



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 06:02 pm BST

PDB ID : 9G6H / pdb\_00009g6h  
EMDB ID : EMD-51102  
Title : active PSII dimer from native Peak4 PSII dimers  
Authors : Zhao, Z.; Vercellino, I.; Nixon, P.J.; Sazanov, L.A.  
Deposited on : 2024-07-18  
Resolution : 2.20 Å(reported)  
Based on initial model : 3KZI

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

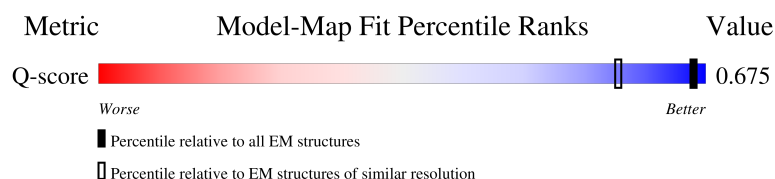
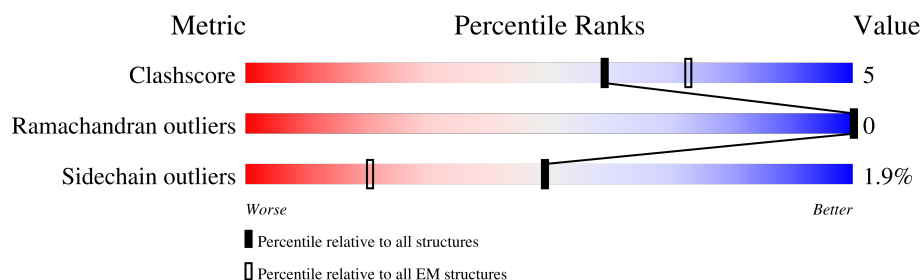
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 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.



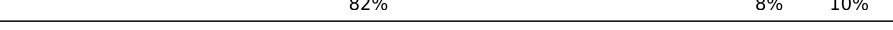
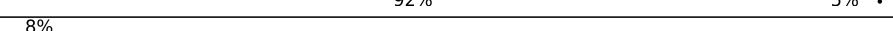
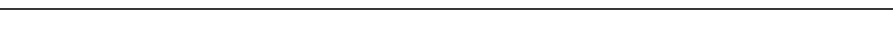
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 3184 ( 1.71 - 2.70 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 360    | <br>80% 12% 8%   |
| 1   | a     | 360    | <br>81% 12% 8%   |
| 2   | B     | 510    | <br>89% 10% .    |
| 2   | b     | 510    | <br>89% 9% .     |

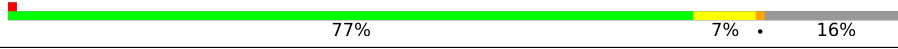
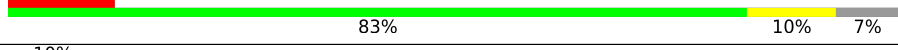
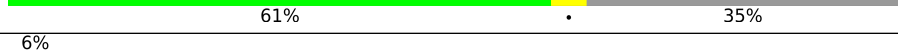
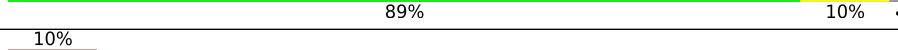
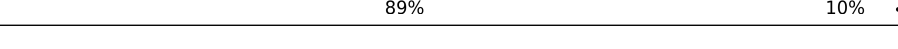
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| Mol | Chain | Length | Quality of chain                                                                                     |
|-----|-------|--------|------------------------------------------------------------------------------------------------------|
| 3   | C     | 461    |  88% 9% ..         |
| 3   | c     | 461    |  89% 9% .          |
| 4   | D     | 352    |  87% 10% .         |
| 4   | d     | 352    |  82% 14% .         |
| 5   | E     | 84     |  85% 12% .         |
| 5   | e     | 84     |  89% 7% .          |
| 6   | F     | 45     |  71% . 24%         |
| 6   | f     | 45     |  71% . 24%         |
| 7   | H     | 66     |  91% . 6%          |
| 7   | h     | 66     |  91% . 6%          |
| 8   | I     | 38     |  87% 8% 5%         |
| 8   | i     | 38     |  84% 8% 8%        |
| 9   | J     | 40     |  85% 5% 10%      |
| 9   | j     | 40     |  82% 8% 10%      |
| 10  | K     | 46     |  70% 11% 20%     |
| 10  | k     | 46     |  74% 7% 20%      |
| 11  | L     | 37     |  92% 5% .        |
| 11  | l     | 37     |  89% 8% .        |
| 12  | M     | 36     |  81% 11% 8%      |
| 12  | m     | 36     |  81% 11% 8%      |
| 13  | O     | 272    |  11% 79% 10% 11% |
| 13  | o     | 272    |  9% 82% 7% 11%   |
| 14  | T     | 32     |  78% 16% 6%      |
| 14  | t     | 32     |  78% 16% 6%      |
| 15  | U     | 134    |  66% 6% . 28%    |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 15  | u     | 134    |  |
| 16  | V     | 163    |  |
| 16  | v     | 163    |  |
| 17  | X     | 41     |  |
| 17  | x     | 41     |  |
| 18  | Y     | 46     |  |
| 18  | y     | 46     |  |
| 19  | Z     | 62     |  |
| 19  | z     | 62     |  |



## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 51092 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 333      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2597  | 1706 | 429 | 447 | 15 |         |       |
| 1   | a     | 333      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2597  | 1706 | 429 | 447 | 15 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 505      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3935  | 2586 | 660 | 676 | 13 |         |       |
| 2   | b     | 505      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3929  | 2583 | 657 | 676 | 13 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 450      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3458  | 2267 | 583 | 595 | 13 |         |       |
| 3   | c     | 450      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3461  | 2268 | 583 | 597 | 13 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 341      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2710  | 1797 | 444 | 457 | 12 |         |       |
| 4   | d     | 341      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2710  | 1797 | 444 | 457 | 12 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 5   | E     | 81       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 650   | 425 | 106 | 119 |         |       |
| 5   | e     | 81       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 650   | 425 | 106 | 119 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | F     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 275   | 187 | 45 | 42 | 1 |         |       |
| 6   | f     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 275   | 187 | 45 | 42 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | H     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 489   | 327 | 78 | 82 | 2 |         |       |
| 7   | h     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 489   | 327 | 78 | 82 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | I     | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 293   | 199 | 46 | 47 | 1 |         |       |
| 8   | i     | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 288   | 196 | 45 | 46 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | J     | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 257   | 174 | 40 | 42 | 1 |         |       |
| 9   | j     | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 257   | 174 | 40 | 42 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | K     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 289   | 201 | 42 | 46 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | k     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 289   | 201 | 42 | 46 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 11  | L     | 36       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 286   | 192 | 44 | 50 |         |       |
| 11  | l     | 36       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 286   | 192 | 44 | 50 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | M     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 254   | 170 | 38 | 45 | 1 |         |       |
| 12  | m     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 254   | 170 | 38 | 45 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | O     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1799  | 1131 | 306 | 358 | 4 |         |       |
| 13  | o     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1794  | 1128 | 303 | 359 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14  | T     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 256   | 180 | 36 | 38 | 2 |         |       |
| 14  | t     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 256   | 180 | 36 | 38 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 15  | U     | 97       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 758   | 483 | 129 | 146 |         |       |
| 15  | u     | 97       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 758   | 483 | 129 | 146 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | V     | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1052  | 668 | 176 | 204 | 4 |         |       |
| 16  | v     | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1052  | 668 | 176 | 204 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 17  | X     | 38       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 279   | 187 | 45 | 47 |         |       |
| 17  | x     | 38       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 275   | 185 | 44 | 46 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 18  | Y     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 214   | 142 | 35 | 35 | 2 |         |       |
| 18  | y     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 214   | 142 | 35 | 35 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19  | Z     | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 458   | 317 | 67 | 72 | 2 |         |       |
| 19  | z     | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 458   | 317 | 67 | 72 | 2 |         |       |

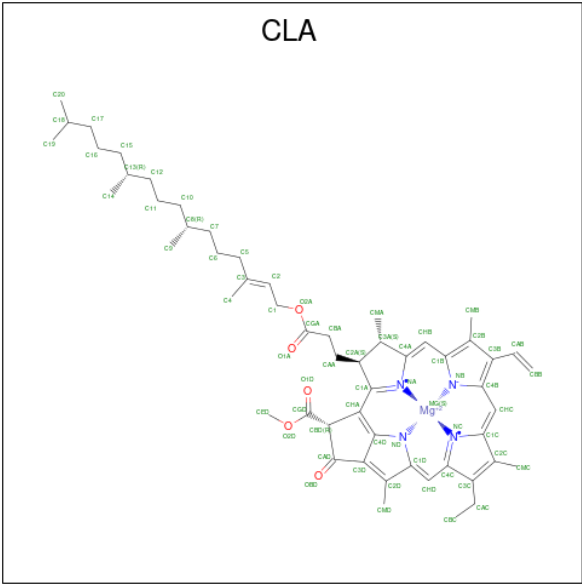
- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 20  | A     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 20  | a     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 21  | A     | 2        | Total | Cl | 0       |
|     |       |          | 2     | 2  |         |
| 21  | a     | 2        | Total | Cl | 0       |
|     |       |          | 2     | 2  |         |

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



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

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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

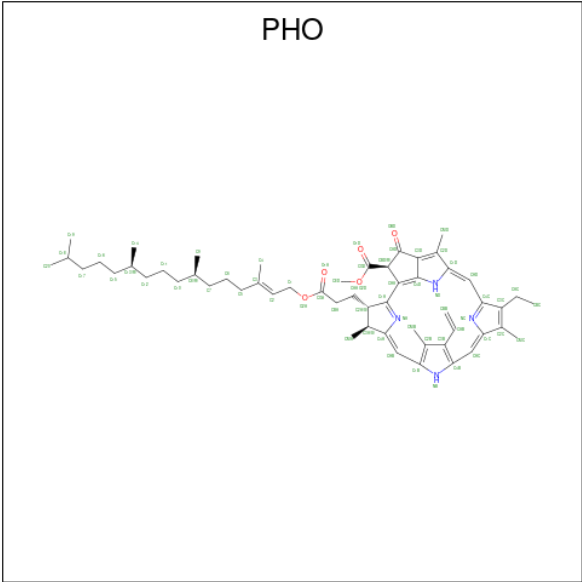
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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

