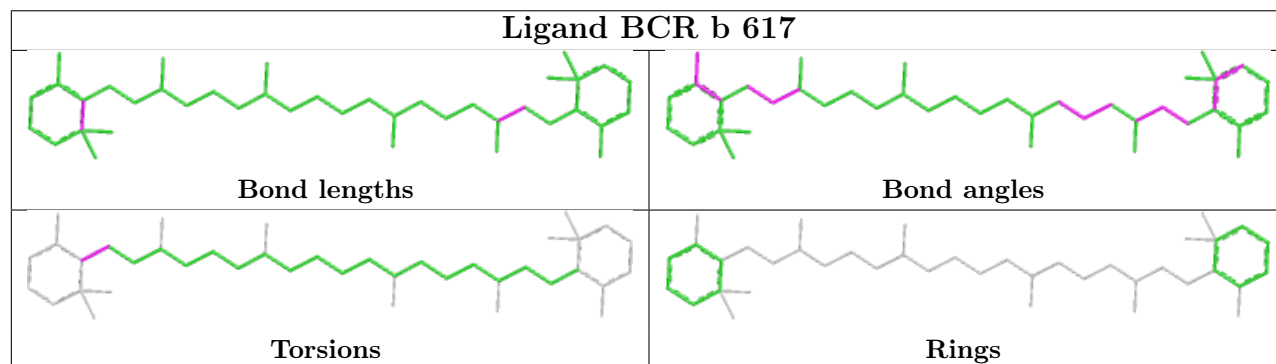
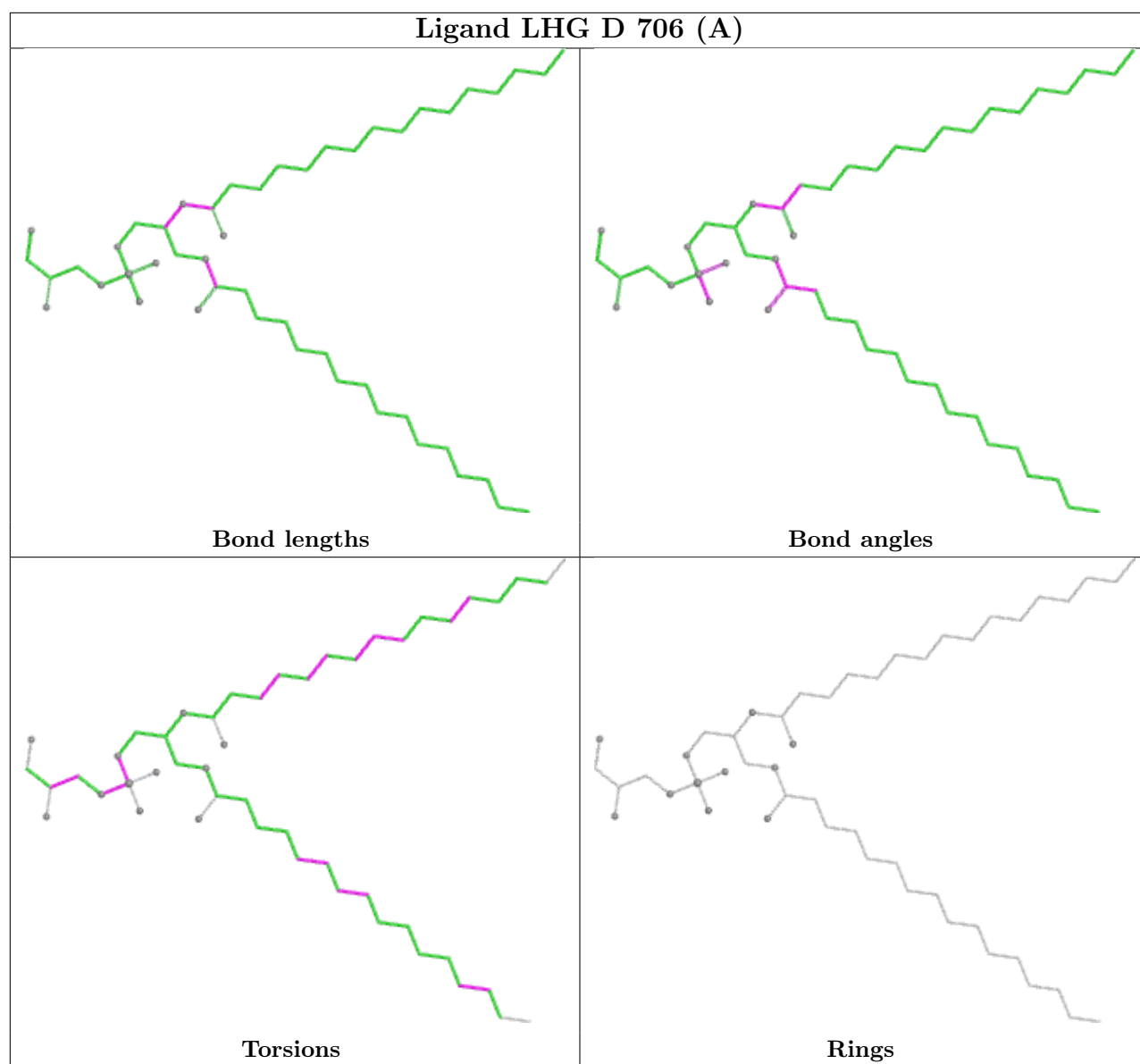


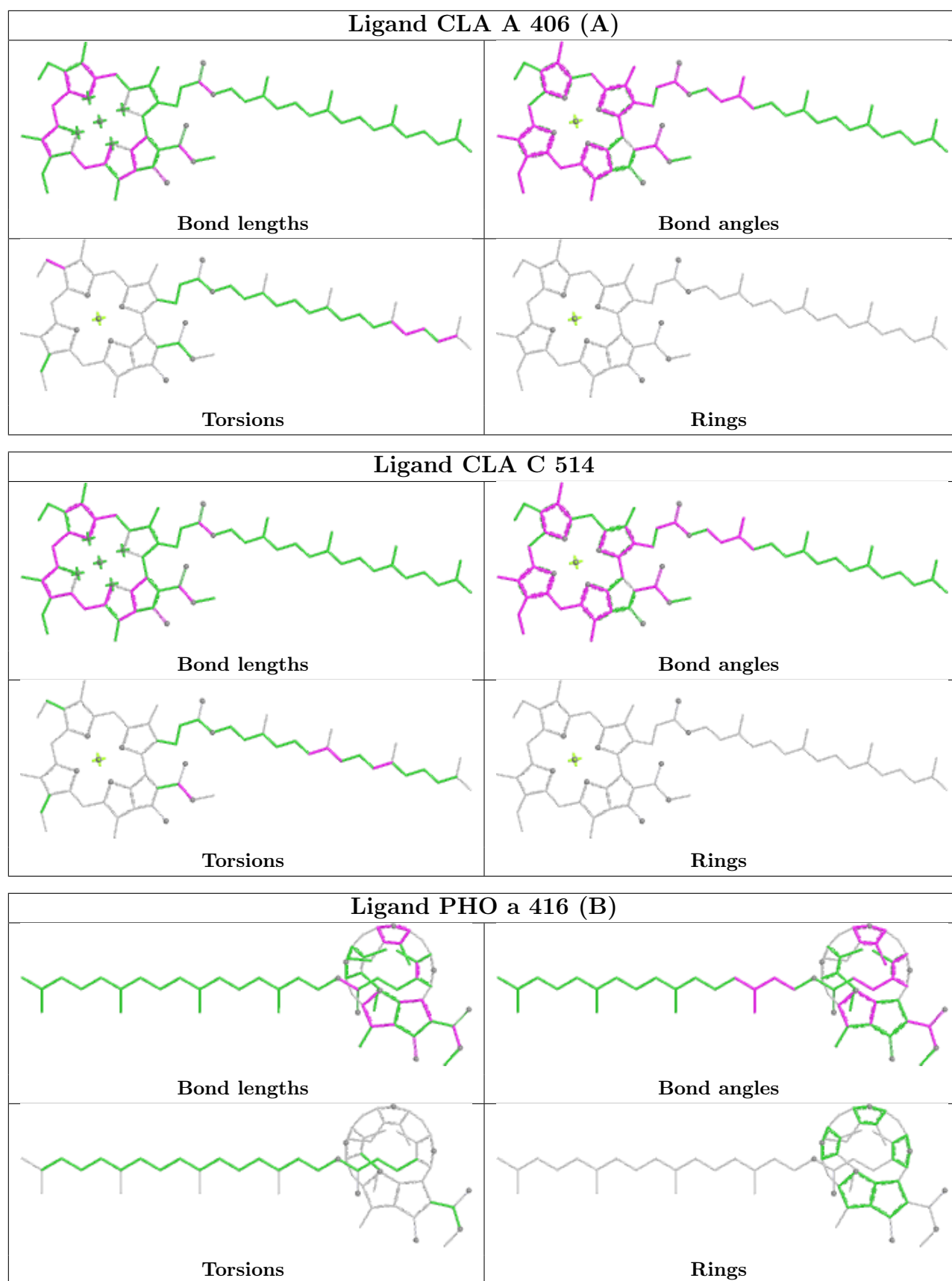
## Ligand CLA b 615

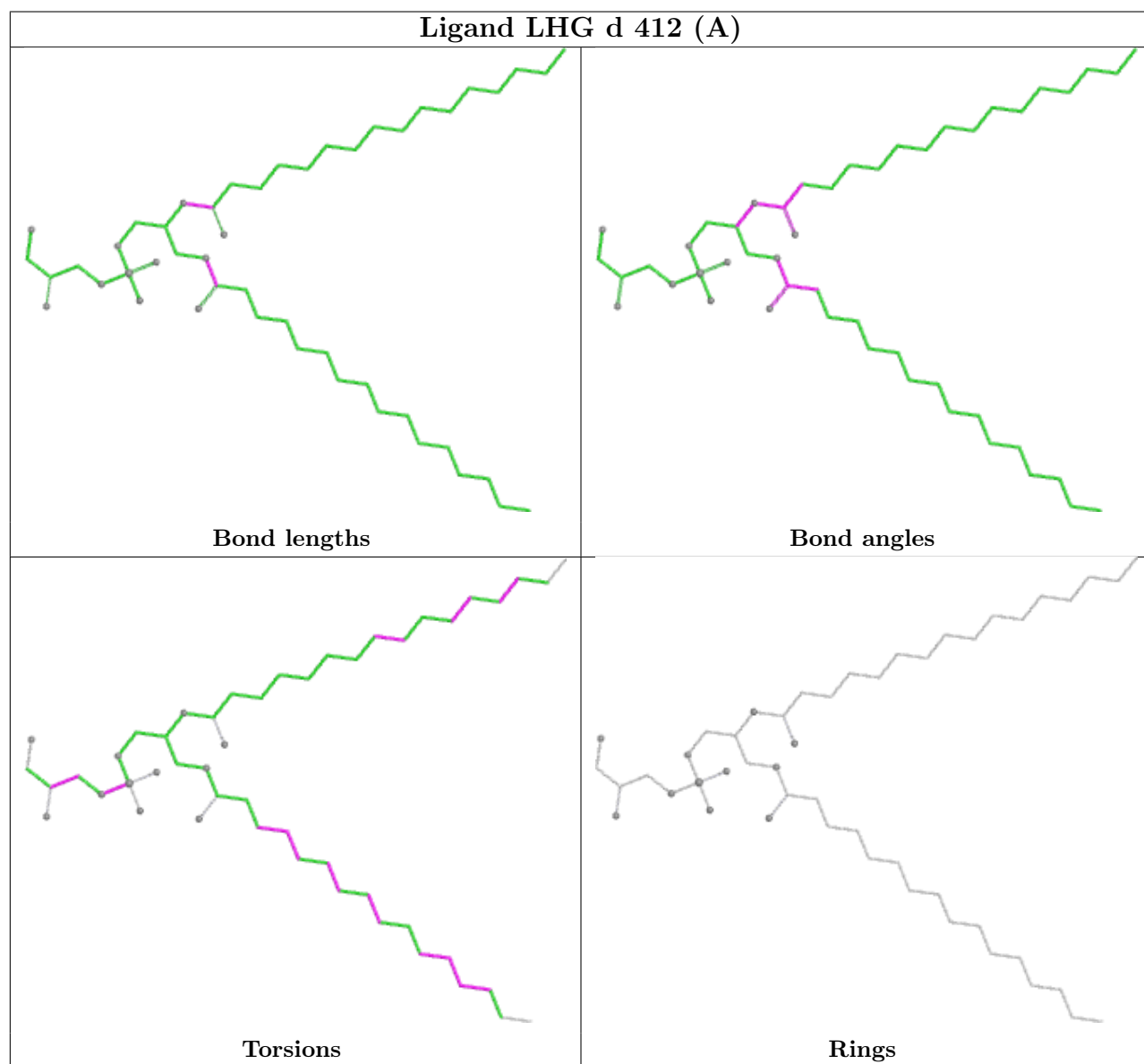
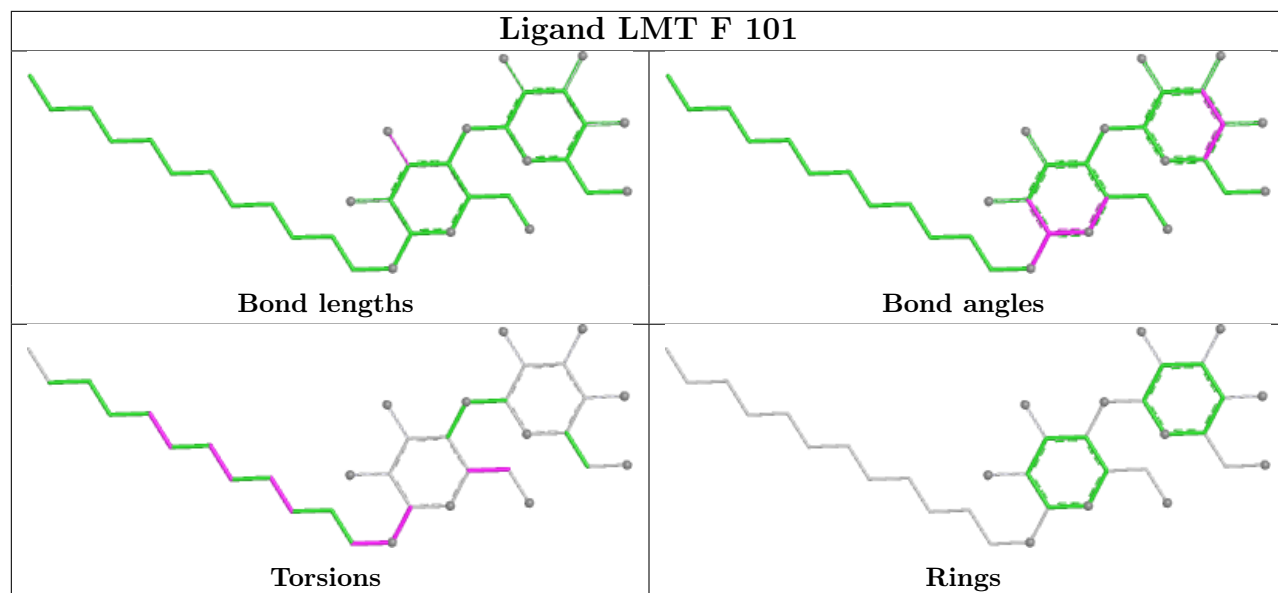


## Ligand LMG c 520

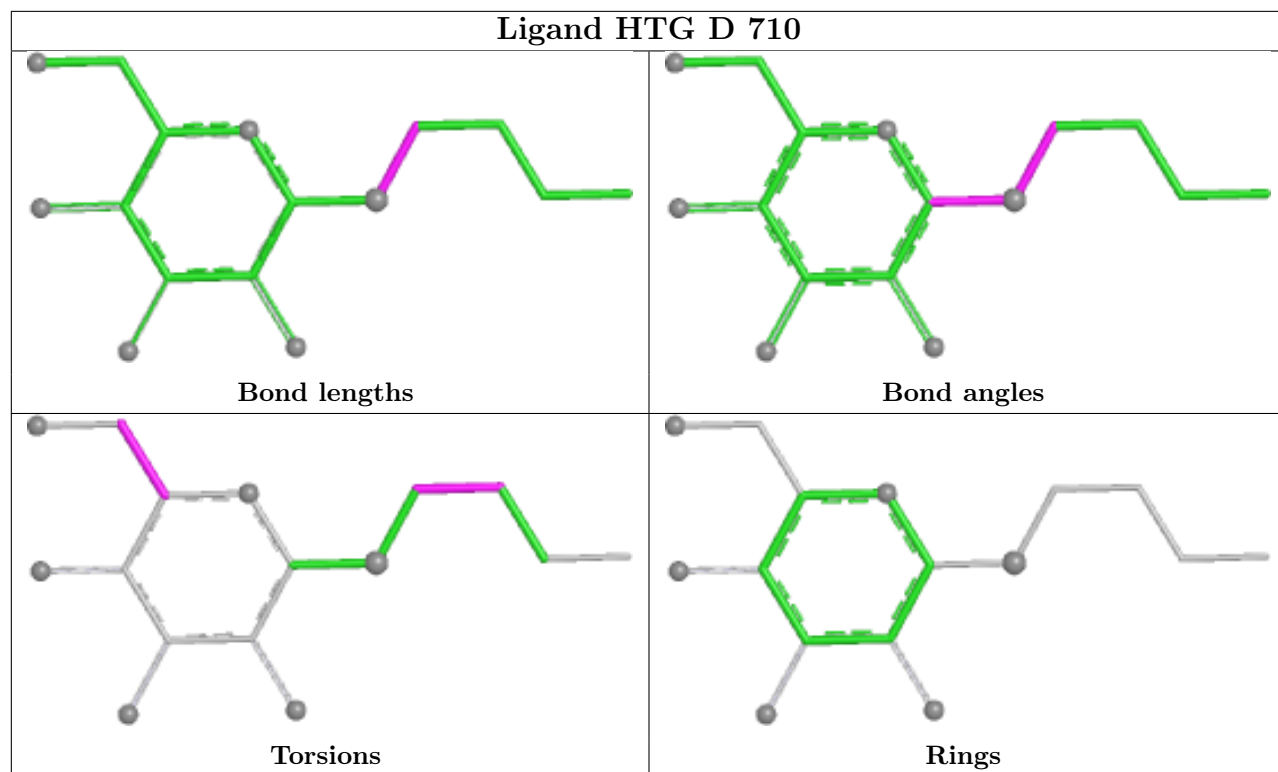




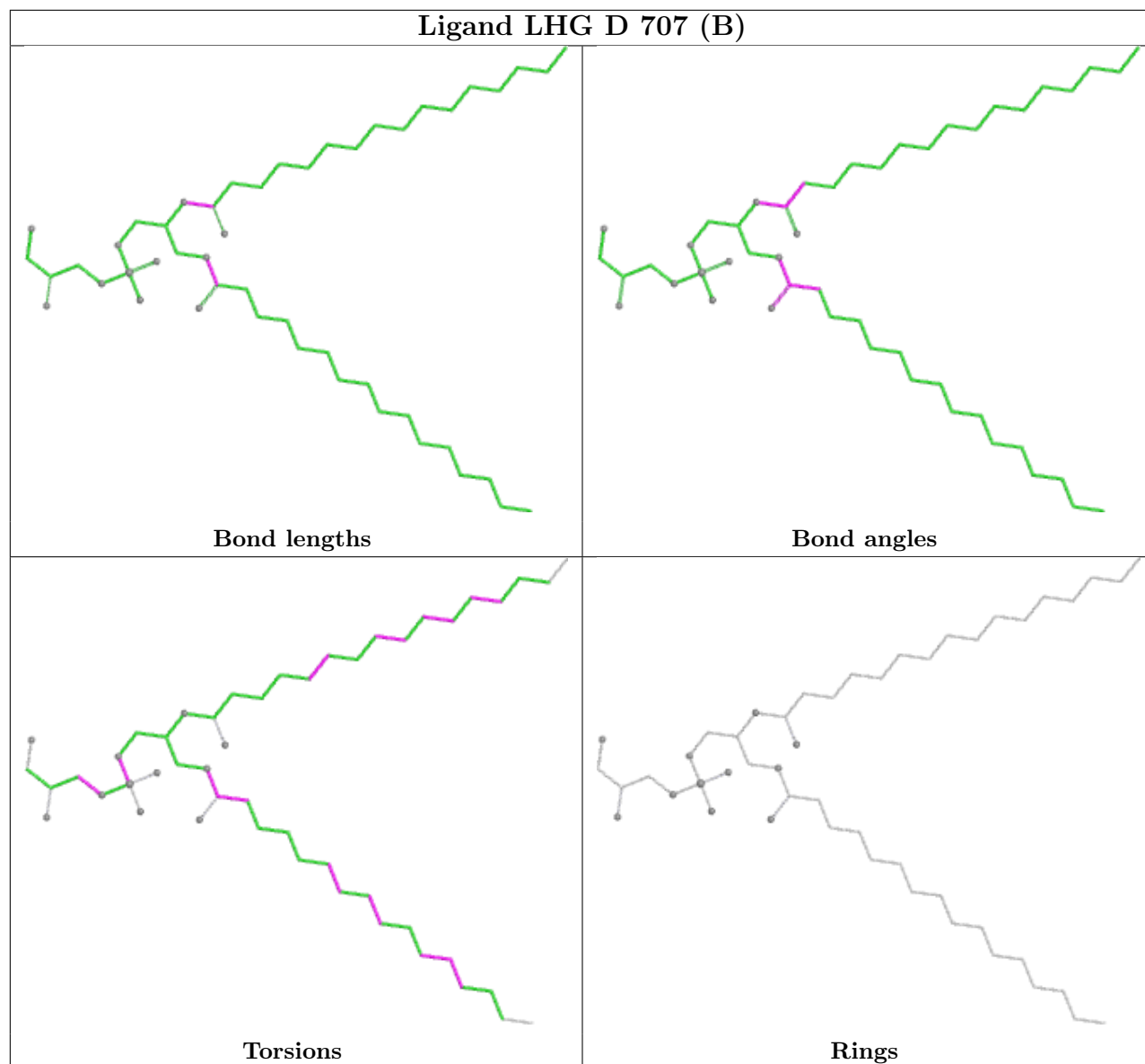




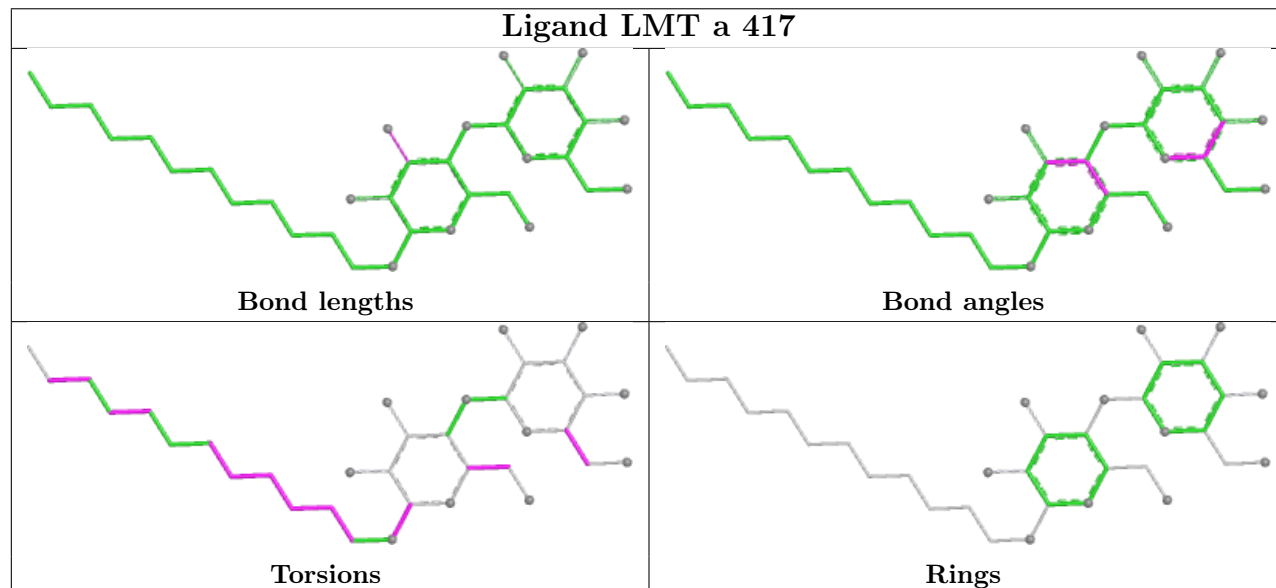




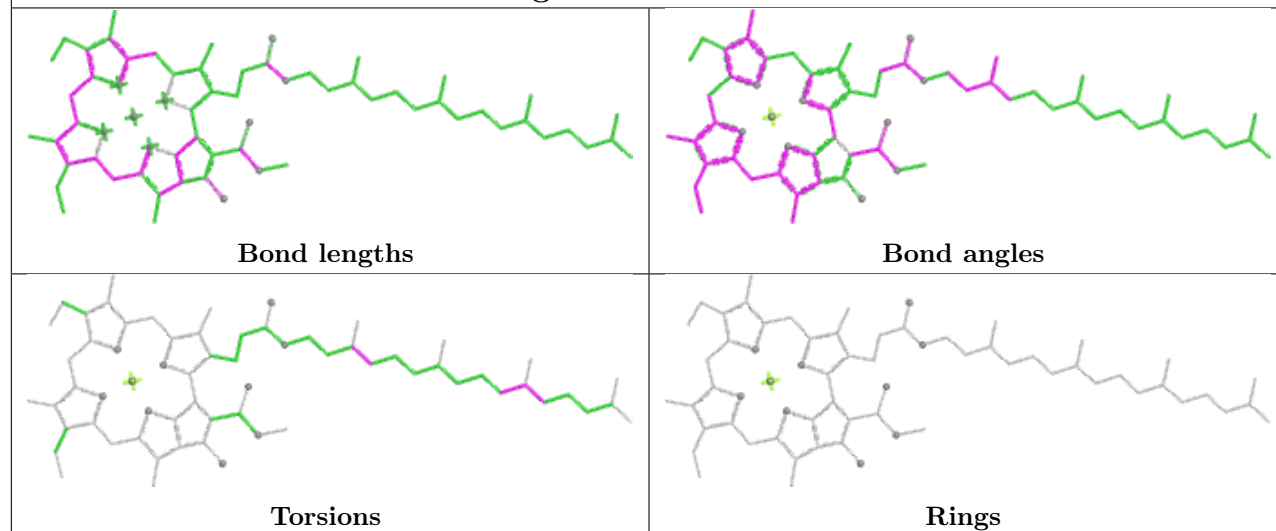
## Ligand LHG D 707 (B)



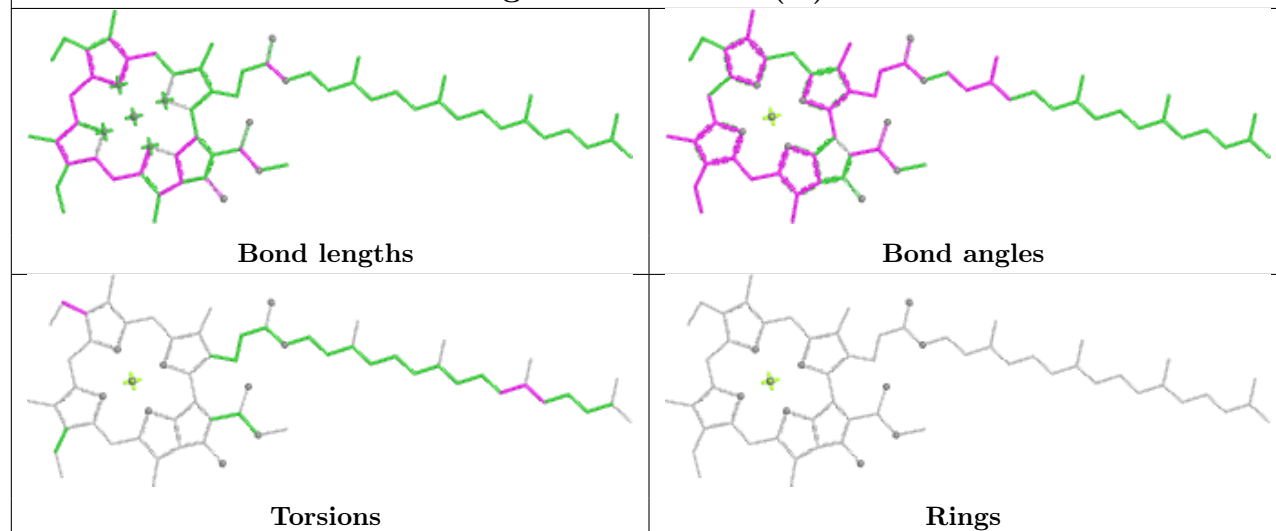
## Ligand LMT a 417



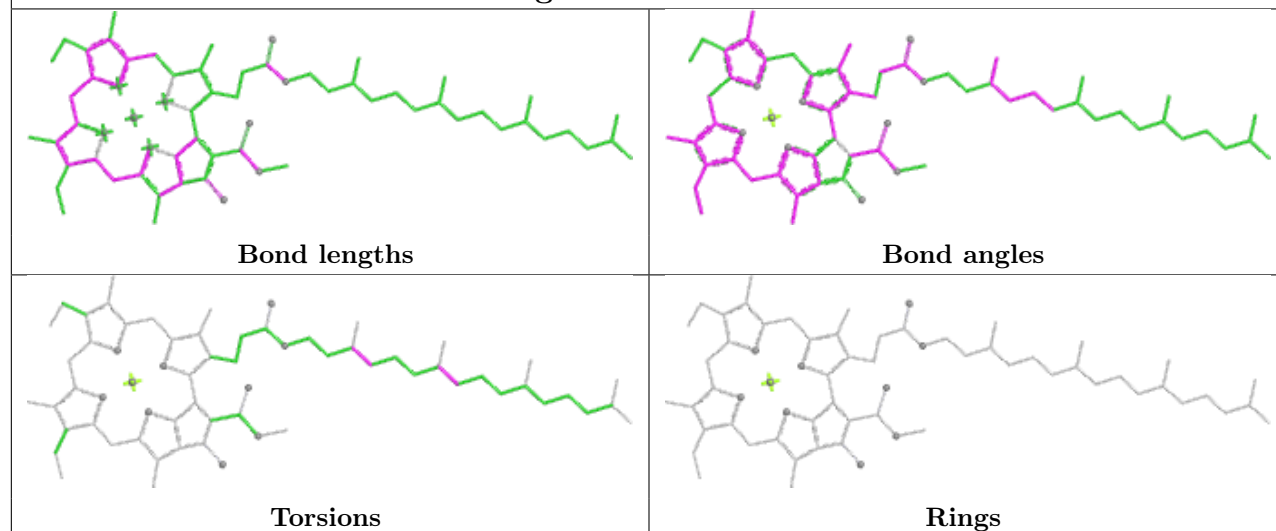
## Ligand CLA C 506



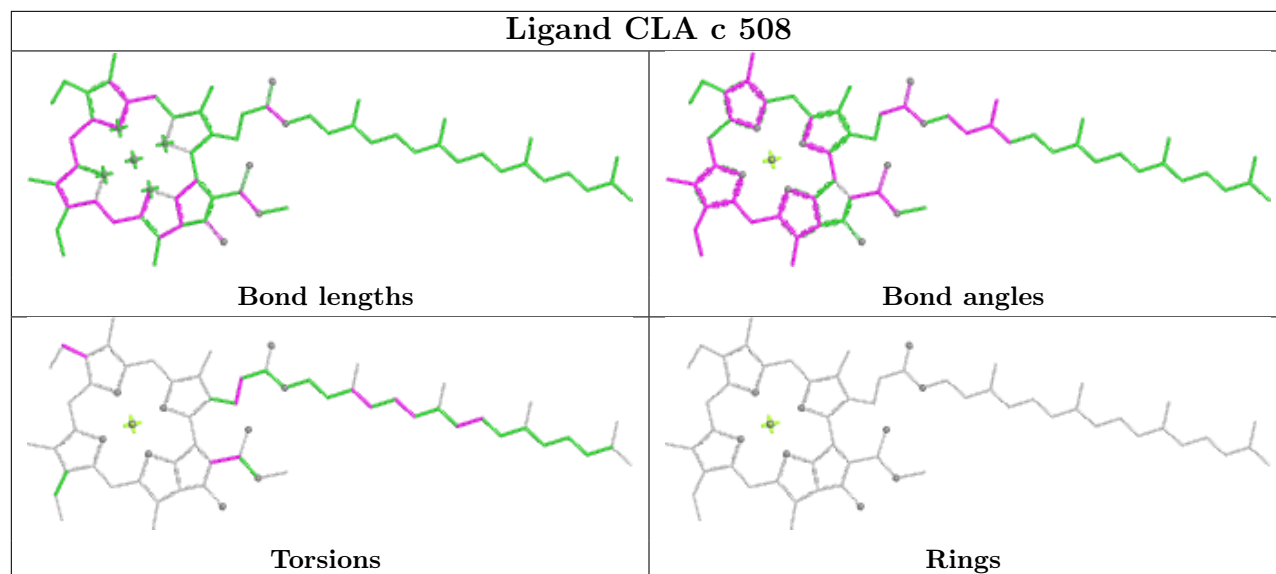
## Ligand CLA a 407 (A)



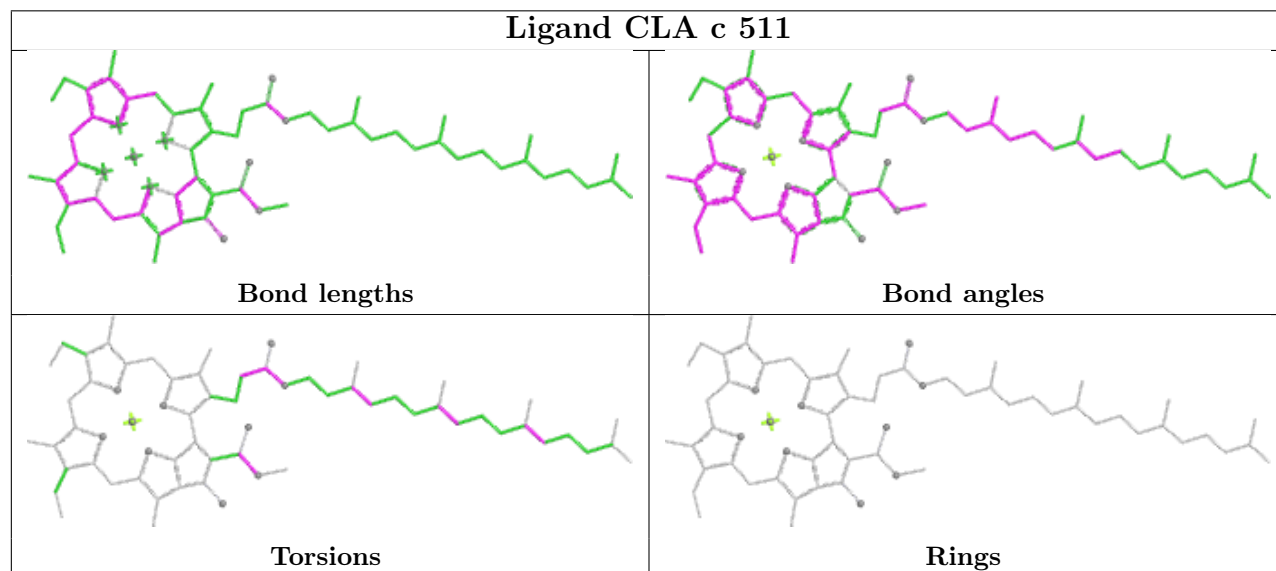
## Ligand CLA b 603



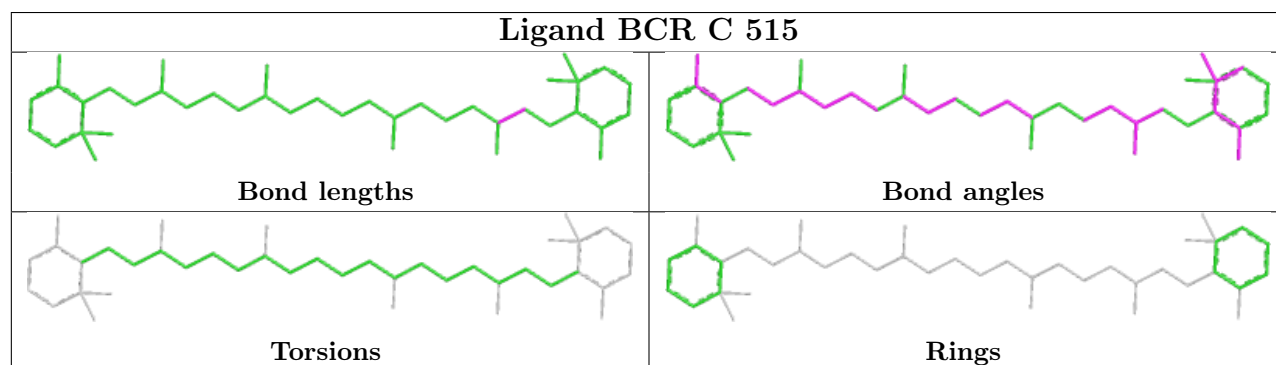
## Ligand CLA c 508

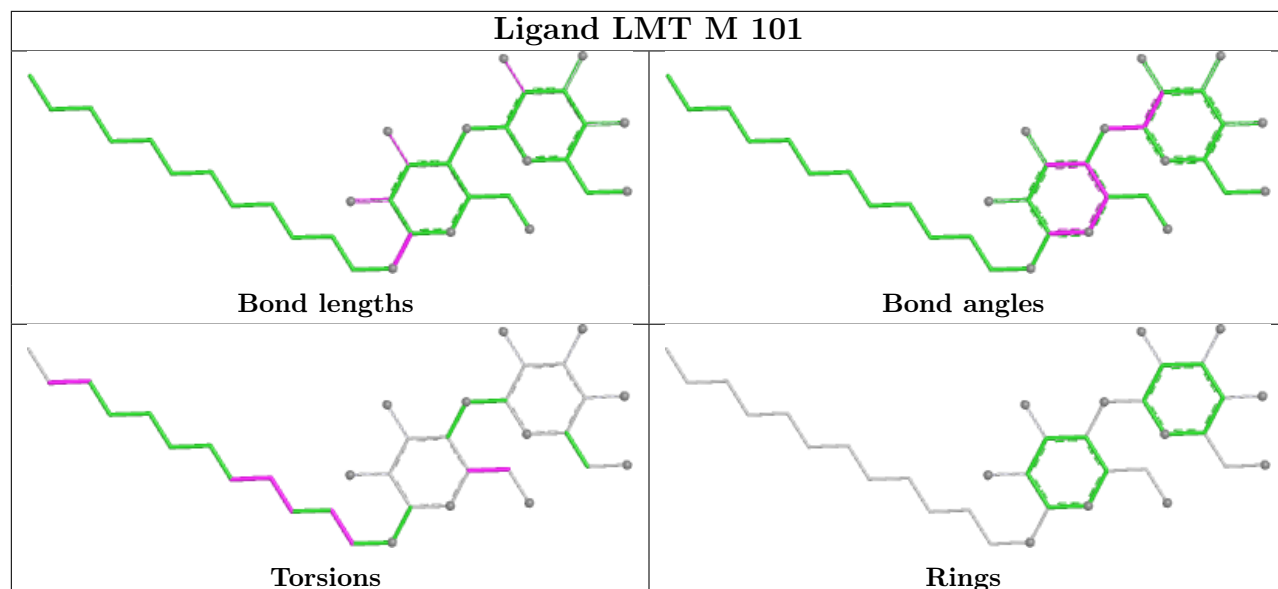
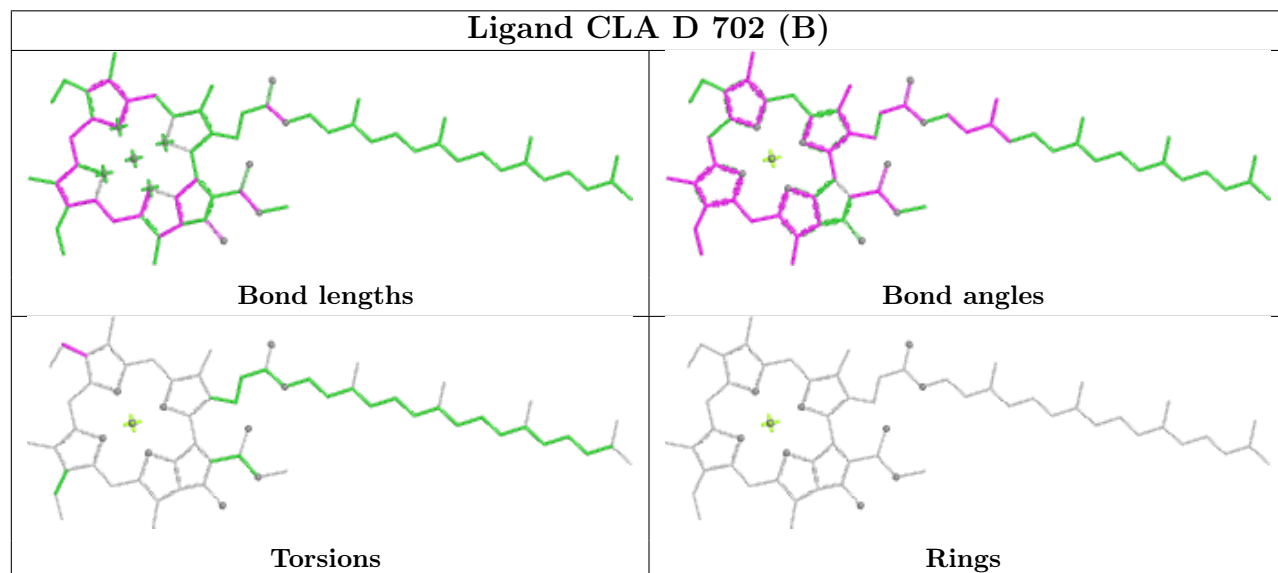
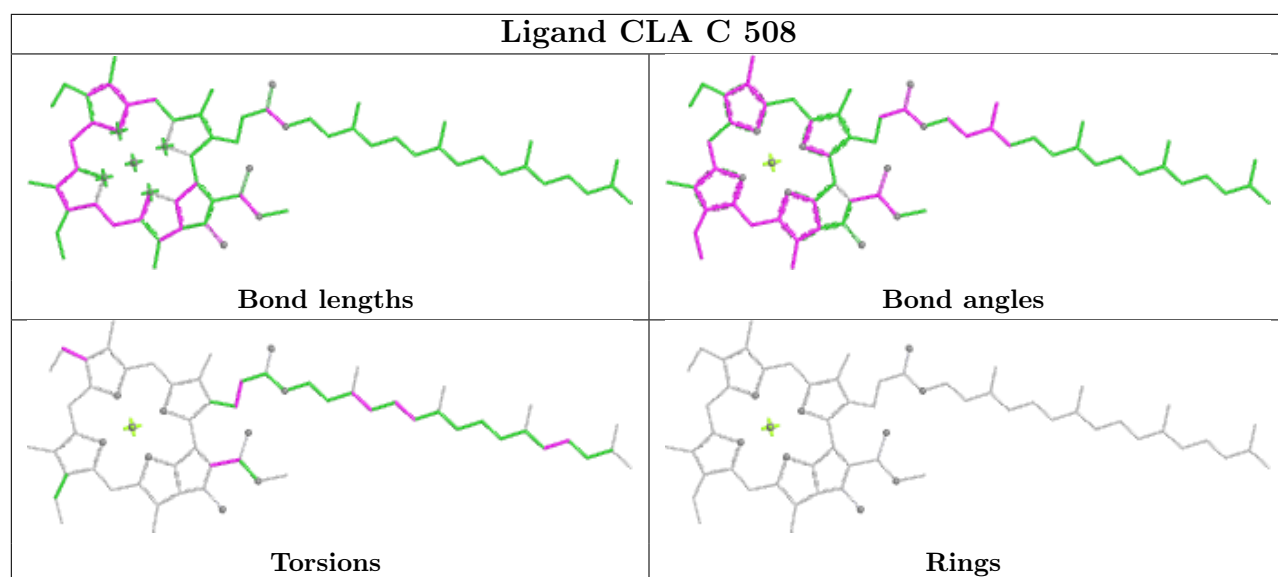


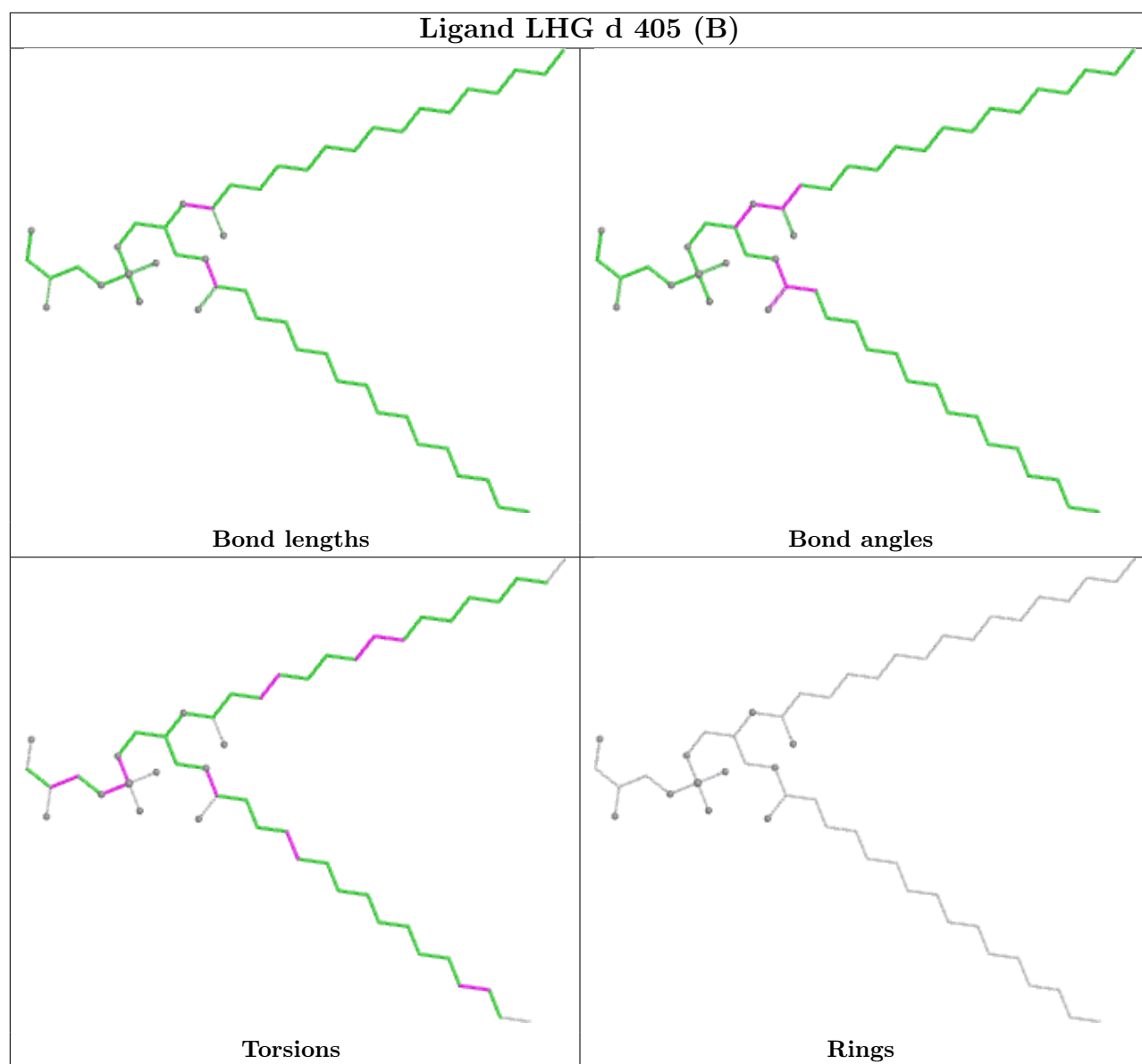
## Ligand CLA c 511

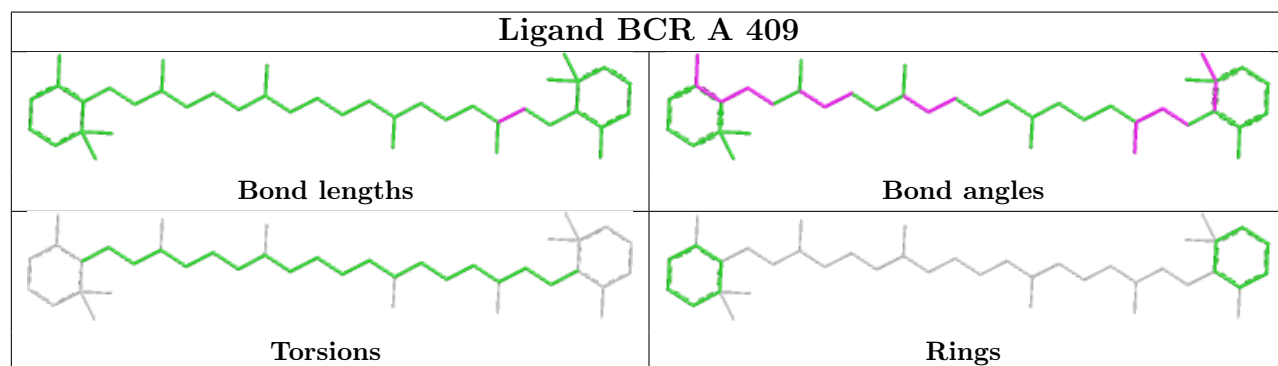
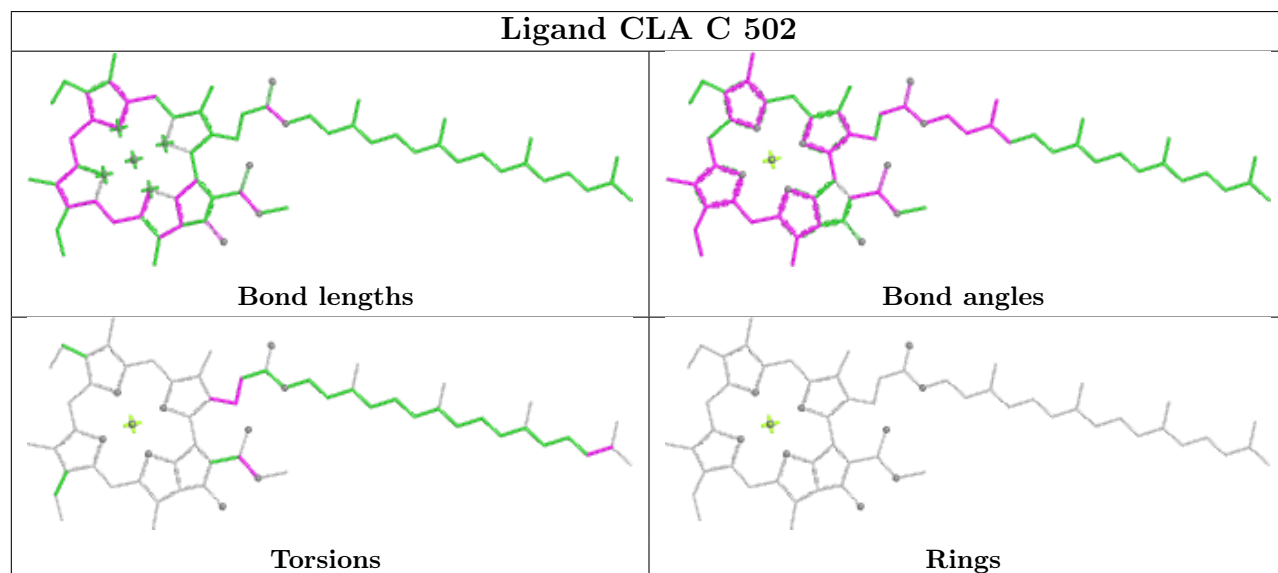
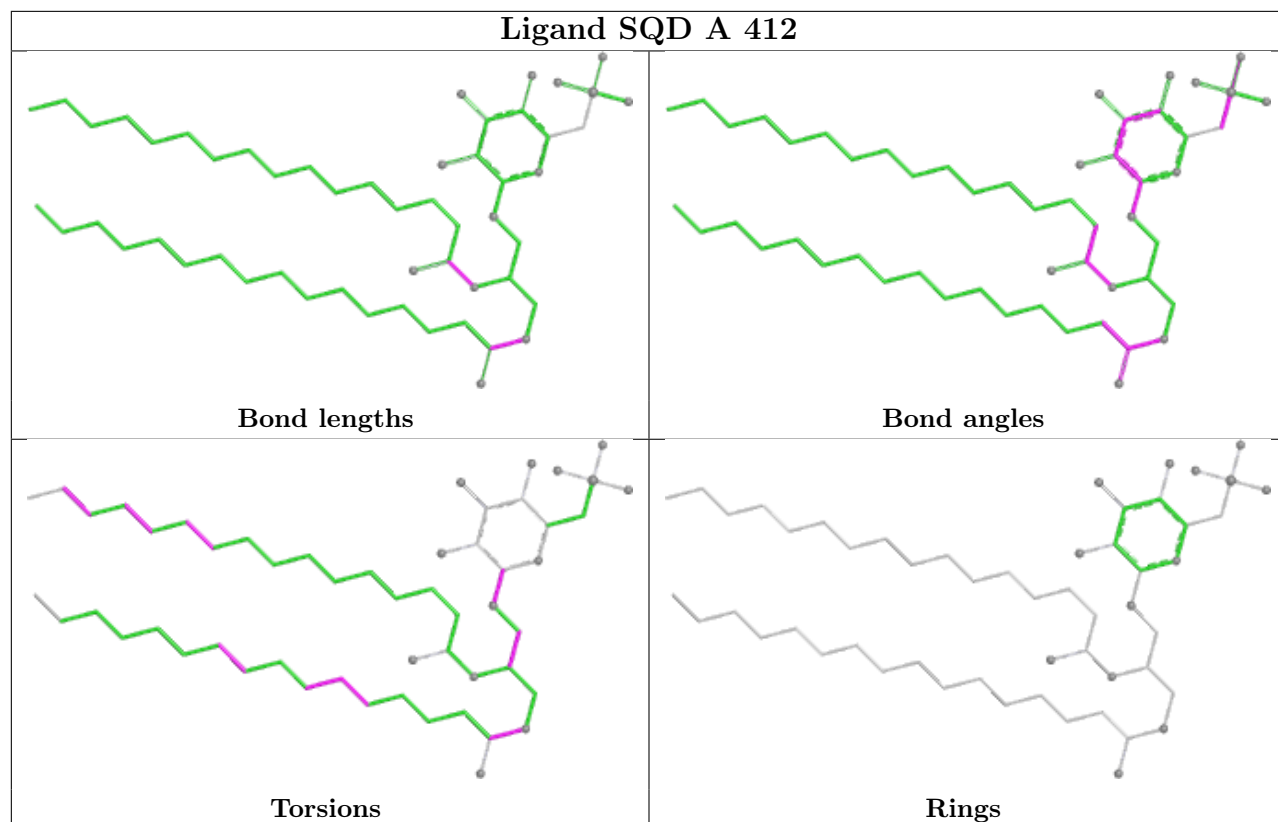


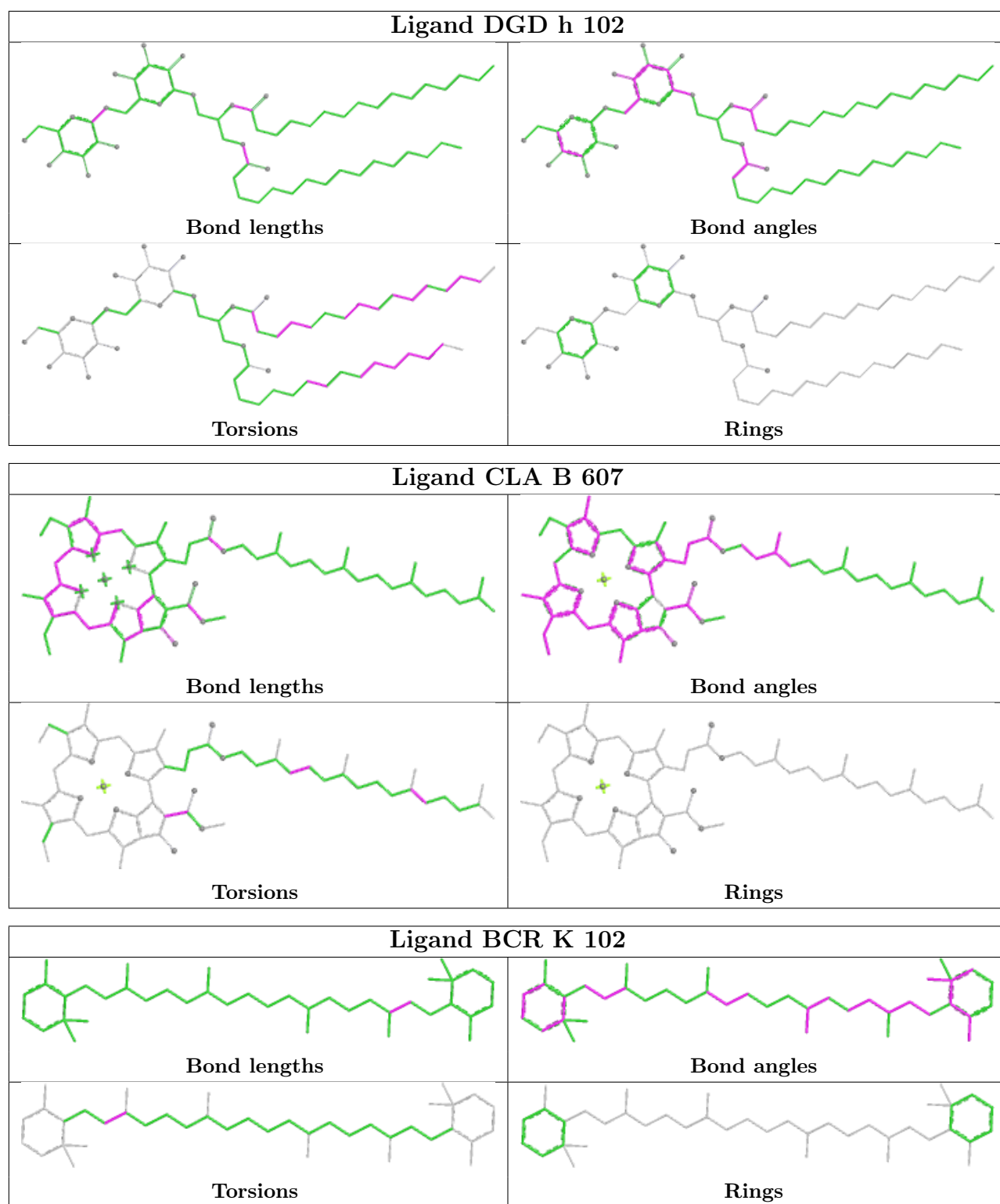
## Ligand BCR C 515



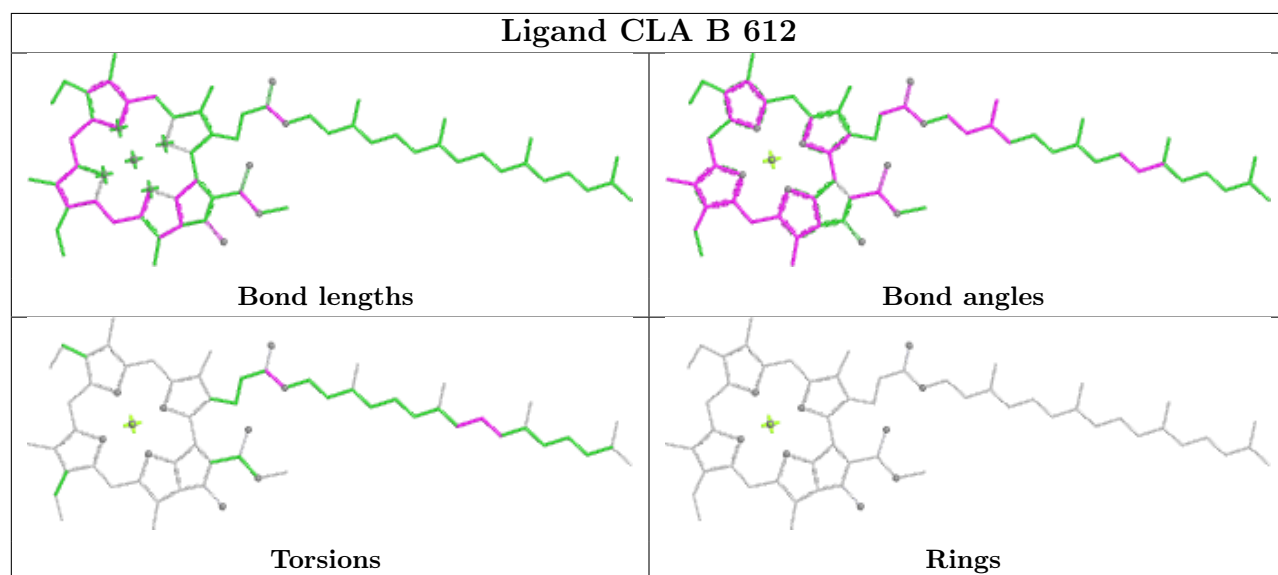
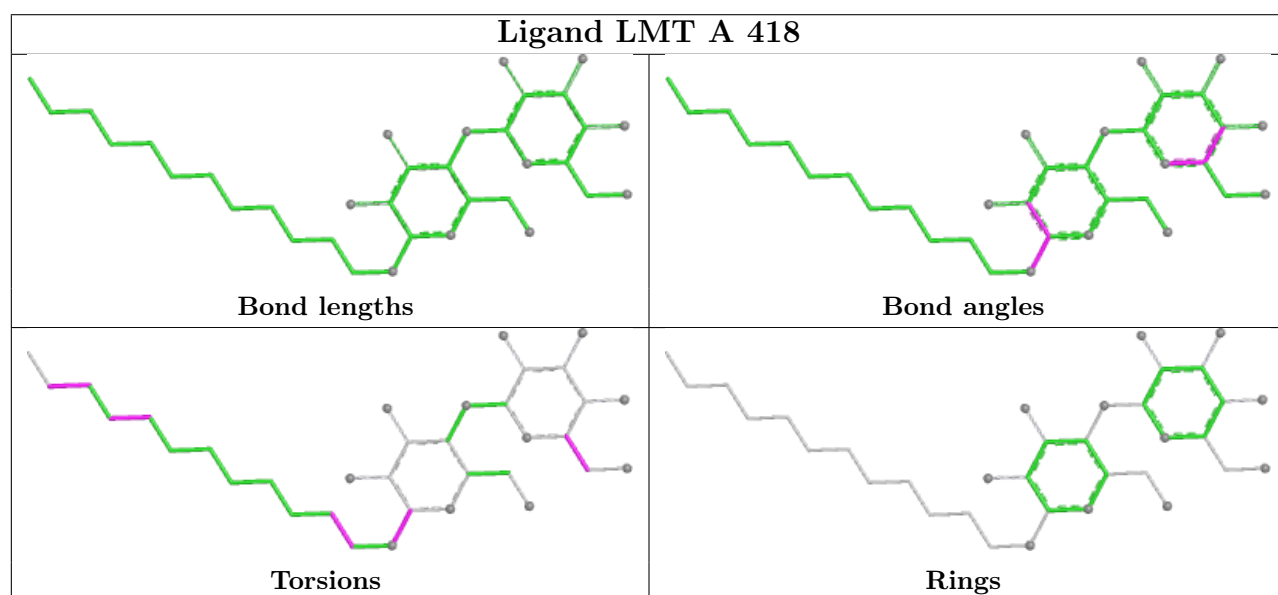
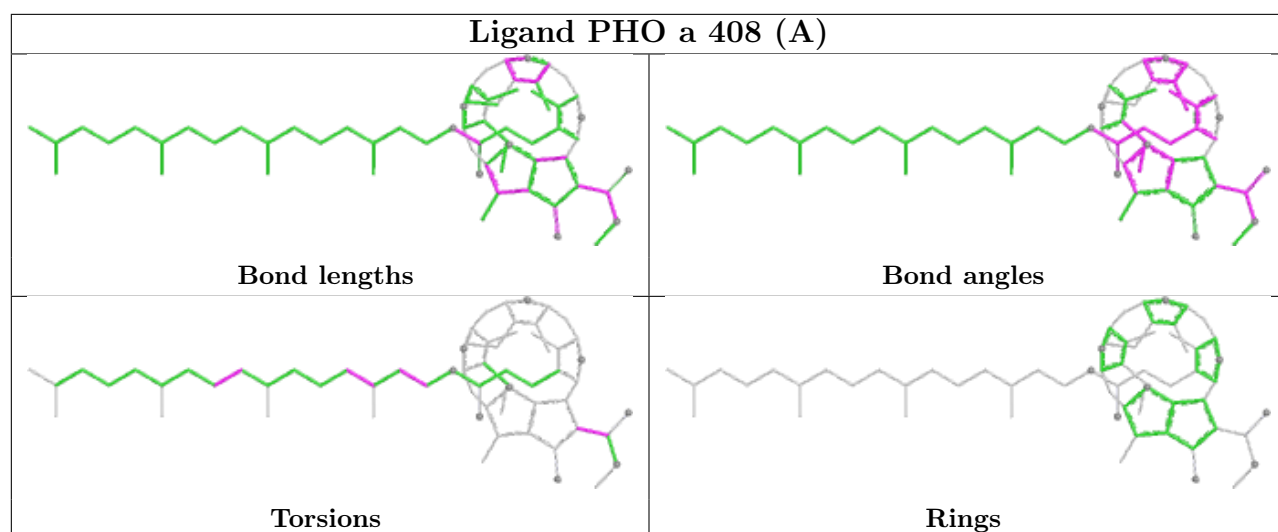




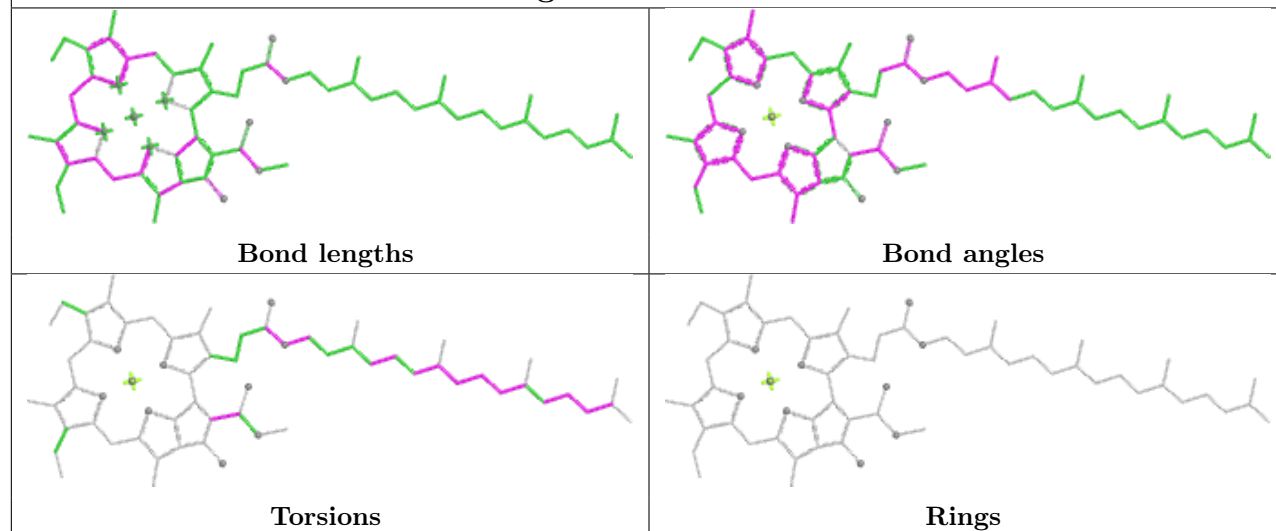




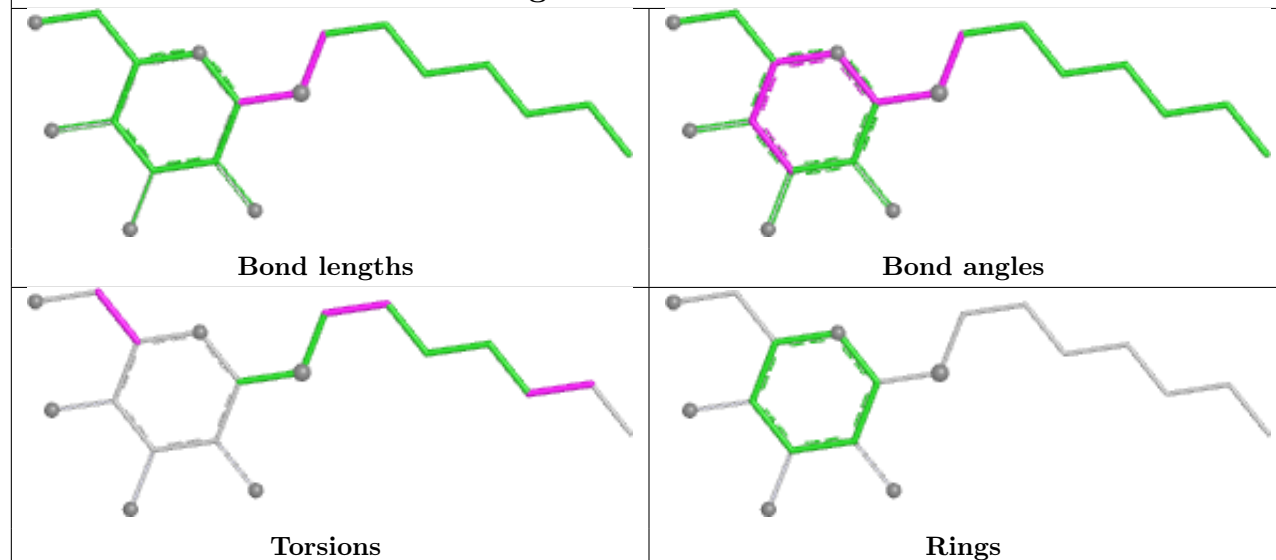




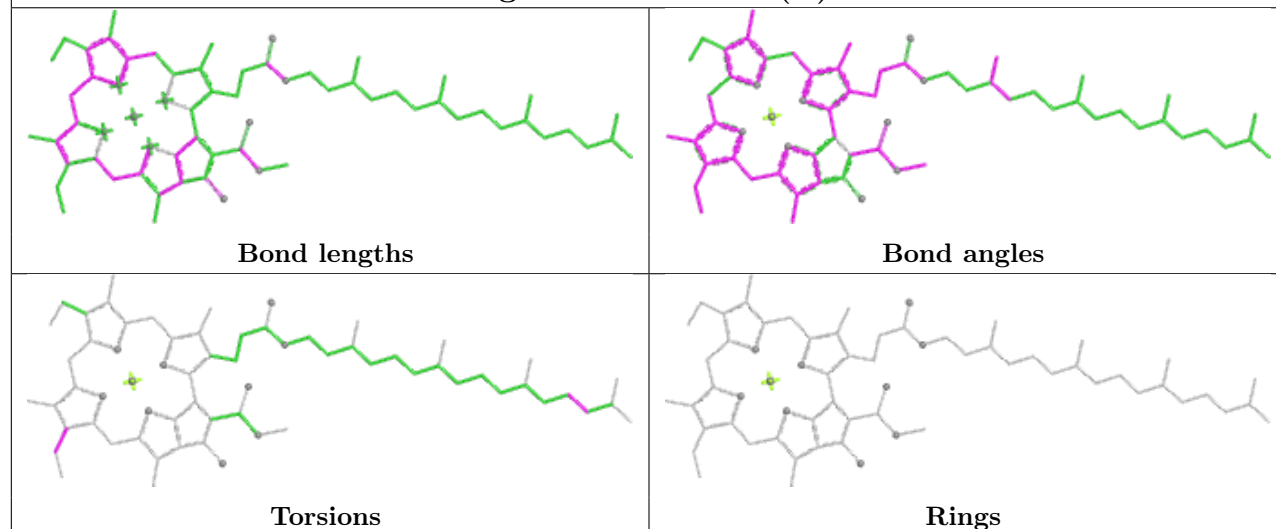
## Ligand CLA c 510

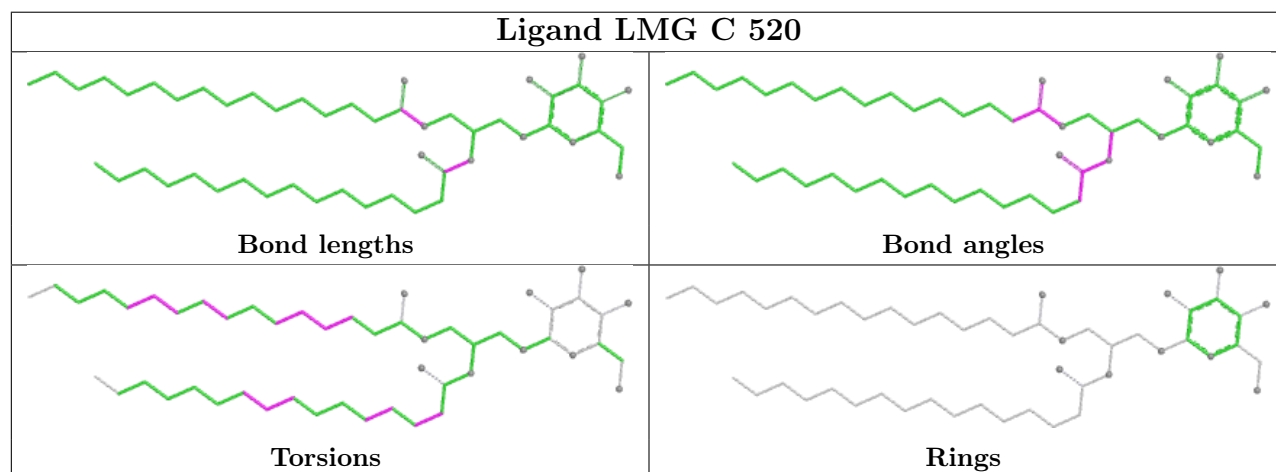
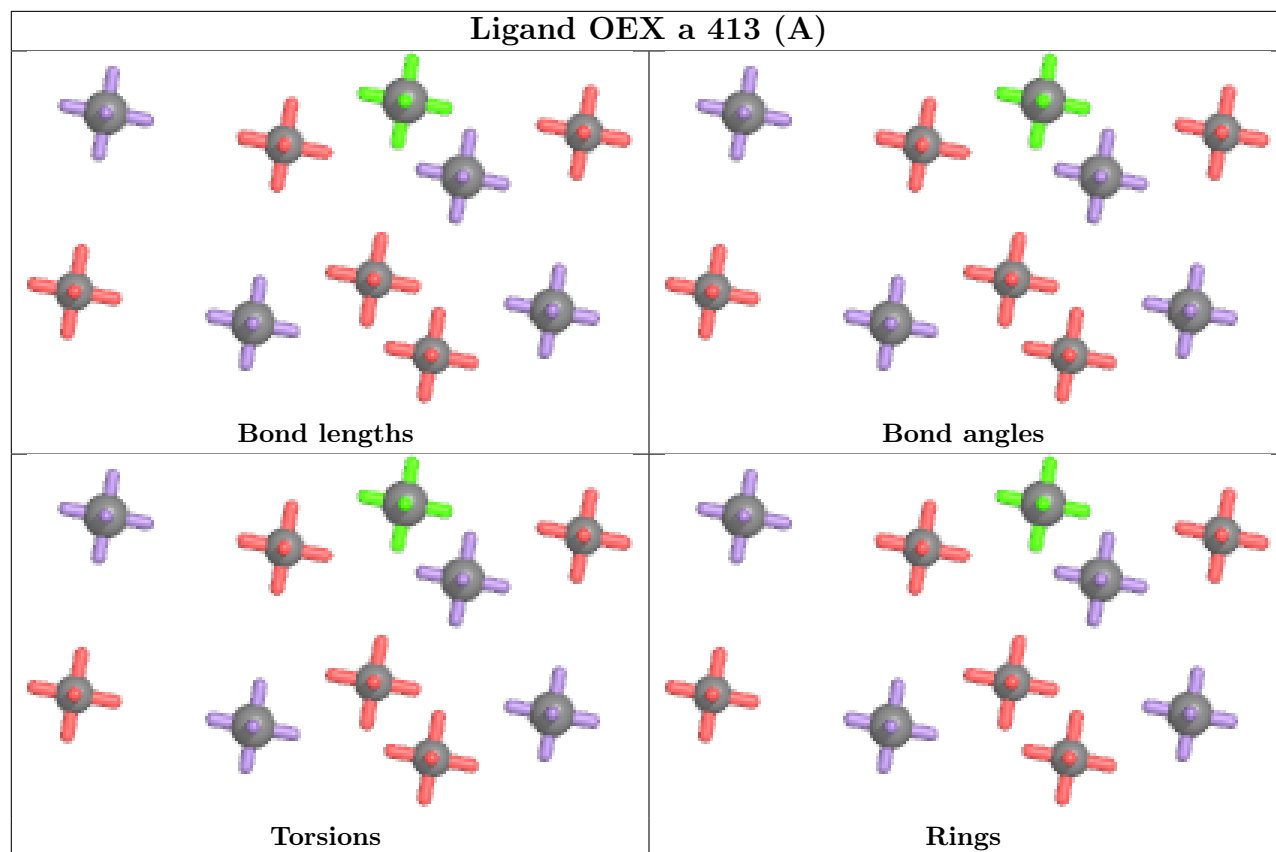


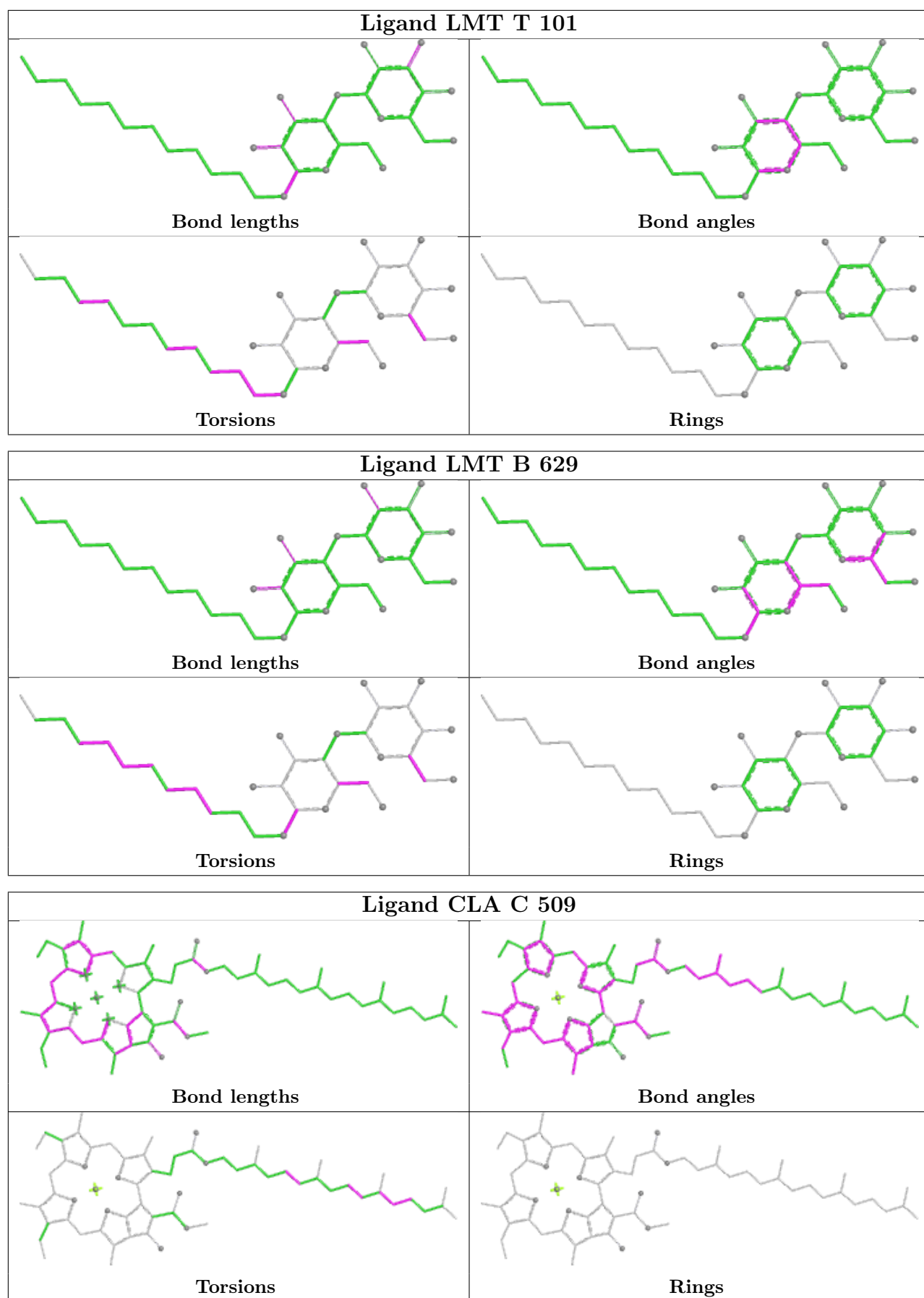
## Ligand HTG B 624

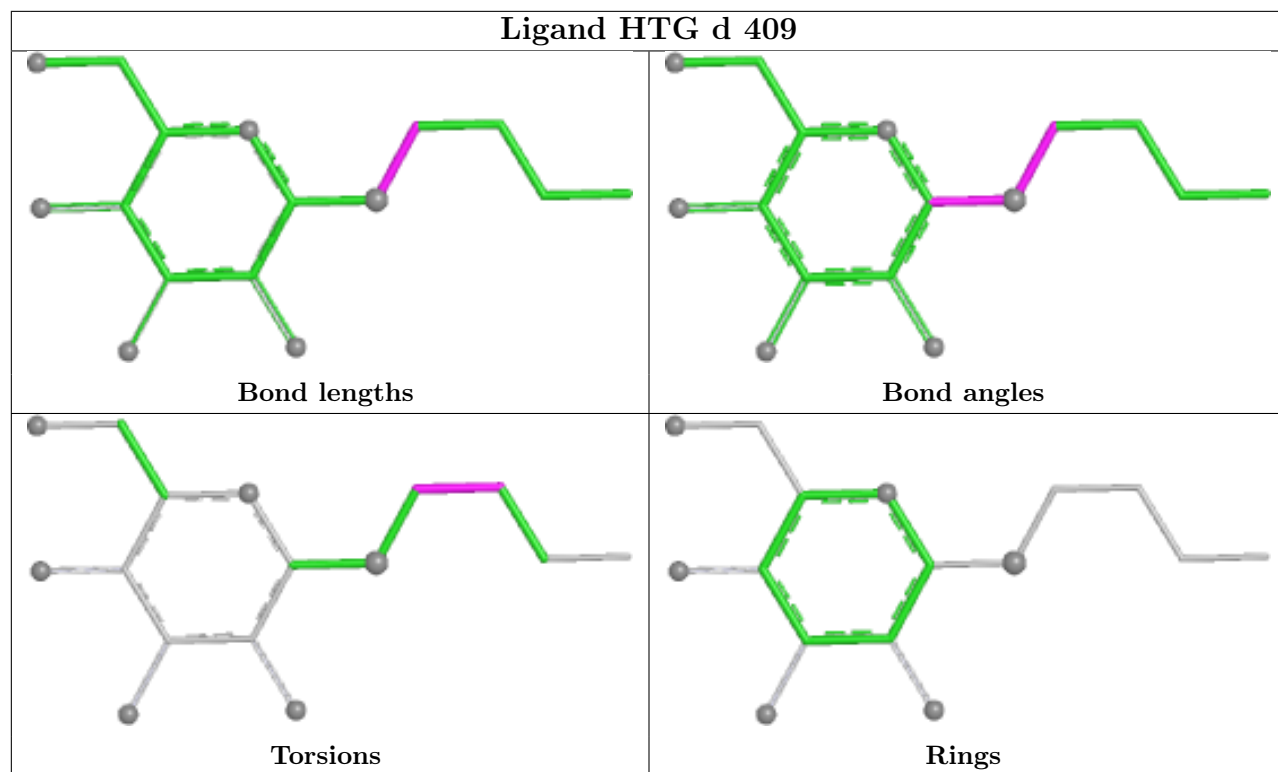


## Ligand CLA A 405 (B)

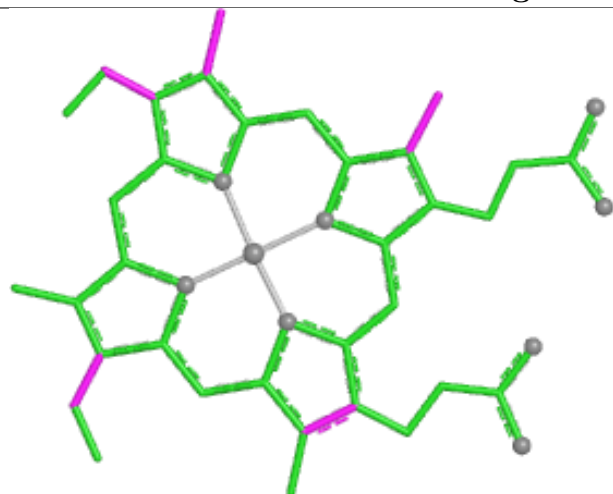




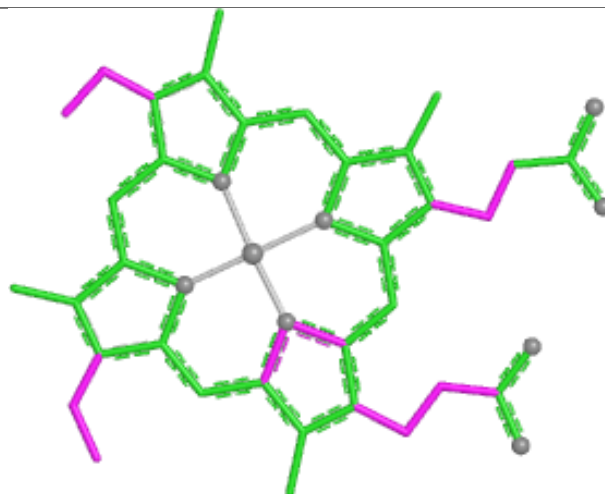




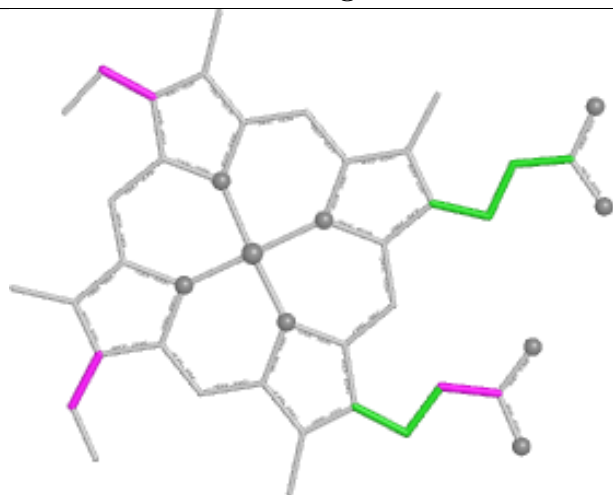
## Ligand HEC V 201



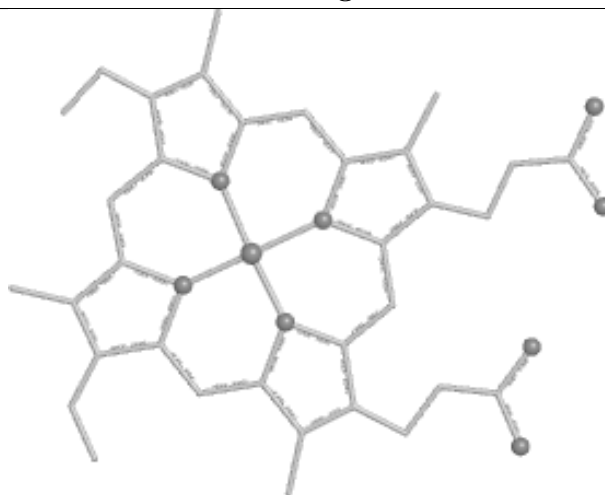
Bond lengths



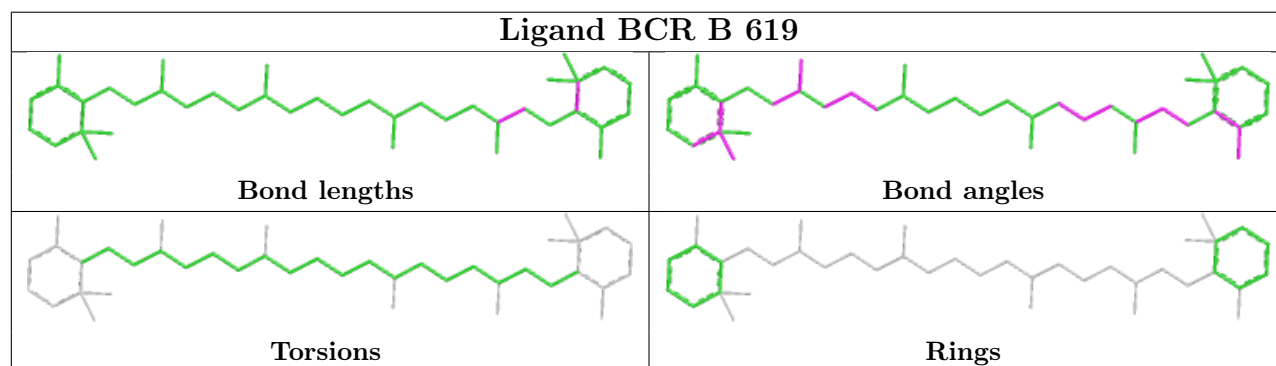
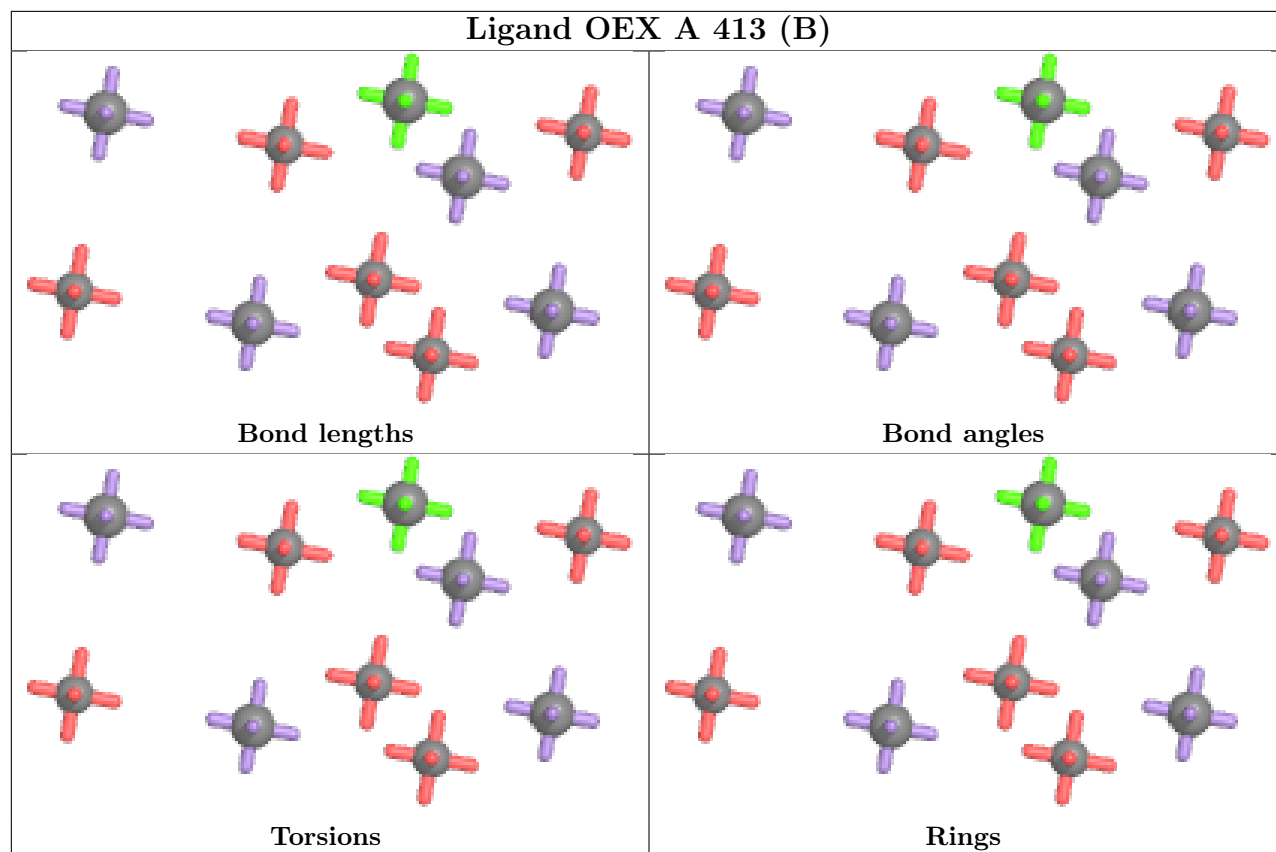
Bond angles

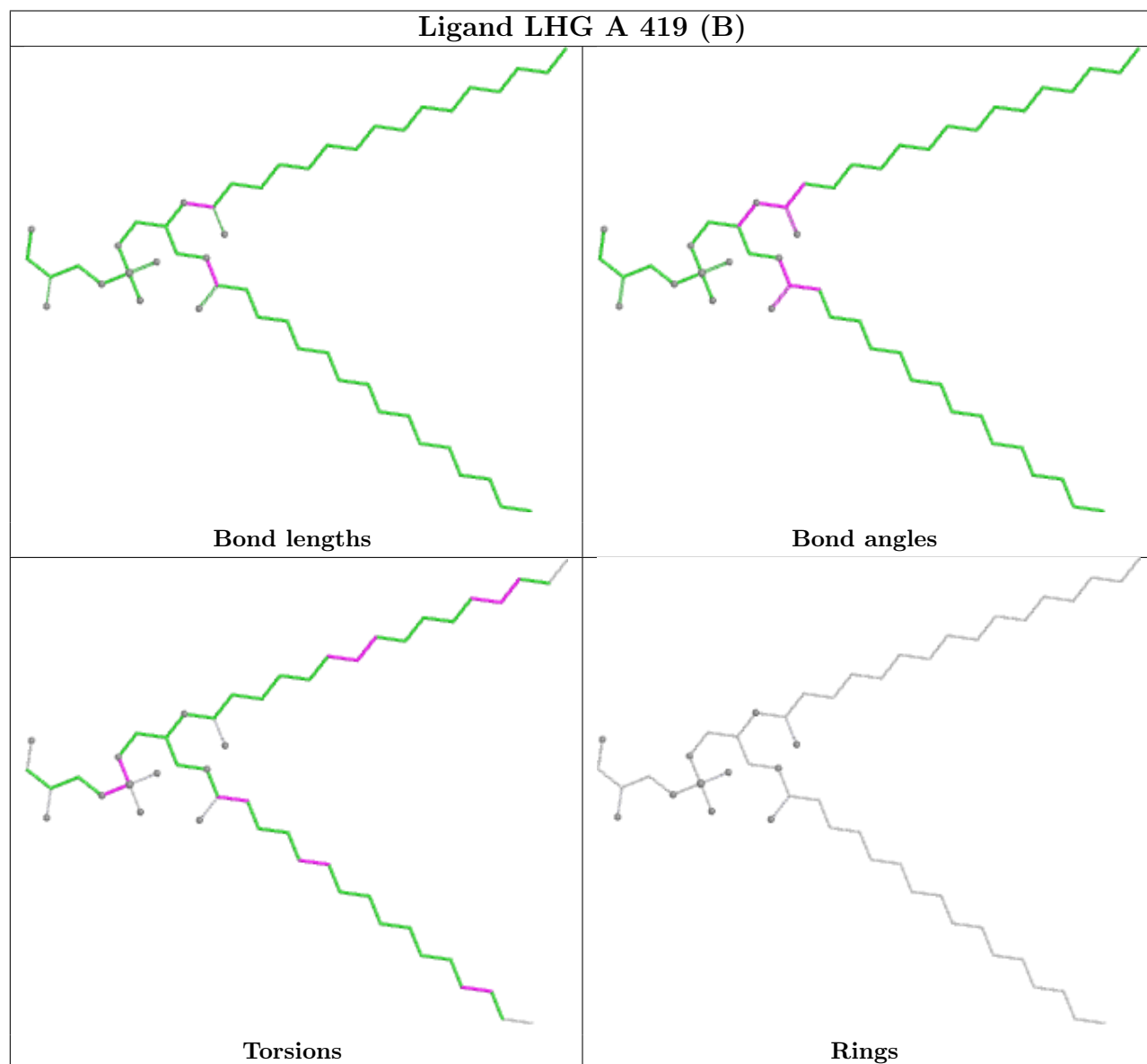
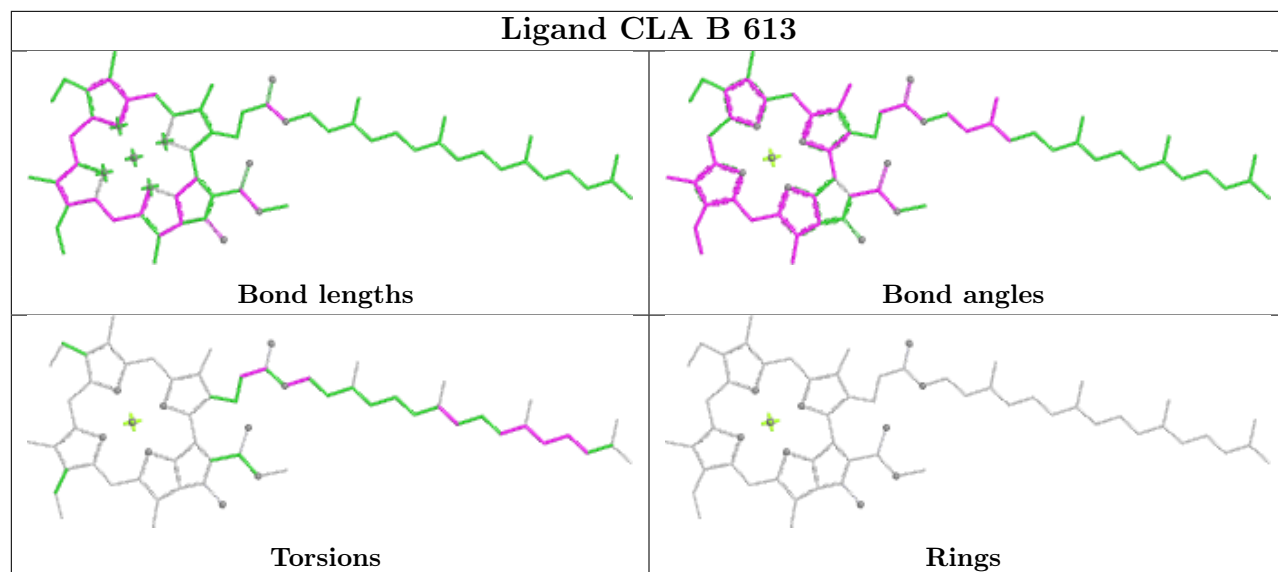


Torsions



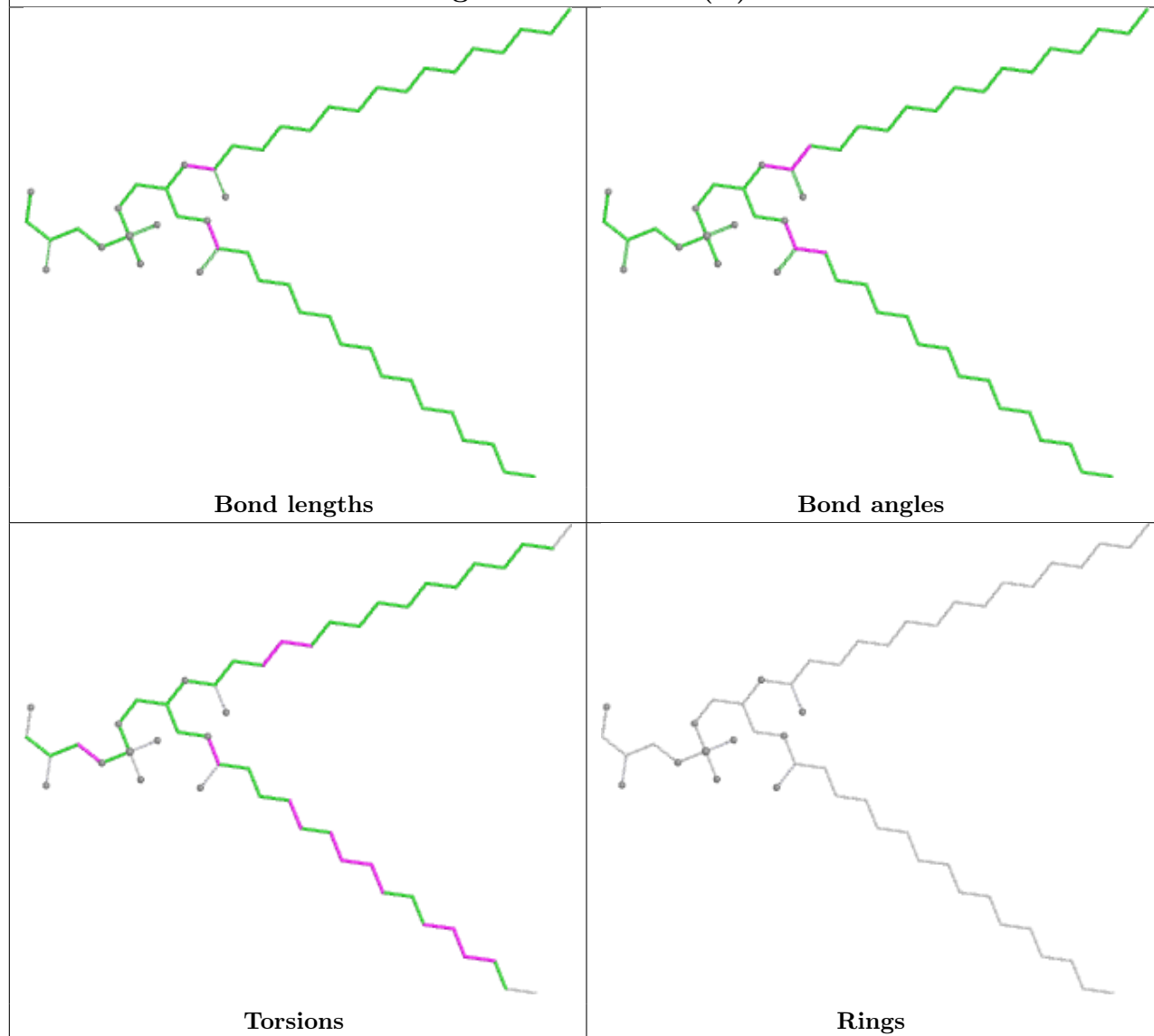
Rings



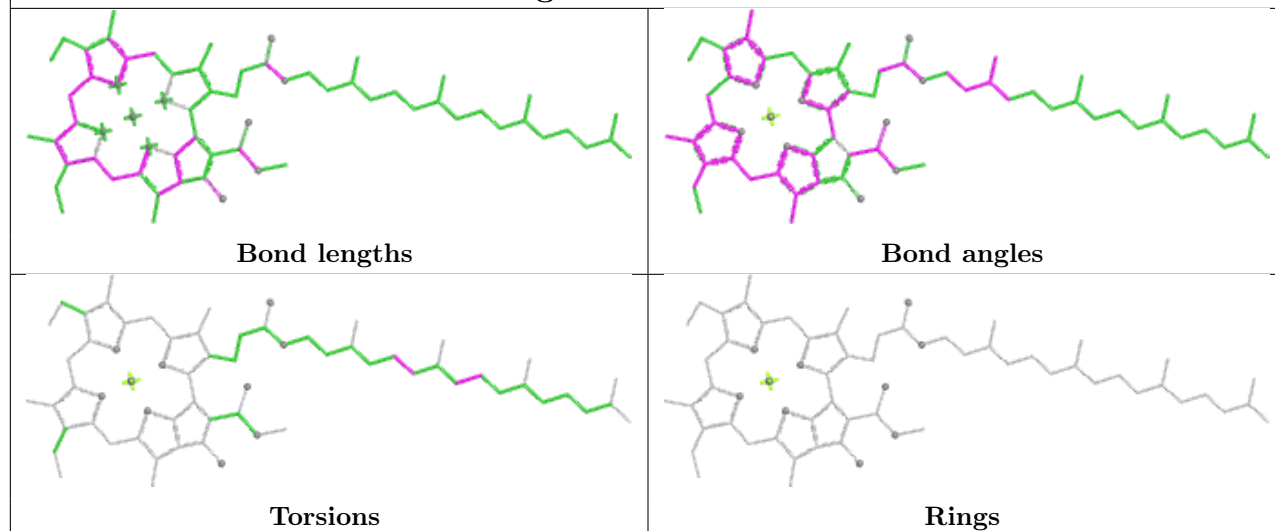


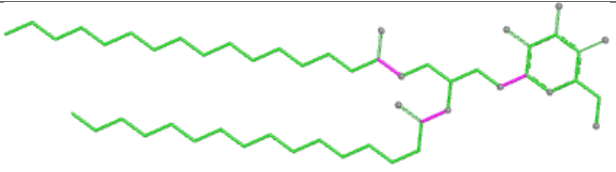
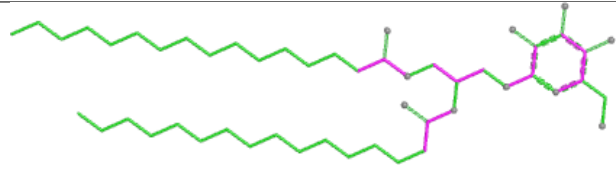
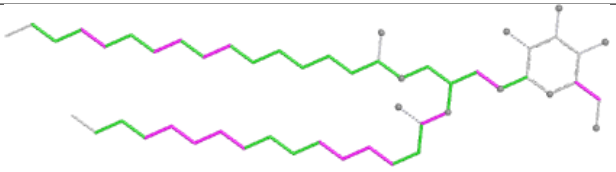
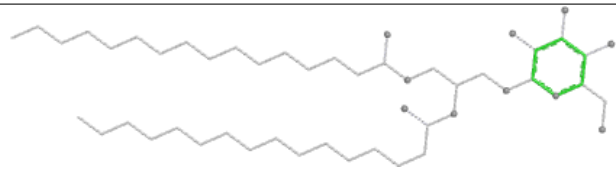