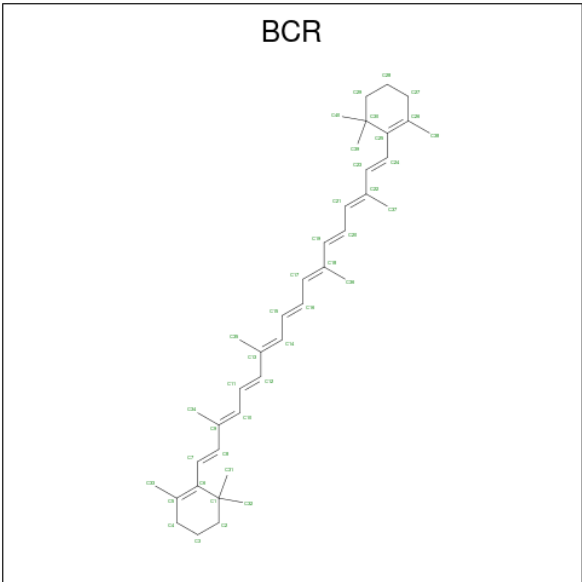
- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).





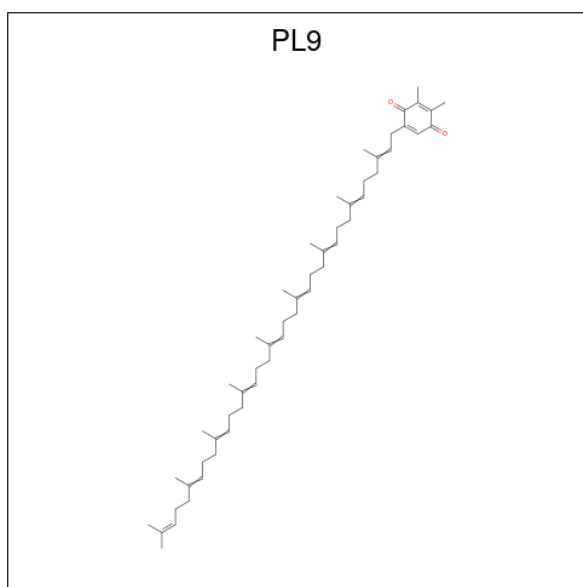
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 23  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 23  | D     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 23  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 23  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



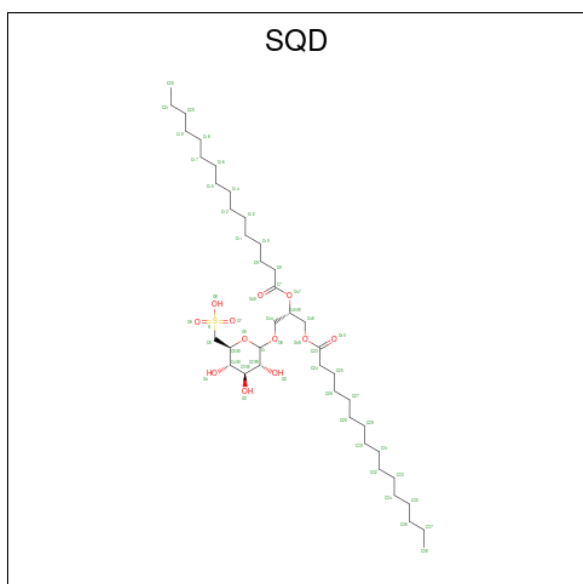
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 24  | A     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | C     | 1        | Total C<br>40 40 | 0       |
| 24  | C     | 1        | Total C<br>40 40 | 0       |
| 24  | F     | 1        | Total C<br>40 40 | 0       |
| 24  | K     | 1        | Total C<br>40 40 | 0       |
| 24  | T     | 1        | Total C<br>40 40 | 0       |
| 24  | Y     | 1        | Total C<br>40 40 | 0       |
| 24  | a     | 1        | Total C<br>40 40 | 0       |
| 24  | b     | 1        | Total C<br>40 40 | 0       |
| 24  | b     | 1        | Total C<br>40 40 | 0       |
| 24  | b     | 1        | Total C<br>40 40 | 0       |
| 24  | c     | 1        | Total C<br>40 40 | 0       |
| 24  | c     | 1        | Total C<br>40 40 | 0       |
| 24  | f     | 1        | Total C<br>40 40 | 0       |
| 24  | k     | 1        | Total C<br>40 40 | 0       |
| 24  | y     | 1        | Total C<br>40 40 | 0       |

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



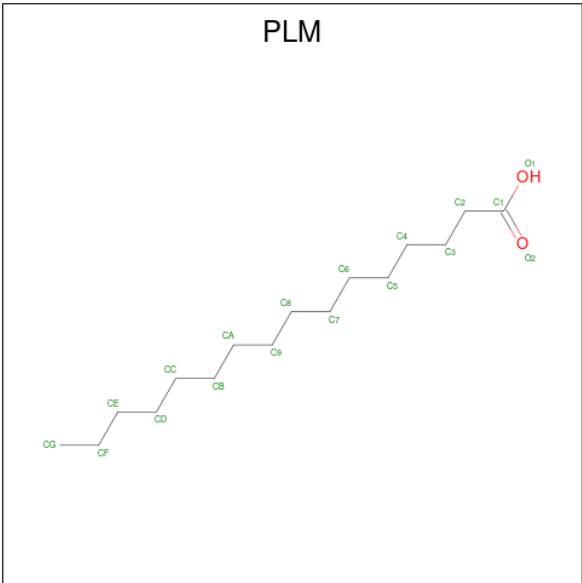
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |
| 25  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |
| 25  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |
| 25  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |

- 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 |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 26  | A     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 26  | A     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 51    | 38 | 12 | 1 |         |
| 26  | D     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 45    | 32 | 12 | 1 |         |
| 26  | a     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 26  | a     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 51    | 38 | 12 | 1 |         |
| 26  | b     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 26  | d     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 45    | 32 | 12 | 1 |         |
| 26  | l     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |

- Molecule 27 is PALMITIC ACID (CCD ID: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 27  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 12    | 10 | 2 |         |
| 27  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 14    | 12 | 2 |         |

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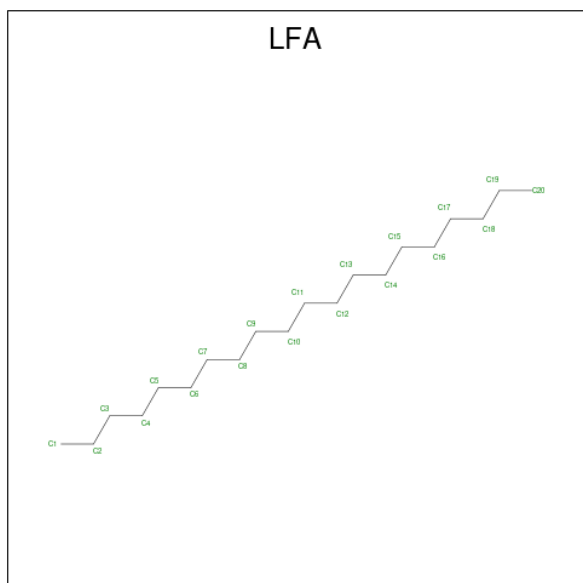
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 27  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 12    | 10 | 2 |         |
| 27  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 17    | 15 | 2 |         |
| 27  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 15    | 13 | 2 |         |
| 27  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 16    | 14 | 2 |         |
| 27  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 13    | 11 | 2 |         |
| 27  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 13    | 11 | 2 |         |
| 27  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 14    | 12 | 2 |         |
| 27  | H     | 1        | Total | C  | O | 0       |
|     |       |          | 12    | 10 | 2 |         |
| 27  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 16    | 14 | 2 |         |
| 27  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 17    | 15 | 2 |         |
| 27  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 13    | 11 | 2 |         |
| 27  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 16    | 14 | 2 |         |
| 27  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 27  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 16    | 14 | 2 |         |
| 27  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | c     | 1        | Total | C  | O | 0       |
|     |       |          | 17    | 15 | 2 |         |
| 27  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 12    | 10 | 2 |         |
| 27  | e     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | e     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | j     | 1        | Total | C  | O | 0       |
|     |       |          | 17    | 15 | 2 |         |
| 27  | j     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 27  | t     | 1        | Total | C  |   | 0       |
|     |       |          | 15    | 15 |   |         |
| 27  | x     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |

- Molecule 28 is EICOSANE (CCD ID: LFA) (formula:  $C_{20}H_{42}$ ).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 28  | A     | 1        | Total | C  | 0       |
|     |       |          | 12    | 12 |         |

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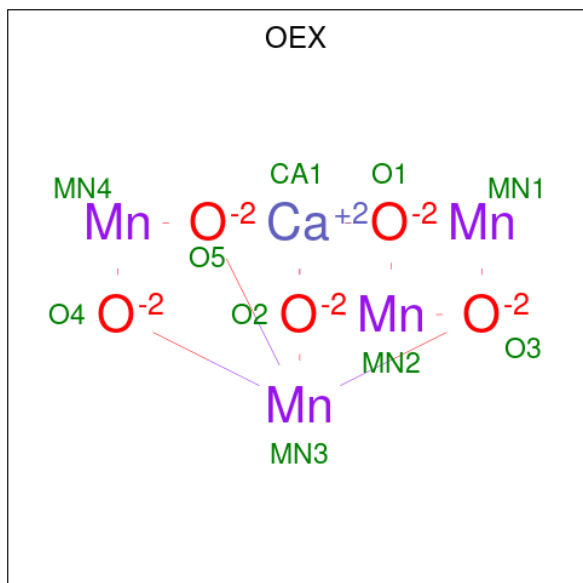
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 28  | B     | 1        | Total C<br>8 8   | 0       |
| 28  | B     | 1        | Total C<br>7 7   | 0       |
| 28  | B     | 1        | Total C<br>8 8   | 0       |
| 28  | B     | 1        | Total C<br>5 5   | 0       |
| 28  | C     | 1        | Total C<br>9 9   | 0       |
| 28  | E     | 1        | Total C<br>20 20 | 0       |
| 28  | H     | 1        | Total C<br>10 10 | 0       |
| 28  | I     | 1        | Total C<br>20 20 | 0       |
| 28  | I     | 1        | Total C<br>11 11 | 0       |
| 28  | I     | 1        | Total C<br>8 8   | 0       |
| 28  | J     | 1        | Total C<br>20 20 | 0       |
| 28  | J     | 1        | Total C<br>11 11 | 0       |
| 28  | T     | 1        | Total C<br>17 17 | 0       |
| 28  | a     | 1        | Total C<br>7 7   | 0       |
| 28  | a     | 1        | Total C<br>11 11 | 0       |
| 28  | a     | 1        | Total C<br>7 7   | 0       |
| 28  | b     | 1        | Total C<br>8 8   | 0       |
| 28  | b     | 1        | Total C<br>4 4   | 0       |
| 28  | d     | 1        | Total C<br>13 13 | 0       |
| 28  | d     | 1        | Total C<br>14 14 | 0       |
| 28  | i     | 1        | Total C<br>20 20 | 0       |