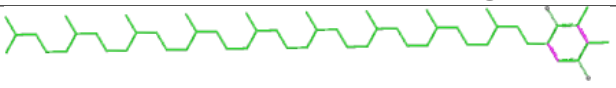
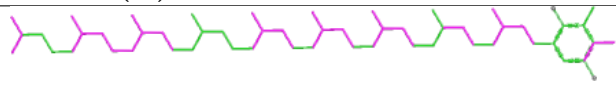
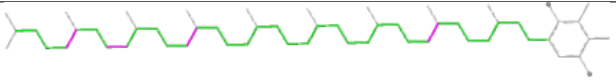
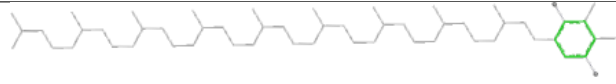
## Ligand LHG d 406 (B)

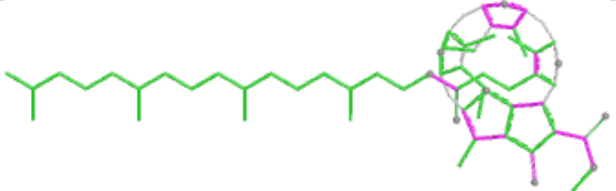
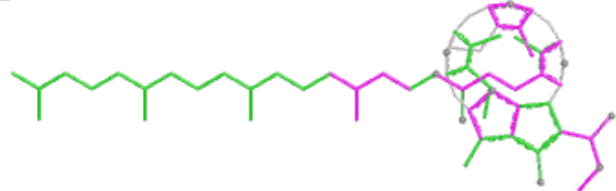
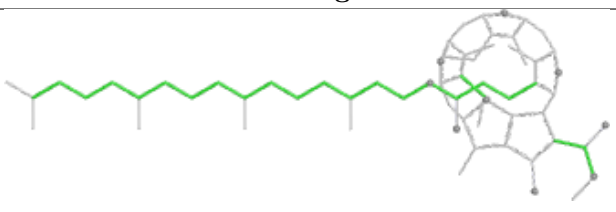
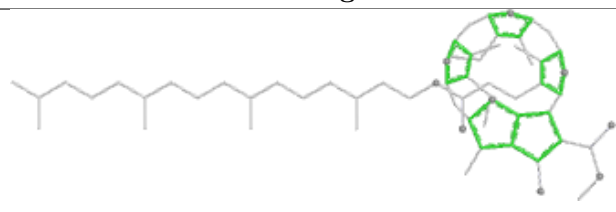


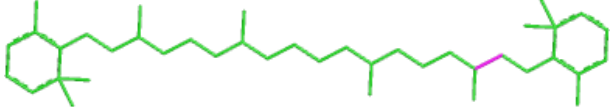
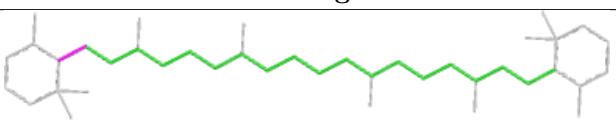
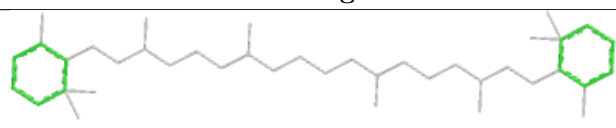
## Ligand CLA c 504

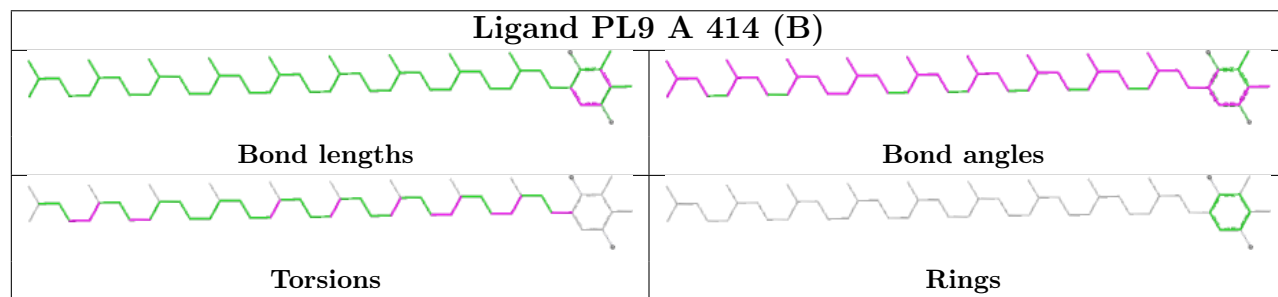
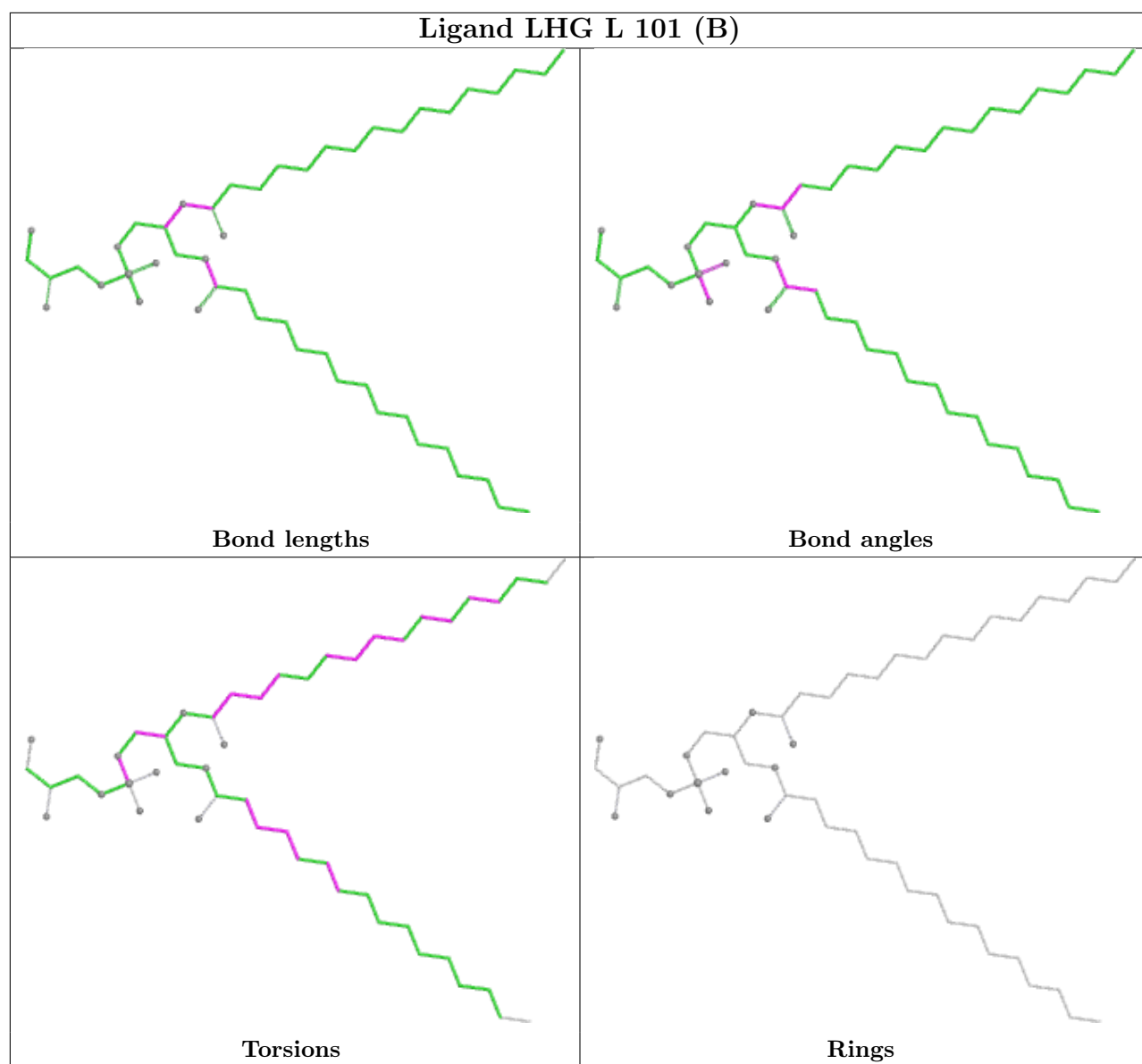


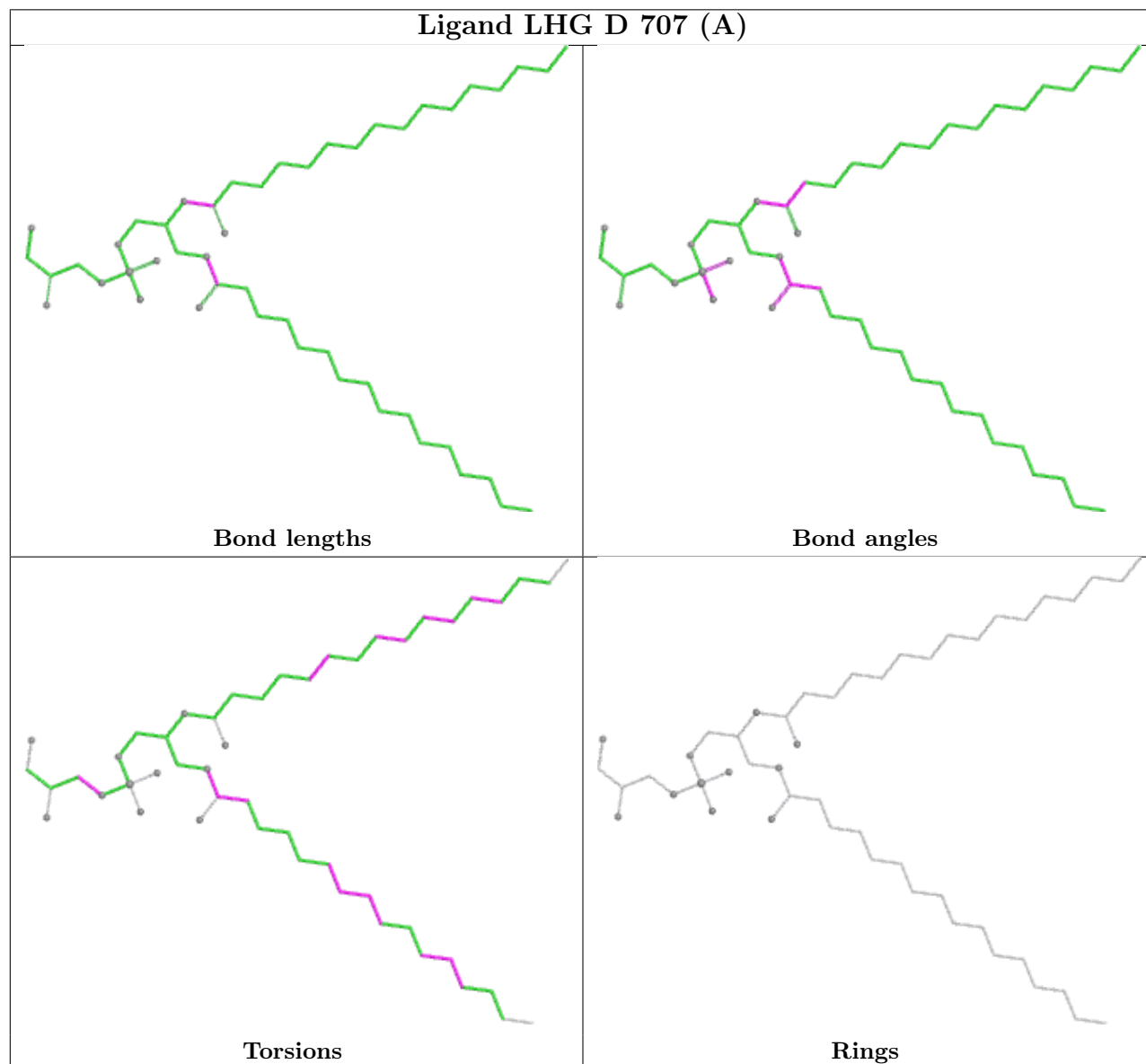
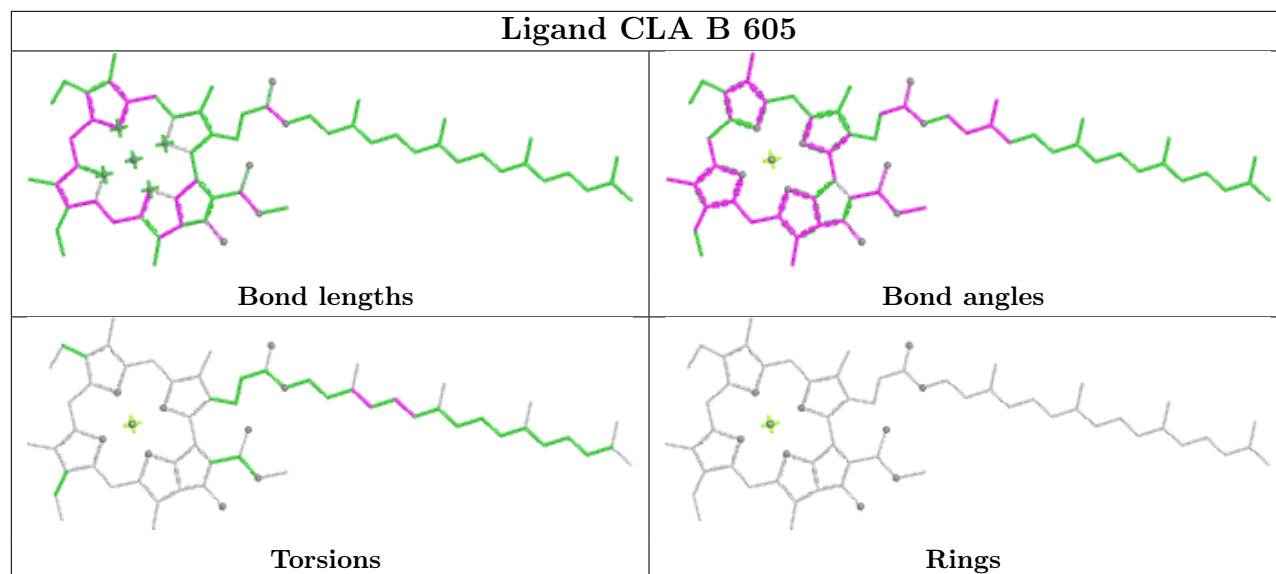
| Ligand LMG C 521                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

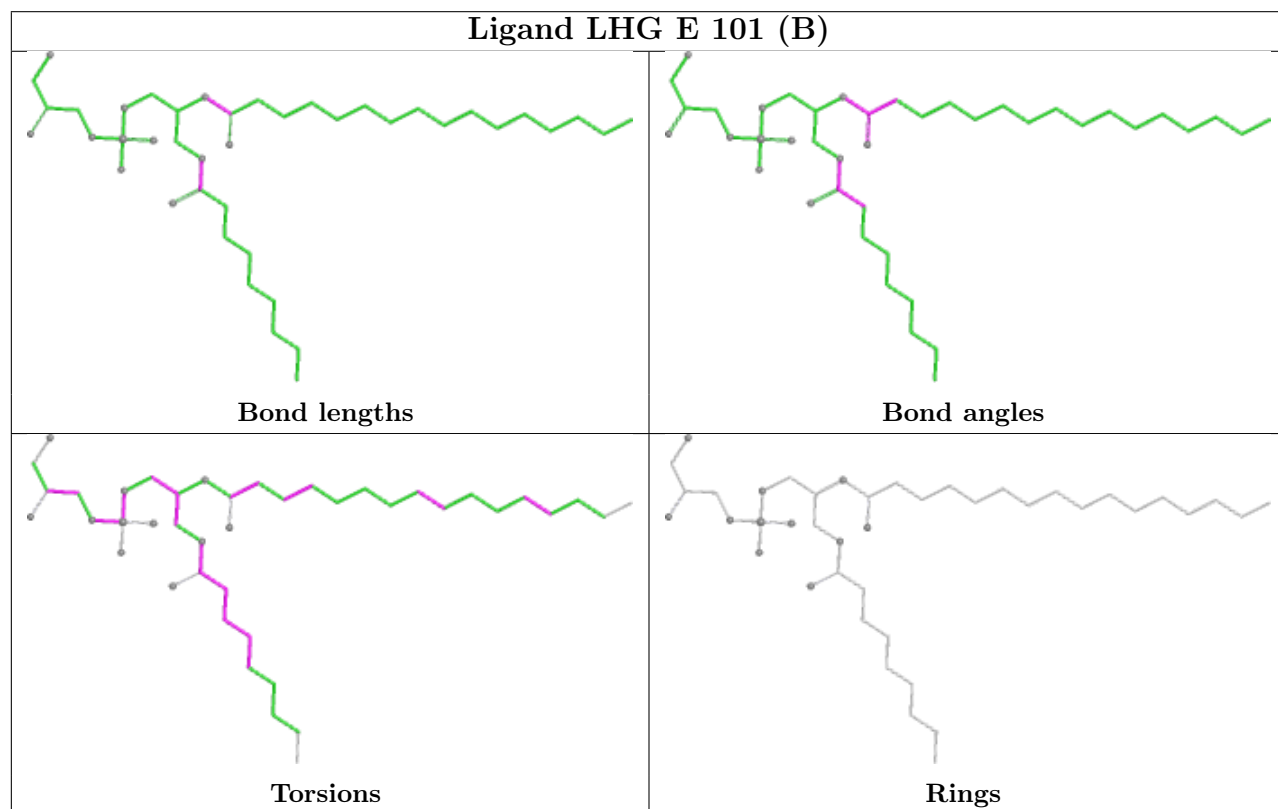
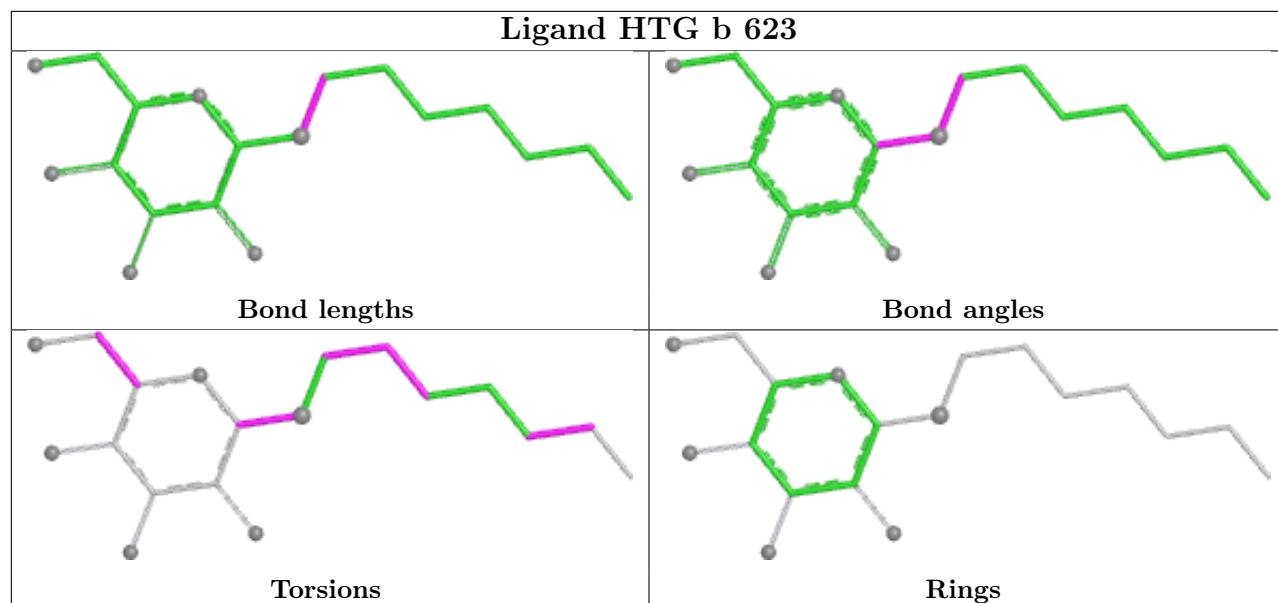
| Ligand PL9 D 705 (B)                                                              |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

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

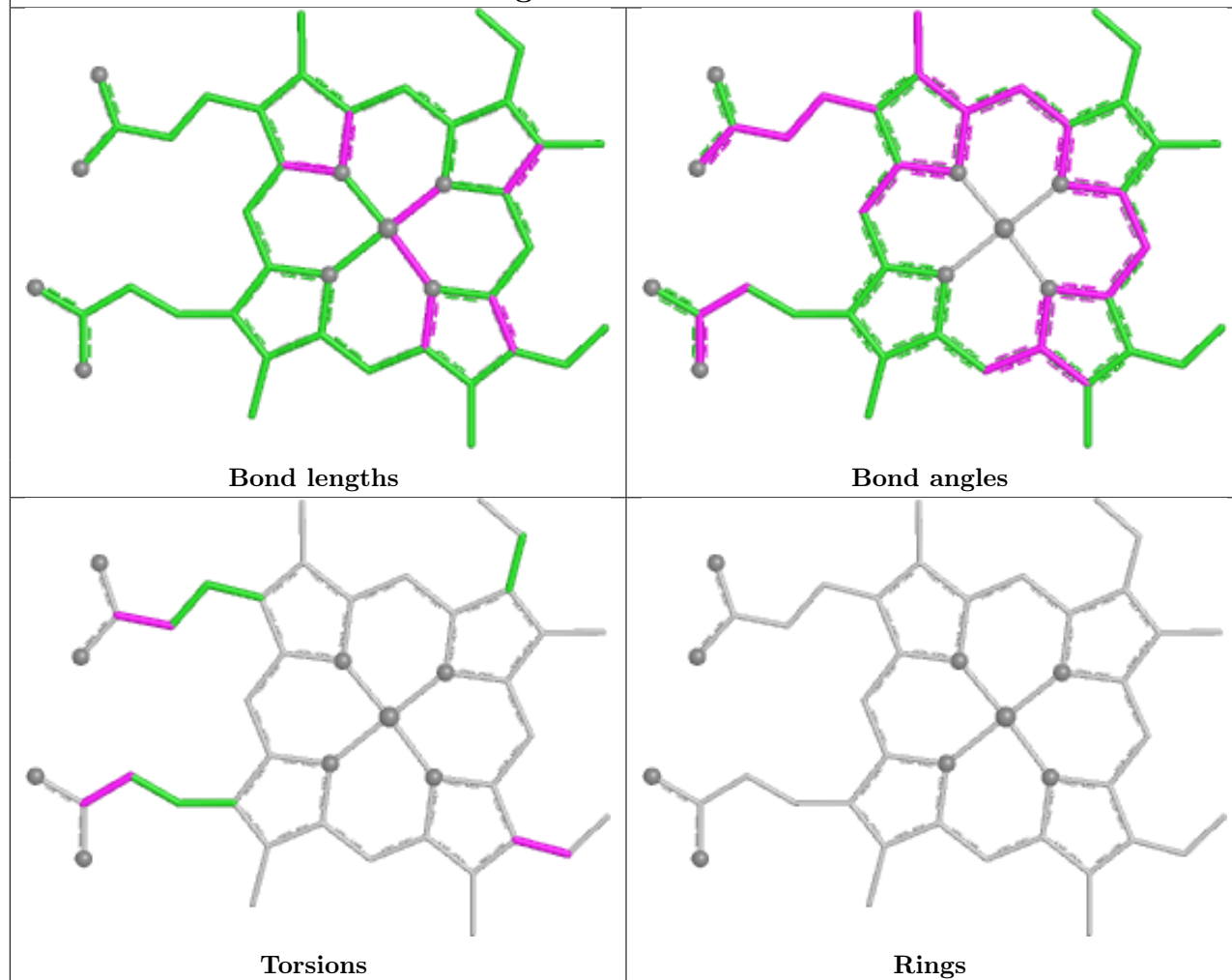
| Ligand BCR B 617                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|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



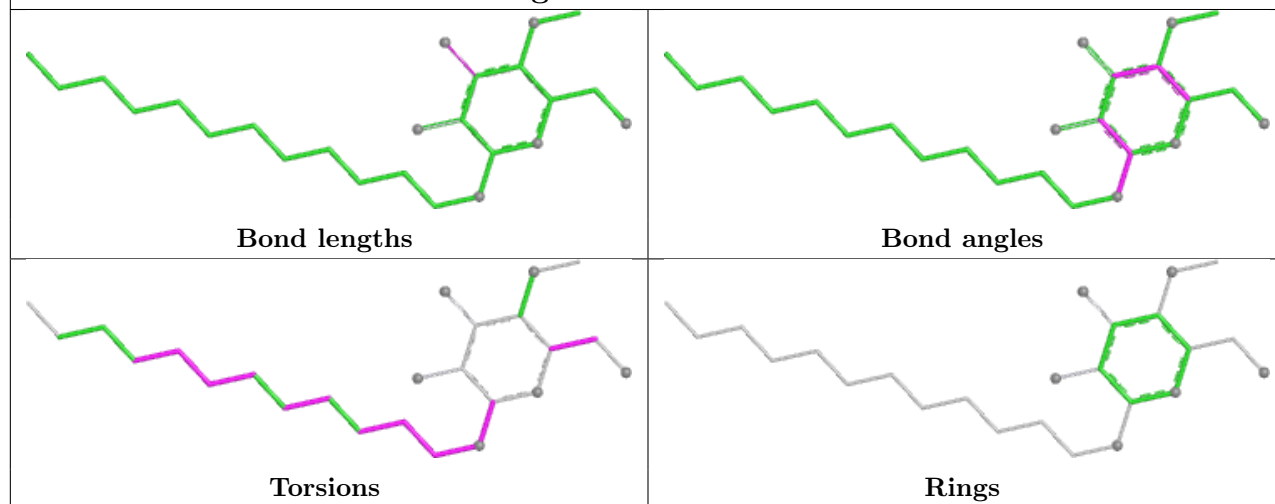


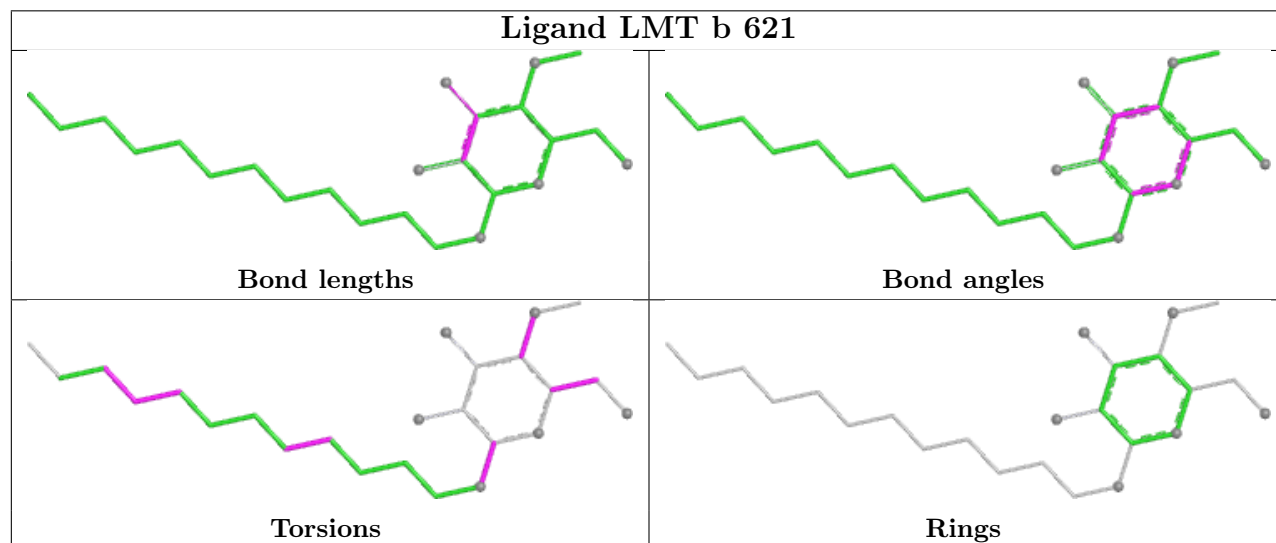
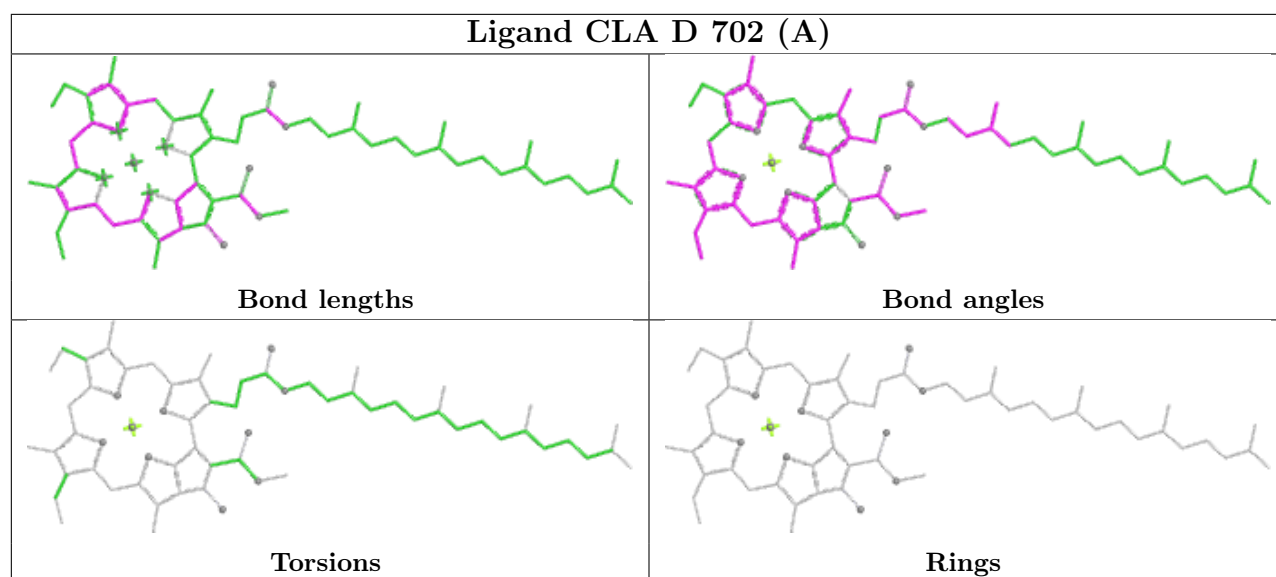


## Ligand HEM f 101

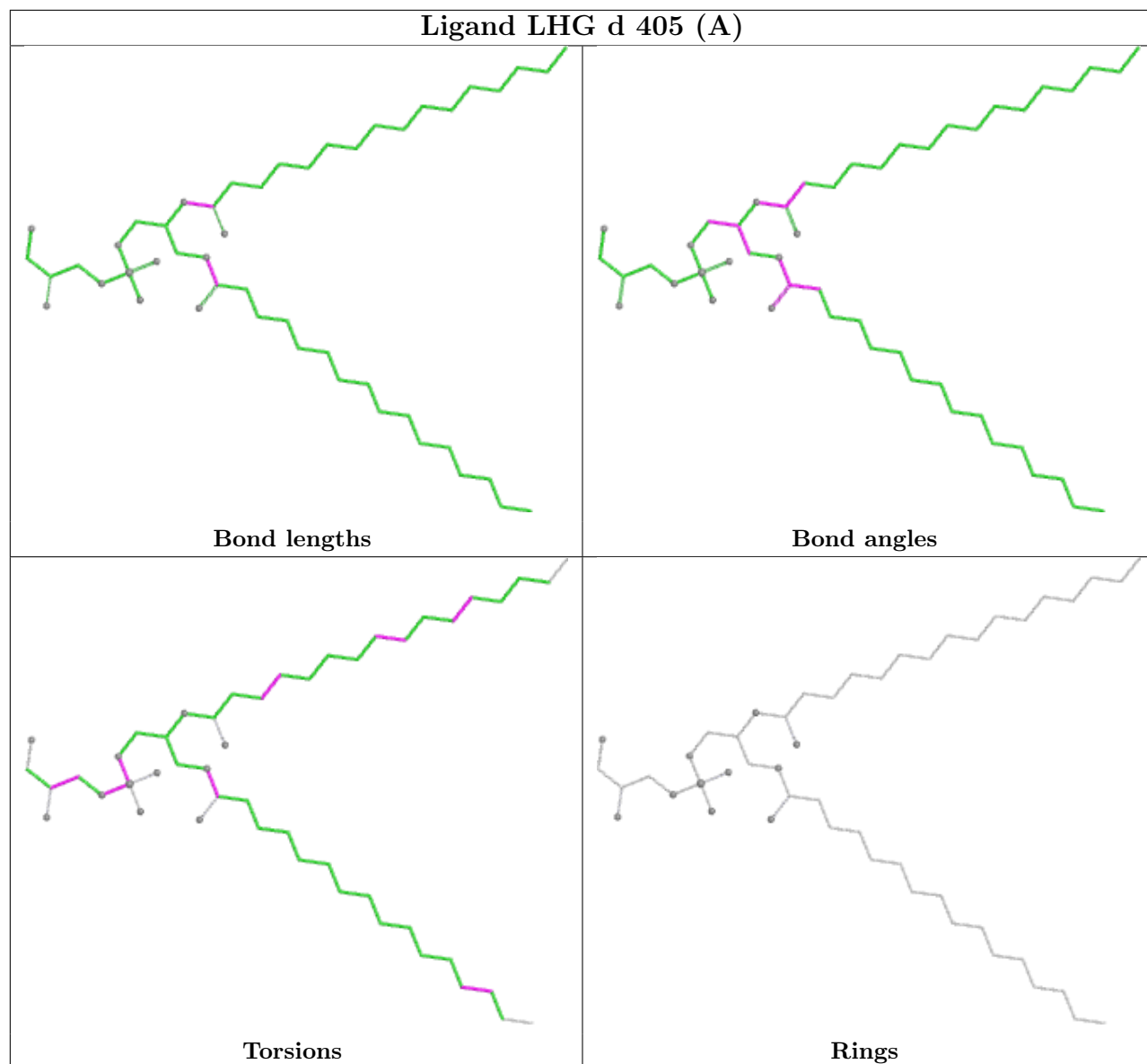


## Ligand LMT b 627

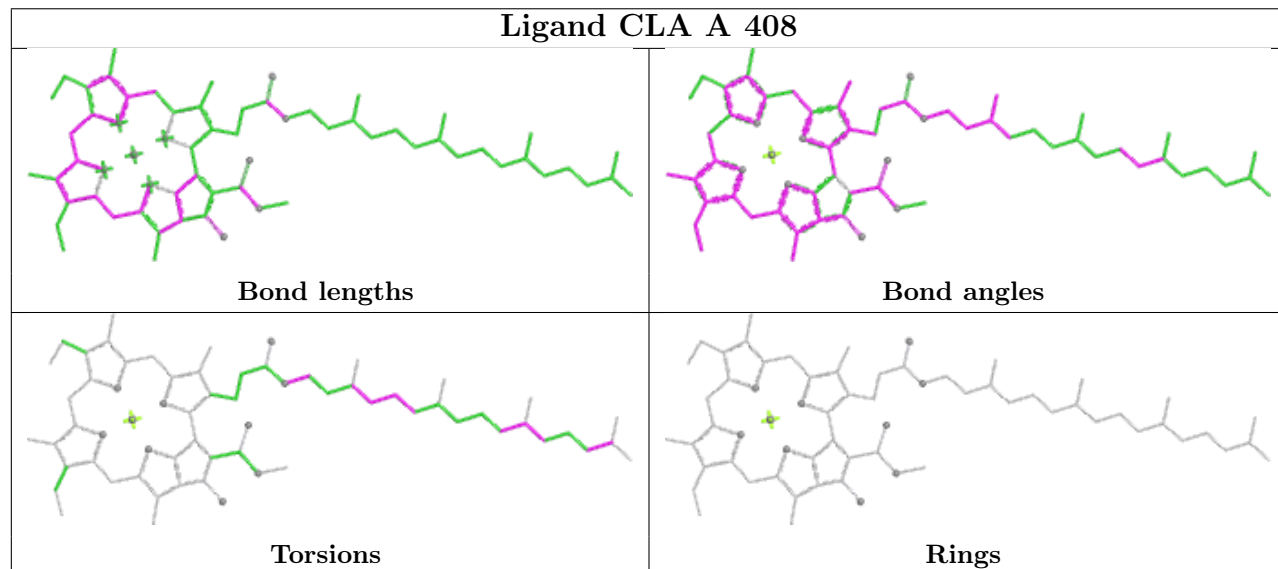




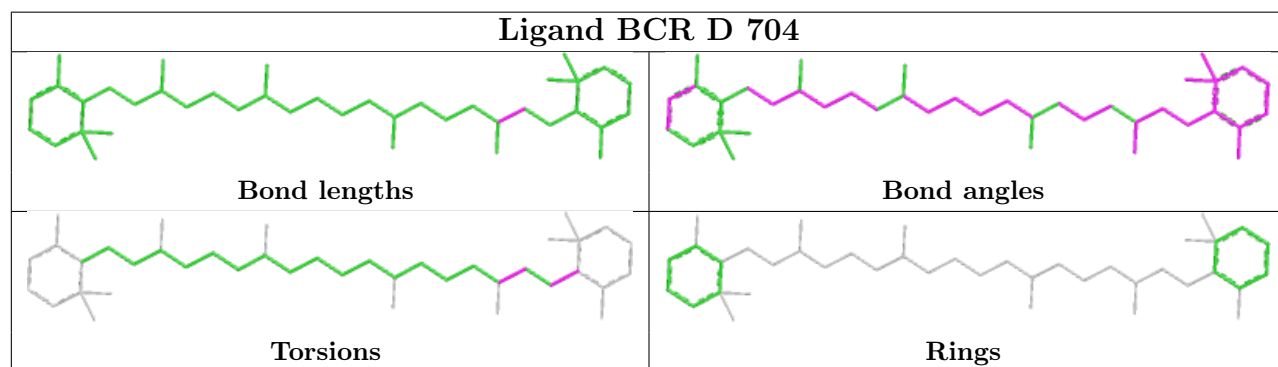
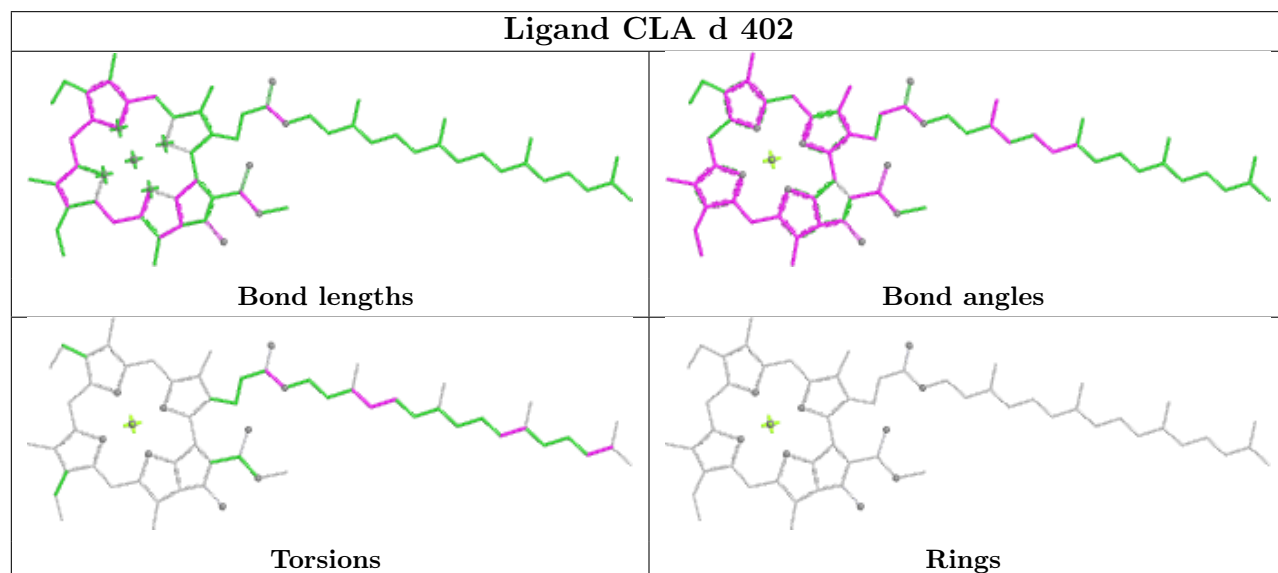
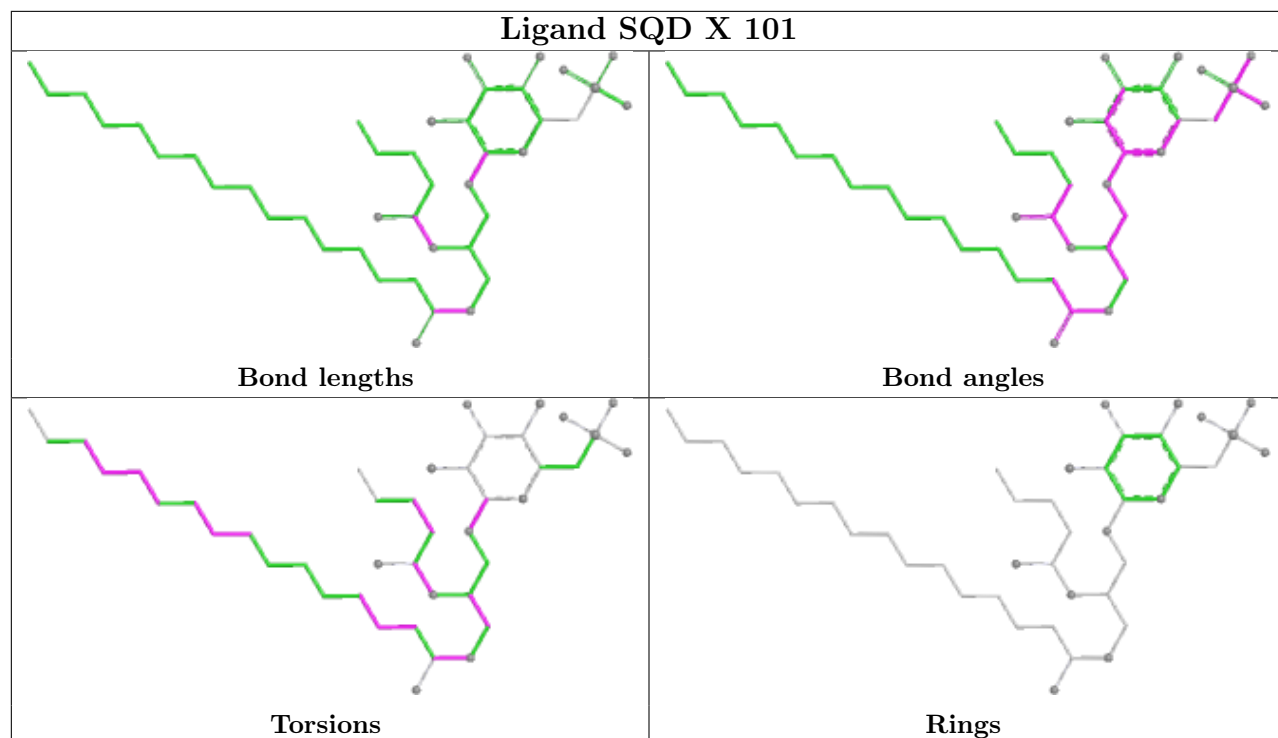
## Ligand LHG d 405 (A)

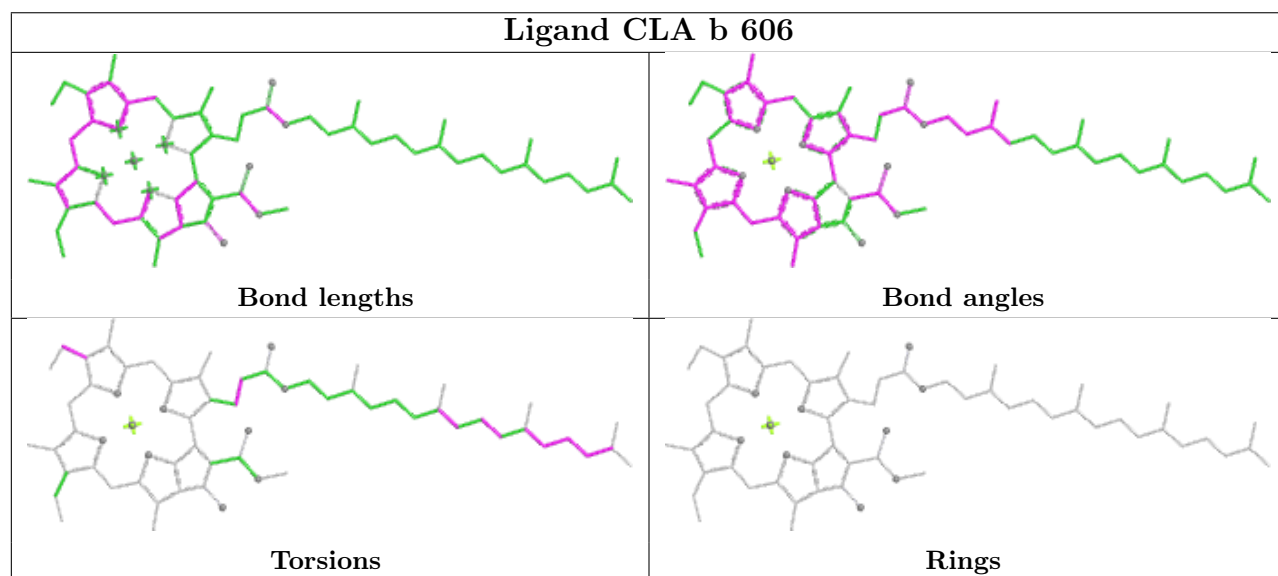
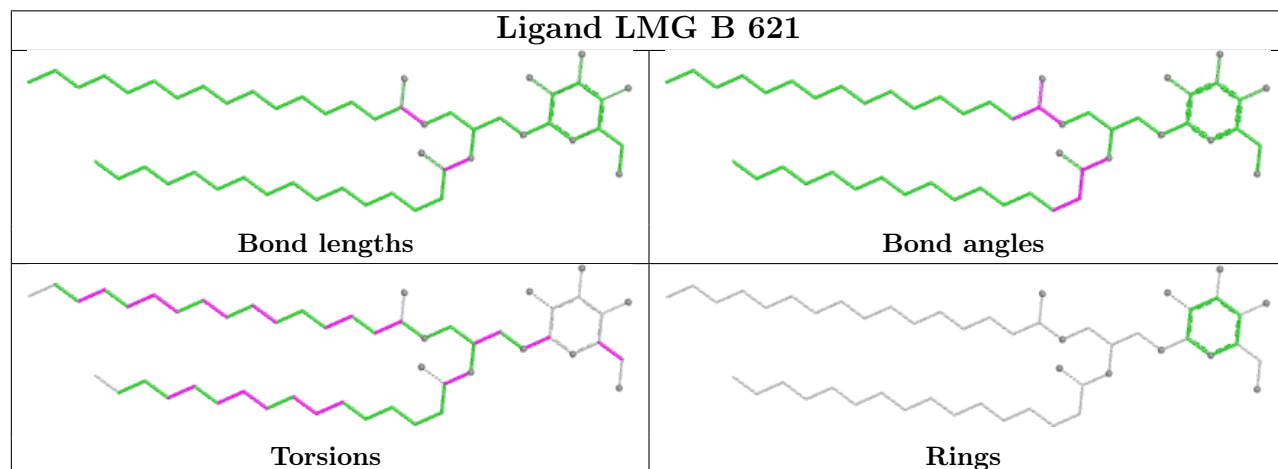
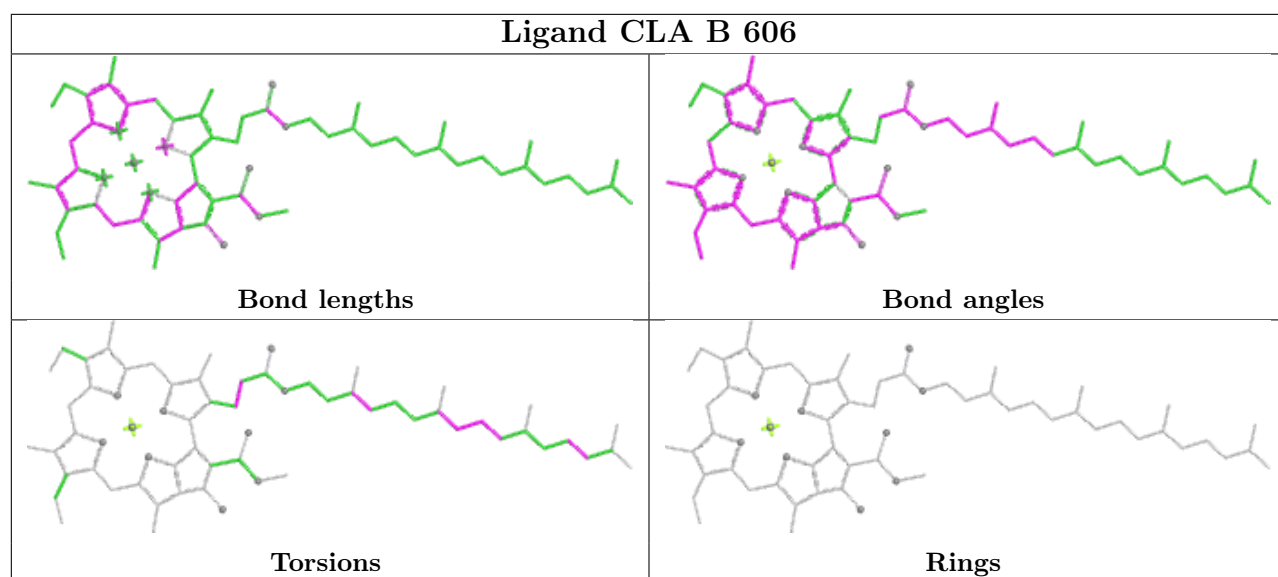


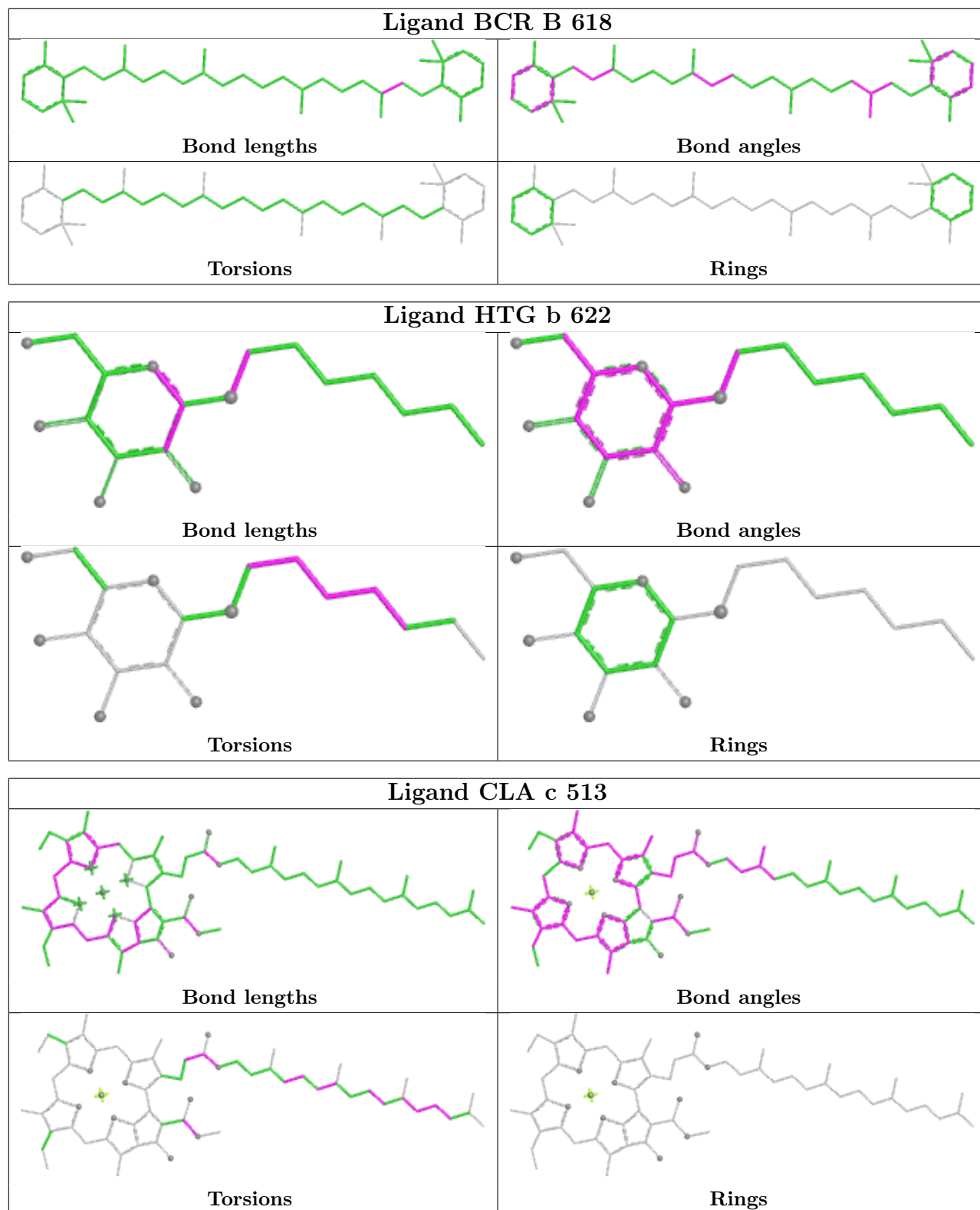
## Ligand CLA A 408

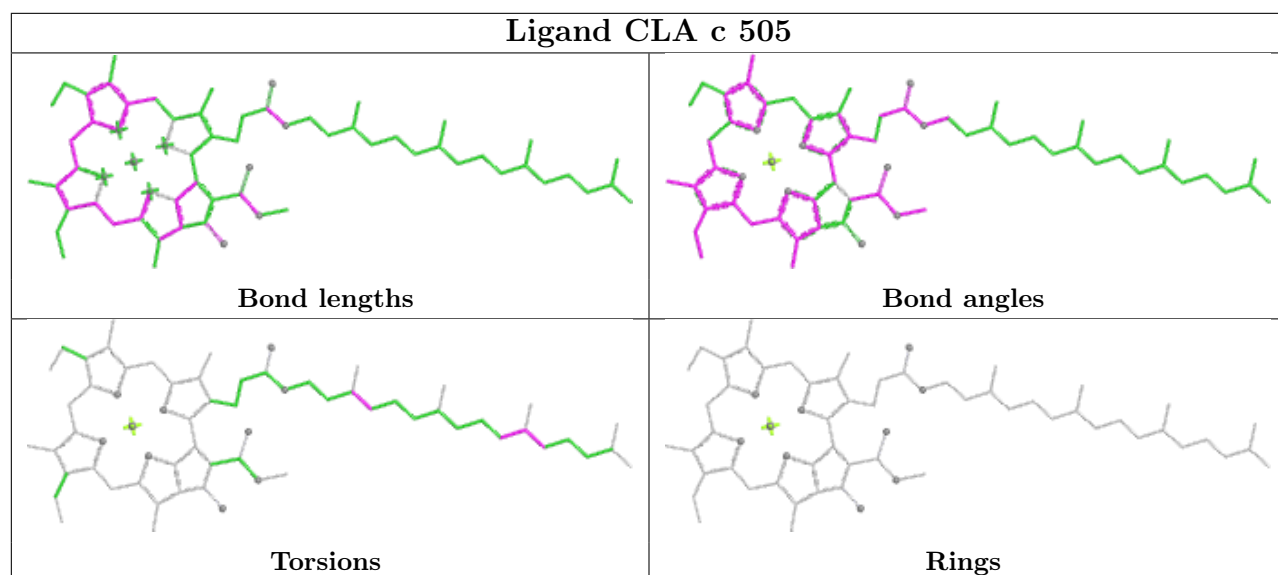
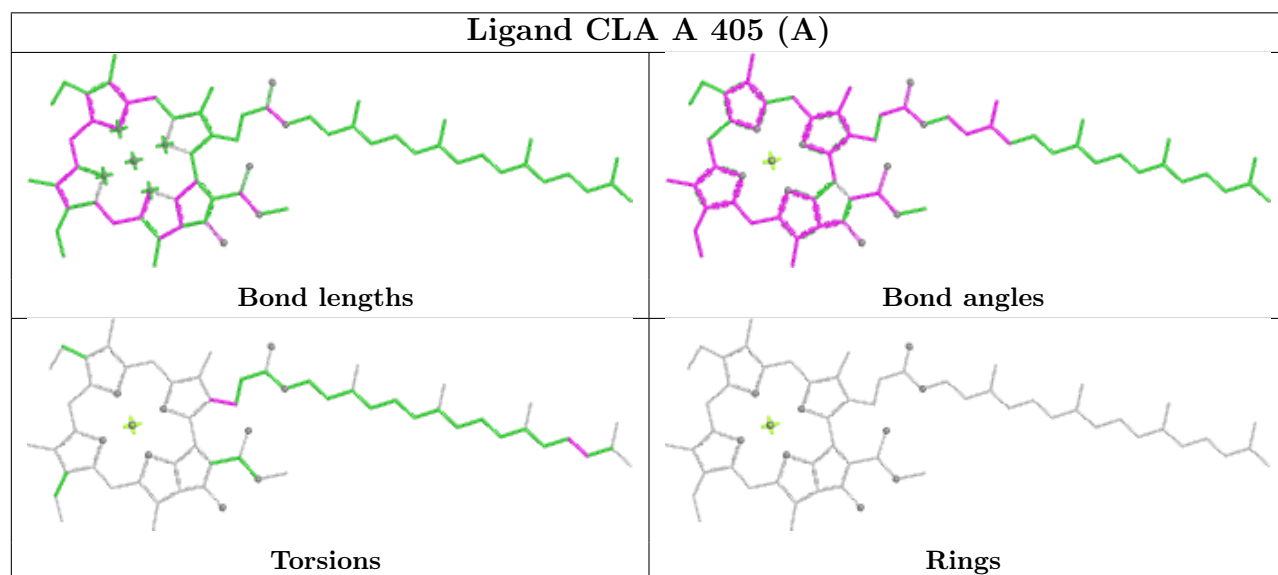
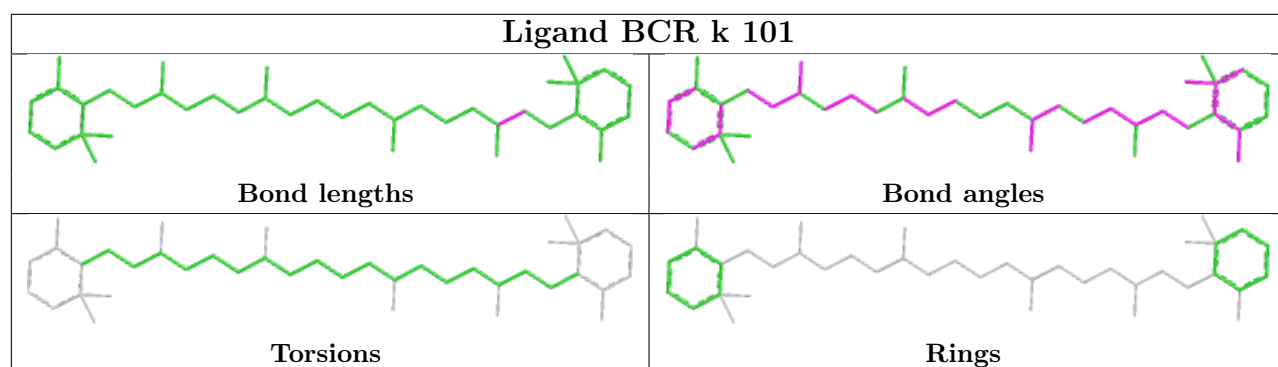


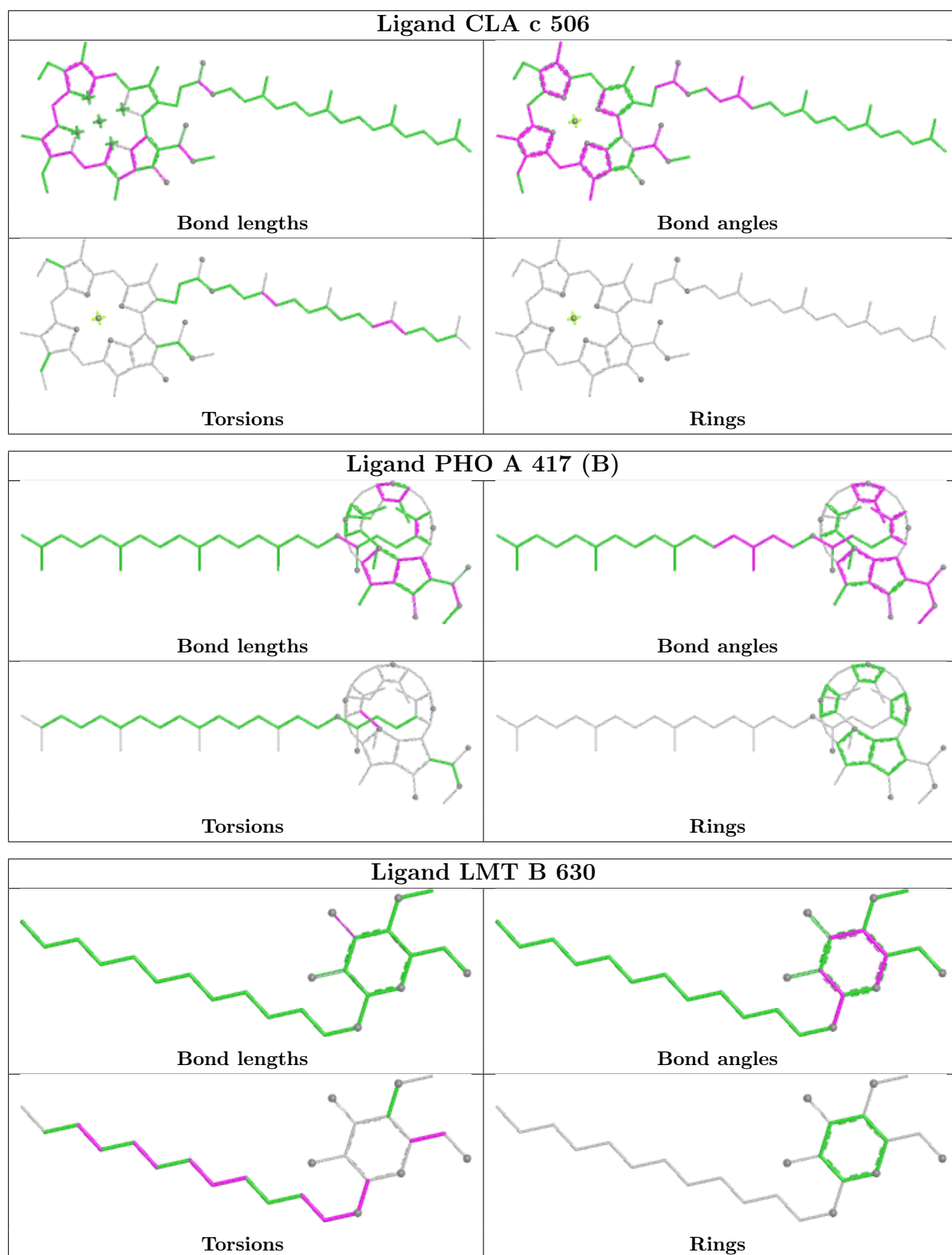


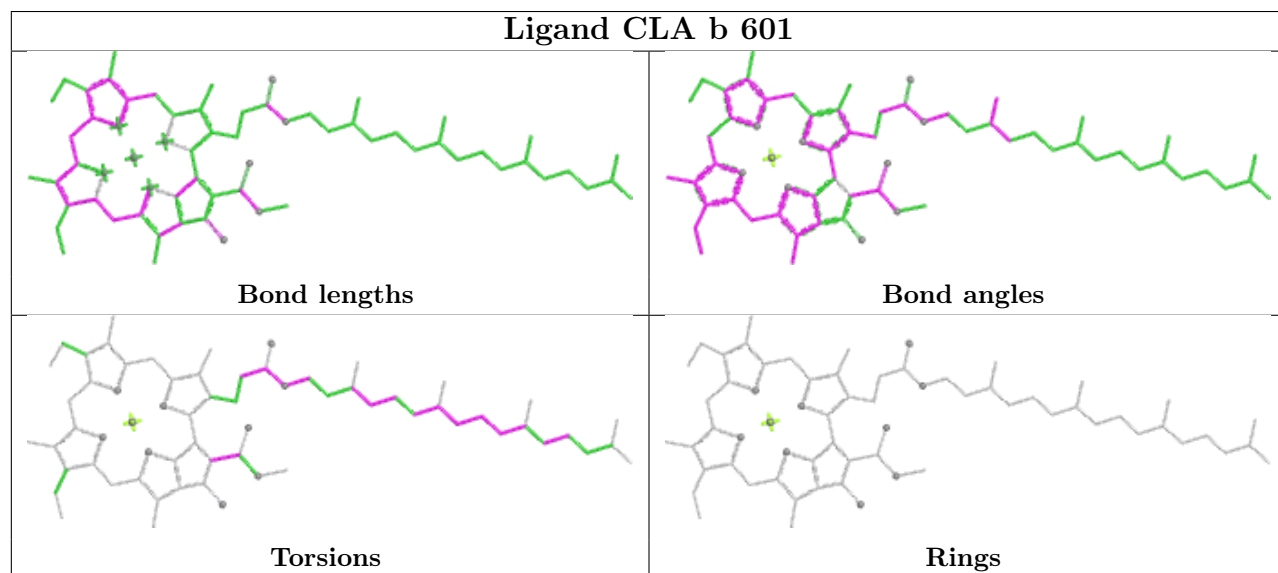
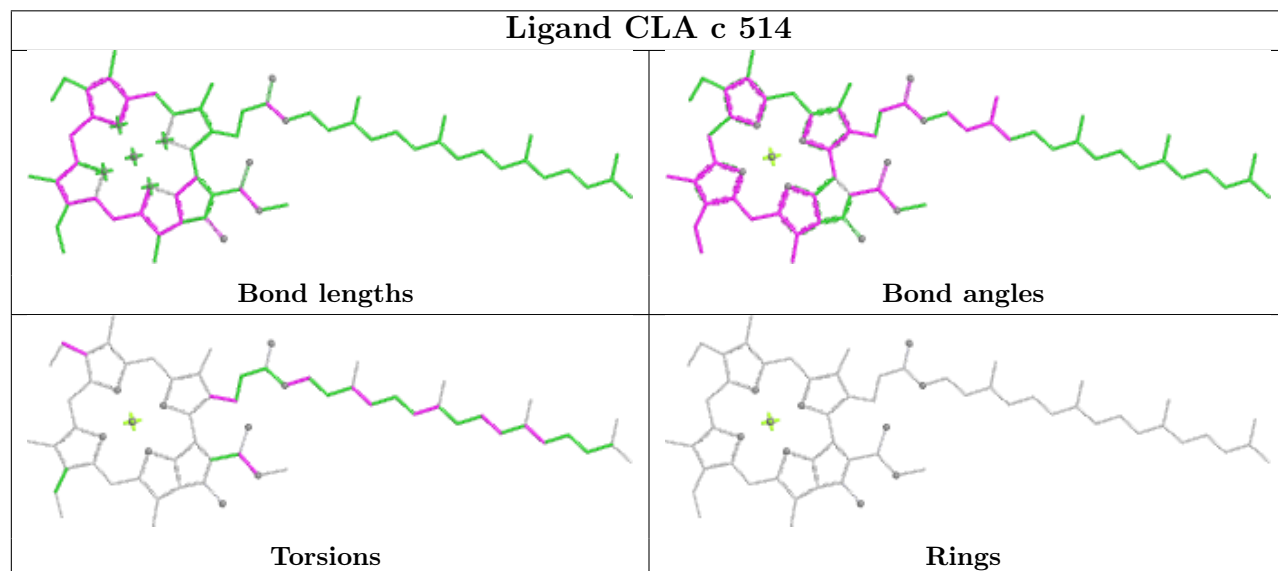
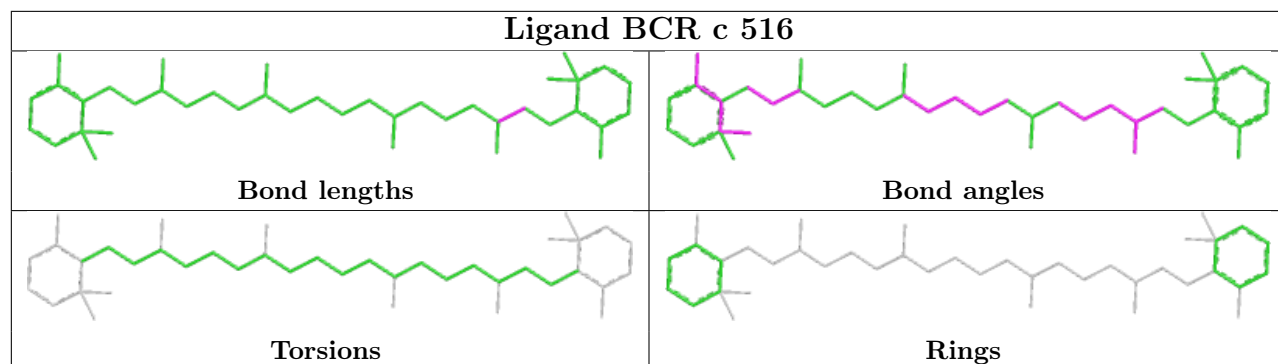




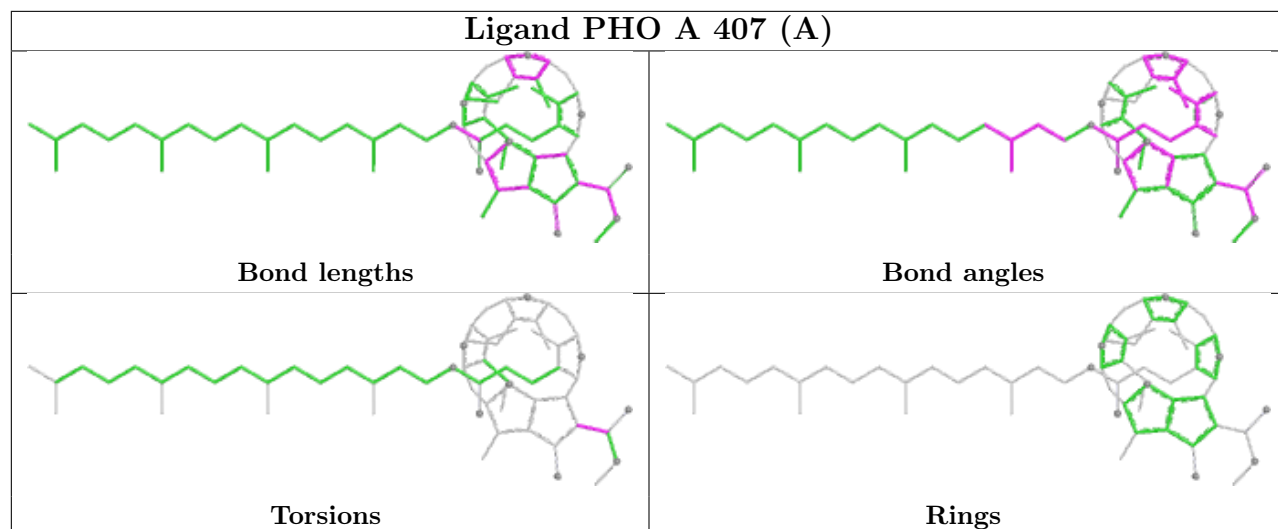




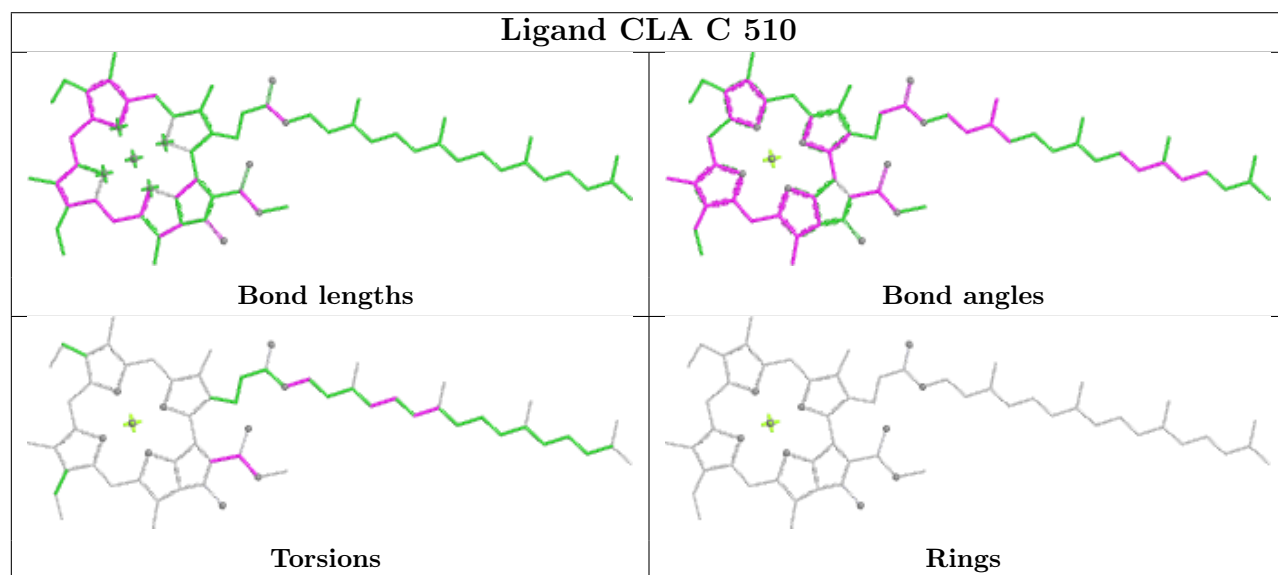




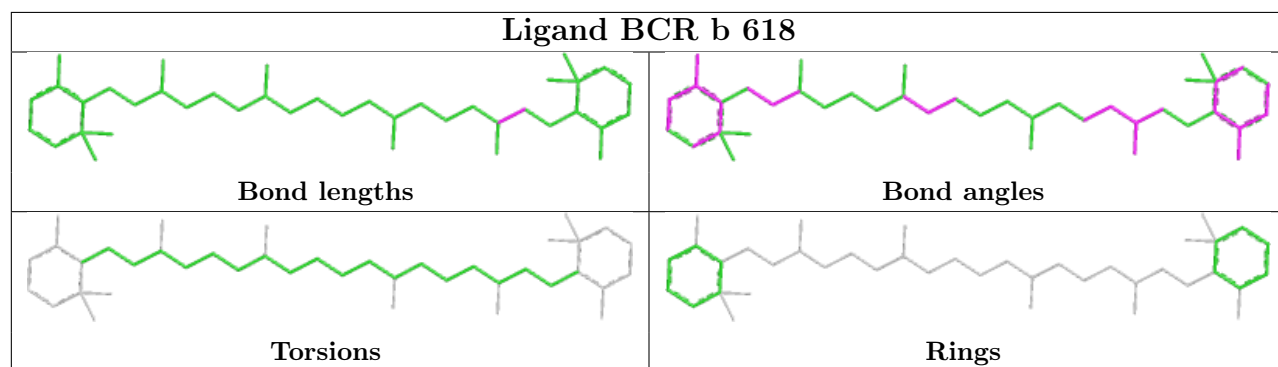
## Ligand PHO A 407 (A)

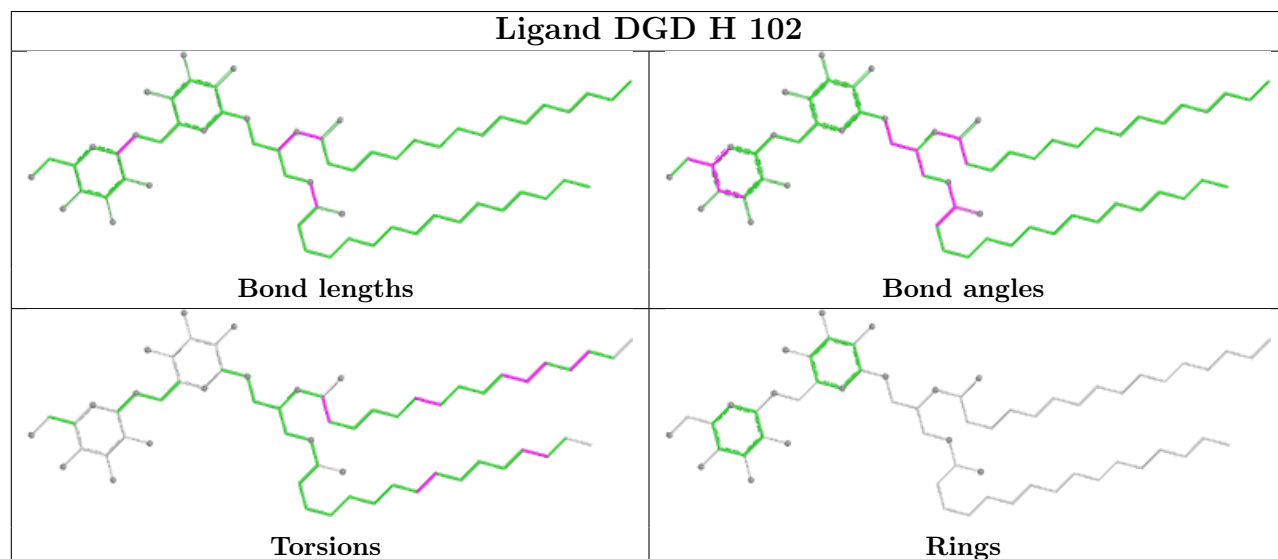
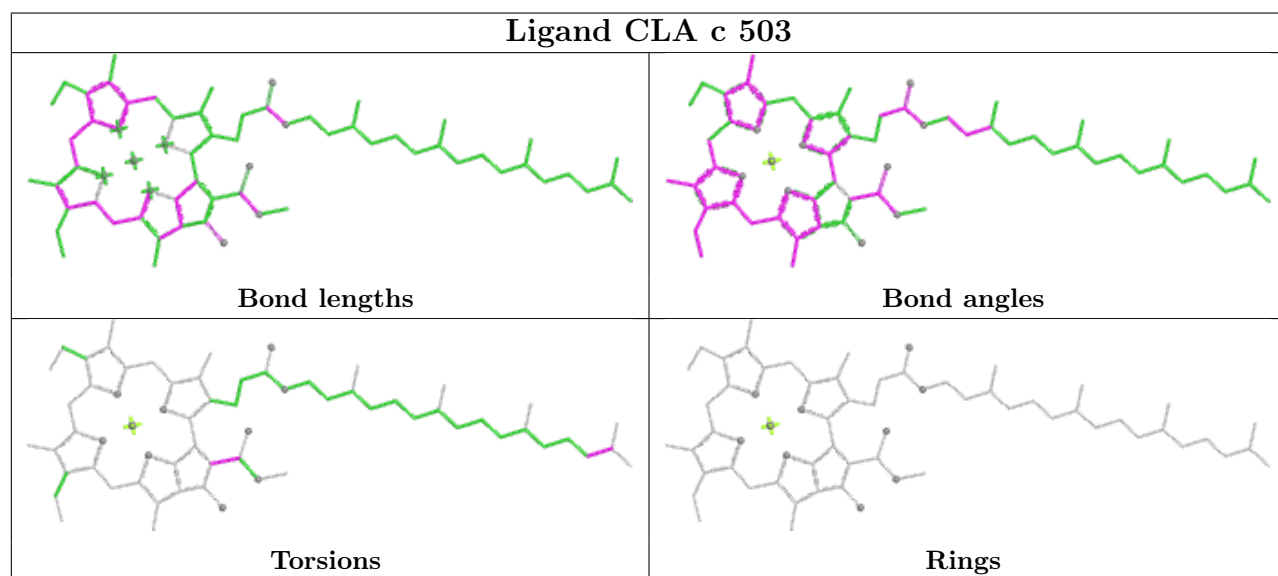
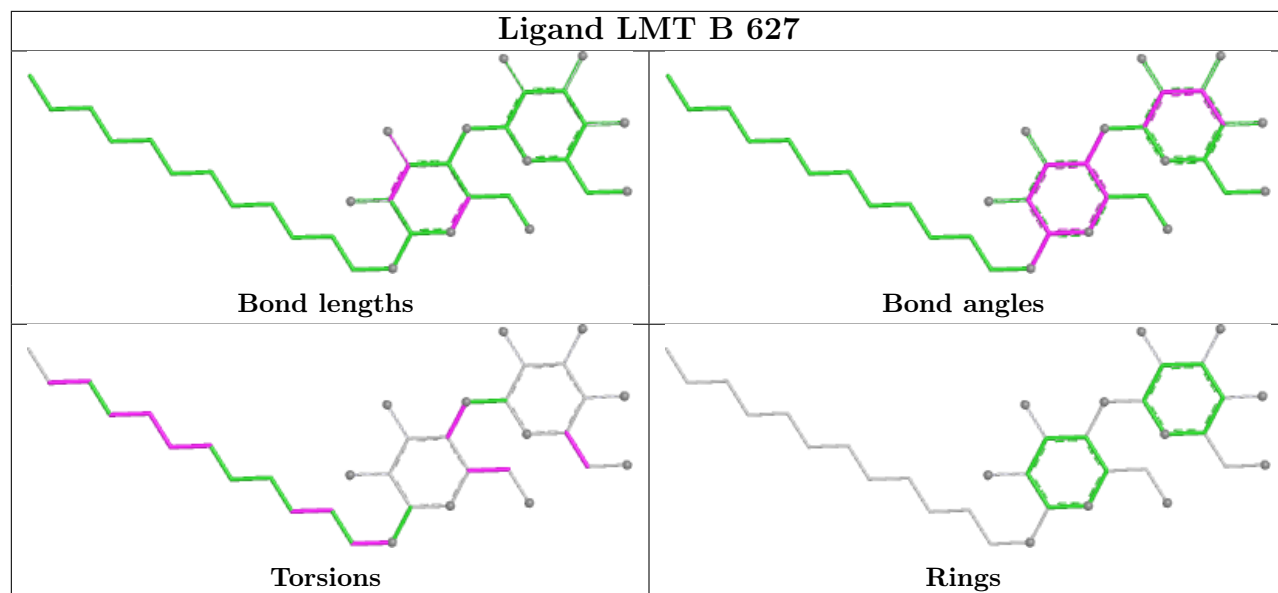


## Ligand CLA C 510



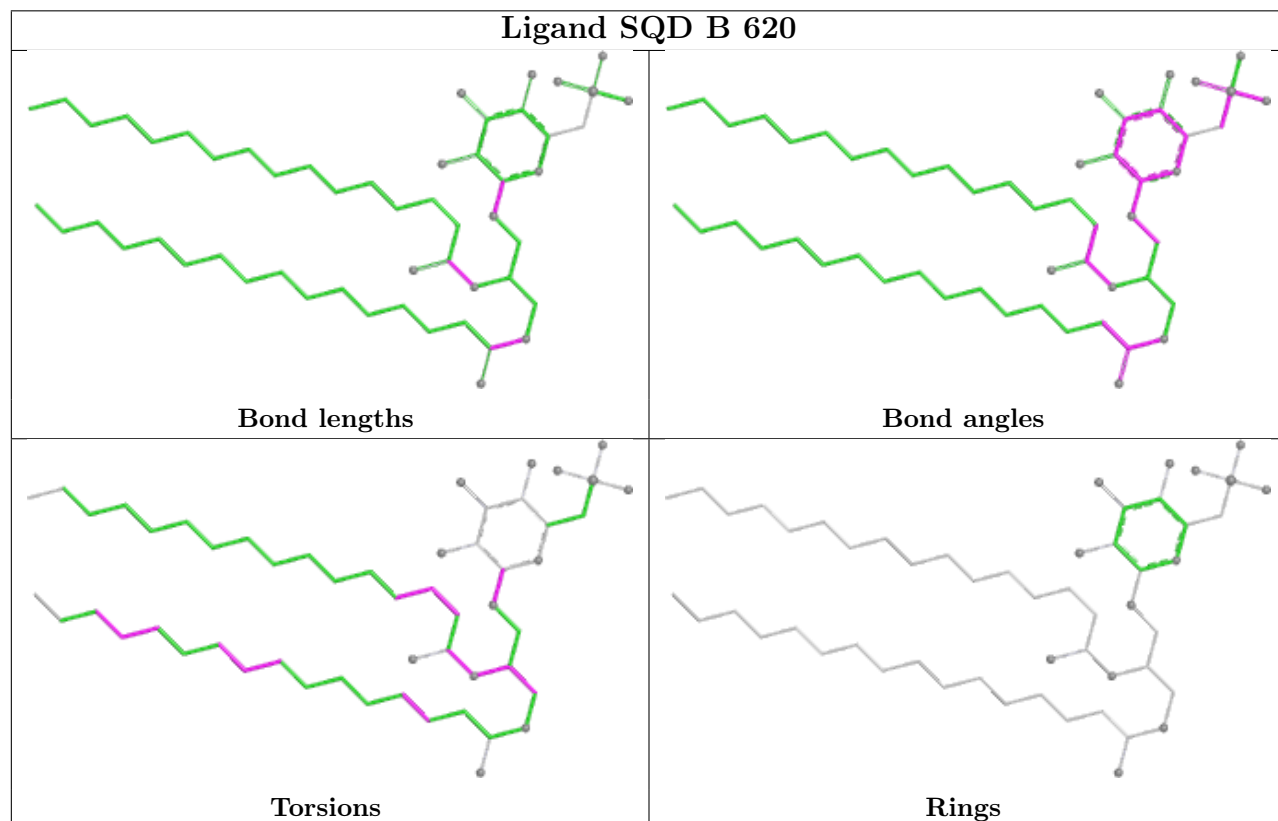
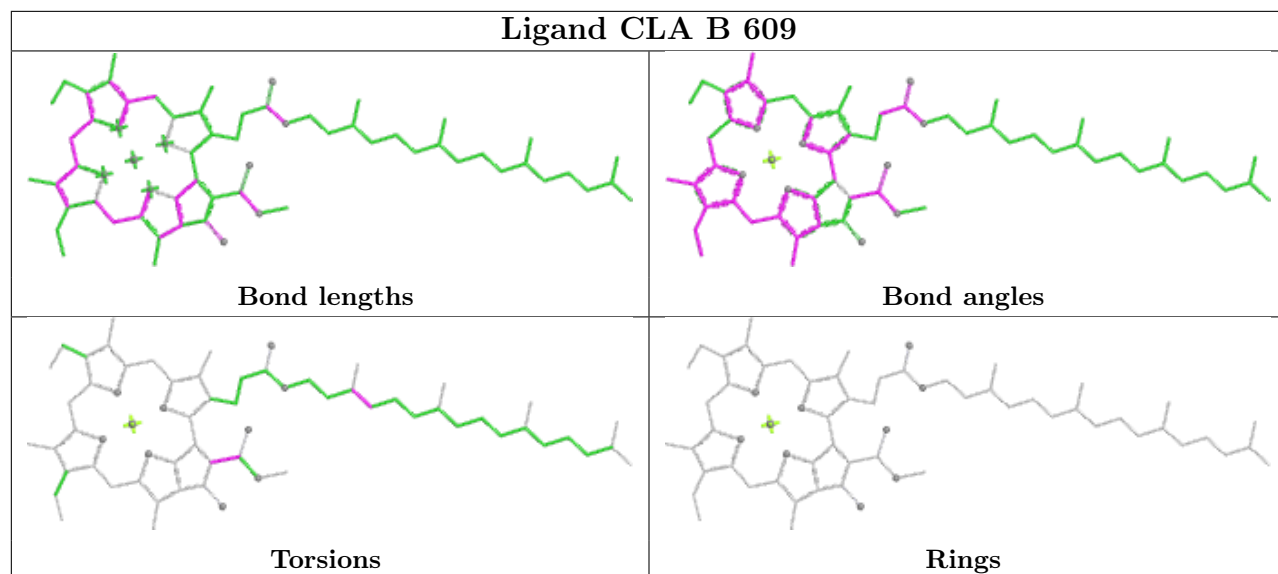
## Ligand BCR b 618

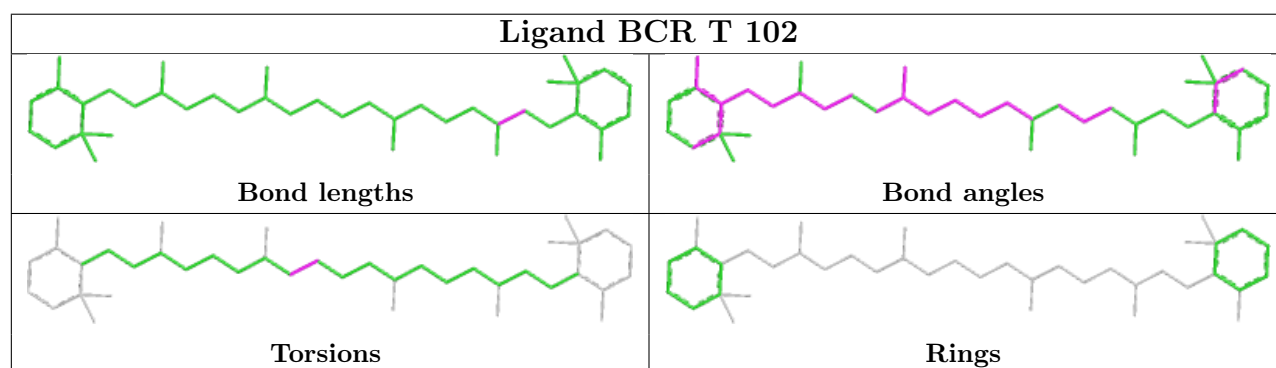
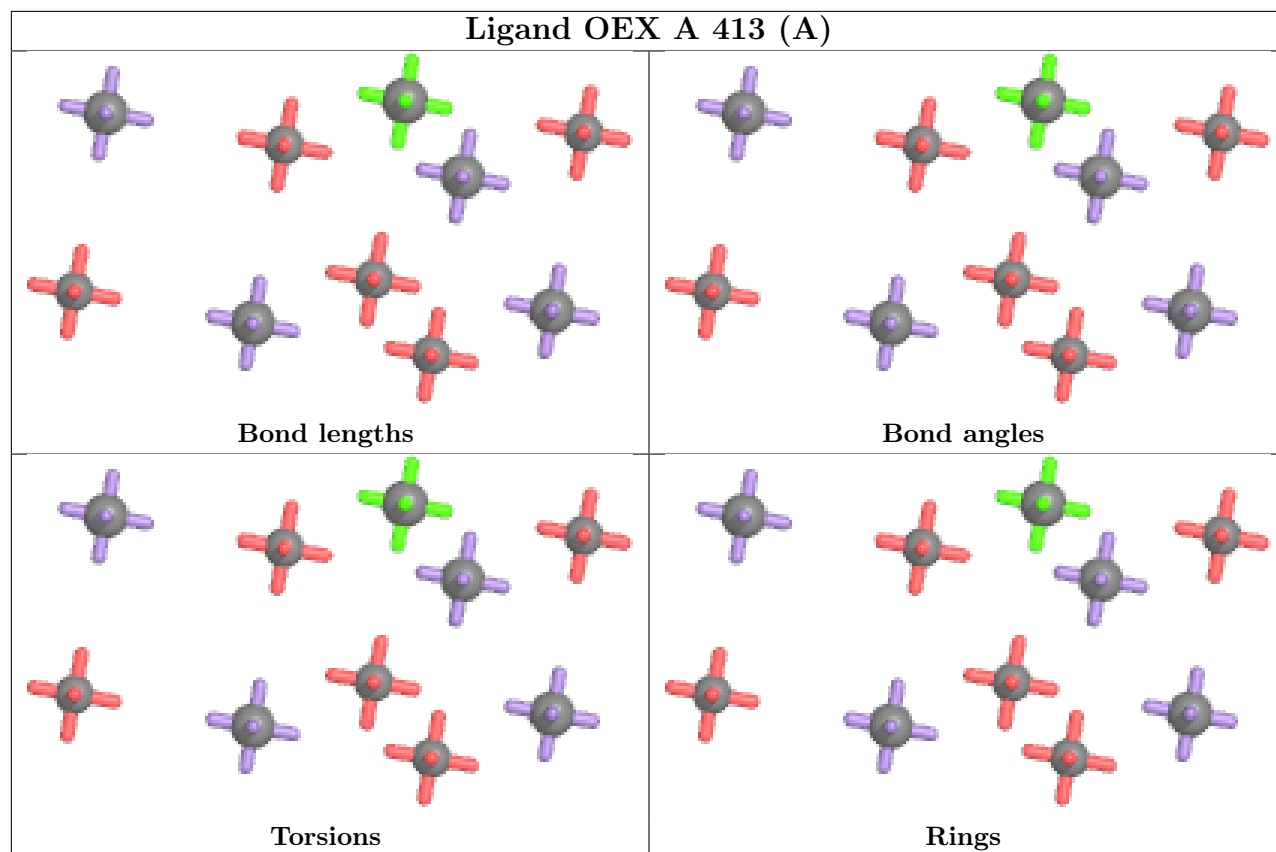


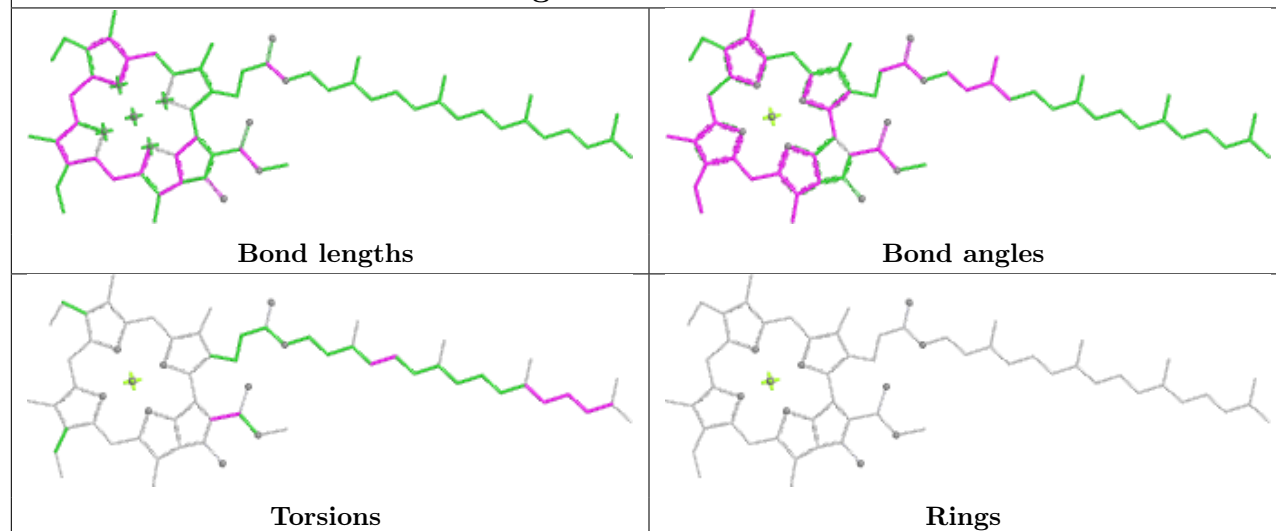
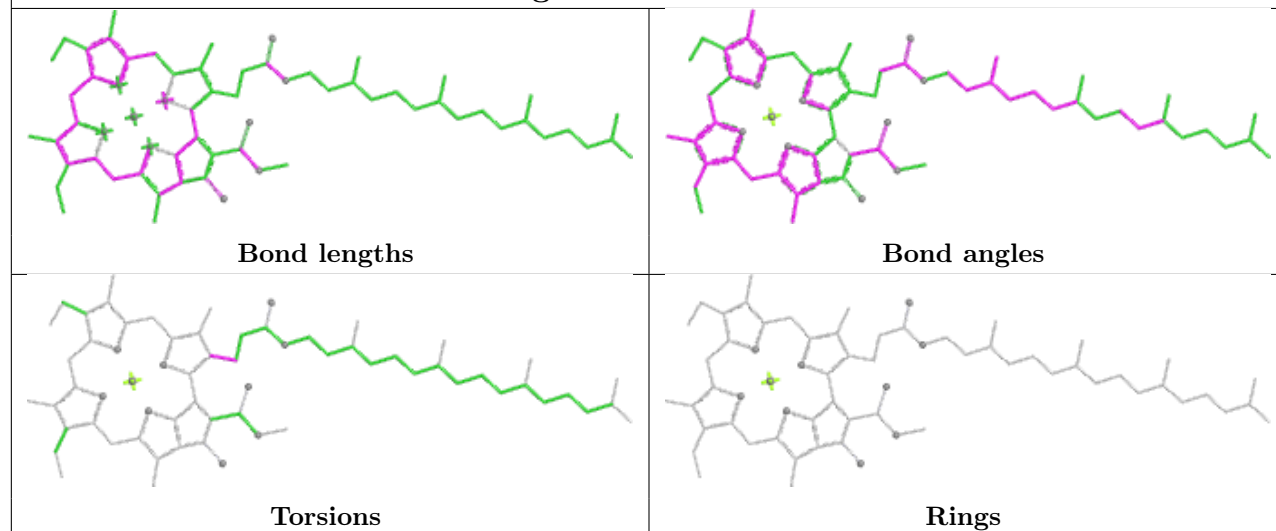


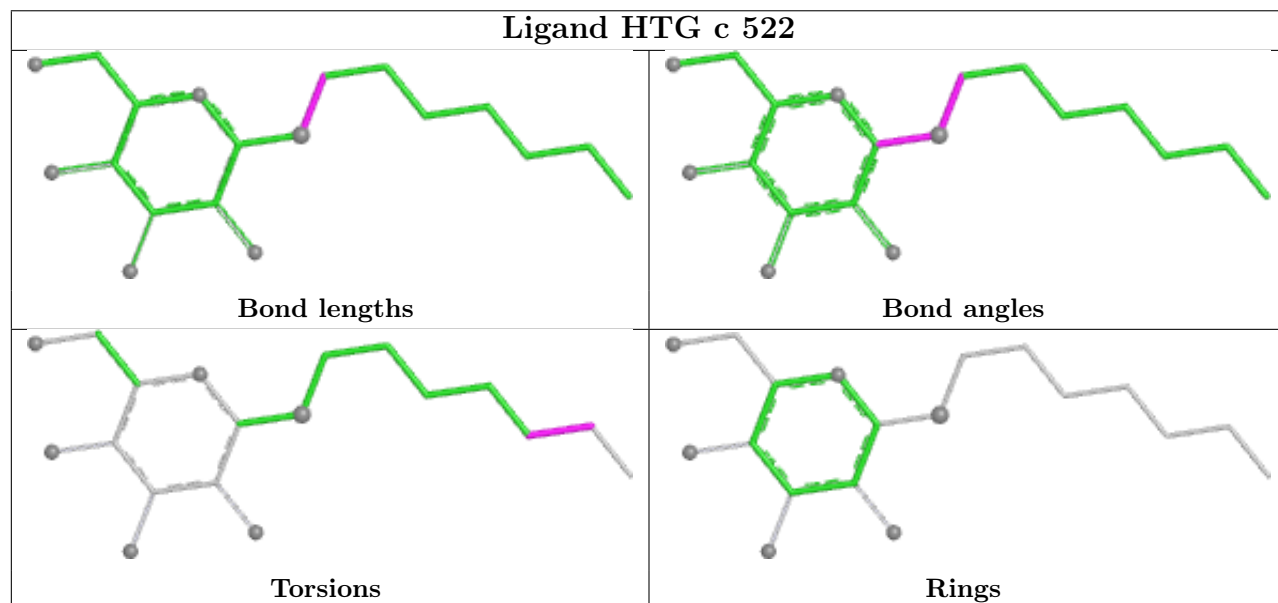
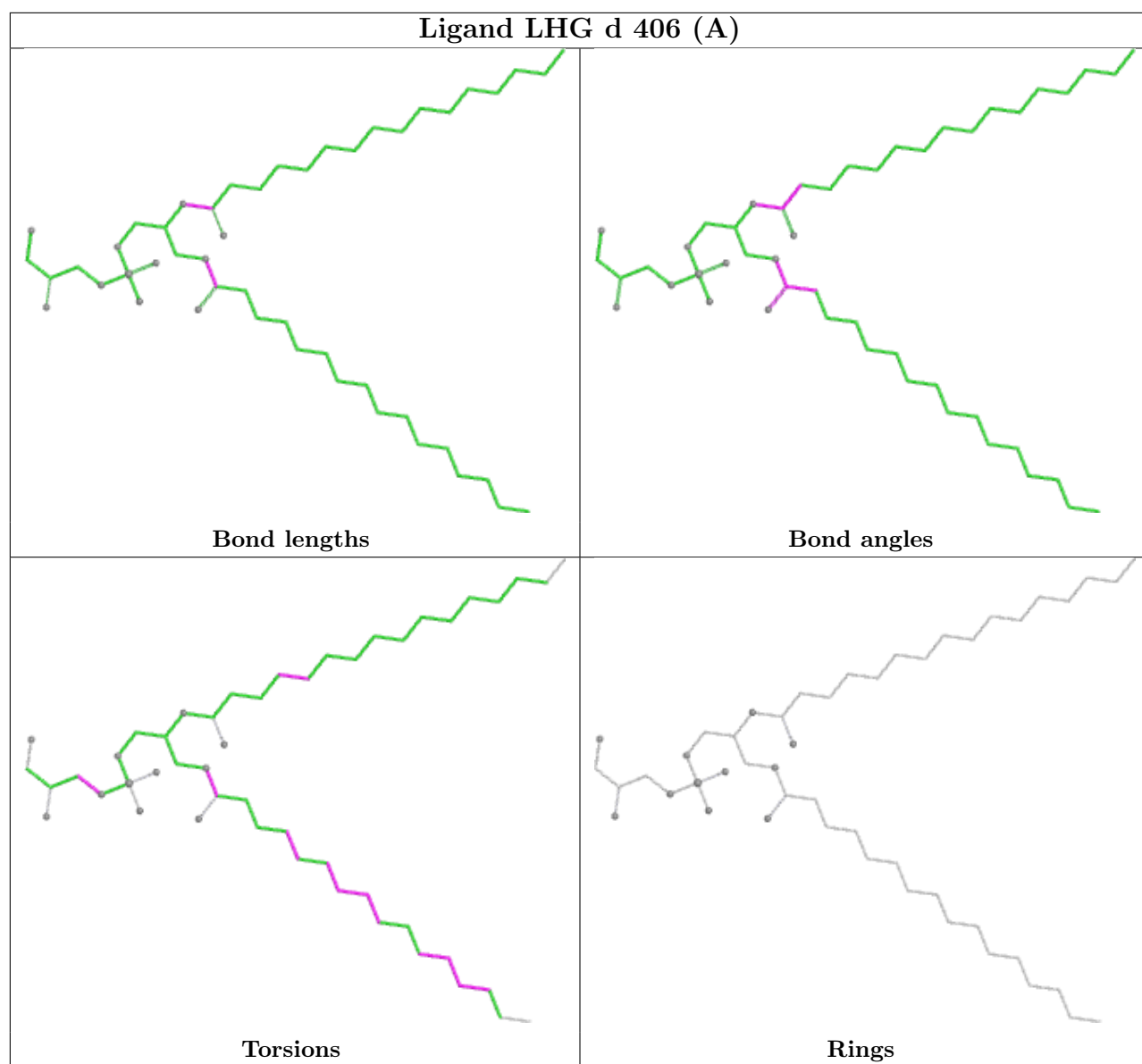