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| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 28  | i     | 1        | Total C<br>9 9 | 0       |
| 28  | i     | 1        | Total C<br>8 8 | 0       |

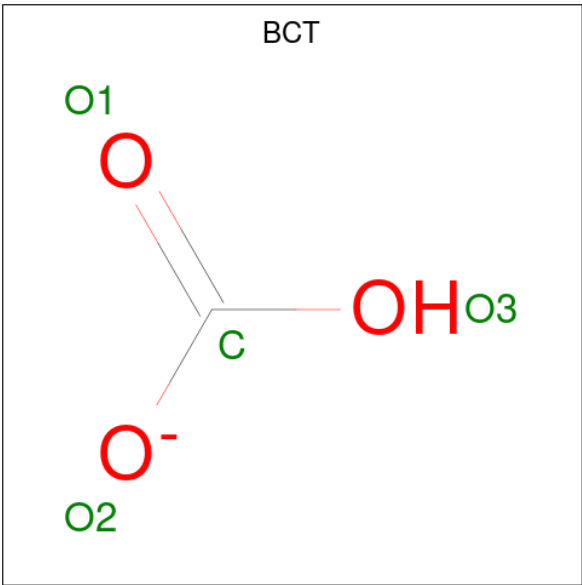
- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms                     | AltConf |
|-----|-------|----------|---------------------------|---------|
| 29  | A     | 1        | Total Ca Mn O<br>10 1 4 5 | 0       |
| 29  | a     | 1        | Total Ca Mn O<br>10 1 4 5 | 0       |

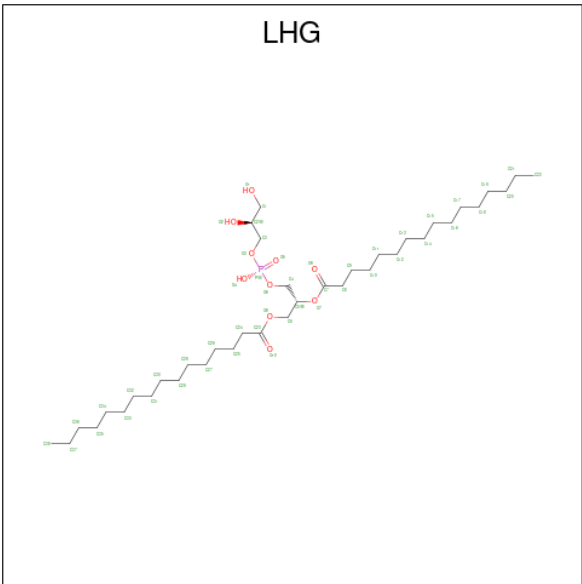
- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).





| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 30  | A     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |
| 30  | a     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



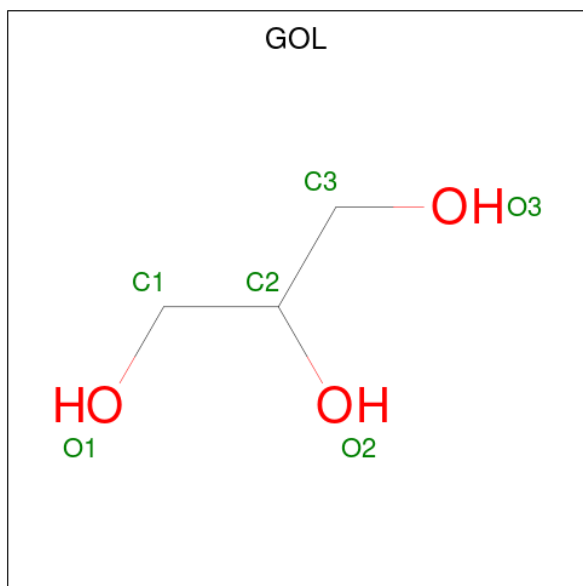
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 31  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 46    | 35 | 10 | 1 |         |

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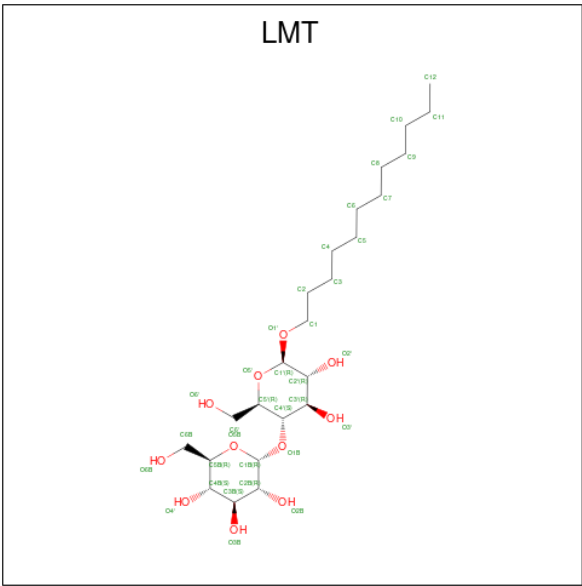
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 31  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 31  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 31  | E     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 40    | 29 | 10 | 1 |         |
| 31  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 31  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 31  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 46    | 35 | 10 | 1 |         |
| 31  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 31  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 48    | 37 | 10 | 1 |         |
| 31  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