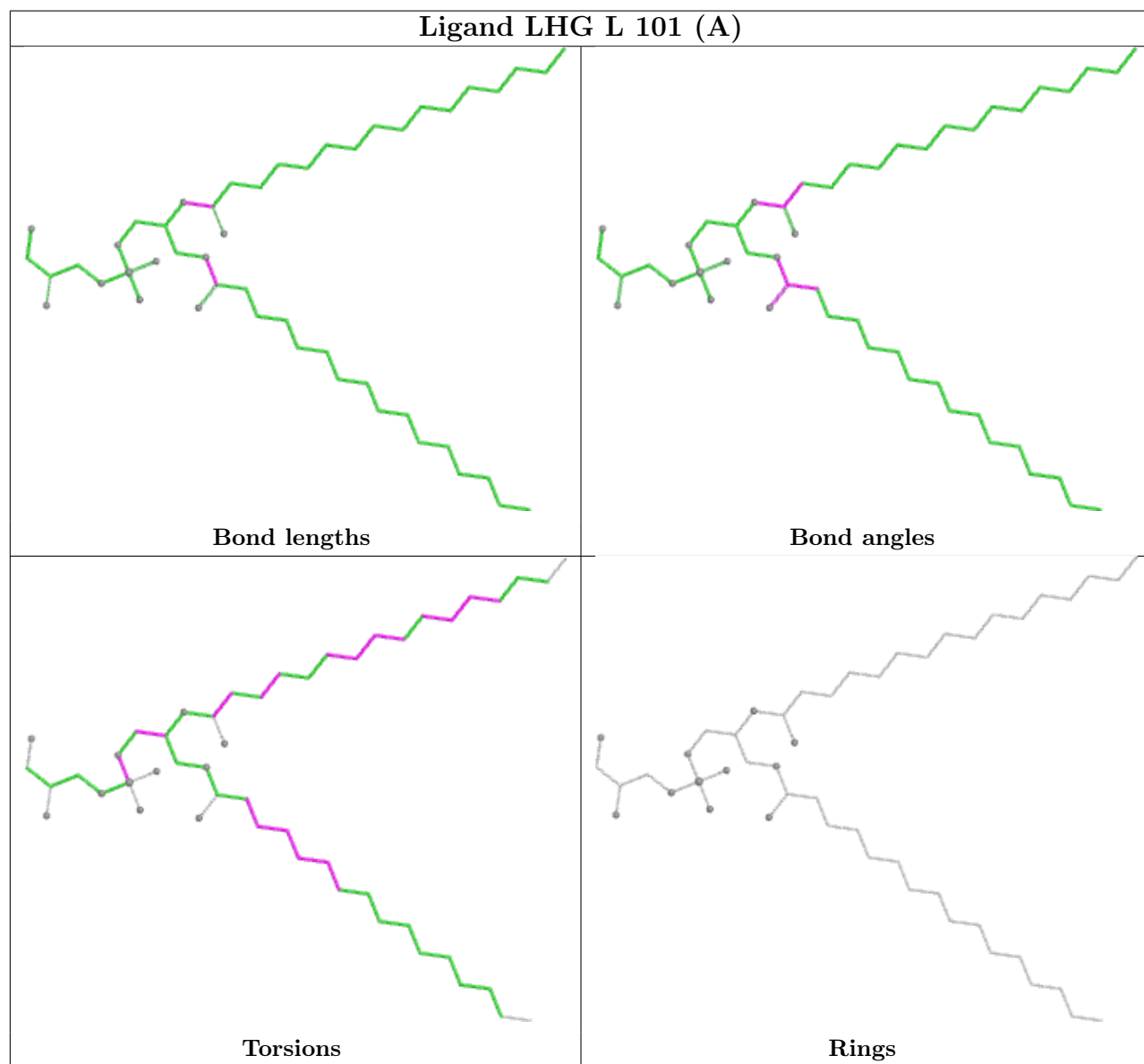
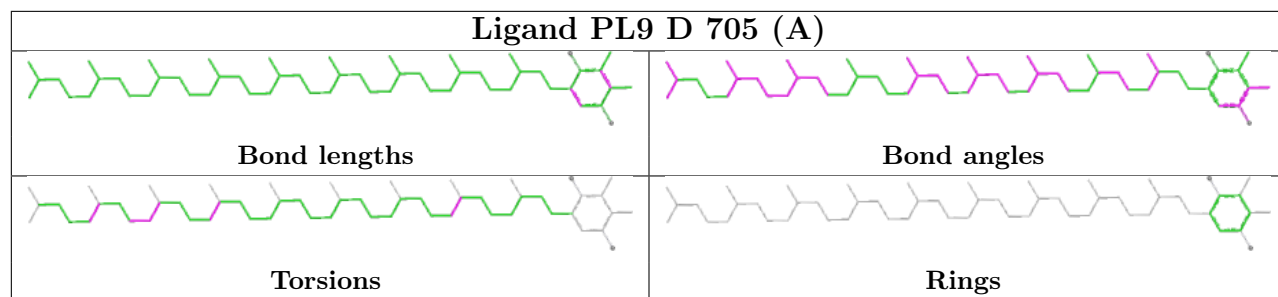
| Ligand CLA A 404 (B) |                    |
|----------------------|--------------------|
| <p>Bond lengths</p>  | <p>Bond angles</p> |
| <p>Torsions</p>      | <p>Rings</p>       |
| Ligand BCR y 101     |                    |
| <p>Bond lengths</p>  | <p>Bond angles</p> |
| <p>Torsions</p>      | <p>Rings</p>       |
| Ligand PL9 a 414 (B) |                    |
| <p>Bond lengths</p>  | <p>Bond angles</p> |
| <p>Torsions</p>      | <p>Rings</p>       |

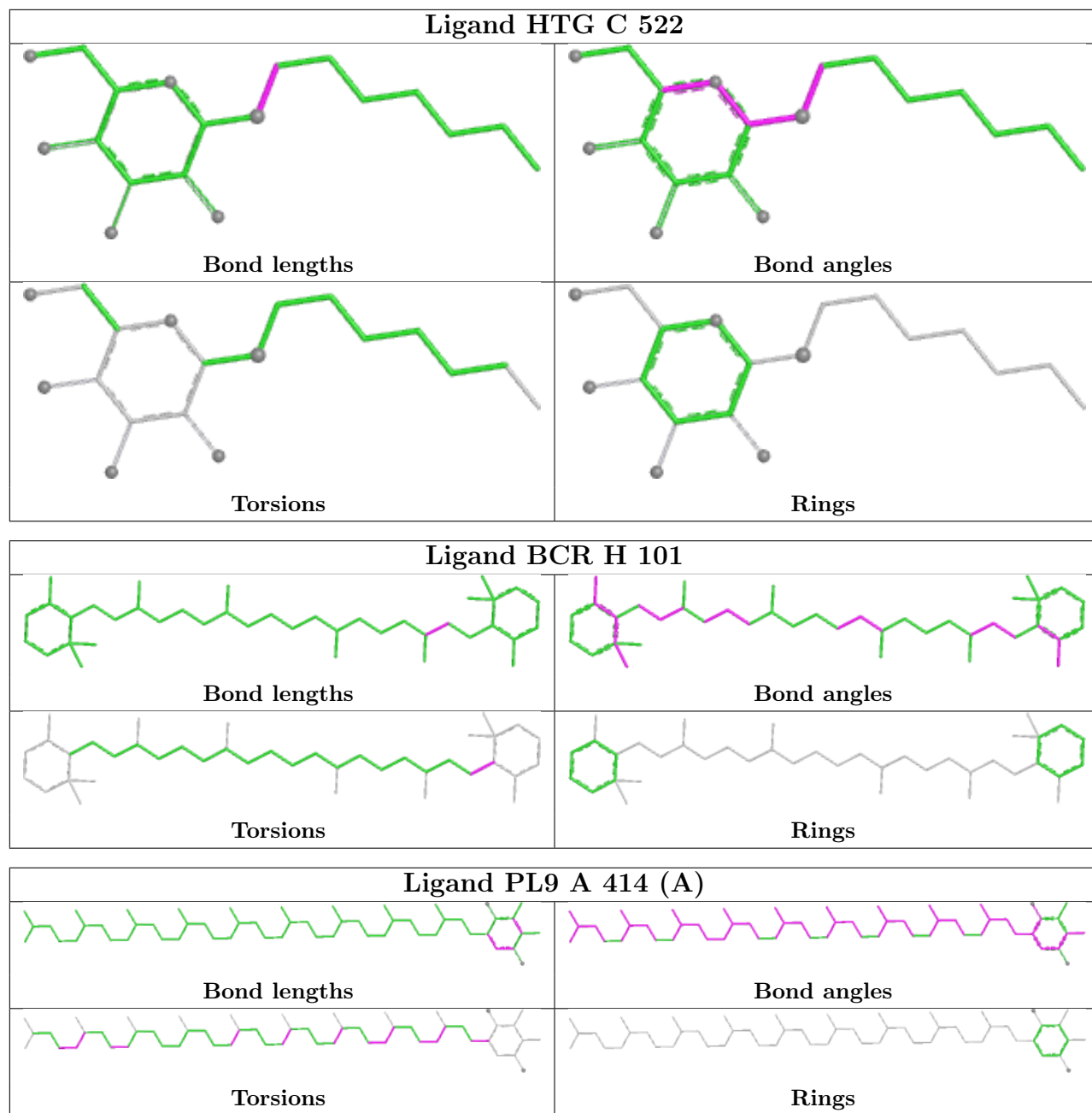




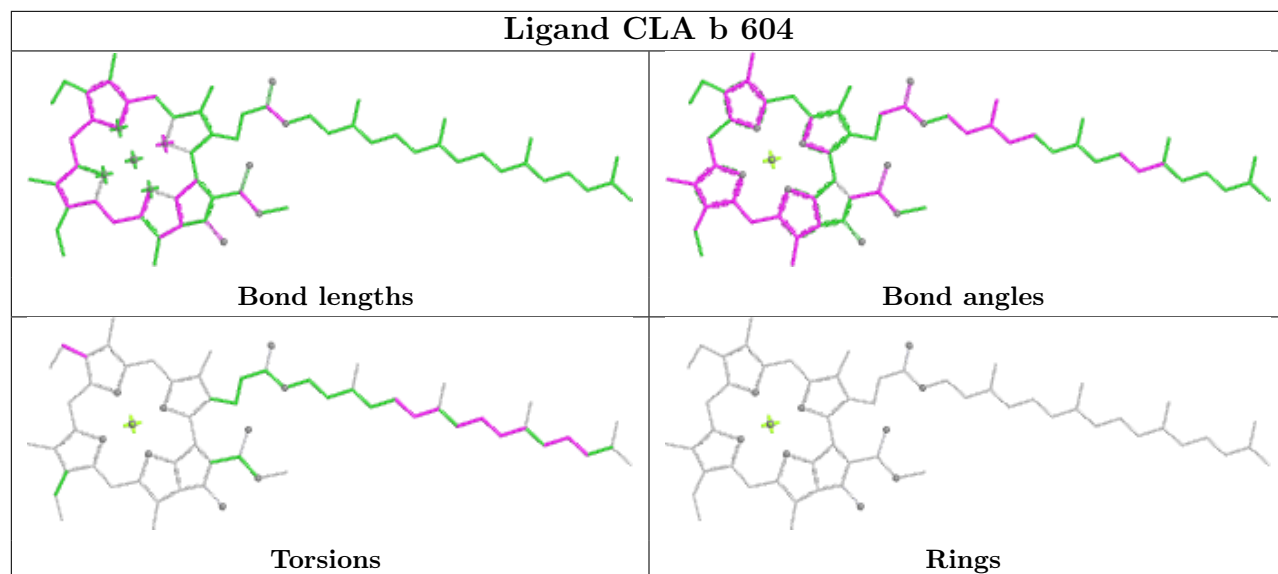
**Ligand CLA C 503****Ligand CLA B 604**



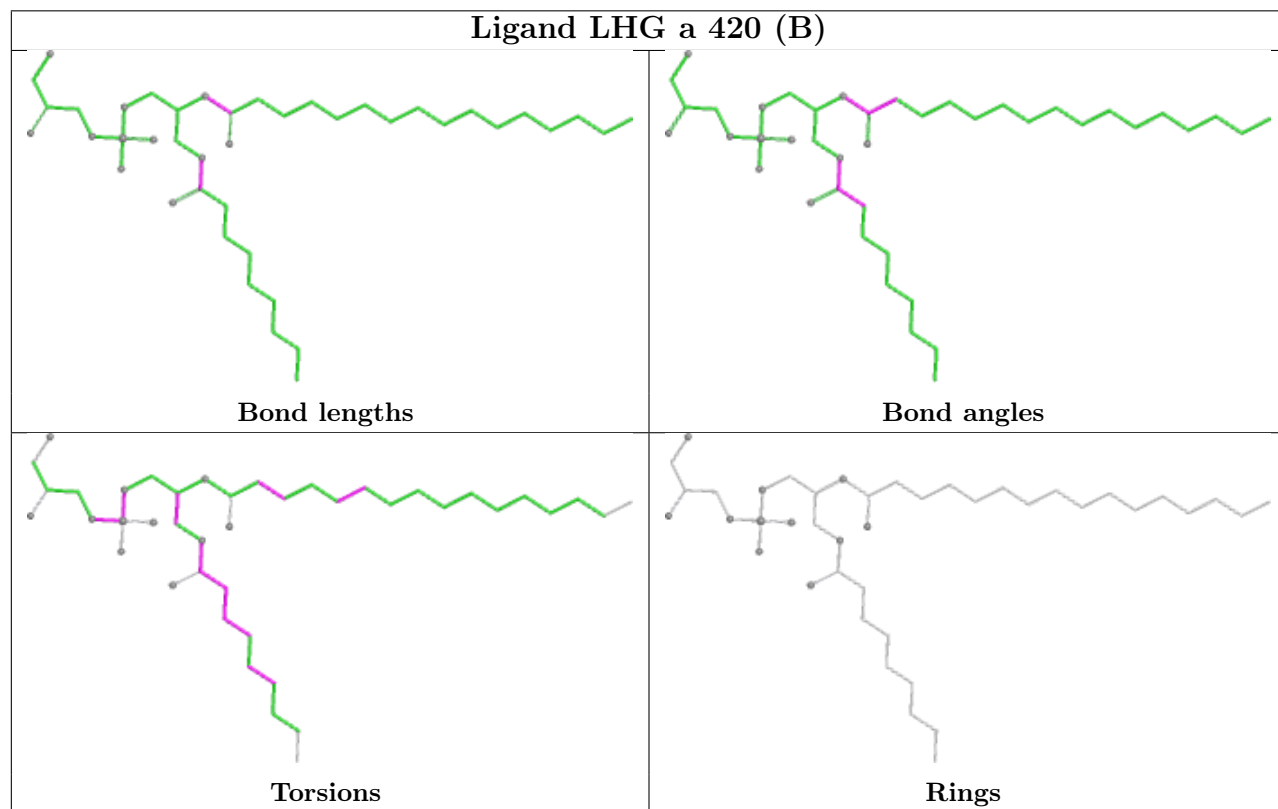




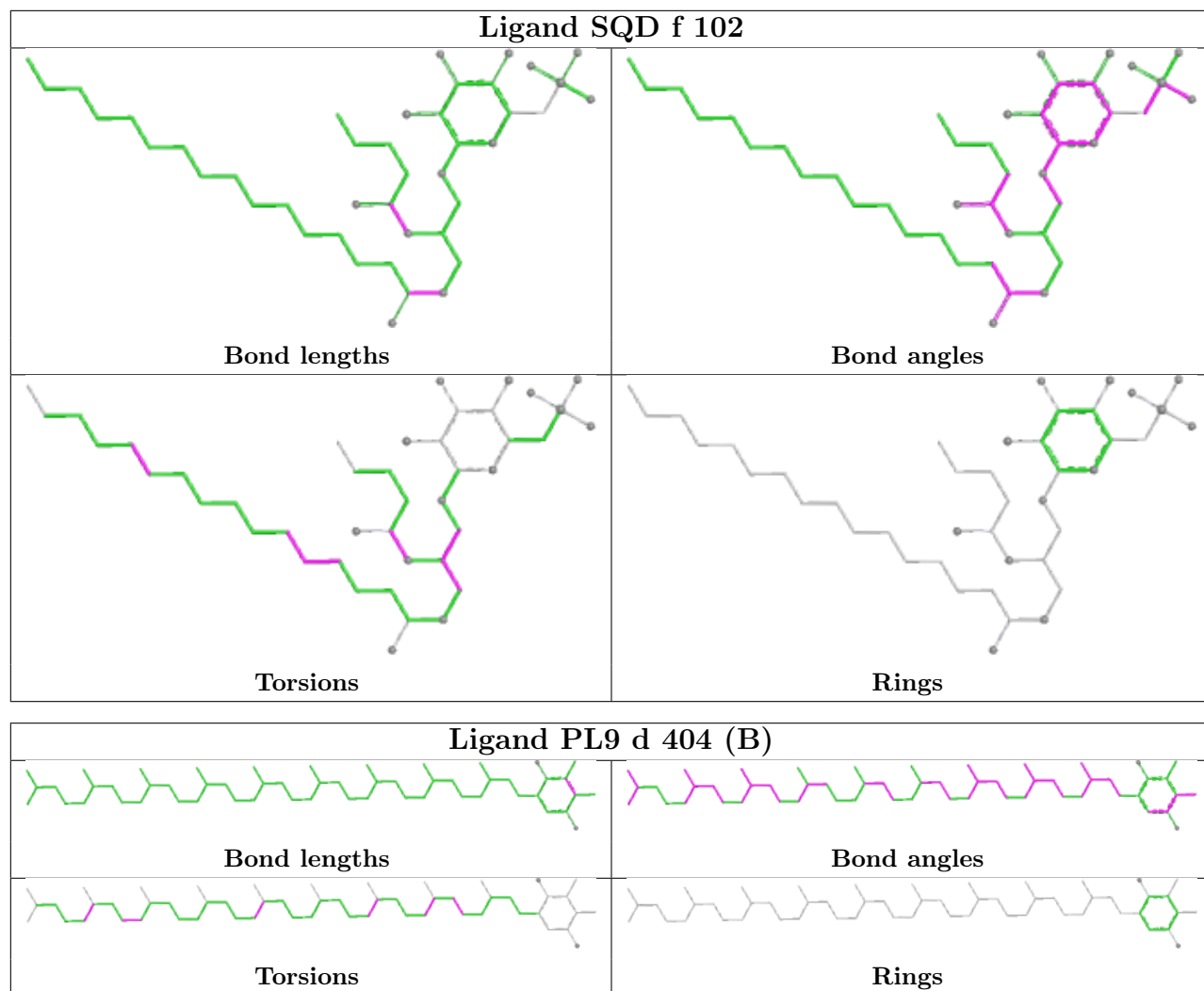
## Ligand CLA b 604

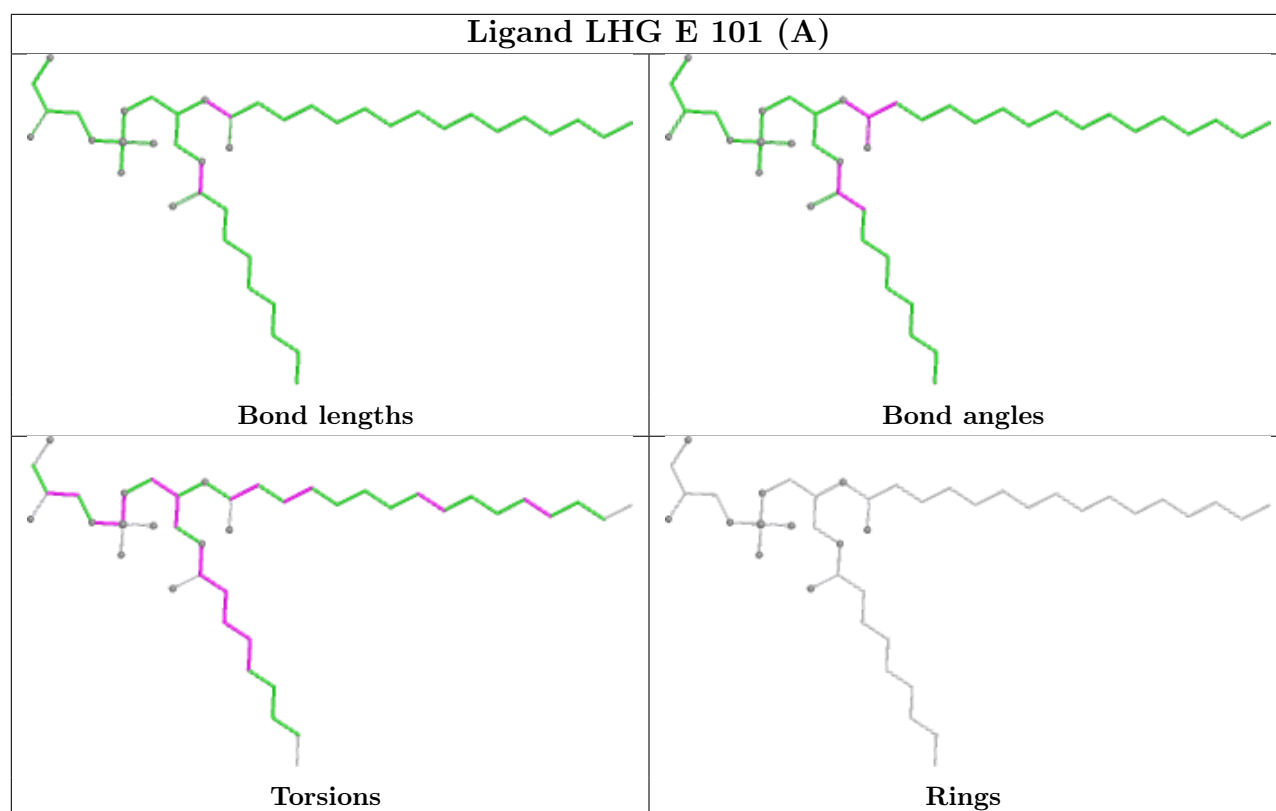


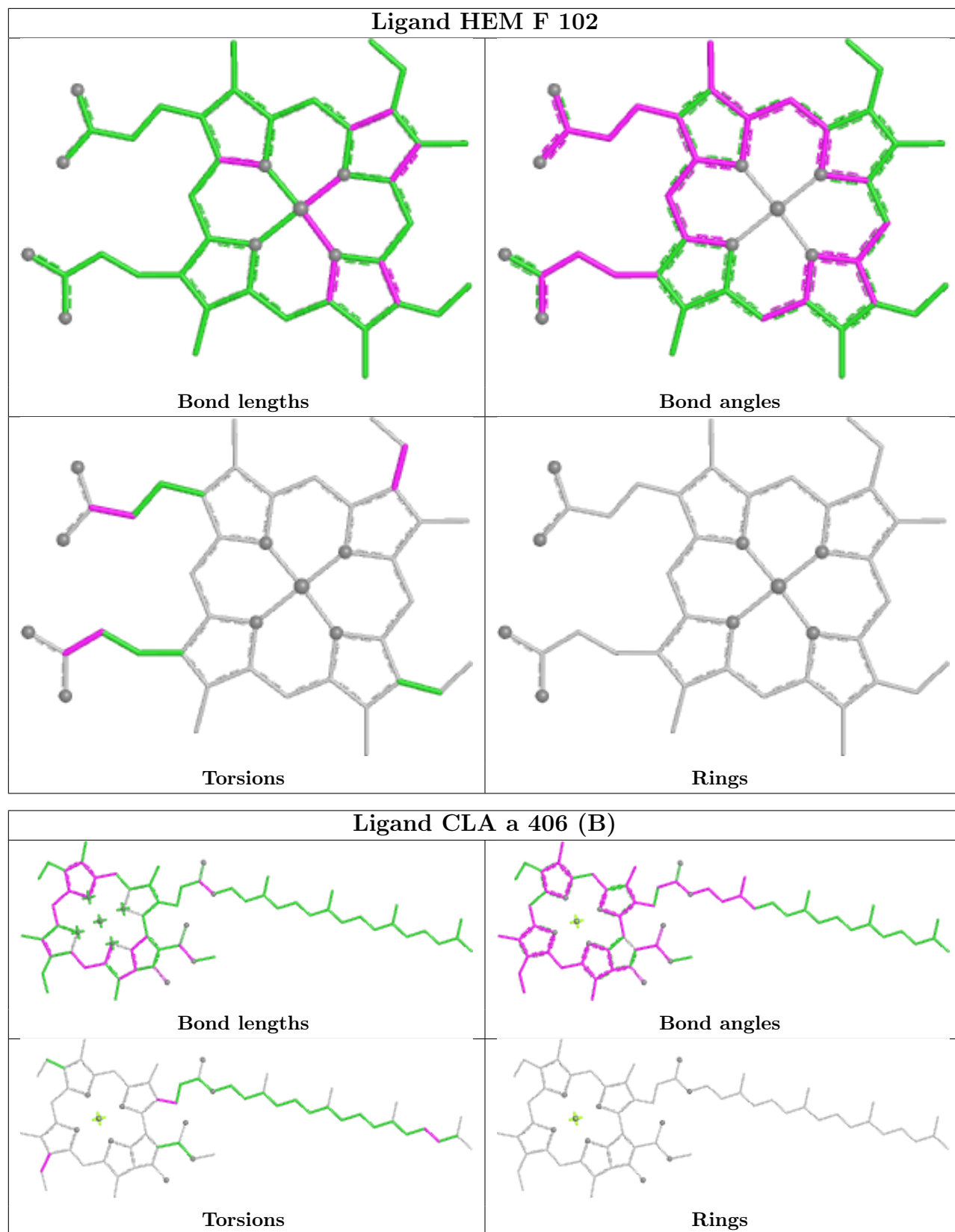
## Ligand LHG a 420 (B)

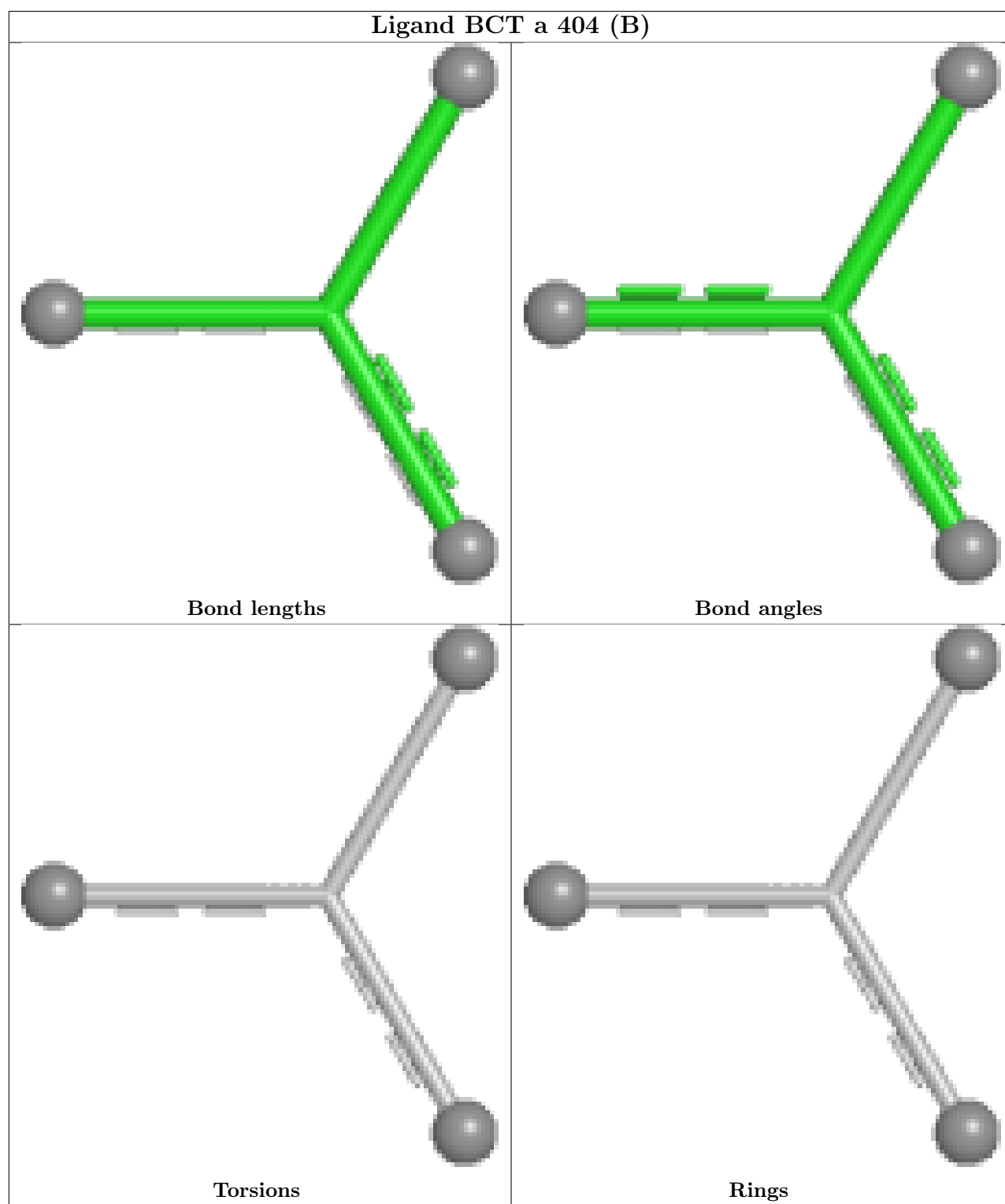


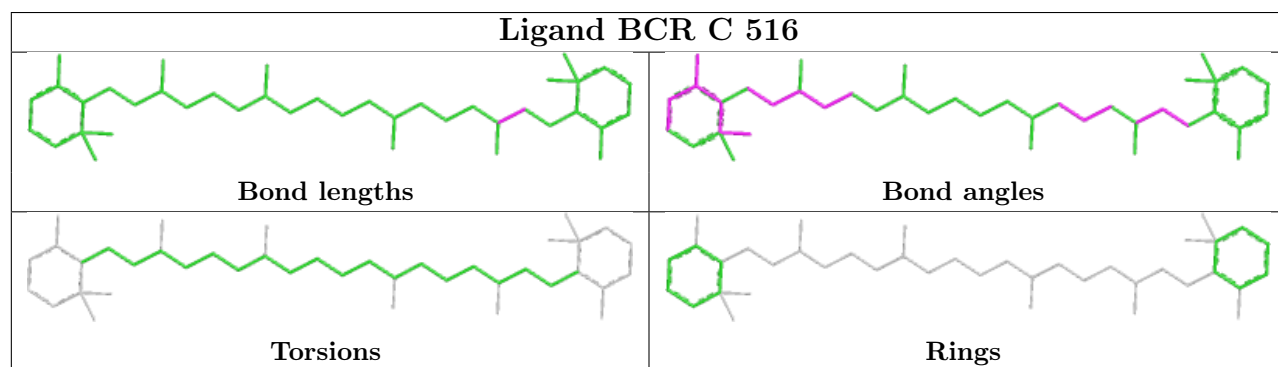
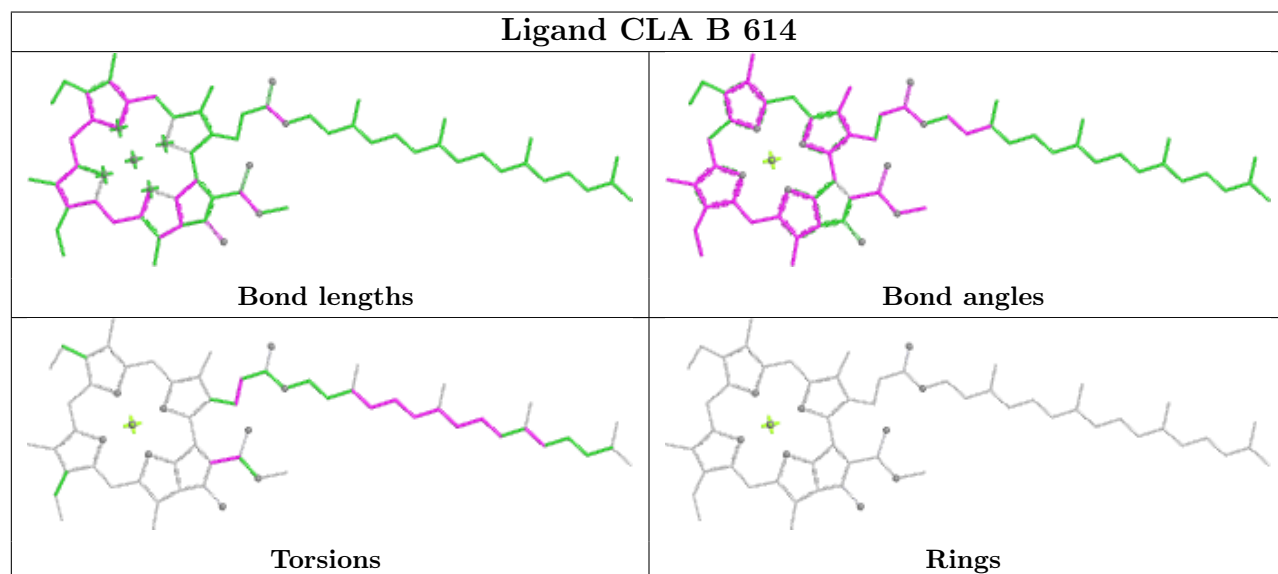
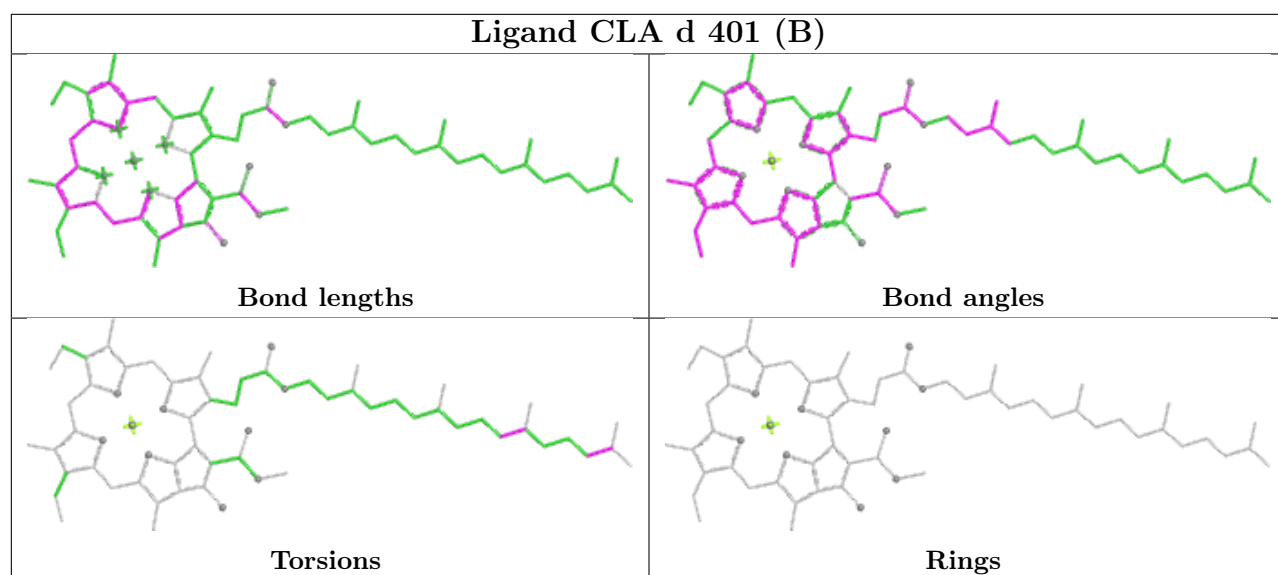


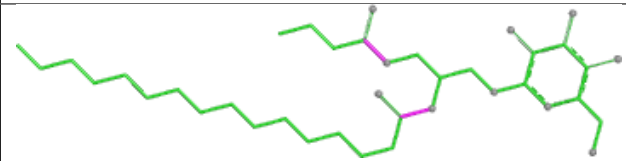
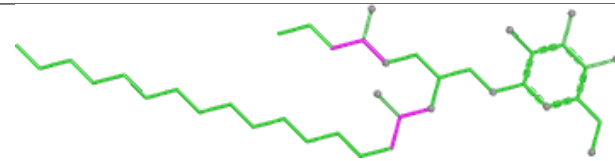
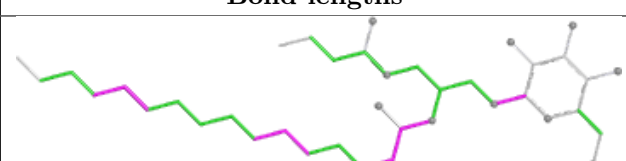
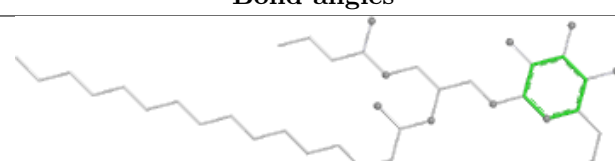
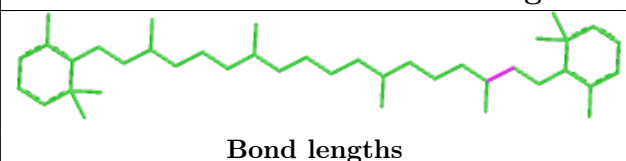
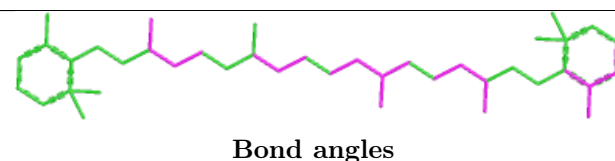
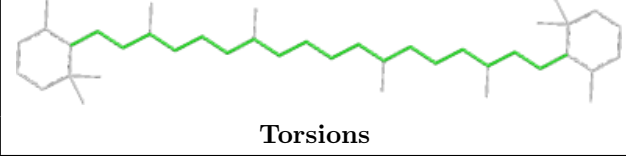
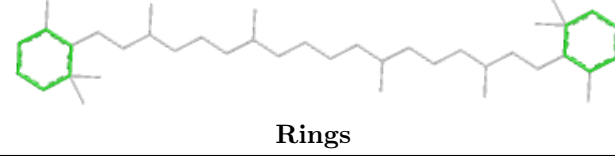
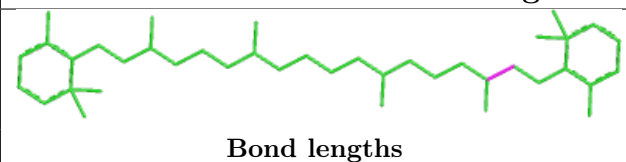
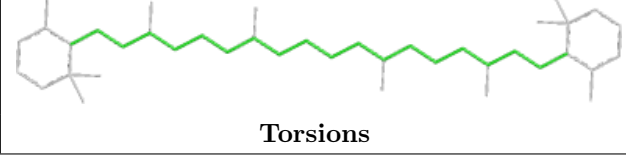
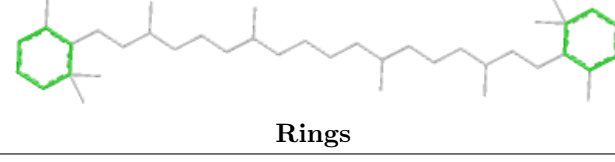
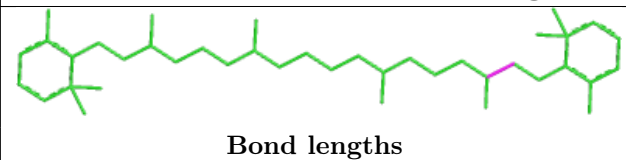
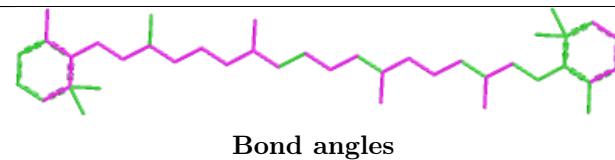
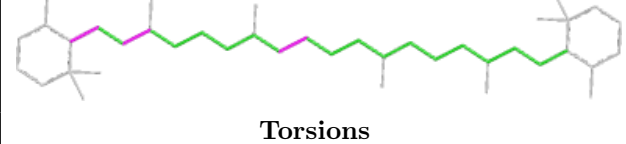
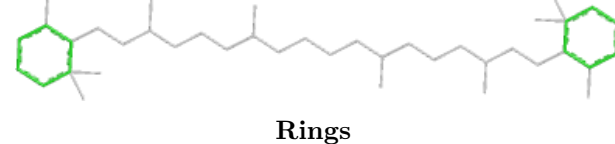


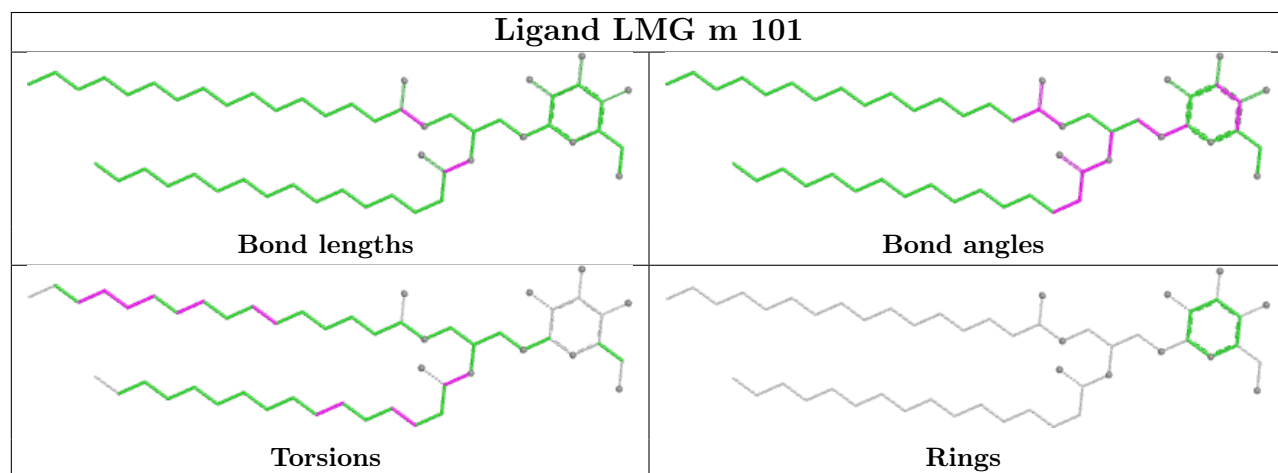
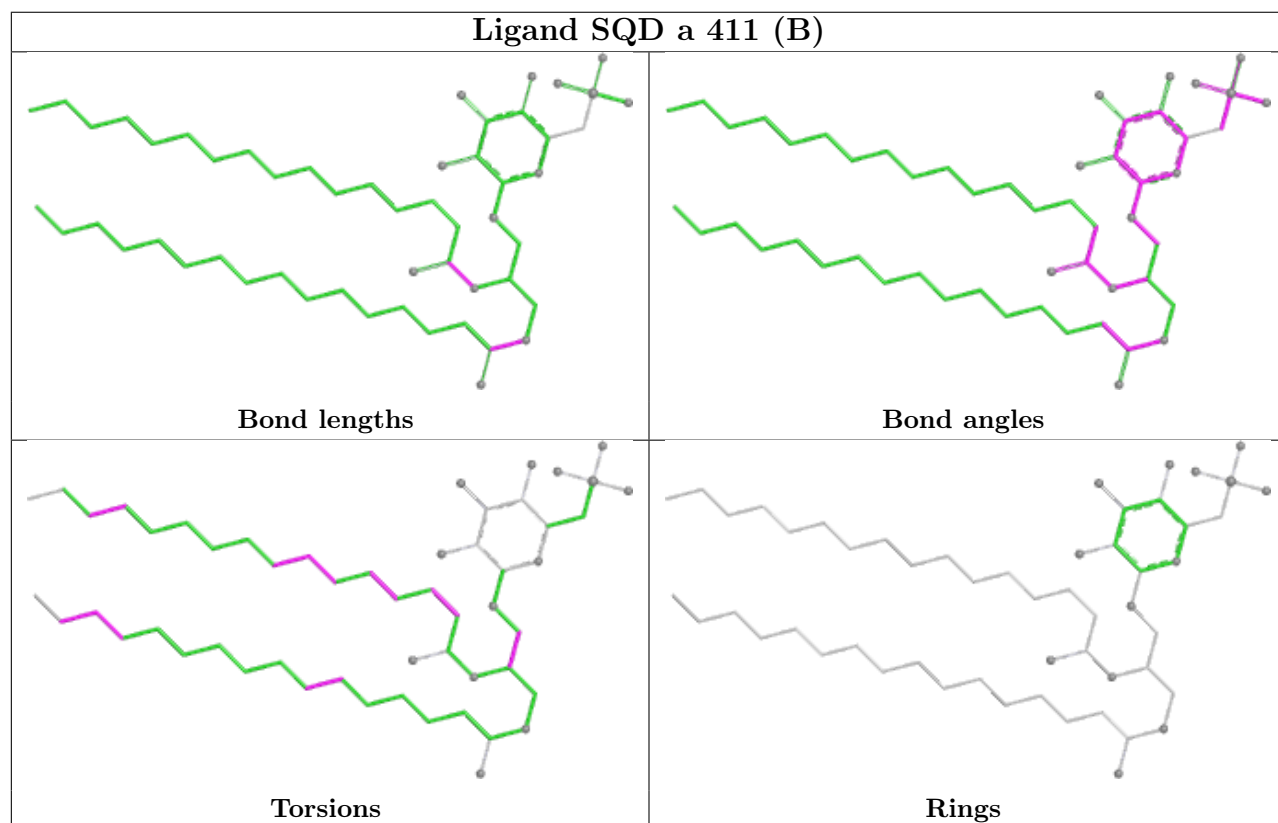
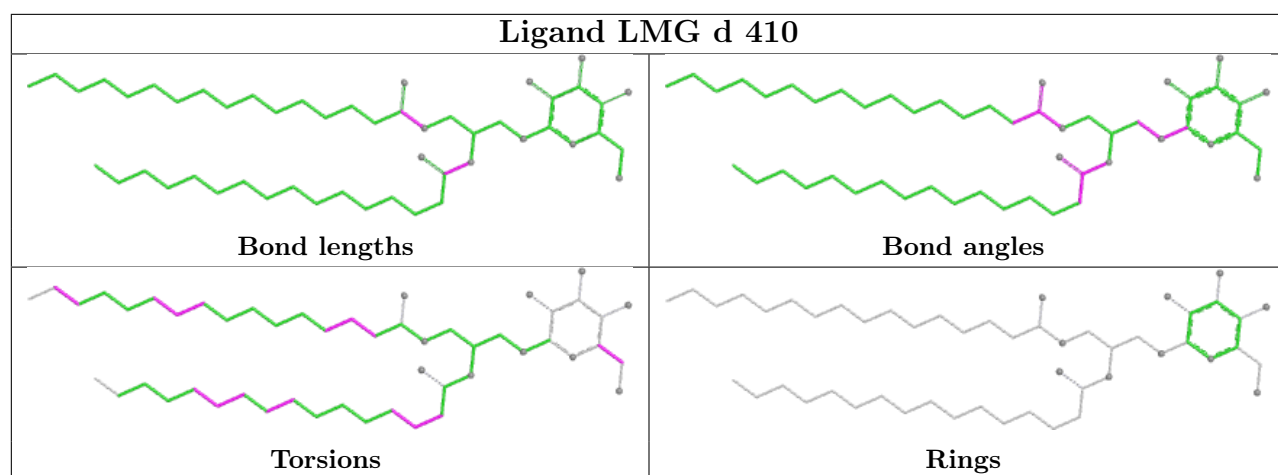




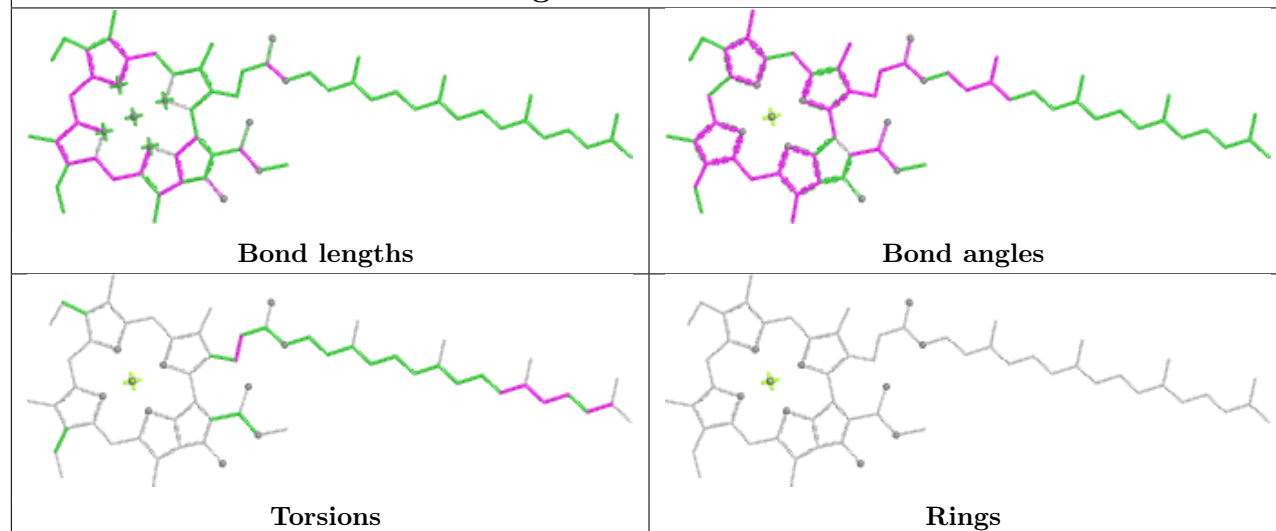




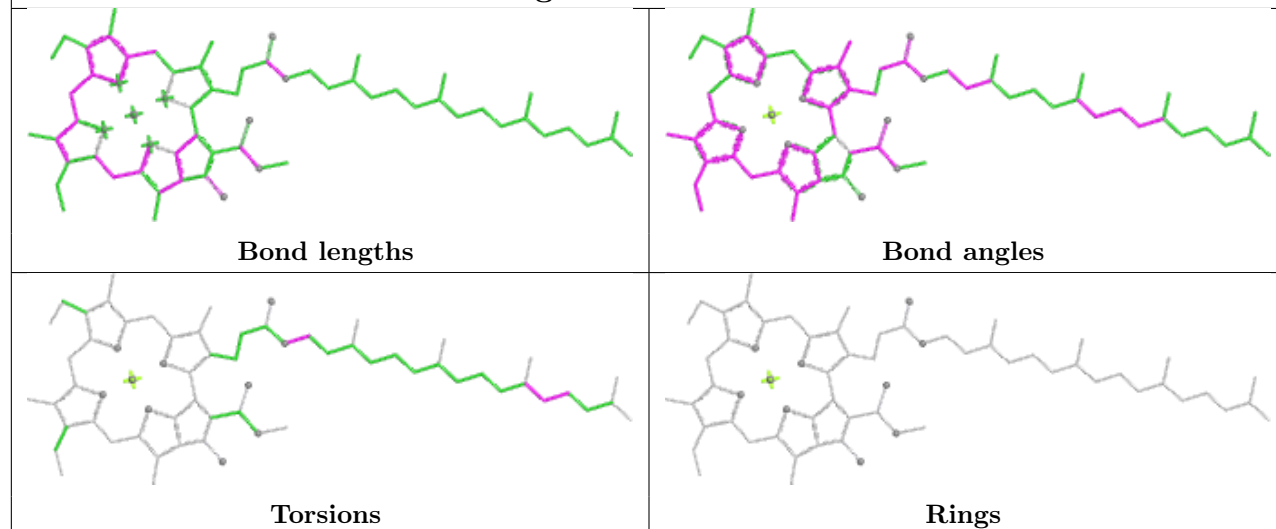
| Ligand LMG z 101                                                                                    |                                                                                                     |
|-----------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------|
| <br>Bond lengths   | <br>Bond angles   |
| <br>Torsions       | <br>Rings         |
| Ligand BCR c 515                                                                                    |                                                                                                     |
| <br>Bond lengths   | <br>Bond angles   |
| <br>Torsions       | <br>Rings         |
| Ligand BCR h 101                                                                                    |                                                                                                     |
| <br>Bond lengths | <br>Bond angles |
| <br>Torsions     | <br>Rings       |
| Ligand BCR t 102                                                                                    |                                                                                                     |
| <br>Bond lengths | <br>Bond angles |
| <br>Torsions     | <br>Rings       |



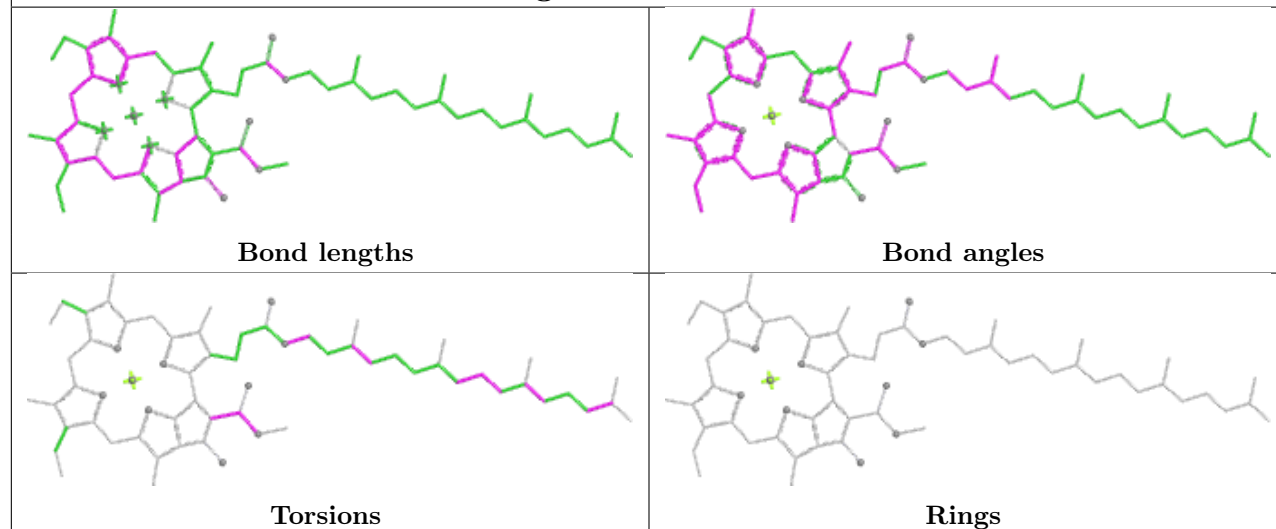
## Ligand CLA B 610



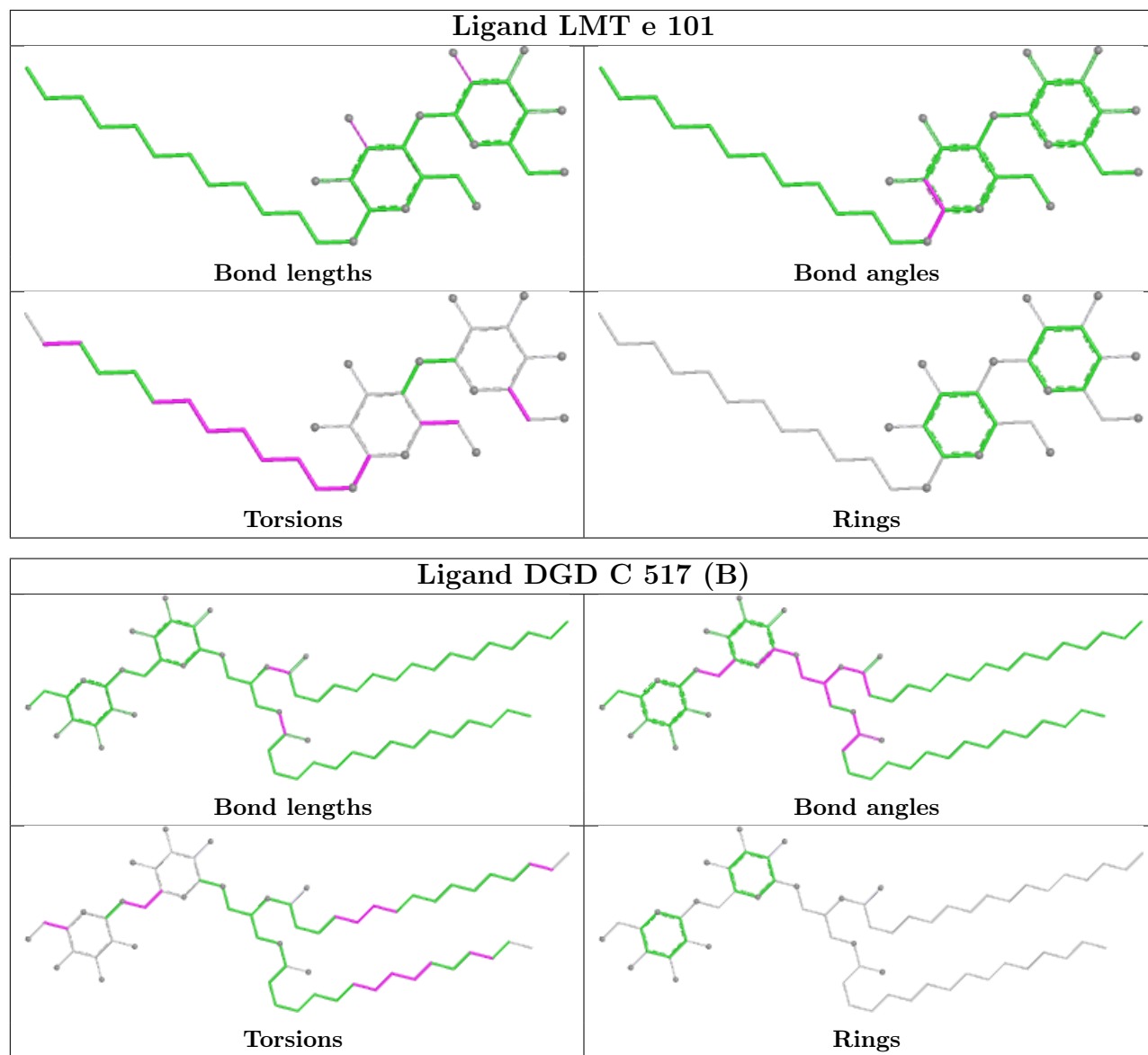
## Ligand CLA b 608



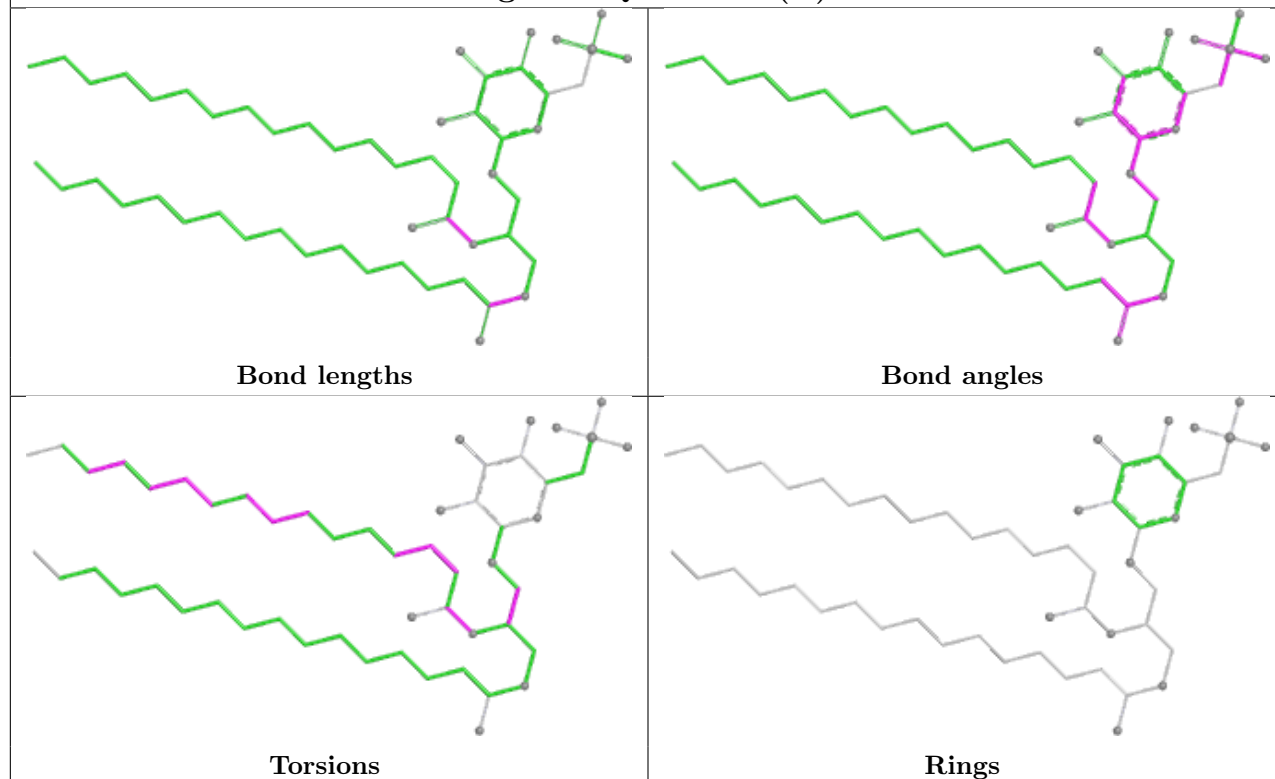
## Ligand CLA b 614



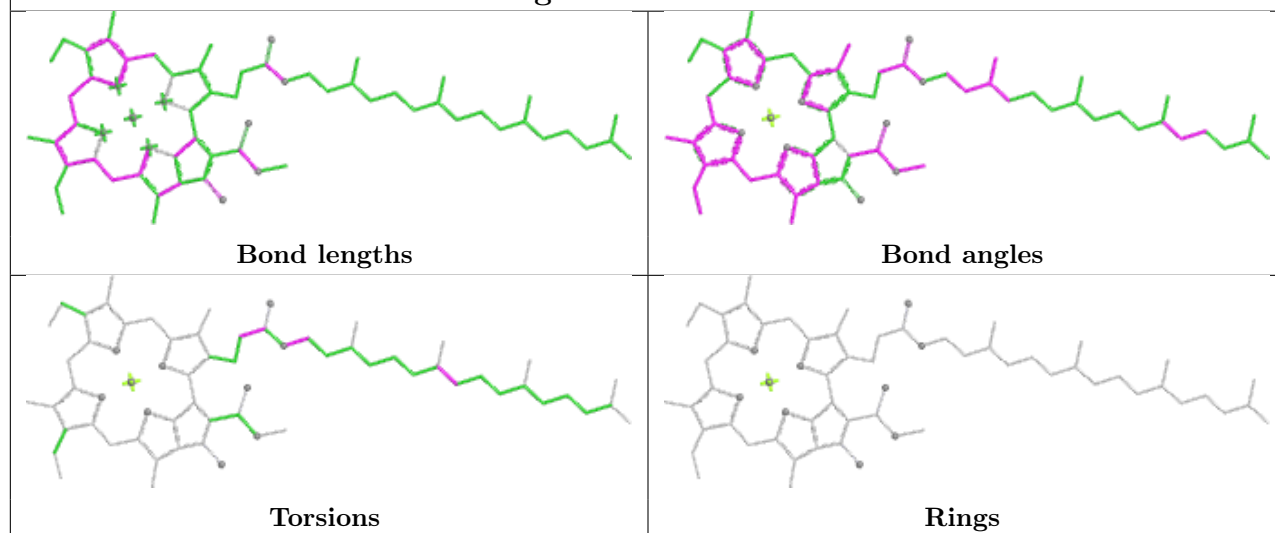


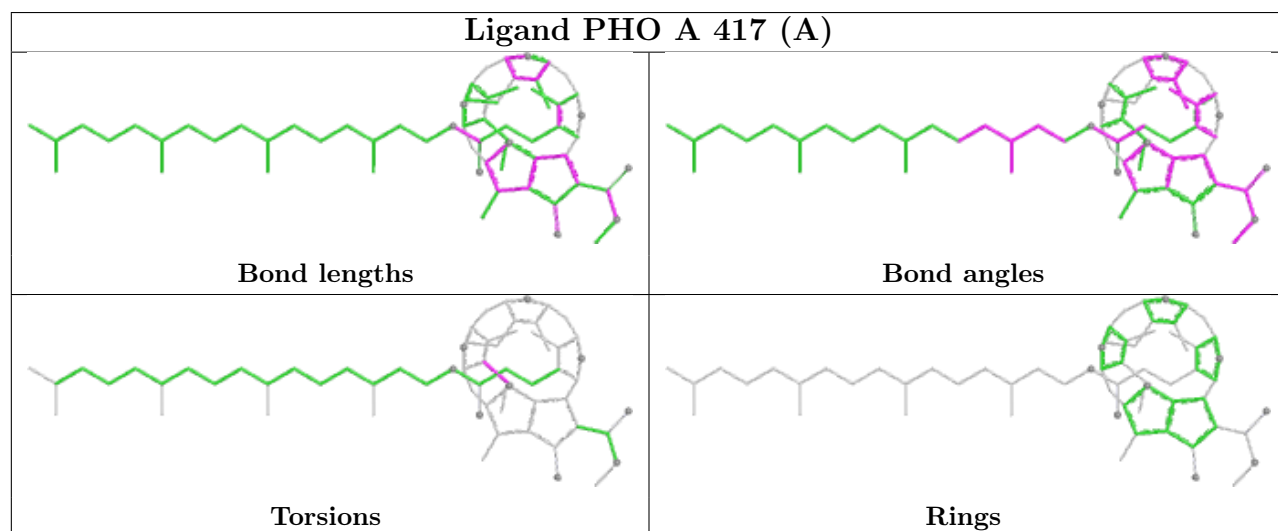
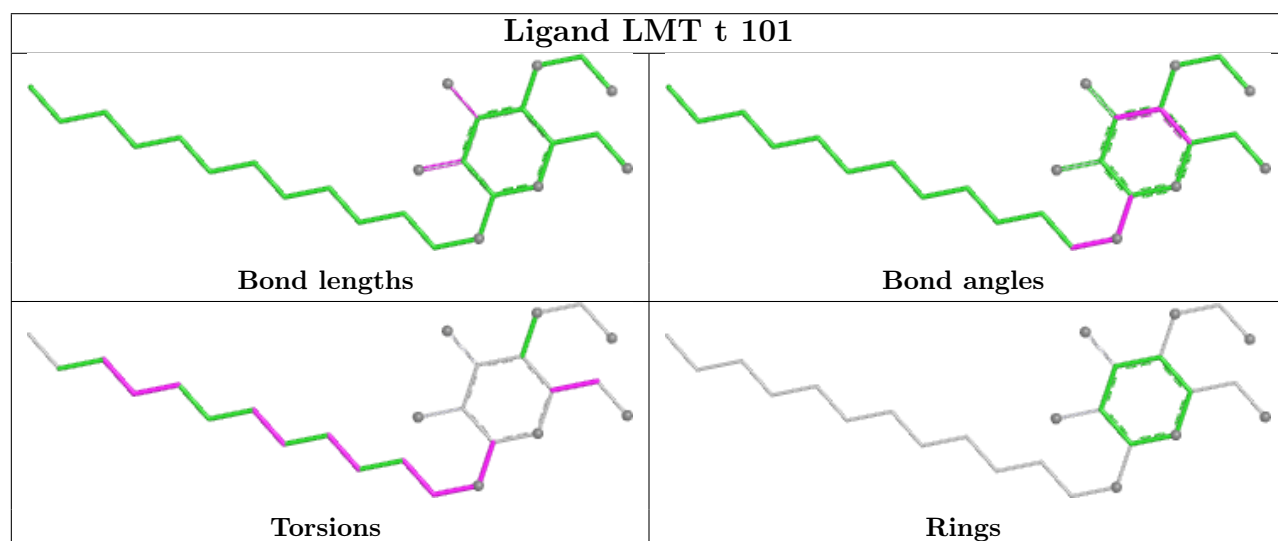
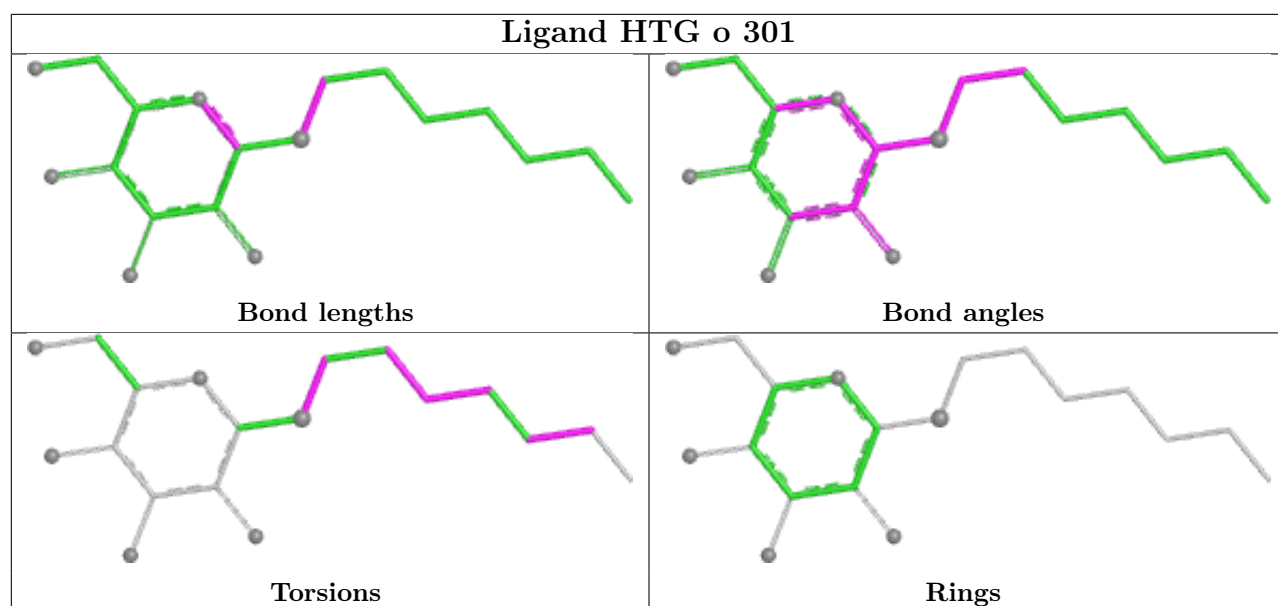


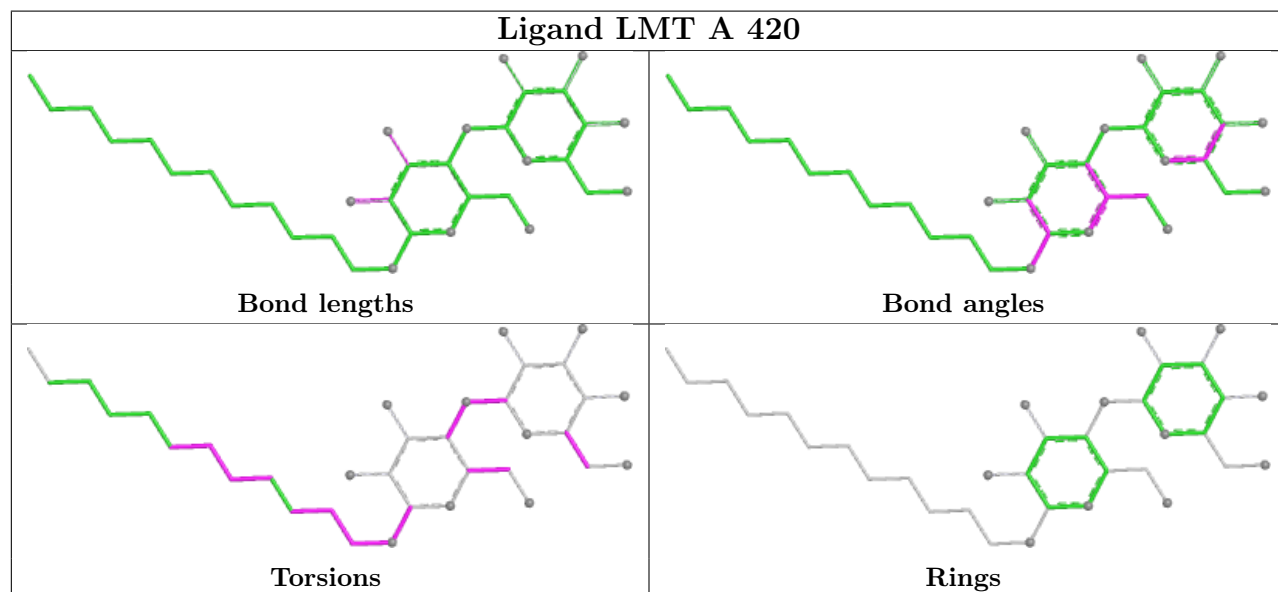
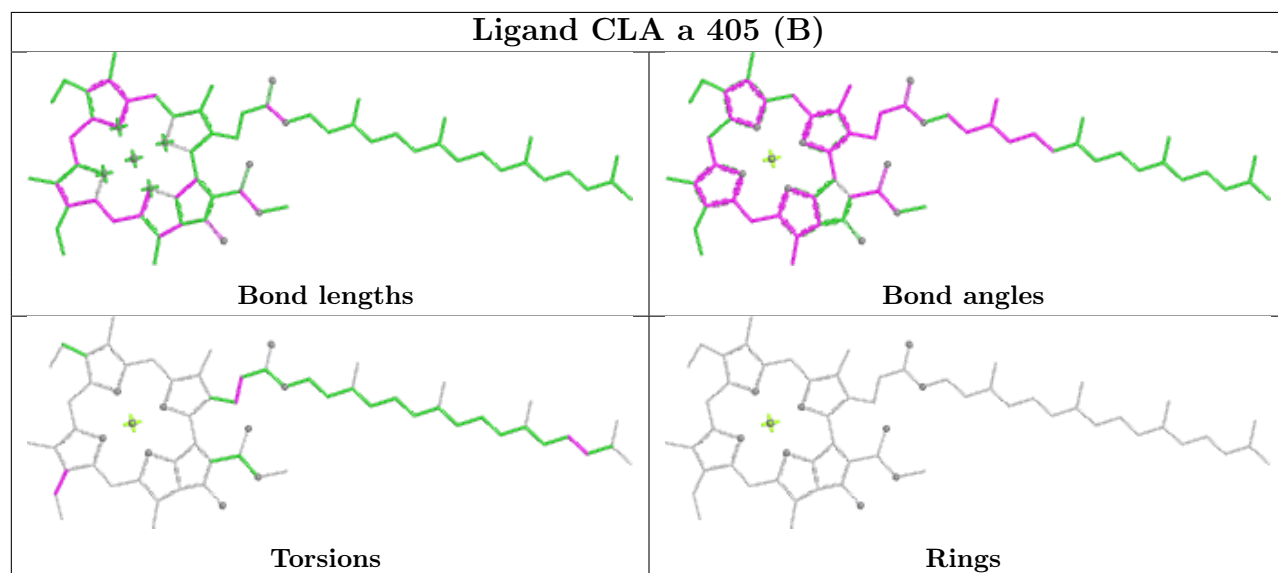
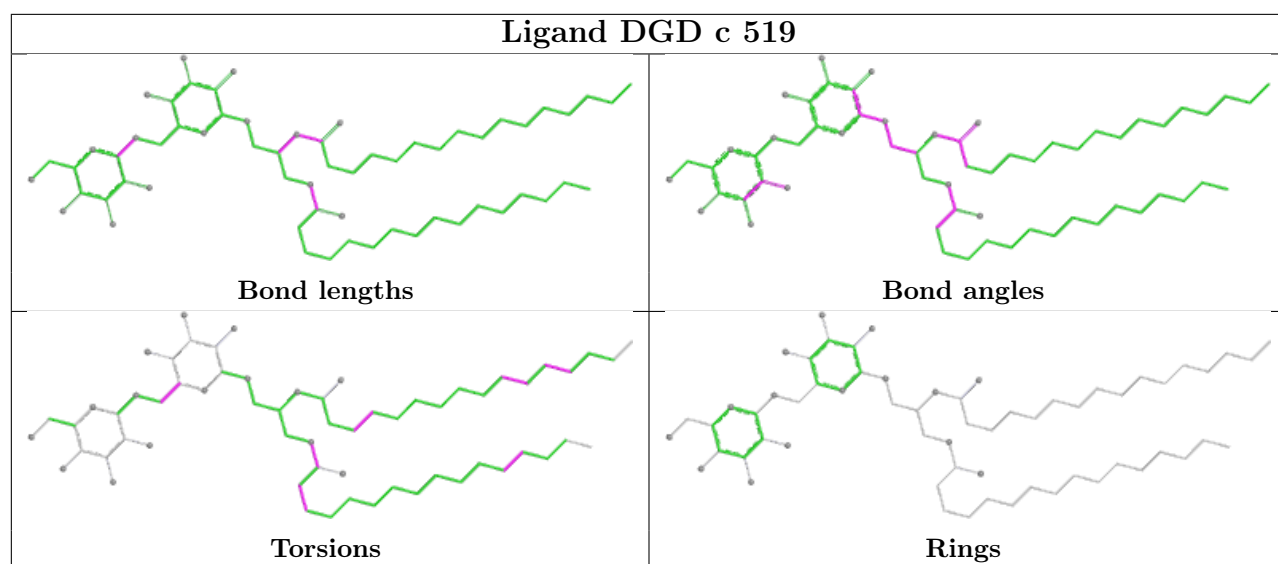
## Ligand SQD A 410 (B)



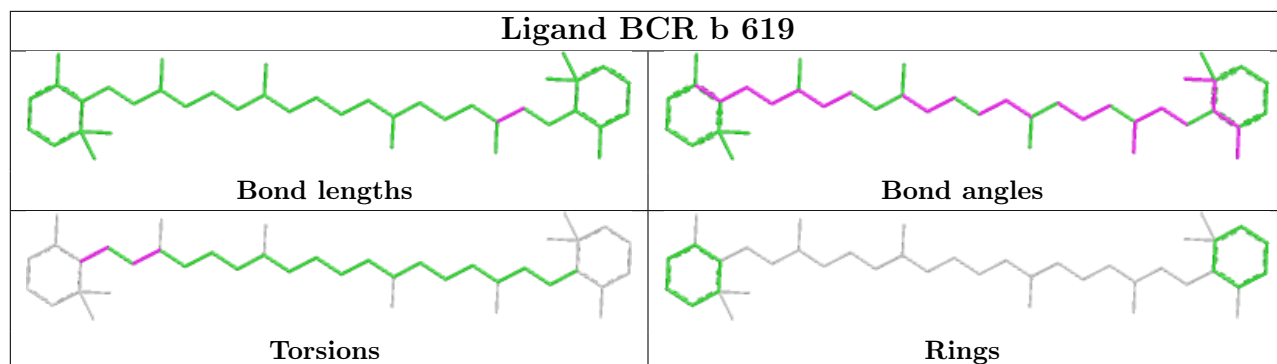
## Ligand CLA b 613



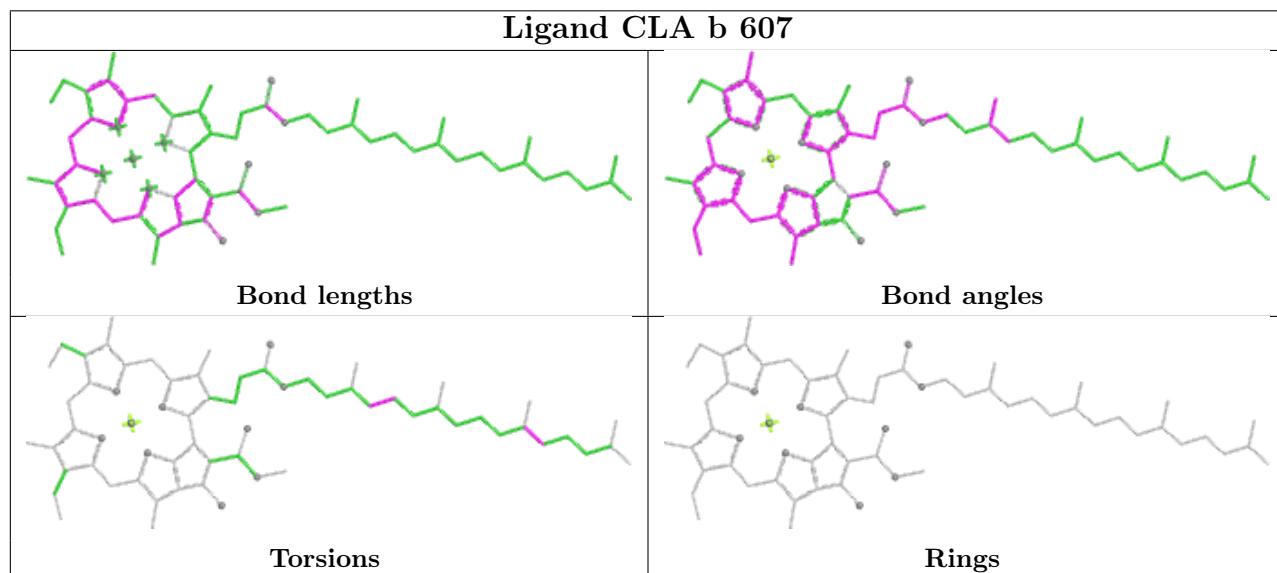




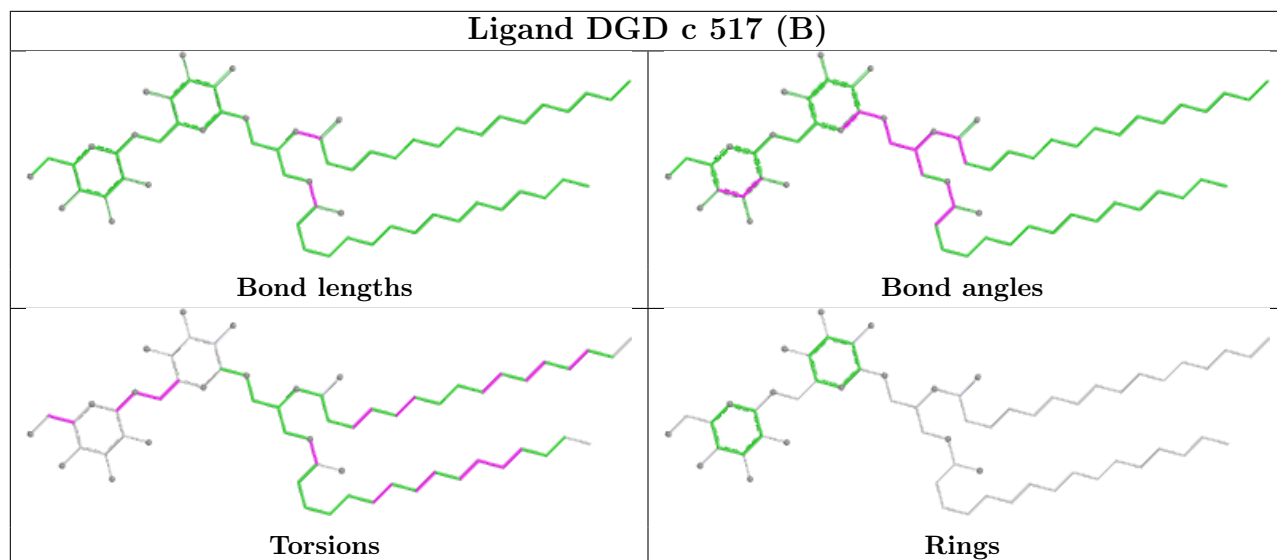
## Ligand BCR b 619



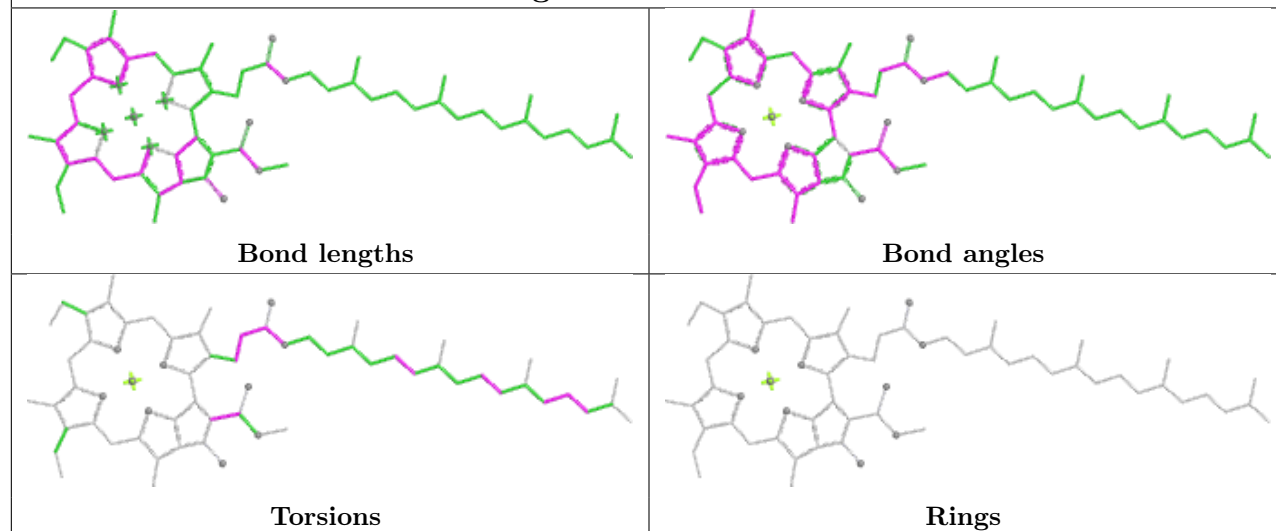
## Ligand CLA b 607



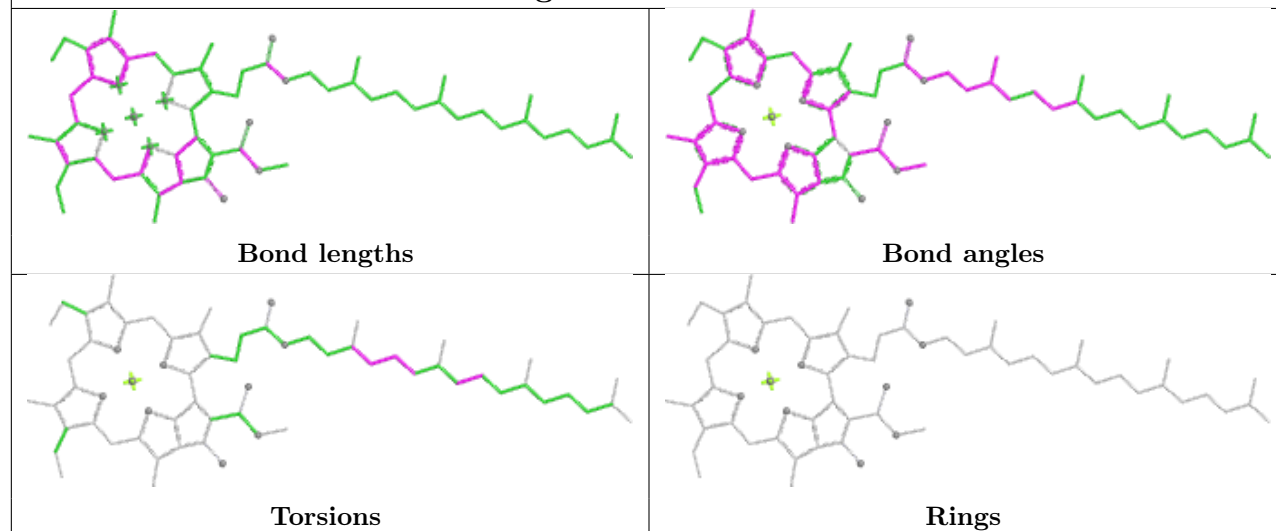
## Ligand DGD c 517 (B)



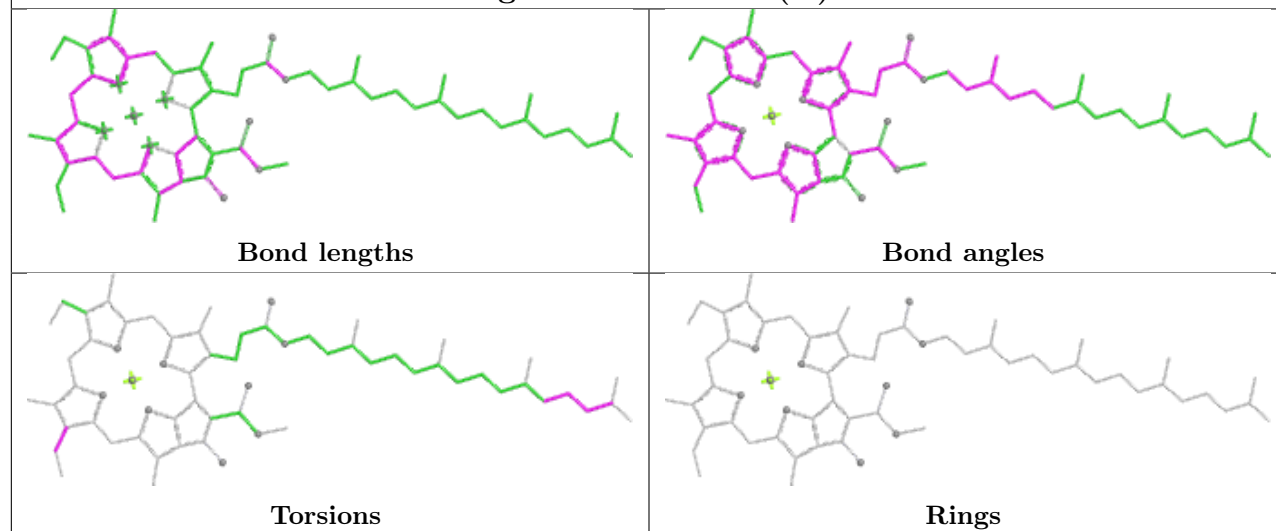
## Ligand CLA B 601

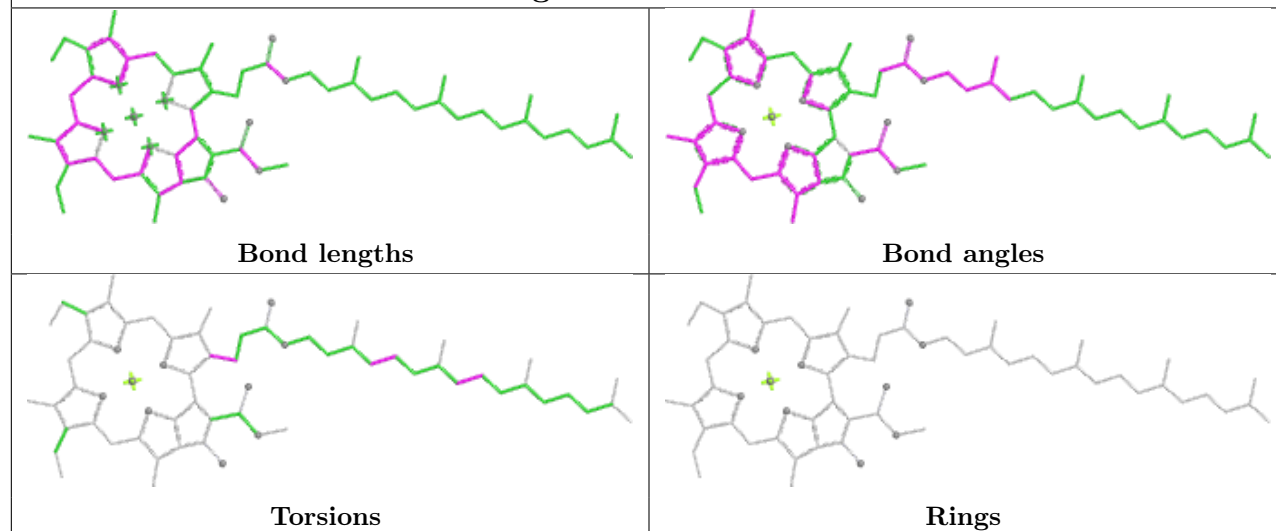
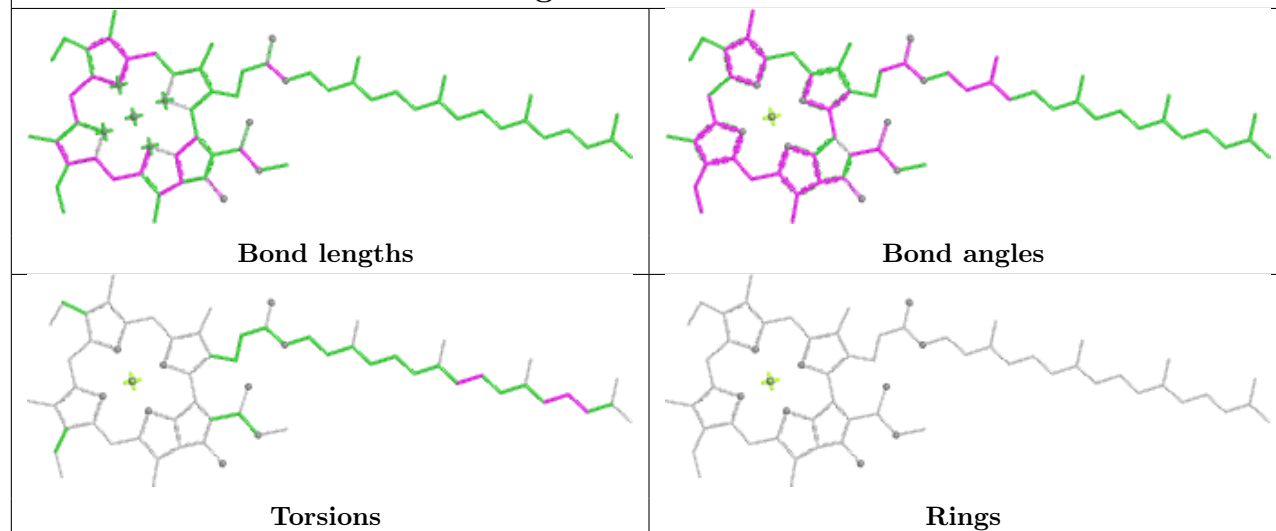


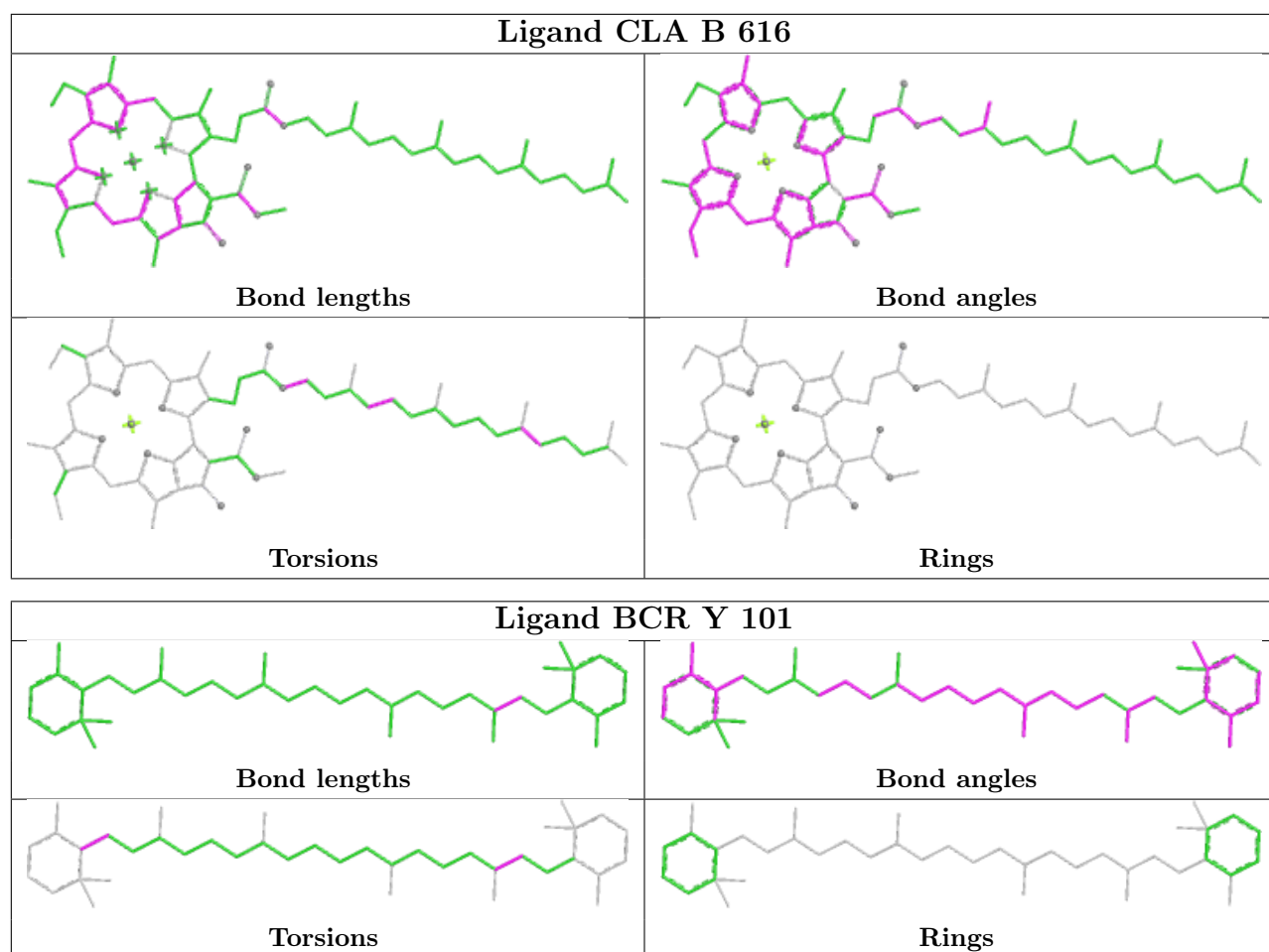
## Ligand CLA b 605



## Ligand CLA A 404 (A)

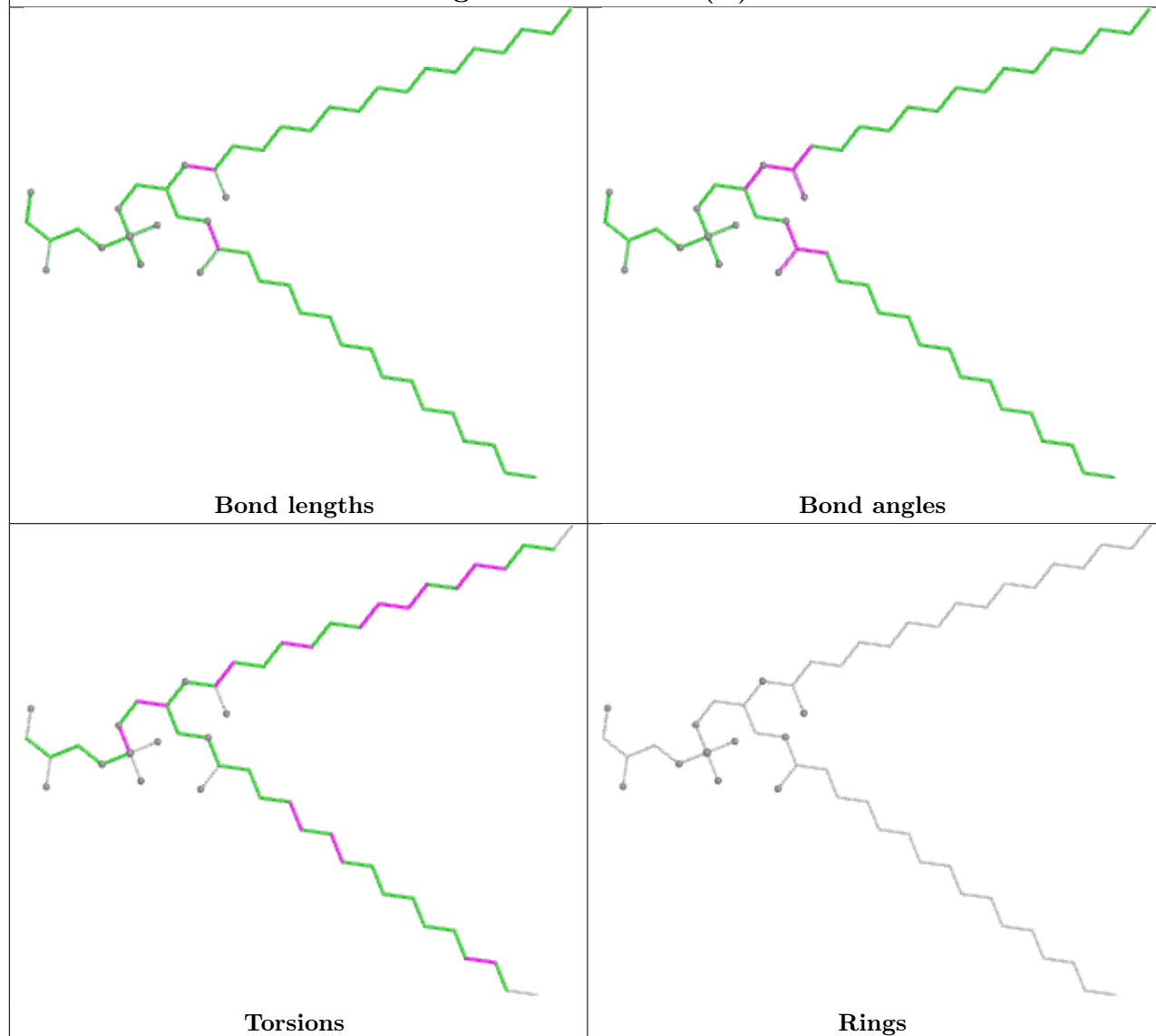


**Ligand CLA C 512****Ligand CLA b 611****Ligand PL9 a 414 (A)**

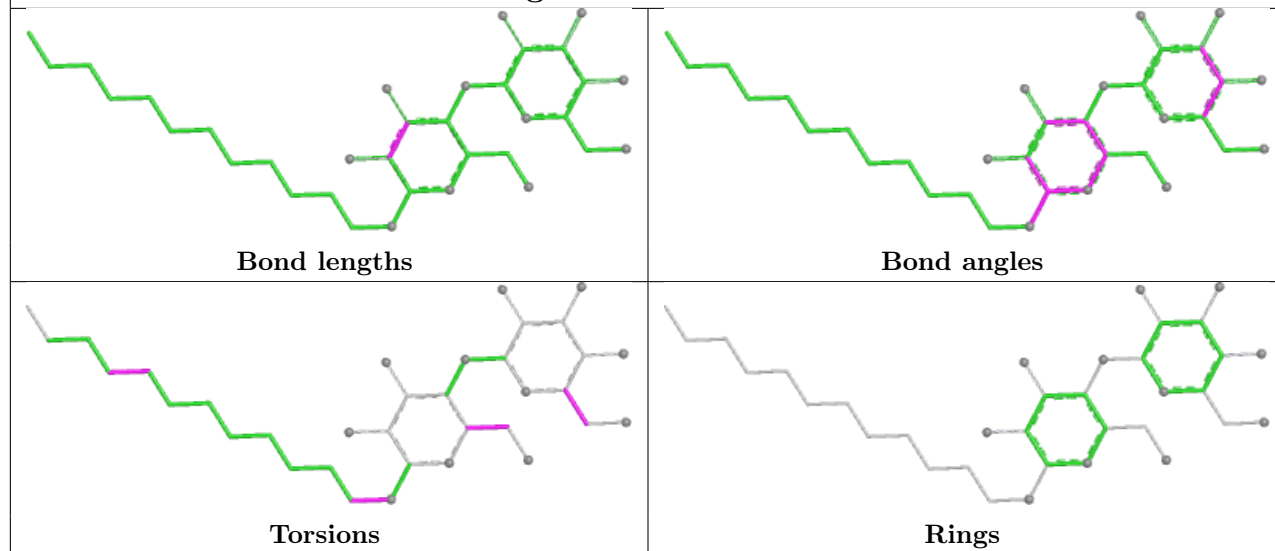




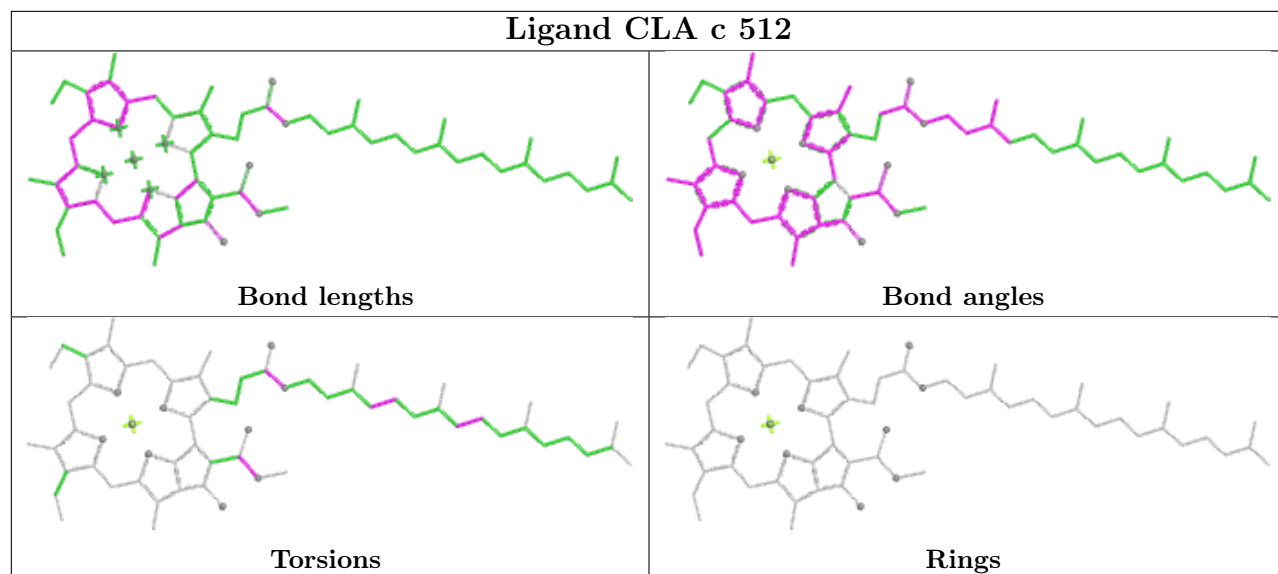
## Ligand LHG b 629 (B)



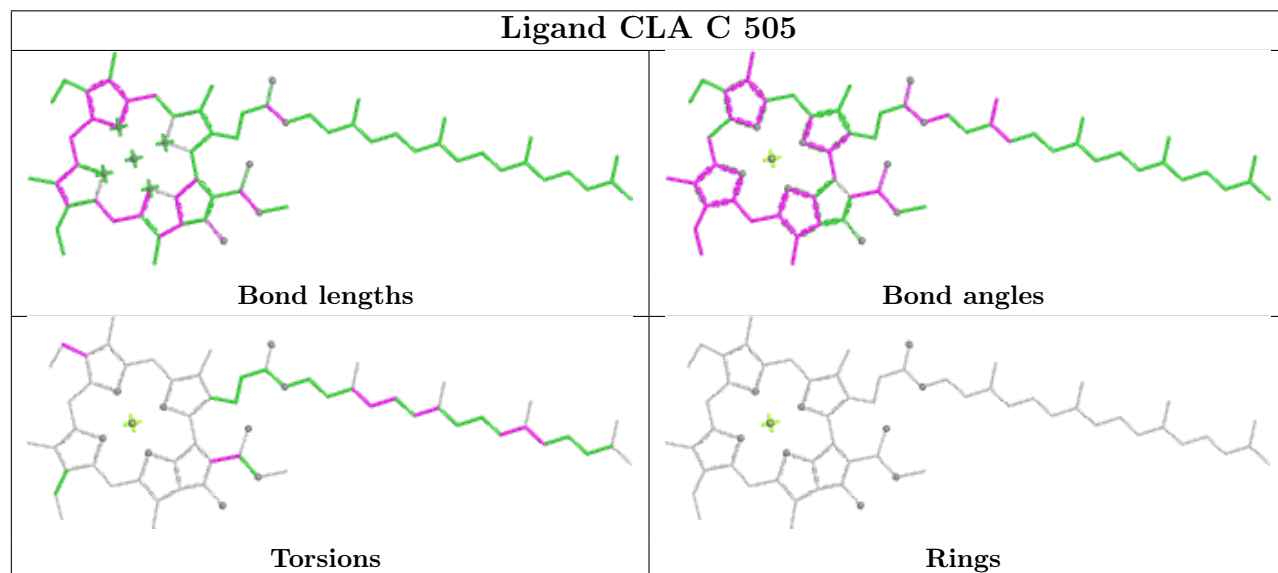
## Ligand LMT m 103

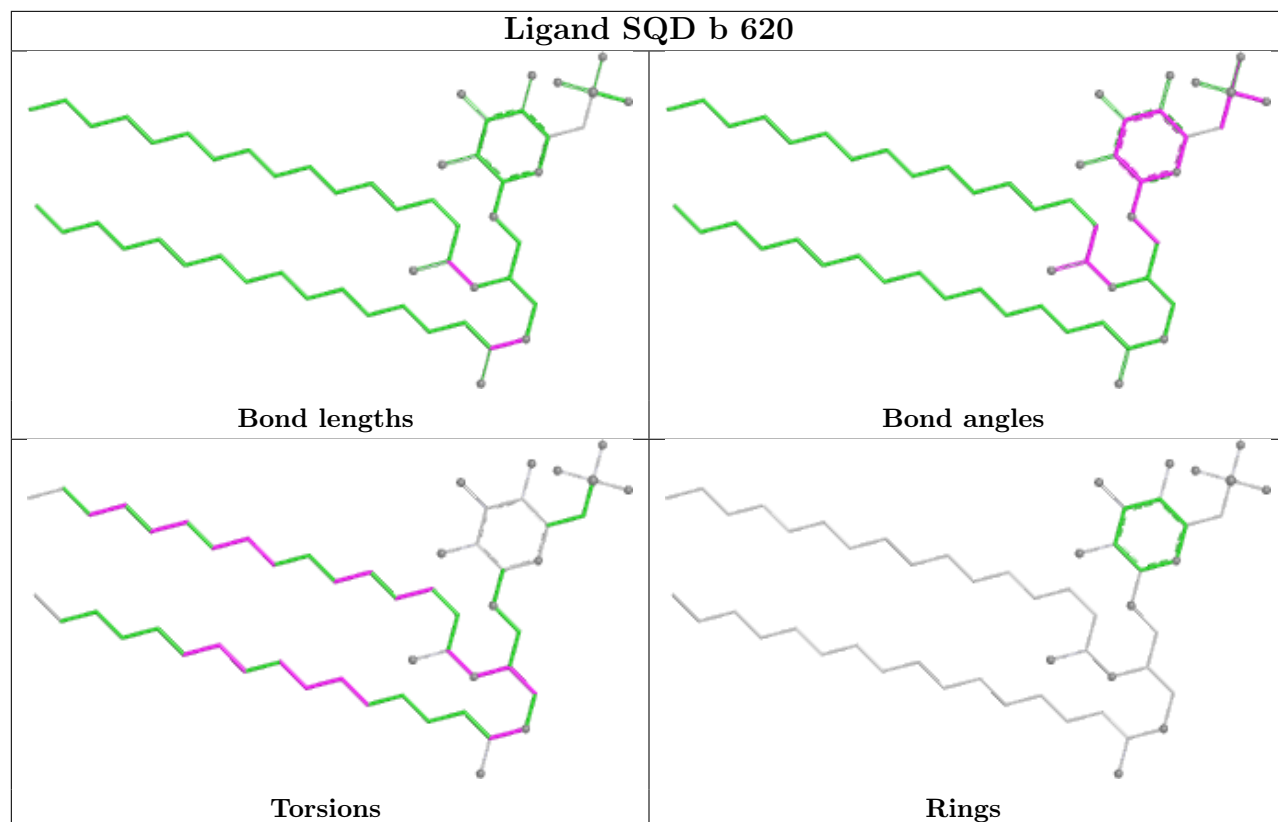


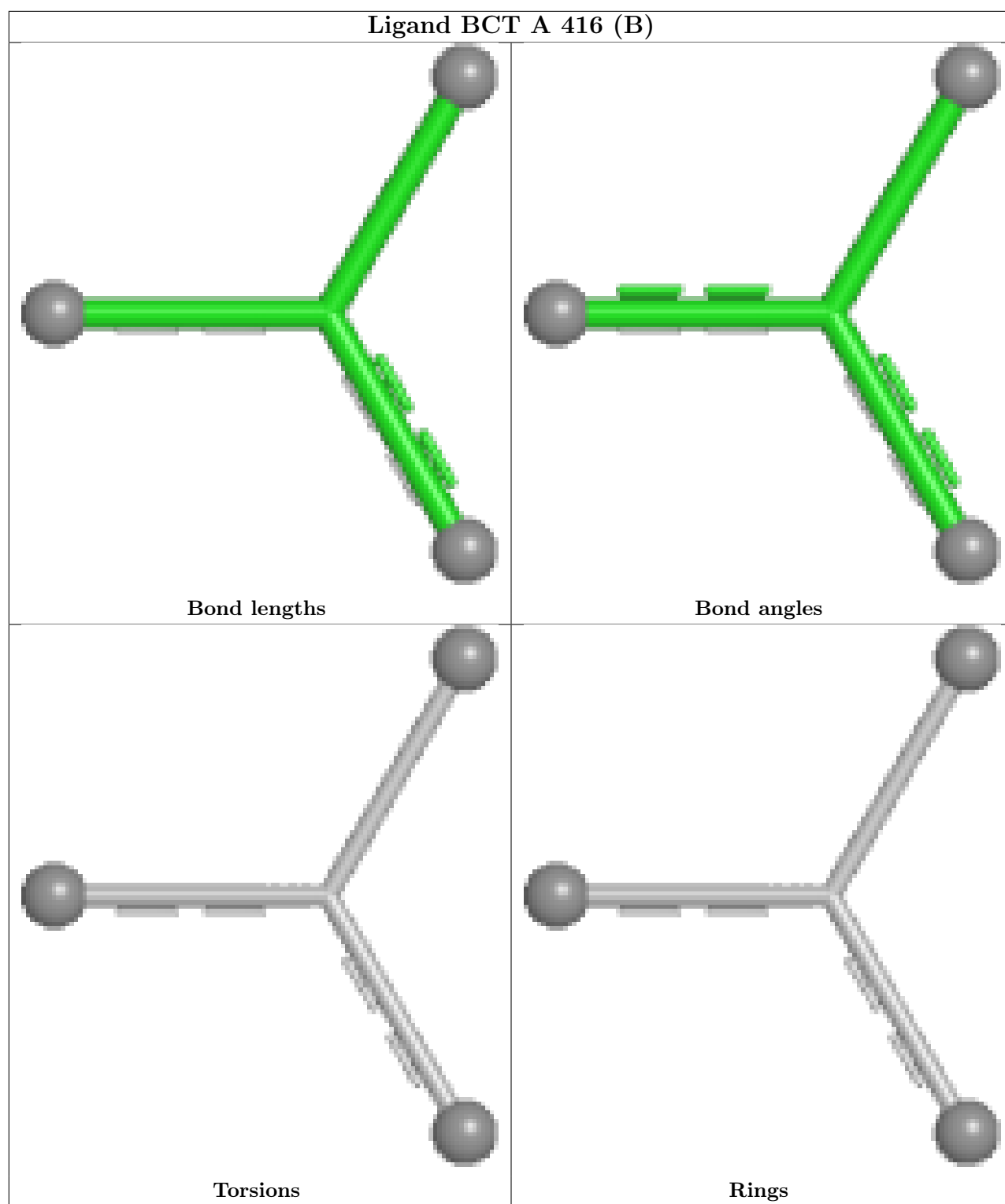
## Ligand CLA c 512



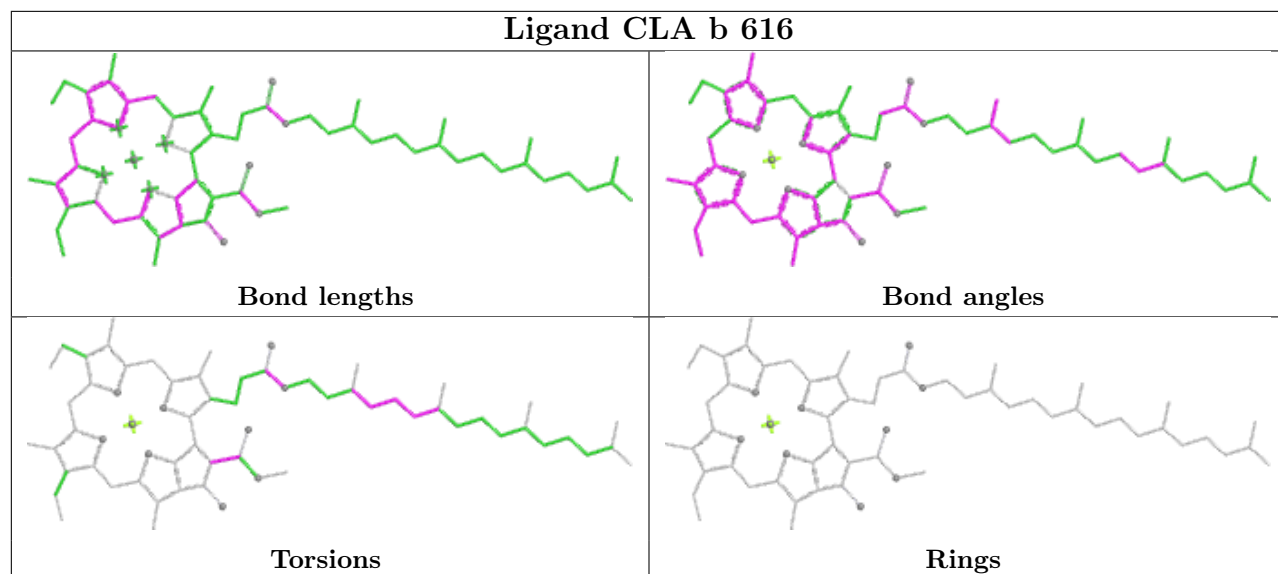
## Ligand CLA C 505



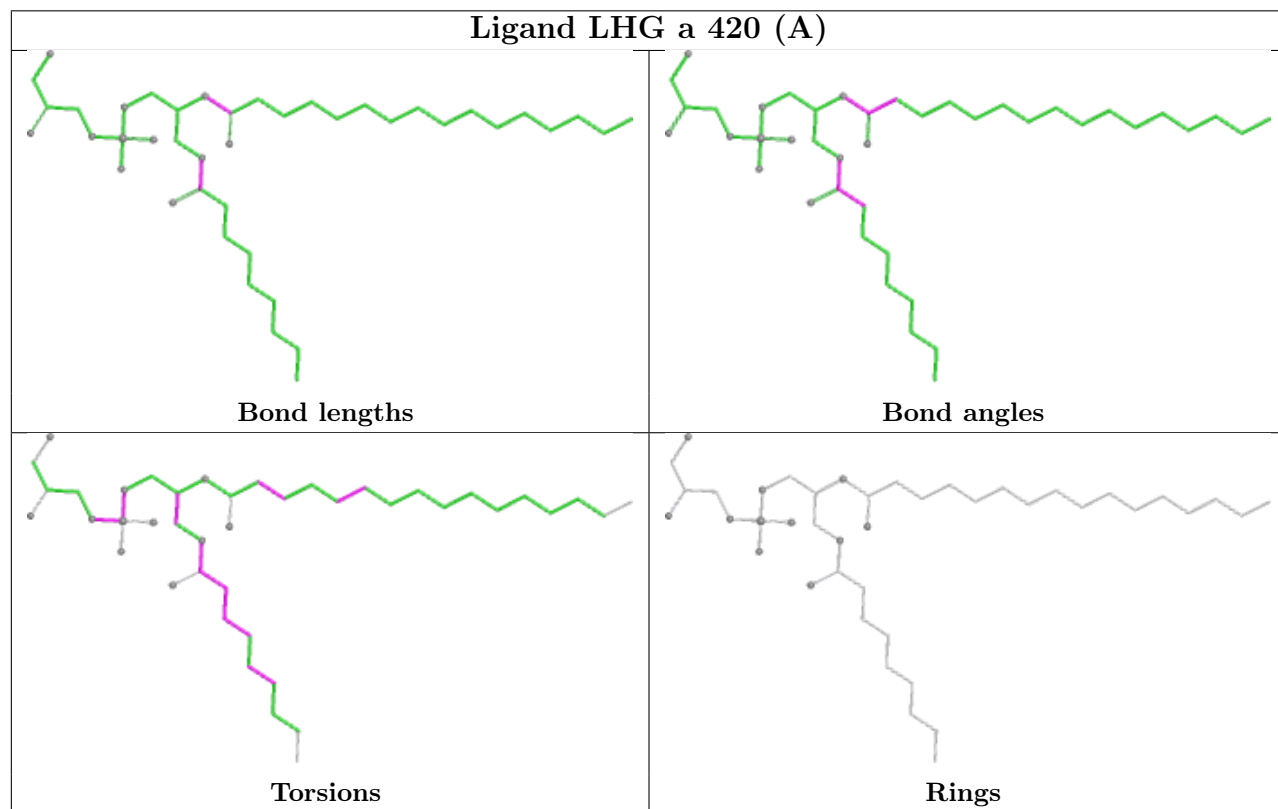


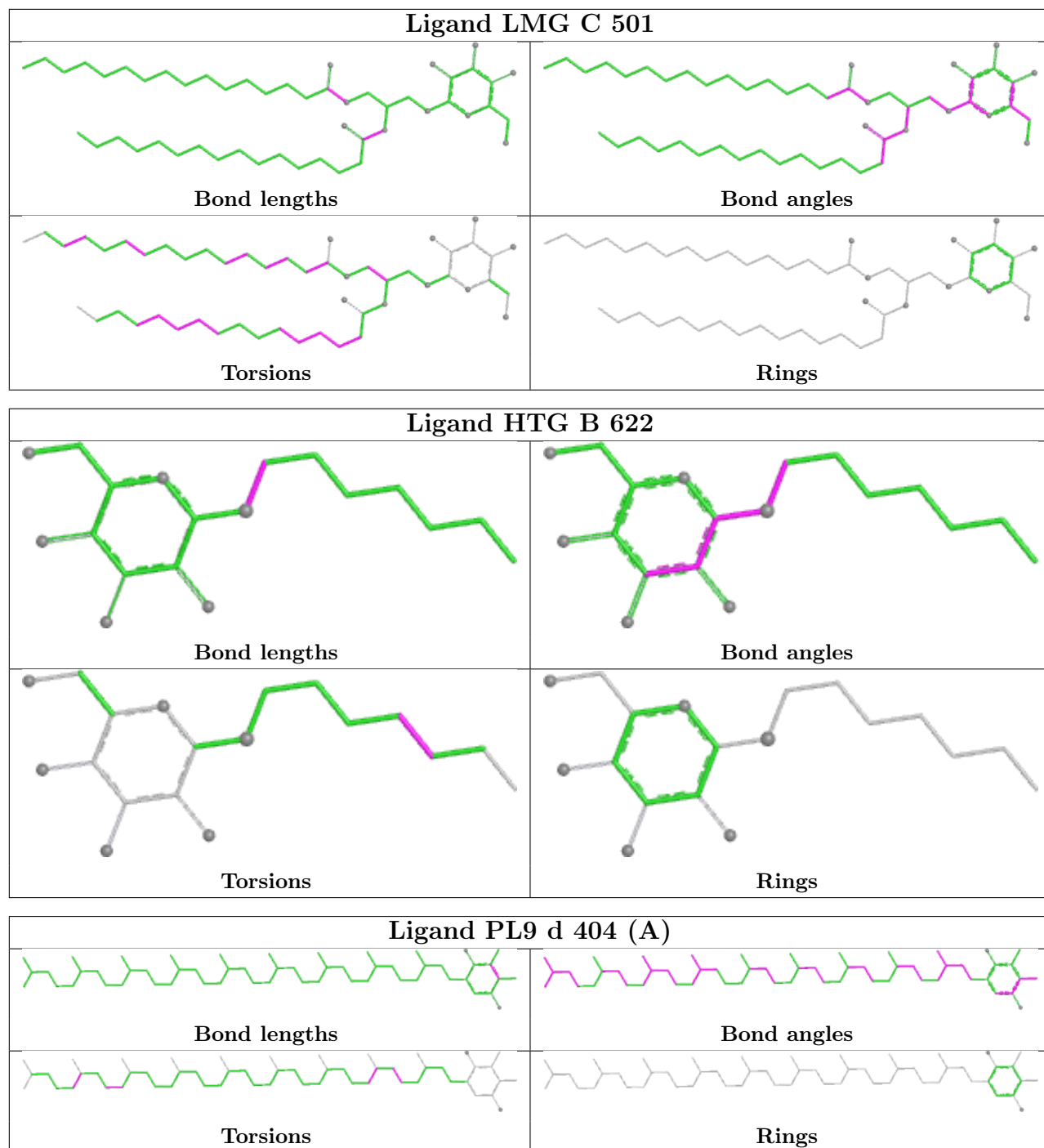


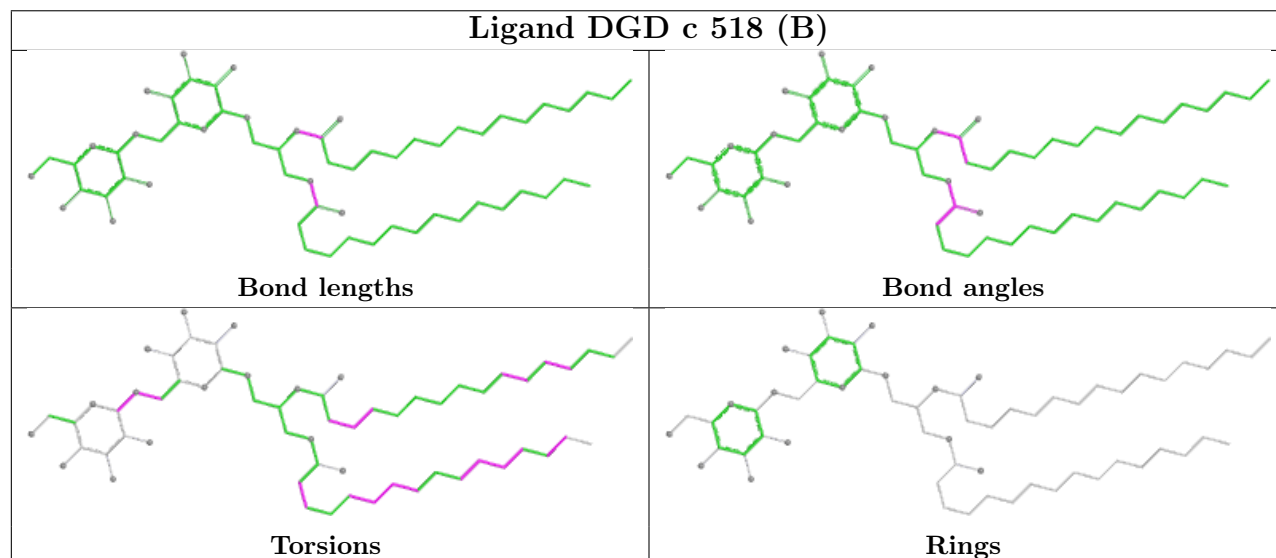
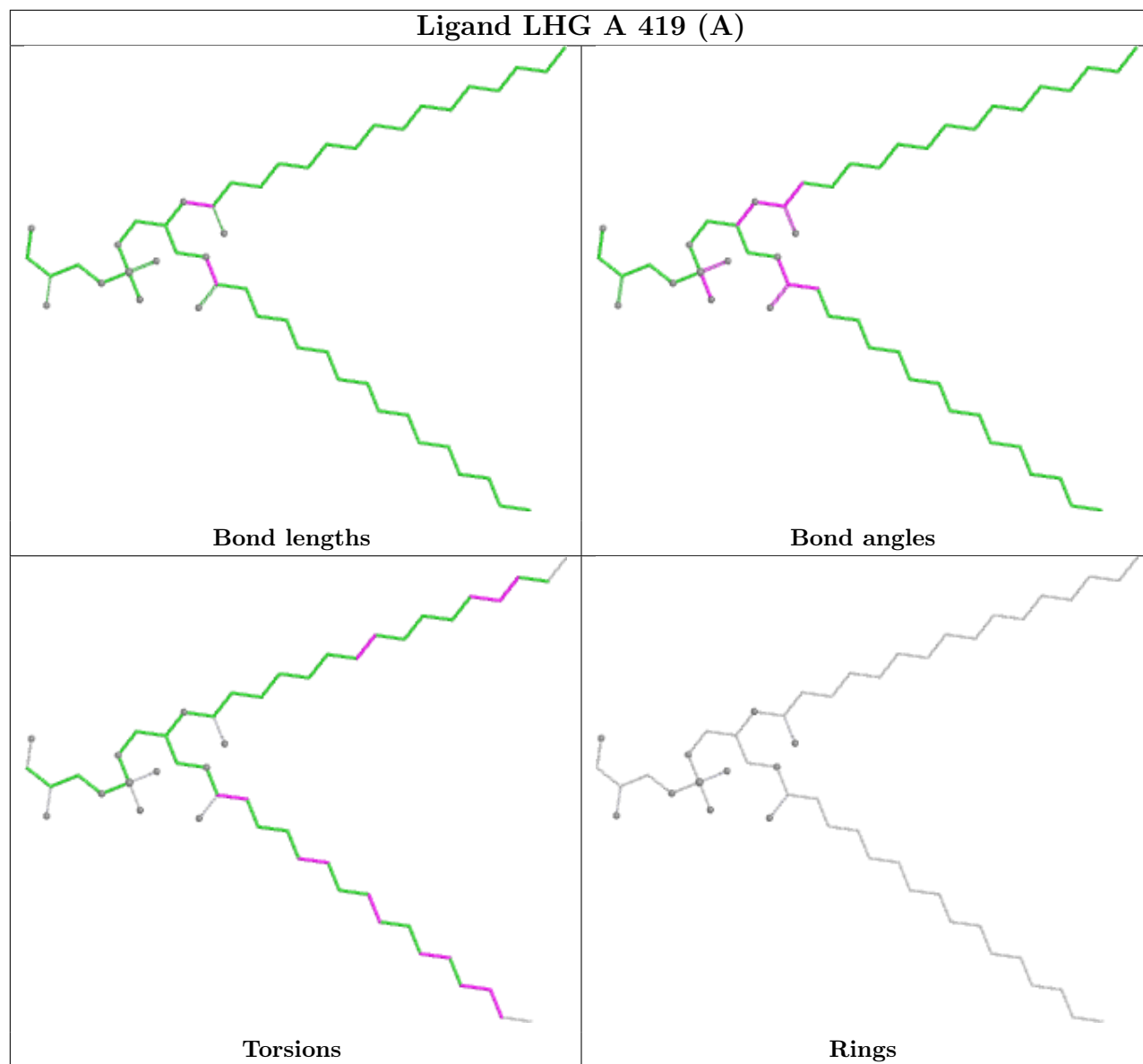
## Ligand CLA b 616

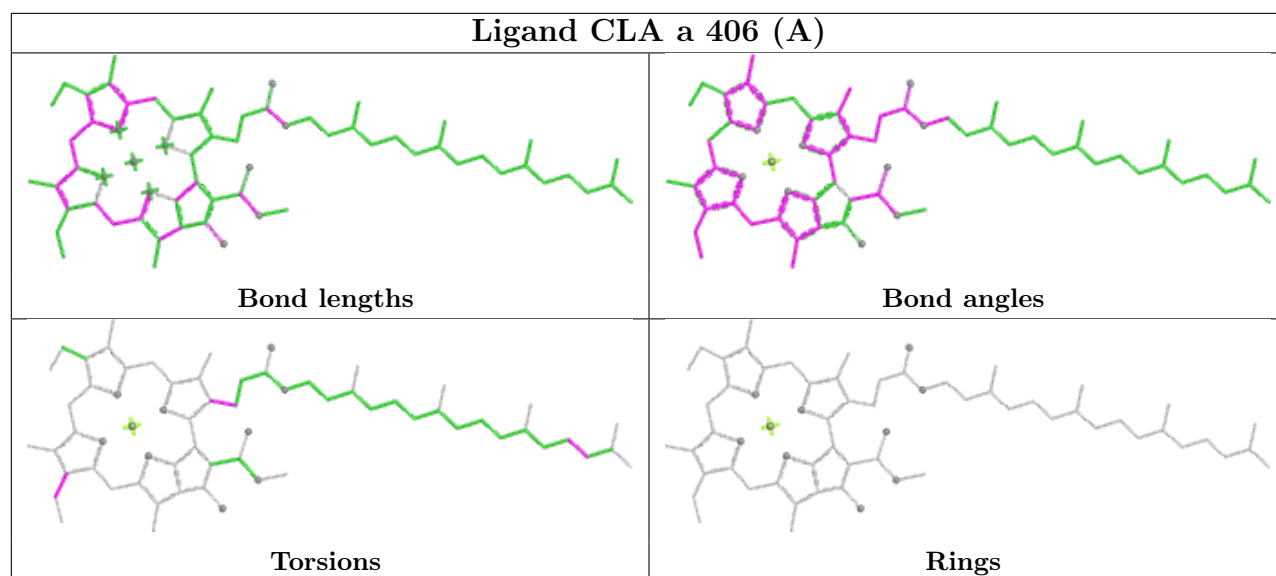
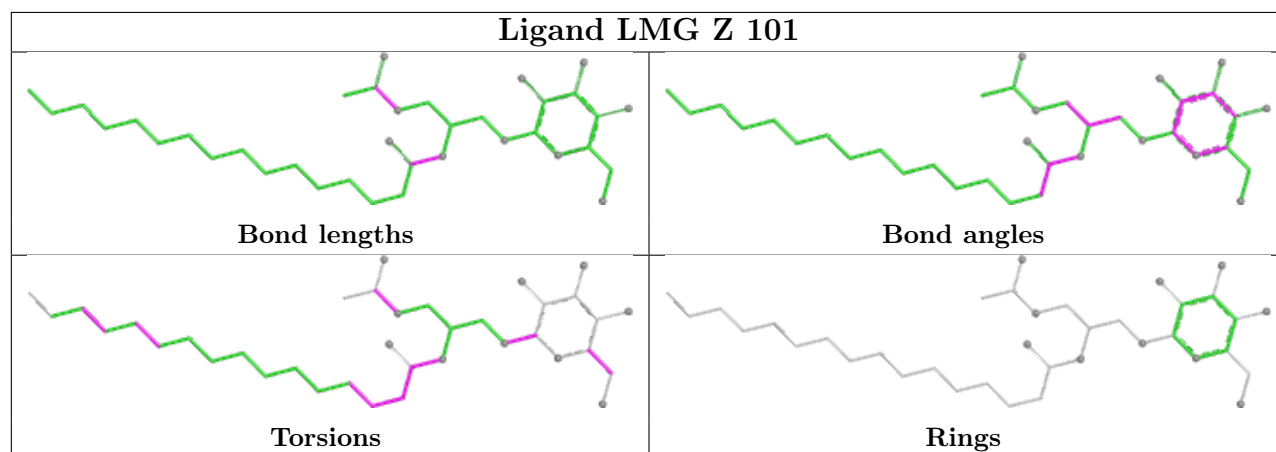
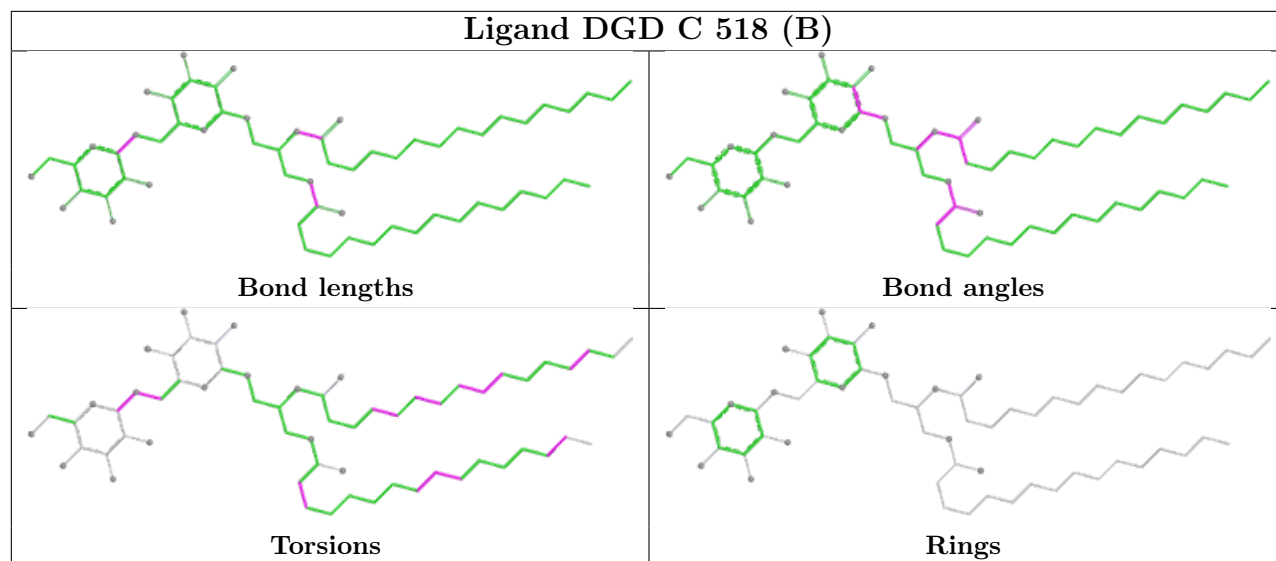


## Ligand LHG a 420 (A)



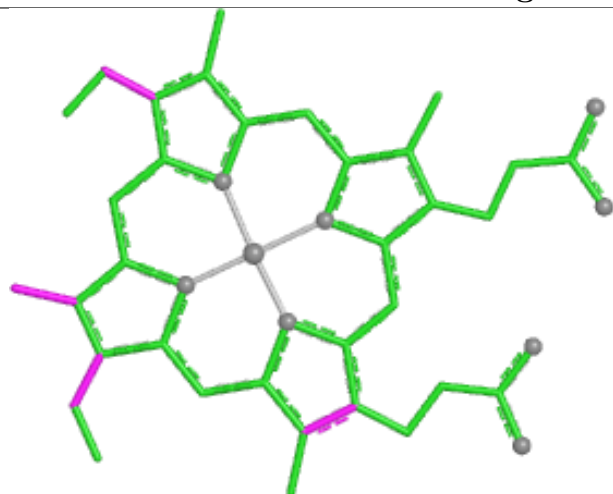




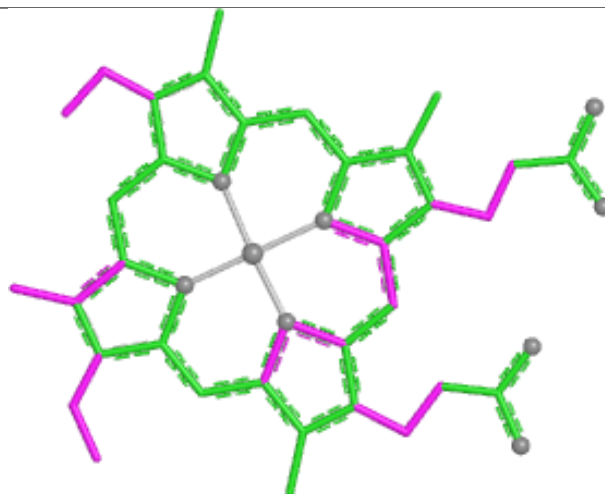




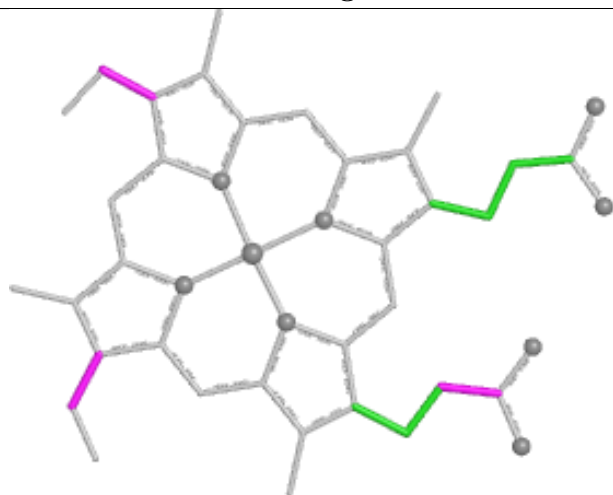
## Ligand HEC v 201



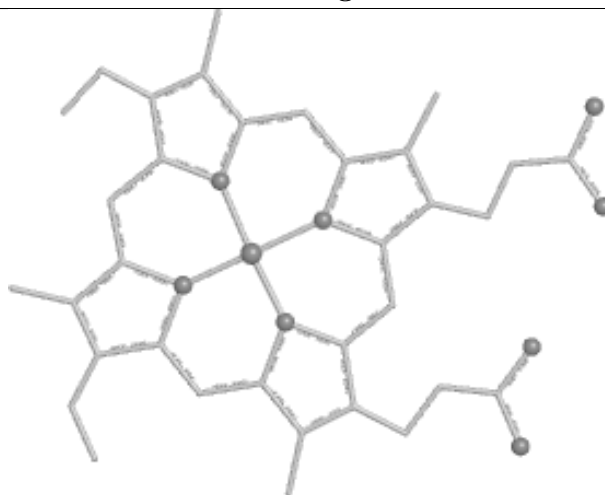
Bond lengths



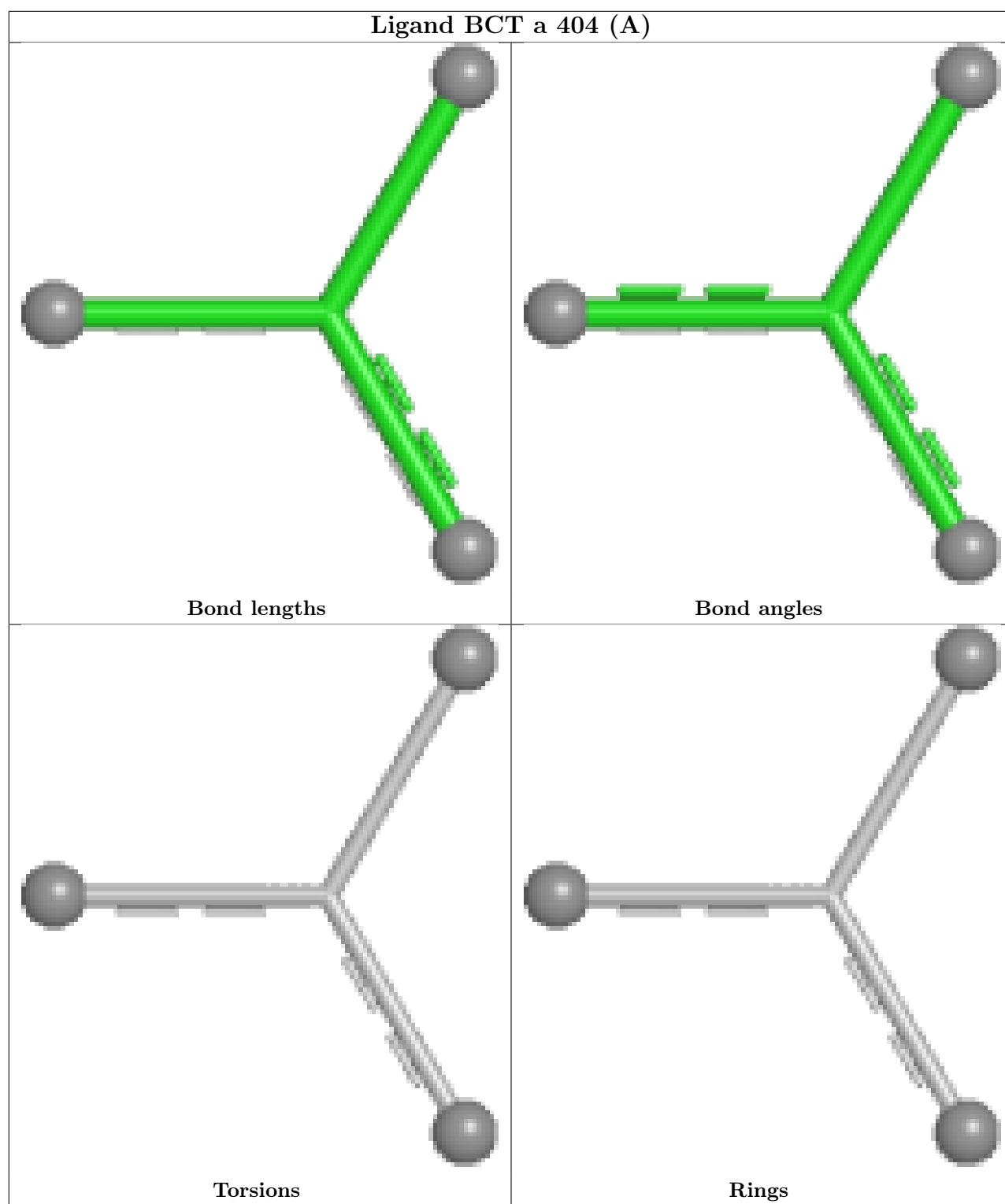
Bond angles

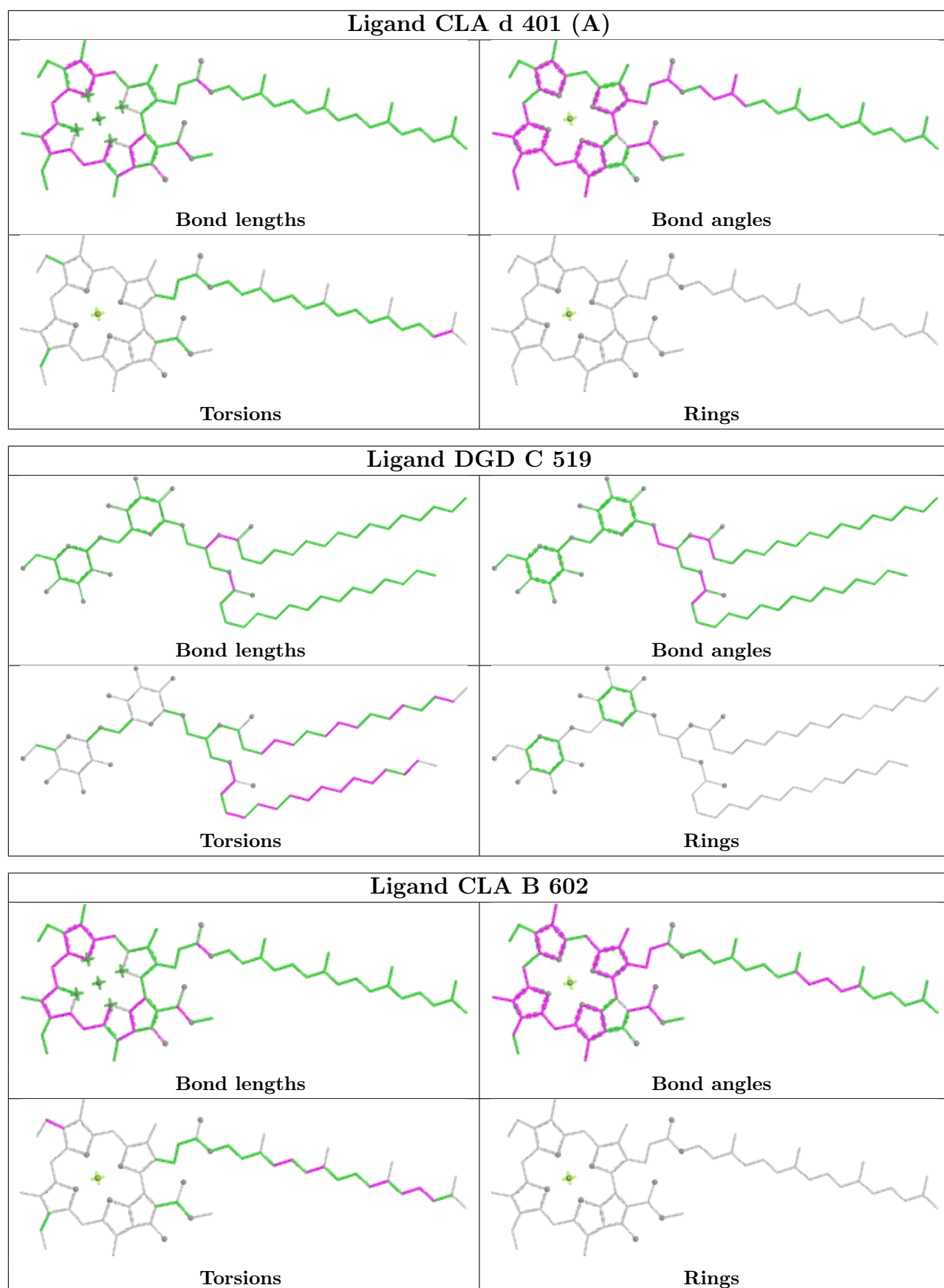


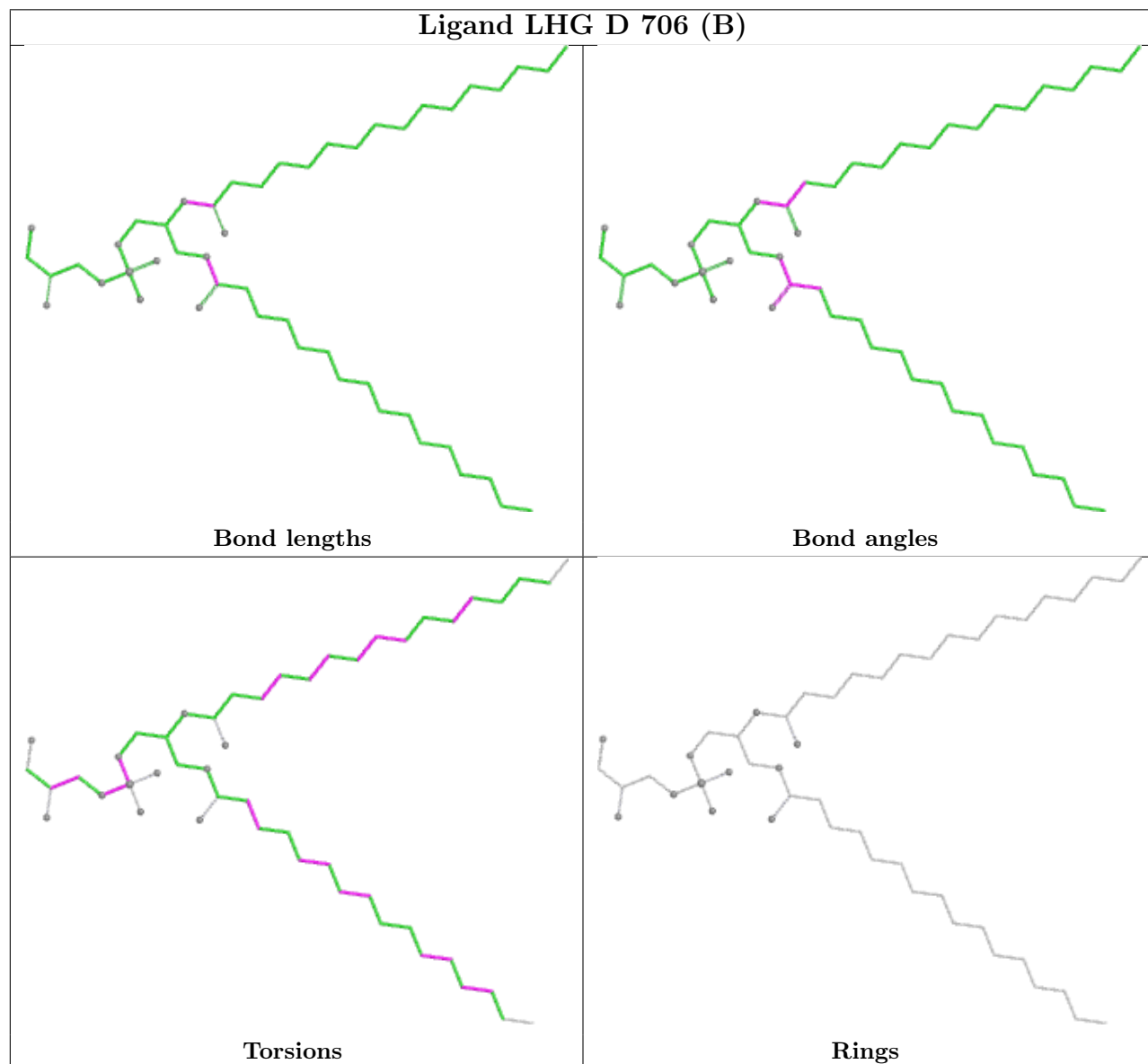
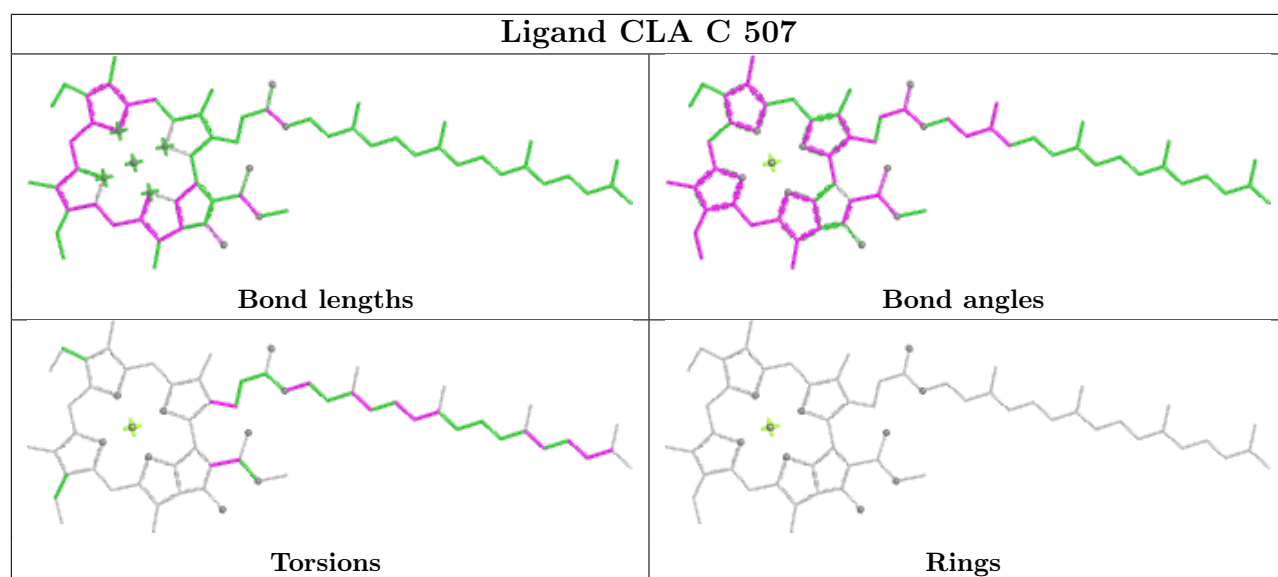
Torsions

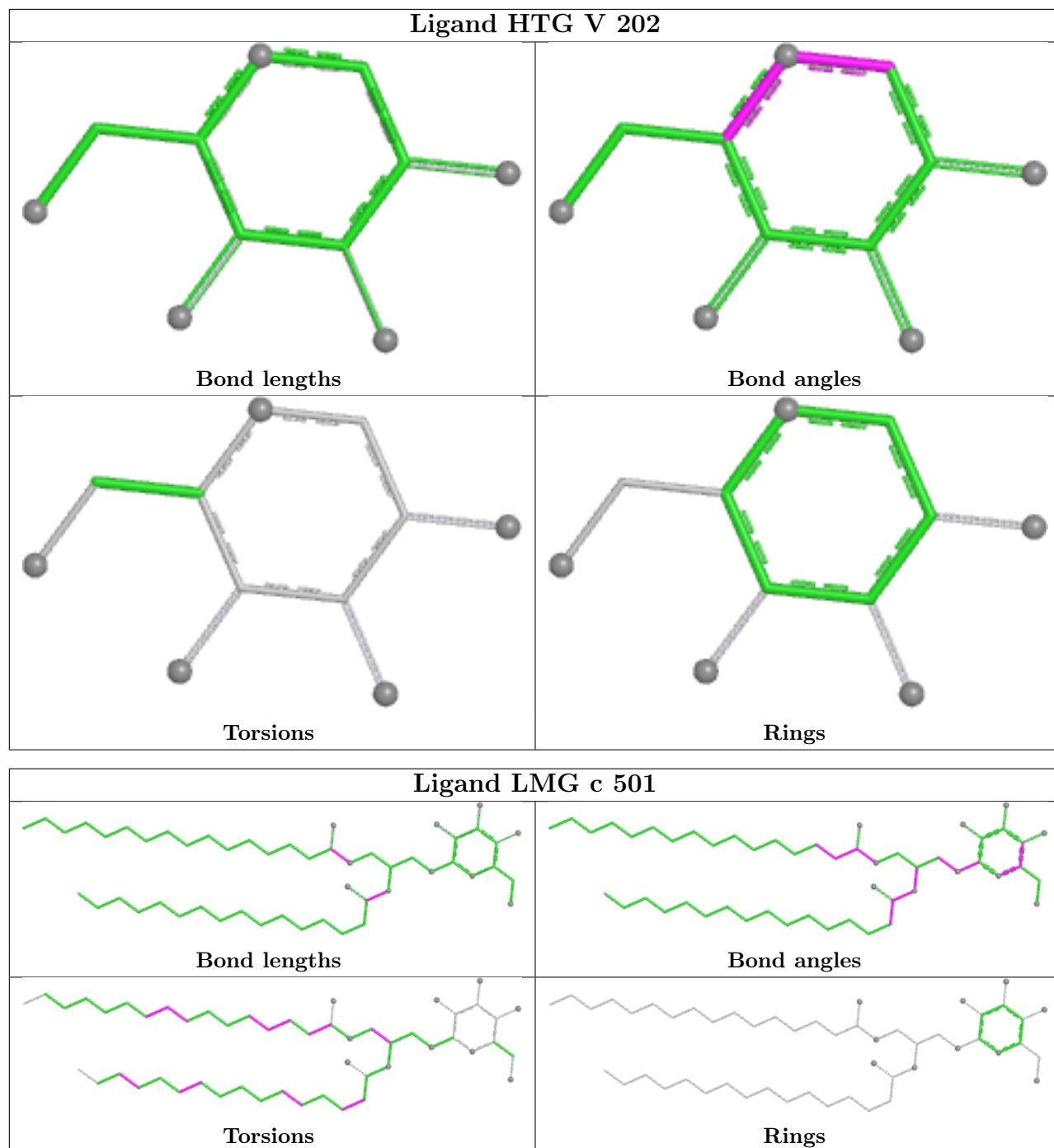


Rings

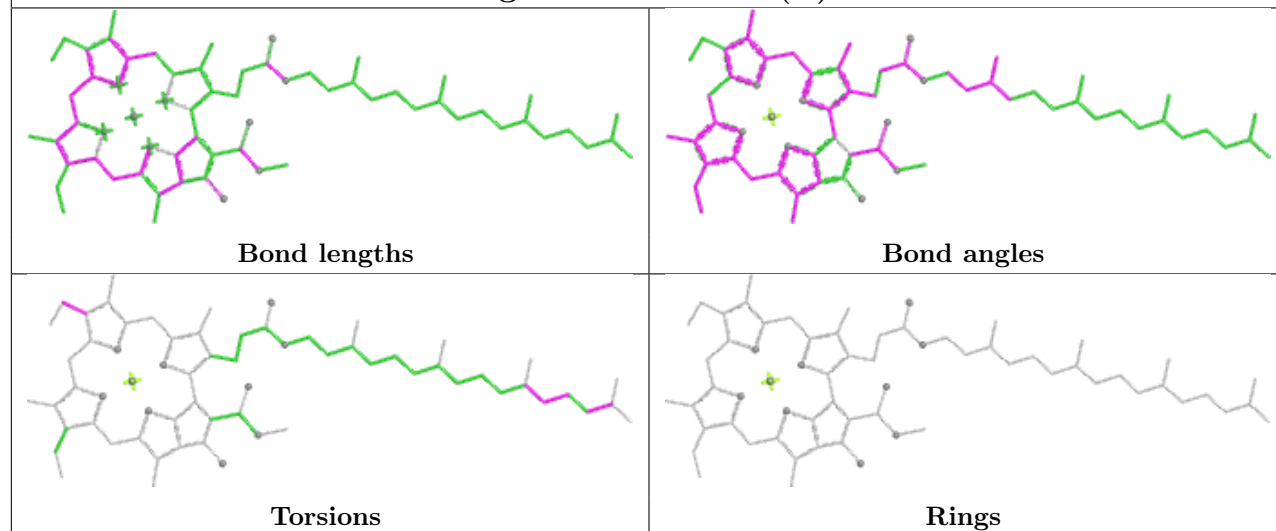




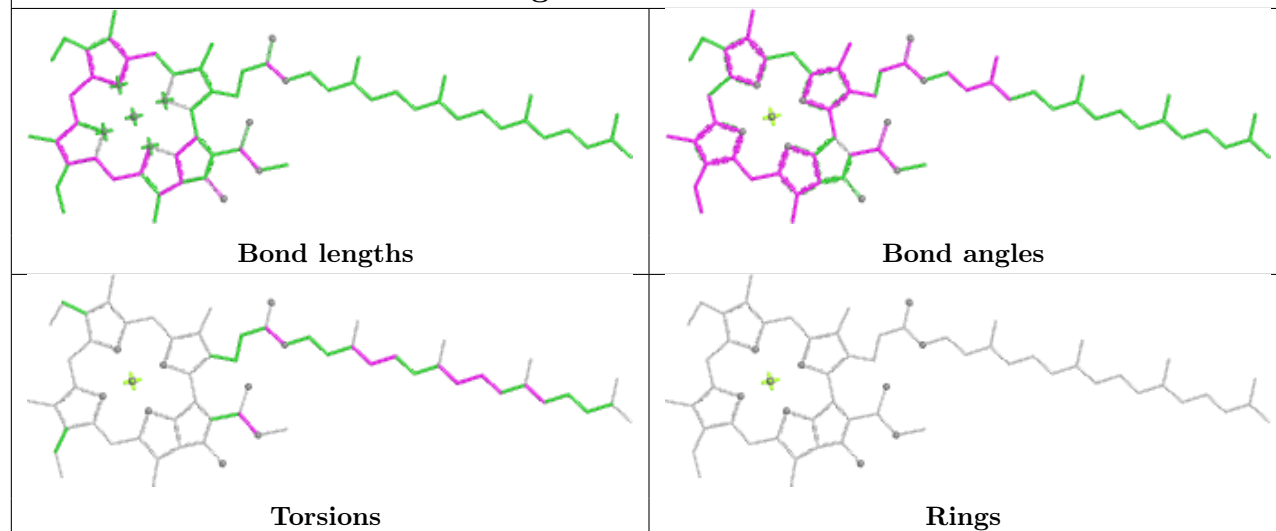


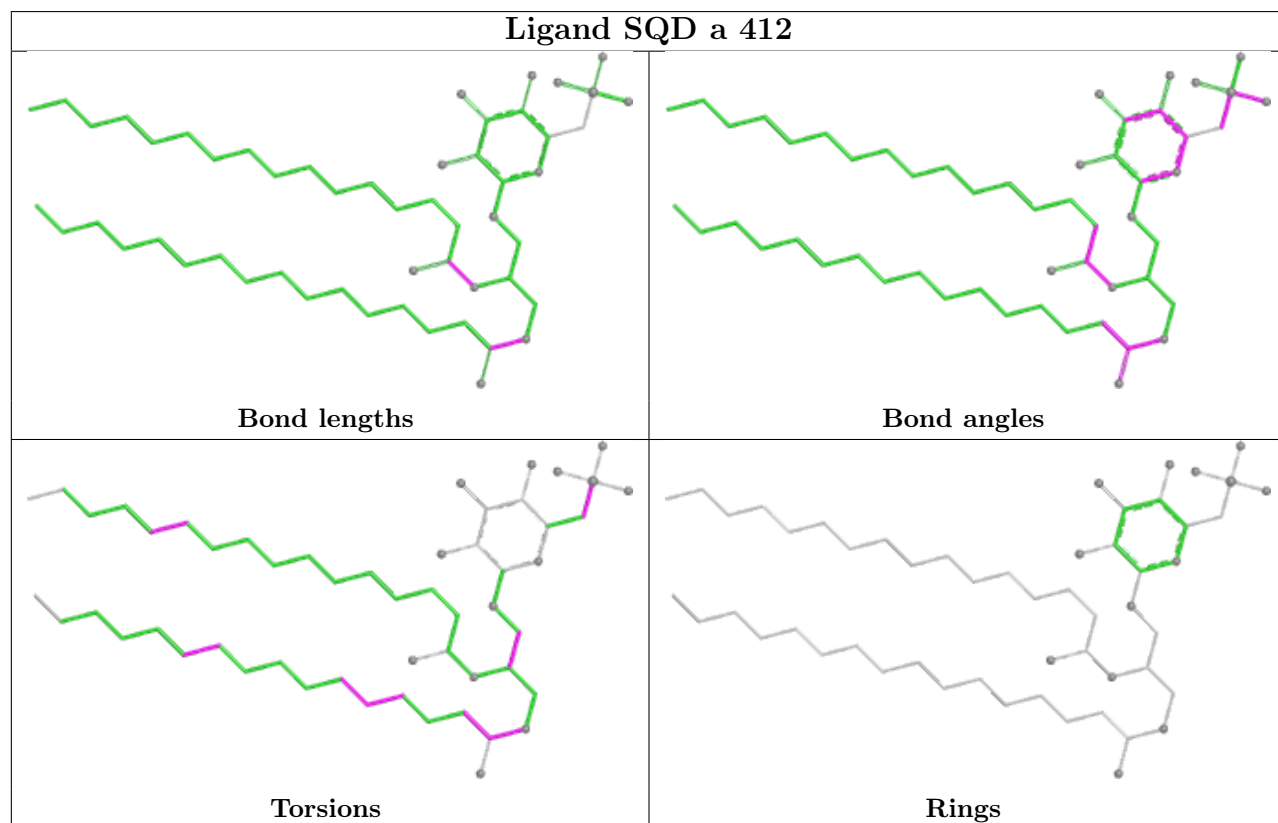
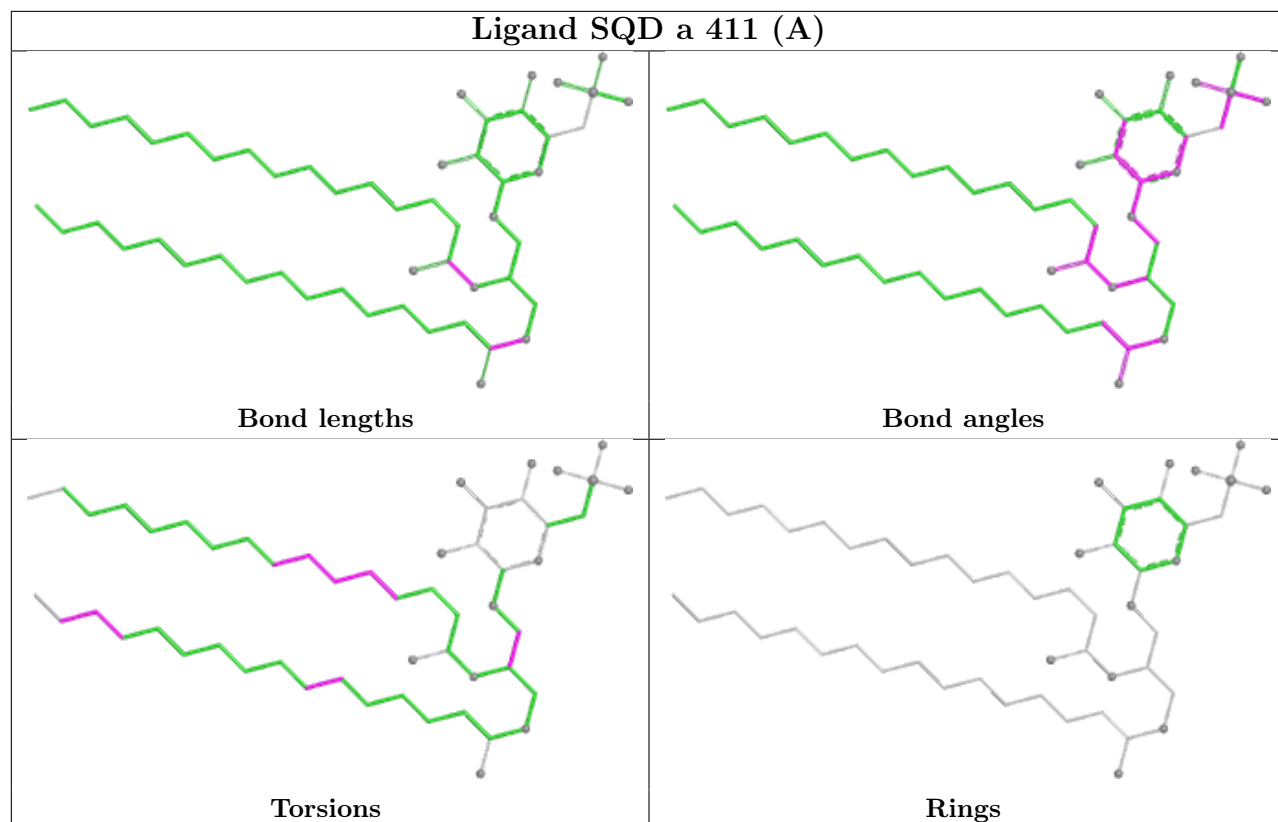


## Ligand CLA A 406 (B)

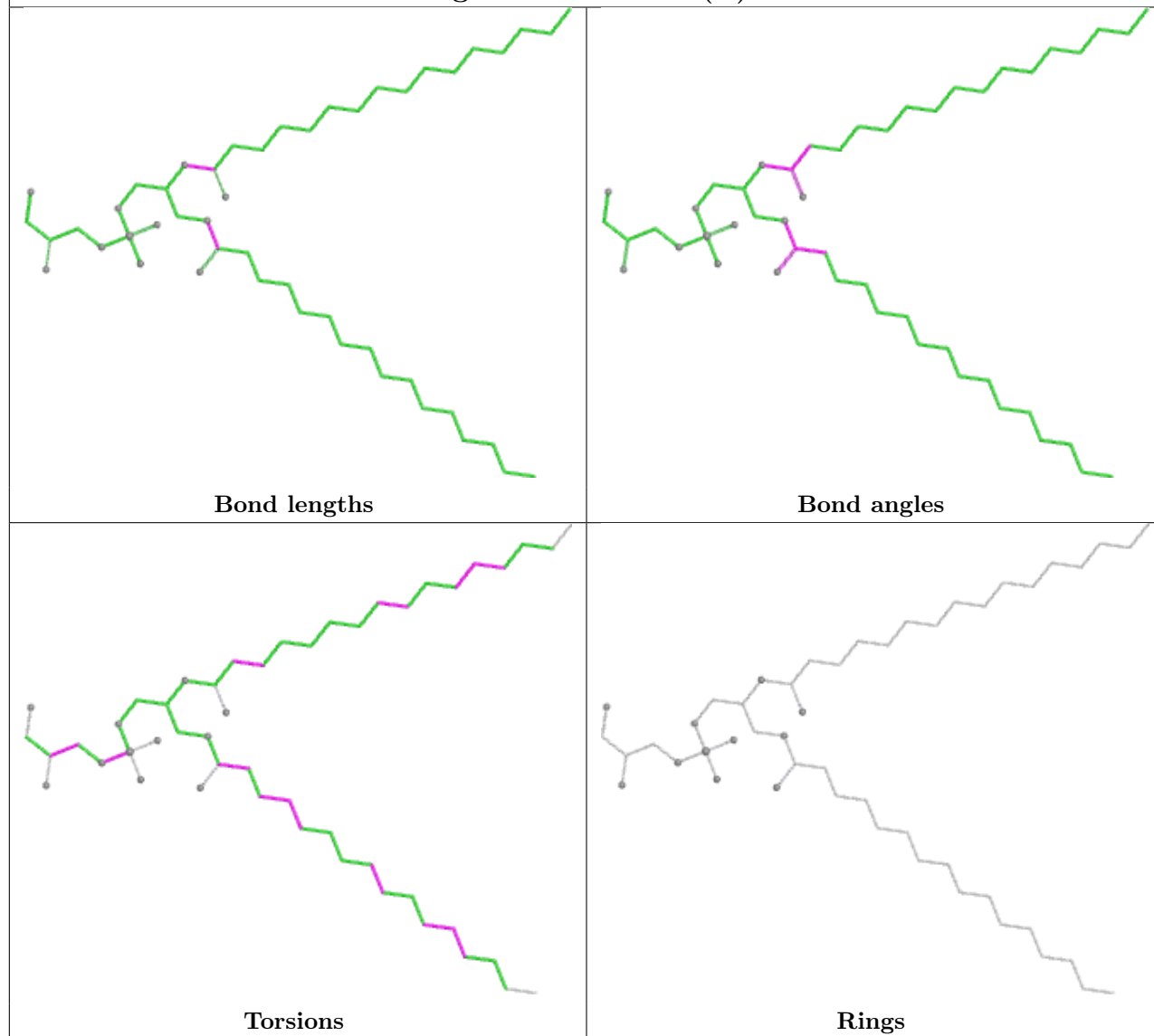


## Ligand CLA D 703

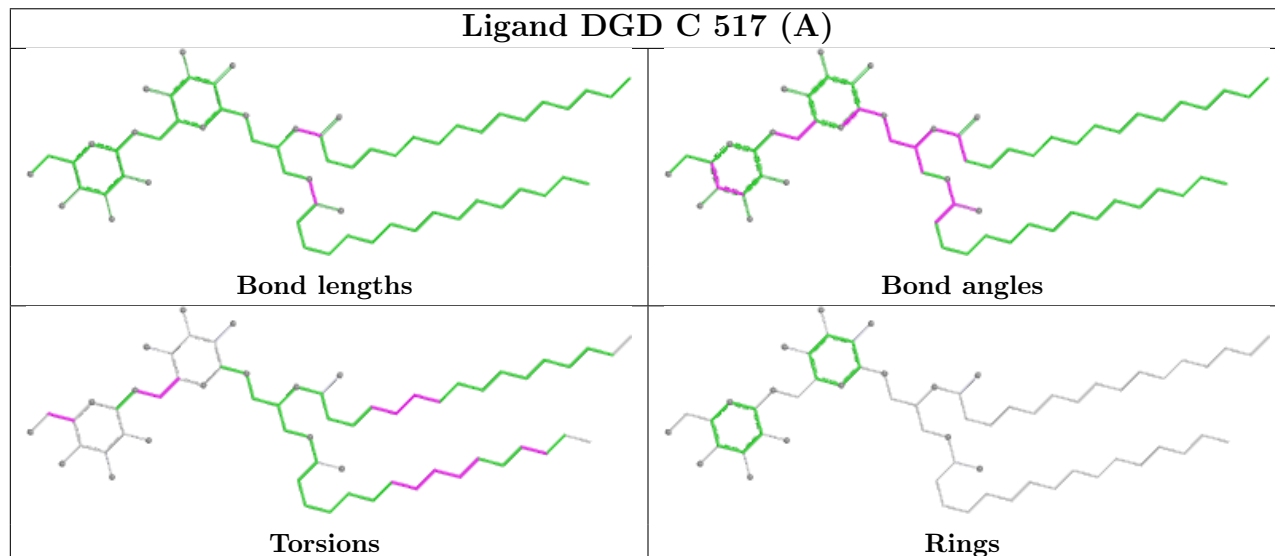




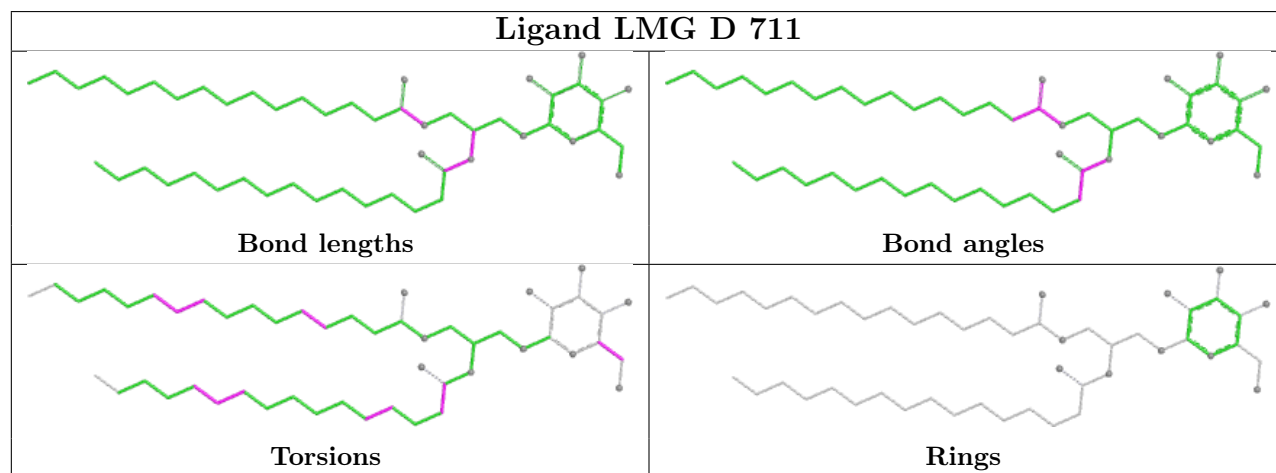
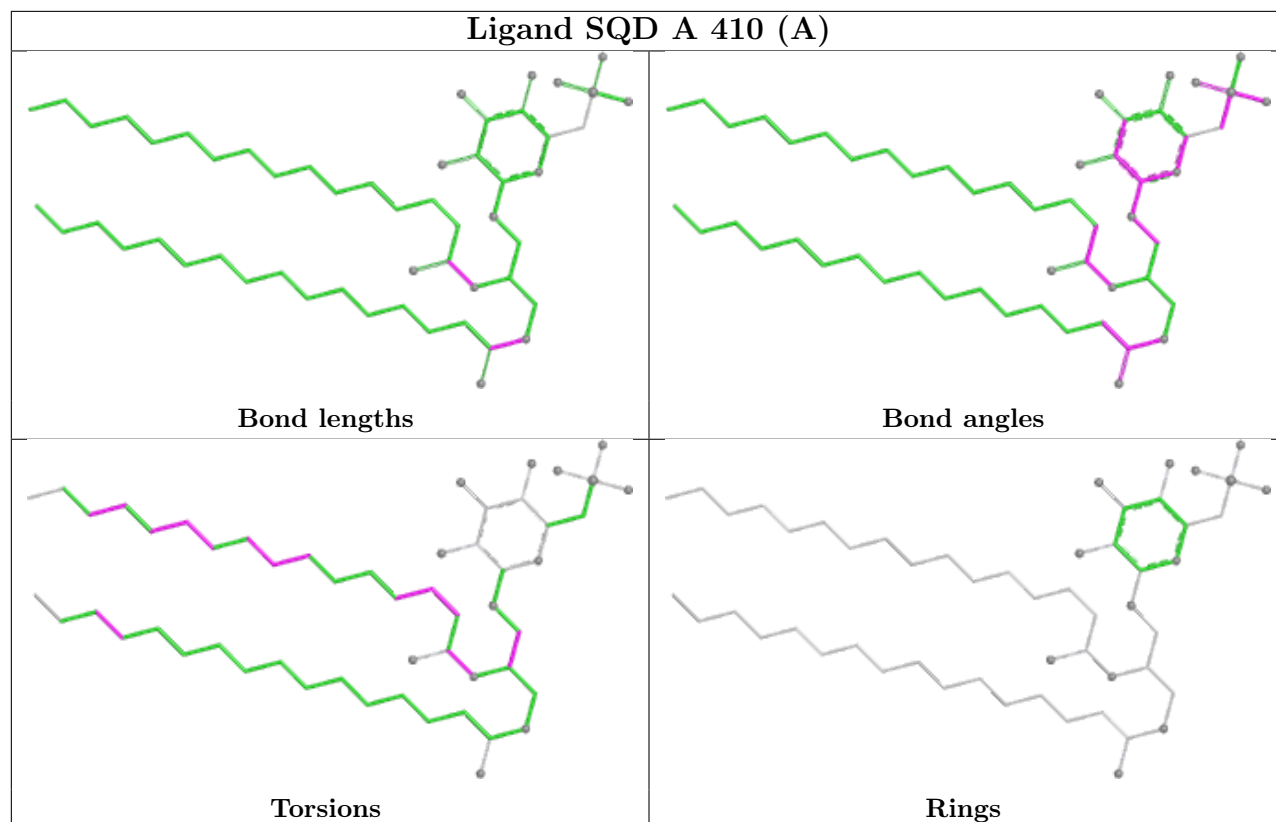
## Ligand LHG d 412 (B)

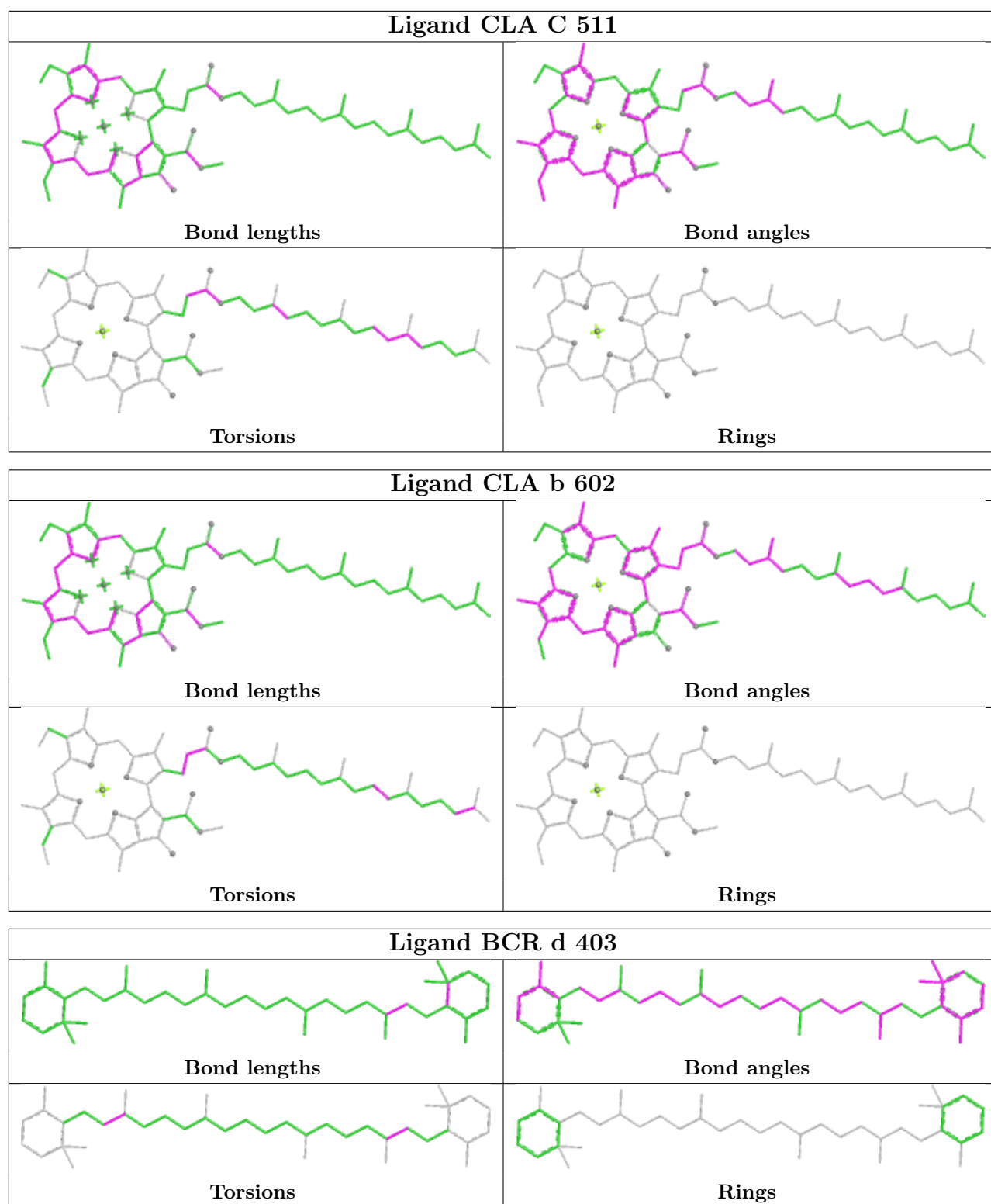


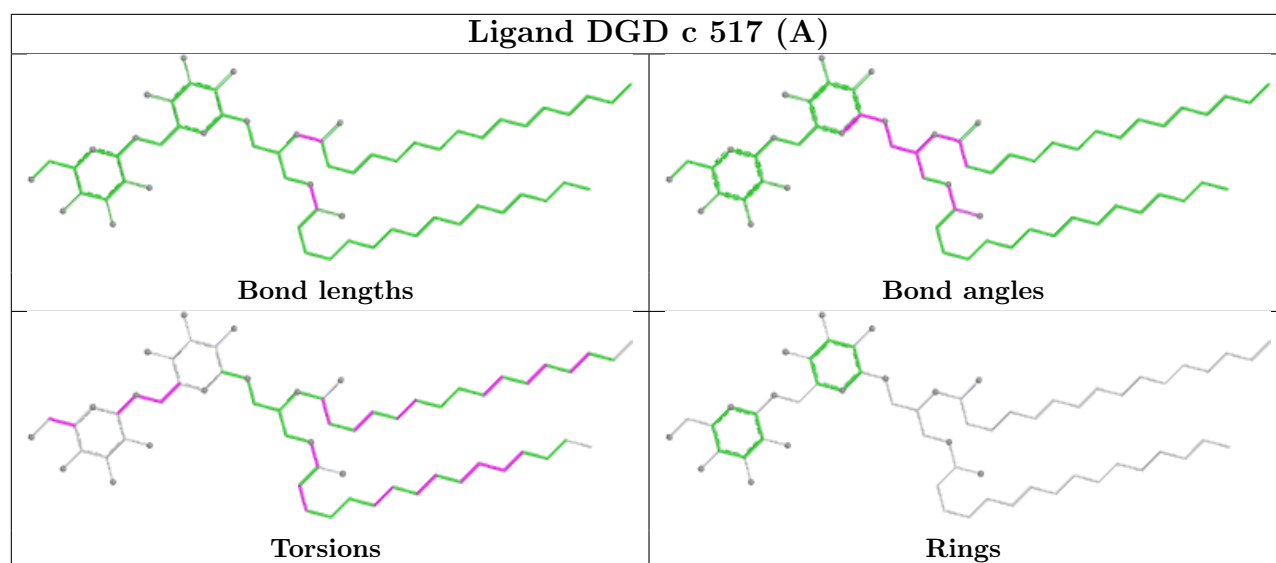
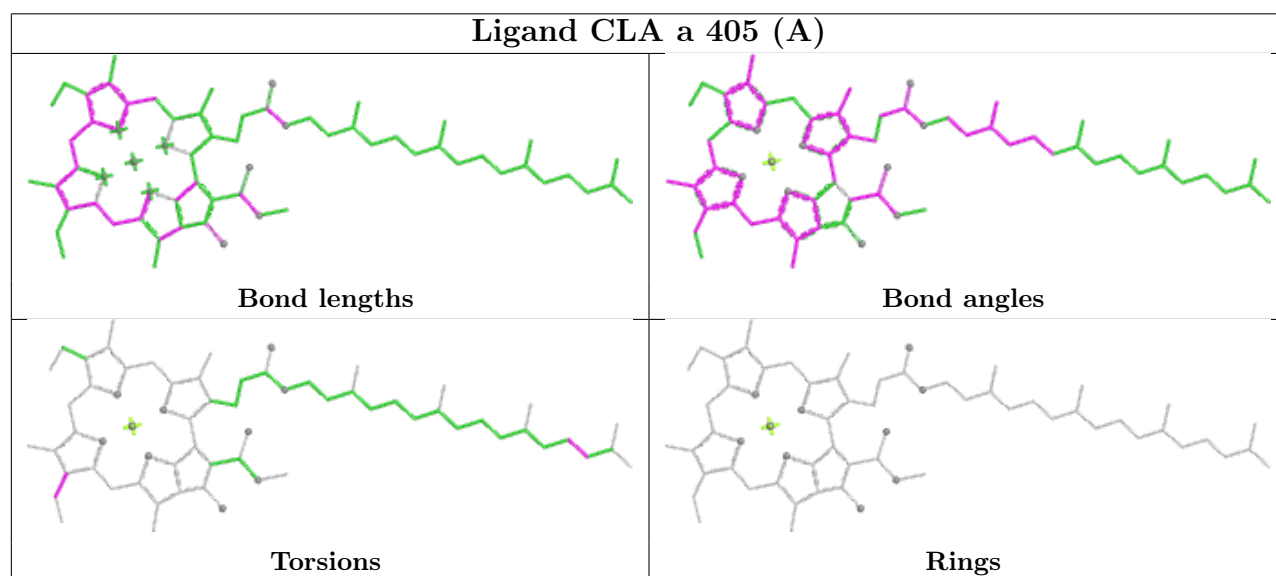
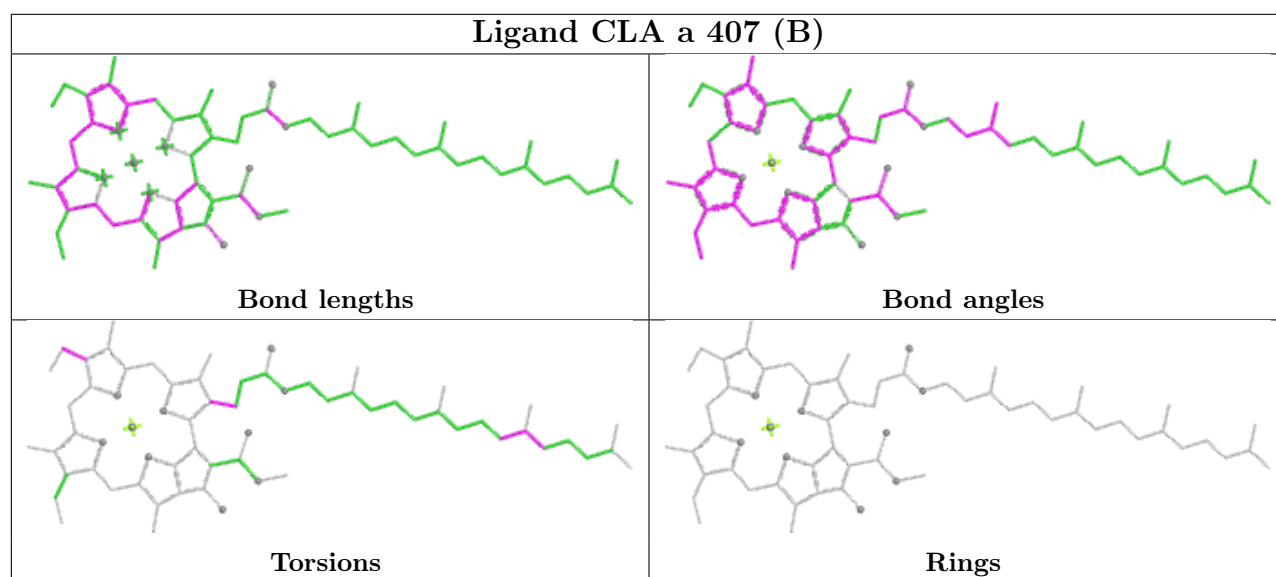
## Ligand DGD C 517 (A)



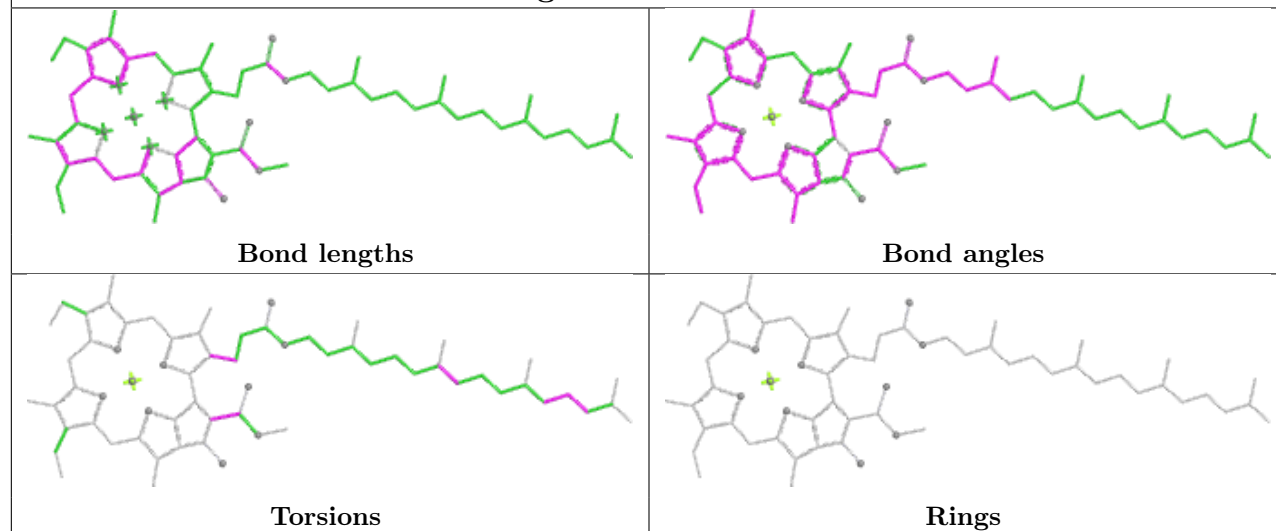




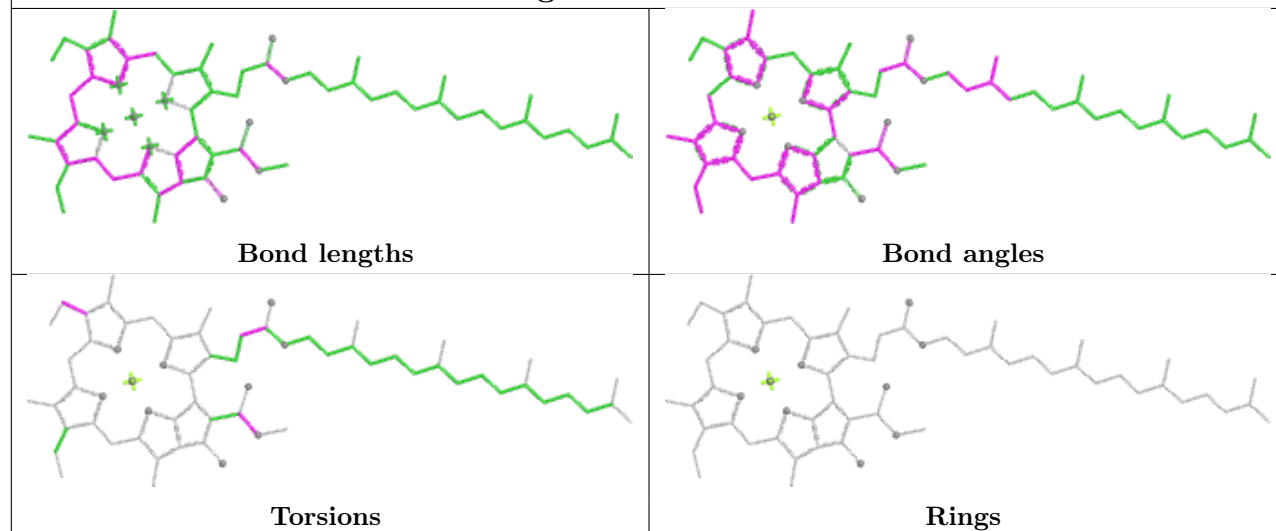




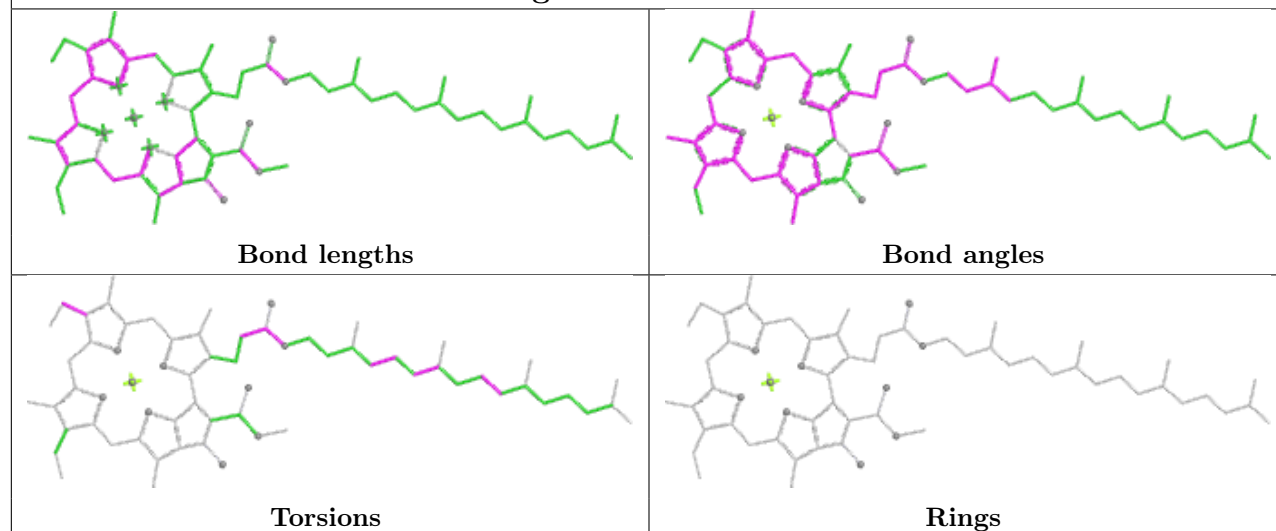
## Ligand CLA c 507

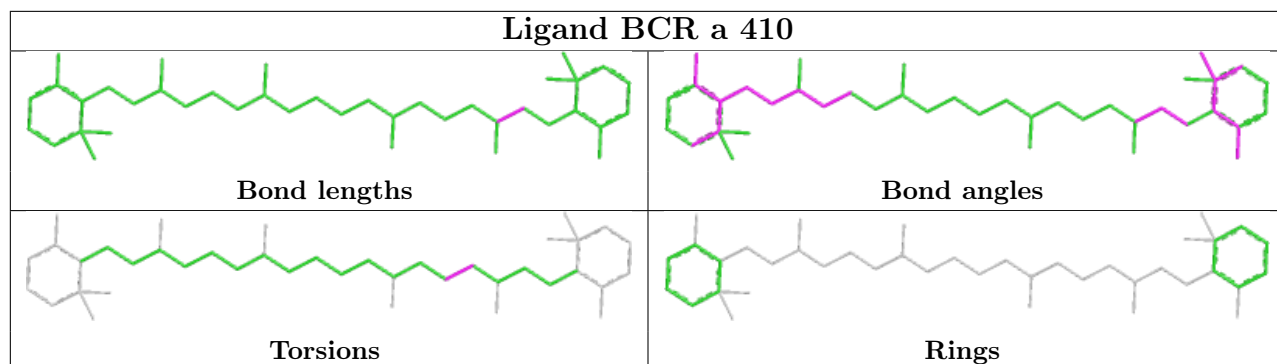
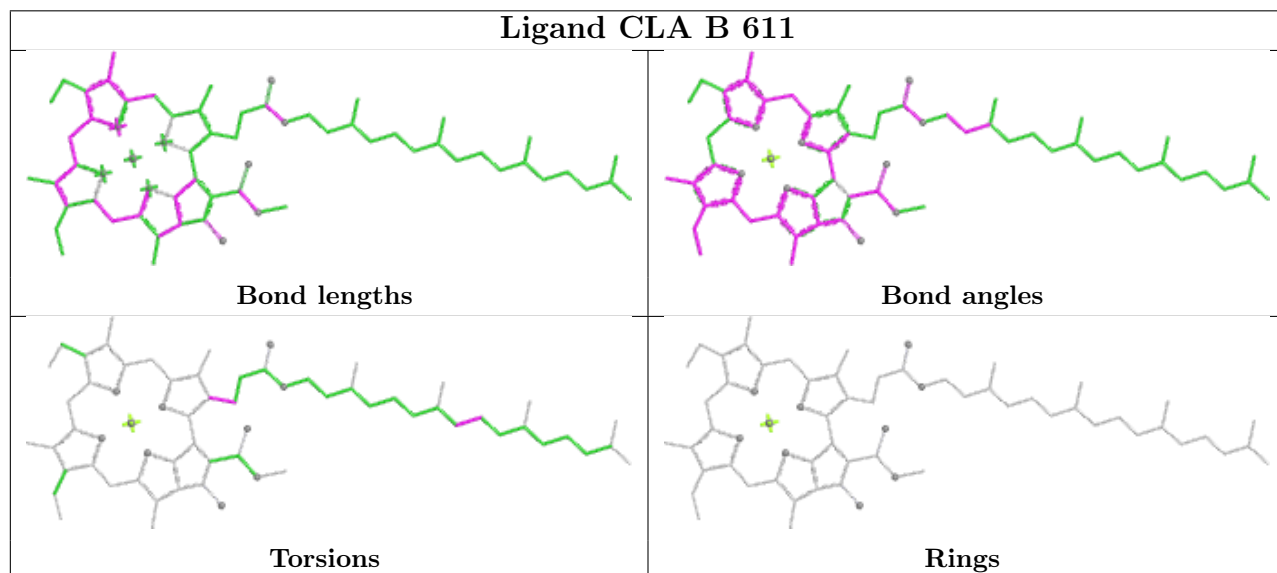
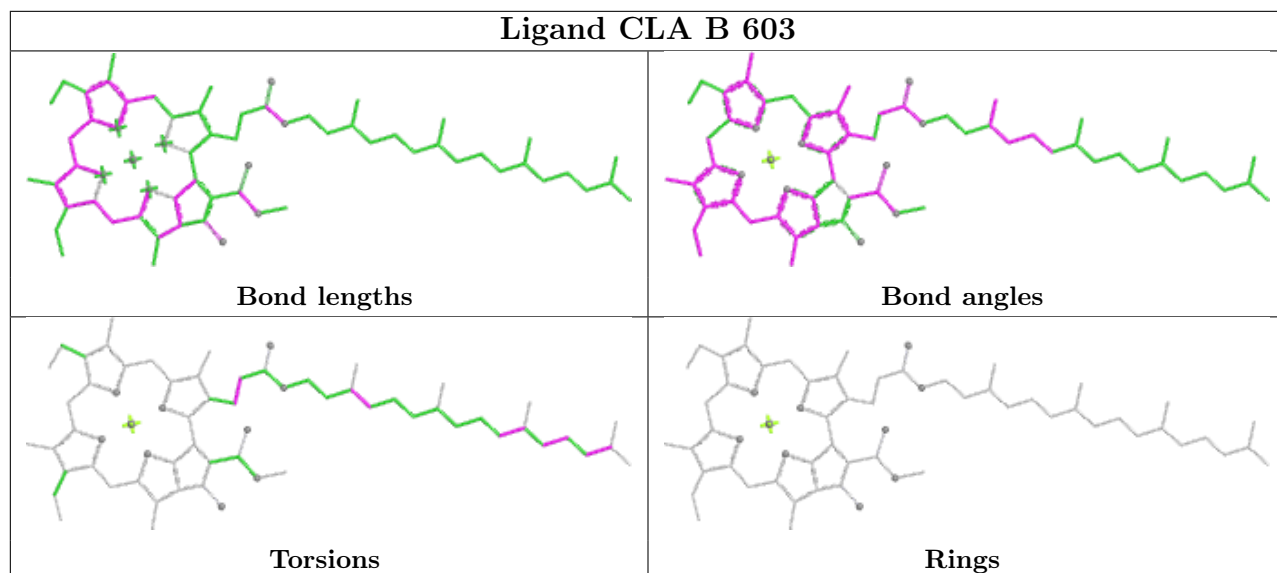


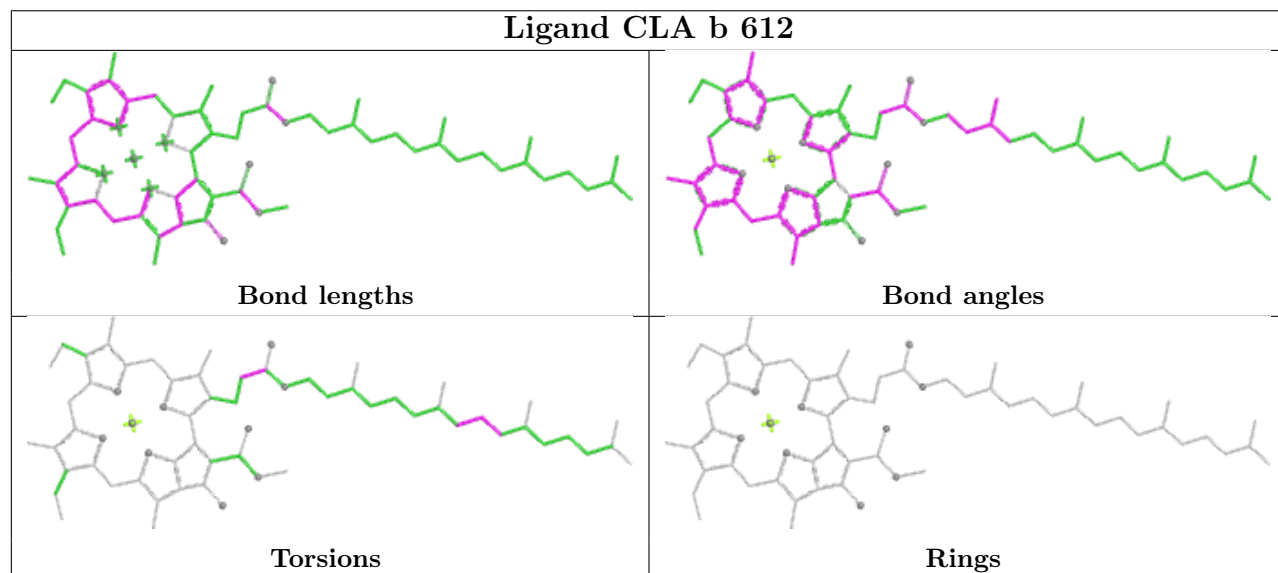
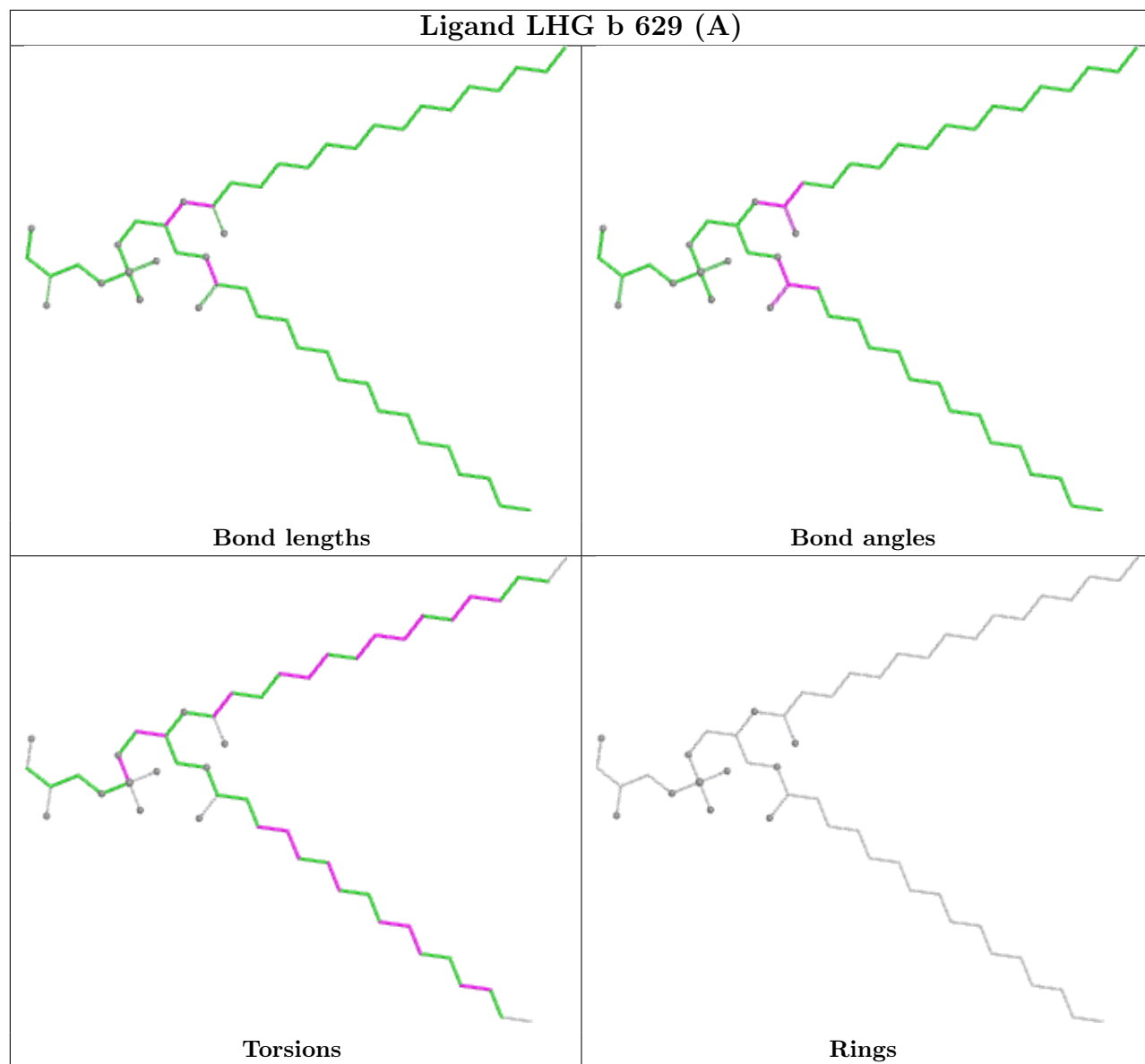
## Ligand CLA c 502



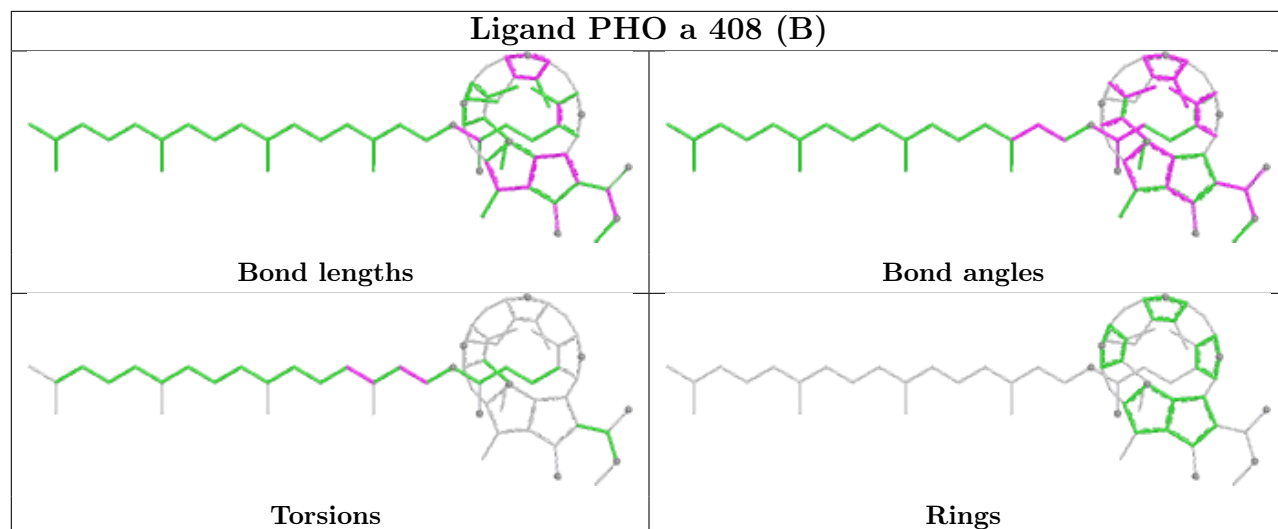
## Ligand CLA C 513



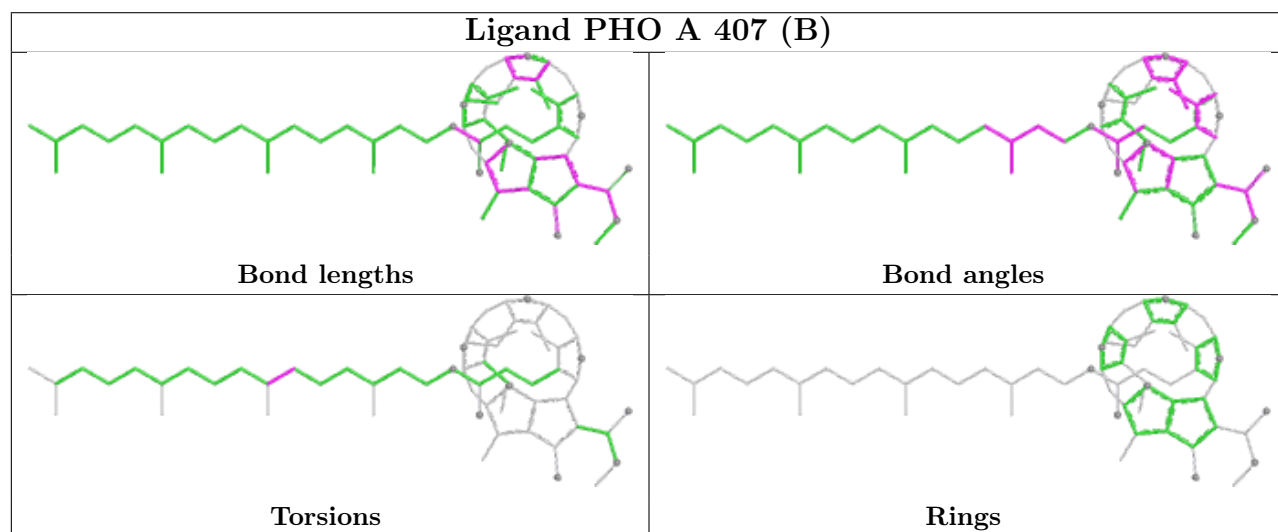
**Ligand BCR a 410****Ligand CLA B 611****Ligand CLA B 603**