- Molecule 32 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 32  | A     | 1        | Total | C | O | 0       |
|     |       |          | 6     | 3 | 3 |         |
| 32  | a     | 1        | Total | C | O | 0       |
|     |       |          | 6     | 3 | 3 |         |

- Molecule 33 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



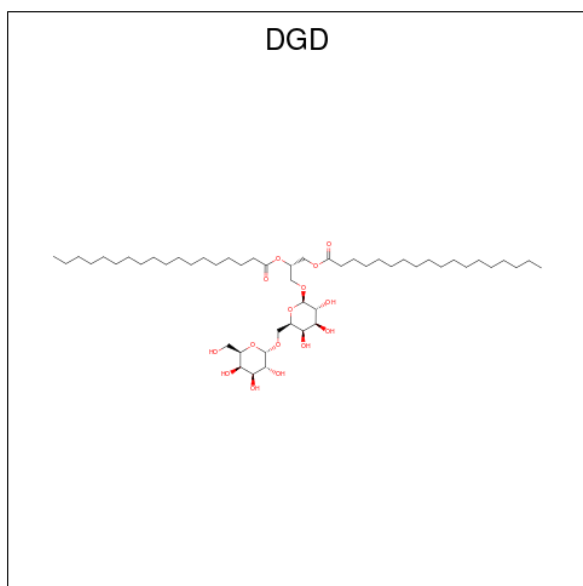
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 33  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 18 | 6  |         |
| 33  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 18 | 6  |         |
| 33  | M     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | T     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 18 | 6  |         |
| 33  | T     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | Z     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 18 | 6  |         |
| 33  | f     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 33  | i     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | j     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 18 | 6  |         |
| 33  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | z     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



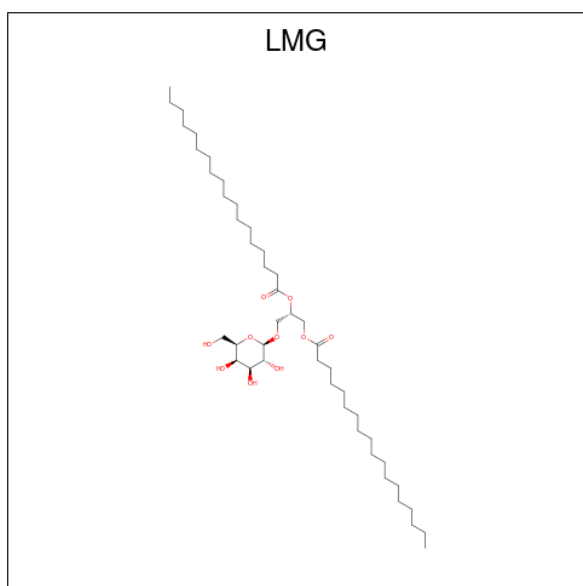
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 34  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 53    | 38 | 15 |         |
| 34  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 54    | 39 | 15 |         |
| 34  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 44    | 35 | 9  |         |
| 34  | H     | 1        | Total | C  | O  | 0       |
|     |       |          | 58    | 43 | 15 |         |
| 34  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 61    | 46 | 15 |         |
| 34  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 53    | 38 | 15 |         |
| 34  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 40 | 15 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 34  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 61    | 46 | 15 |         |
| 34  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 36 | 11 |         |
| 34  | h     | 1        | Total | C  | O  | 0       |
|     |       |          | 58    | 43 | 15 |         |

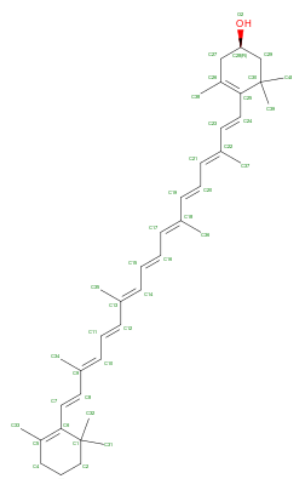
- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 35  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 35  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 35  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 37 | 10 |         |
| 35  | M     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 35  | Y     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 35  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |
| 35  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 35  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 37 | 10 |         |

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| Mol | Chain | Residues | Atoms       |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
| 37  | H     | 1        | Total<br>41 | C<br>40 | O<br>1 | 0       |
| 37  | h     | 1        | Total<br>41 | C<br>40 | O<br>1 | 0       |

- Molecule 38 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 38  | O     | 1        | Total Ca<br>1 1 | 0       |
| 38  | o     | 1        | Total Ca<br>1 1 | 0       |

- Molecule 39 is water.

| Mol | Chain | Residues | Atoms              | AltConf |
|-----|-------|----------|--------------------|---------|
| 39  | A     | 92       | Total O<br>92 92   | 0       |
| 39  | B     | 133      | Total O<br>133 133 | 0       |
| 39  | C     | 101      | Total O<br>101 101 | 1       |
| 39  | D     | 91       | Total O<br>91 91   | 0       |
| 39  | E     | 14       | Total O<br>14 14   | 0       |