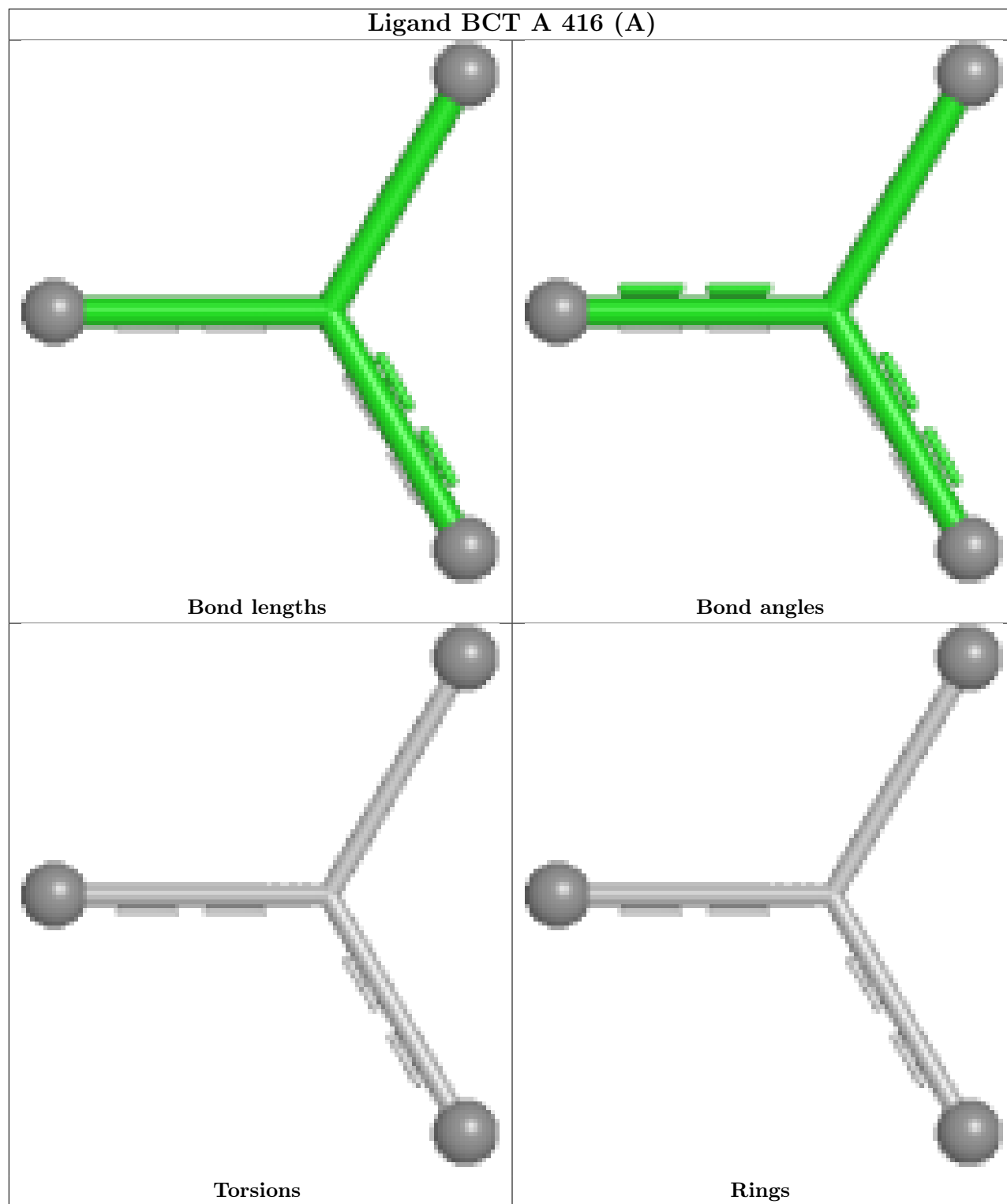


## Ligand PHO a 408 (B)



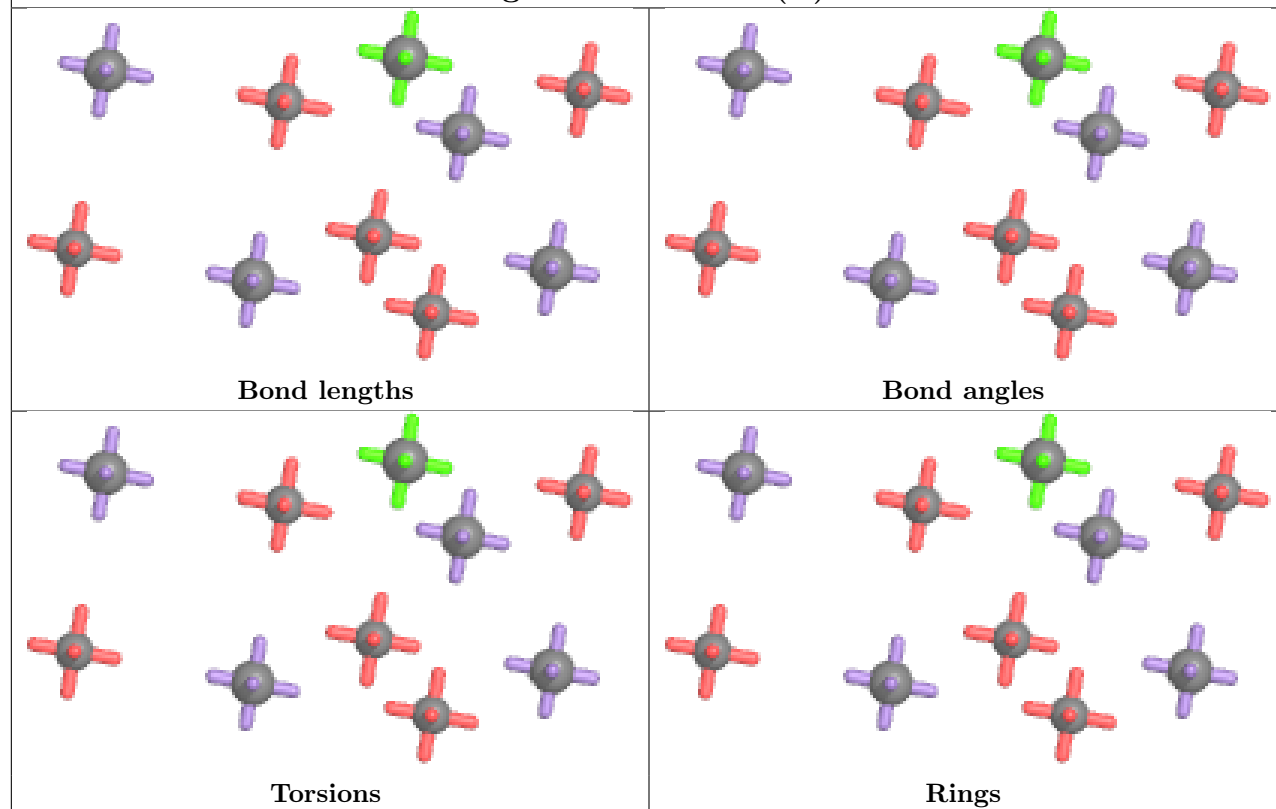
## Ligand PHO A 407 (B)



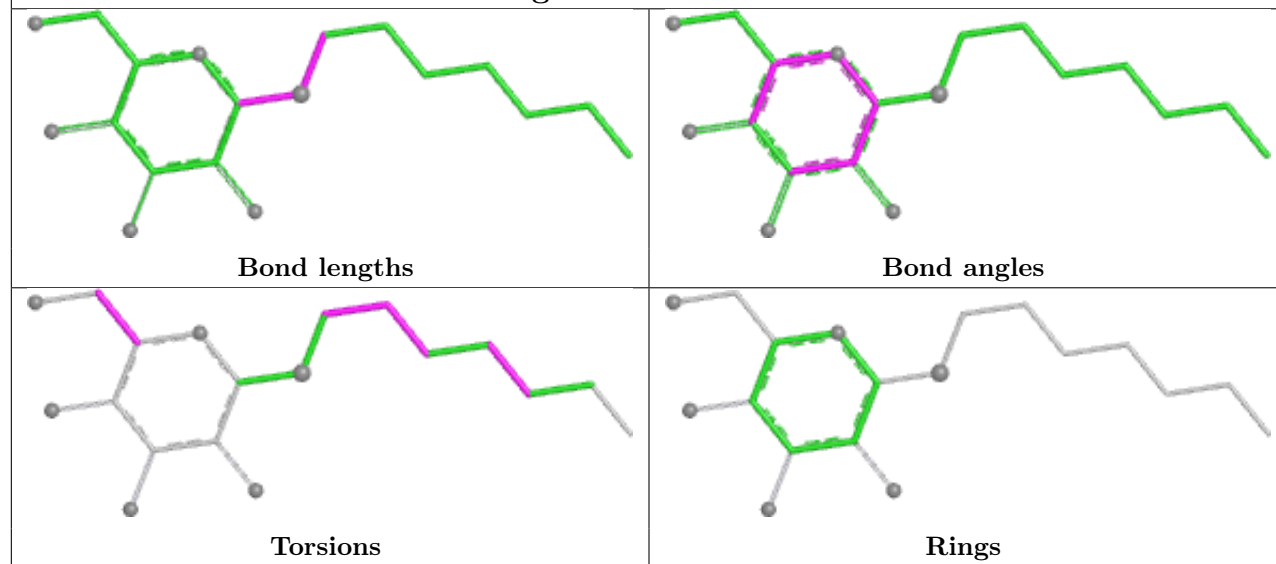




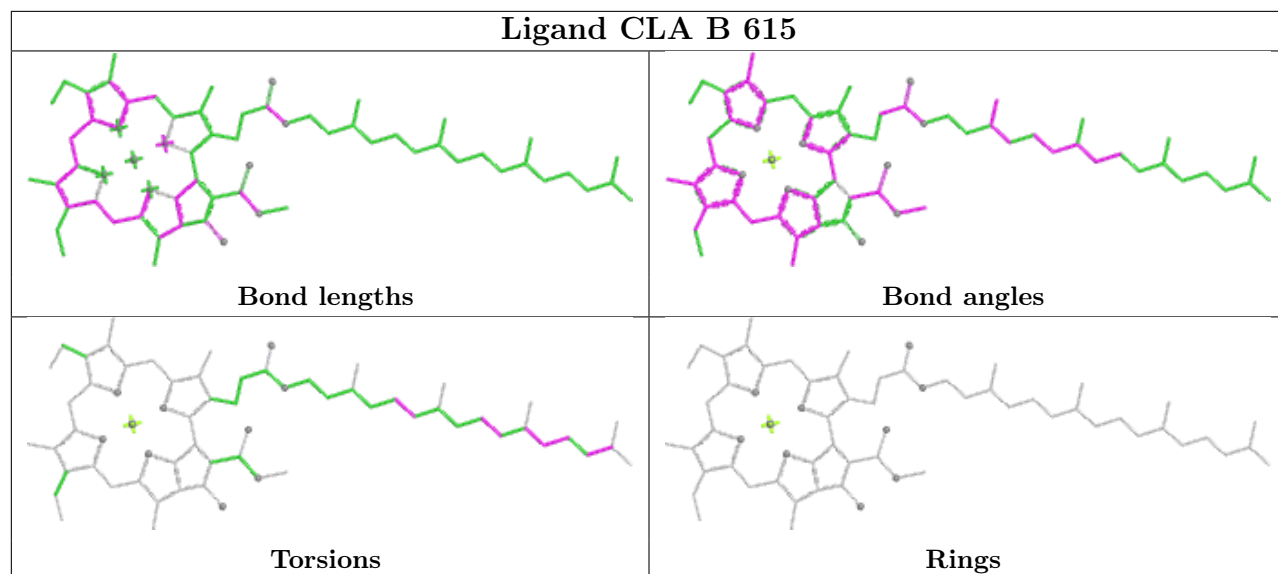
## Ligand OEX a 413 (B)



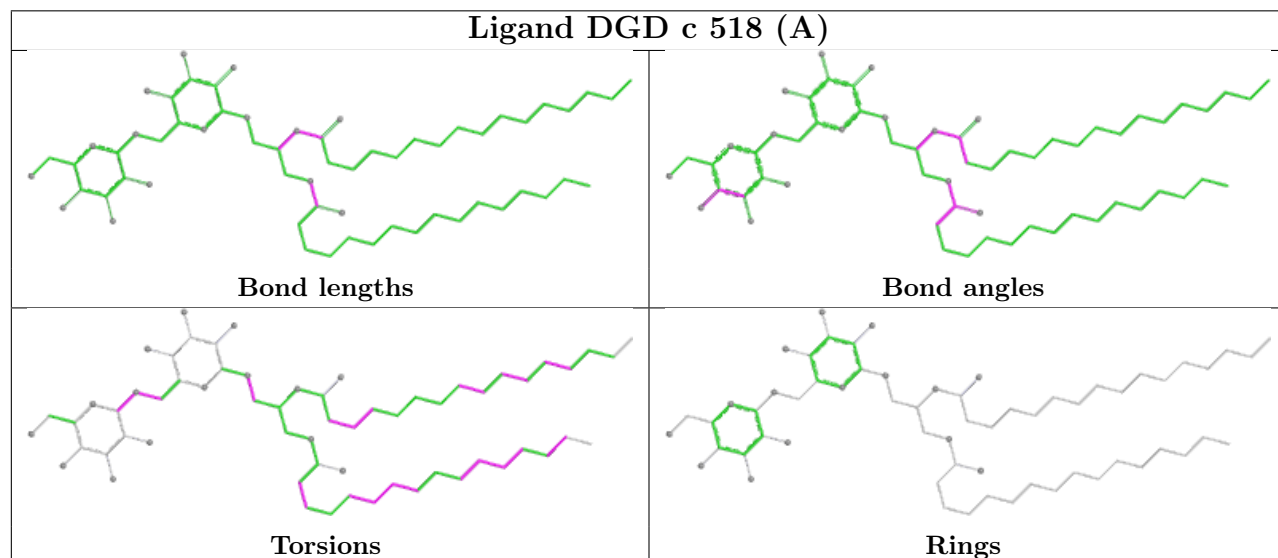
## Ligand HTG b 625



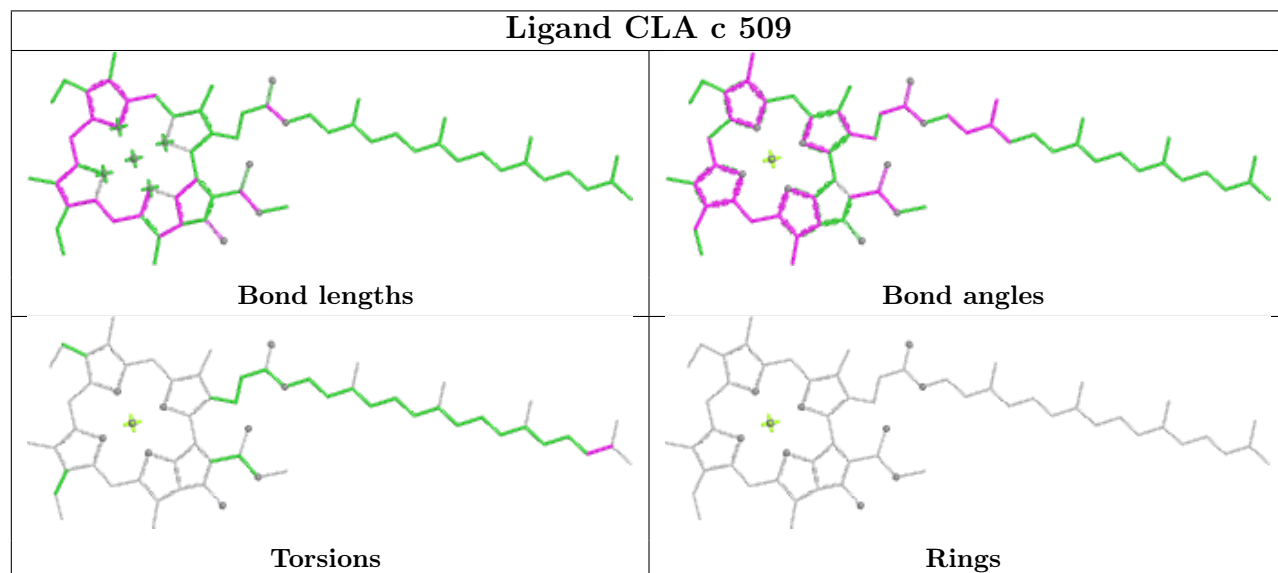
## Ligand CLA B 615



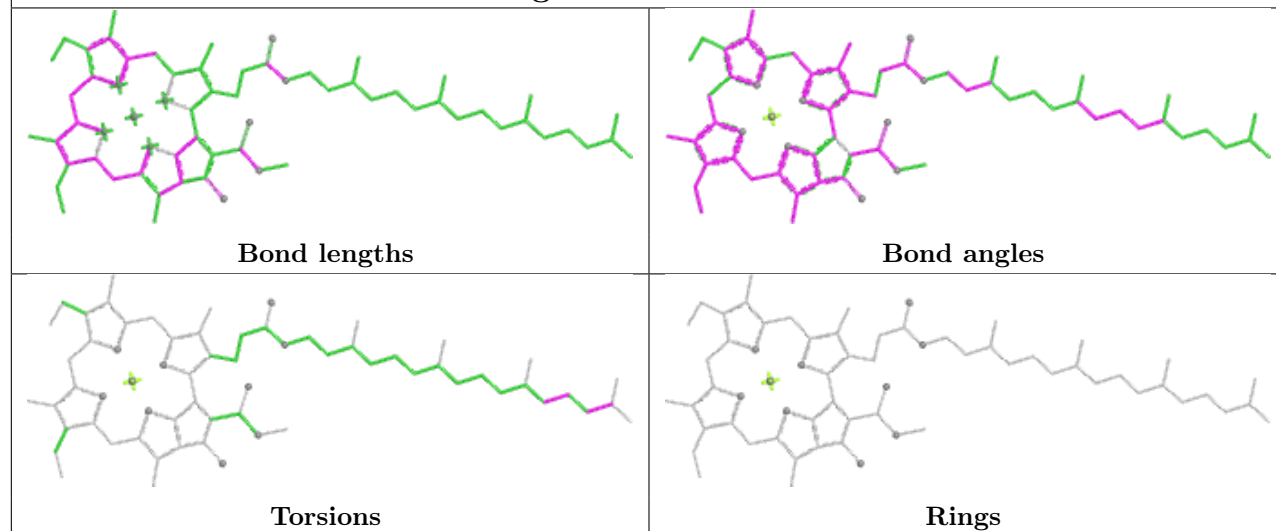
## Ligand DGD c 518 (A)



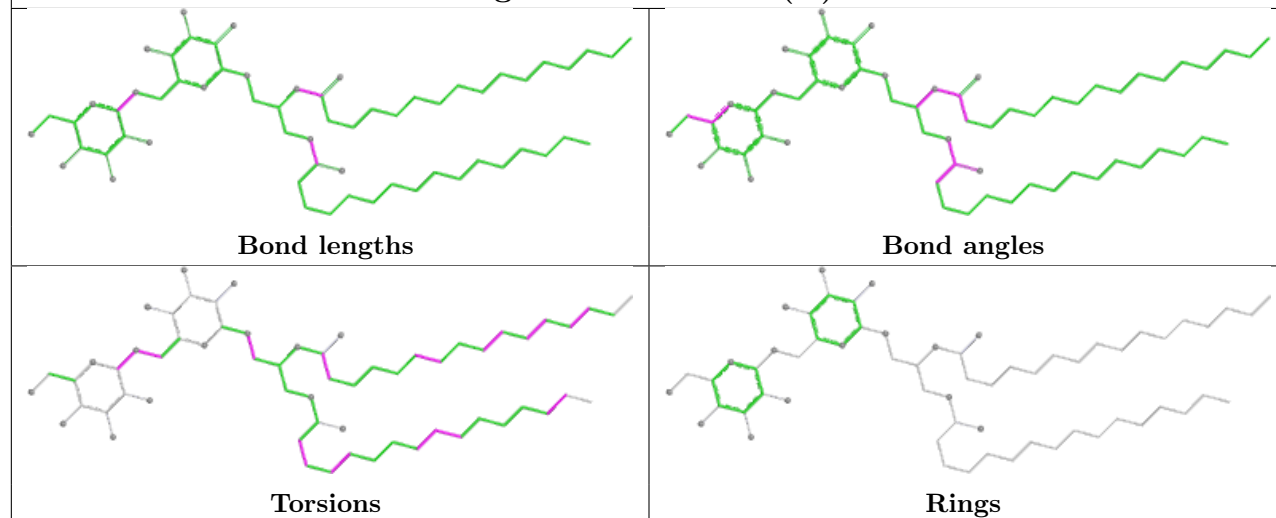
## Ligand CLA c 509



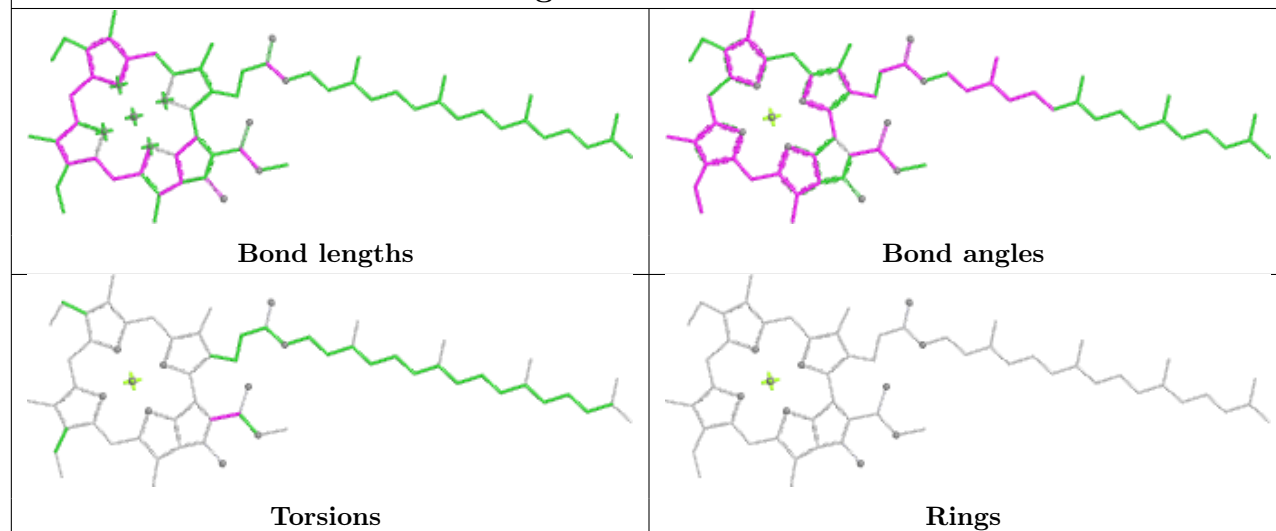
## Ligand CLA B 608

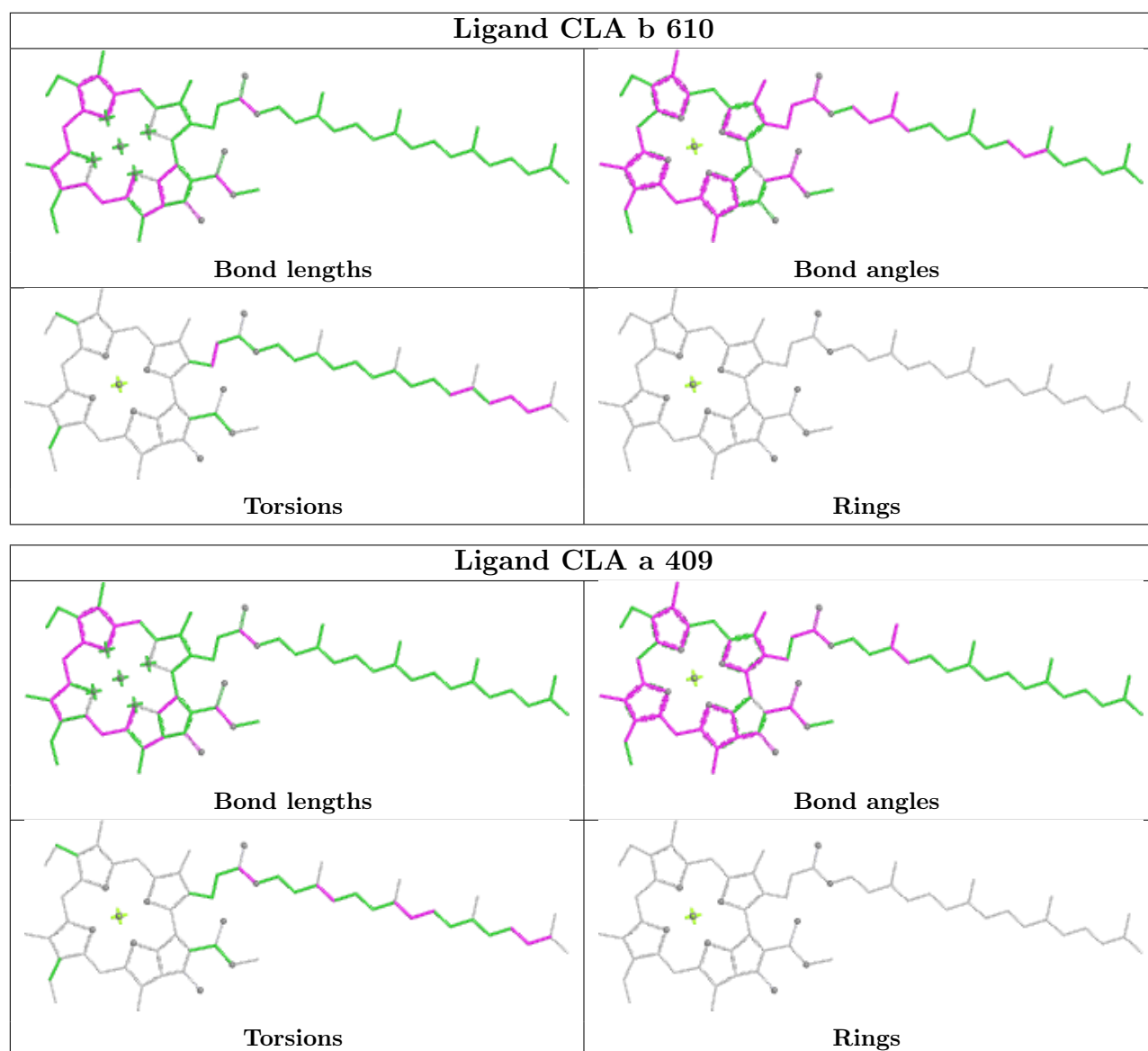


## Ligand DGD C 518 (A)



## Ligand CLA b 609





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)  | -0.56  | 1 (0%) 90 90 | 21, 27, 60, 128       | 222 (66%) |
| 1   | a     | 334/344 (97%)  | -0.53  | 1 (0%) 90 90 | 22, 29, 65, 124       | 220 (65%) |
| 2   | B     | 504/505 (99%)  | -0.51  | 1 (0%) 91 91 | 23, 54, 81, 119       | 22 (4%)   |
| 2   | b     | 504/505 (99%)  | -0.45  | 0 100 100    | 24, 58, 92, 169       | 19 (3%)   |
| 3   | C     | 451/455 (99%)  | -0.54  | 0 100 100    | 22, 60, 81, 160       | 99 (21%)  |
| 3   | c     | 455/455 (100%) | -0.45  | 1 (0%) 91 91 | 25, 66, 86, 130       | 101 (22%) |
| 4   | D     | 342/342 (100%) | -0.60  | 0 100 100    | 21, 47, 65, 136       | 115 (33%) |
| 4   | d     | 341/342 (99%)  | -0.60  | 0 100 100    | 22, 51, 75, 133       | 119 (34%) |
| 5   | E     | 81/84 (96%)    | -0.34  | 1 (1%) 76 77 | 53, 70, 99, 165       | 0         |
| 5   | e     | 79/84 (94%)    | -0.32  | 1 (1%) 75 76 | 32, 77, 114, 152      | 2 (2%)    |
| 6   | F     | 34/44 (77%)    | -0.59  | 0 100 100    | 54, 62, 86, 117       | 0         |
| 6   | f     | 31/44 (70%)    | -0.36  | 1 (3%) 50 52 | 55, 68, 94, 155       | 1 (3%)    |
| 7   | H     | 64/65 (98%)    | -0.31  | 1 (1%) 70 72 | 53, 64, 85, 106       | 0         |
| 7   | h     | 64/65 (98%)    | -0.41  | 1 (1%) 70 72 | 41, 70, 95, 115       | 1 (1%)    |
| 8   | I     | 37/38 (97%)    | -0.21  | 0 100 100    | 54, 63, 127, 162      | 0         |
| 8   | i     | 37/38 (97%)    | -0.27  | 0 100 100    | 55, 65, 122, 143      | 0         |
| 9   | J     | 38/39 (97%)    | -0.32  | 0 100 100    | 51, 70, 124, 180      | 0         |
| 9   | j     | 39/39 (100%)   | -0.31  | 0 100 100    | 60, 76, 128, 171      | 0         |
| 10  | K     | 37/37 (100%)   | -0.61  | 0 100 100    | 59, 68, 89, 113       | 0         |
| 10  | k     | 37/37 (100%)   | -0.46  | 0 100 100    | 68, 75, 98, 112       | 0         |
| 11  | L     | 36/37 (97%)    | -0.57  | 0 100 100    | 24, 48, 100, 142      | 2 (5%)    |
| 11  | l     | 36/37 (97%)    | -0.52  | 0 100 100    | 25, 49, 104, 136      | 2 (5%)    |
| 12  | M     | 32/36 (88%)    | -0.57  | 0 100 100    | 27, 49, 76, 147       | 1 (3%)    |
| 12  | m     | 33/36 (91%)    | -0.43  | 0 100 100    | 25, 51, 73, 154       | 2 (6%)    |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9     |
|-----|-------|-----------------|--------|---------------|-----------------------|-----------|
| 13  | O     | 243/244 (99%)   | -0.48  | 0 100 100     | 21, 64, 116, 187      | 10 (4%)   |
| 13  | o     | 243/244 (99%)   | -0.49  | 0 100 100     | 23, 67, 129, 174      | 8 (3%)    |
| 14  | T     | 29/32 (90%)     | -0.60  | 0 100 100     | 27, 47, 59, 65        | 6 (20%)   |
| 14  | t     | 29/32 (90%)     | -0.59  | 1 (3%) 48 50  | 28, 49, 66, 73        | 5 (17%)   |
| 15  | U     | 96/104 (92%)    | -0.58  | 0 100 100     | 25, 59, 91, 102       | 4 (4%)    |
| 15  | u     | 97/104 (93%)    | -0.61  | 0 100 100     | 28, 62, 84, 138       | 5 (5%)    |
| 16  | V     | 137/137 (100%)  | -0.64  | 0 100 100     | 24, 58, 83, 107       | 6 (4%)    |
| 16  | v     | 137/137 (100%)  | -0.56  | 0 100 100     | 27, 71, 104, 139      | 6 (4%)    |
| 17  | X     | 38/40 (95%)     | -0.32  | 0 100 100     | 35, 72, 94, 113       | 1 (2%)    |
| 17  | x     | 38/40 (95%)     | -0.09  | 0 100 100     | 64, 79, 124, 162      | 0         |
| 18  | Y     | 29/30 (96%)     | 0.03   | 0 100 100     | 69, 87, 124, 125      | 0         |
| 18  | y     | 29/30 (96%)     | -0.21  | 0 100 100     | 76, 92, 113, 116      | 0         |
| 19  | Z     | 62/62 (100%)    | -0.34  | 0 100 100     | 65, 80, 134, 159      | 0         |
| 19  | z     | 62/62 (100%)    | 0.09   | 0 100 100     | 81, 95, 146, 205      | 0         |
| 20  | R     | 34/34 (100%)    | 0.37   | 2 (5%) 28 30  | 82, 103, 134, 144     | 0         |
| All | All   | 5283/5384 (98%) | -0.49  | 12 (0%) 91 91 | 21, 58, 99, 205       | 979 (18%) |

All (12) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 5   | e     | 79[A] | PHE  | 3.9  |
| 7   | H     | 65    | LEU  | 3.2  |
| 6   | f     | 16[A] | PHE  | 3.1  |
| 14  | t     | 30[A] | THR  | 2.8  |
| 1   | A     | 11    | ALA  | 2.7  |
| 20  | R     | 28    | VAL  | 2.5  |
| 2   | B     | 494   | GLY  | 2.5  |
| 3   | c     | 20    | SER  | 2.3  |
| 7   | h     | 65    | LEU  | 2.3  |
| 1   | a     | 11    | ALA  | 2.2  |
| 20  | R     | 35    | LEU  | 2.1  |
| 5   | E     | 4     | THR  | 2.0  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 14  | FME  | T     | 1   | 10/11 | 0.94 | 0.07 | 47,58,69,72                | 0     |
| 14  | FME  | t     | 1   | 10/11 | 0.95 | 0.08 | 43,50,69,76                | 0     |
| 8   | FME  | i     | 1   | 10/11 | 0.96 | 0.06 | 50,68,83,87                | 0     |
| 8   | FME  | I     | 1   | 10/11 | 0.96 | 0.07 | 60,68,82,83                | 0     |
| 12  | FME  | m     | 1   | 10/11 | 0.97 | 0.07 | 50,64,91,120               | 0     |
| 12  | FME  | M     | 1   | 10/11 | 0.97 | 0.06 | 49,61,93,102               | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 27  | GOL  | a     | 418    | 6/6   | 0.63 | 0.15 | 80,108,110,120             | 0     |
| 30  | UNL  | j     | 101    | 10/-  | 0.66 | 0.20 | 83,96,103,107              | 0     |
| 30  | UNL  | A     | 415    | 28/-  | 0.69 | 0.15 | 89,115,132,142             | 0     |
| 30  | UNL  | J     | 101    | 10/-  | 0.70 | 0.28 | 69,81,97,105               | 0     |
| 32  | LMT  | B     | 629    | 35/35 | 0.70 | 0.15 | 65,117,147,151             | 0     |
| 32  | LMT  | A     | 418    | 35/35 | 0.71 | 0.14 | 72,119,140,144             | 0     |
| 32  | LMT  | F     | 101    | 35/35 | 0.71 | 0.15 | 104,135,179,184            | 0     |
| 30  | UNL  | a     | 415    | 30/-  | 0.72 | 0.12 | 92,122,144,155             | 0     |
| 35  | HTG  | B     | 622    | 19/19 | 0.73 | 0.16 | 66,99,118,134              | 0     |
| 32  | LMT  | a     | 417    | 35/35 | 0.74 | 0.14 | 112,138,151,161            | 0     |
| 32  | LMT  | A     | 420    | 35/35 | 0.74 | 0.12 | 96,138,157,172             | 0     |
| 30  | UNL  | I     | 101    | 40/-  | 0.75 | 0.15 | 75,109,159,173             | 0     |
| 30  | UNL  | m     | 102    | 10/-  | 0.75 | 0.20 | 75,77,102,106              | 0     |
| 30  | UNL  | K     | 101[B] | 34/-  | 0.76 | 0.14 | 90,113,127,130             | 34    |
| 32  | LMT  | e     | 101    | 35/35 | 0.76 | 0.14 | 107,142,187,194            | 0     |
| 30  | UNL  | K     | 101[A] | 34/-  | 0.76 | 0.14 | 90,113,127,130             | 34    |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 26  | SQD  | f     | 102    | 43/54 | 0.77 | 0.12 | 97,131,176,184              | 0     |
| 30  | UNL  | l     | 101    | 10/-  | 0.77 | 0.17 | 71,79,95,97                 | 0     |
| 27  | GOL  | O     | 302    | 6/6   | 0.78 | 0.10 | 67,88,100,104               | 0     |
| 34  | LMG  | C     | 521    | 51/55 | 0.78 | 0.11 | 59,121,157,175              | 0     |
| 30  | UNL  | i     | 101    | 40/-  | 0.78 | 0.13 | 74,107,162,167              | 0     |
| 35  | HTG  | C     | 522    | 19/19 | 0.78 | 0.12 | 111,128,143,152             | 0     |
| 37  | CA   | F     | 103    | 1/1   | 0.78 | 0.23 | 128,128,128,128             | 0     |
| 27  | GOL  | o     | 304    | 6/6   | 0.79 | 0.15 | 89,93,102,106               | 0     |
| 30  | UNL  | b     | 626    | 33/-  | 0.79 | 0.13 | 69,96,158,173               | 0     |
| 27  | GOL  | d     | 411    | 6/6   | 0.80 | 0.24 | 52,68,77,89                 | 0     |
| 30  | UNL  | c     | 525[A] | 32/-  | 0.80 | 0.15 | 98,115,128,135              | 32    |
| 30  | UNL  | c     | 525[B] | 32/-  | 0.80 | 0.15 | 98,115,128,135              | 32    |
| 27  | GOL  | A     | 411    | 6/6   | 0.80 | 0.14 | 63,80,85,90                 | 0     |
| 32  | LMT  | b     | 621    | 25/35 | 0.80 | 0.13 | 86,120,162,172              | 0     |
| 27  | GOL  | B     | 626    | 6/6   | 0.81 | 0.13 | 68,87,96,119                | 0     |
| 30  | UNL  | D     | 709    | 40/-  | 0.81 | 0.13 | 67,98,145,157               | 0     |
| 30  | UNL  | d     | 408    | 36/-  | 0.81 | 0.12 | 68,97,136,143               | 0     |
| 29  | PL9  | A     | 414[A] | 55/55 | 0.82 | 0.15 | 66,96,110,116               | 55    |
| 29  | PL9  | A     | 414[B] | 55/55 | 0.82 | 0.15 | 66,96,111,117               | 55    |
| 27  | GOL  | o     | 303    | 6/6   | 0.82 | 0.17 | 85,106,121,123              | 0     |
| 35  | HTG  | b     | 623    | 19/19 | 0.82 | 0.11 | 83,133,157,164              | 0     |
| 27  | GOL  | b     | 624    | 6/6   | 0.82 | 0.16 | 93,103,110,118              | 0     |
| 35  | HTG  | D     | 710    | 16/19 | 0.83 | 0.11 | 86,105,131,151              | 0     |
| 27  | GOL  | a     | 419    | 6/6   | 0.83 | 0.15 | 60,80,88,94                 | 0     |
| 35  | HTG  | d     | 409    | 16/19 | 0.83 | 0.11 | 79,122,141,161              | 0     |
| 32  | LMT  | B     | 627    | 35/35 | 0.83 | 0.11 | 61,108,138,152              | 0     |
| 33  | LHG  | a     | 420[B] | 42/49 | 0.84 | 0.11 | 99,148,163,168              | 42    |
| 35  | HTG  | V     | 202    | 11/19 | 0.84 | 0.09 | 81,115,121,129              | 0     |
| 26  | SQD  | a     | 412    | 54/54 | 0.84 | 0.10 | 67,97,137,156               | 0     |
| 35  | HTG  | c     | 522    | 19/19 | 0.84 | 0.09 | 104,126,145,148             | 0     |
| 30  | UNL  | B     | 625    | 33/-  | 0.84 | 0.13 | 58,109,143,152              | 0     |
| 33  | LHG  | a     | 420[A] | 42/49 | 0.84 | 0.11 | 99,148,163,168              | 42    |
| 32  | LMT  | T     | 101    | 35/35 | 0.85 | 0.11 | 76,131,174,184              | 0     |
| 34  | LMG  | Z     | 101    | 37/55 | 0.85 | 0.13 | 66,119,147,176              | 0     |
| 32  | LMT  | b     | 627    | 25/35 | 0.86 | 0.12 | 53,101,149,156              | 0     |
| 35  | HTG  | b     | 622    | 19/19 | 0.86 | 0.12 | 58,83,125,127               | 0     |
| 34  | LMG  | z     | 101    | 39/55 | 0.86 | 0.12 | 75,130,153,169              | 0     |
| 26  | SQD  | A     | 412    | 54/54 | 0.86 | 0.10 | 66,89,136,163               | 0     |
| 32  | LMT  | t     | 101    | 26/35 | 0.86 | 0.12 | 75,114,149,159              | 0     |
| 34  | LMG  | c     | 521    | 51/55 | 0.86 | 0.10 | 72,137,167,189              | 0     |
| 27  | GOL  | O     | 303    | 6/6   | 0.87 | 0.12 | 88,102,106,117              | 0     |
| 29  | PL9  | a     | 414[A] | 55/55 | 0.87 | 0.15 | 87,109,123,130              | 55    |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 29  | PL9  | a     | 414[B] | 55/55 | 0.87 | 0.15 | 87,109,124,130              | 55    |
| 32  | LMT  | B     | 630    | 25/35 | 0.87 | 0.11 | 57,92,148,164               | 0     |
| 32  | LMT  | m     | 103    | 35/35 | 0.87 | 0.10 | 55,95,109,123               | 0     |
| 27  | GOL  | l     | 102[A] | 6/6   | 0.87 | 0.17 | 71,105,107,108              | 6     |
| 35  | HTG  | o     | 301    | 19/19 | 0.87 | 0.12 | 58,86,117,132               | 0     |
| 27  | GOL  | l     | 102[B] | 6/6   | 0.87 | 0.17 | 70,107,107,108              | 6     |
| 26  | SQD  | X     | 101    | 43/54 | 0.88 | 0.11 | 73,104,134,142              | 0     |
| 26  | SQD  | b     | 620    | 54/54 | 0.88 | 0.10 | 68,98,127,133               | 0     |
| 33  | LHG  | E     | 101[A] | 42/49 | 0.88 | 0.12 | 70,107,122,131              | 42    |
| 33  | LHG  | E     | 101[B] | 42/49 | 0.88 | 0.12 | 70,107,123,131              | 42    |
| 26  | SQD  | B     | 620    | 54/54 | 0.89 | 0.10 | 64,98,139,146               | 0     |
| 31  | BCT  | A     | 416[A] | 4/4   | 0.89 | 0.10 | 54,56,61,64                 | 4     |
| 31  | BCT  | A     | 416[B] | 4/4   | 0.89 | 0.10 | 54,54,63,63                 | 4     |
| 30  | UNL  | D     | 708    | 17/-  | 0.89 | 0.11 | 65,78,110,128               | 0     |
| 32  | LMT  | M     | 101    | 35/35 | 0.89 | 0.10 | 64,95,120,130               | 0     |
| 23  | CLA  | b     | 601    | 65/65 | 0.89 | 0.10 | 60,88,131,160               | 0     |
| 37  | CA   | f     | 103    | 1/1   | 0.89 | 0.12 | 123,123,123,123             | 0     |
| 27  | GOL  | c     | 527    | 6/6   | 0.90 | 0.16 | 103,117,127,128             | 0     |
| 27  | GOL  | D     | 701    | 6/6   | 0.90 | 0.28 | 56,77,86,93                 | 0     |
| 27  | GOL  | v     | 202[A] | 6/6   | 0.90 | 0.11 | 68,79,85,87                 | 6     |
| 27  | GOL  | v     | 202[B] | 6/6   | 0.90 | 0.11 | 68,79,85,88                 | 6     |
| 27  | GOL  | V     | 203[A] | 6/6   | 0.90 | 0.12 | 59,73,76,83                 | 6     |
| 27  | GOL  | V     | 203[B] | 6/6   | 0.90 | 0.12 | 58,73,76,83                 | 6     |
| 23  | CLA  | c     | 514    | 65/65 | 0.91 | 0.09 | 68,93,130,148               | 0     |
| 34  | LMG  | c     | 501    | 51/55 | 0.91 | 0.08 | 67,90,114,134               | 0     |
| 34  | LMG  | c     | 520    | 51/55 | 0.91 | 0.09 | 63,91,137,157               | 0     |
| 27  | GOL  | B     | 628    | 6/6   | 0.91 | 0.12 | 73,79,89,102                | 0     |
| 34  | LMG  | m     | 101    | 51/55 | 0.91 | 0.09 | 60,76,98,112                | 0     |
| 23  | CLA  | B     | 601    | 65/65 | 0.91 | 0.09 | 55,78,119,156               | 0     |
| 27  | GOL  | D     | 712    | 6/6   | 0.91 | 0.15 | 51,66,78,101                | 0     |
| 27  | GOL  | B     | 623    | 6/6   | 0.91 | 0.09 | 71,85,90,90                 | 0     |
| 34  | LMG  | C     | 501    | 51/55 | 0.91 | 0.09 | 61,90,118,132               | 0     |
| 37  | CA   | o     | 302    | 1/1   | 0.91 | 0.07 | 111,111,111,111             | 0     |
| 27  | GOL  | b     | 628    | 6/6   | 0.92 | 0.08 | 84,86,95,96                 | 0     |
| 35  | HTG  | b     | 625    | 19/19 | 0.92 | 0.08 | 64,78,100,111               | 0     |
| 33  | LHG  | A     | 419[A] | 49/49 | 0.92 | 0.10 | 51,65,85,93                 | 49    |
| 35  | HTG  | B     | 624    | 19/19 | 0.92 | 0.07 | 66,78,100,107               | 0     |
| 33  | LHG  | A     | 419[B] | 49/49 | 0.92 | 0.10 | 51,66,85,93                 | 49    |
| 34  | LMG  | B     | 621    | 51/55 | 0.92 | 0.09 | 56,72,94,121                | 0     |
| 30  | UNL  | d     | 407    | 17/-  | 0.92 | 0.10 | 67,84,111,112               | 0     |
| 34  | LMG  | C     | 520    | 51/55 | 0.92 | 0.09 | 57,87,123,129               | 0     |
| 34  | LMG  | D     | 711    | 51/55 | 0.93 | 0.09 | 50,68,126,141               | 0     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 25  | BCR  | T     | 102    | 40/40 | 0.93 | 0.07 | 44,61,75,80                 | 0     |
| 25  | BCR  | d     | 403    | 40/40 | 0.93 | 0.08 | 53,65,102,114               | 0     |
| 25  | BCR  | t     | 102    | 40/40 | 0.93 | 0.07 | 43,63,83,98                 | 0     |
| 34  | LMG  | d     | 410    | 51/55 | 0.93 | 0.08 | 52,69,126,154               | 0     |
| 23  | CLA  | b     | 616    | 65/65 | 0.93 | 0.08 | 49,63,130,145               | 0     |
| 23  | CLA  | C     | 514    | 65/65 | 0.93 | 0.08 | 57,84,113,118               | 0     |
| 25  | BCR  | D     | 704    | 40/40 | 0.93 | 0.09 | 47,60,103,111               | 0     |
| 36  | DGD  | c     | 518[A] | 62/66 | 0.93 | 0.08 | 57,70,121,139               | 62    |
| 36  | DGD  | c     | 518[B] | 62/66 | 0.93 | 0.08 | 57,70,121,139               | 62    |
| 26  | SQD  | a     | 411[A] | 54/54 | 0.93 | 0.10 | 59,82,124,129               | 54    |
| 37  | CA   | c     | 523    | 1/1   | 0.93 | 0.09 | 76,76,76,76                 | 0     |
| 26  | SQD  | a     | 411[B] | 54/54 | 0.93 | 0.10 | 59,82,124,129               | 54    |
| 25  | BCR  | K     | 102    | 40/40 | 0.93 | 0.10 | 55,67,79,82                 | 0     |
| 31  | BCT  | a     | 404[B] | 4/4   | 0.94 | 0.09 | 61,61,71,85                 | 4     |
| 23  | CLA  | c     | 505    | 65/65 | 0.94 | 0.07 | 50,63,111,139               | 0     |
| 23  | CLA  | c     | 507    | 65/65 | 0.94 | 0.08 | 53,69,127,138               | 0     |
| 23  | CLA  | c     | 513    | 65/65 | 0.94 | 0.09 | 63,81,130,137               | 0     |
| 23  | CLA  | A     | 408    | 65/65 | 0.94 | 0.09 | 42,54,132,155               | 0     |
| 23  | CLA  | d     | 402    | 65/65 | 0.94 | 0.09 | 51,67,133,149               | 0     |
| 25  | BCR  | B     | 619    | 40/40 | 0.94 | 0.08 | 47,60,90,98                 | 0     |
| 30  | UNL  | X     | 102    | 18/-  | 0.94 | 0.10 | 62,75,114,115               | 0     |
| 25  | BCR  | C     | 515    | 40/40 | 0.94 | 0.08 | 57,75,89,93                 | 0     |
| 23  | CLA  | D     | 703    | 65/65 | 0.94 | 0.08 | 47,59,126,136               | 0     |
| 25  | BCR  | H     | 101    | 40/40 | 0.94 | 0.07 | 47,64,80,89                 | 0     |
| 23  | CLA  | a     | 409    | 65/65 | 0.94 | 0.10 | 43,56,143,159               | 0     |
| 23  | CLA  | C     | 505    | 65/65 | 0.94 | 0.07 | 40,57,96,128                | 0     |
| 25  | BCR  | c     | 515    | 40/40 | 0.94 | 0.08 | 71,83,93,95                 | 0     |
| 23  | CLA  | b     | 614    | 65/65 | 0.94 | 0.07 | 42,51,105,124               | 0     |
| 25  | BCR  | h     | 101    | 40/40 | 0.94 | 0.08 | 55,65,91,97                 | 0     |
| 23  | CLA  | C     | 507    | 65/65 | 0.94 | 0.08 | 56,72,124,142               | 0     |
| 33  | LHG  | D     | 707[A] | 49/49 | 0.94 | 0.09 | 51,61,108,113               | 49    |
| 33  | LHG  | D     | 707[B] | 49/49 | 0.94 | 0.09 | 51,61,108,113               | 49    |
| 25  | BCR  | y     | 101    | 40/40 | 0.94 | 0.07 | 56,72,86,96                 | 0     |
| 26  | SQD  | A     | 410[A] | 54/54 | 0.94 | 0.09 | 58,79,110,117               | 54    |
| 26  | SQD  | A     | 410[B] | 54/54 | 0.94 | 0.09 | 58,79,110,118               | 54    |
| 31  | BCT  | a     | 404[A] | 4/4   | 0.94 | 0.09 | 60,61,69,82                 | 4     |
| 36  | DGD  | C     | 518[A] | 62/66 | 0.94 | 0.08 | 51,67,115,122               | 62    |
| 36  | DGD  | C     | 518[B] | 62/66 | 0.94 | 0.08 | 51,67,116,122               | 62    |
| 36  | DGD  | c     | 517[A] | 62/66 | 0.94 | 0.07 | 49,64,104,113               | 62    |
| 36  | DGD  | c     | 517[B] | 62/66 | 0.94 | 0.07 | 48,64,104,113               | 62    |
| 33  | LHG  | b     | 629[A] | 49/49 | 0.94 | 0.09 | 53,61,68,92                 | 49    |
| 33  | LHG  | b     | 629[B] | 49/49 | 0.94 | 0.09 | 52,61,68,93                 | 49    |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 36  | DGD  | c     | 519    | 62/66 | 0.94 | 0.07 | 50,68,104,134               | 0     |
| 33  | LHG  | d     | 406[A] | 49/49 | 0.94 | 0.10 | 54,66,114,132               | 49    |
| 33  | LHG  | d     | 406[B] | 49/49 | 0.94 | 0.10 | 54,66,114,132               | 49    |
| 33  | LHG  | d     | 412[A] | 49/49 | 0.94 | 0.09 | 52,68,81,90                 | 49    |
| 33  | LHG  | d     | 412[B] | 49/49 | 0.94 | 0.09 | 52,68,82,90                 | 49    |
| 27  | GOL  | C     | 523[B] | 6/6   | 0.95 | 0.09 | 59,64,69,73                 | 6     |
| 25  | BCR  | b     | 619    | 40/40 | 0.95 | 0.07 | 48,62,86,89                 | 0     |
| 23  | CLA  | C     | 509    | 65/65 | 0.95 | 0.07 | 47,56,121,146               | 0     |
| 23  | CLA  | c     | 506    | 65/65 | 0.95 | 0.07 | 48,65,88,99                 | 0     |
| 23  | CLA  | C     | 513    | 65/65 | 0.95 | 0.08 | 54,74,115,133               | 0     |
| 25  | BCR  | k     | 101    | 40/40 | 0.95 | 0.08 | 56,74,83,91                 | 0     |
| 23  | CLA  | c     | 508    | 65/65 | 0.95 | 0.09 | 52,70,82,92                 | 0     |
| 23  | CLA  | c     | 509    | 65/65 | 0.95 | 0.07 | 43,66,128,150               | 0     |
| 23  | CLA  | B     | 611    | 65/65 | 0.95 | 0.07 | 38,48,65,76                 | 0     |
| 23  | CLA  | B     | 614    | 65/65 | 0.95 | 0.07 | 39,51,111,124               | 0     |
| 23  | CLA  | a     | 407[A] | 65/65 | 0.95 | 0.07 | 43,56,128,136               | 65    |
| 25  | BCR  | A     | 409    | 40/40 | 0.95 | 0.07 | 41,53,67,69                 | 0     |
| 25  | BCR  | B     | 618    | 40/40 | 0.95 | 0.06 | 43,57,73,83                 | 0     |
| 23  | CLA  | a     | 407[B] | 65/65 | 0.95 | 0.07 | 43,56,128,136               | 65    |
| 23  | CLA  | B     | 616    | 65/65 | 0.95 | 0.09 | 50,63,135,143               | 0     |
| 23  | CLA  | B     | 603    | 65/65 | 0.95 | 0.08 | 42,54,74,83                 | 0     |
| 23  | CLA  | b     | 606    | 65/65 | 0.95 | 0.07 | 40,59,109,127               | 0     |
| 23  | CLA  | B     | 606    | 65/65 | 0.95 | 0.08 | 44,58,110,134               | 0     |
| 23  | CLA  | C     | 508    | 65/65 | 0.95 | 0.08 | 50,63,87,96                 | 0     |
| 36  | DGD  | C     | 517[A] | 62/66 | 0.95 | 0.07 | 47,59,99,108                | 62    |
| 36  | DGD  | C     | 517[B] | 62/66 | 0.95 | 0.07 | 47,59,99,108                | 62    |
| 30  | UNL  | x     | 101    | 18/-  | 0.95 | 0.10 | 73,81,134,142               | 0     |
| 33  | LHG  | d     | 405[A] | 49/49 | 0.95 | 0.08 | 50,59,71,78                 | 49    |
| 36  | DGD  | C     | 519    | 62/66 | 0.95 | 0.07 | 44,61,99,122                | 0     |
| 36  | DGD  | H     | 102    | 62/66 | 0.95 | 0.08 | 48,63,76,88                 | 0     |
| 33  | LHG  | d     | 405[B] | 49/49 | 0.95 | 0.08 | 50,59,71,79                 | 49    |
| 25  | BCR  | Y     | 101    | 40/40 | 0.95 | 0.07 | 51,64,84,89                 | 0     |
| 25  | BCR  | a     | 410    | 40/40 | 0.95 | 0.07 | 44,56,67,73                 | 0     |
| 29  | PL9  | D     | 705[A] | 55/55 | 0.95 | 0.07 | 38,51,61,68                 | 55    |
| 29  | PL9  | D     | 705[B] | 55/55 | 0.95 | 0.07 | 37,51,61,69                 | 55    |
| 36  | DGD  | h     | 102    | 62/66 | 0.95 | 0.08 | 50,66,80,86                 | 0     |
| 25  | BCR  | b     | 617    | 40/40 | 0.95 | 0.06 | 46,57,65,70                 | 0     |
| 27  | GOL  | C     | 523[A] | 6/6   | 0.95 | 0.09 | 59,64,68,73                 | 6     |
| 29  | PL9  | d     | 404[A] | 55/55 | 0.95 | 0.07 | 41,52,62,69                 | 55    |
| 29  | PL9  | d     | 404[B] | 55/55 | 0.95 | 0.07 | 41,52,63,70                 | 55    |
| 25  | BCR  | b     | 618    | 40/40 | 0.96 | 0.06 | 47,61,78,83                 | 0     |
| 27  | GOL  | c     | 526[A] | 6/6   | 0.96 | 0.08 | 72,74,80,83                 | 6     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 27  | GOL  | c     | 526[B] | 6/6   | 0.96 | 0.08 | 72,75,81,83                 | 6     |
| 23  | CLA  | c     | 502    | 65/65 | 0.96 | 0.07 | 54,67,80,89                 | 0     |
| 23  | CLA  | c     | 504    | 65/65 | 0.96 | 0.07 | 49,71,86,103                | 0     |
| 25  | BCR  | c     | 516    | 40/40 | 0.96 | 0.07 | 53,67,80,90                 | 0     |
| 23  | CLA  | A     | 405[A] | 65/65 | 0.96 | 0.06 | 36,46,58,71                 | 65    |
| 23  | CLA  | A     | 405[B] | 65/65 | 0.96 | 0.06 | 35,46,58,71                 | 65    |
| 23  | CLA  | D     | 702[A] | 65/65 | 0.96 | 0.07 | 36,45,68,81                 | 65    |
| 23  | CLA  | D     | 702[B] | 65/65 | 0.96 | 0.07 | 36,45,68,83                 | 65    |
| 23  | CLA  | B     | 602    | 65/65 | 0.96 | 0.06 | 46,56,71,86                 | 0     |
| 23  | CLA  | c     | 512    | 65/65 | 0.96 | 0.08 | 57,71,87,114                | 0     |
| 23  | CLA  | C     | 502    | 65/65 | 0.96 | 0.06 | 49,60,74,85                 | 0     |
| 23  | CLA  | C     | 504    | 65/65 | 0.96 | 0.06 | 47,62,72,85                 | 0     |
| 23  | CLA  | A     | 406[A] | 65/65 | 0.96 | 0.06 | 40,49,114,130               | 65    |
| 24  | PHO  | A     | 407[A] | 64/64 | 0.96 | 0.06 | 40,46,53,59                 | 64    |
| 24  | PHO  | A     | 407[B] | 64/64 | 0.96 | 0.06 | 40,46,53,60                 | 64    |
| 24  | PHO  | A     | 417[A] | 64/64 | 0.96 | 0.06 | 37,50,58,62                 | 64    |
| 24  | PHO  | A     | 417[B] | 64/64 | 0.96 | 0.06 | 37,50,58,62                 | 64    |
| 24  | PHO  | a     | 408[A] | 64/64 | 0.96 | 0.06 | 42,49,54,57                 | 64    |
| 24  | PHO  | a     | 408[B] | 64/64 | 0.96 | 0.06 | 41,49,55,57                 | 64    |
| 24  | PHO  | a     | 416[A] | 64/64 | 0.96 | 0.07 | 44,56,63,67                 | 64    |
| 24  | PHO  | a     | 416[B] | 64/64 | 0.96 | 0.07 | 43,56,63,67                 | 64    |
| 33  | LHG  | D     | 706[A] | 49/49 | 0.96 | 0.08 | 48,55,68,77                 | 49    |
| 33  | LHG  | D     | 706[B] | 49/49 | 0.96 | 0.08 | 47,55,68,78                 | 49    |
| 23  | CLA  | C     | 506    | 65/65 | 0.96 | 0.07 | 45,61,91,102                | 0     |
| 25  | BCR  | B     | 617    | 40/40 | 0.96 | 0.06 | 41,55,63,71                 | 0     |
| 23  | CLA  | b     | 602    | 65/65 | 0.96 | 0.07 | 48,61,84,94                 | 0     |
| 23  | CLA  | b     | 604    | 65/65 | 0.96 | 0.07 | 43,53,103,127               | 0     |
| 33  | LHG  | L     | 101[A] | 49/49 | 0.96 | 0.07 | 51,59,70,92                 | 49    |
| 33  | LHG  | L     | 101[B] | 49/49 | 0.96 | 0.07 | 50,59,70,92                 | 49    |
| 23  | CLA  | A     | 406[B] | 65/65 | 0.96 | 0.06 | 40,49,114,130               | 65    |
| 25  | BCR  | C     | 516    | 40/40 | 0.96 | 0.06 | 51,63,77,84                 | 0     |
| 23  | CLA  | b     | 607    | 65/65 | 0.96 | 0.07 | 38,50,81,91                 | 0     |
| 23  | CLA  | b     | 609    | 65/65 | 0.96 | 0.07 | 47,64,75,91                 | 0     |
| 23  | CLA  | b     | 611    | 65/65 | 0.96 | 0.07 | 38,51,72,80                 | 0     |
| 23  | CLA  | b     | 612    | 65/65 | 0.96 | 0.07 | 40,54,65,72                 | 0     |
| 37  | CA   | O     | 301    | 1/1   | 0.96 | 0.06 | 113,113,113,113             | 0     |
| 23  | CLA  | B     | 607    | 65/65 | 0.96 | 0.06 | 36,48,74,86                 | 0     |
| 23  | CLA  | b     | 615    | 65/65 | 0.96 | 0.06 | 49,61,84,94                 | 0     |
| 23  | CLA  | B     | 610    | 65/65 | 0.96 | 0.08 | 43,55,68,89                 | 0     |
| 21  | FE2  | a     | 401[A] | 1/1   | 0.97 | 0.04 | 54,54,54,54                 | 1     |
| 23  | CLA  | B     | 615    | 65/65 | 0.97 | 0.06 | 44,55,83,97                 | 0     |
| 23  | CLA  | a     | 405[A] | 65/65 | 0.97 | 0.07 | 41,48,64,76                 | 65    |

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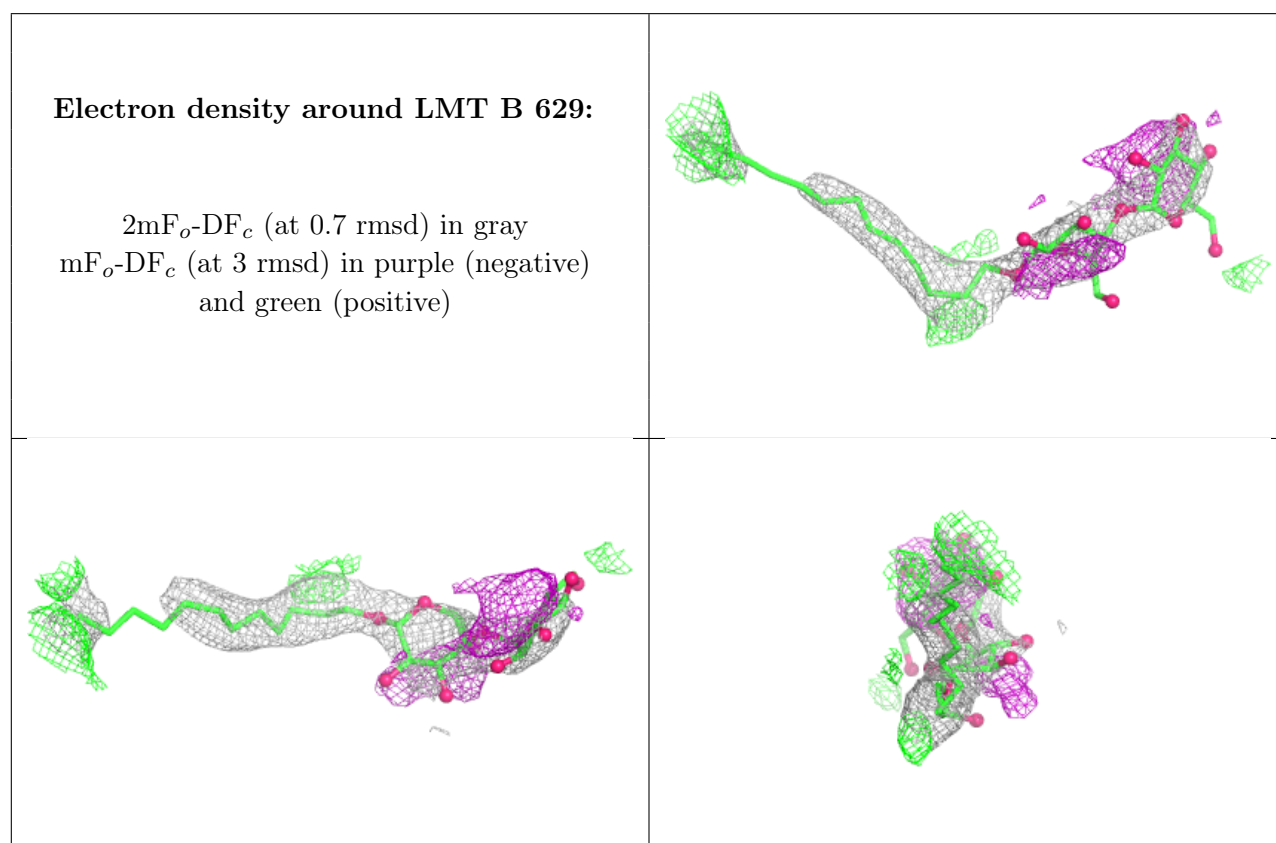
| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 23  | CLA  | a     | 405[B] | 65/65 | 0.97 | 0.07 | 40,47,64,77                 | 65    |
| 23  | CLA  | a     | 406[A] | 65/65 | 0.97 | 0.06 | 39,46,67,71                 | 65    |
| 23  | CLA  | a     | 406[B] | 65/65 | 0.97 | 0.06 | 39,47,67,71                 | 65    |
| 23  | CLA  | c     | 510    | 65/65 | 0.97 | 0.08 | 50,63,92,98                 | 0     |
| 23  | CLA  | c     | 511    | 65/65 | 0.97 | 0.06 | 50,64,77,90                 | 0     |
| 21  | FE2  | a     | 401[B] | 1/1   | 0.97 | 0.04 | 54,54,54,54                 | 1     |
| 23  | CLA  | B     | 604    | 65/65 | 0.97 | 0.06 | 38,48,118,132               | 0     |
| 23  | CLA  | C     | 503    | 65/65 | 0.97 | 0.06 | 43,55,81,92                 | 0     |
| 23  | CLA  | d     | 401[A] | 65/65 | 0.97 | 0.06 | 41,47,71,91                 | 65    |
| 23  | CLA  | d     | 401[B] | 65/65 | 0.97 | 0.06 | 41,47,72,91                 | 65    |
| 23  | CLA  | B     | 605    | 65/65 | 0.97 | 0.06 | 40,50,68,85                 | 0     |
| 22  | CL   | A     | 403[A] | 1/1   | 0.97 | 0.03 | 47,47,47,47                 | 1     |
| 23  | CLA  | b     | 603    | 65/65 | 0.97 | 0.06 | 45,57,83,95                 | 0     |
| 22  | CL   | A     | 403[B] | 1/1   | 0.97 | 0.03 | 47,47,47,47                 | 1     |
| 23  | CLA  | b     | 605    | 65/65 | 0.97 | 0.07 | 39,52,78,83                 | 0     |
| 23  | CLA  | B     | 608    | 65/65 | 0.97 | 0.05 | 41,52,71,79                 | 0     |
| 23  | CLA  | B     | 609    | 65/65 | 0.97 | 0.06 | 45,60,74,78                 | 0     |
| 23  | CLA  | b     | 608    | 65/65 | 0.97 | 0.05 | 42,58,79,96                 | 0     |
| 23  | CLA  | A     | 404[A] | 65/65 | 0.97 | 0.06 | 38,44,62,71                 | 65    |
| 23  | CLA  | b     | 610    | 65/65 | 0.97 | 0.07 | 49,58,71,83                 | 0     |
| 23  | CLA  | C     | 510    | 65/65 | 0.97 | 0.08 | 46,59,84,88                 | 0     |
| 23  | CLA  | C     | 511    | 65/65 | 0.97 | 0.06 | 48,59,79,85                 | 0     |
| 23  | CLA  | b     | 613    | 65/65 | 0.97 | 0.05 | 42,52,88,102                | 0     |
| 37  | CA   | C     | 524    | 1/1   | 0.97 | 0.06 | 71,71,71,71                 | 0     |
| 23  | CLA  | C     | 512    | 65/65 | 0.97 | 0.07 | 52,64,81,91                 | 0     |
| 23  | CLA  | A     | 404[B] | 65/65 | 0.97 | 0.06 | 37,44,63,71                 | 65    |
| 23  | CLA  | B     | 612    | 65/65 | 0.97 | 0.06 | 36,50,64,75                 | 0     |
| 23  | CLA  | B     | 613    | 65/65 | 0.97 | 0.06 | 40,48,97,105                | 0     |
| 23  | CLA  | c     | 503    | 65/65 | 0.97 | 0.07 | 44,60,91,109                | 0     |
| 22  | CL   | a     | 402[B] | 1/1   | 0.98 | 0.06 | 50,50,50,50                 | 1     |
| 22  | CL   | A     | 402[A] | 1/1   | 0.98 | 0.06 | 43,43,43,43                 | 1     |
| 22  | CL   | A     | 402[B] | 1/1   | 0.98 | 0.06 | 44,44,44,44                 | 1     |
| 22  | CL   | a     | 402[A] | 1/1   | 0.98 | 0.06 | 49,49,49,49                 | 1     |
| 38  | HEM  | F     | 102    | 43/43 | 0.98 | 0.07 | 54,69,84,91                 | 0     |
| 38  | HEM  | f     | 101    | 43/43 | 0.98 | 0.07 | 58,86,113,139               | 0     |
| 39  | MG   | J     | 102    | 1/1   | 0.98 | 0.03 | 60,60,60,60                 | 0     |
| 40  | HEC  | V     | 201    | 43/43 | 0.98 | 0.06 | 41,52,59,62                 | 0     |
| 40  | HEC  | v     | 201    | 43/43 | 0.98 | 0.07 | 51,62,70,78                 | 0     |
| 21  | FE2  | A     | 401[A] | 1/1   | 0.99 | 0.03 | 52,52,52,52                 | 1     |
| 37  | CA   | c     | 524    | 1/1   | 0.99 | 0.03 | 81,81,81,81                 | 0     |
| 21  | FE2  | A     | 401[B] | 1/1   | 0.99 | 0.03 | 52,52,52,52                 | 1     |
| 22  | CL   | a     | 403[A] | 1/1   | 0.99 | 0.07 | 53,53,53,53                 | 1     |

*Continued on next page...*

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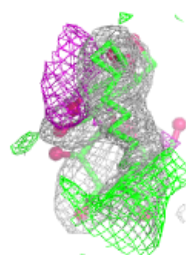
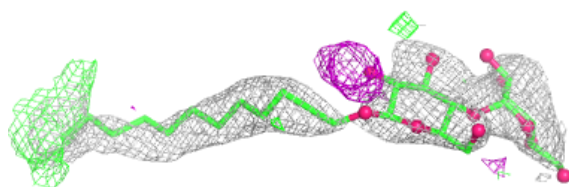
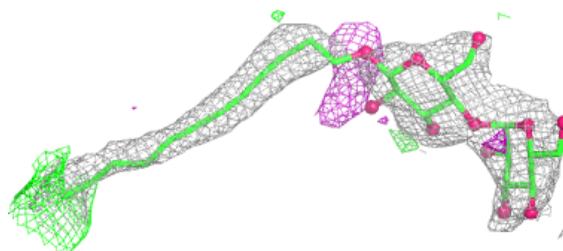
| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 22  | CL   | a     | 403[B] | 1/1   | 0.99 | 0.07 | 53,53,53,53                 | 1     |
| 28  | OEX  | A     | 413[A] | 10/10 | 0.99 | 0.03 | 43,46,49,51                 | 10    |
| 28  | OEX  | A     | 413[B] | 10/10 | 0.99 | 0.03 | 42,46,50,50                 | 10    |
| 39  | MG   | j     | 102    | 1/1   | 0.99 | 0.04 | 67,67,67,67                 | 0     |
| 28  | OEX  | a     | 413[A] | 10/10 | 0.99 | 0.03 | 47,50,54,56                 | 10    |
| 28  | OEX  | a     | 413[B] | 10/10 | 0.99 | 0.03 | 46,50,54,54                 | 10    |

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.

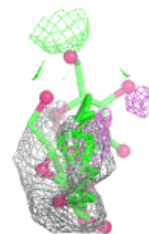
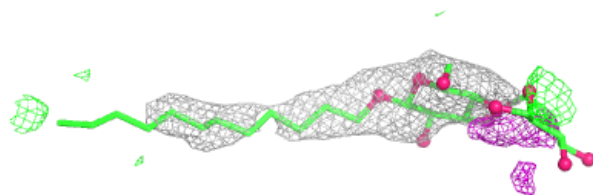
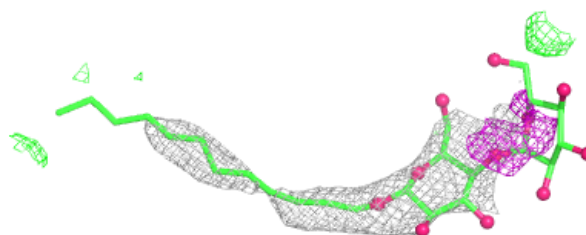


**Electron density around LMT A 418:**

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

**Electron density around LMT F 101:**

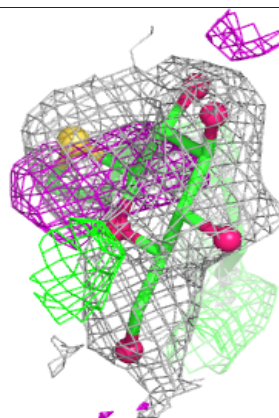
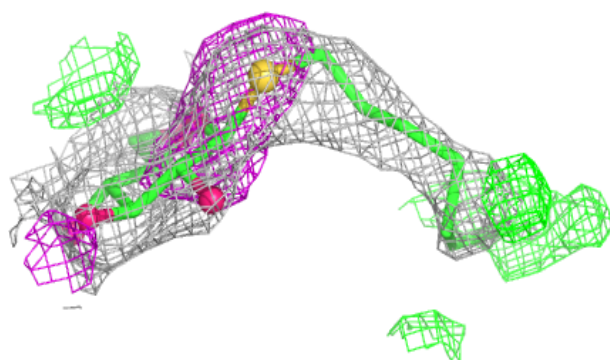
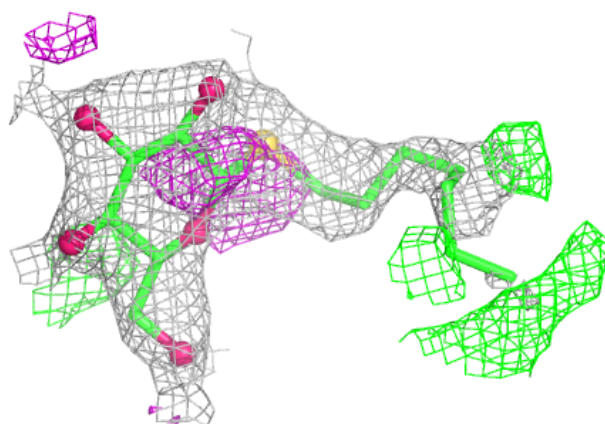
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



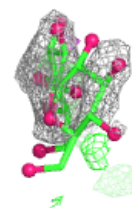
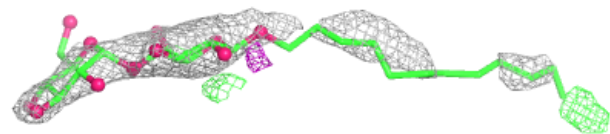
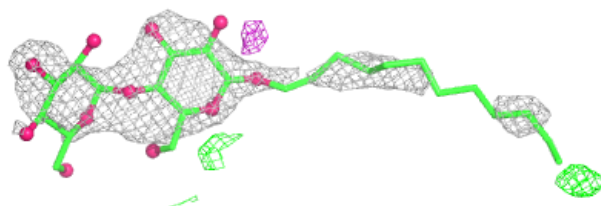


**Electron density around HTG B 622:**

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

**Electron density around LMT a 417:**

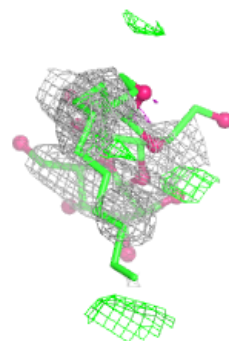
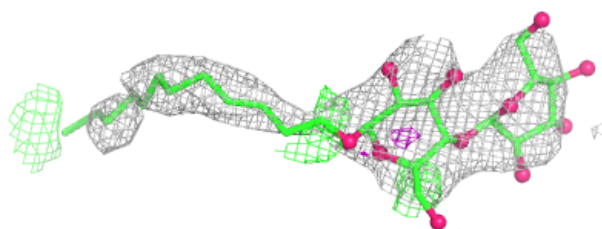
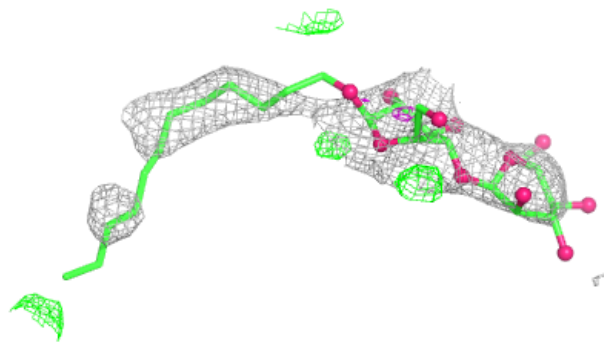
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



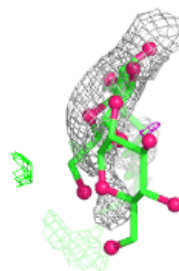
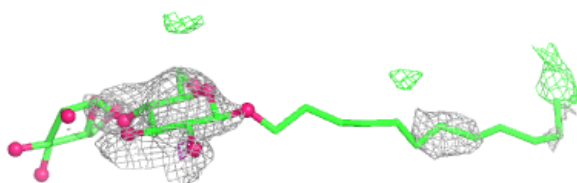
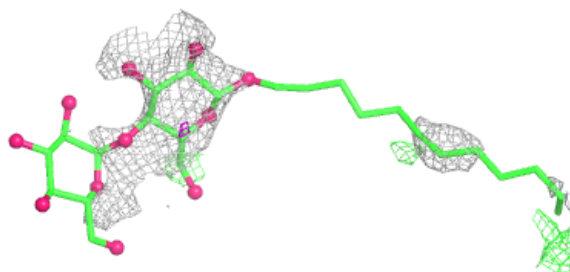


**Electron density around LMT A 420:**

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

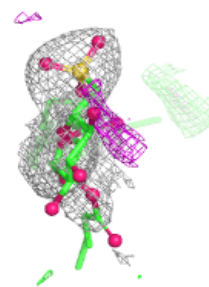
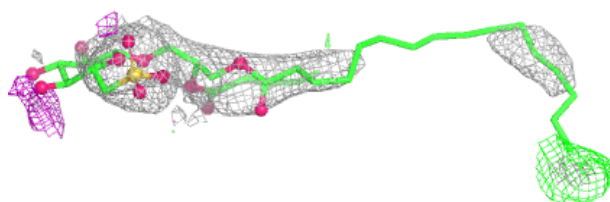
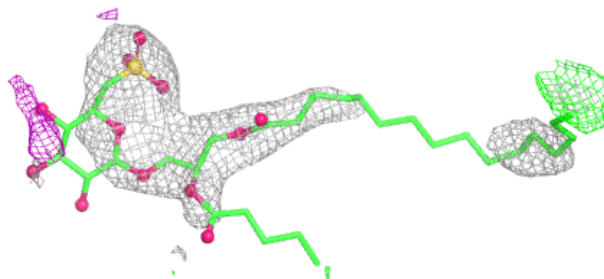
**Electron density around LMT e 101:**

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

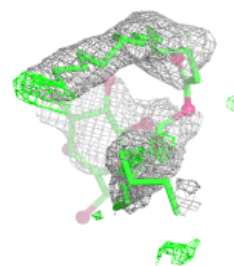
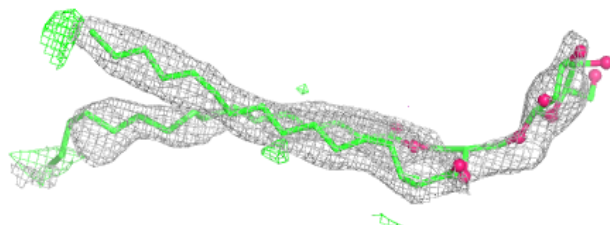
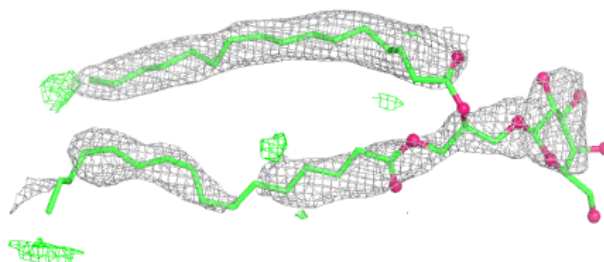


**Electron density around SQD f 102:**

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

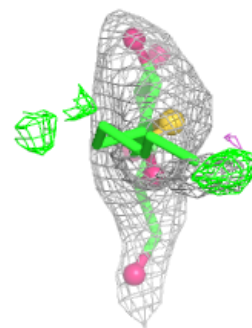
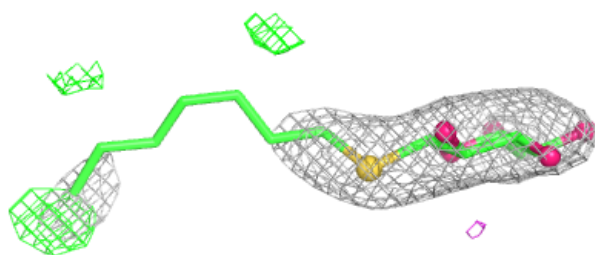
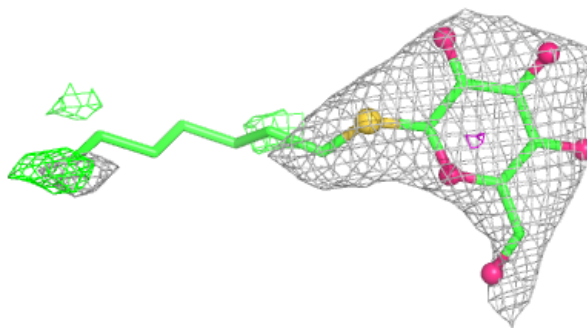
**Electron density around LMG C 521:**

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

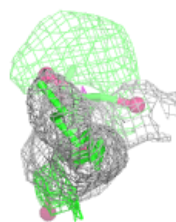
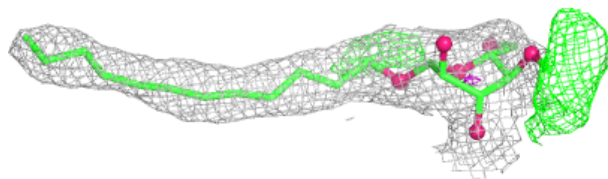
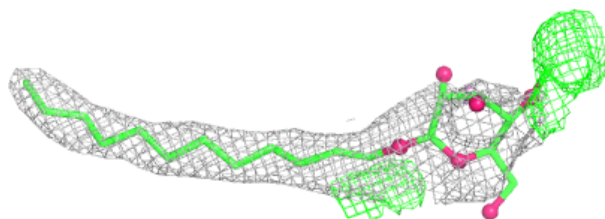


**Electron density around HTG C 522:**

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

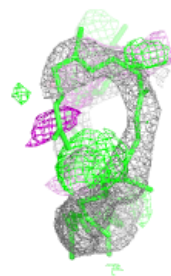
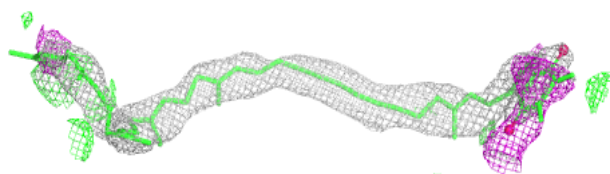
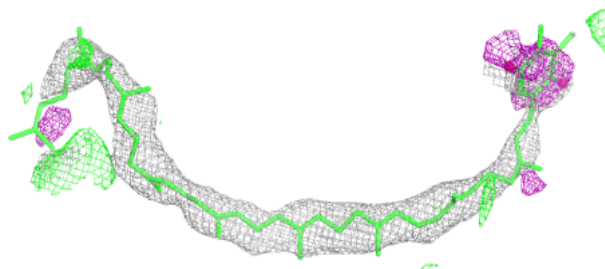
**Electron density around LMT b 621:**

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

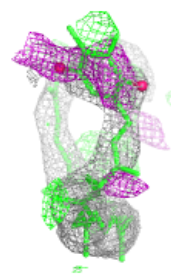
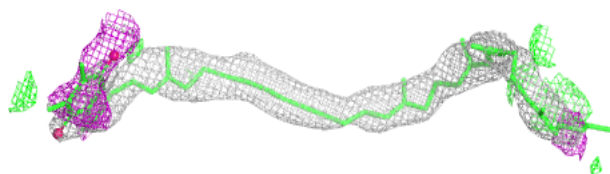
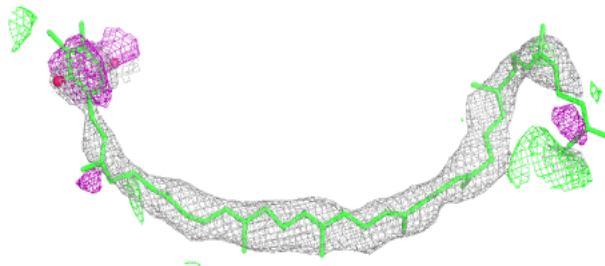


**Electron density around PL9 A 414 (A):**

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

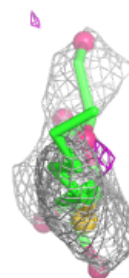
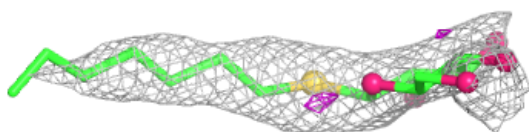
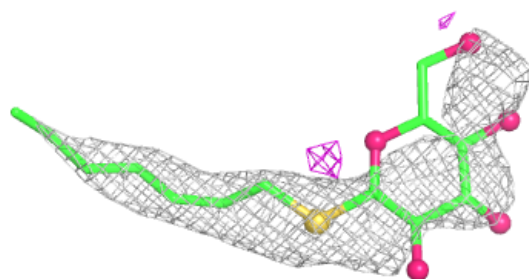
**Electron density around PL9 A 414 (B):**

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

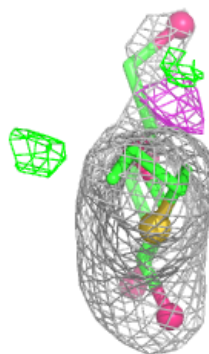
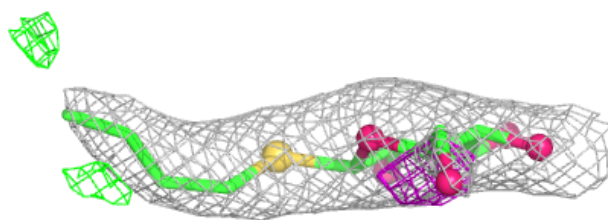
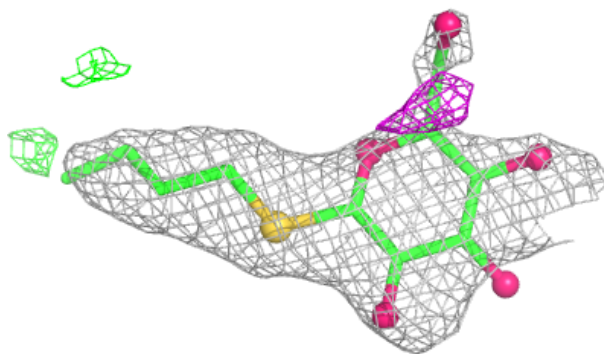


**Electron density around HTG b 623:**

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

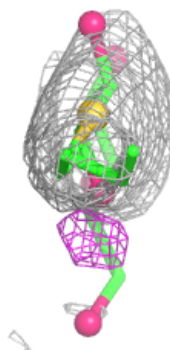
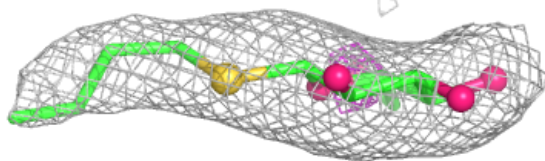
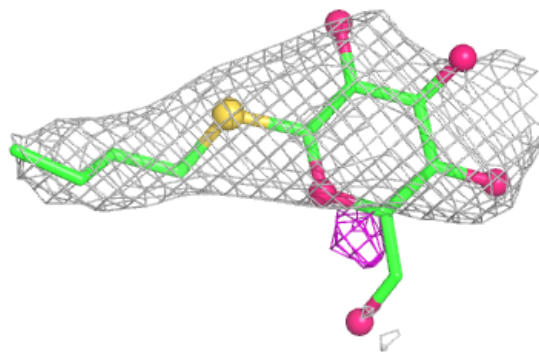
**Electron density around HTG D 710:**

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

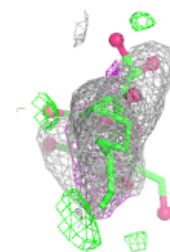
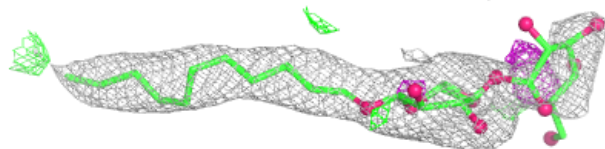
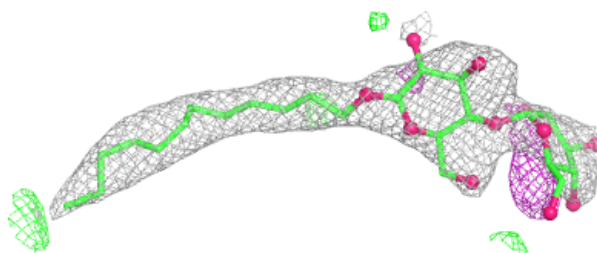


**Electron density around HTG d 409:**

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

**Electron density around LMT B 627:**

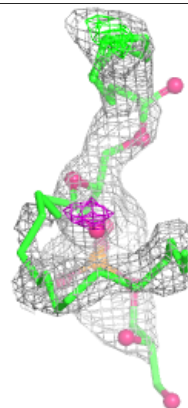
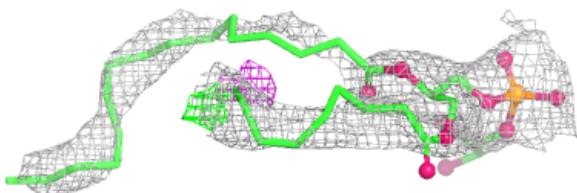
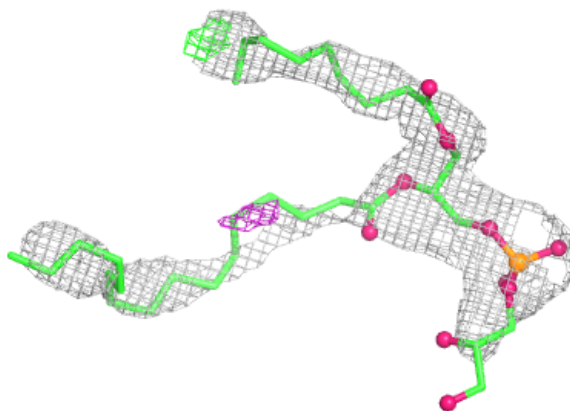
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





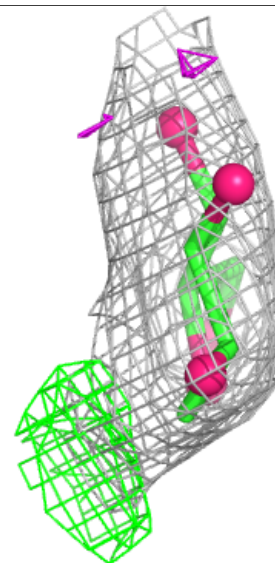
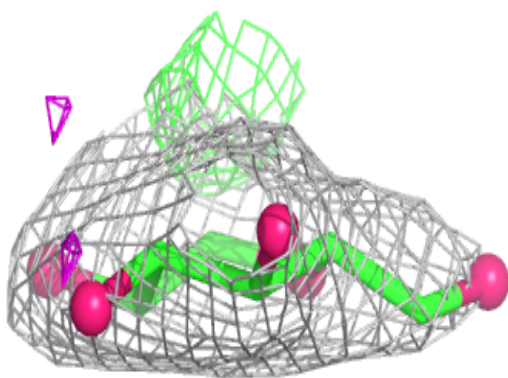
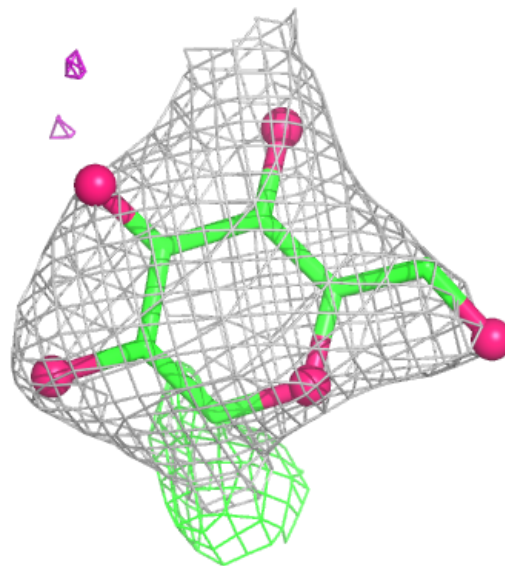
**Electron density around LHG a 420 (B):**

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and green (positive)



**Electron density around HTG V 202:**

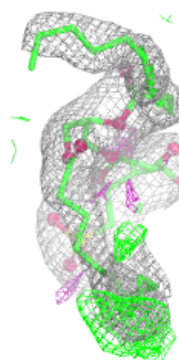
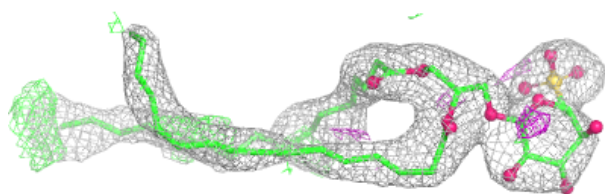
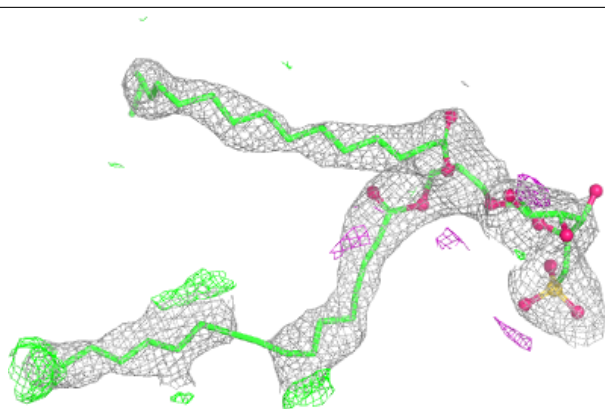
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



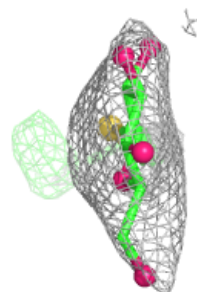
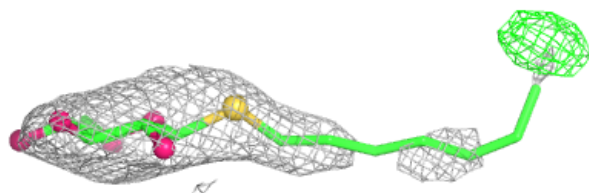
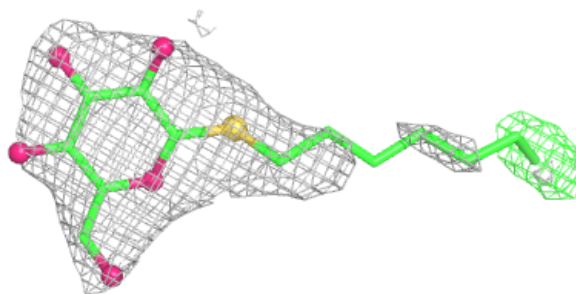


**Electron density around SQD a 412:**

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

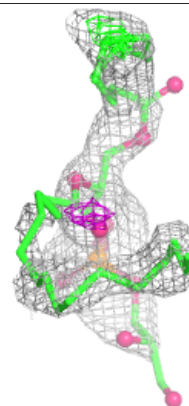
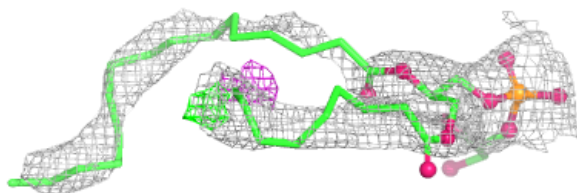
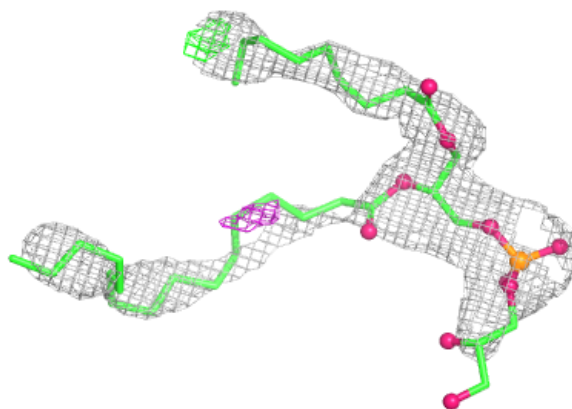
**Electron density around HTG c 522:**

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

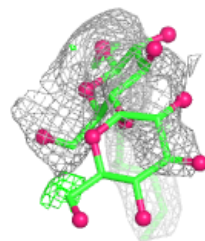
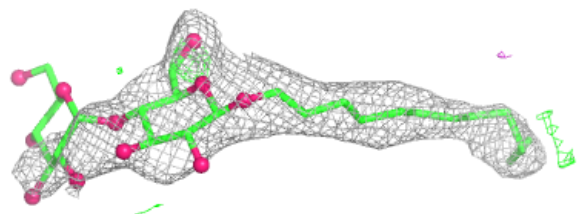
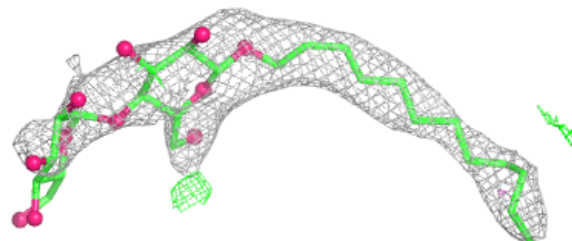


**Electron density around LHG a 420 (A):**

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

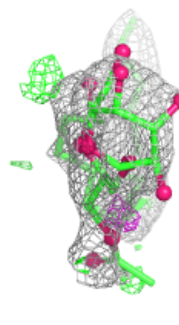
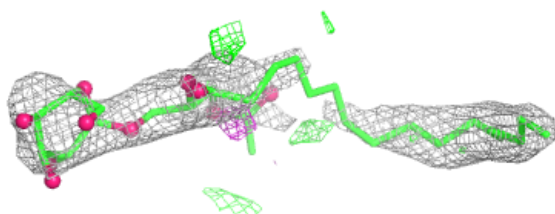
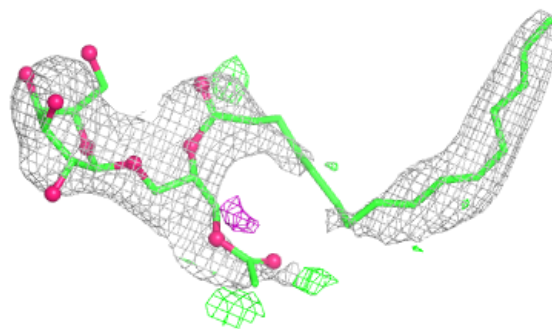
**Electron density around LMT T 101:**

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and green (positive)

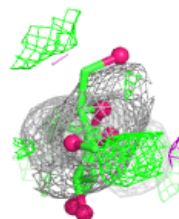
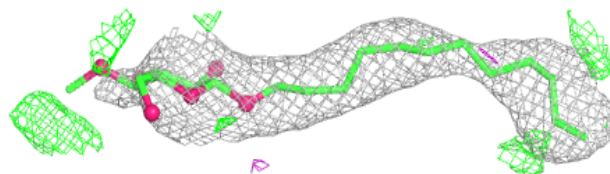
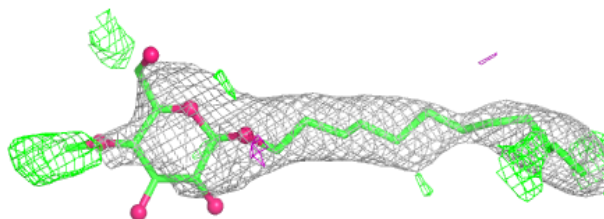


**Electron density around LMG Z 101:**

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

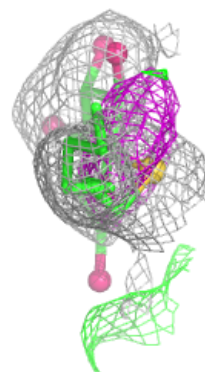
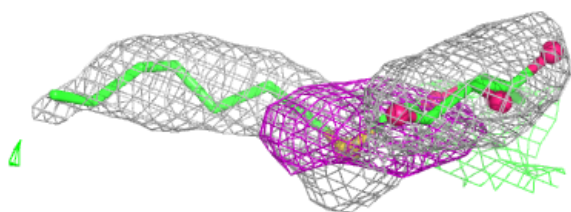
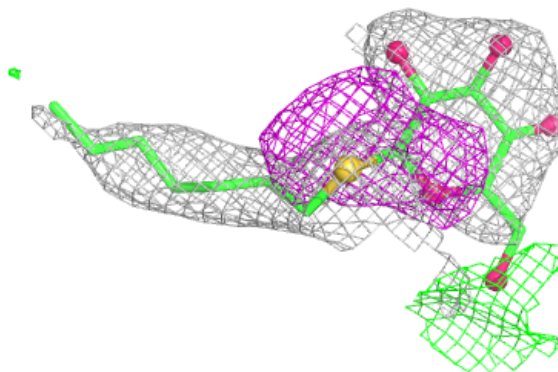
**Electron density around LMT b 627:**

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

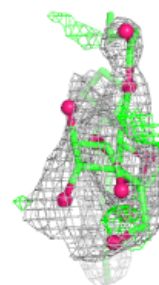
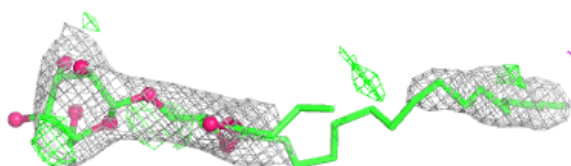
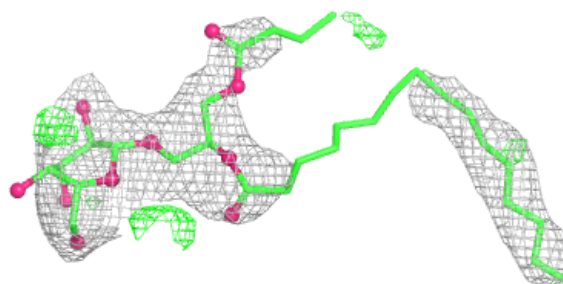


**Electron density around HTG b 622:**

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

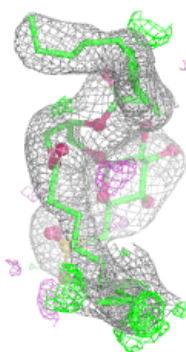
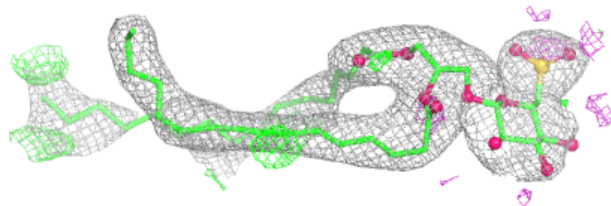
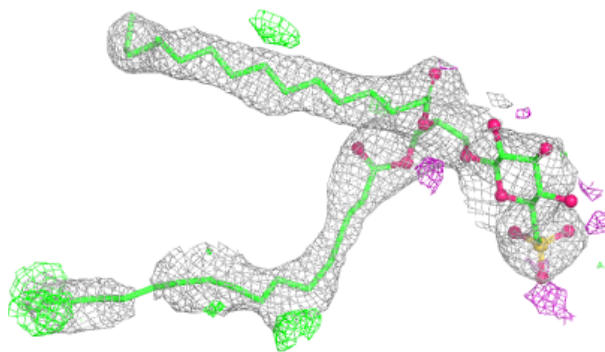
**Electron density around LMG z 101:**

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

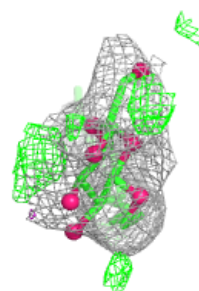
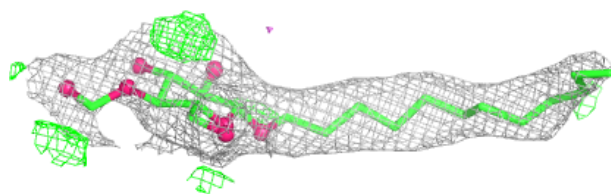
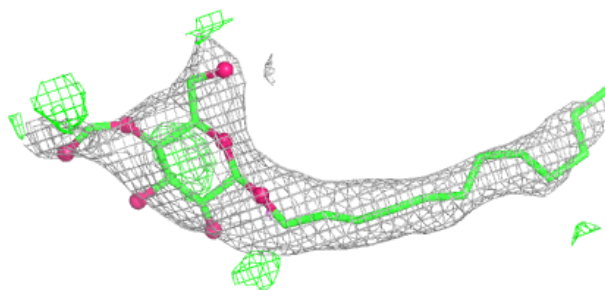


**Electron density around SQD A 412:**

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

**Electron density around LMT t 101:**

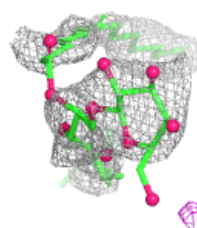
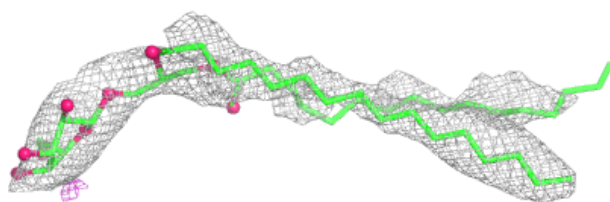
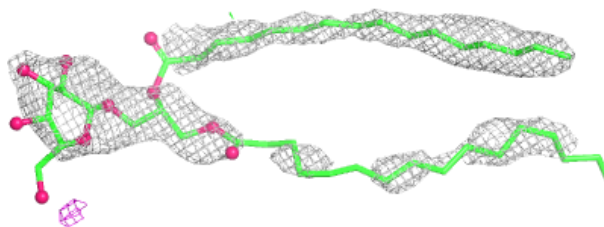
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



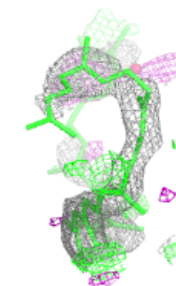
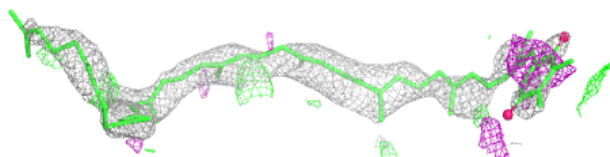
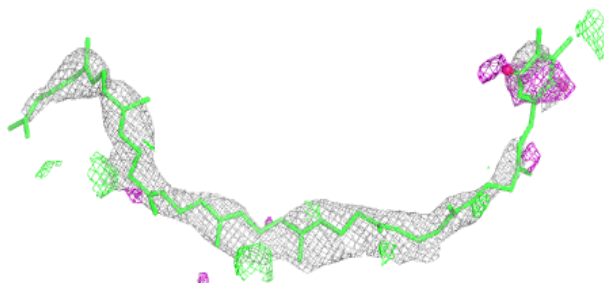


**Electron density around LMG c 521:**

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

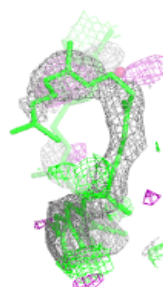
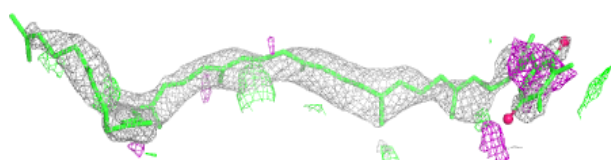
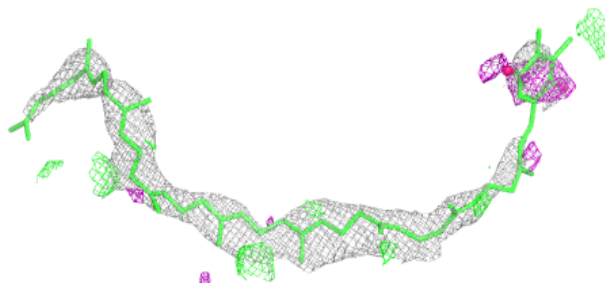
**Electron density around PL9 a 414 (A):**

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

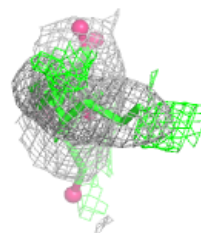
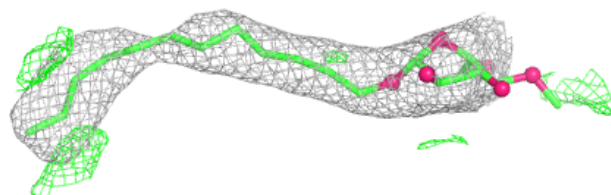
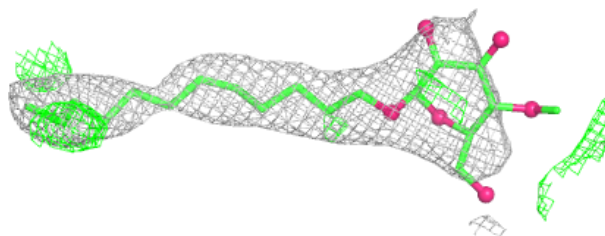


**Electron density around PL9 a 414 (B):**

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

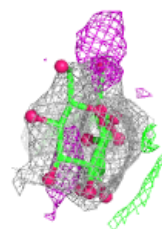
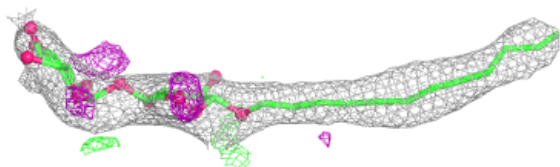
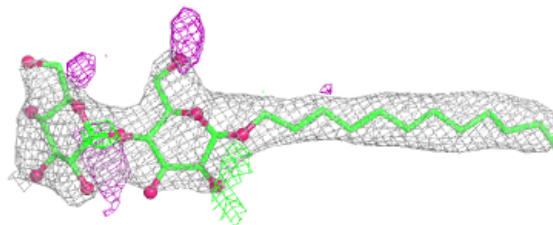
**Electron density around LMT B 630:**

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

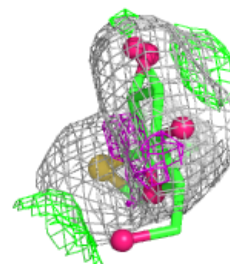
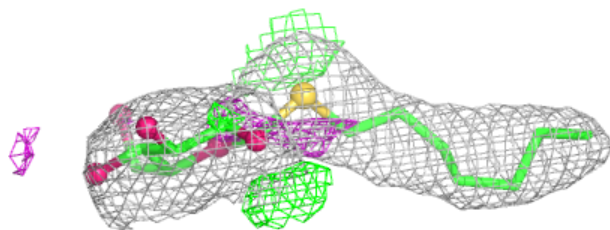
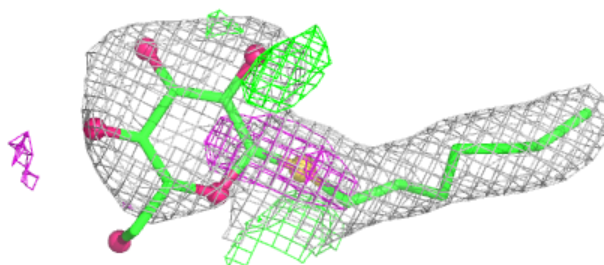


**Electron density around LMT m 103:**

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

**Electron density around HTG o 301:**

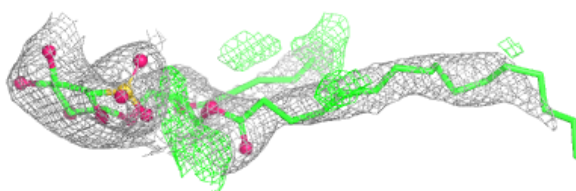
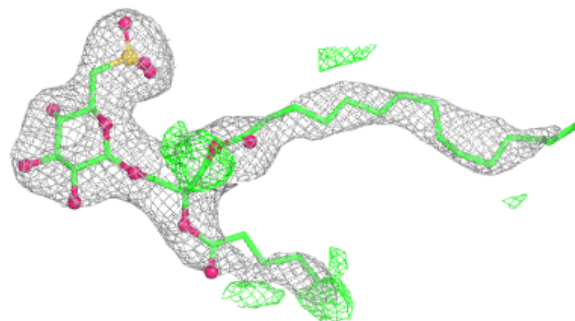
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



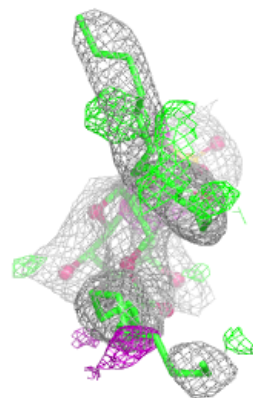
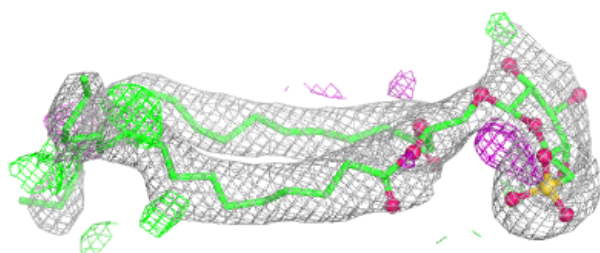
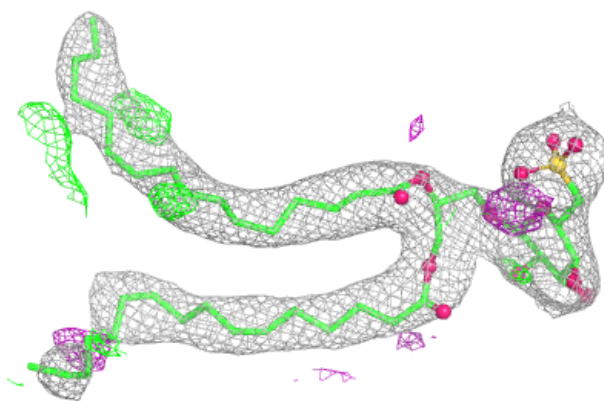


**Electron density around SQD X 101:**

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

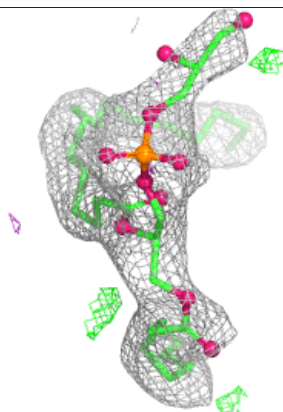
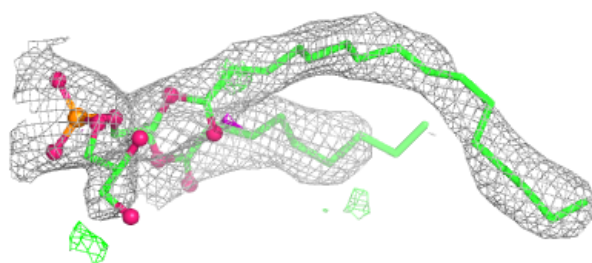
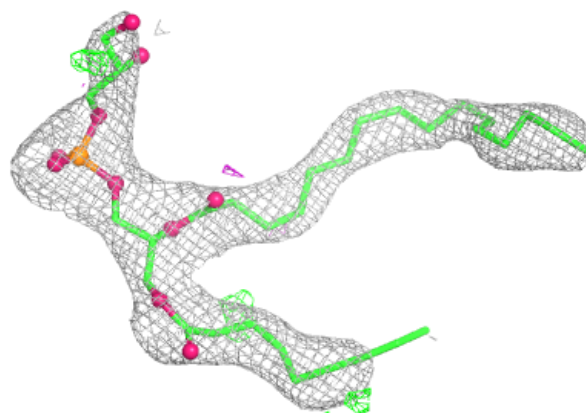
**Electron density around SQD b 620:**

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

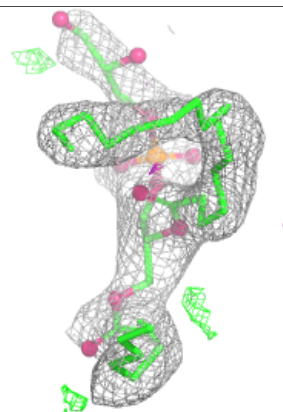
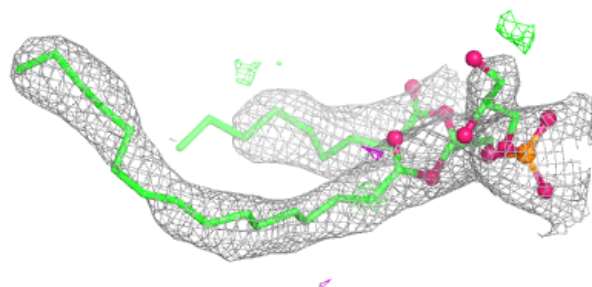
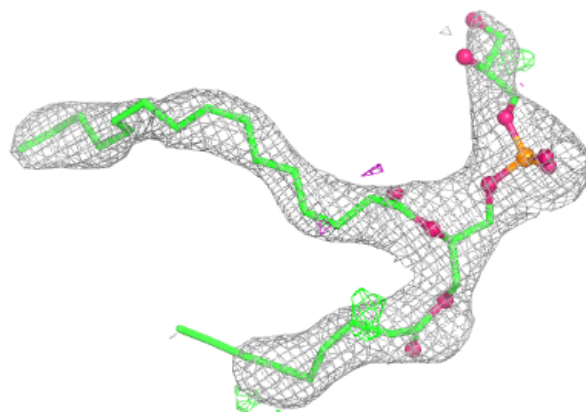


**Electron density around LHG E 101 (A):**

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

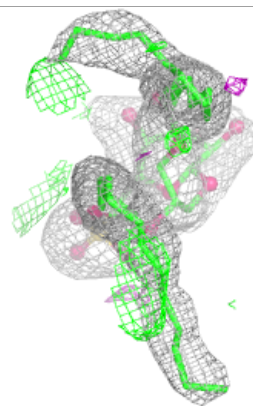
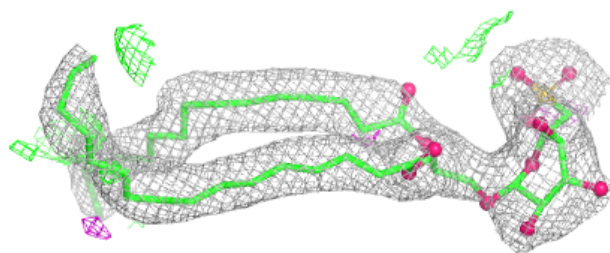
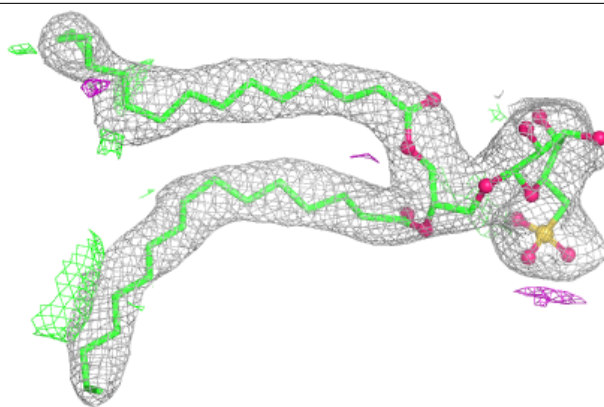
**Electron density around LHG E 101 (B):**

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



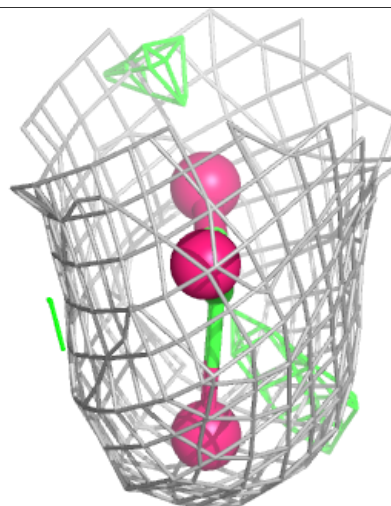
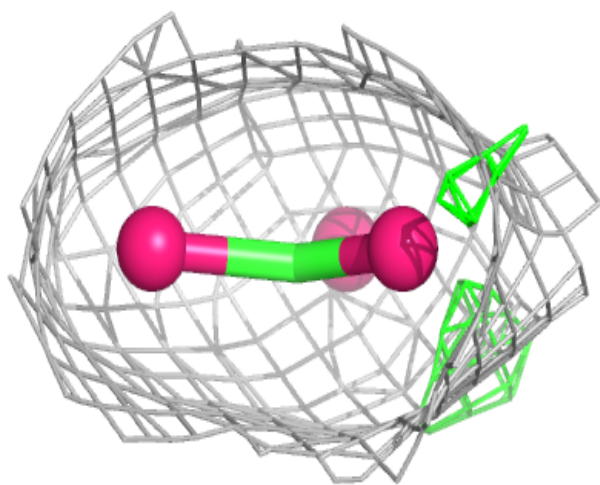
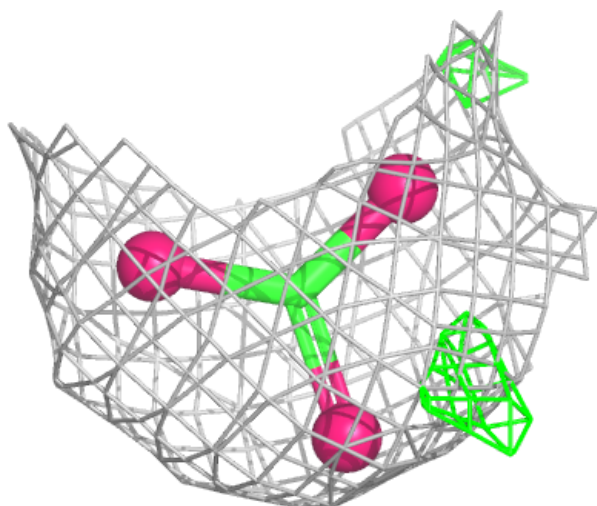
**Electron density around SQD B 620:**

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



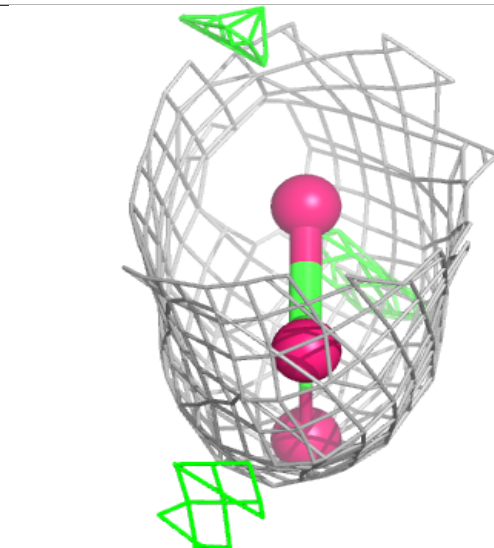
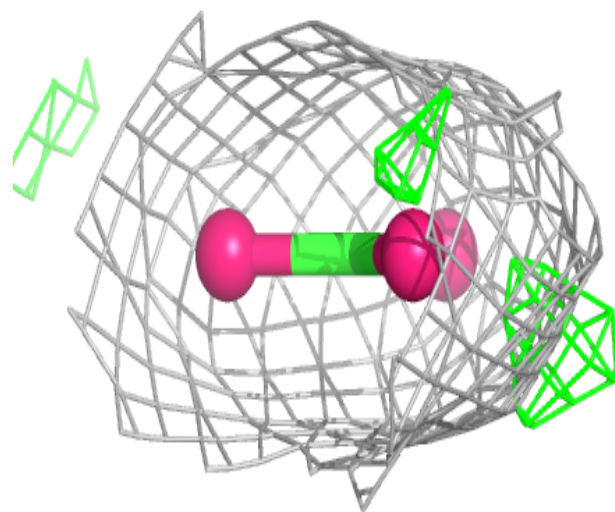
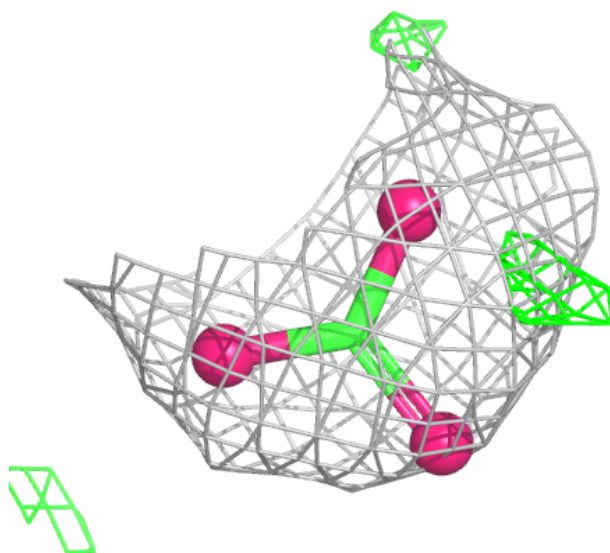
**Electron density around BCT A 416 (A):**

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



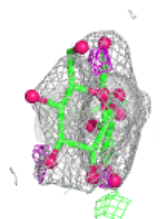
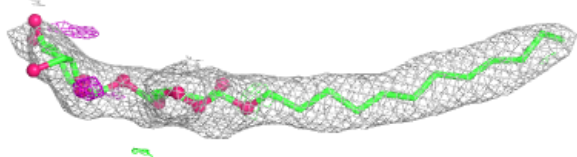
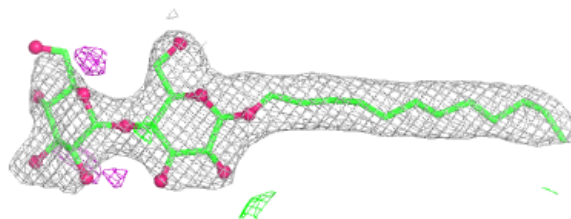
**Electron density around BCT A 416 (B):**

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



**Electron density around LMT M 101:**

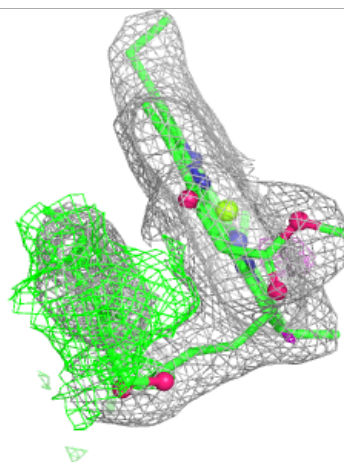
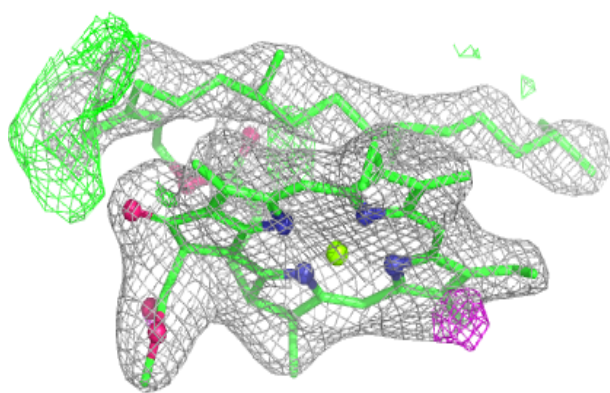
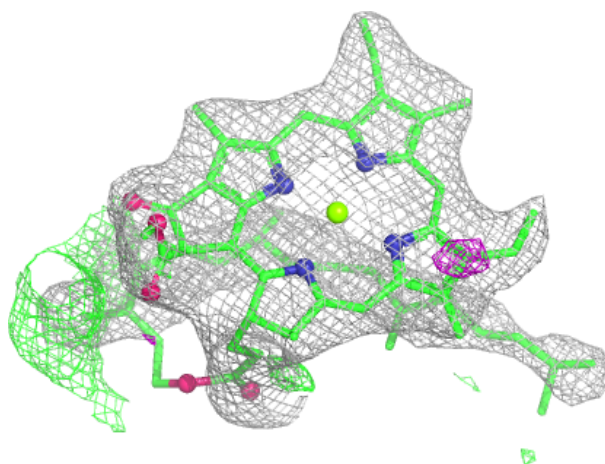
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





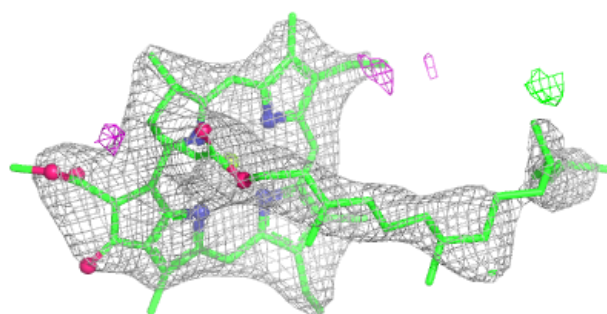
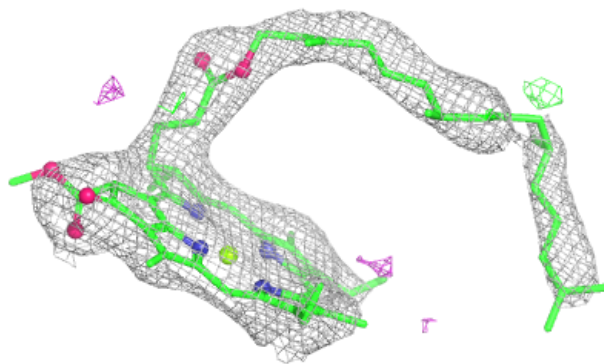
**Electron density around CLA b 601:**

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

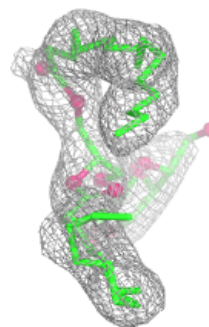
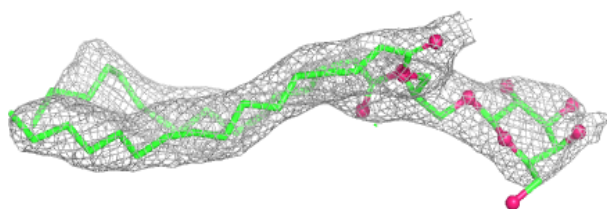
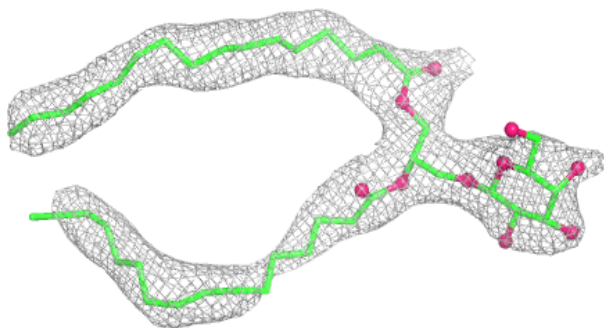


**Electron density around CLA c 514:**

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

**Electron density around LMG c 501:**

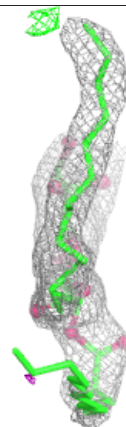
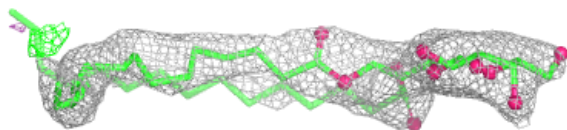
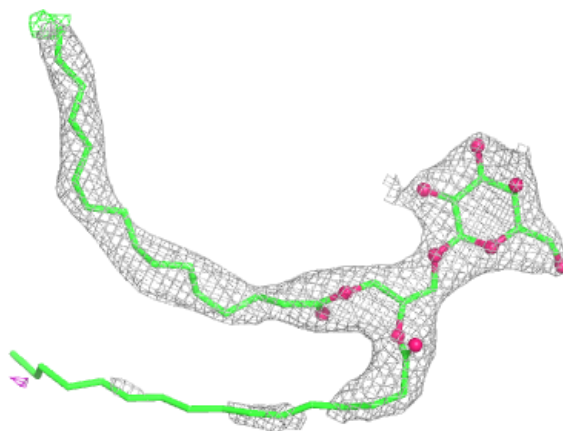
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



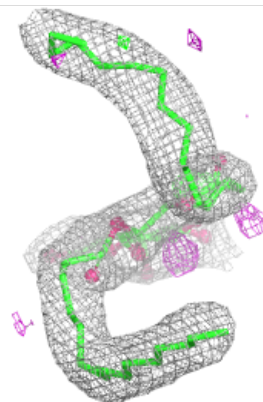
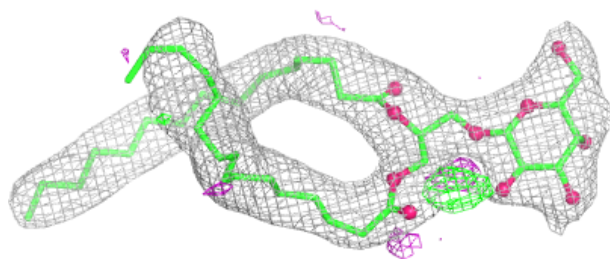
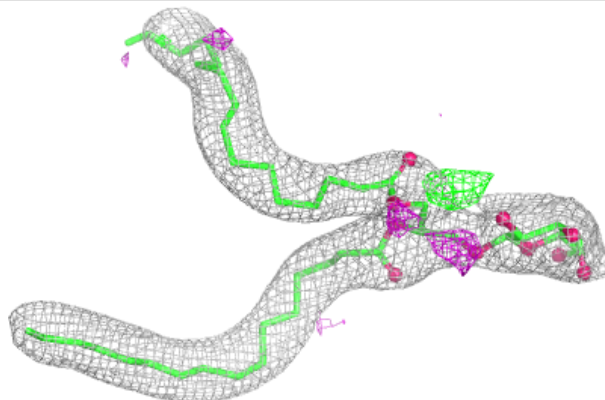


**Electron density around LMG c 520:**

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

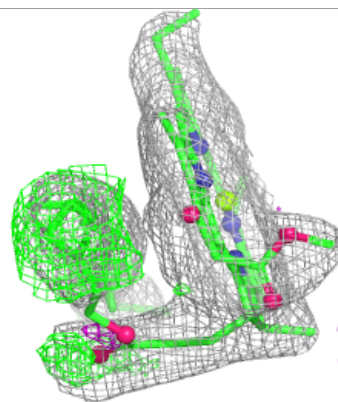
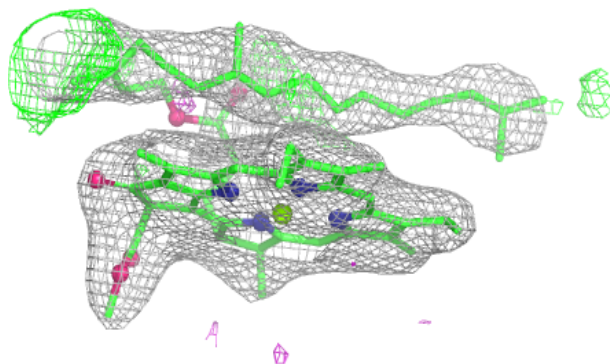
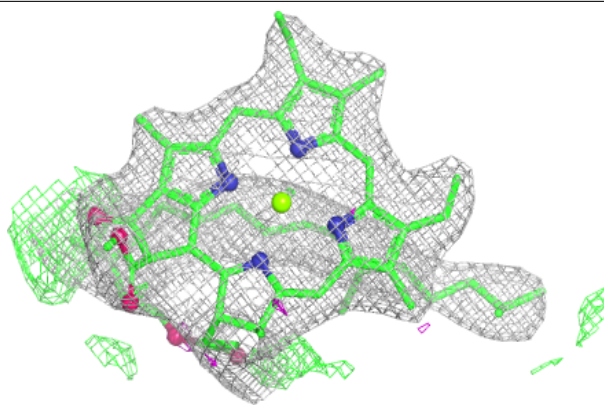
**Electron density around LMG m 101:**

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

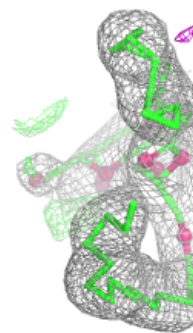
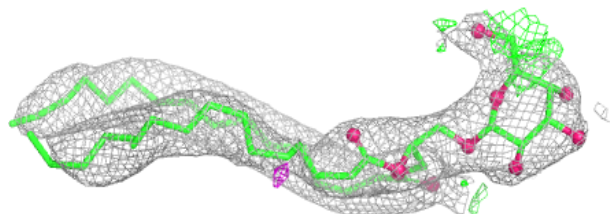
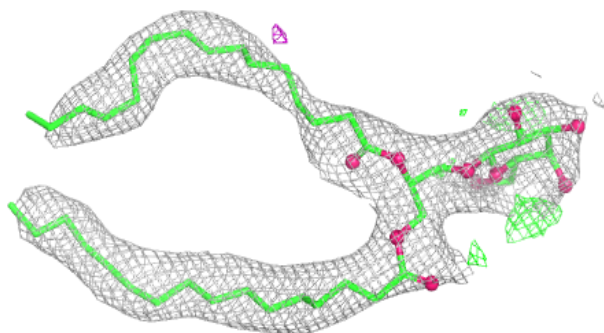


**Electron density around CLA B 601:**

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

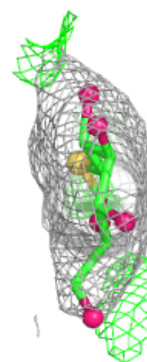
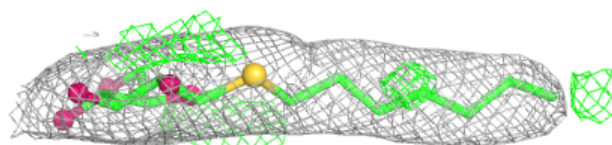
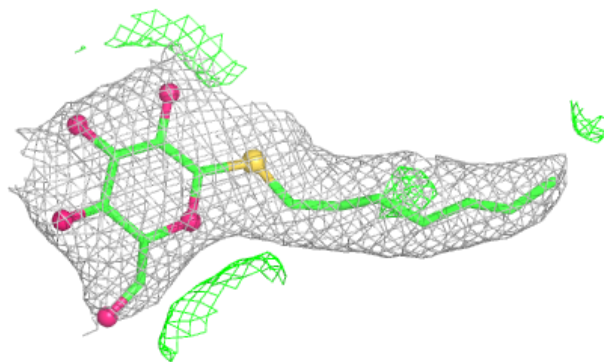
**Electron density around LMG C 501:**

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

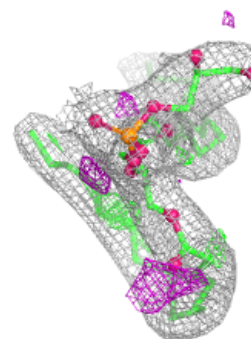
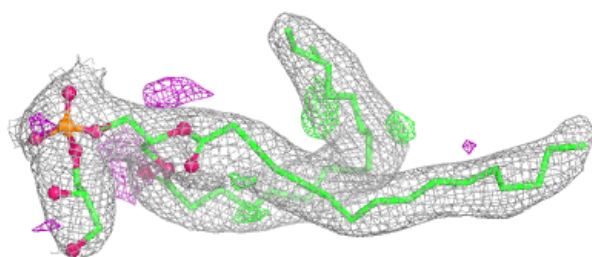
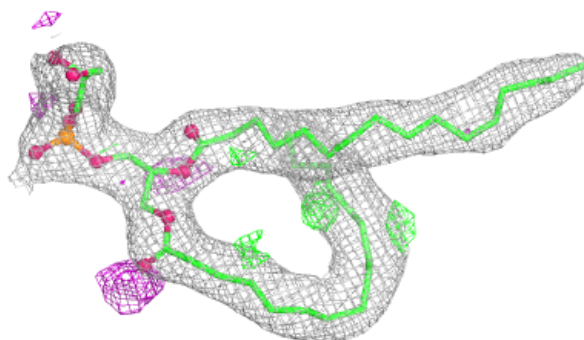


**Electron density around HTG b 625:**

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

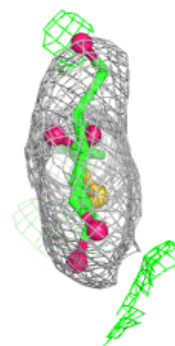
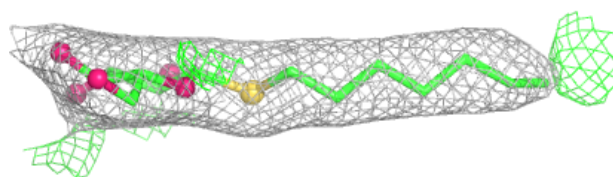
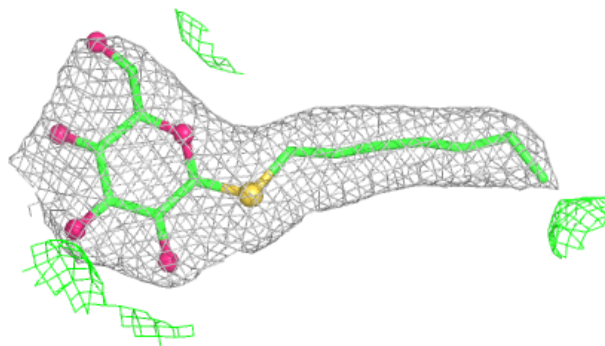
**Electron density around LHG A 419 (A):**

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

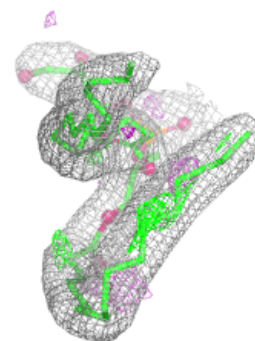
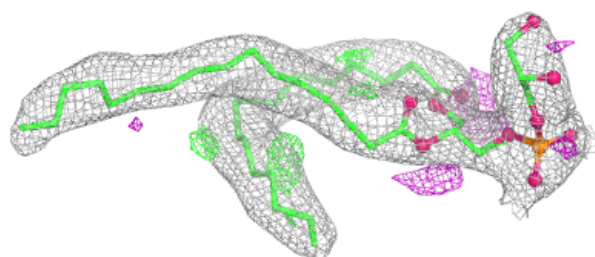
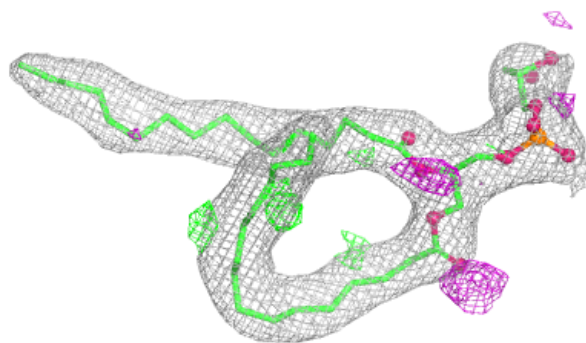


**Electron density around HTG B 624:**

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

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

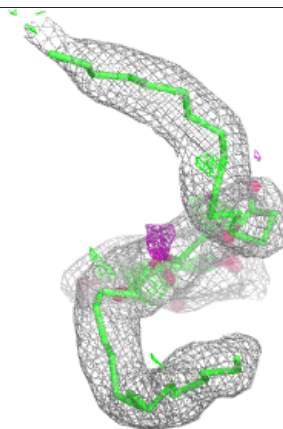
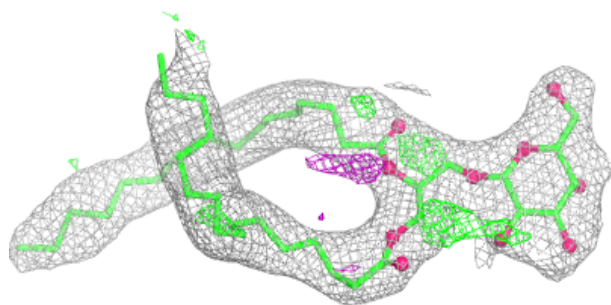
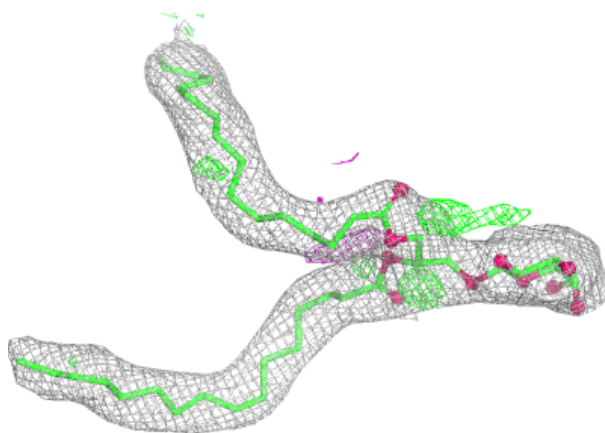
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





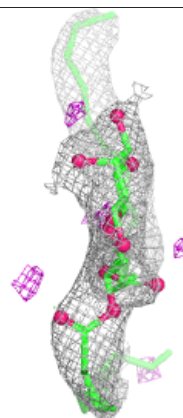
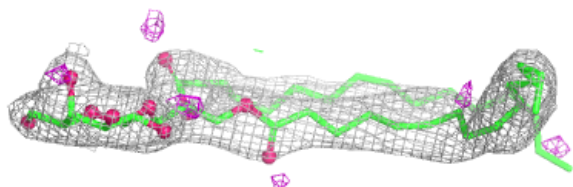
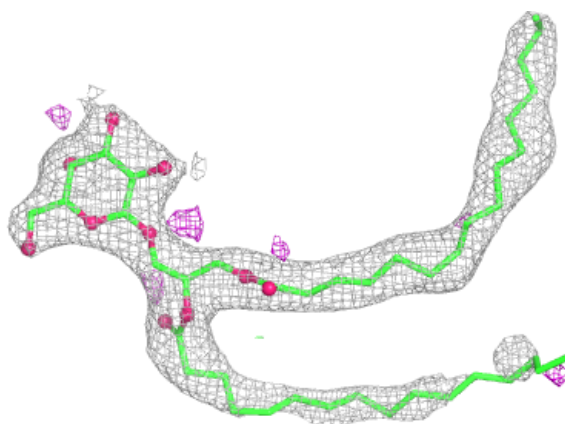
**Electron density around LMG B 621:**

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

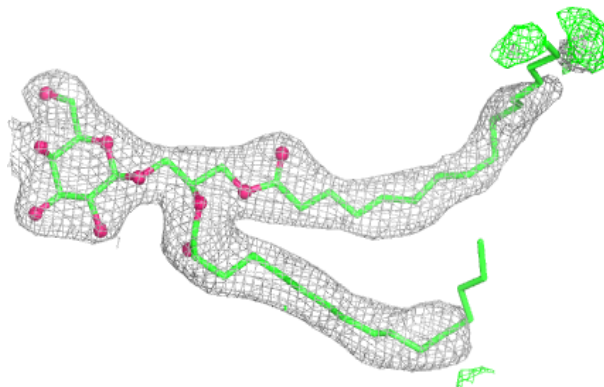


**Electron density around LMG C 520:**

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

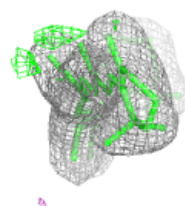
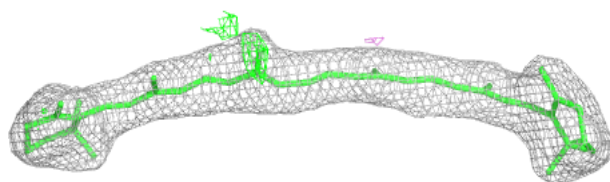
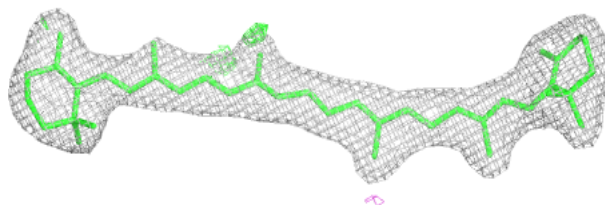
**Electron density around LMG D 711:**

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

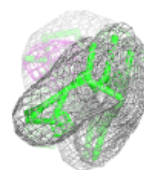
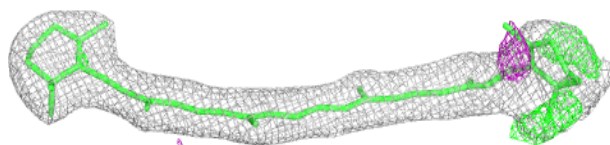
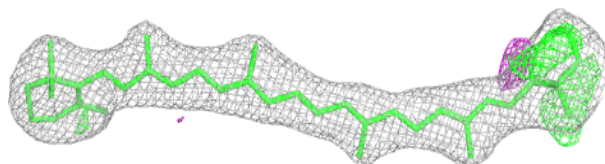


**Electron density around BCR T 102:**

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

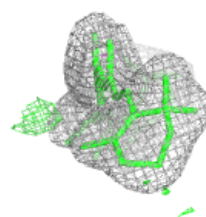
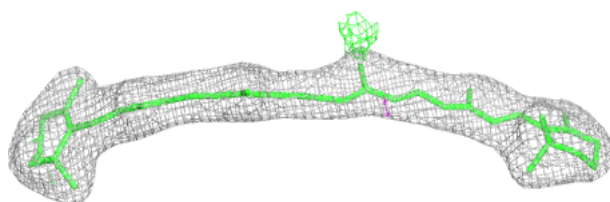
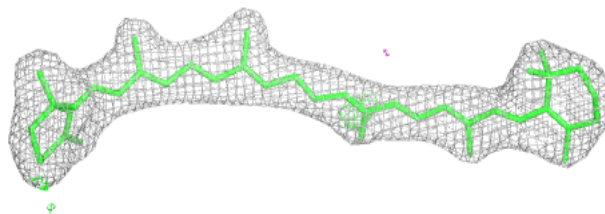
**Electron density around BCR d 403:**

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

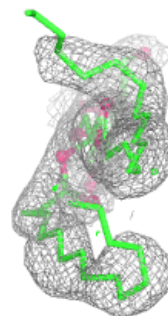
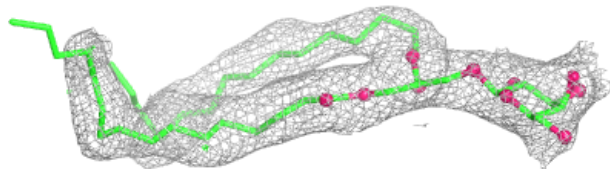
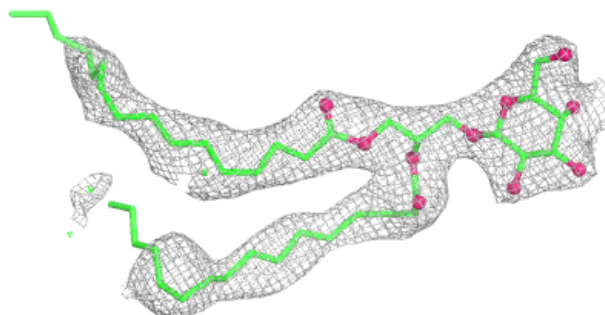


**Electron density around BCR t 102:**

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

**Electron density around LMG d 410:**

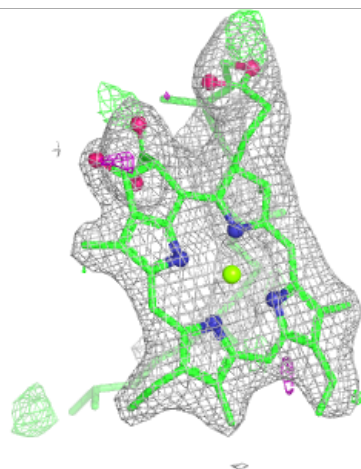
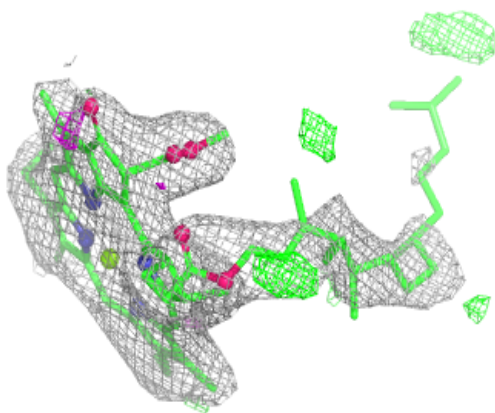
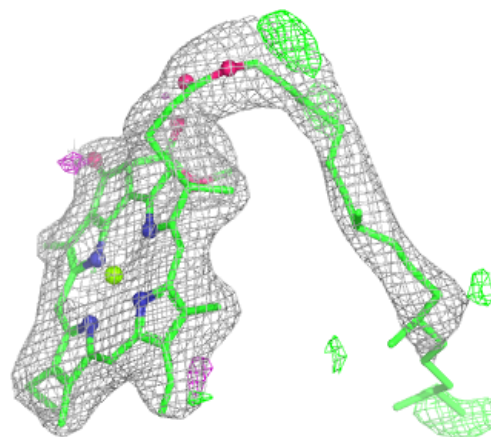
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





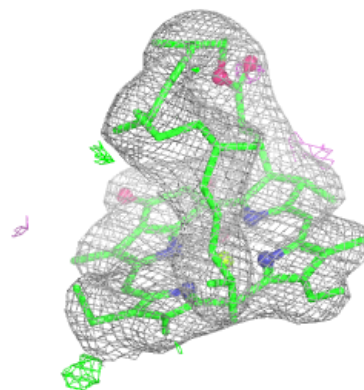
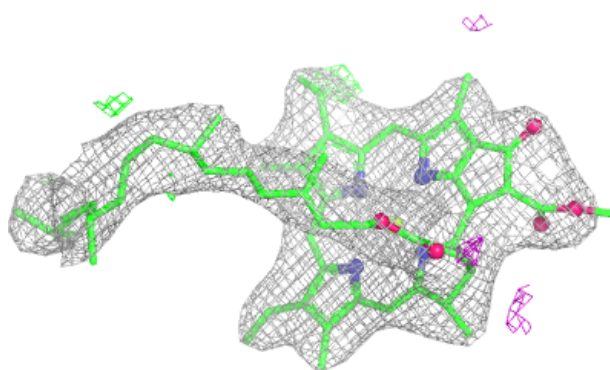
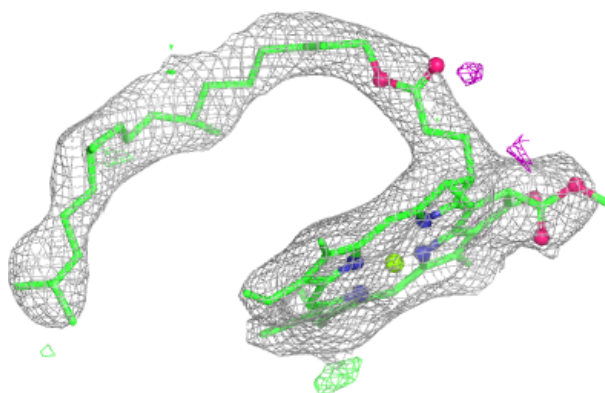
**Electron density around CLA b 616:**

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

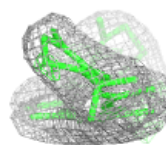
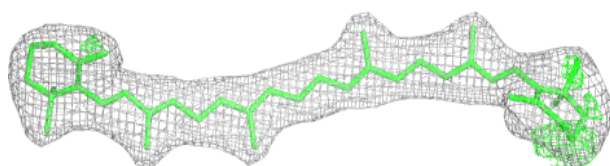
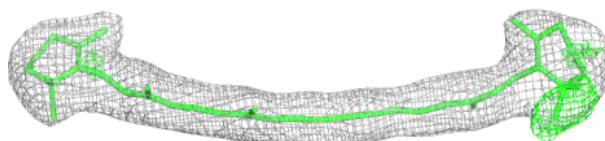


**Electron density around CLA C 514:**

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

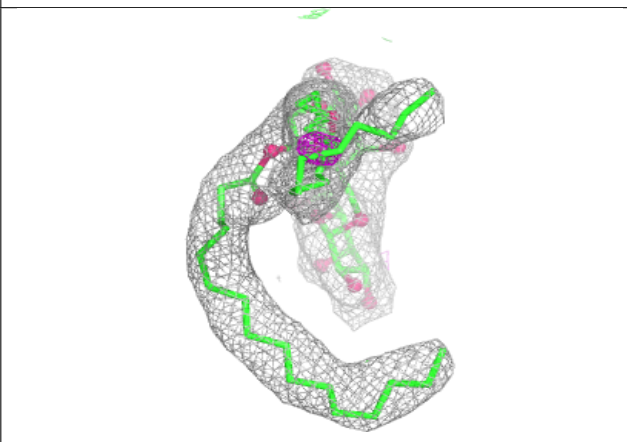
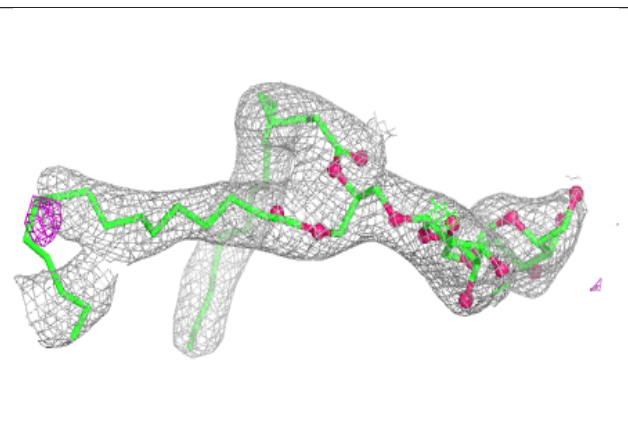
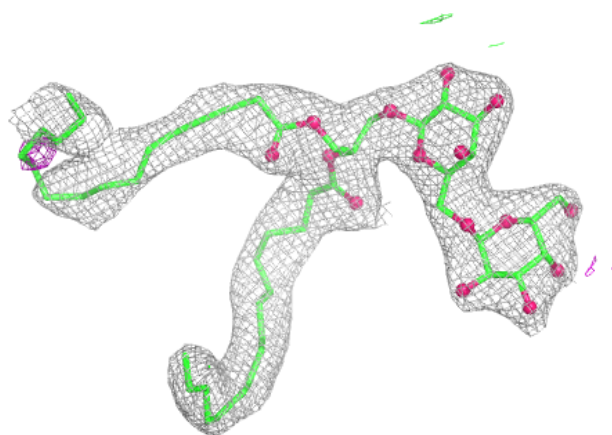
**Electron density around BCR D 704:**

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



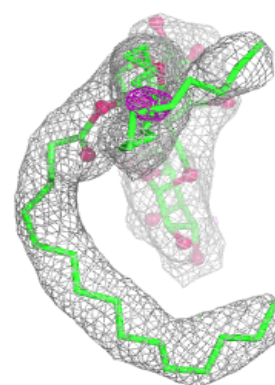
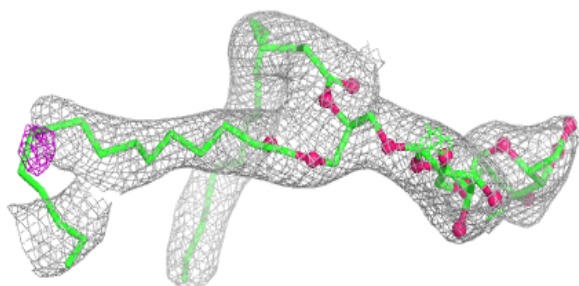
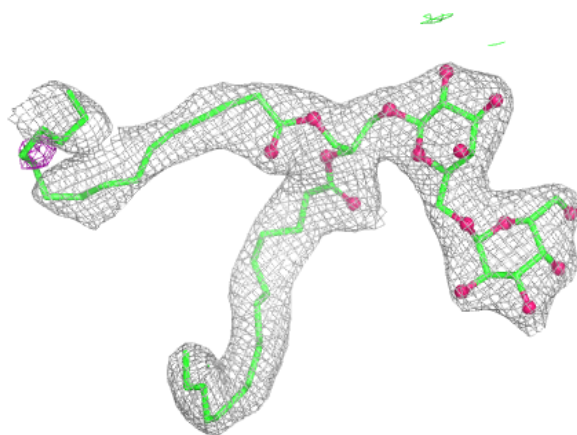
**Electron density around DGD c 518 (A):**

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



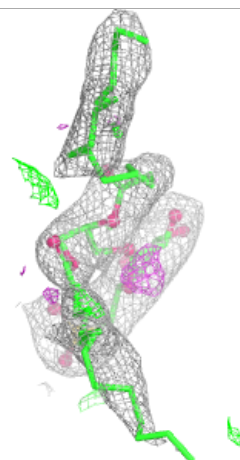
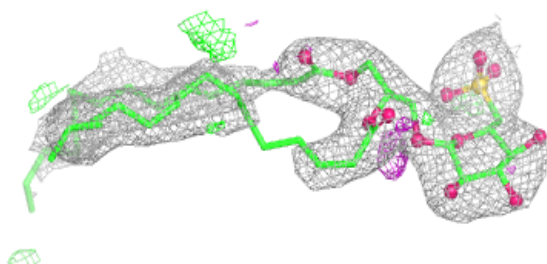
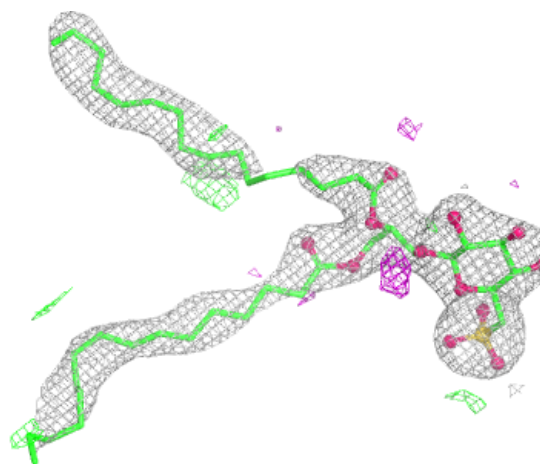
**Electron density around DGD c 518 (B):**

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



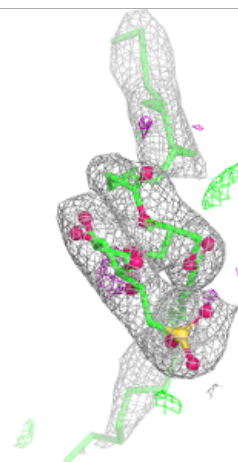
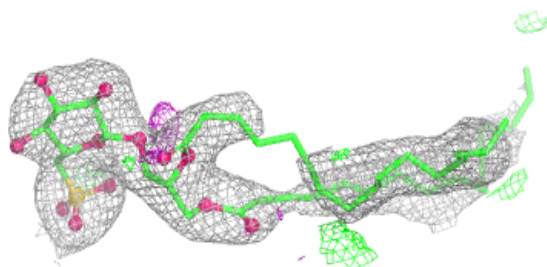
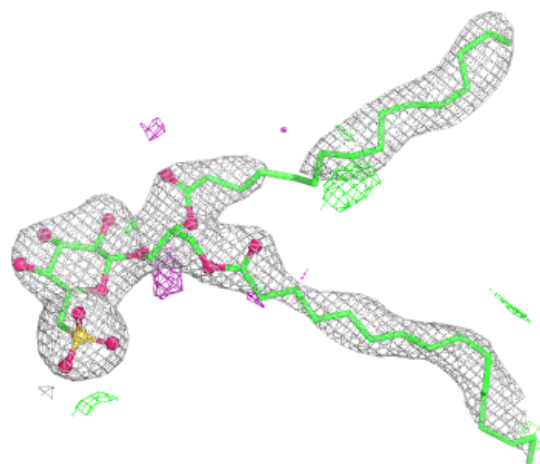
**Electron density around SQD a 411 (A):**

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



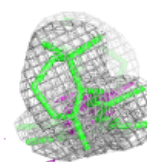
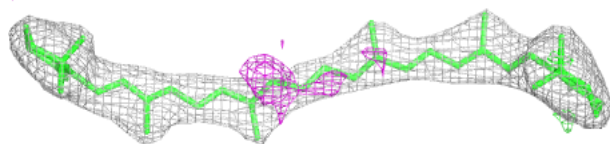
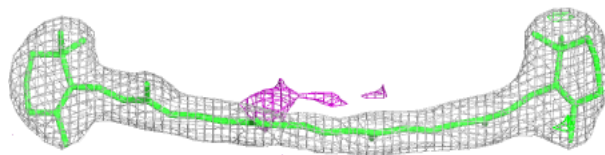
**Electron density around SQD a 411 (B):**

$2mF_o-DF_c$  (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:**

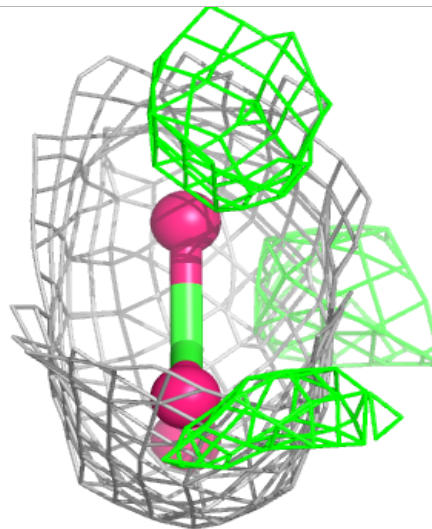
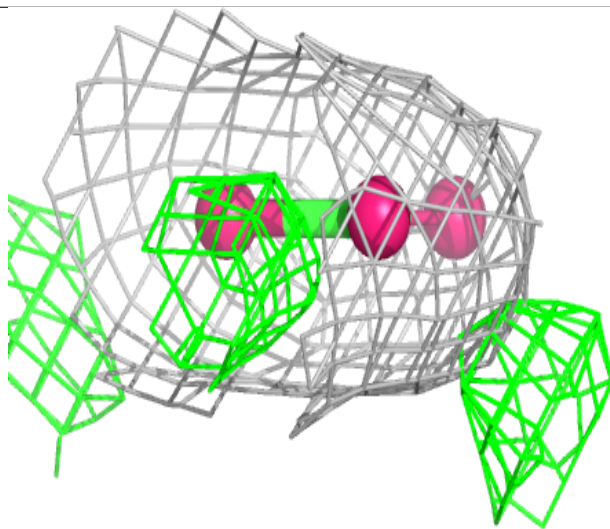
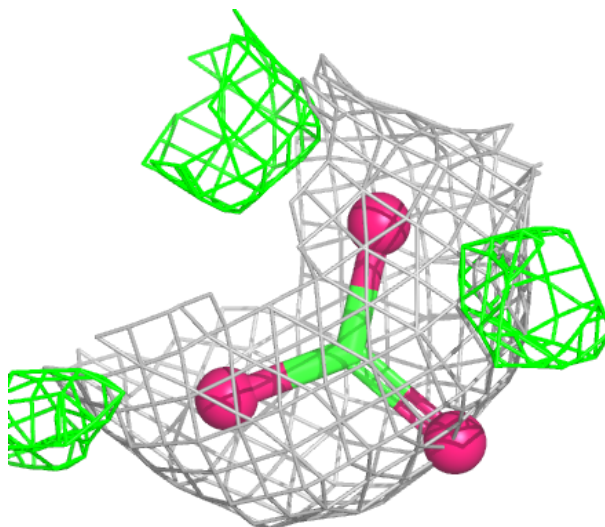
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





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

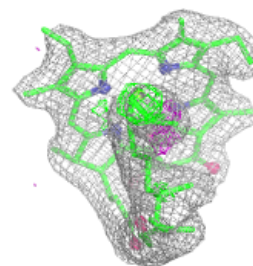
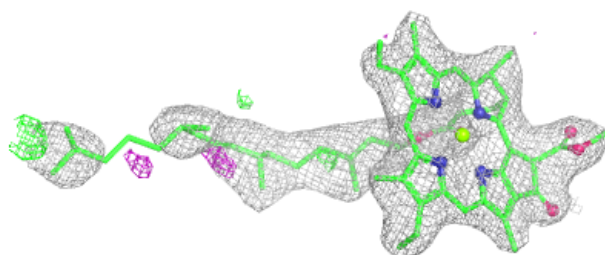
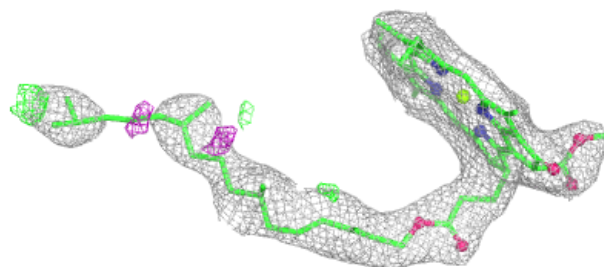
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



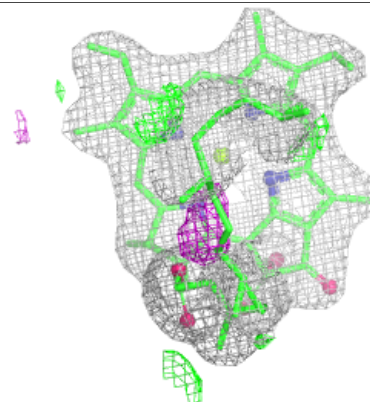
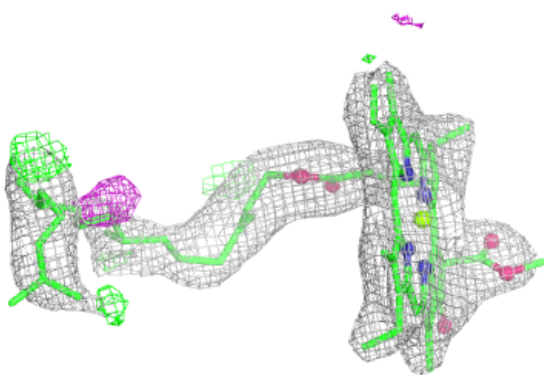
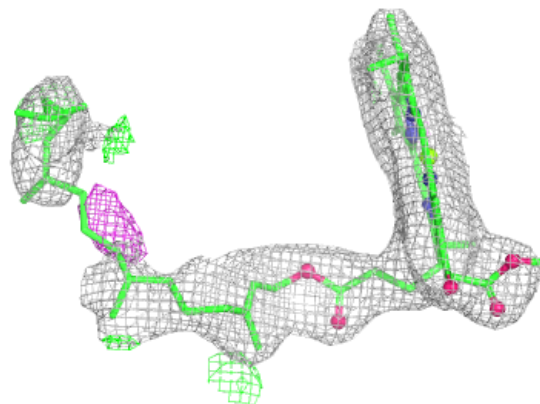


**Electron density around CLA c 505:**

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

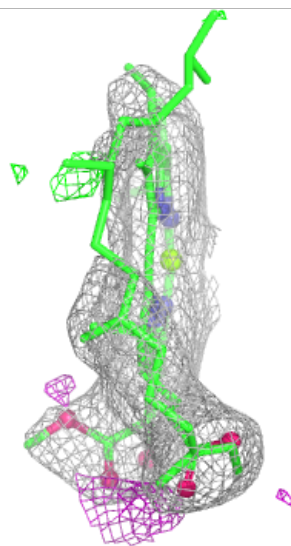
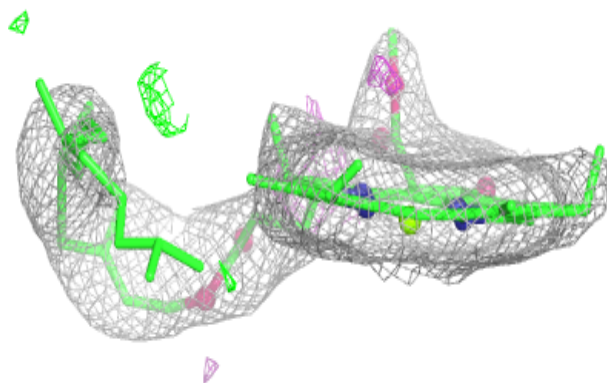
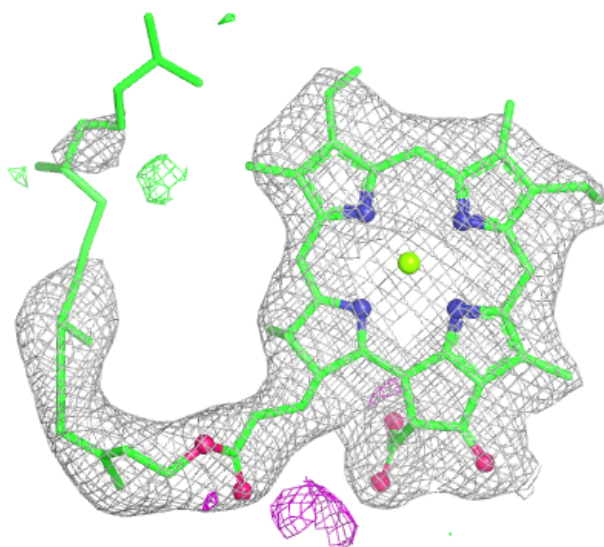
**Electron density around CLA c 507:**

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



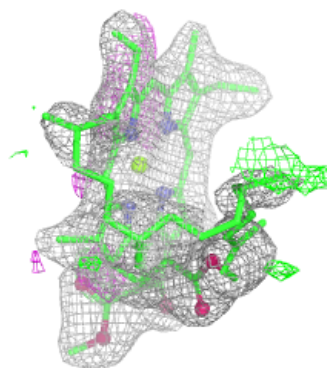
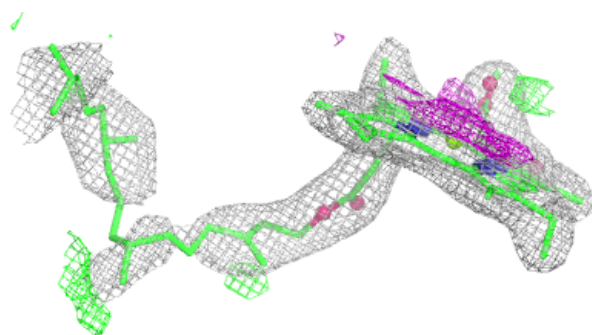
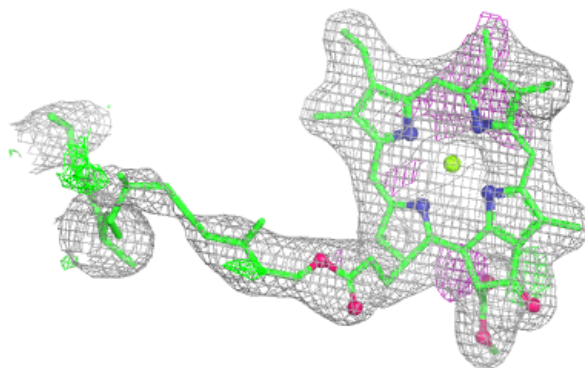
**Electron density around CLA c 513:**

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

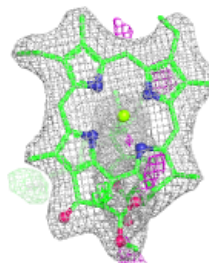
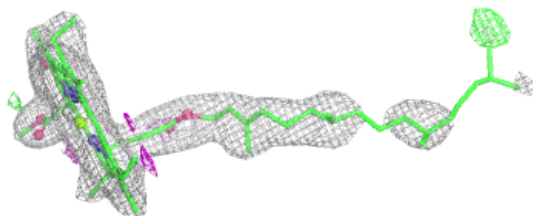
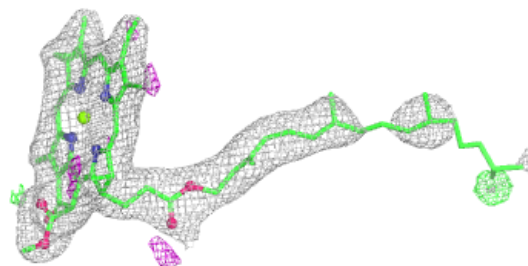


**Electron density around CLA A 408:**

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

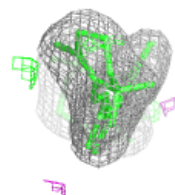
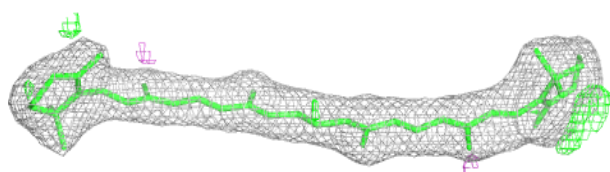
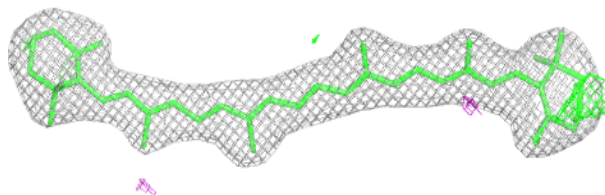
**Electron density around CLA d 402:**

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

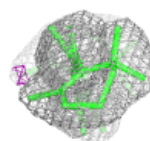
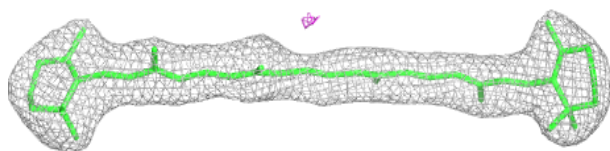
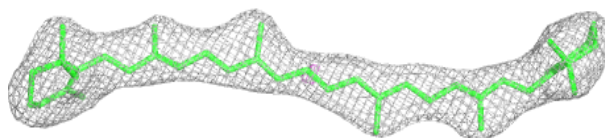


**Electron density around BCR B 619:**

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

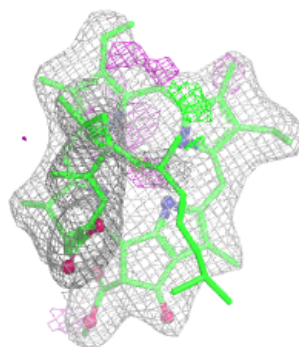
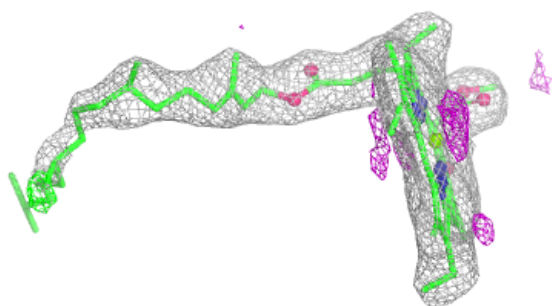
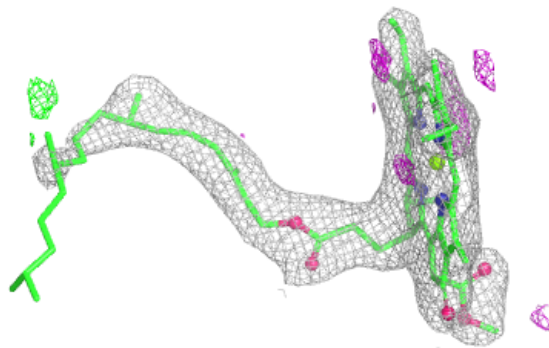
**Electron density around BCR C 515:**

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

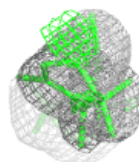
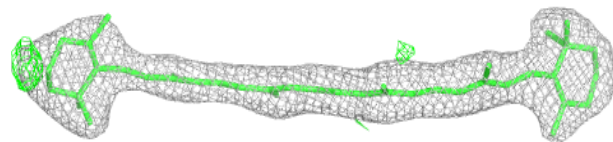
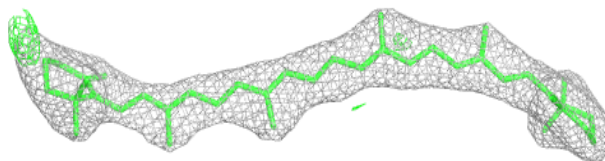


**Electron density around CLA D 703:**

$2mF_o-DF_c$  (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:**

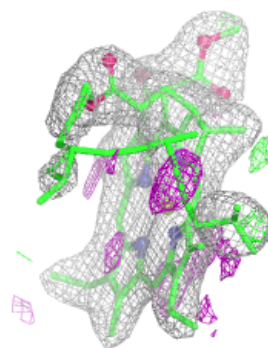
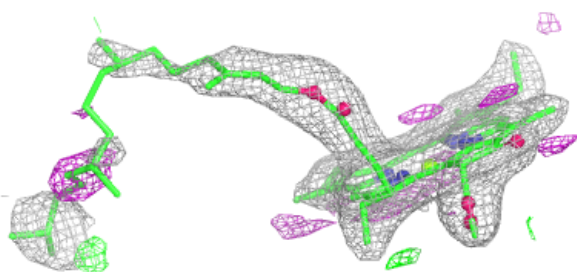
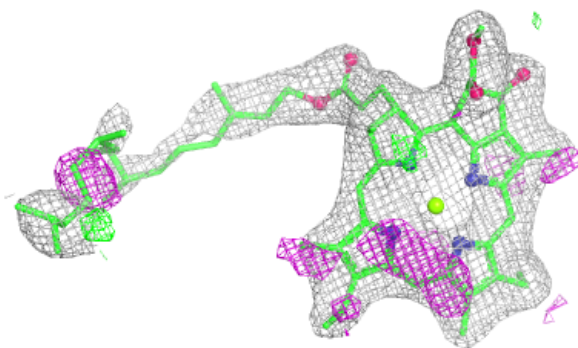
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



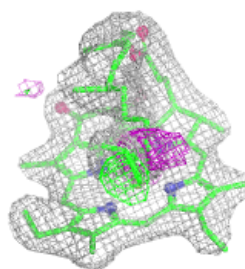
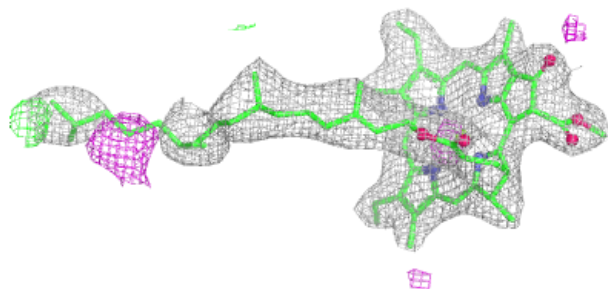
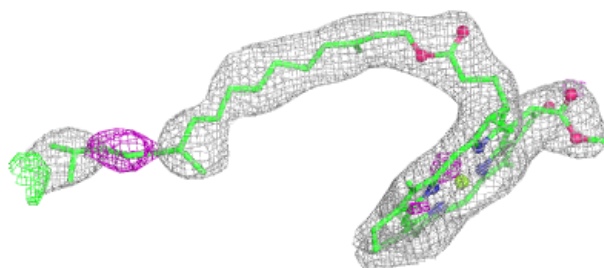


**Electron density around CLA a 409:**

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

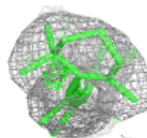
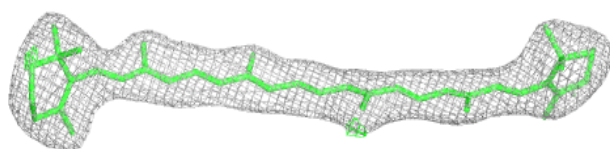
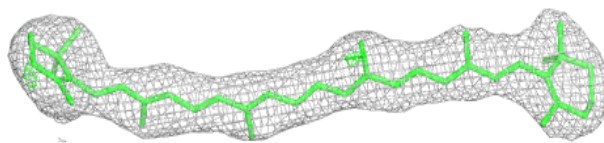
**Electron density around CLA C 505:**

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

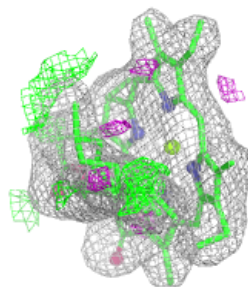
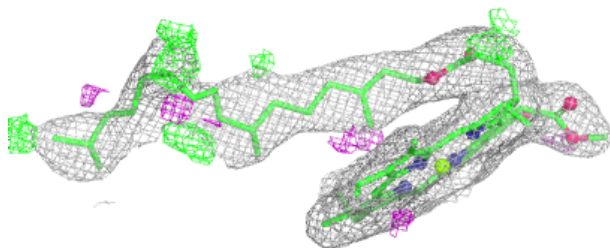
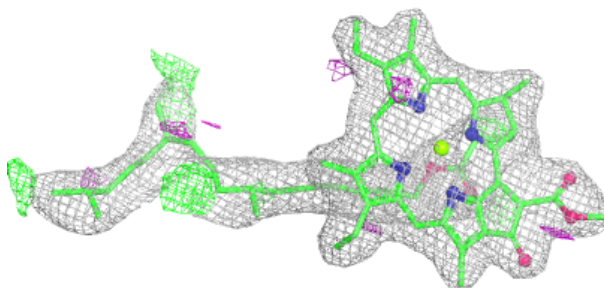


**Electron density around BCR c 515:**

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

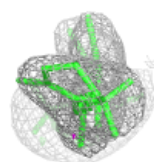
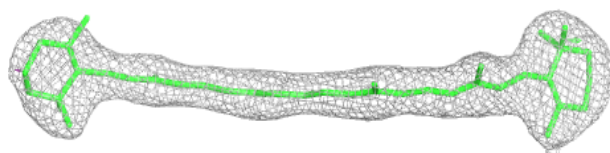
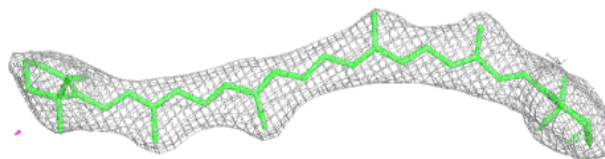
**Electron density around CLA b 614:**

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

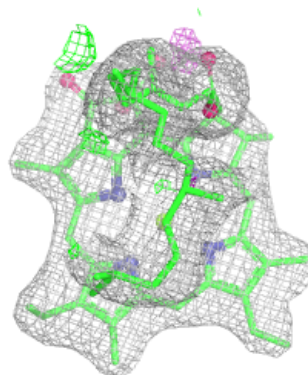
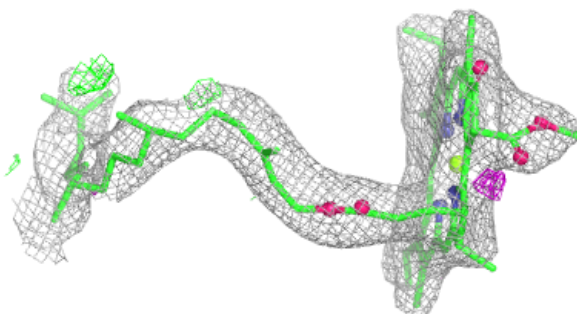
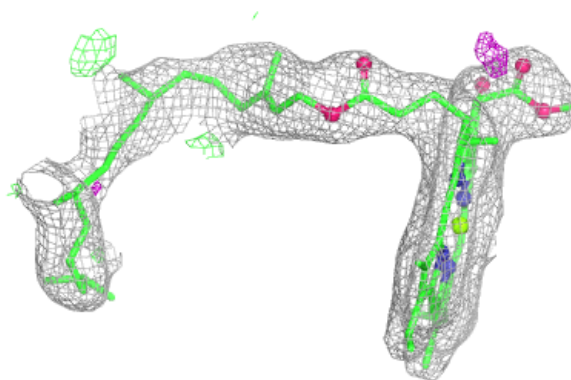


**Electron density around BCR h 101:**

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

**Electron density around CLA C 507:**

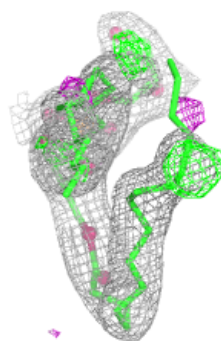
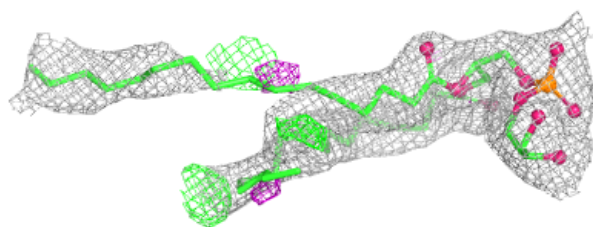
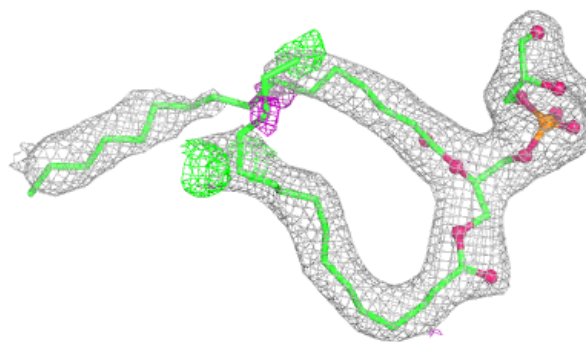
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



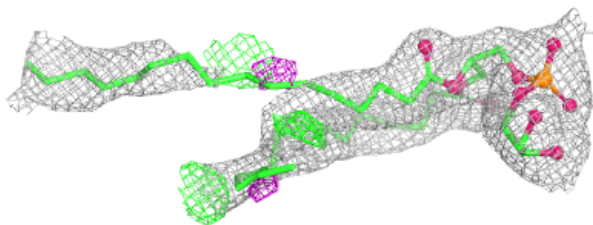
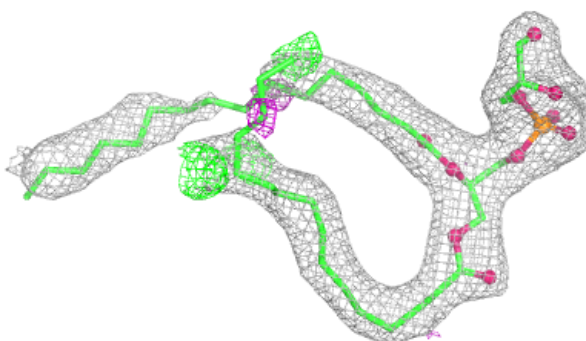


**Electron density around LHG D 707 (A):**

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

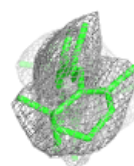
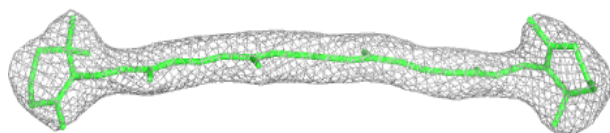
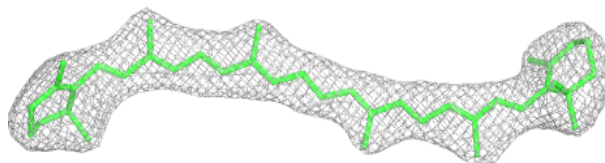
**Electron density around LHG D 707 (B):**

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

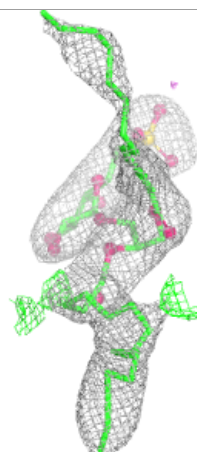
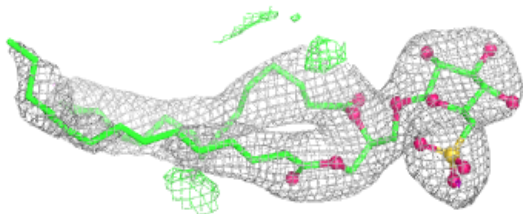
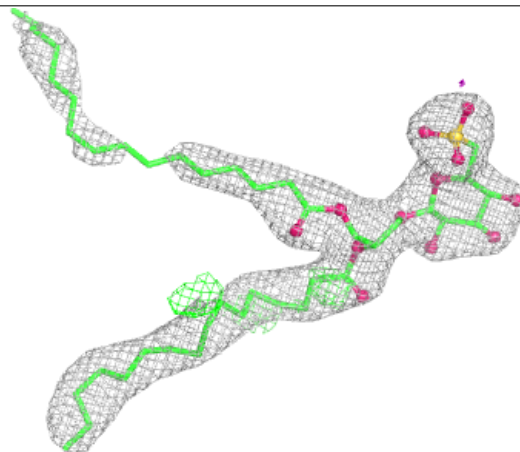


**Electron density around BCR y 101:**

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

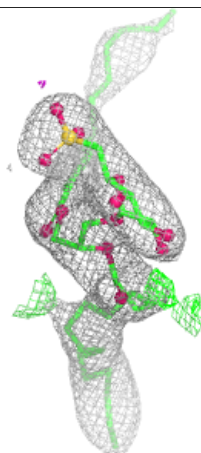
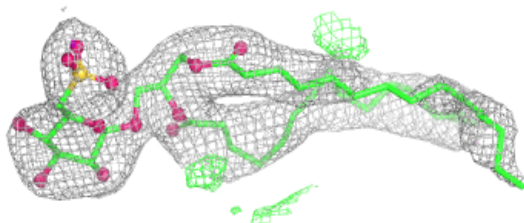
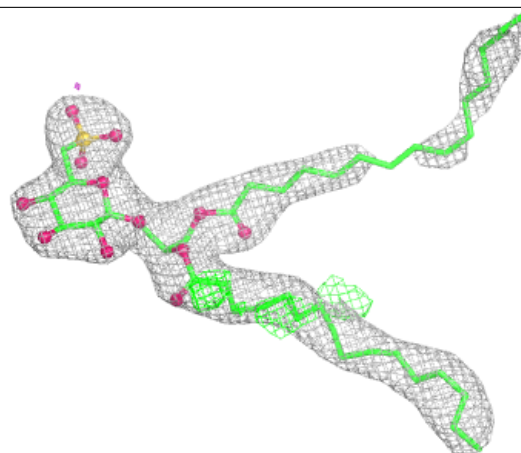
**Electron density around SQD A 410 (A):**

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



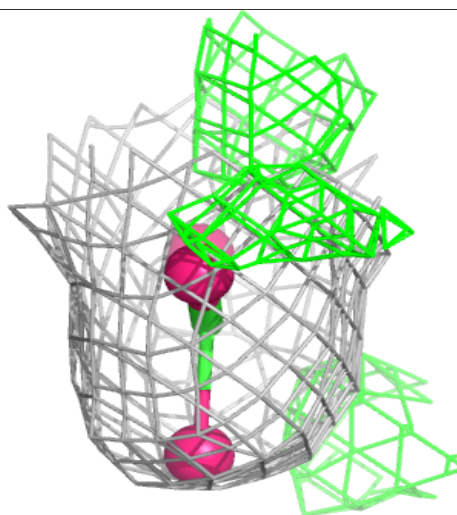
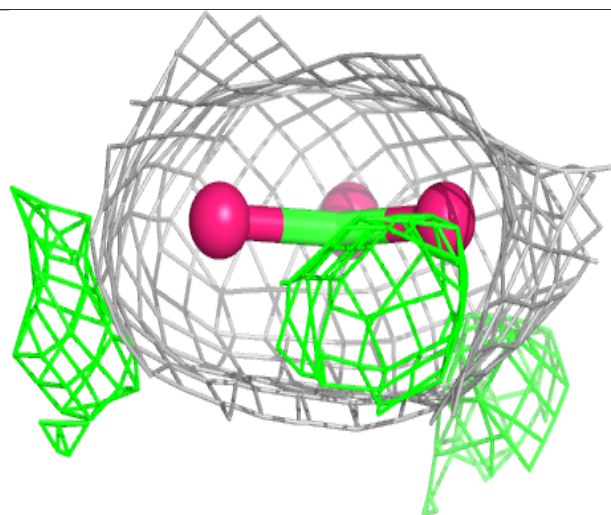
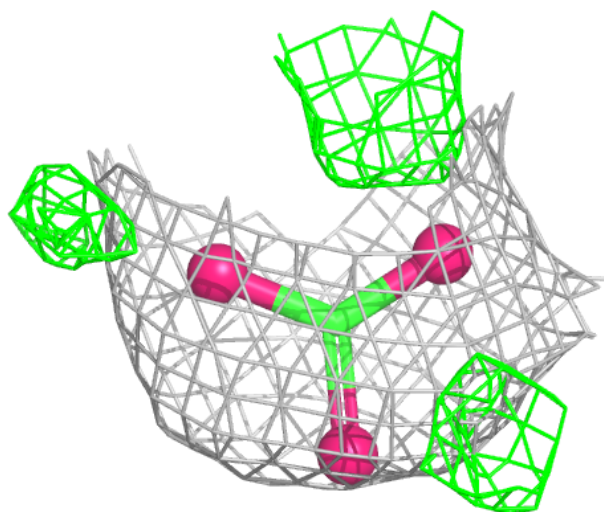
**Electron density around SQD A 410 (B):**

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



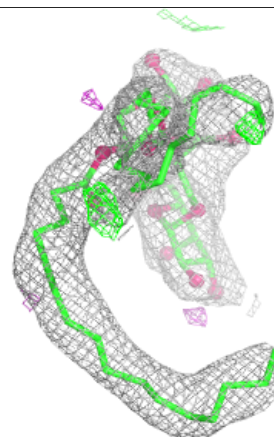
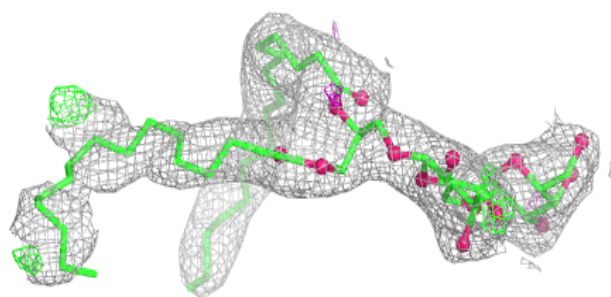
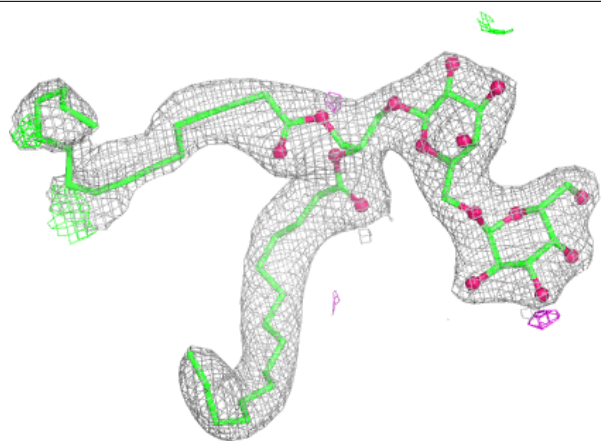
**Electron density around BCT a 404 (A):**

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



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

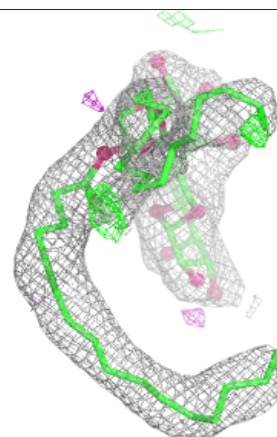
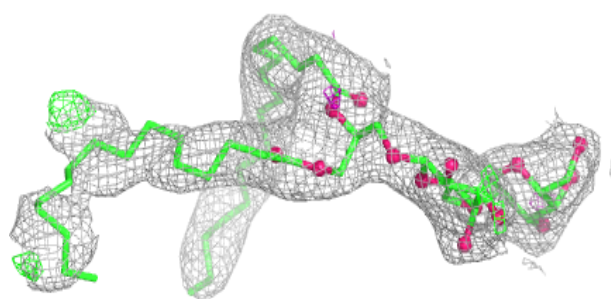
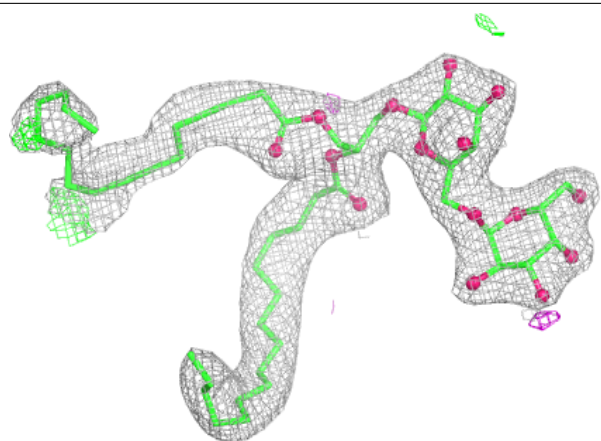
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



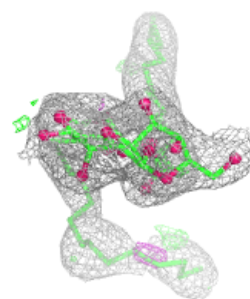
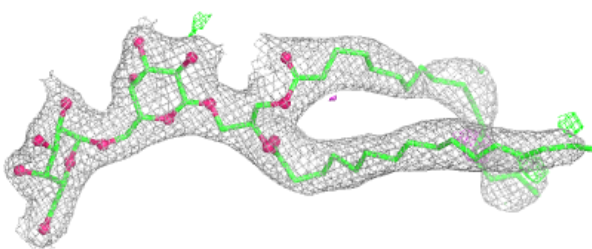
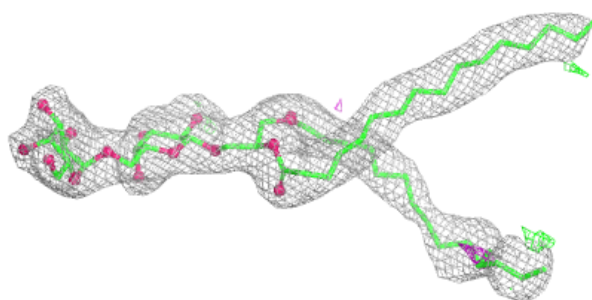


**Electron density around DGD C 518 (B):**

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

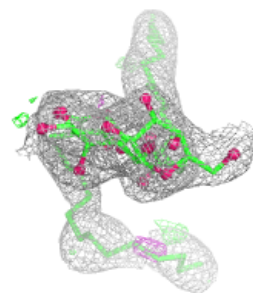
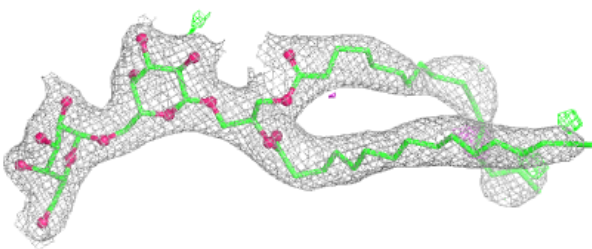
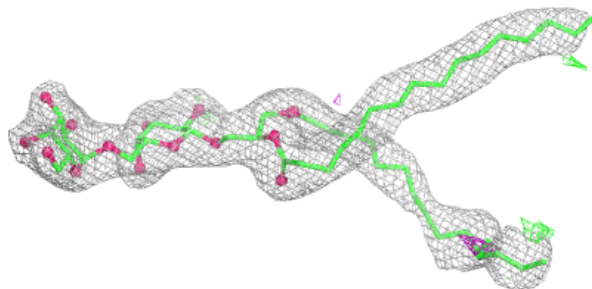
**Electron density around DGD c 517 (A):**

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



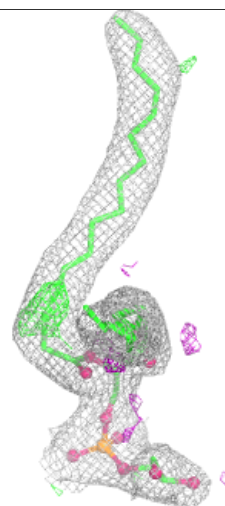
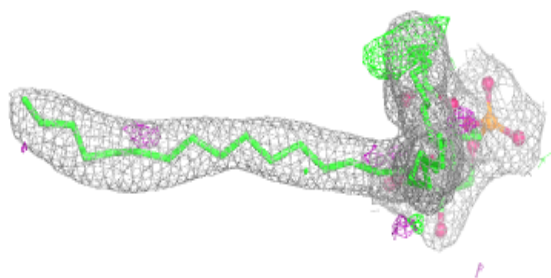
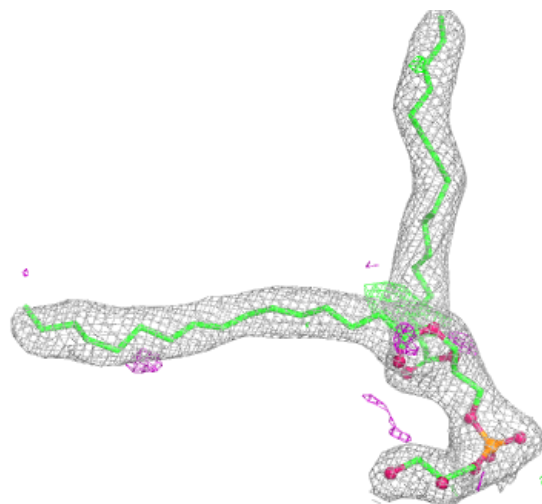
**Electron density around DGD c 517 (B):**

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



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

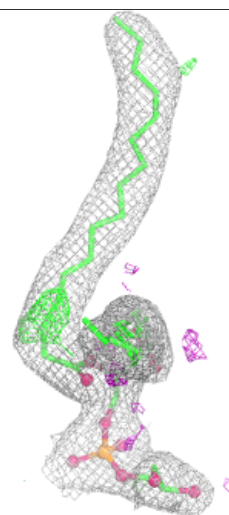
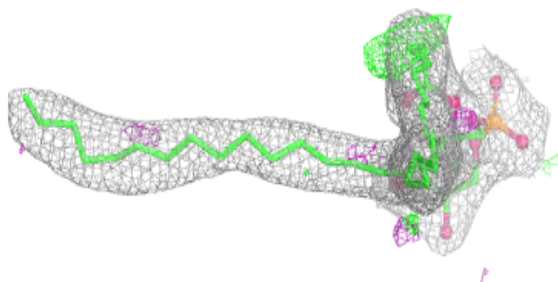
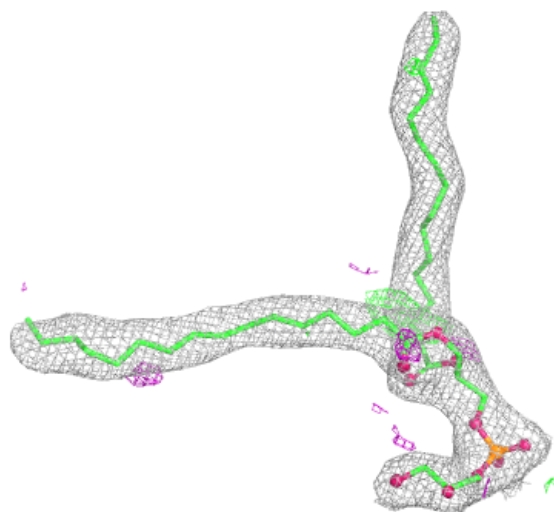
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





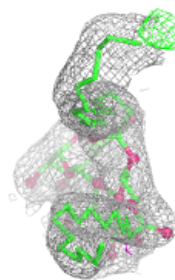
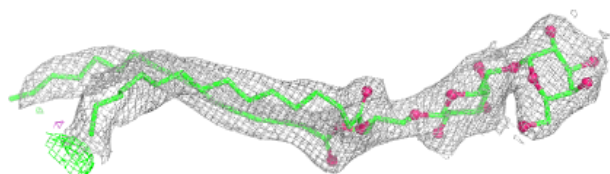
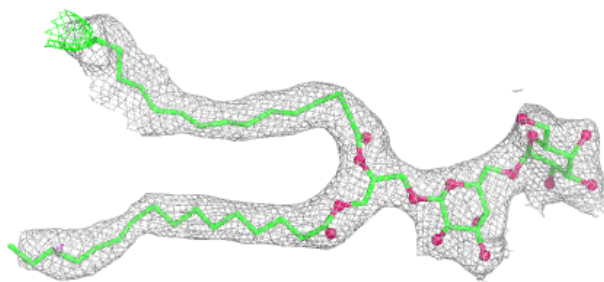
**Electron density around LHG b 629 (B):**

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

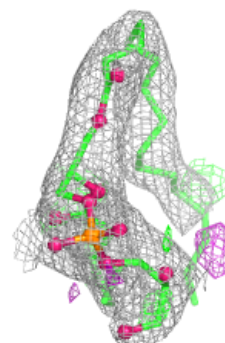
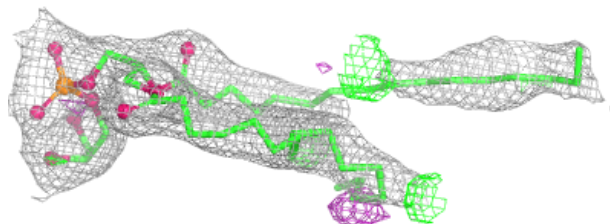
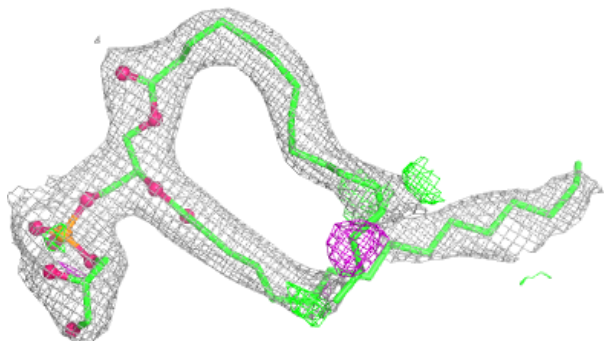


**Electron density around DGD c 519:**

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

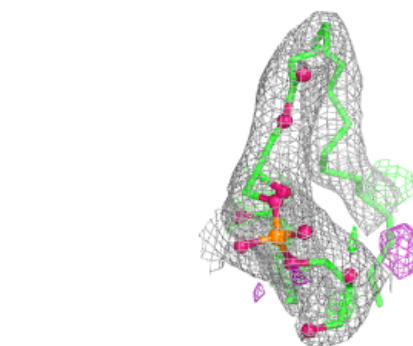
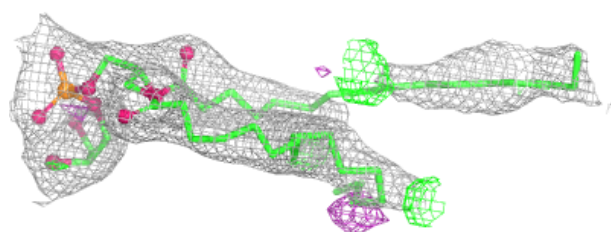
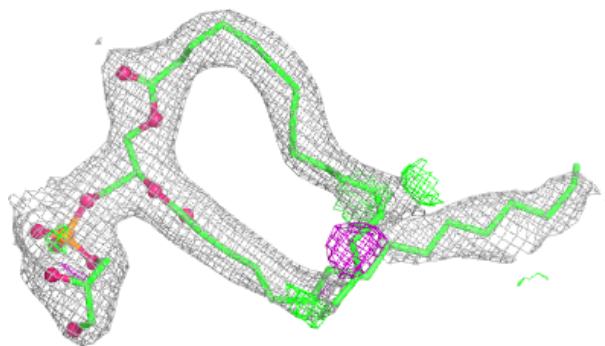
**Electron density around LHG d 406 (A):**