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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 39  | F     | 3        | Total<br>3   | O<br>3   | 0       |
| 39  | H     | 11       | Total<br>11  | O<br>11  | 0       |
| 39  | I     | 1        | Total<br>1   | O<br>1   | 0       |
| 39  | J     | 4        | Total<br>4   | O<br>4   | 0       |
| 39  | K     | 1        | Total<br>1   | O<br>1   | 0       |
| 39  | L     | 8        | Total<br>8   | O<br>8   | 0       |
| 39  | M     | 3        | Total<br>3   | O<br>3   | 0       |
| 39  | O     | 37       | Total<br>37  | O<br>37  | 0       |
| 39  | T     | 4        | Total<br>4   | O<br>4   | 0       |
| 39  | U     | 14       | Total<br>14  | O<br>14  | 0       |
| 39  | V     | 26       | Total<br>26  | O<br>26  | 0       |
| 39  | X     | 3        | Total<br>3   | O<br>3   | 0       |
| 39  | a     | 94       | Total<br>94  | O<br>94  | 0       |
| 39  | b     | 137      | Total<br>137 | O<br>137 | 0       |
| 39  | c     | 104      | Total<br>104 | O<br>104 | 0       |
| 39  | d     | 91       | Total<br>91  | O<br>91  | 0       |
| 39  | e     | 15       | Total<br>15  | O<br>15  | 0       |
| 39  | f     | 4        | Total<br>4   | O<br>4   | 0       |
| 39  | h     | 11       | Total<br>11  | O<br>11  | 0       |
| 39  | i     | 3        | Total<br>3   | O<br>3   | 0       |
| 39  | j     | 4        | Total<br>4   | O<br>4   | 0       |

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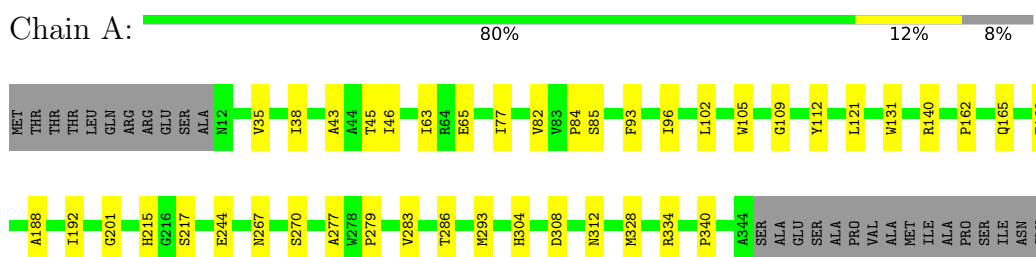
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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 39  | k     | 1        | Total<br>1  | O<br>1  | 0       |
| 39  | l     | 10       | Total<br>10 | O<br>10 | 0       |
| 39  | m     | 3        | Total<br>3  | O<br>3  | 0       |
| 39  | o     | 39       | Total<br>39 | O<br>39 | 0       |
| 39  | t     | 4        | Total<br>4  | O<br>4  | 0       |
| 39  | u     | 13       | Total<br>13 | O<br>13 | 0       |
| 39  | v     | 25       | Total<br>25 | O<br>25 | 0       |
| 39  | x     | 2        | Total<br>2  | O<br>2  | 0       |

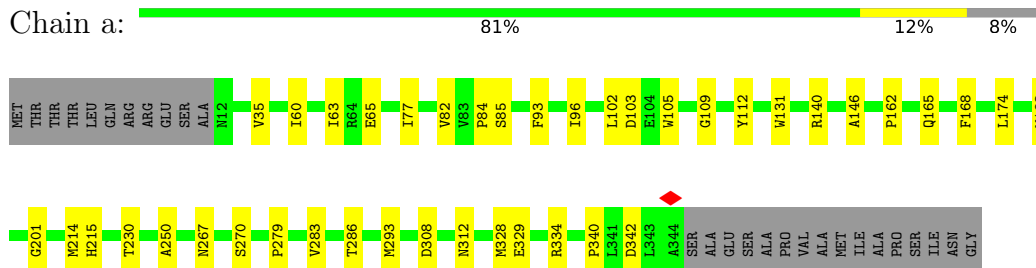
### 3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

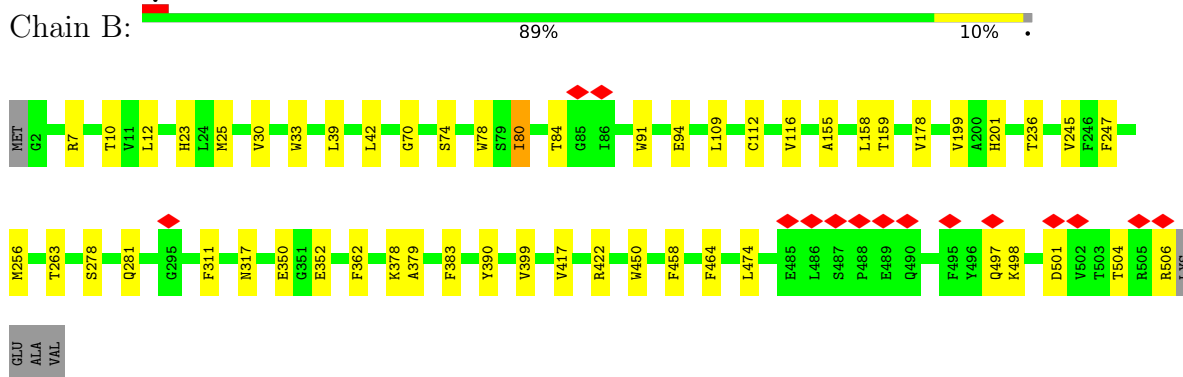
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