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

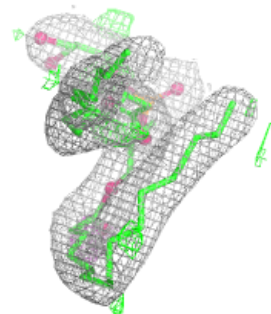
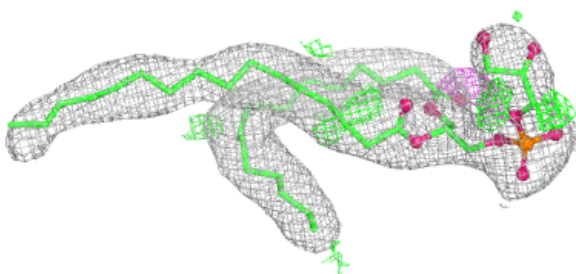
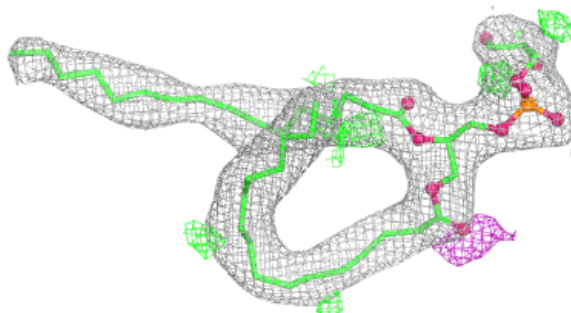


**Electron density around LHG d 406 (B):**

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

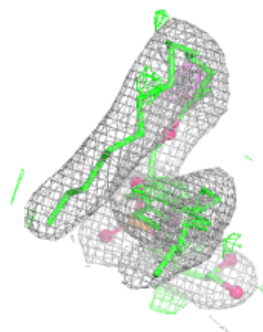
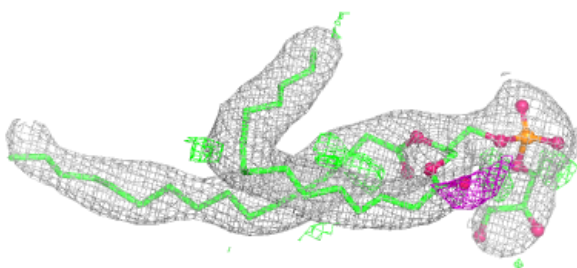
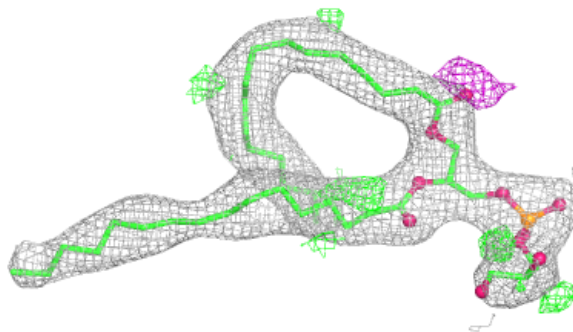
**Electron density around LHG d 412 (A):**

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

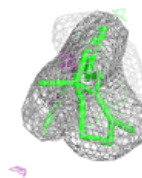
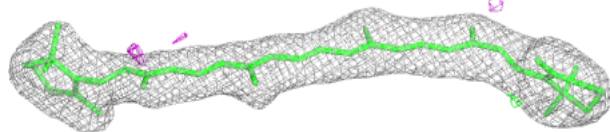
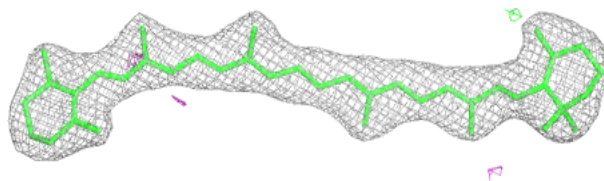


**Electron density around LHG d 412 (B):**

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

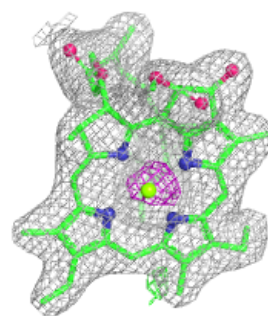
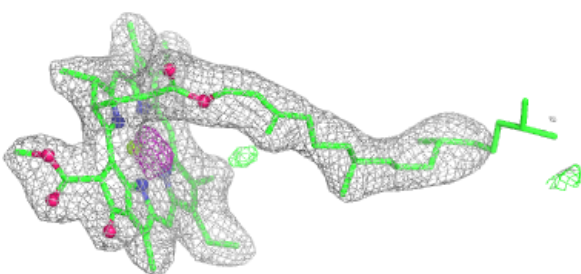
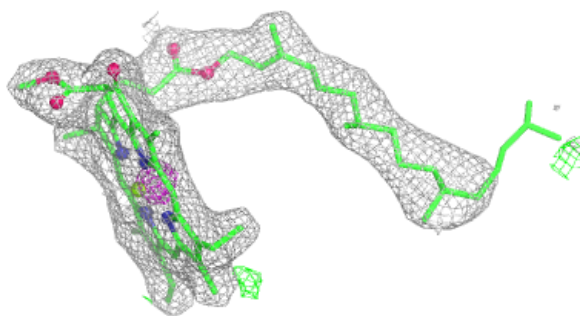
**Electron density around BCR b 619:**

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

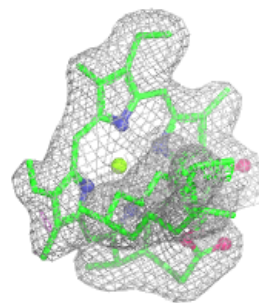
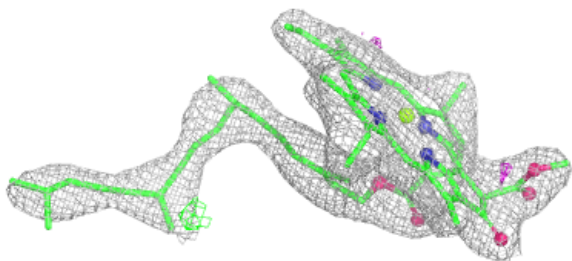
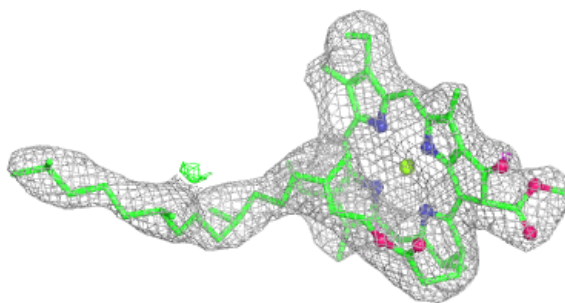


**Electron density around CLA C 509:**

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

**Electron density around CLA c 506:**

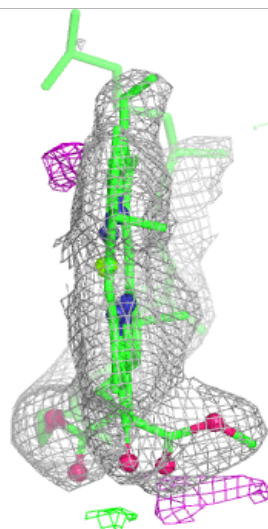
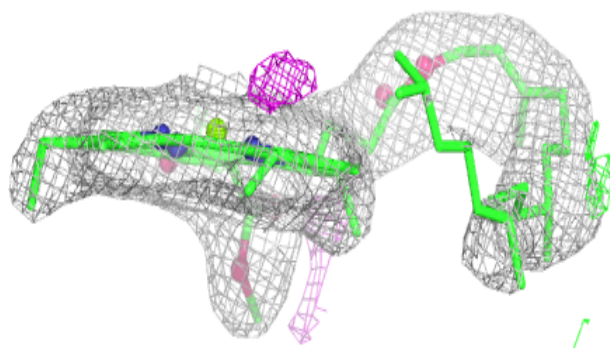
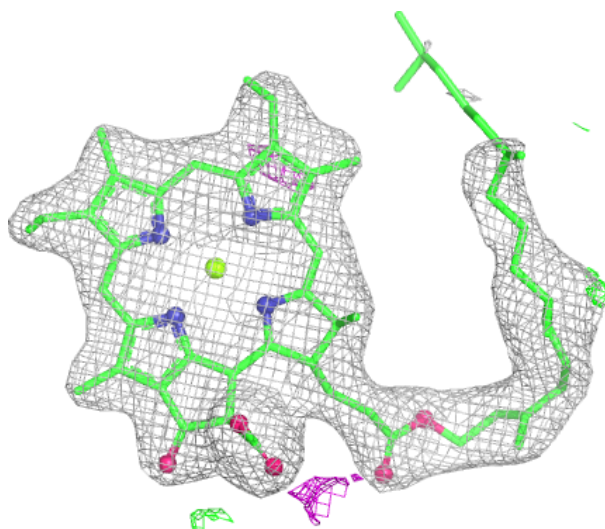
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





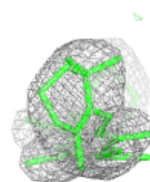
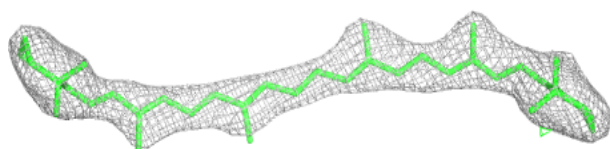
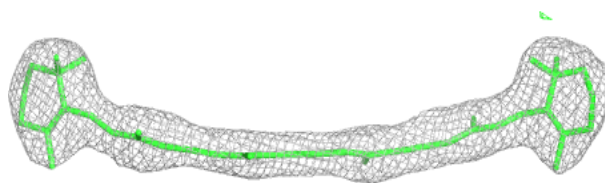
**Electron density around CLA C 513:**

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

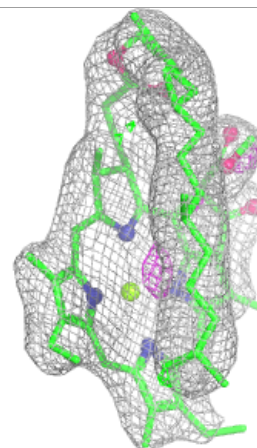
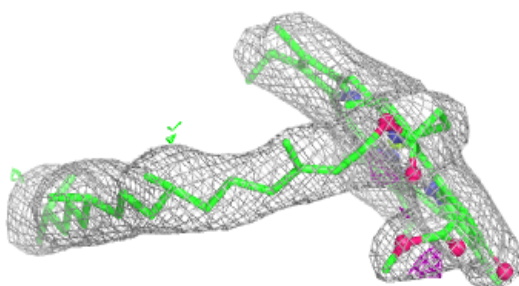
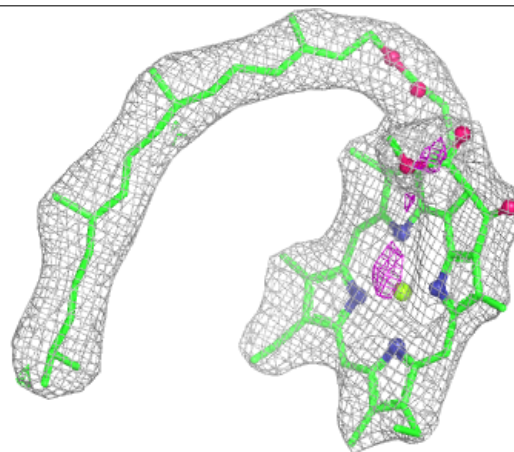


**Electron density around BCR k 101:**

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

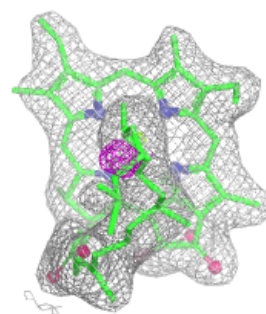
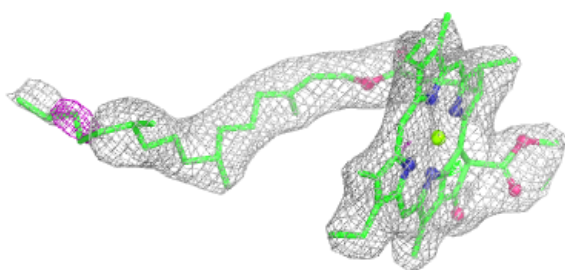
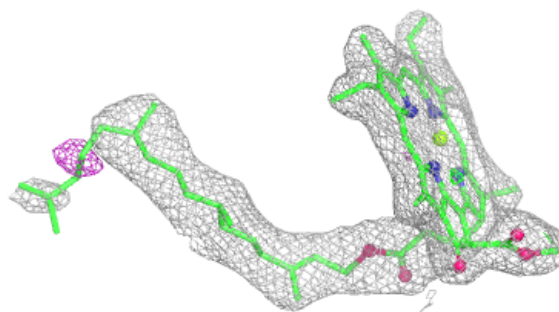
**Electron density around CLA c 508:**

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



**Electron density around CLA c 509:**

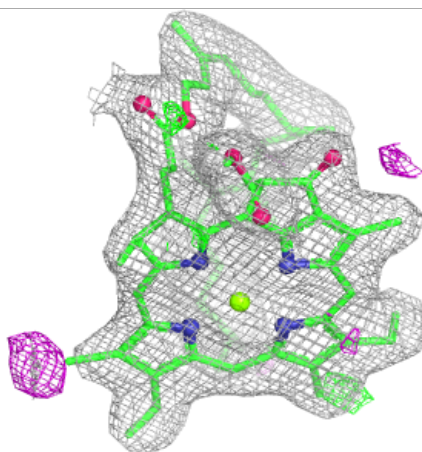
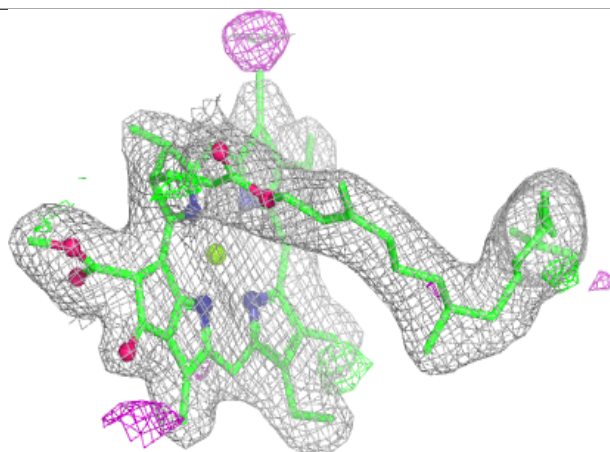
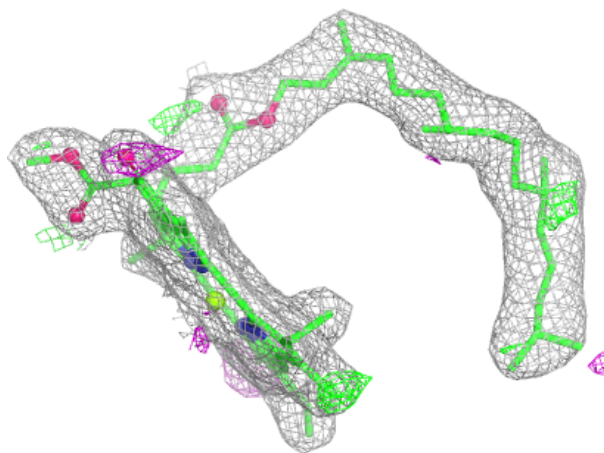
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



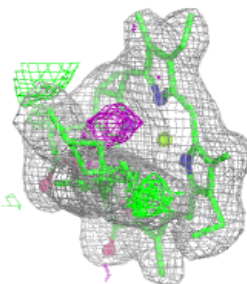
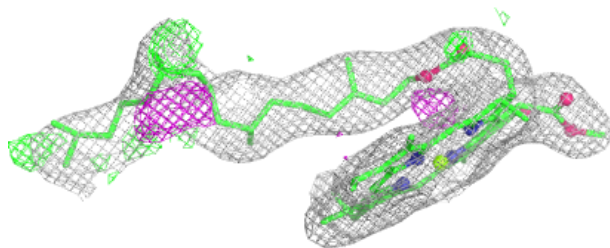
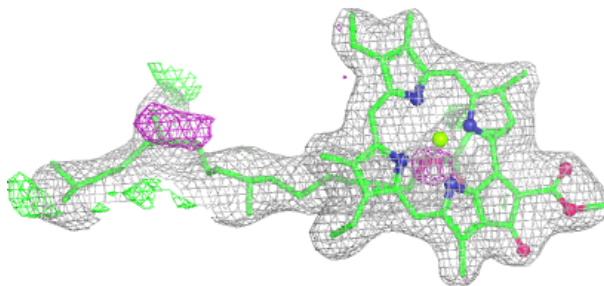


**Electron density around CLA B 611:**

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

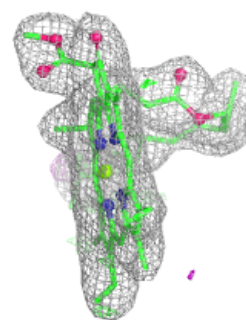
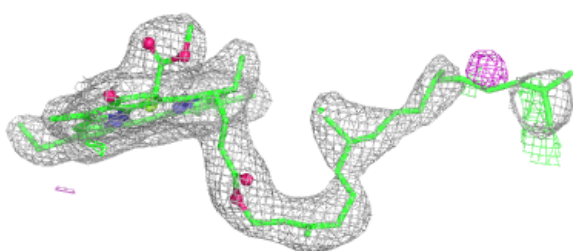
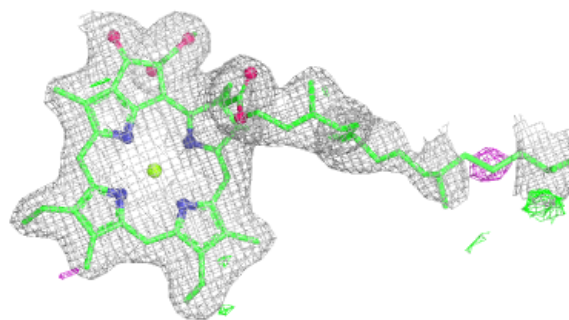
**Electron density around CLA B 614:**

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

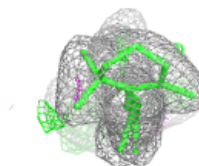
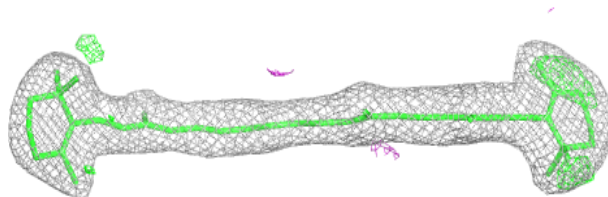
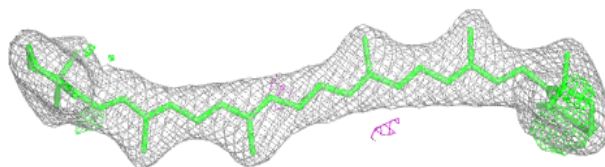


**Electron density around CLA a 407 (A):**

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

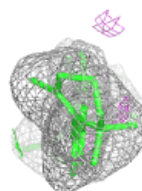
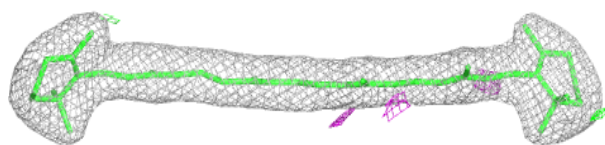
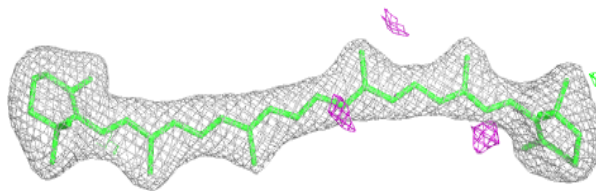
**Electron density around BCR A 409:**

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

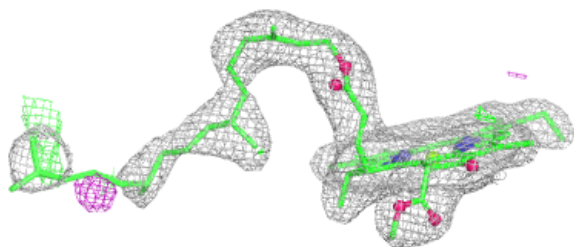
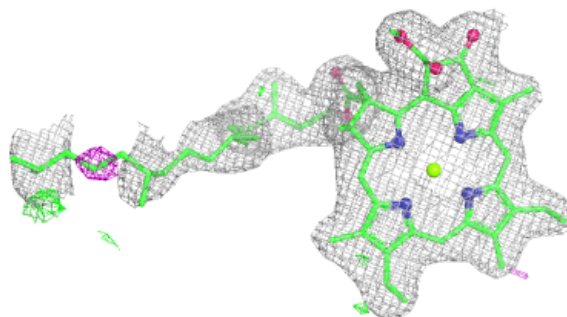


**Electron density around BCR B 618:**

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

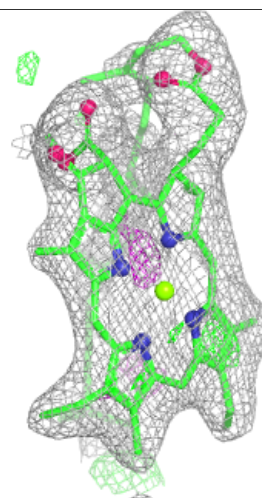
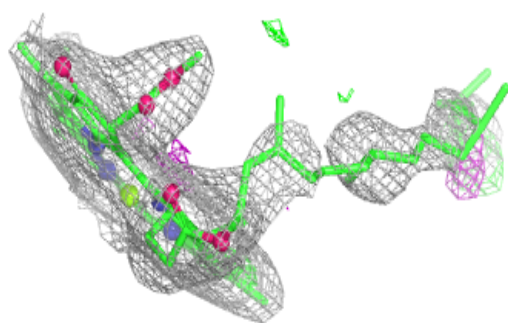
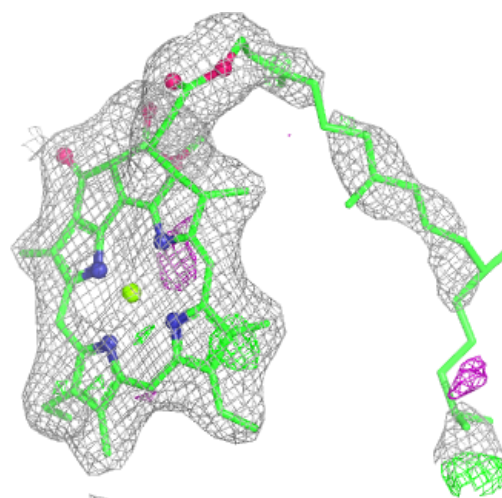
**Electron density around CLA a 407 (B):**

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



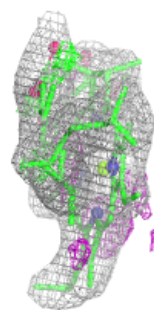
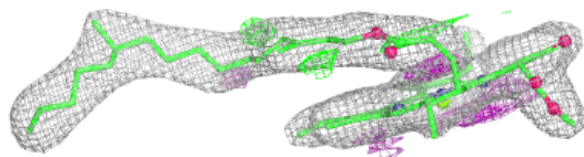
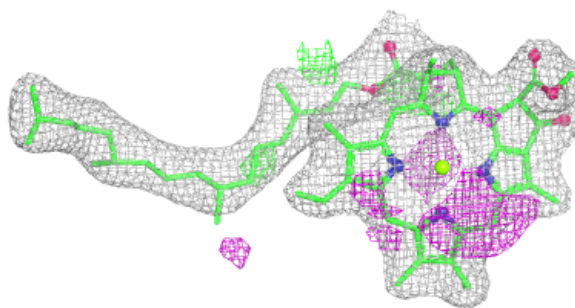
**Electron density around CLA B 616:**

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

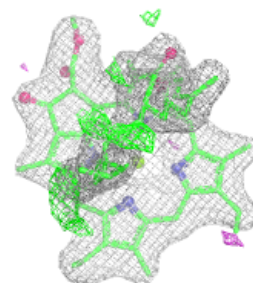
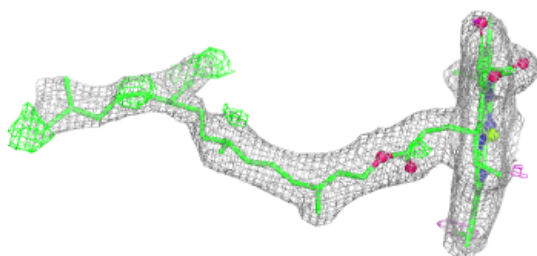
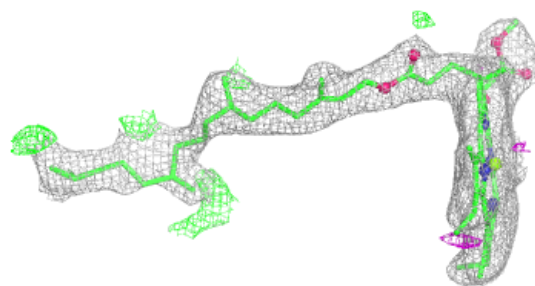


**Electron density around CLA B 603:**

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

**Electron density around CLA b 606:**

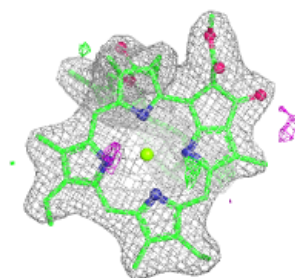
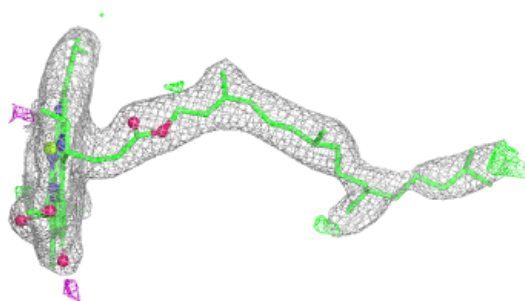
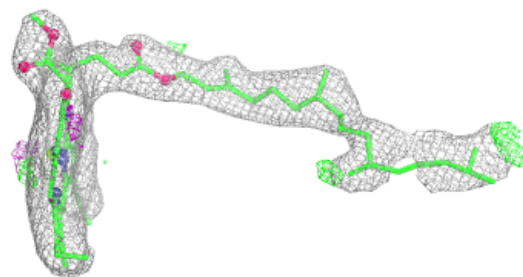
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





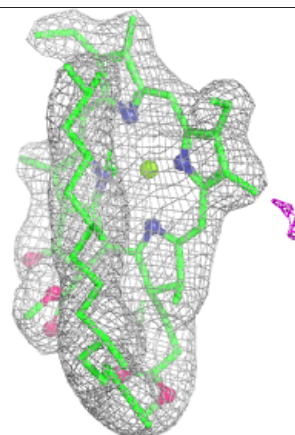
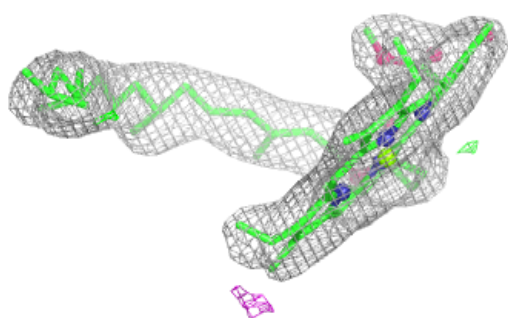
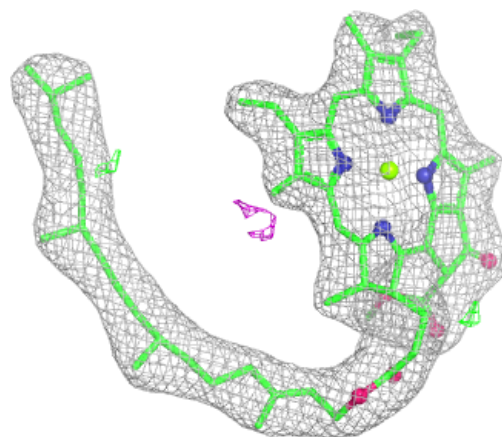
**Electron density around CLA B 606:**

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

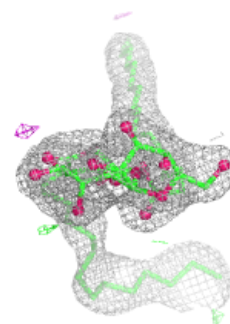
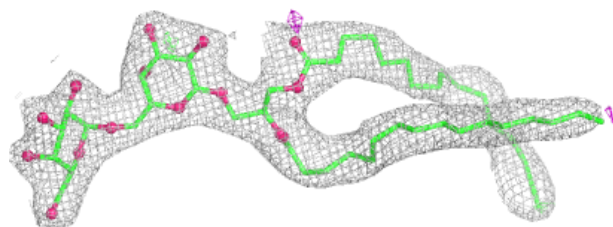
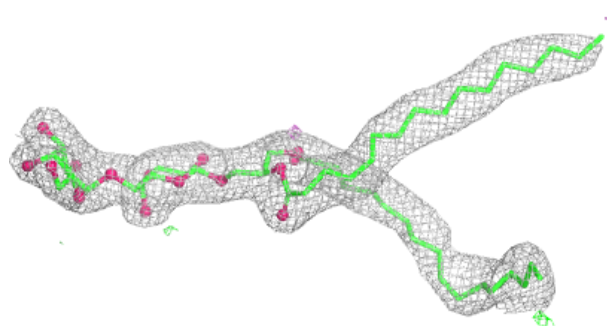


**Electron density around CLA C 508:**

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

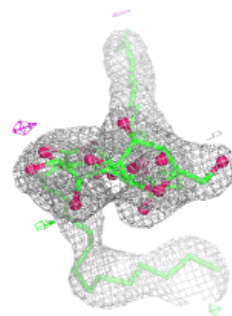
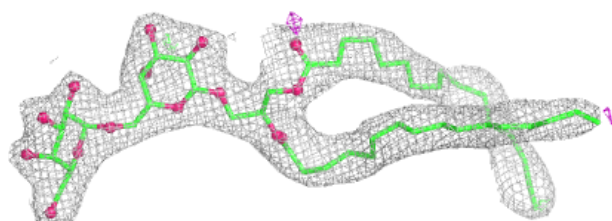
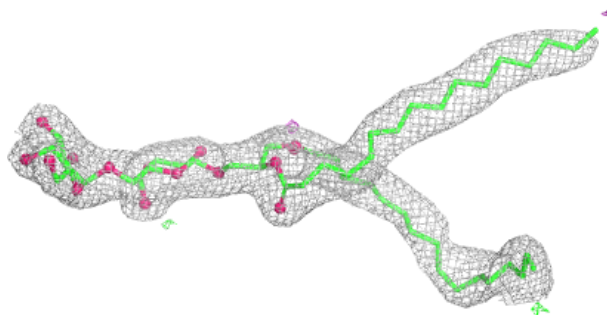
**Electron density around DGD C 517 (A):**

$2mF_o-DF_c$  (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):**

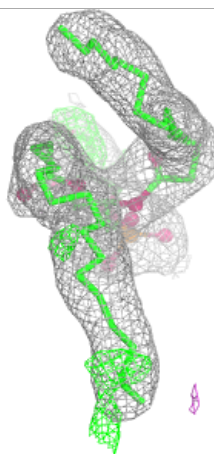
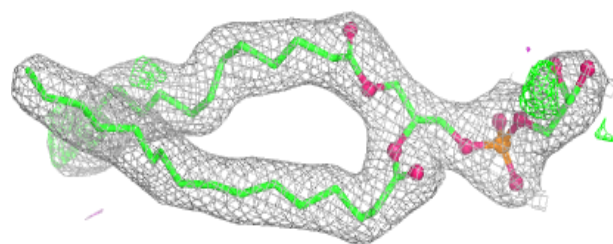
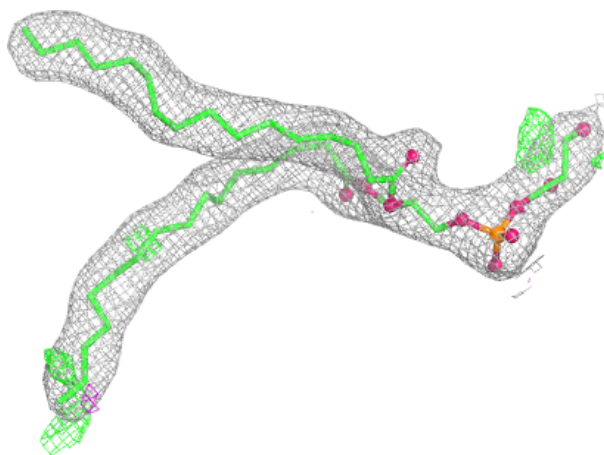
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





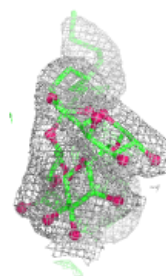
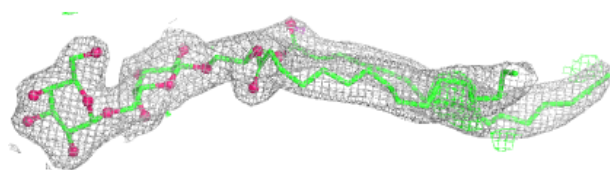
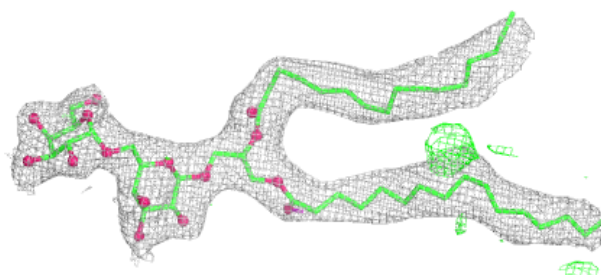
**Electron density around LHG d 405 (A):**

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

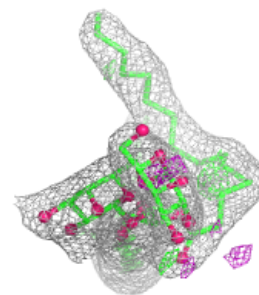
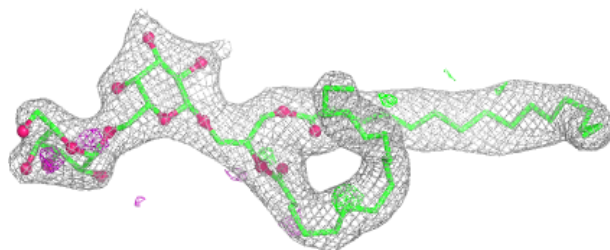
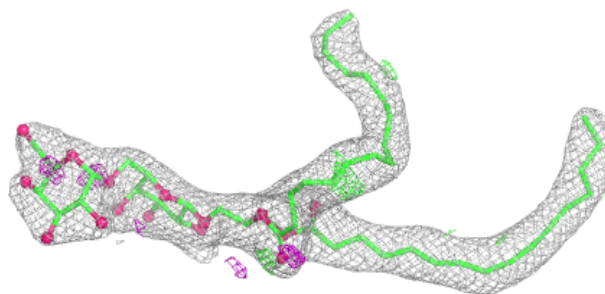


**Electron density around DGD C 519:**

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

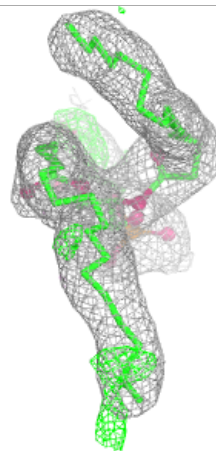
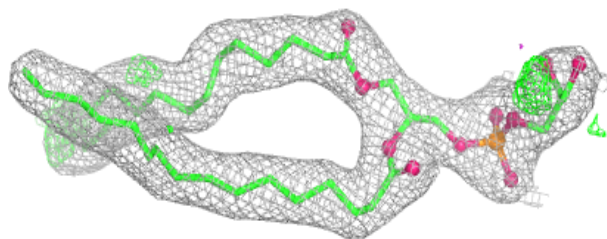
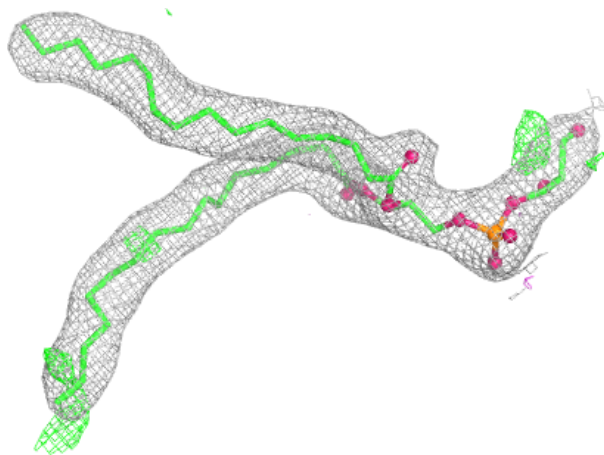
**Electron density around DGD H 102:**

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



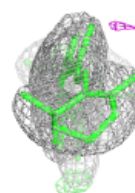
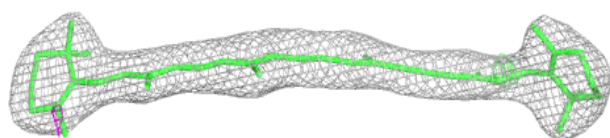
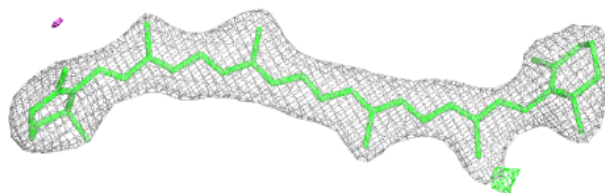
**Electron density around LHG d 405 (B):**

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

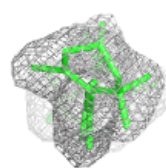
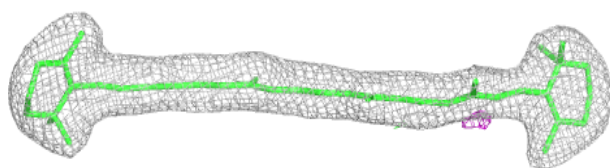
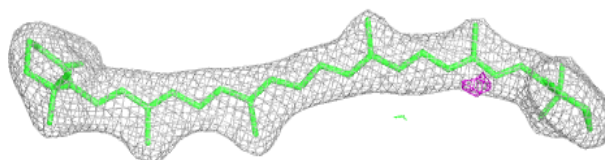


**Electron density around BCR Y 101:**

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

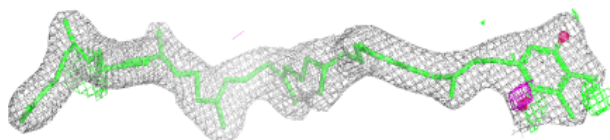
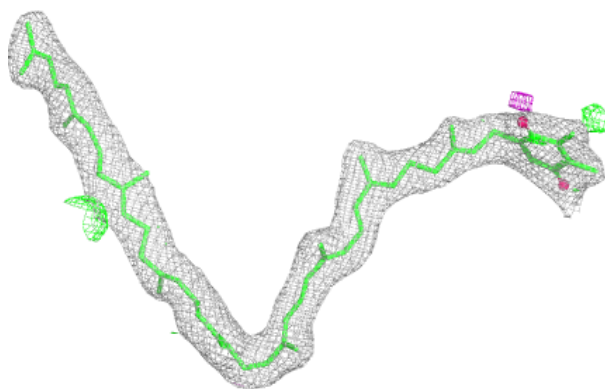
**Electron density around BCR a 410:**

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

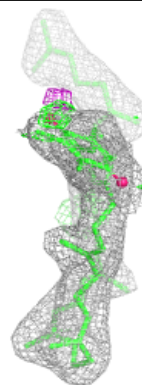
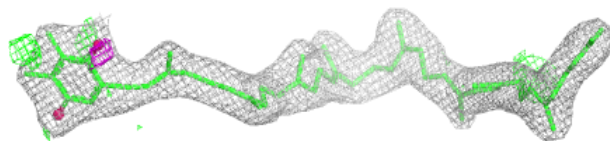
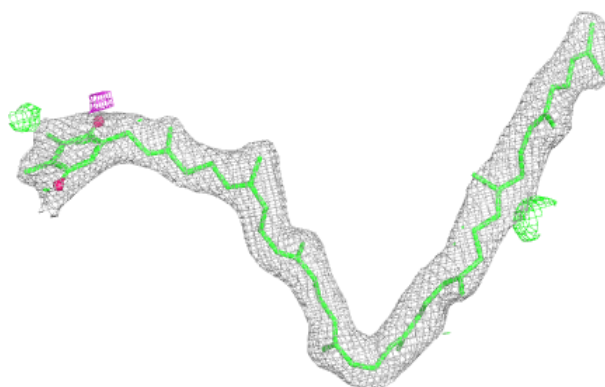


**Electron density around PL9 D 705 (A):**

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

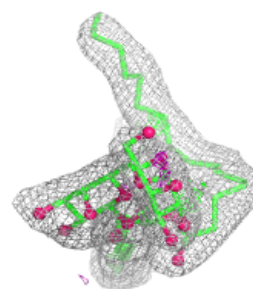
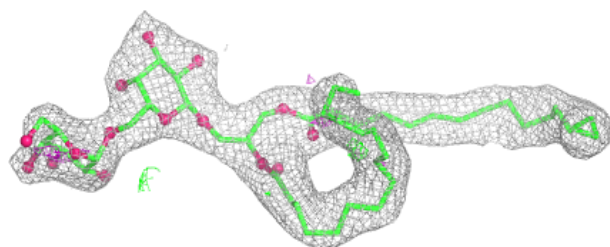
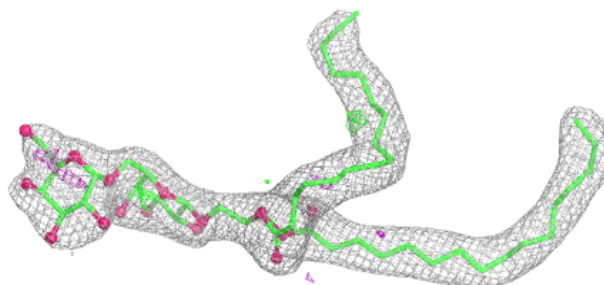
**Electron density around PL9 D 705 (B):**

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

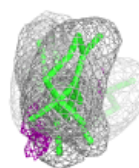
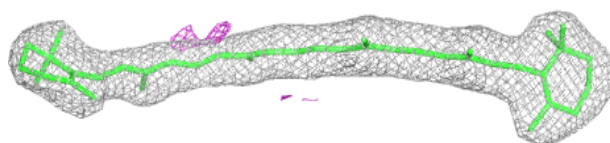
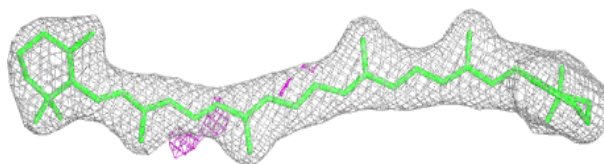


**Electron density around DGD h 102:**

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

**Electron density around BCR b 617:**

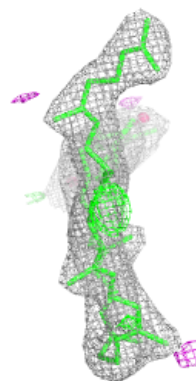
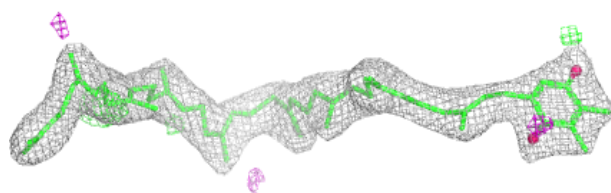
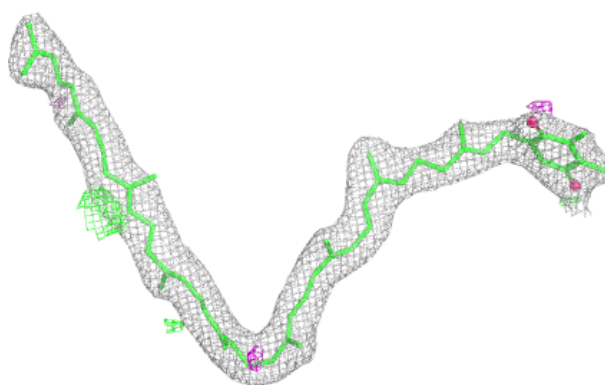
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



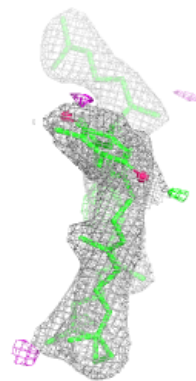
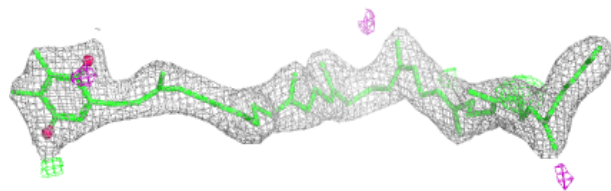
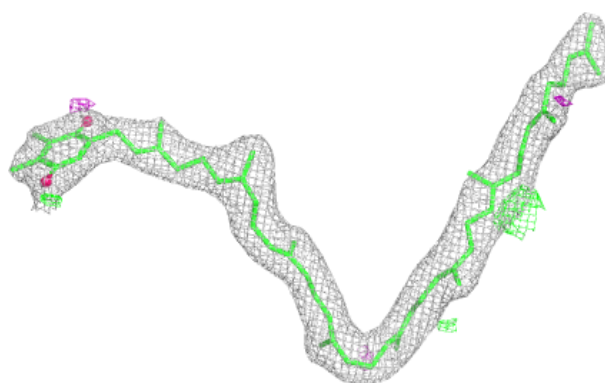


**Electron density around PL9 d 404 (A):**

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

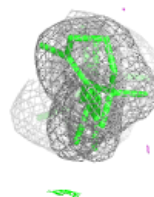
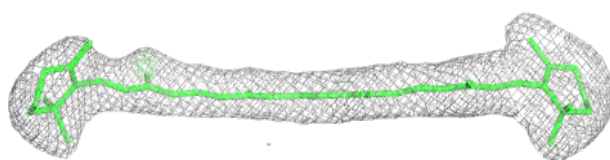
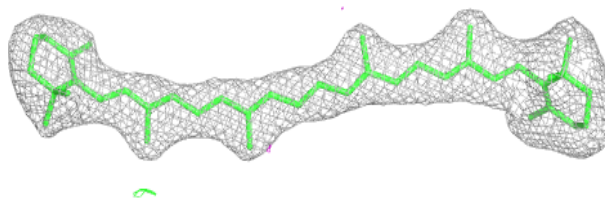
**Electron density around PL9 d 404 (B):**

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

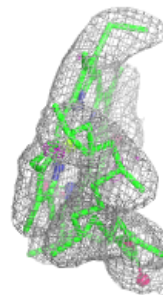
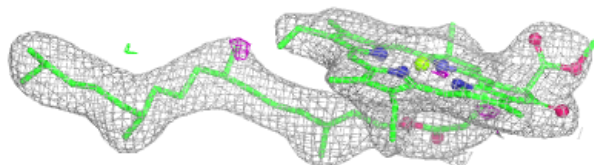
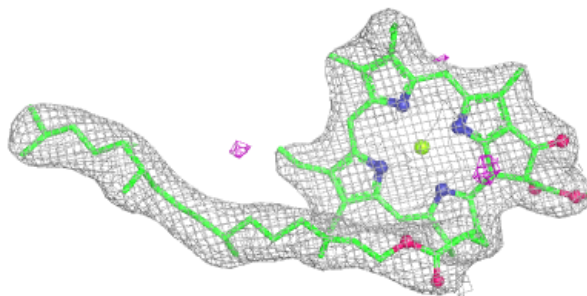


**Electron density around BCR b 618:**

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

**Electron density around CLA c 502:**

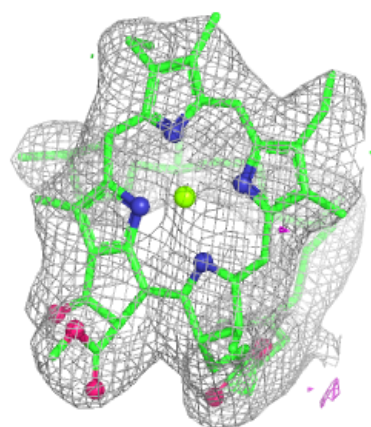
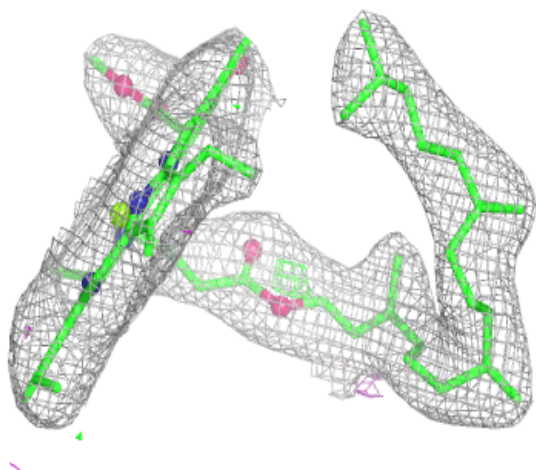
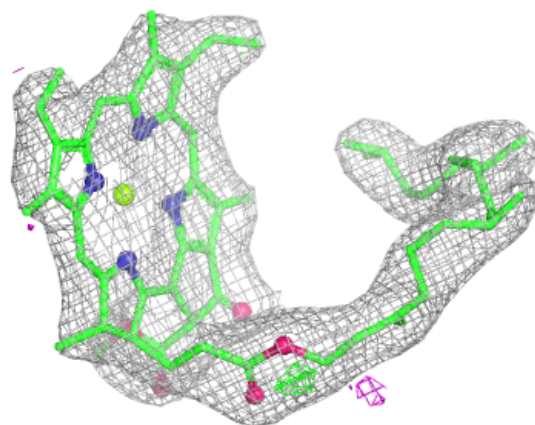
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





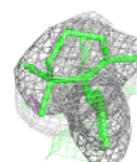
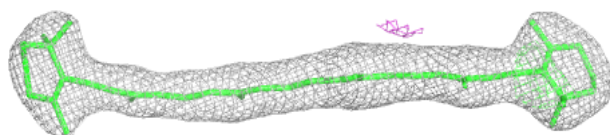
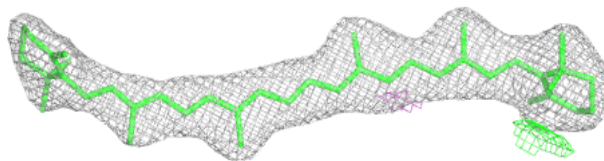
**Electron density around CLA c 504:**

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

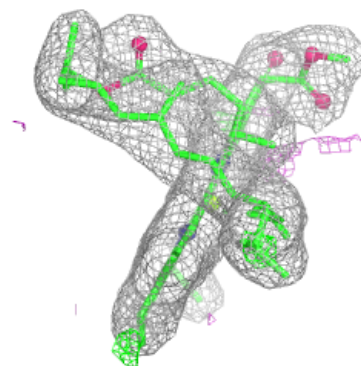
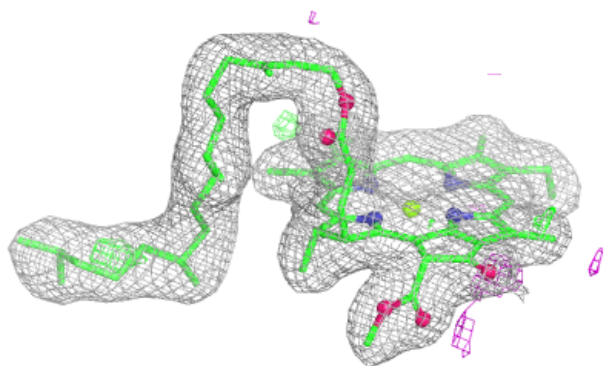
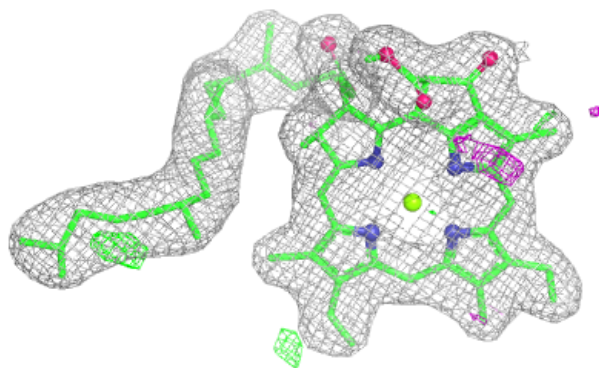


**Electron density around BCR c 516:**

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

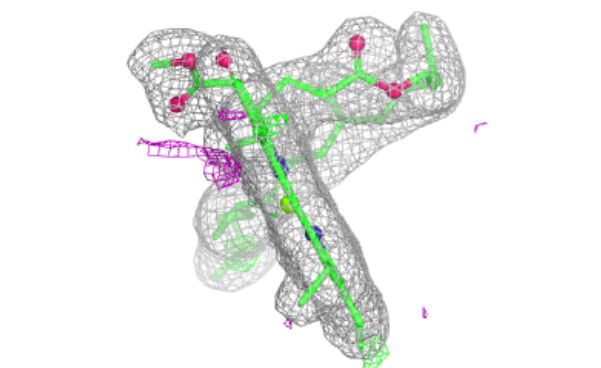
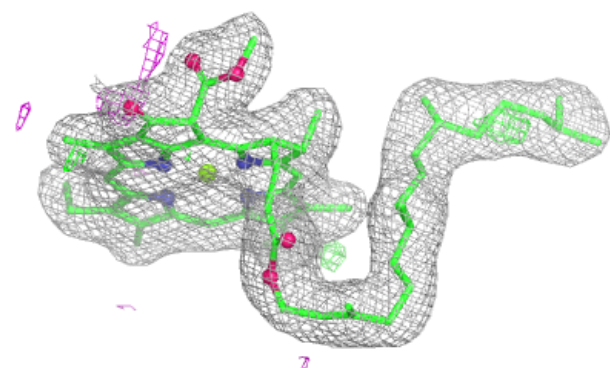
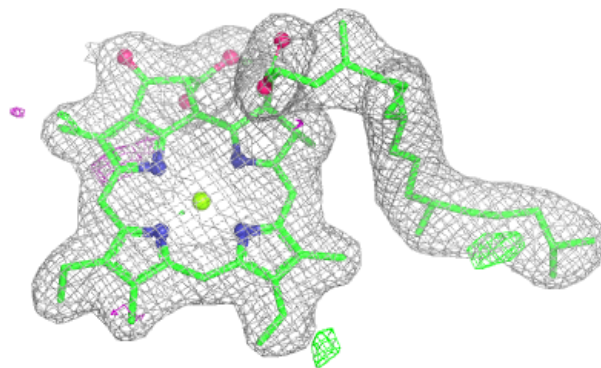
**Electron density around CLA A 405 (A):**

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

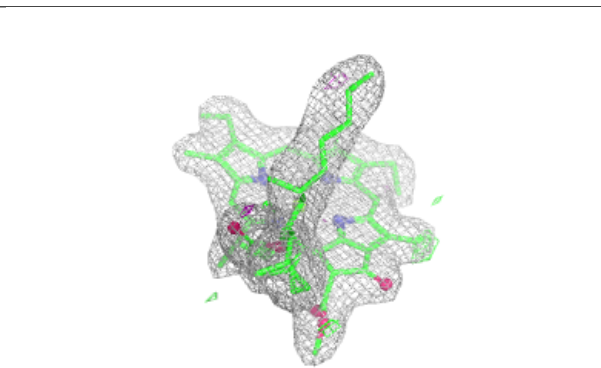
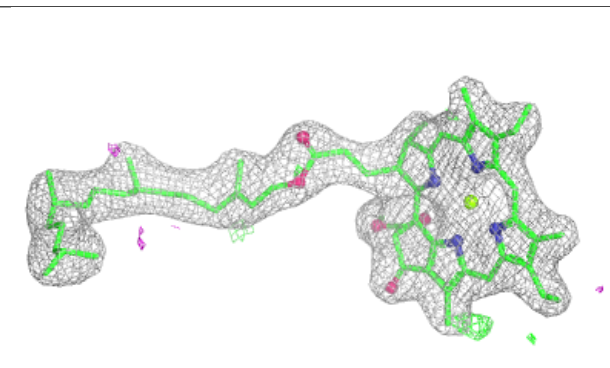
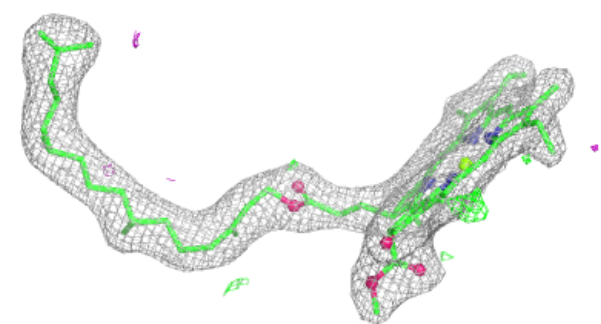


**Electron density around CLA A 405 (B):**

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

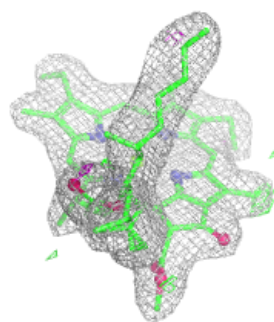
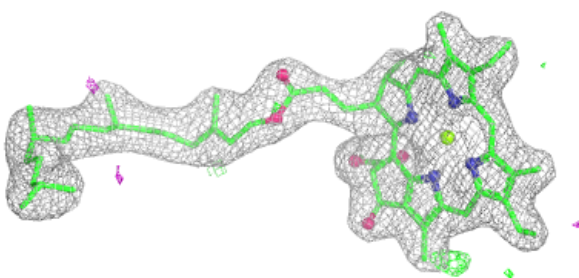
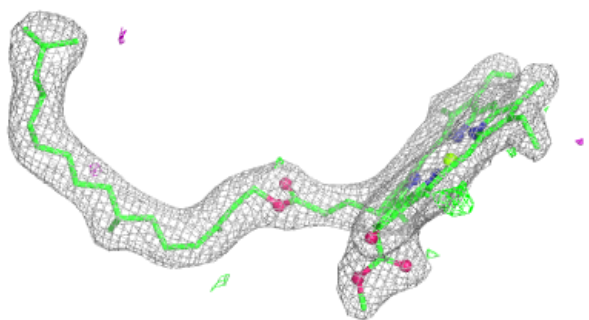
**Electron density around CLA D 702 (A):**

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

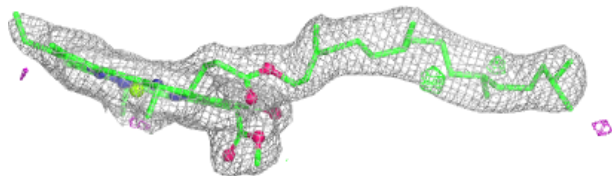
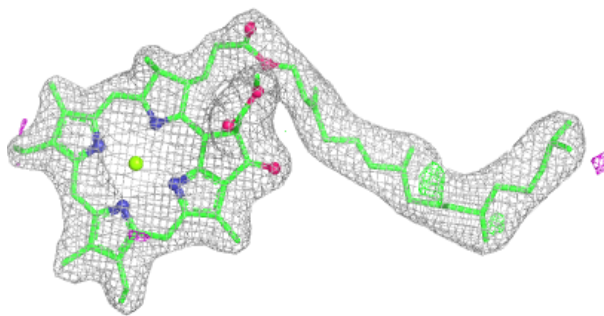


**Electron density around CLA D 702 (B):**

$2mF_o-DF_c$  (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:**

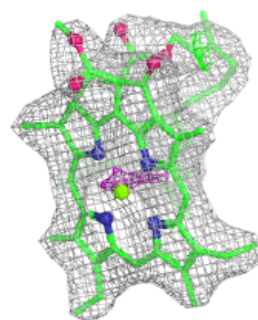
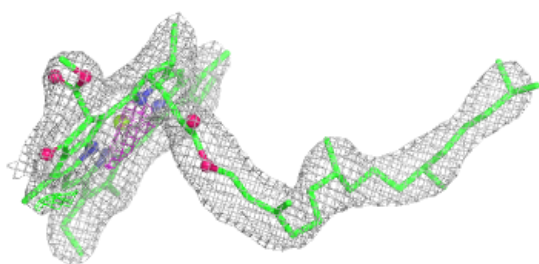
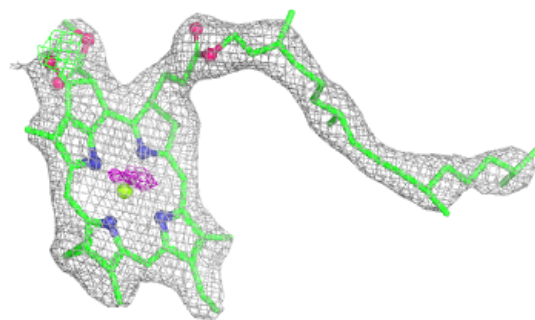
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



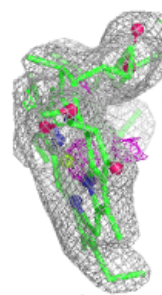
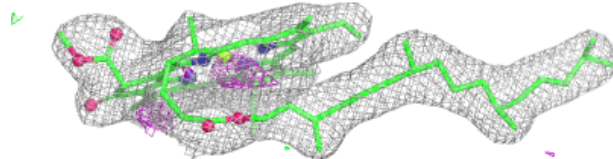
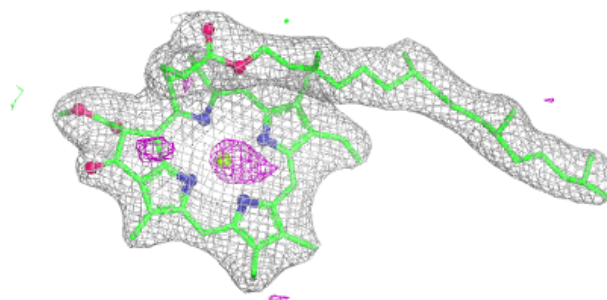


**Electron density around CLA c 512:**

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

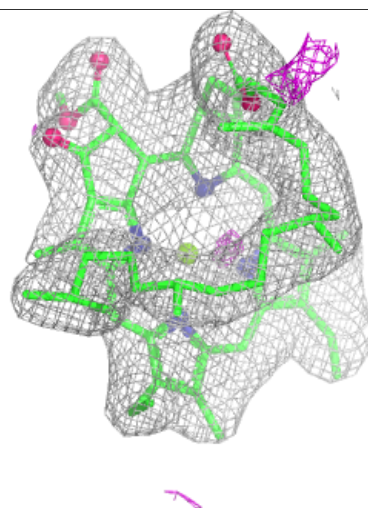
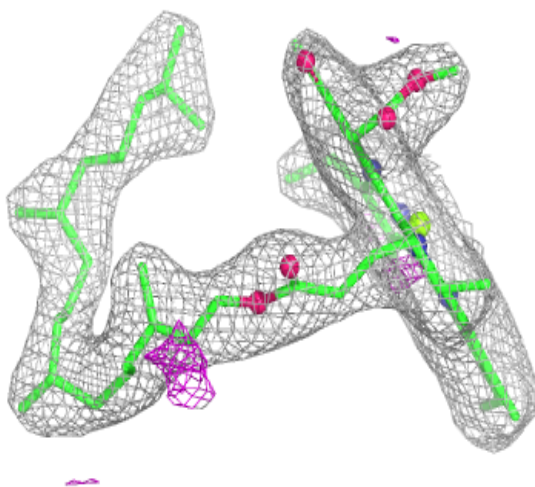
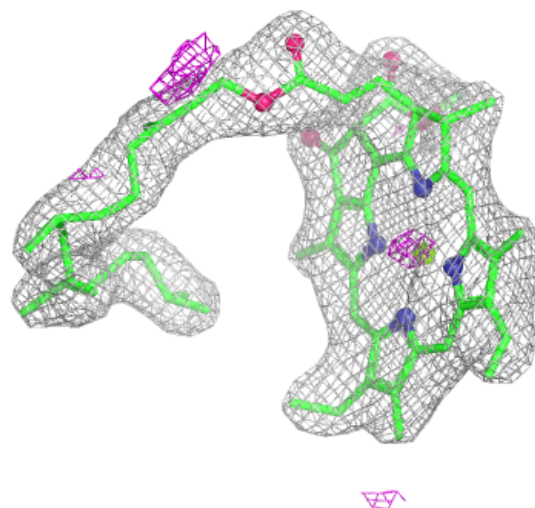
**Electron density around CLA C 502:**

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



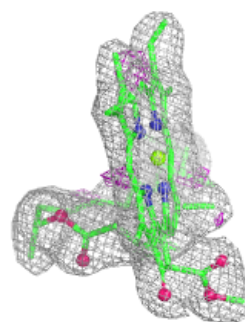
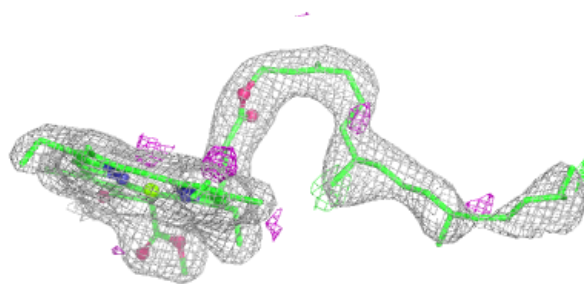
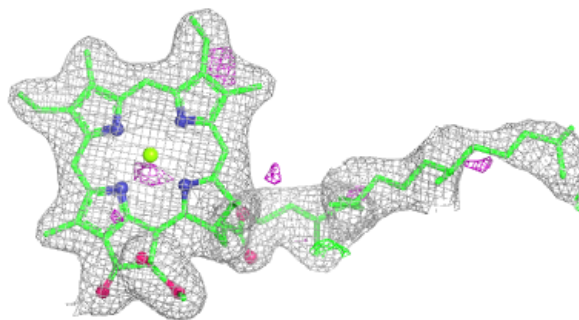
**Electron density around CLA C 504:**

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



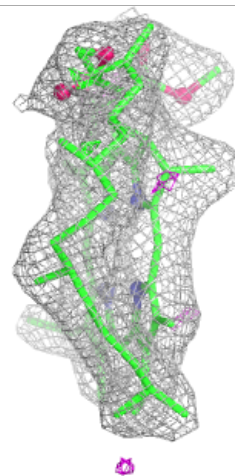
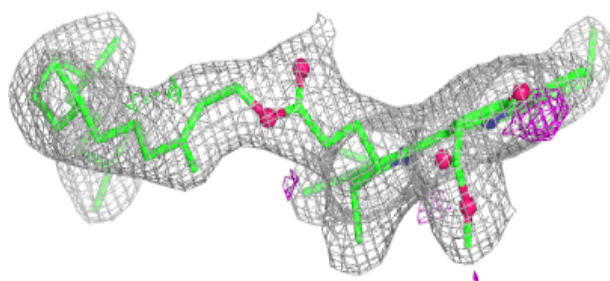
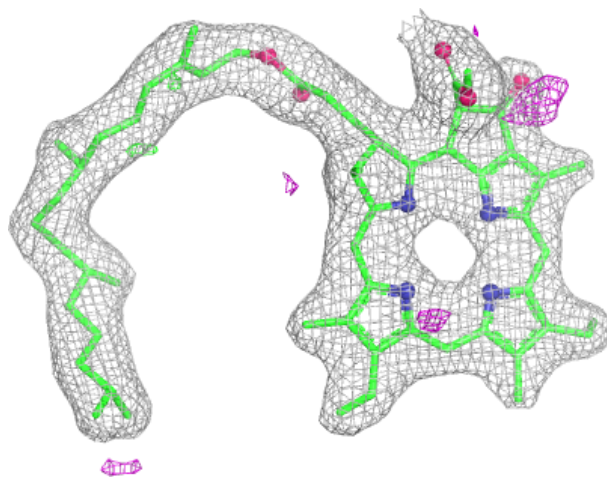
**Electron density around CLA A 406 (A):**

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



**Electron density around PHO A 407 (A):**

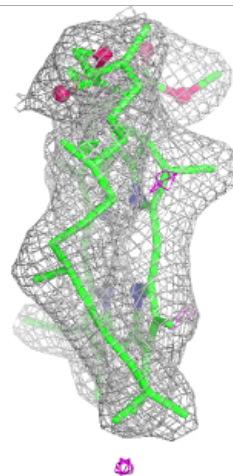
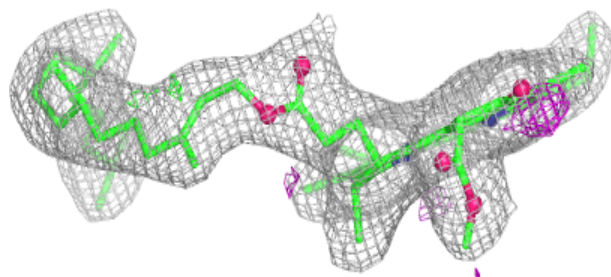
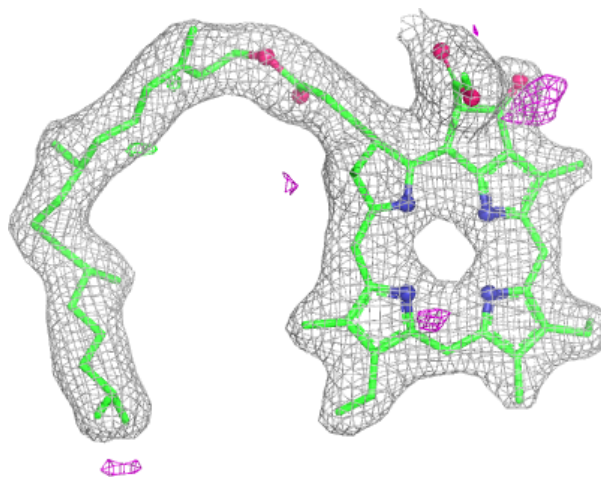
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





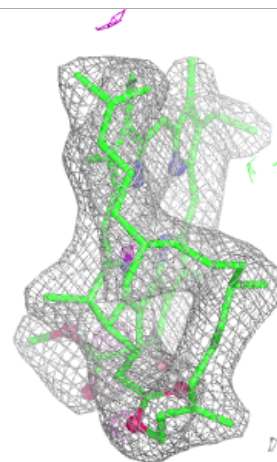
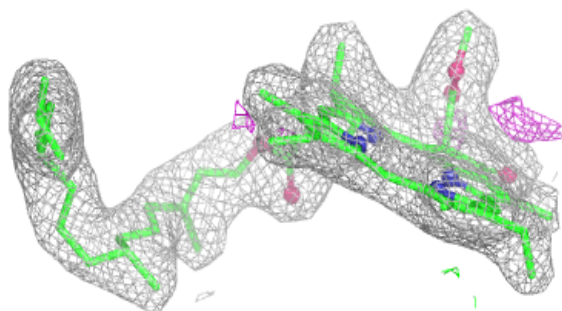
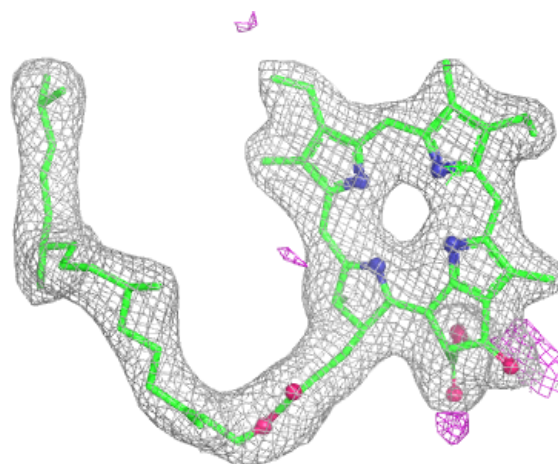
**Electron density around PHO A 407 (B):**

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



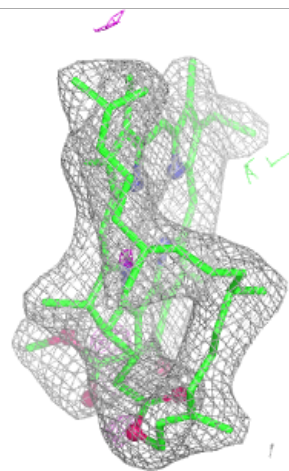
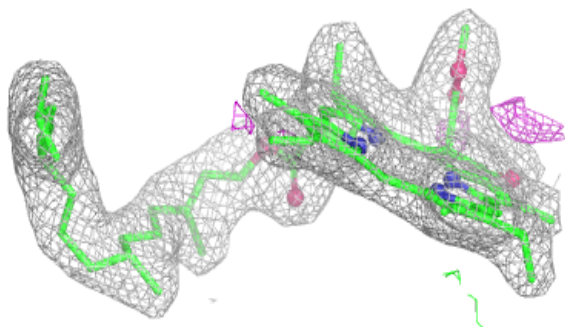
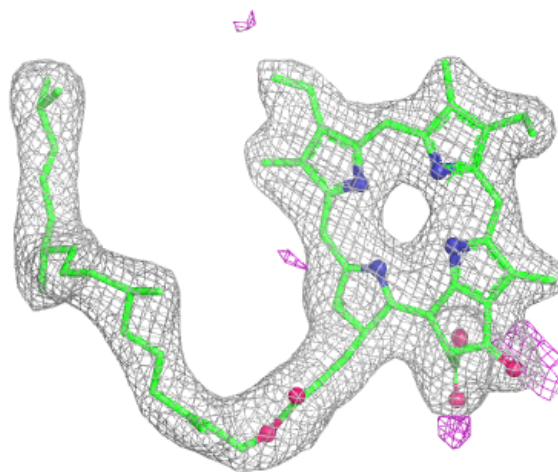
**Electron density around PHO A 417 (A):**

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



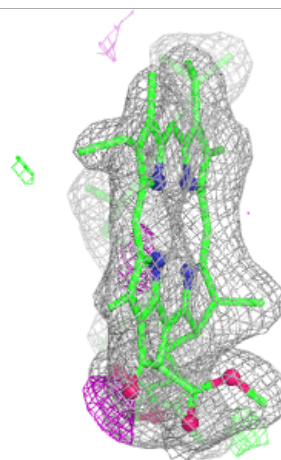
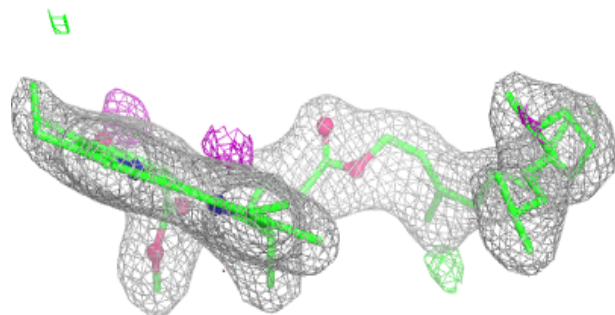
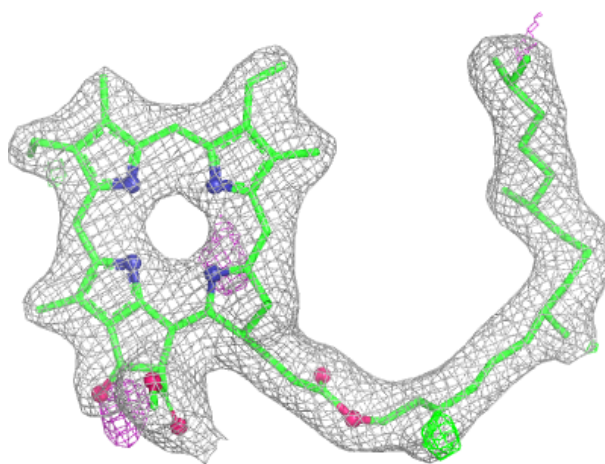
**Electron density around PHO A 417 (B):**

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



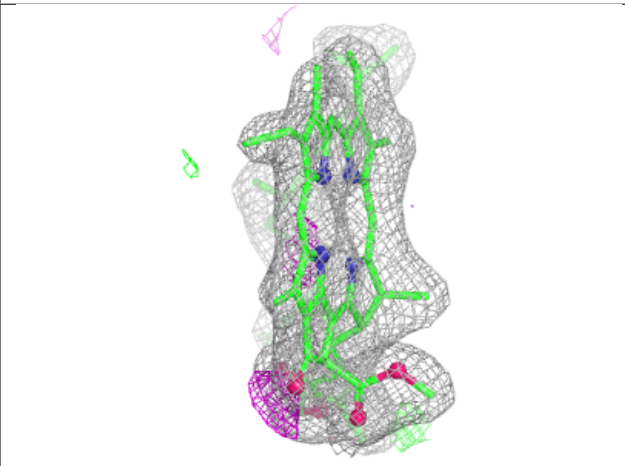
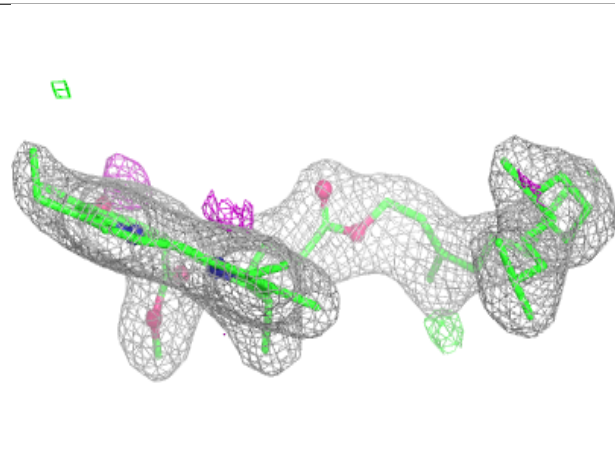
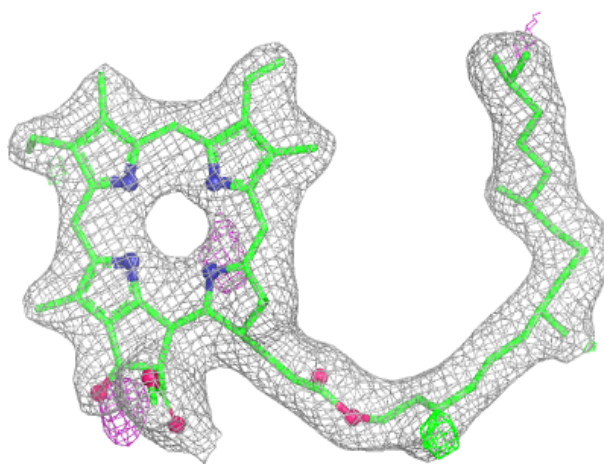
**Electron density around PHO a 408 (A):**

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



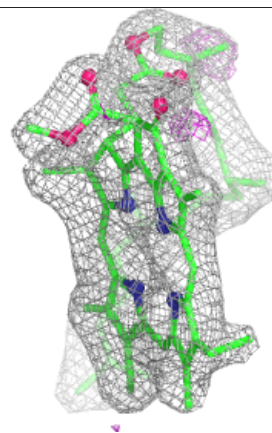
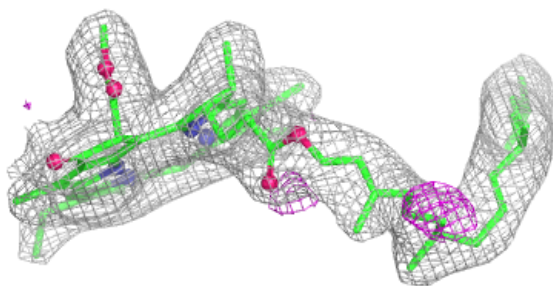
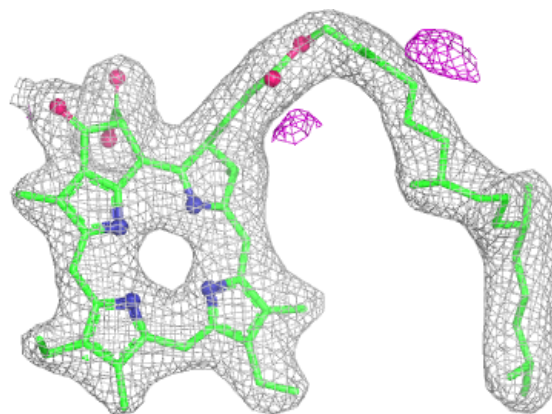
**Electron density around PHO a 408 (B):**

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



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

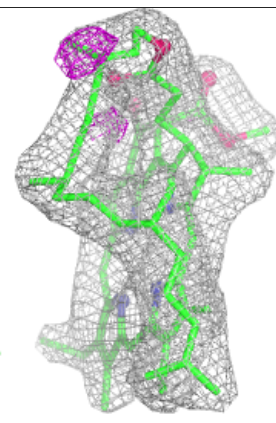
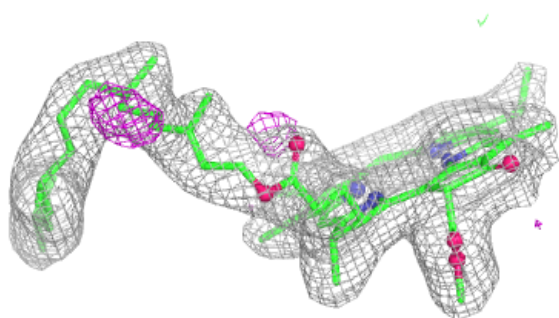
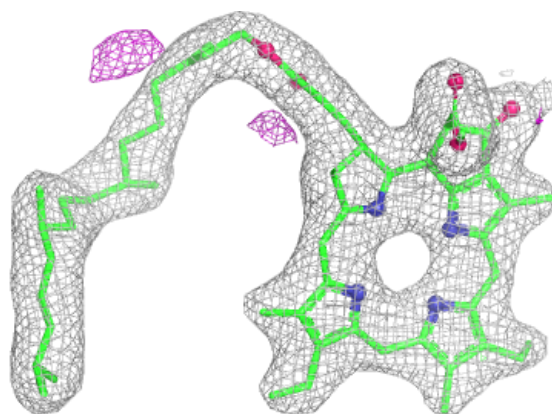
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





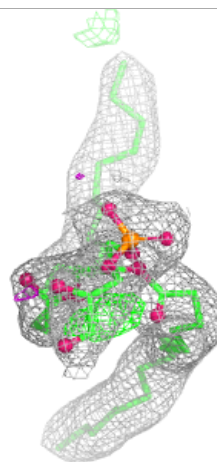
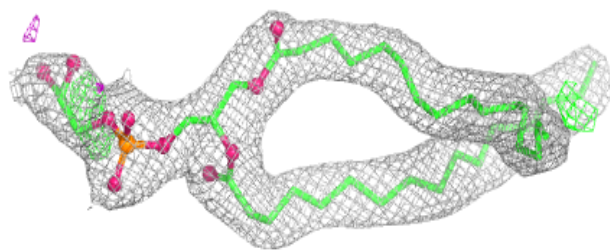
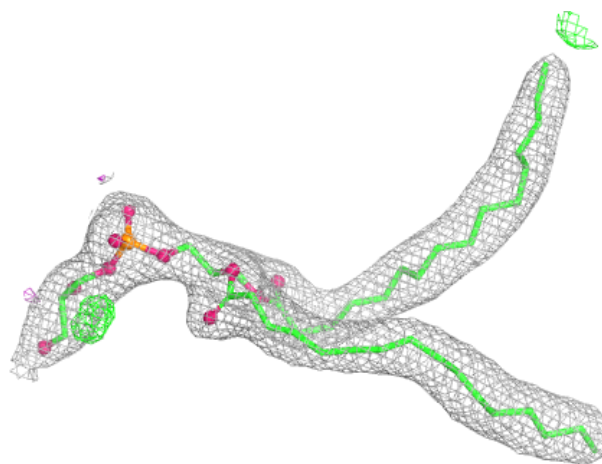
**Electron density around PHO a 416 (B):**

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



**Electron density around LHG D 706 (A):**

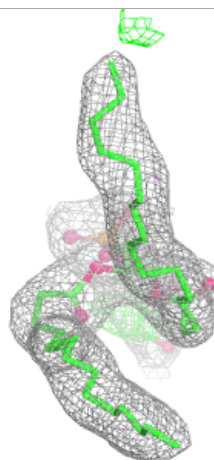
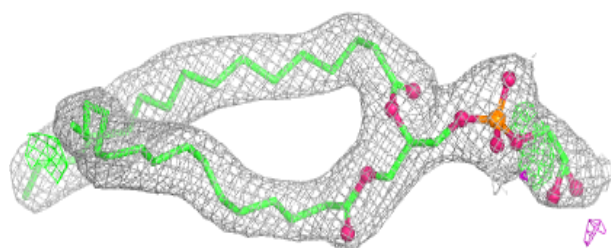
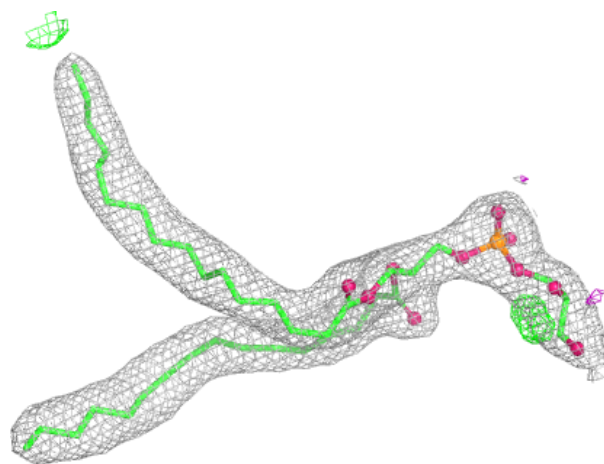
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





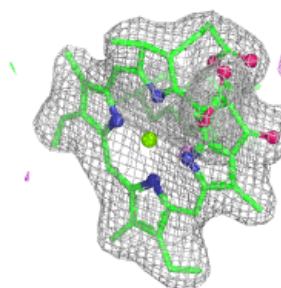
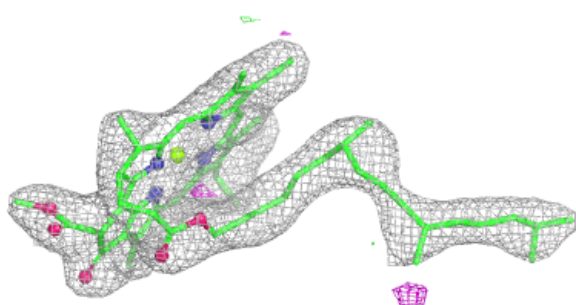
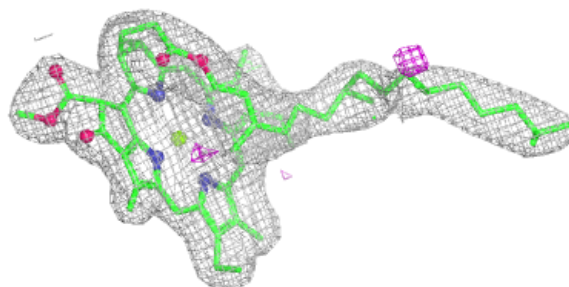
**Electron density around LHG D 706 (B):**

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

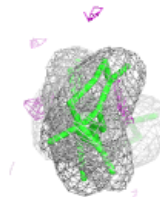
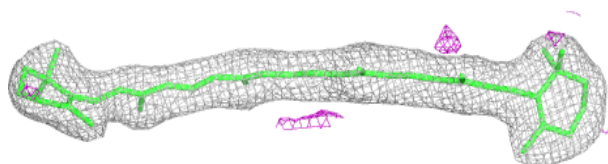
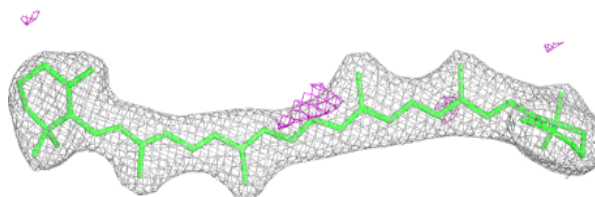


**Electron density around CLA C 506:**

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

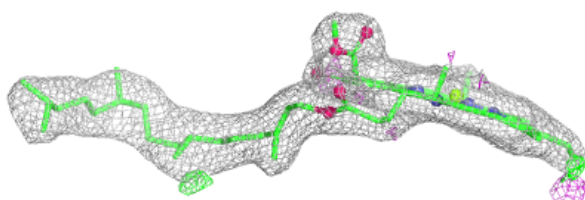
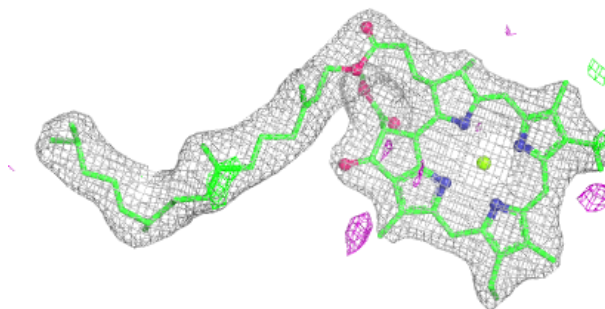
**Electron density around BCR B 617:**

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

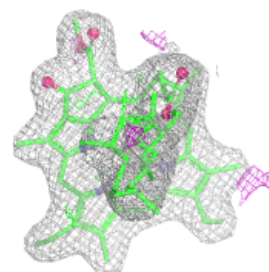
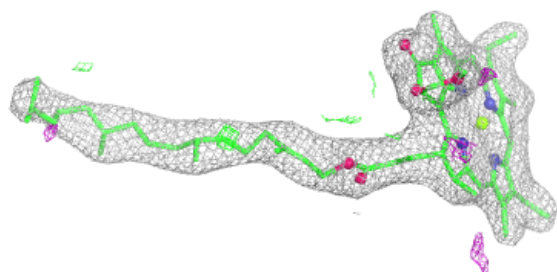
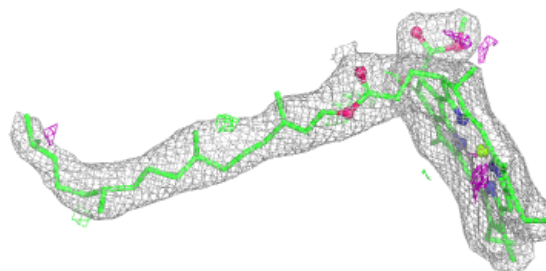


**Electron density around CLA b 602:**

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

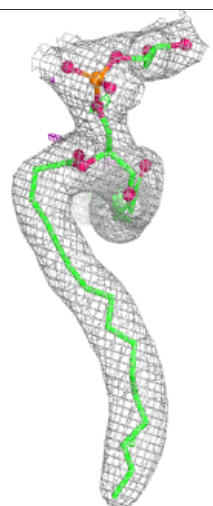
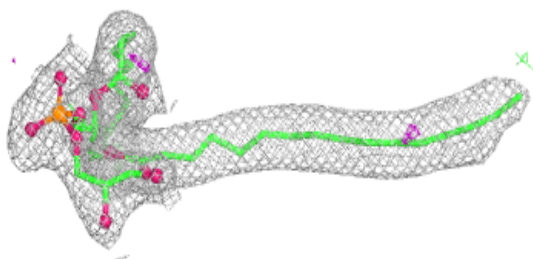
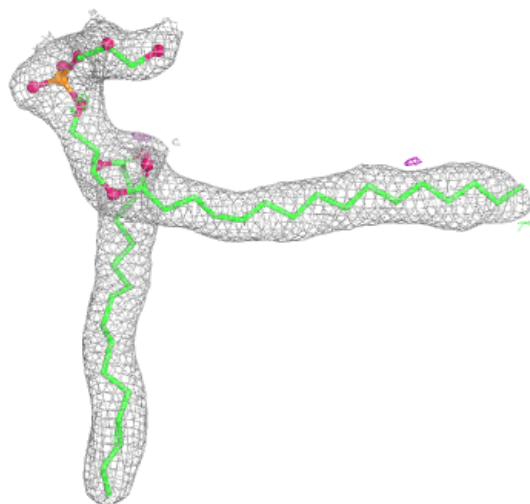
**Electron density around CLA b 604:**

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



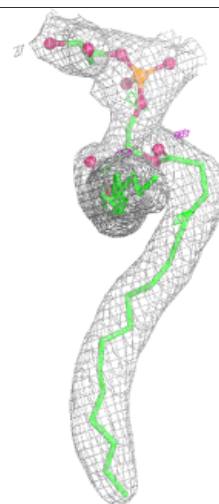
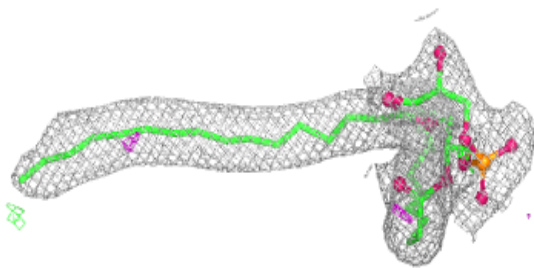
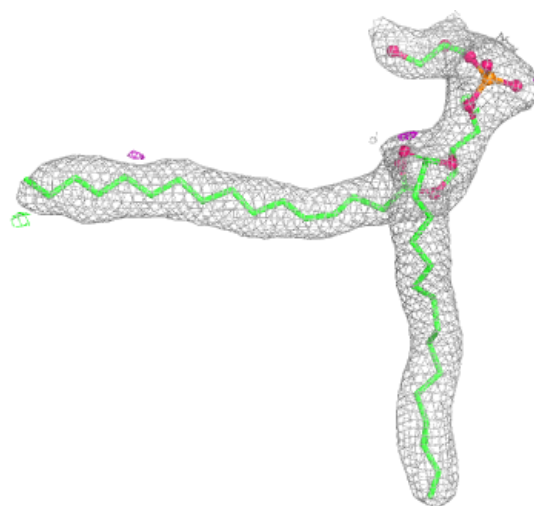
**Electron density around LHG L 101 (A):**

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



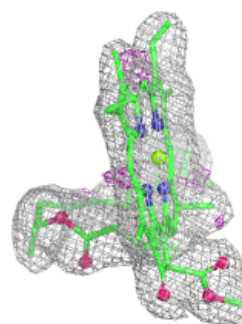
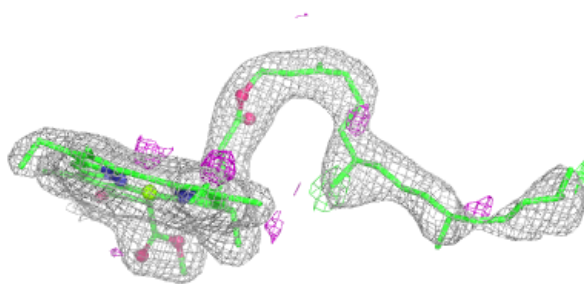
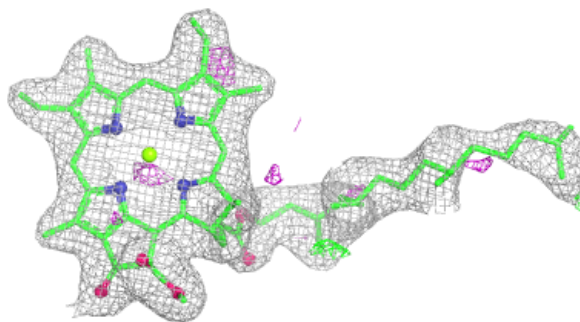
**Electron density around LHG L 101 (B):**

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

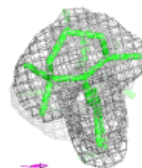
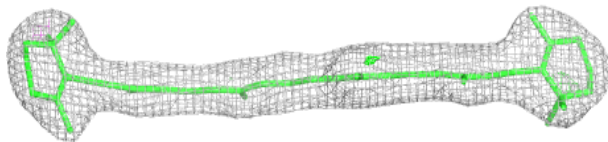
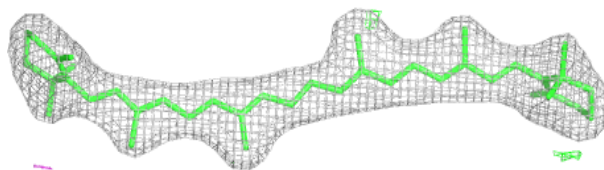


**Electron density around CLA A 406 (B):**

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

**Electron density around BCR C 516:**

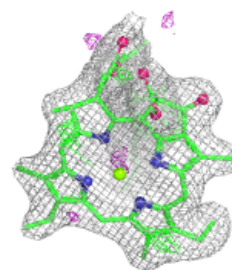
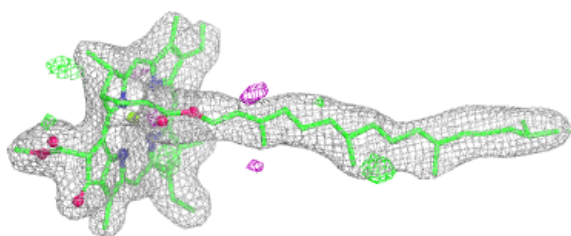
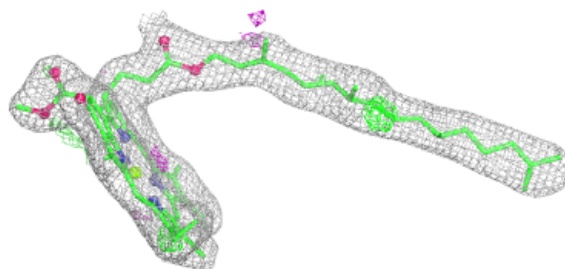
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



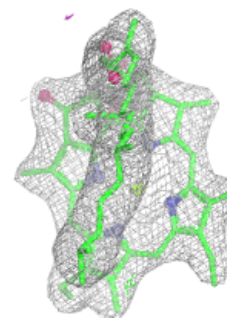
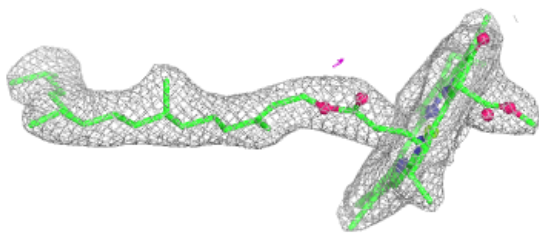
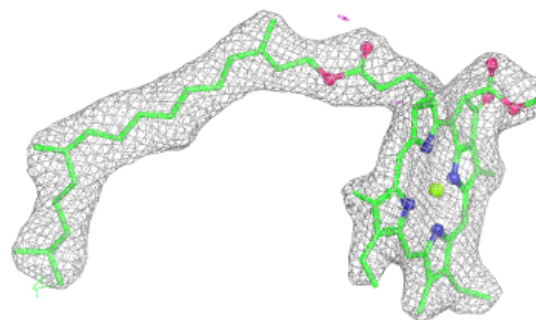


**Electron density around CLA b 607:**

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

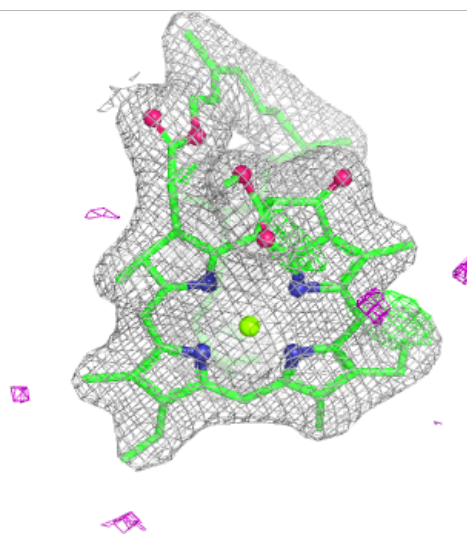
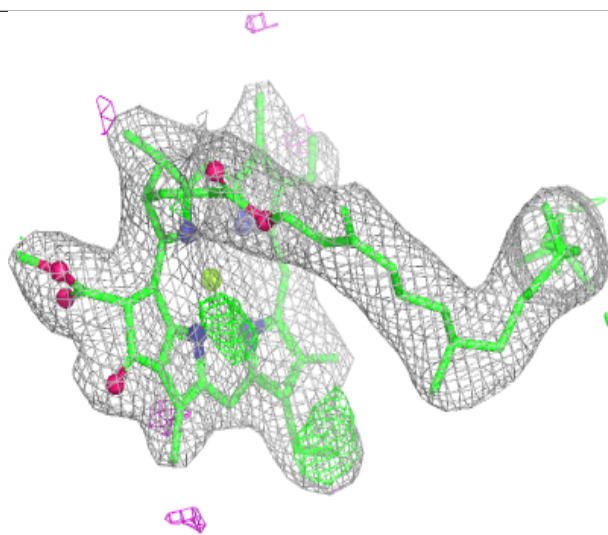
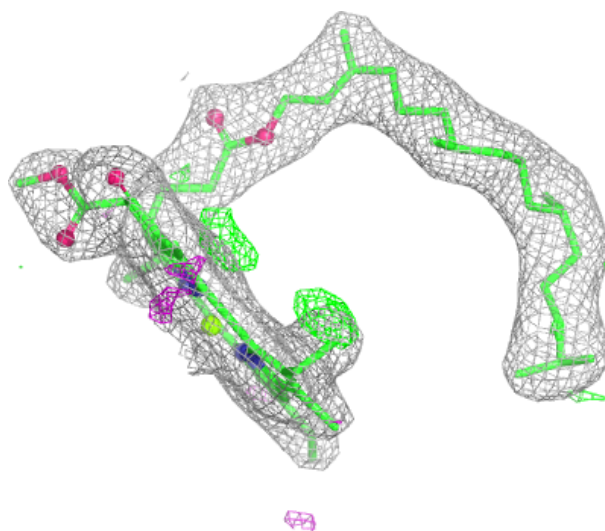
**Electron density around CLA b 609:**

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



**Electron density around CLA b 611:**

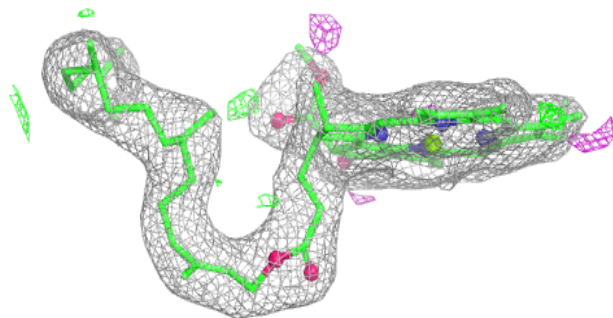
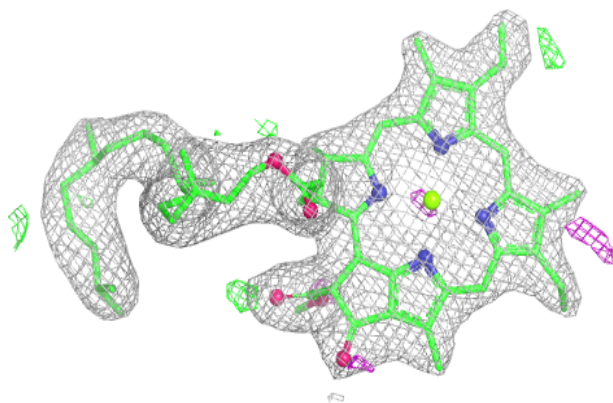
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



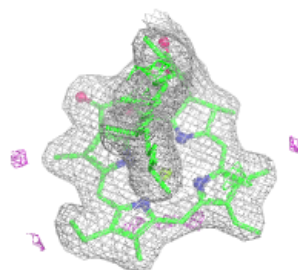
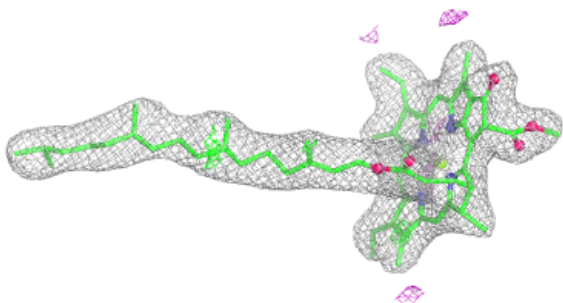
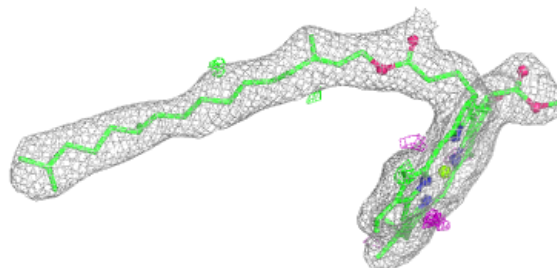


**Electron density around CLA b 612:**

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

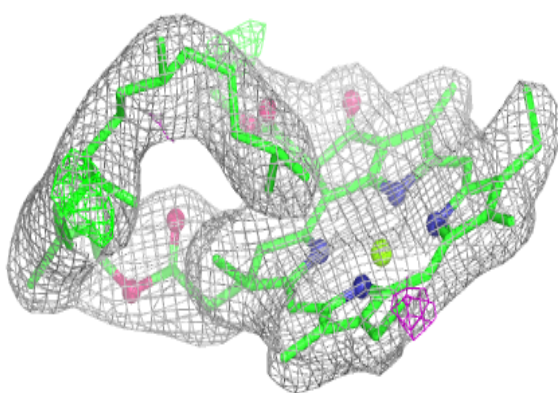
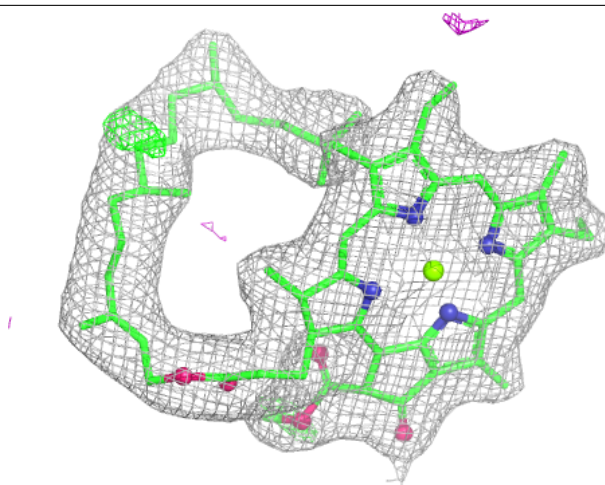
**Electron density around CLA B 607:**

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



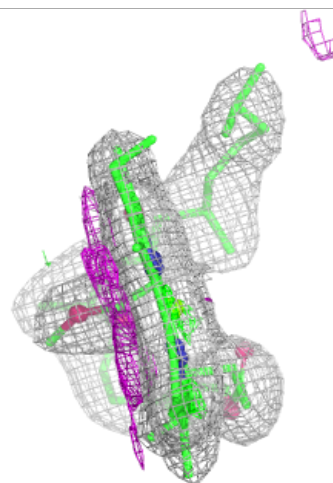
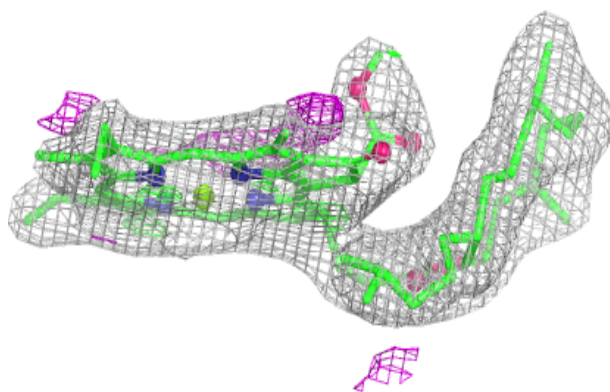
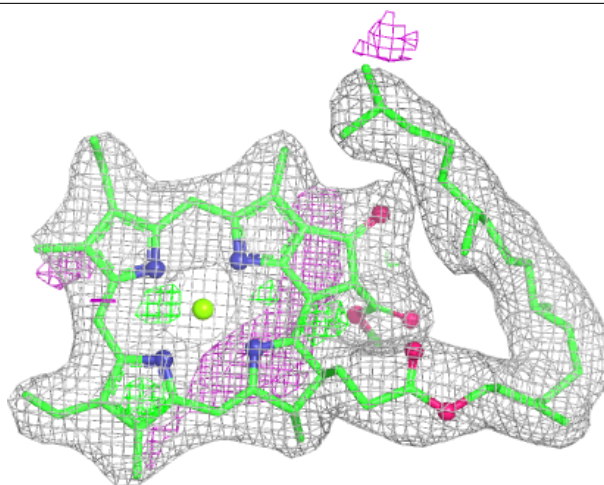
**Electron density around CLA b 615:**

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



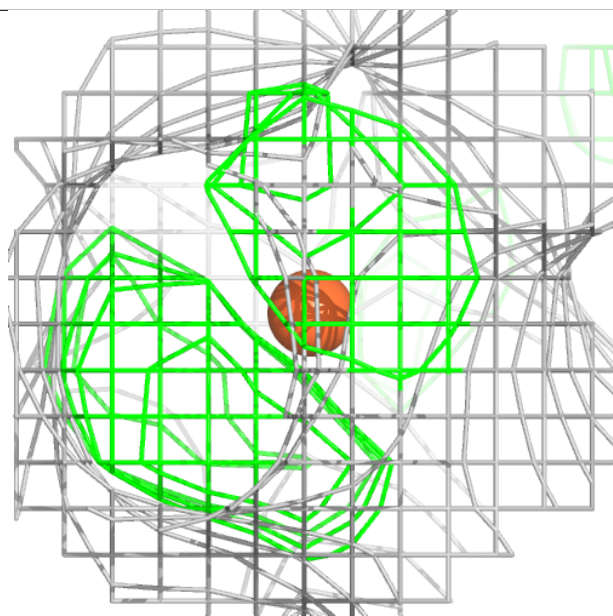
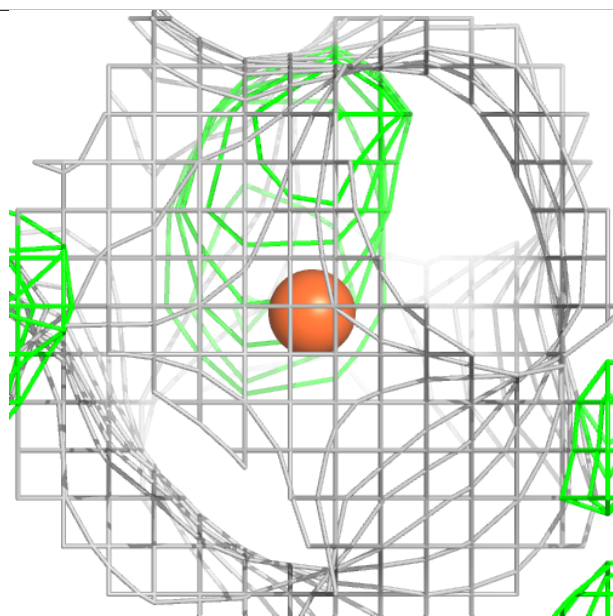
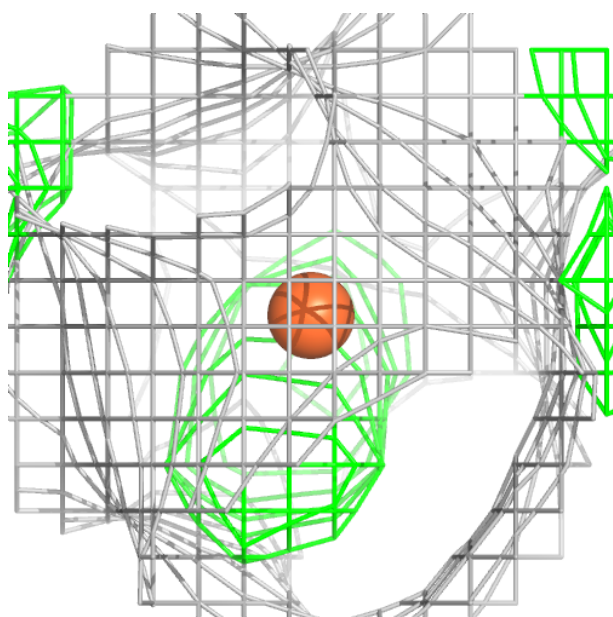
**Electron density around CLA B 610:**

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



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

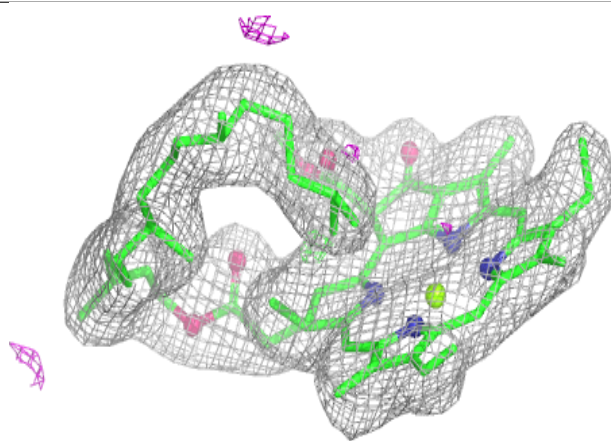
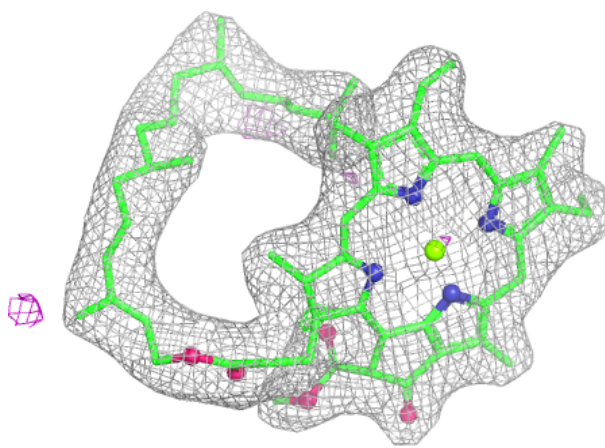
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





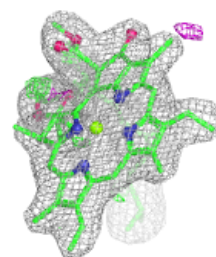
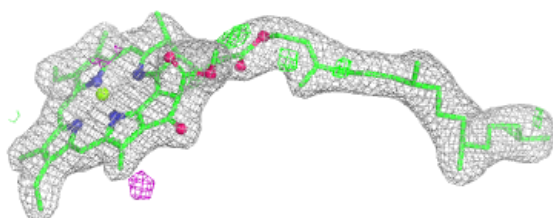
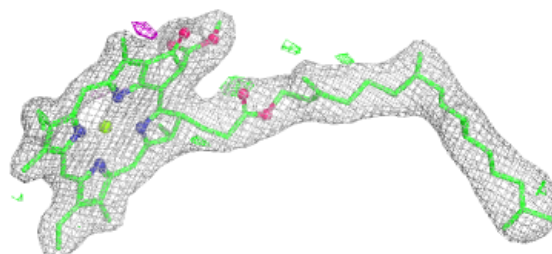
**Electron density around CLA B 615:**

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

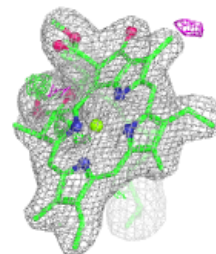
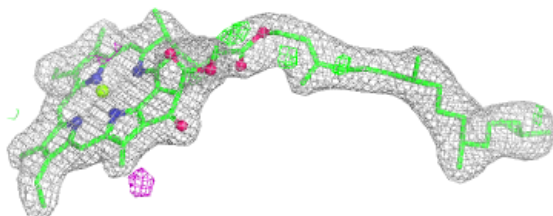
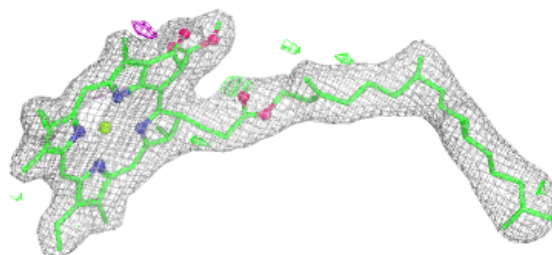


**Electron density around CLA a 405 (A):**

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

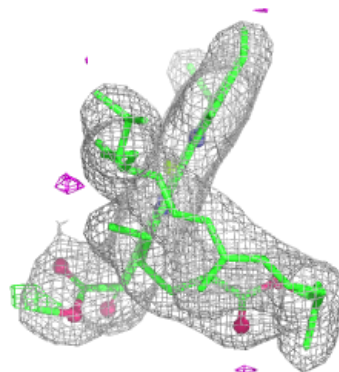
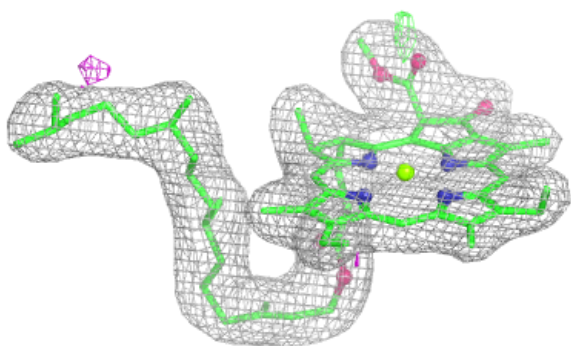
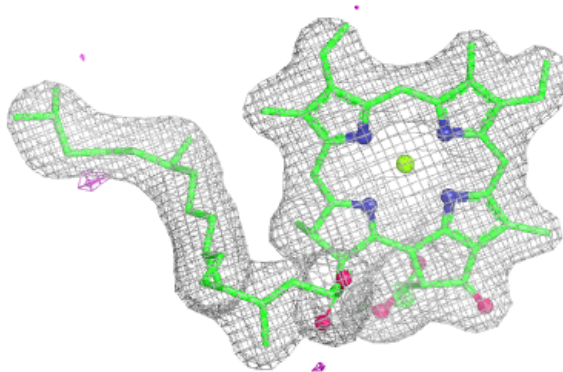
**Electron density around CLA a 405 (B):**

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

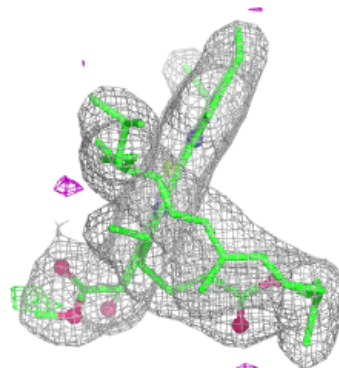
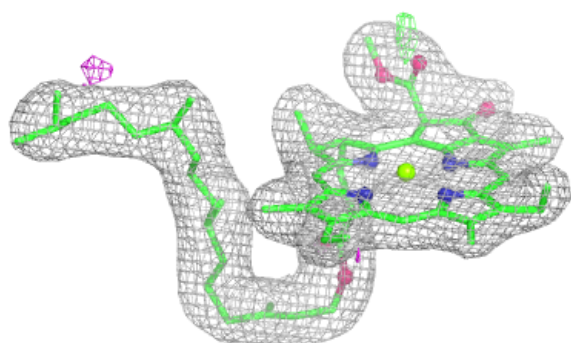
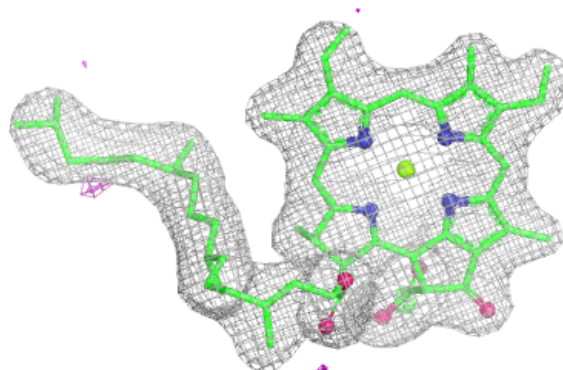


**Electron density around CLA a 406 (A):**

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

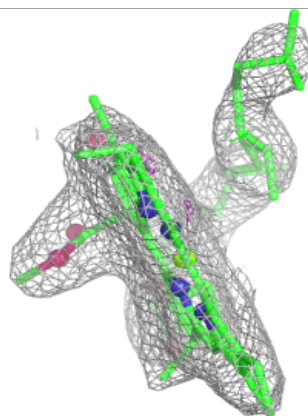
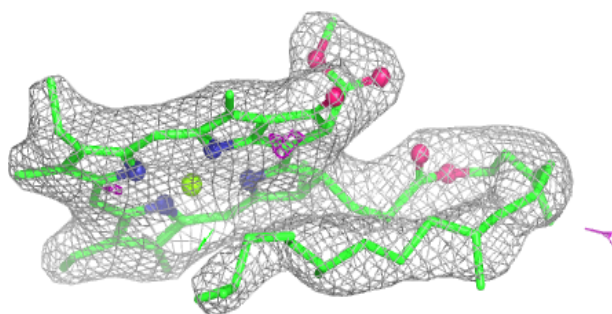
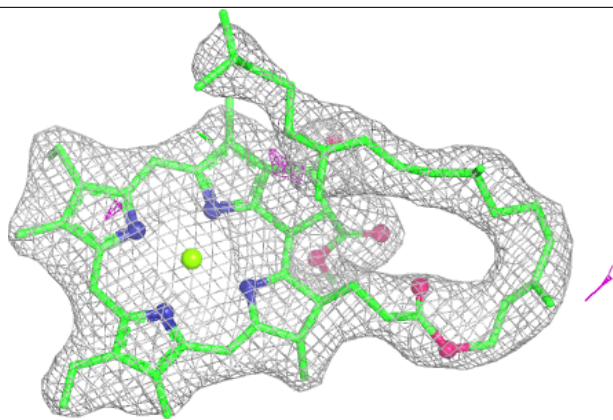
**Electron density around CLA a 406 (B):**

$2mF_o-DF_c$  (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:**

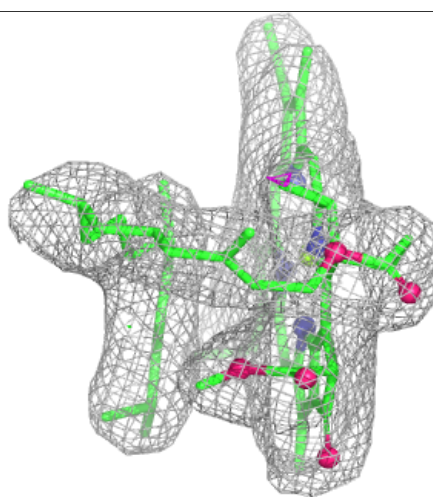
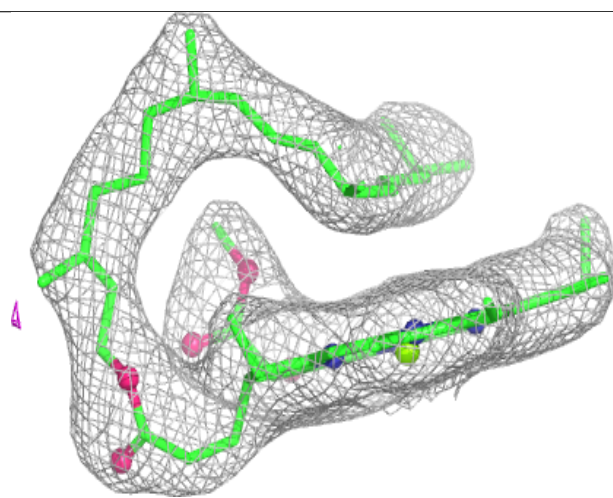
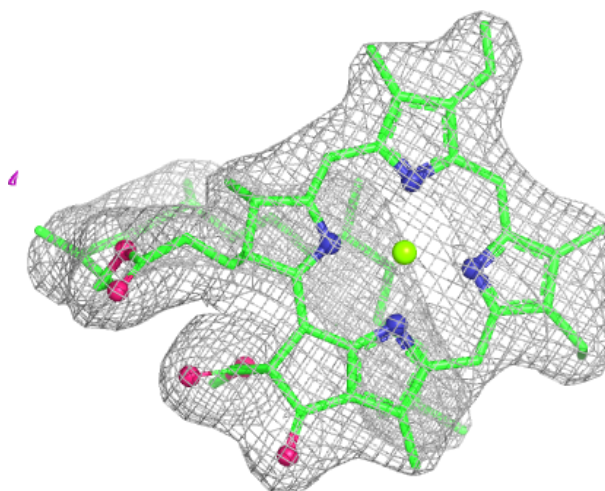
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





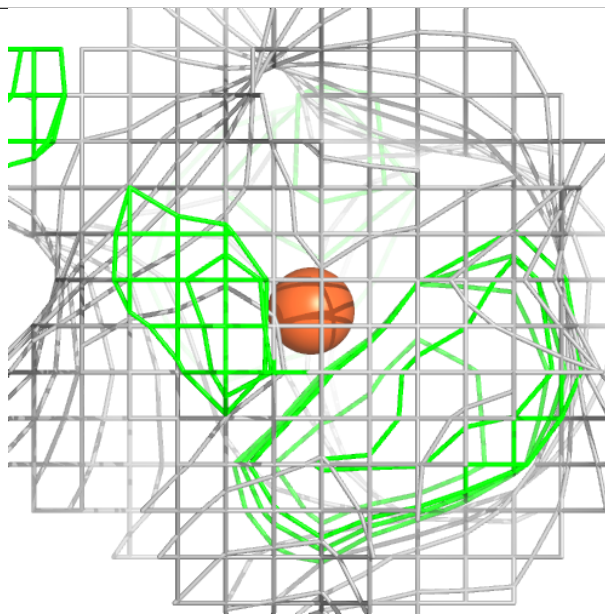
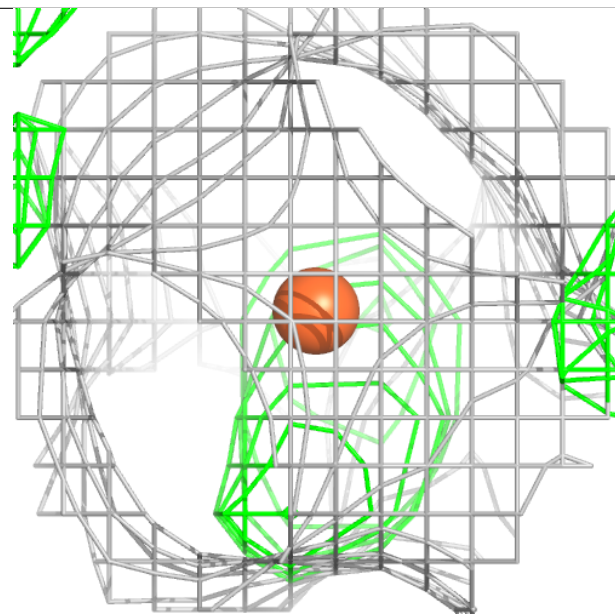
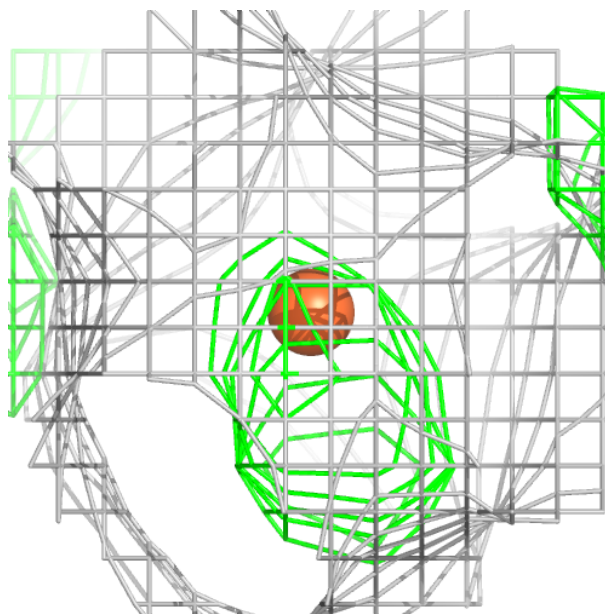
**Electron density around CLA c 511:**

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



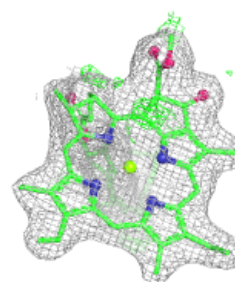
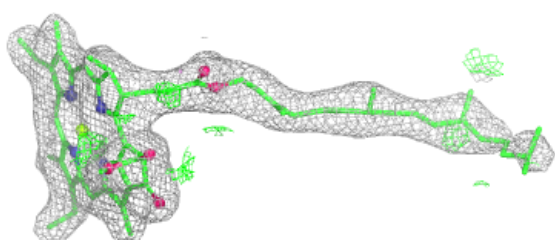
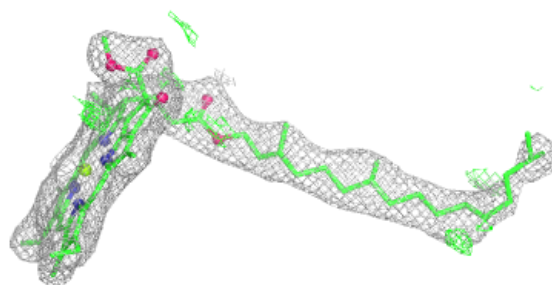
**Electron density around FE2 a 401 (B):**

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

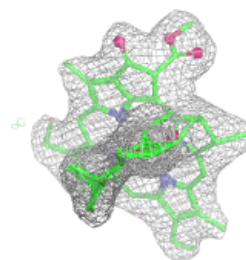
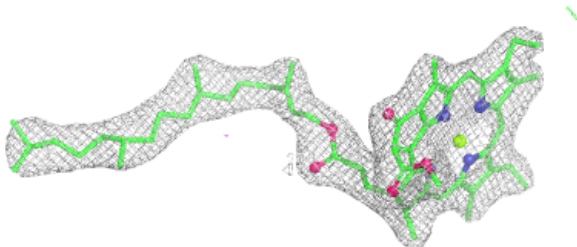
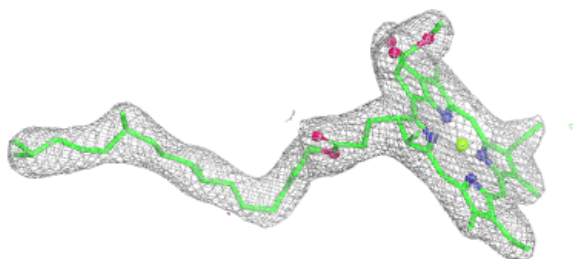


**Electron density around CLA B 604:**

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

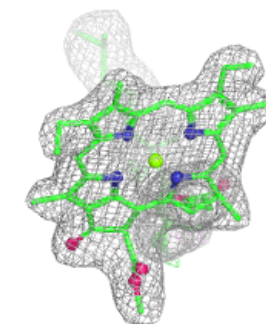
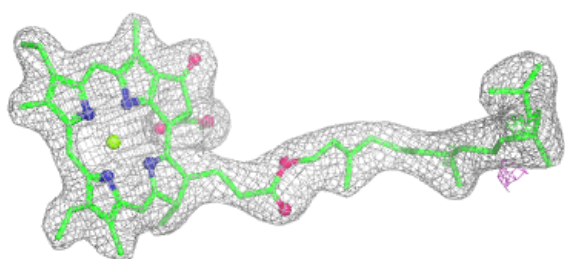
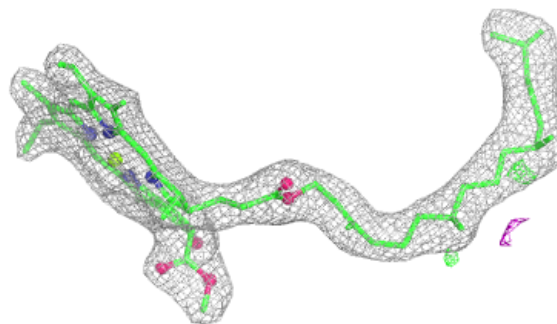
**Electron density around CLA C 503:**

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

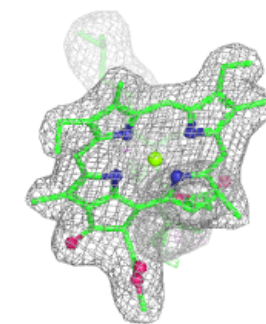
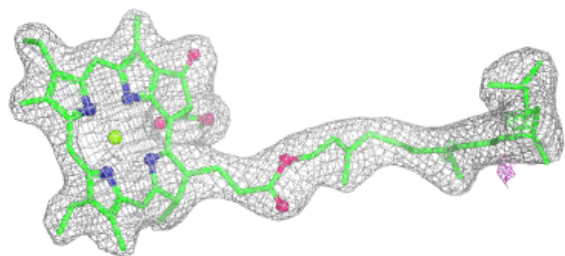
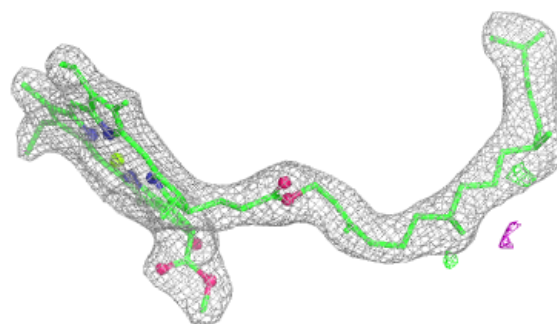


**Electron density around CLA d 401 (A):**

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

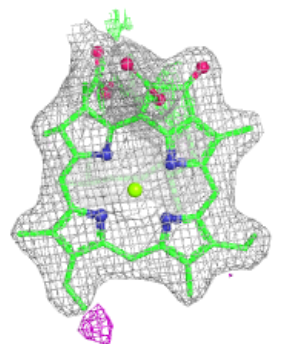
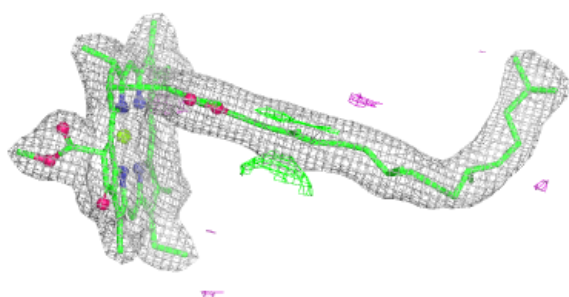
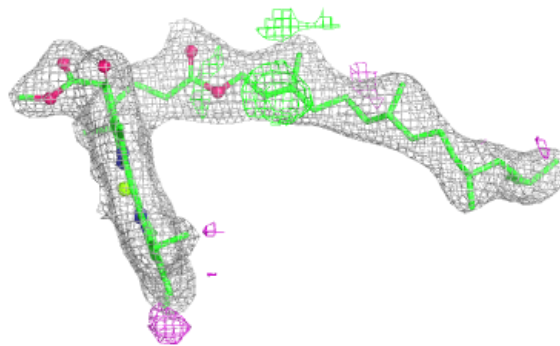
**Electron density around CLA d 401 (B):**

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



**Electron density around CLA B 605:**

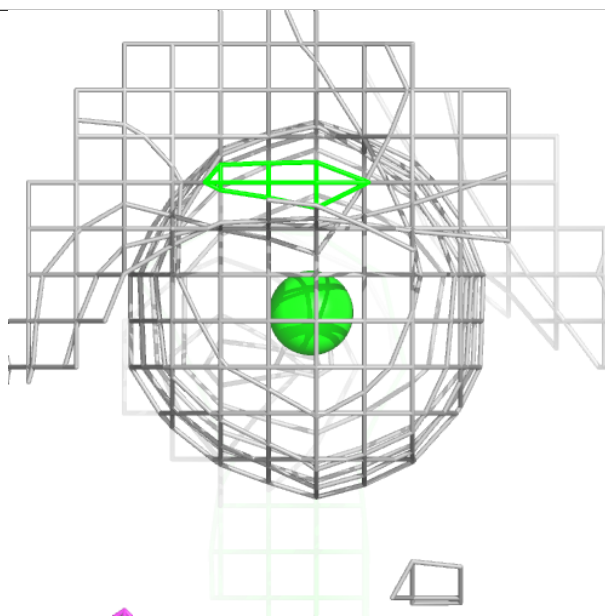
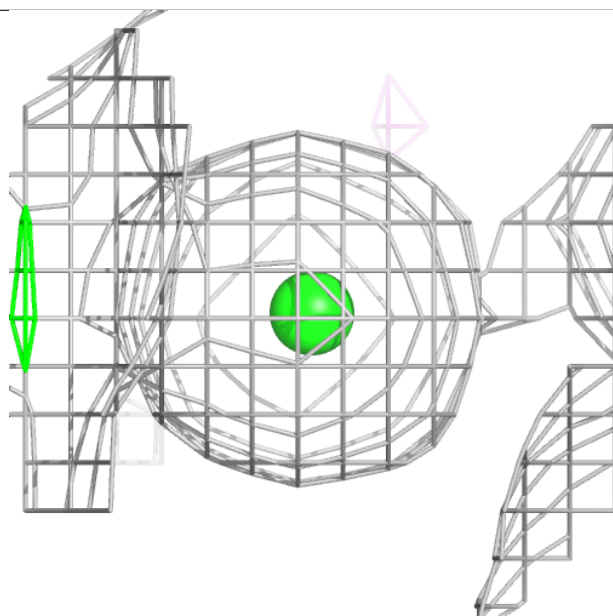
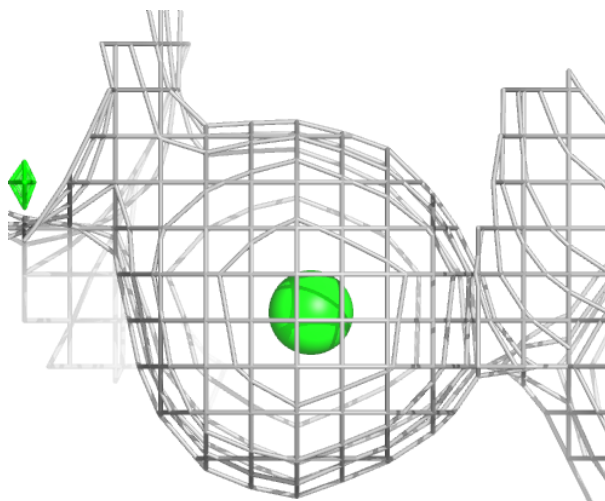
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





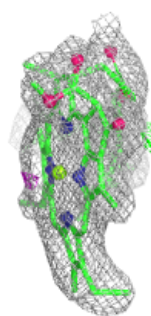
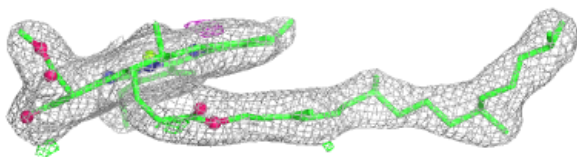
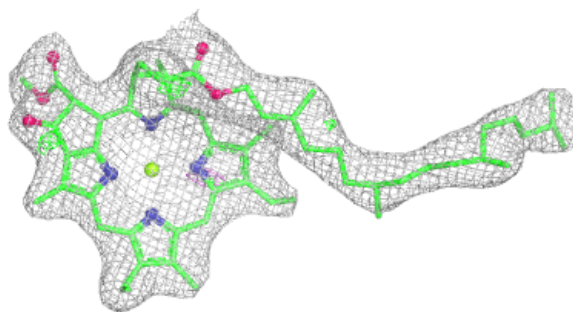
**Electron density around CL A 403 (A):**

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



**Electron density around CLA b 603:**

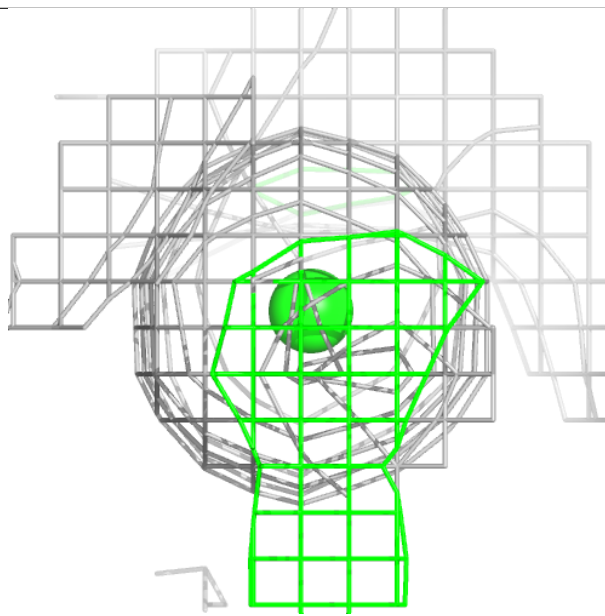
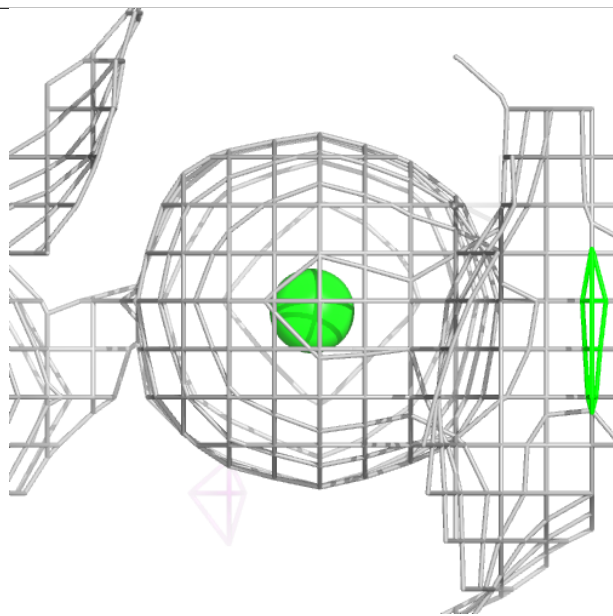
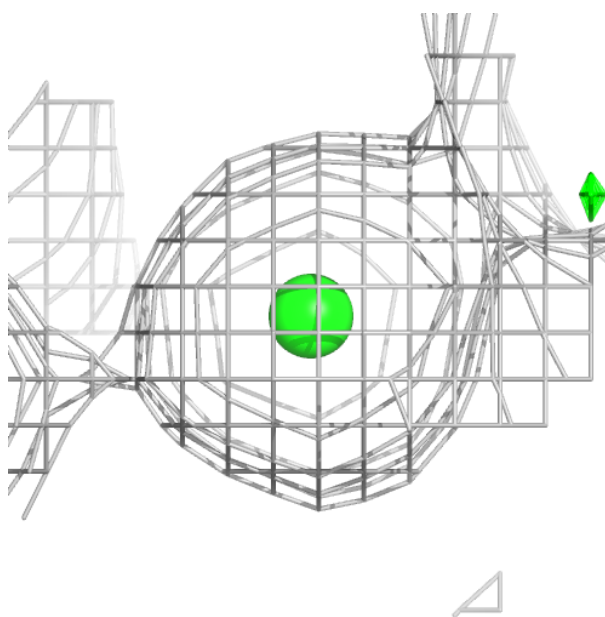
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





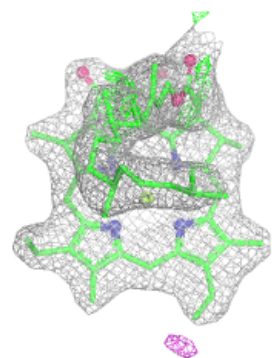
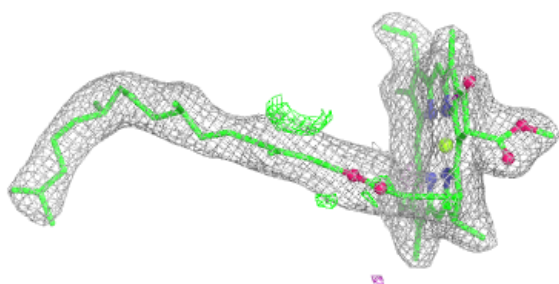
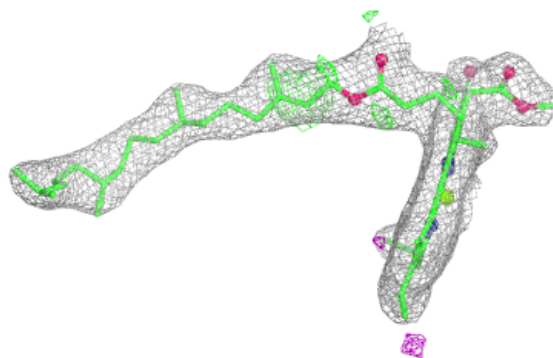
**Electron density around CL A 403 (B):**

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

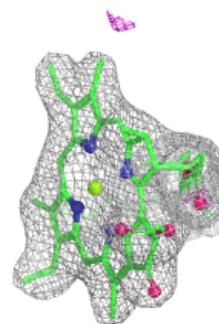
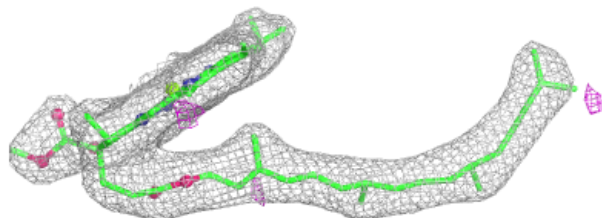
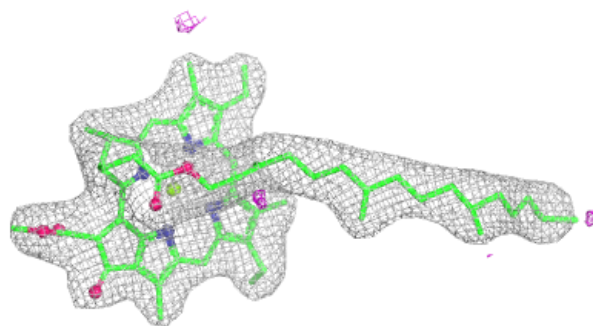


**Electron density around CLA b 605:**

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

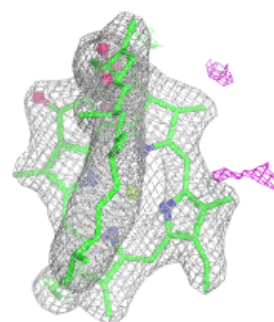
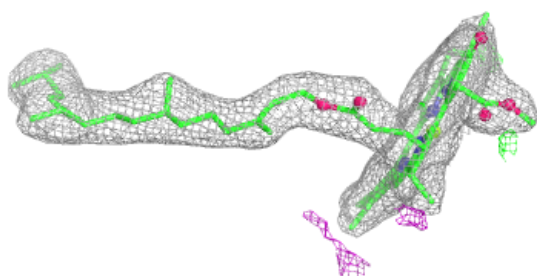
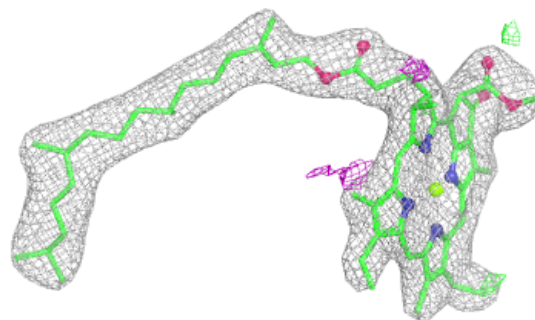
**Electron density around CLA B 608:**

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

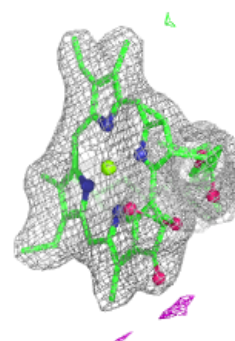
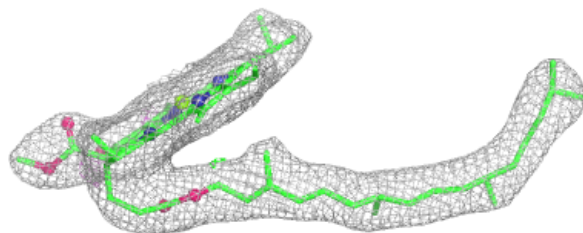
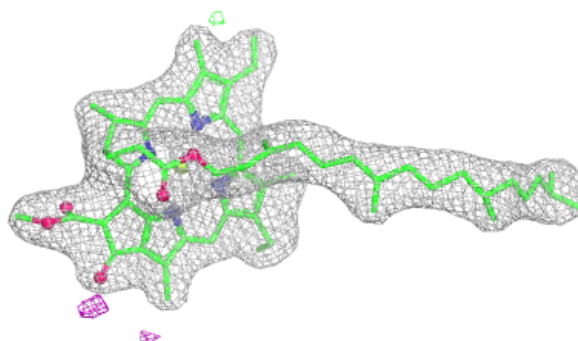


**Electron density around CLA B 609:**

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

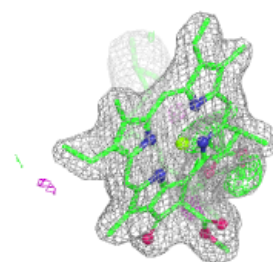
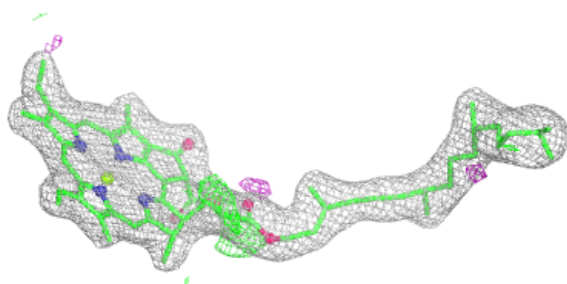
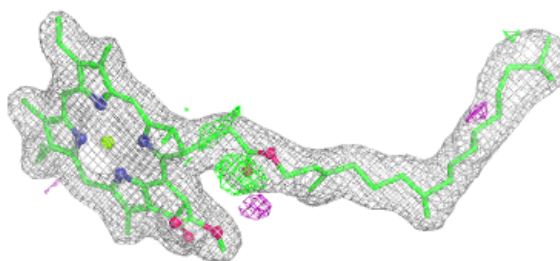
**Electron density around CLA b 608:**

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

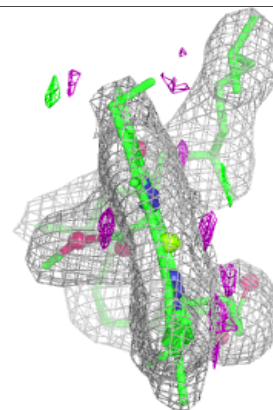
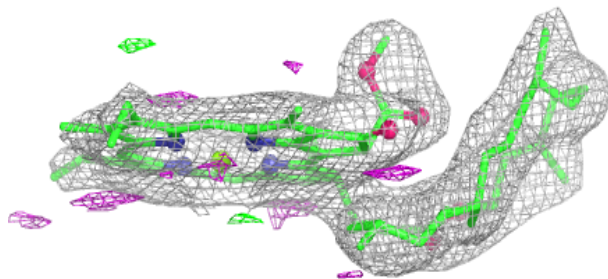
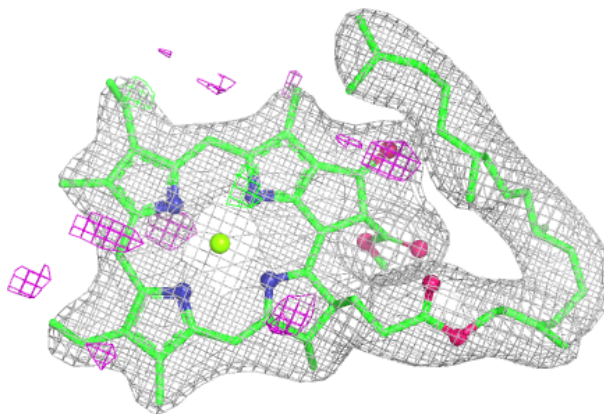


**Electron density around CLA A 404 (A):**

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

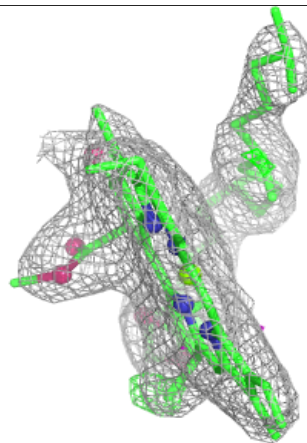
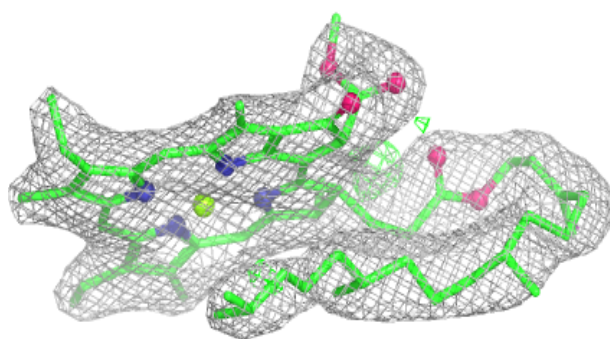
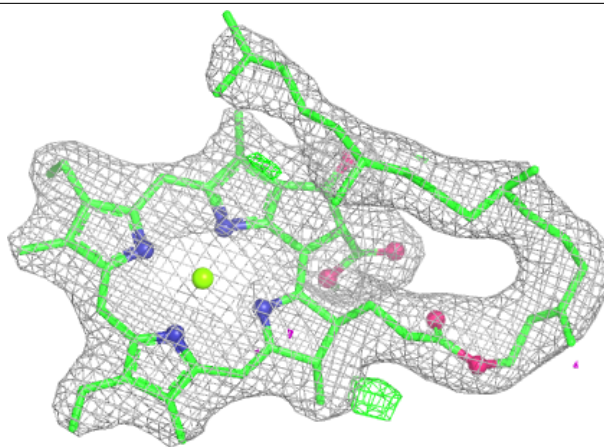
**Electron density around CLA b 610:**

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



**Electron density around CLA C 510:**

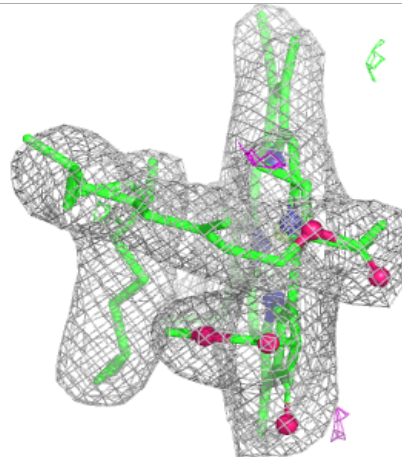
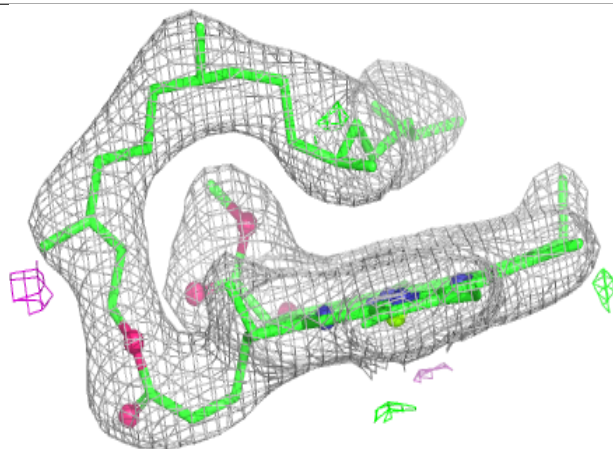
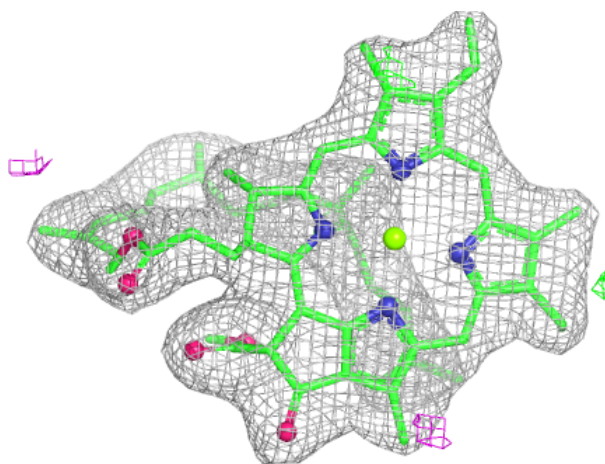
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





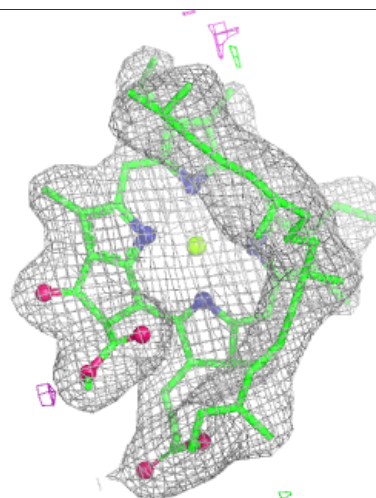
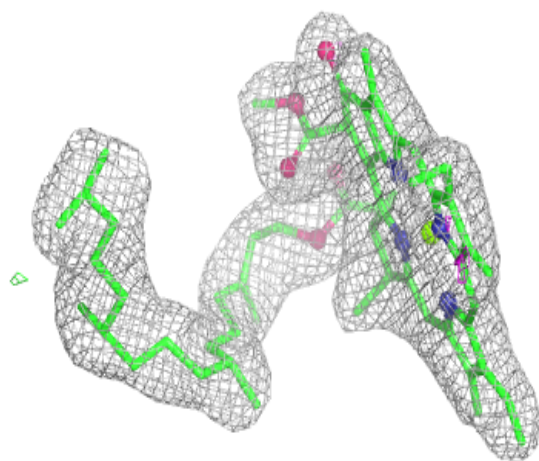
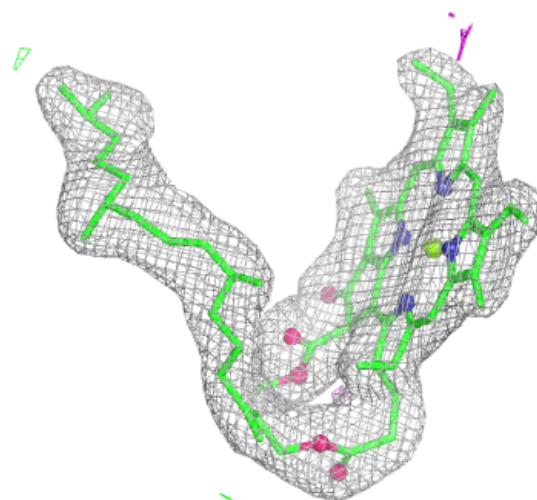
**Electron density around CLA C 511:**

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



**Electron density around CLA b 613:**

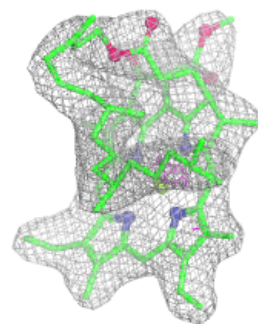
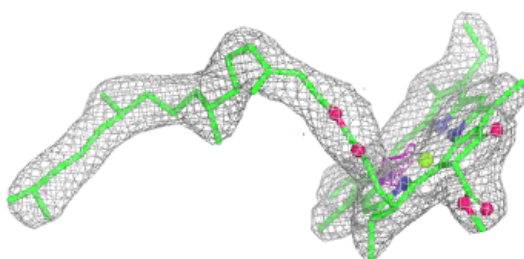
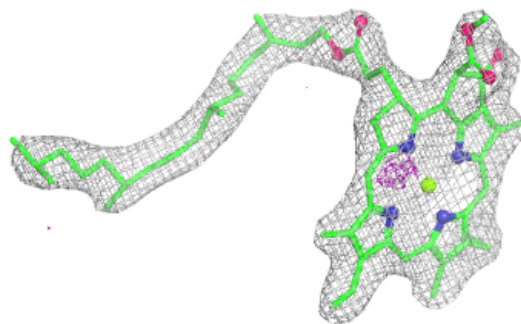
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



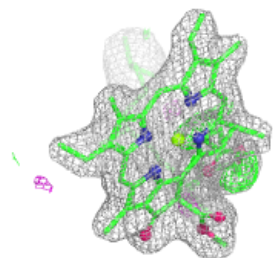
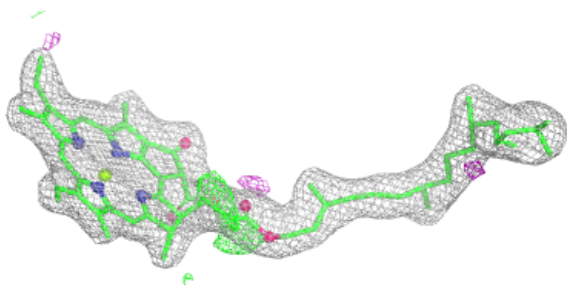
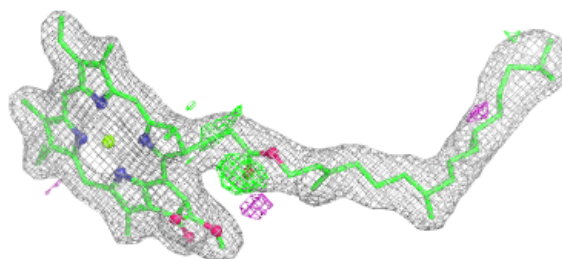


**Electron density around CLA C 512:**

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

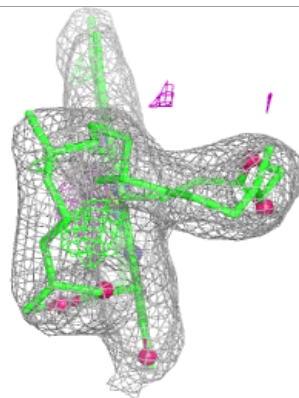
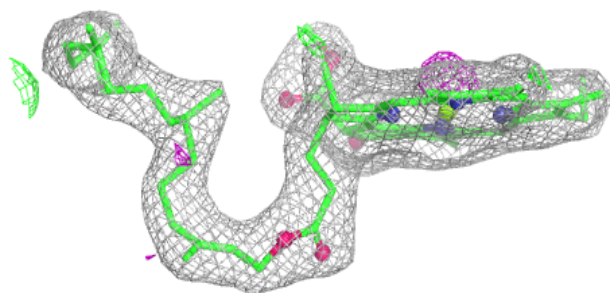
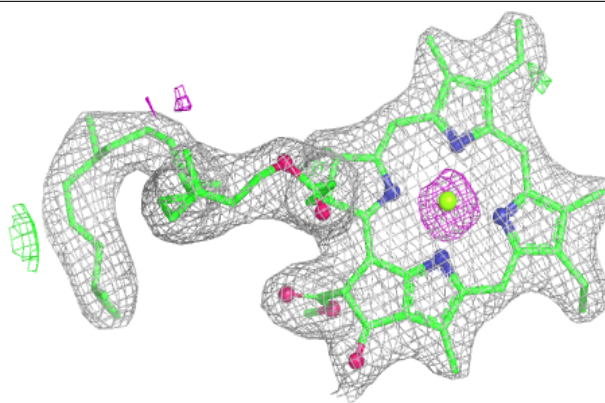
**Electron density around CLA A 404 (B):**

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

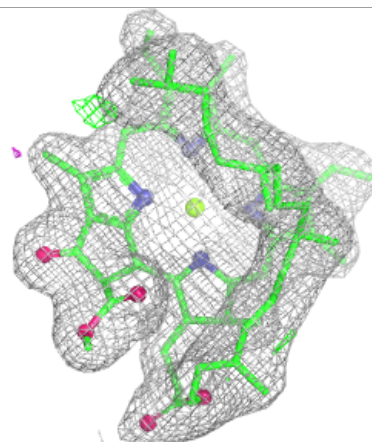
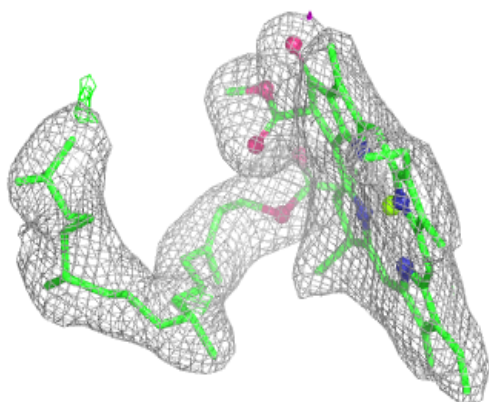
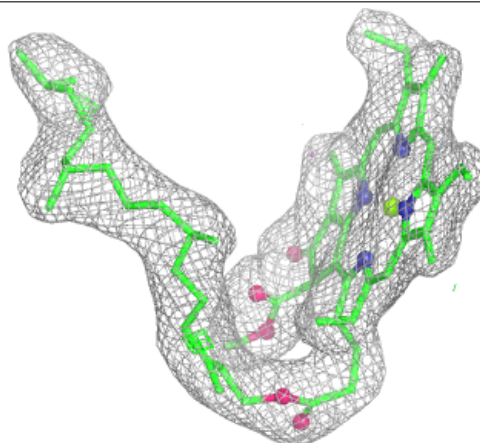


**Electron density around CLA B 612:**

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

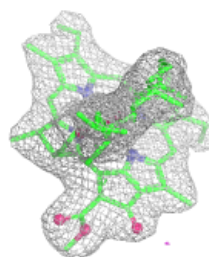
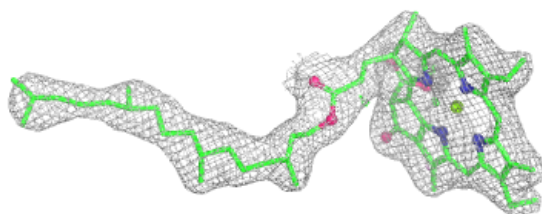
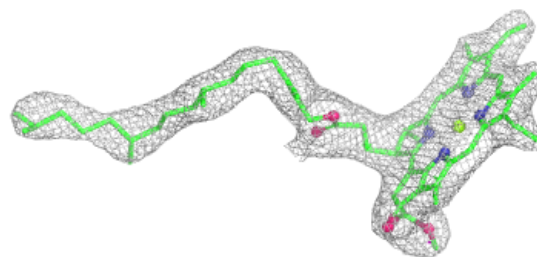
**Electron density around CLA B 613:**

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



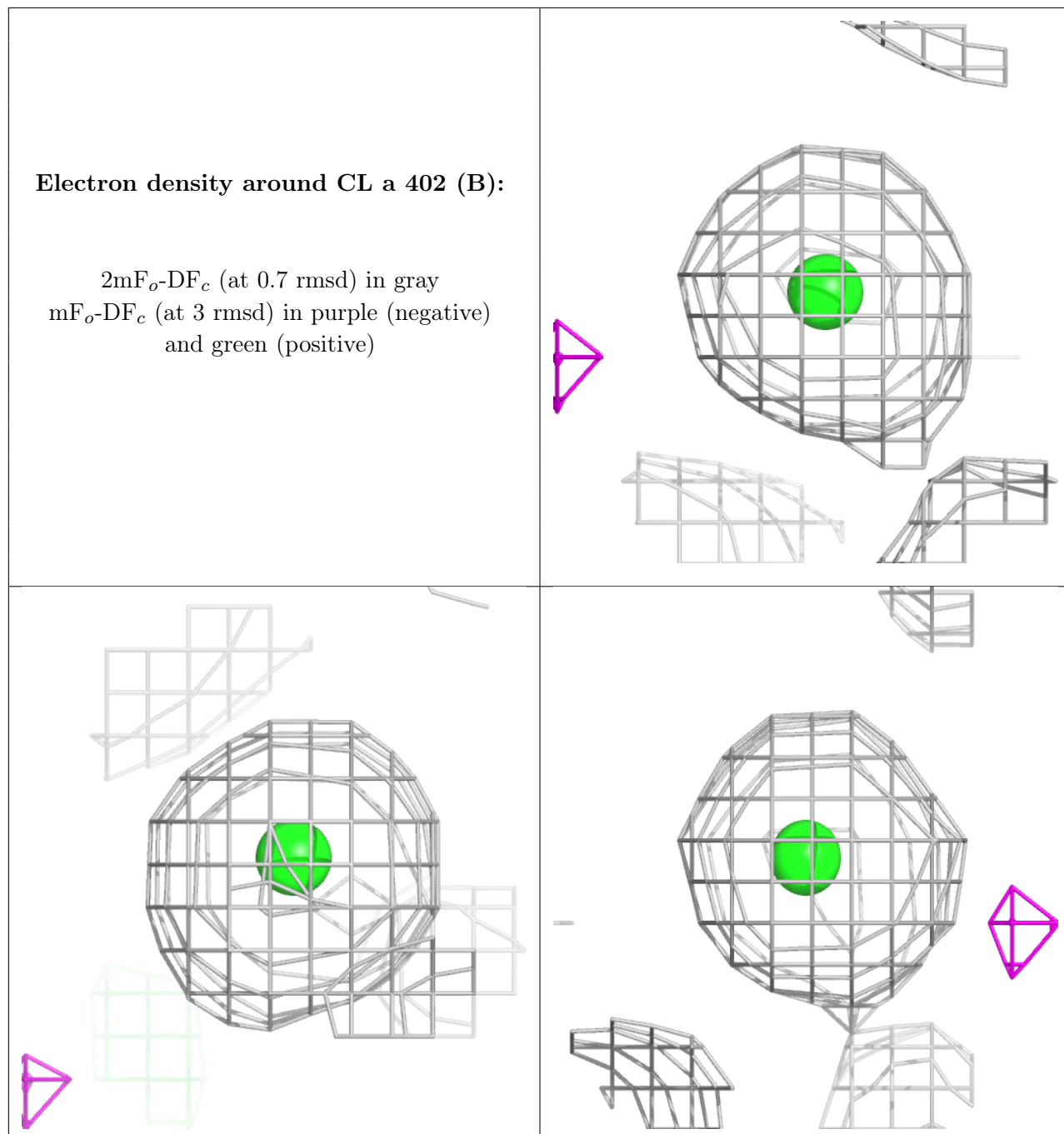
**Electron density around CLA c 503:**

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



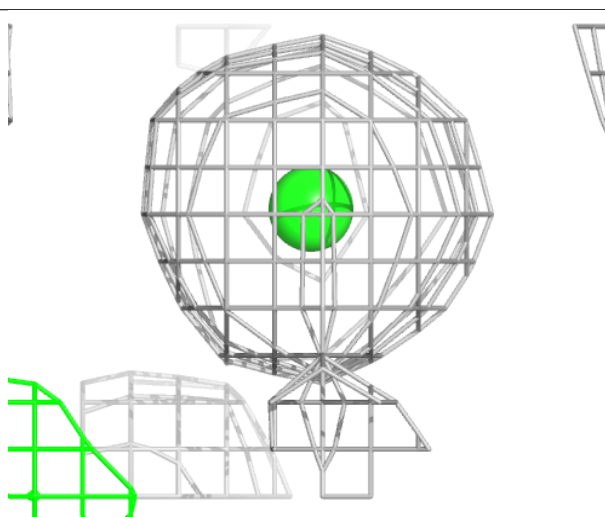
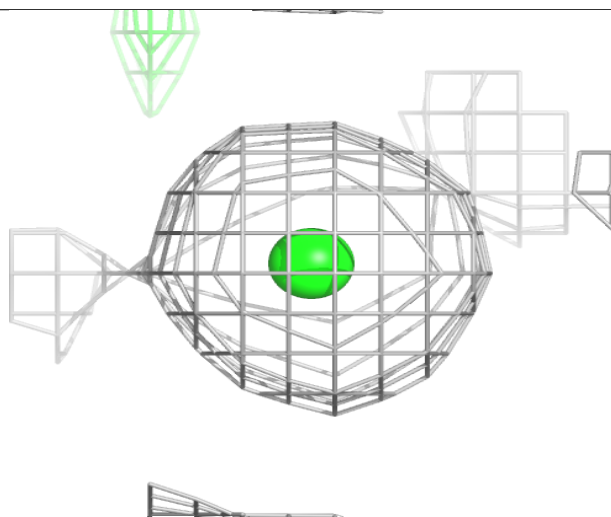
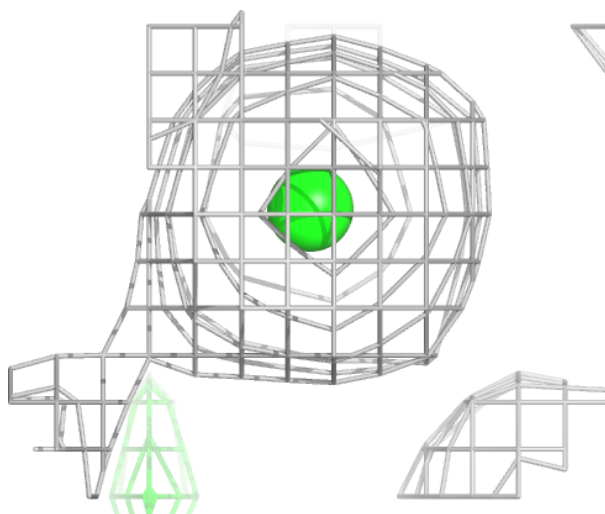
**Electron density around CL a 402 (B):**

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



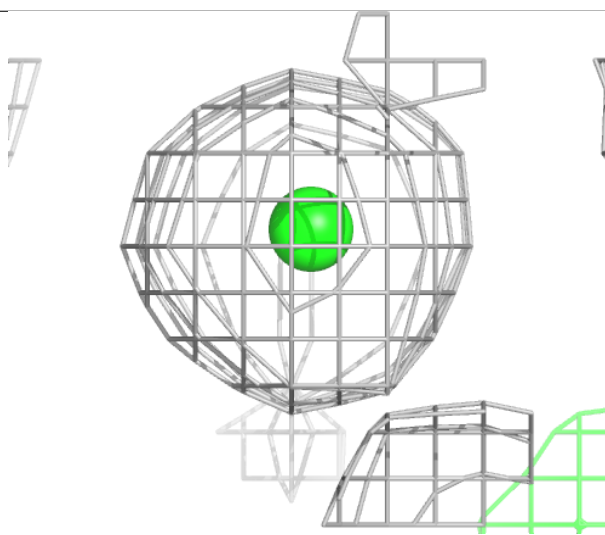
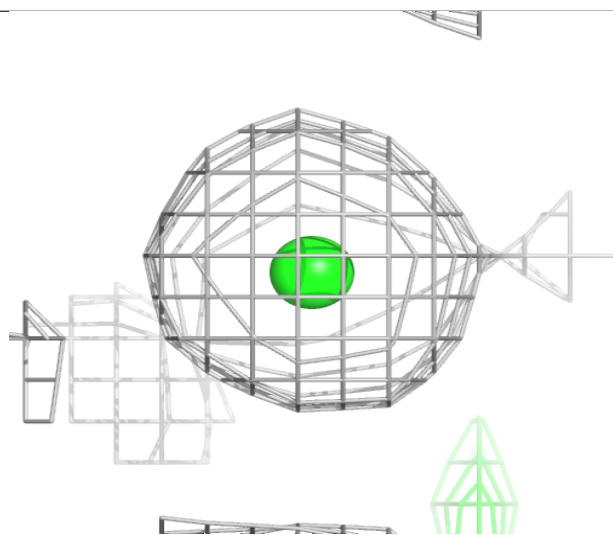
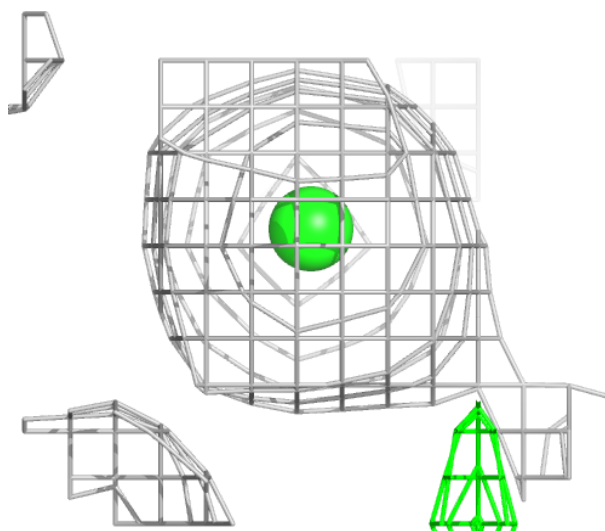
**Electron density around CL A 402 (A):**

$2mF_o-DF_c$  (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):**

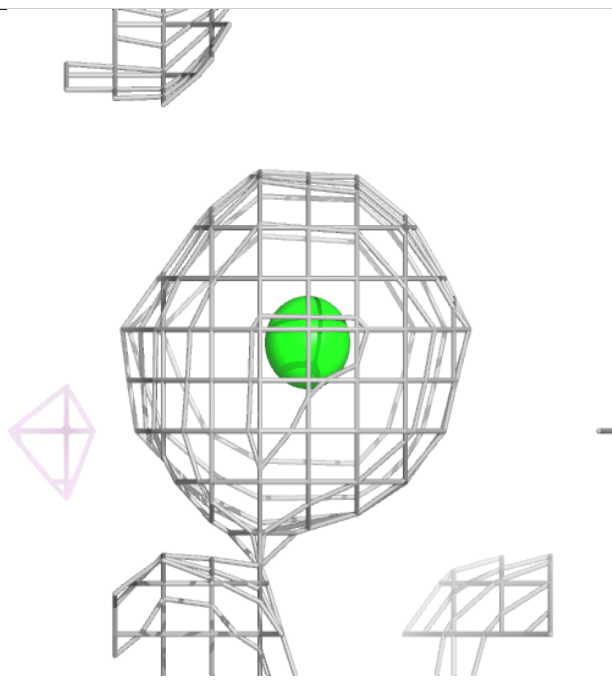
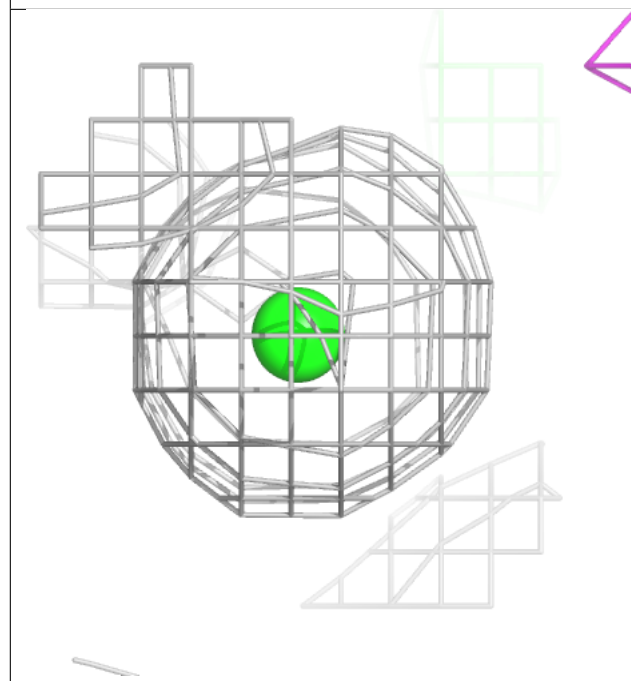
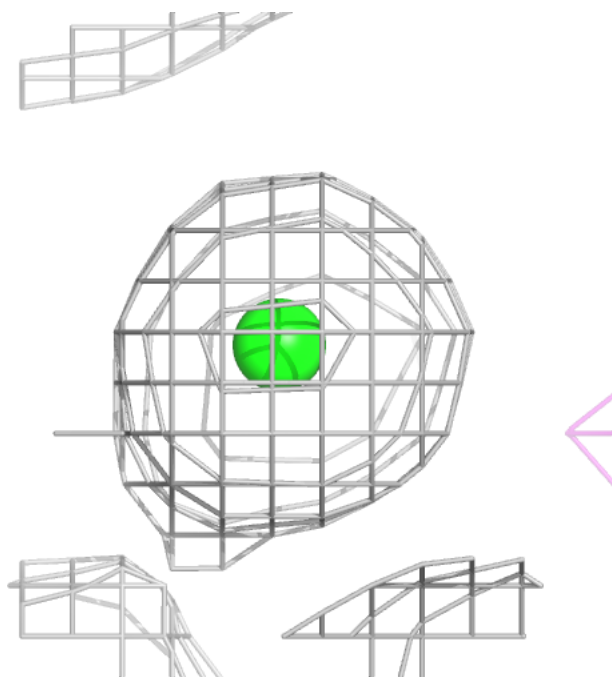
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





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

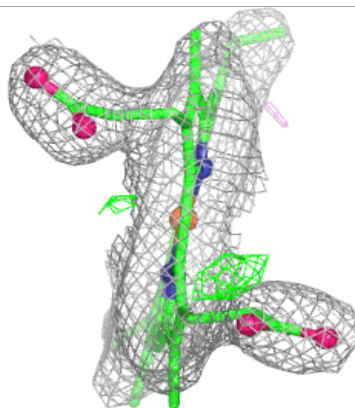
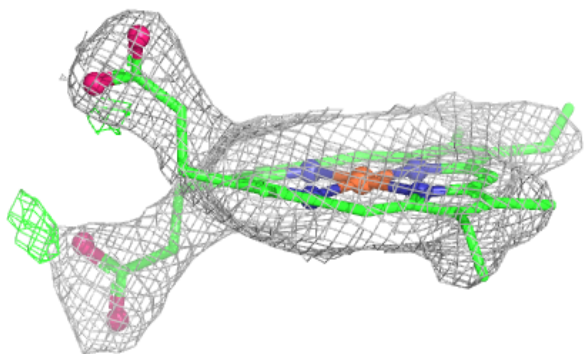
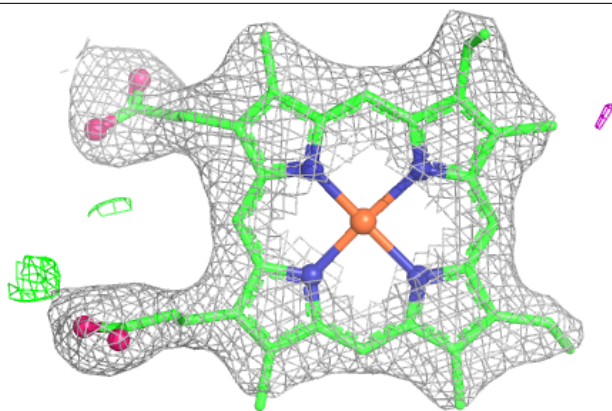
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





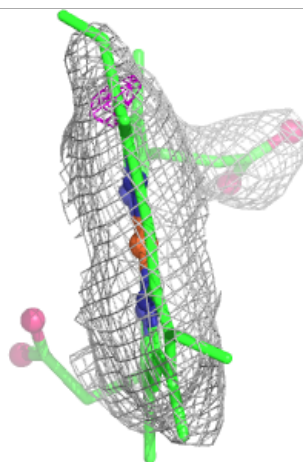
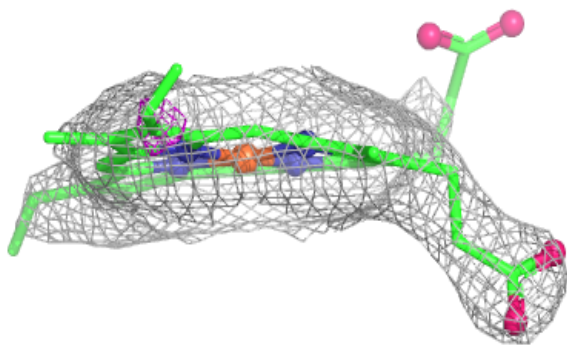
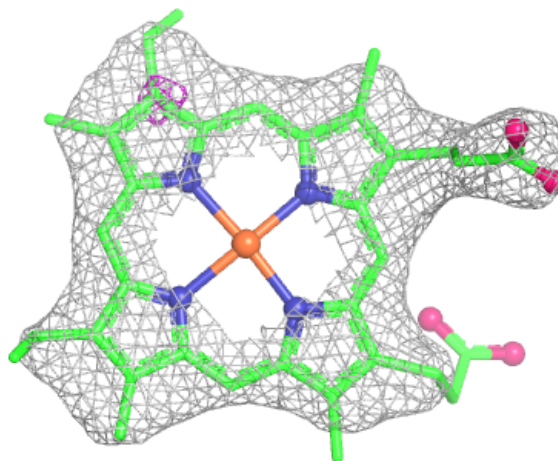
**Electron density around HEM F 102:**

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



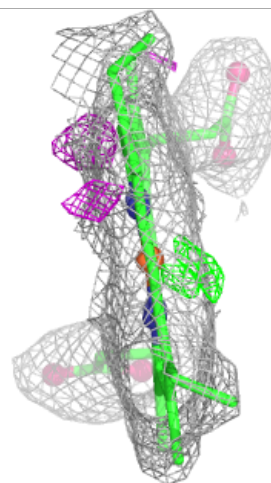
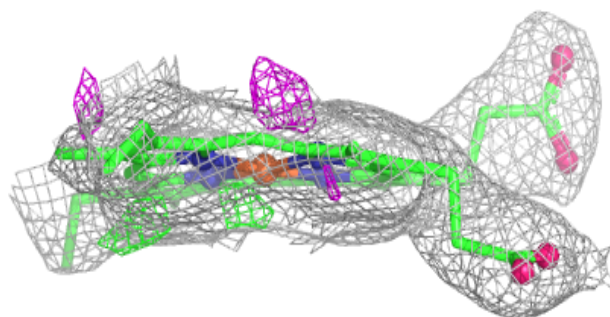
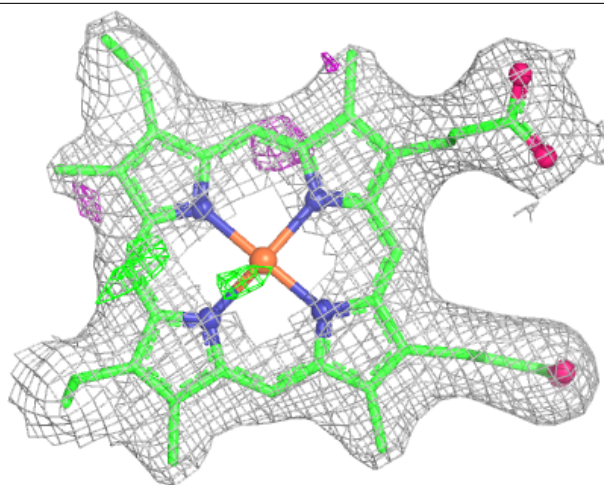
**Electron density around HEM f 101:**

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



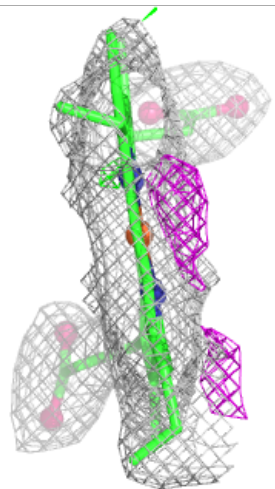
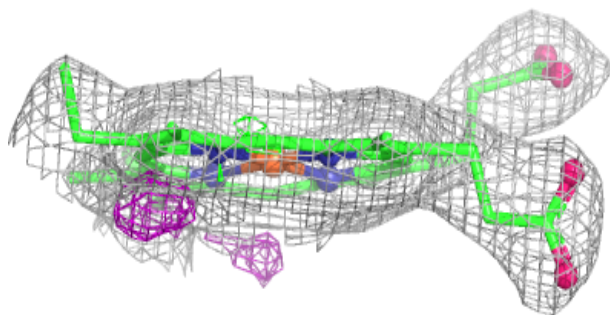
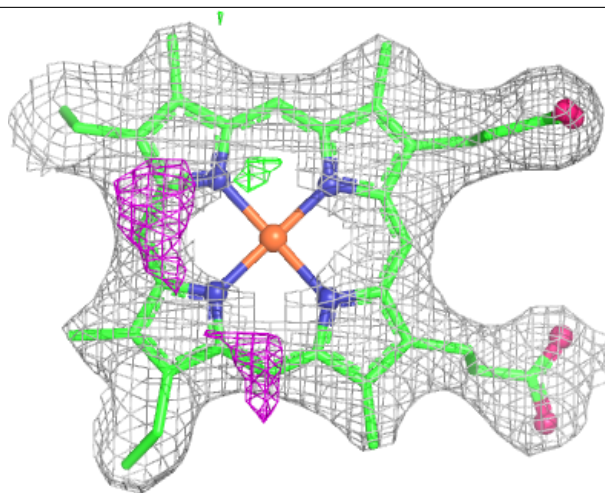
**Electron density around HEC V 201:**

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



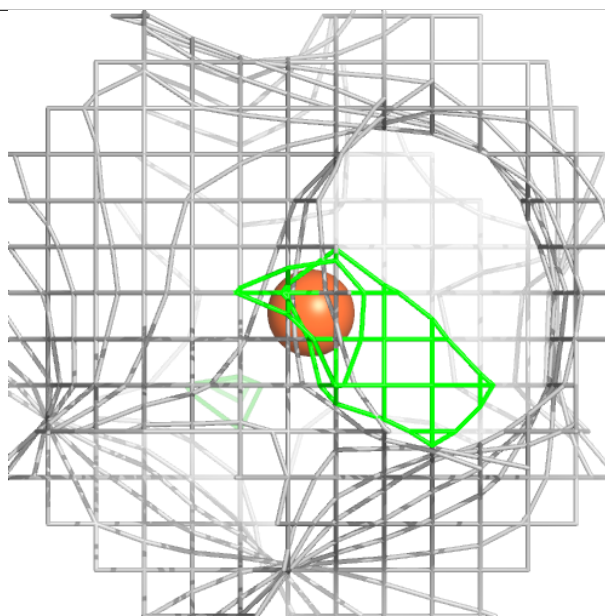
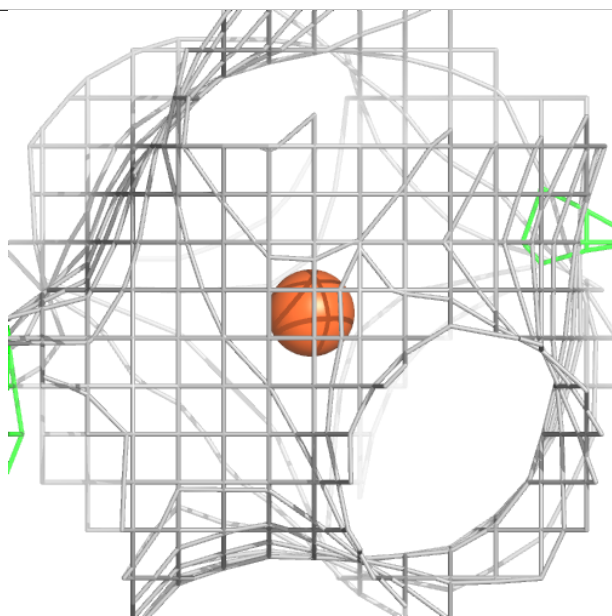
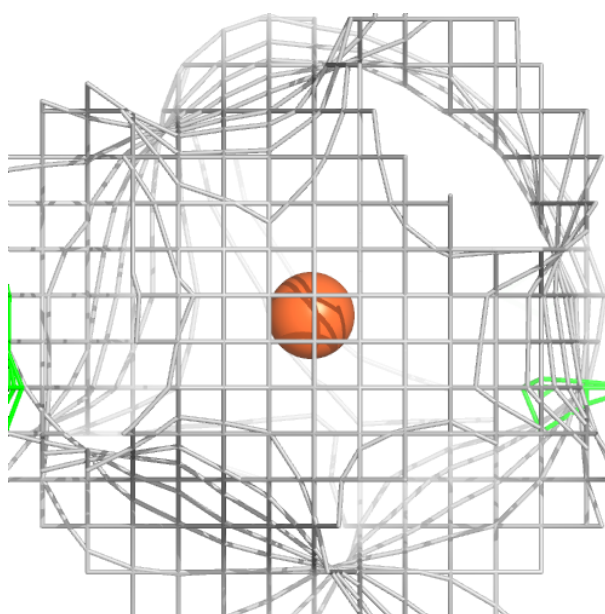
**Electron density around HEC v 201:**

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



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

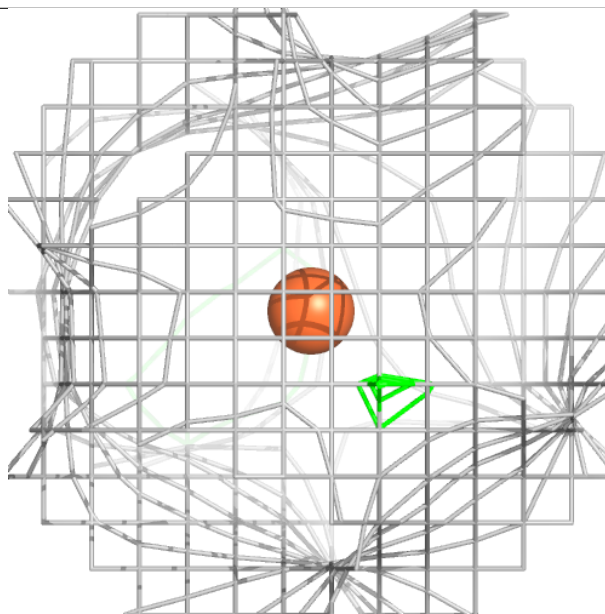
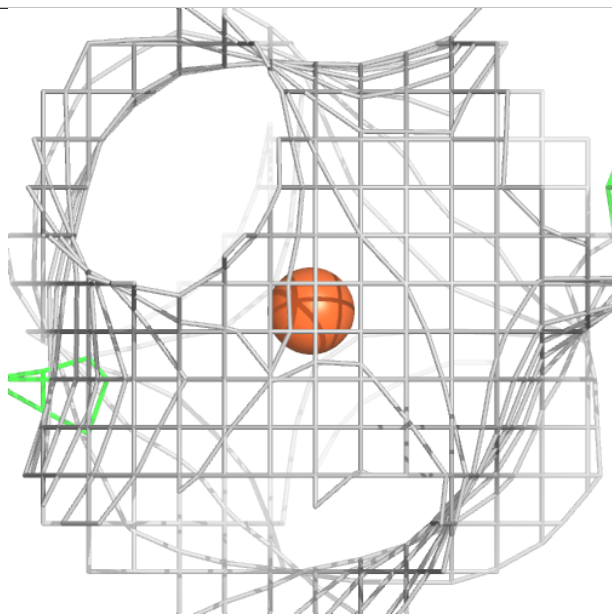
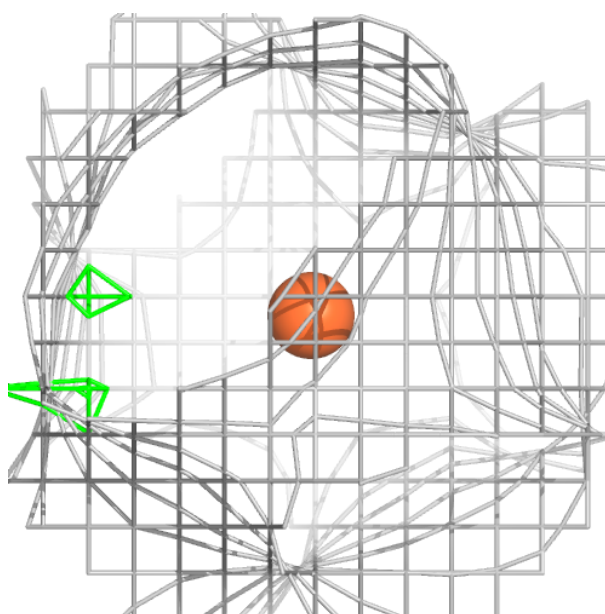
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





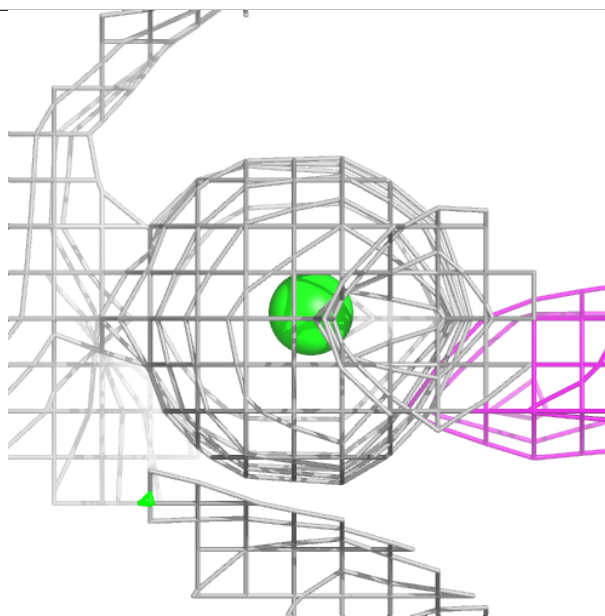
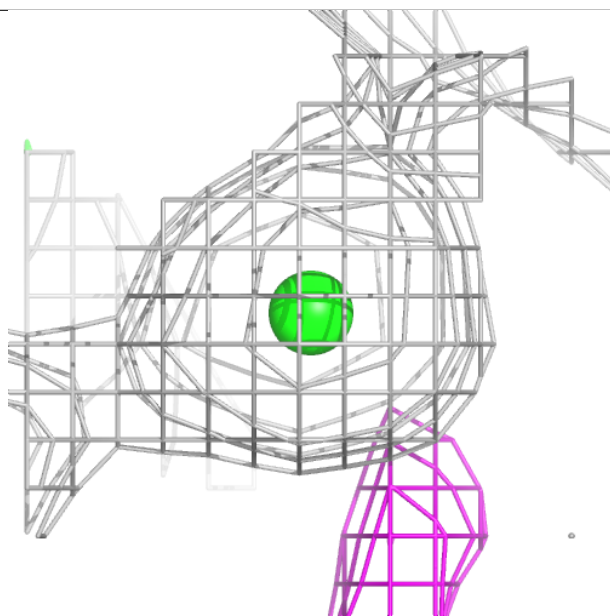
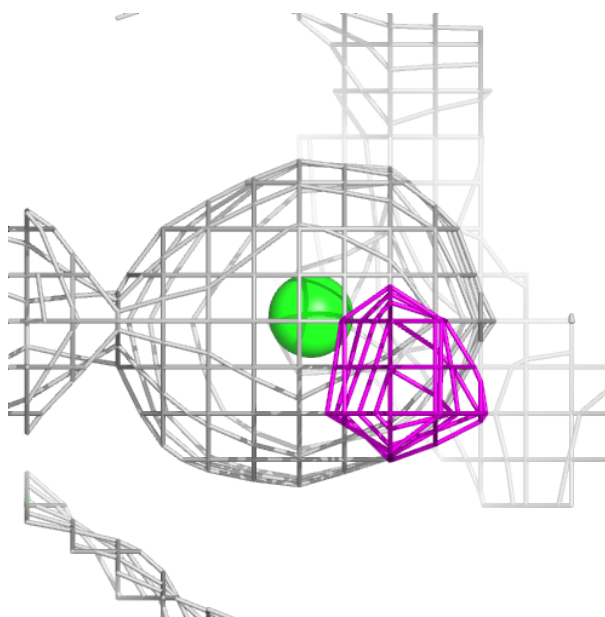
**Electron density around FE2 A 401 (B):**

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



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

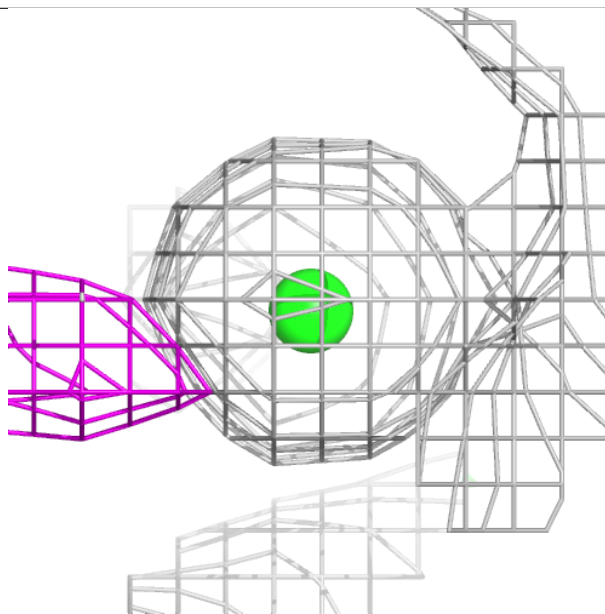
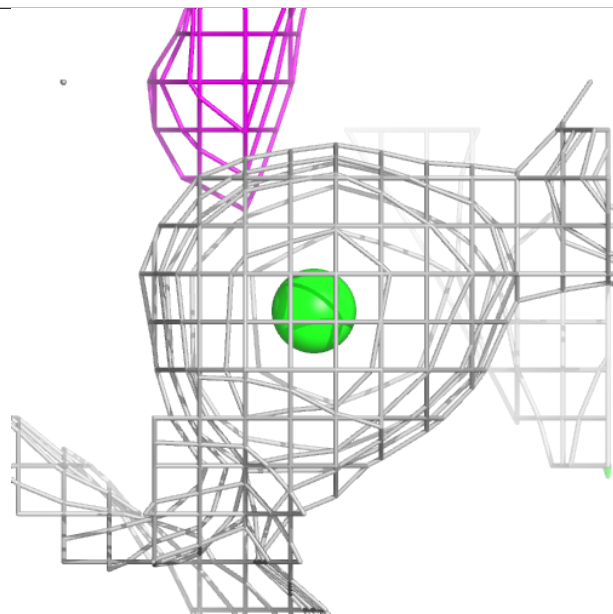
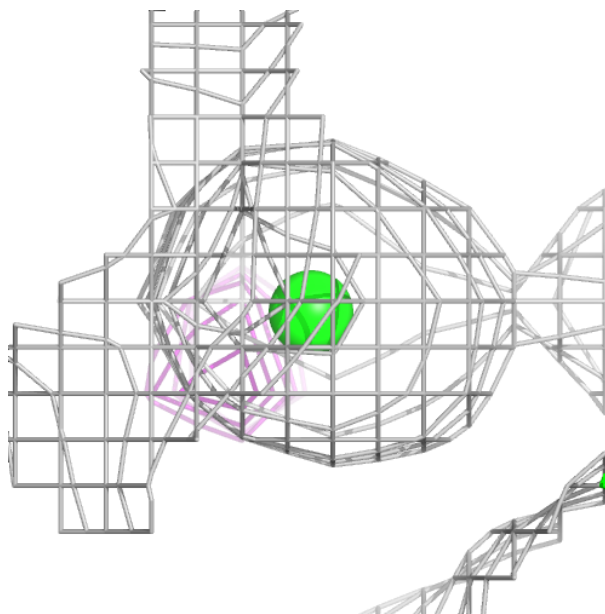
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





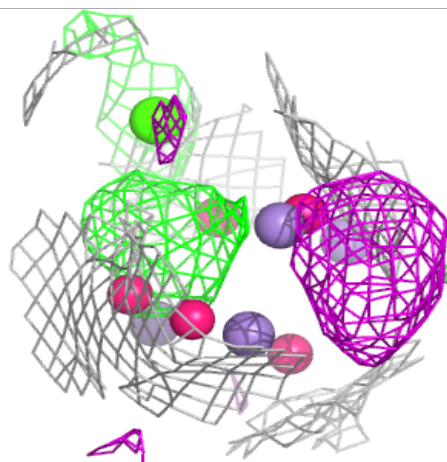
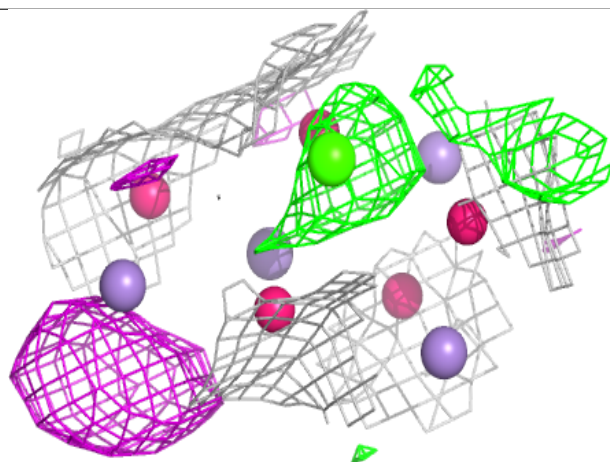
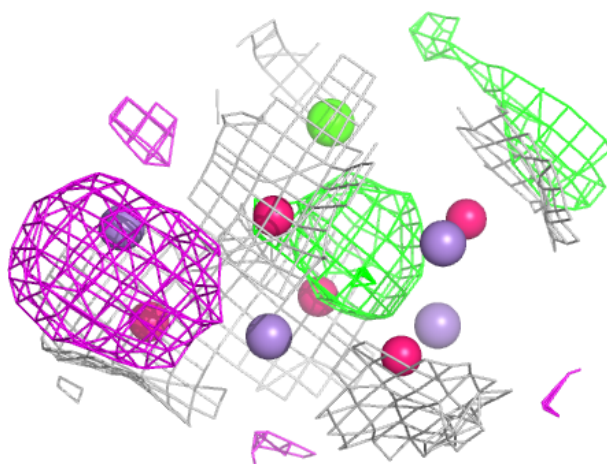
**Electron density around CL a 403 (B):**

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



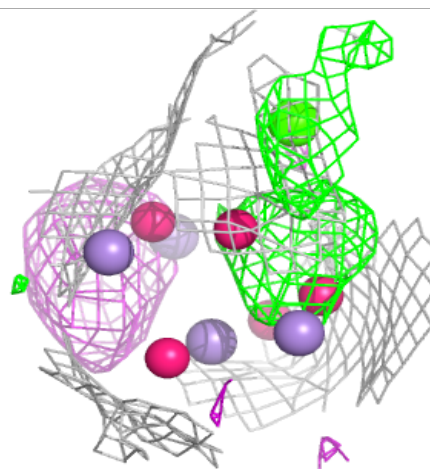
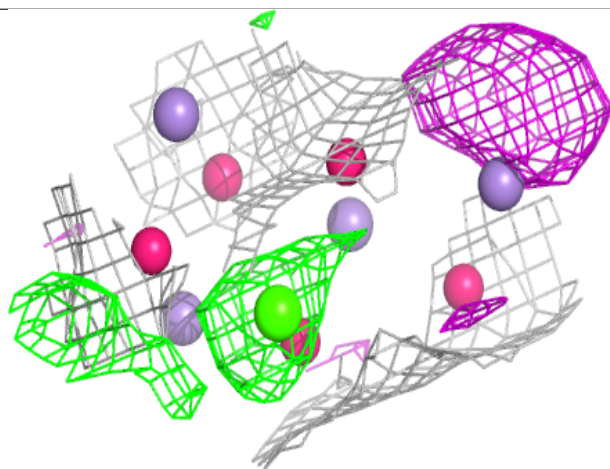
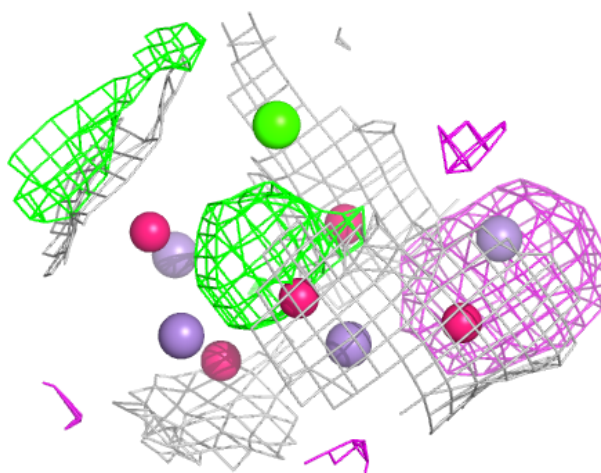
**Electron density around OEX A 413 (A):**

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



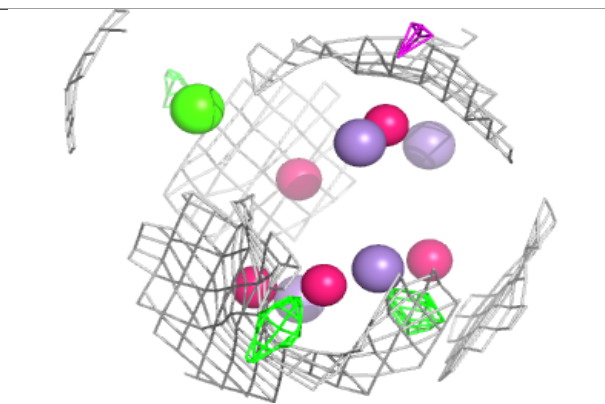
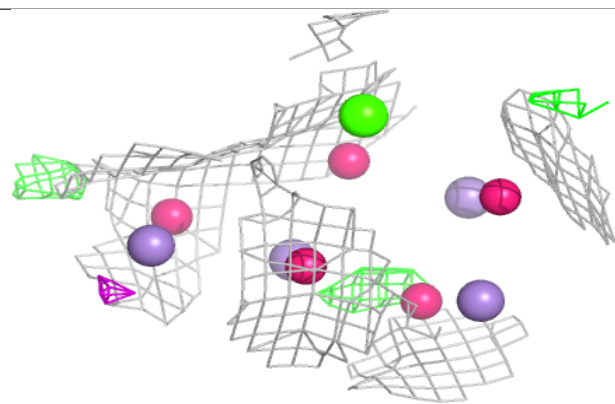
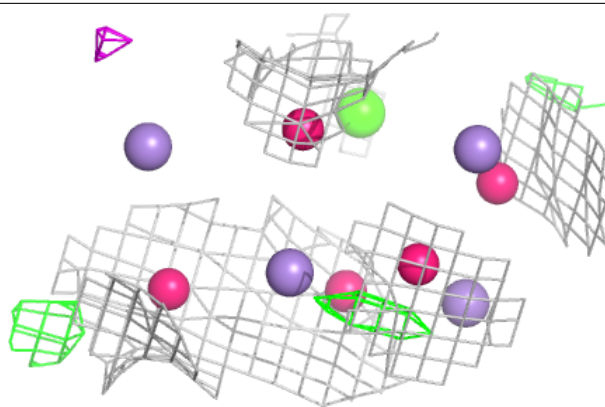
**Electron density around OEX A 413 (B):**

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



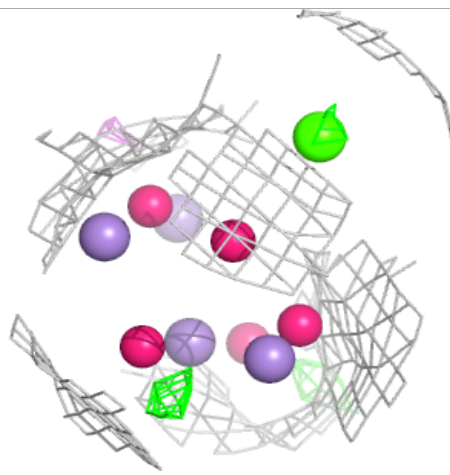
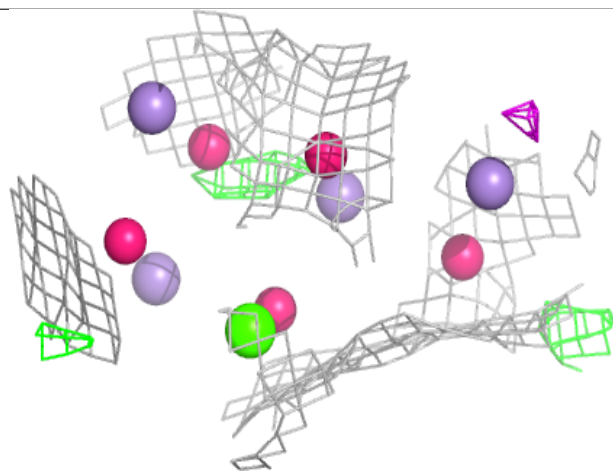
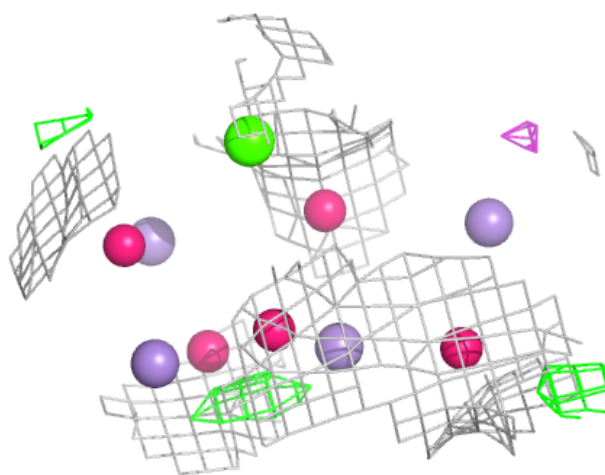
**Electron density around OEX a 413 (A):**

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



**Electron density around OEX 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.