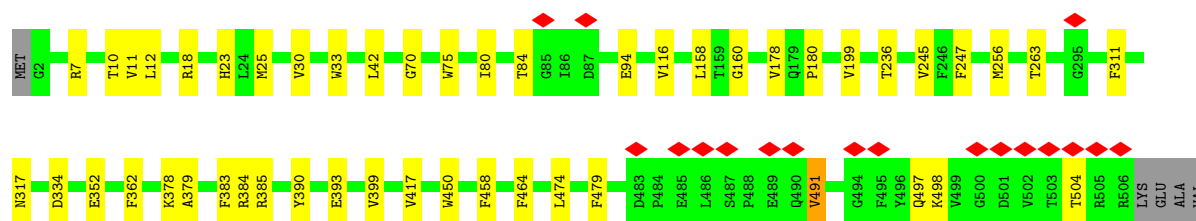


- Molecule 2: Photosystem II CP47 reaction center protein



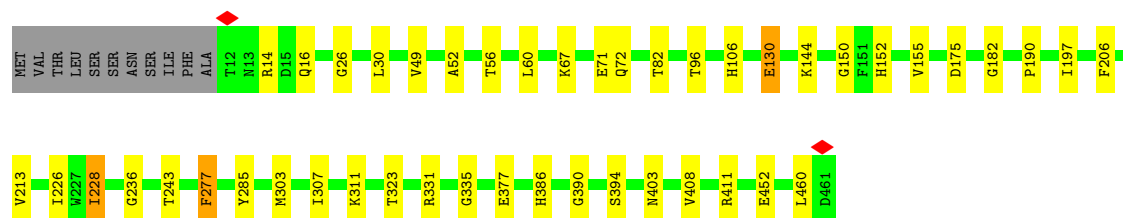
- Molecule 2: Photosystem II CP47 reaction center protein





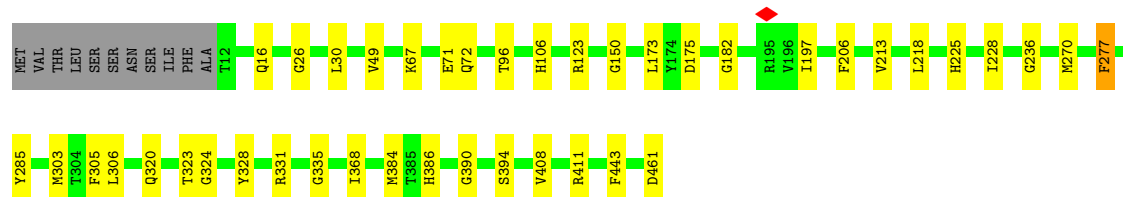
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 88% 9% . .



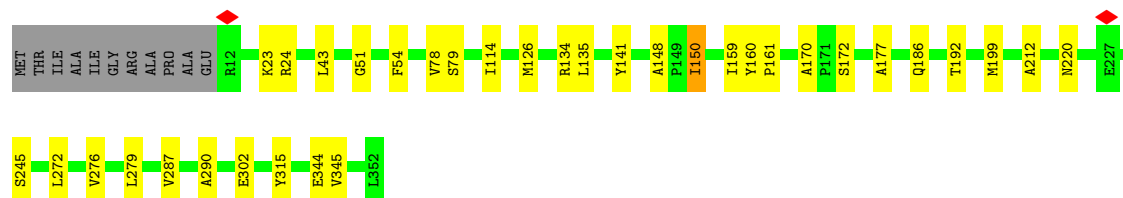
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 9% .



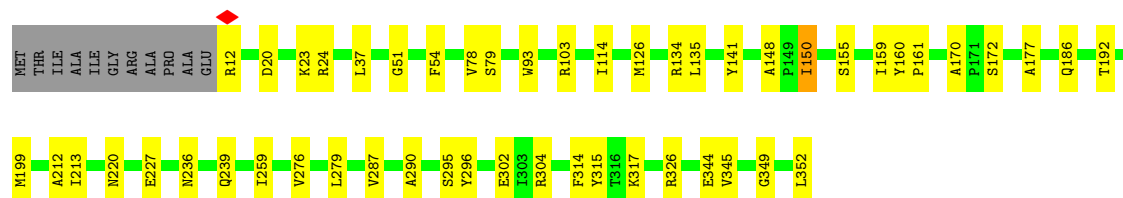
• Molecule 4: Photosystem II D2 protein

Chain D: 87% 10% .

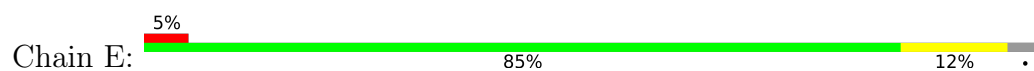


• Molecule 4: Photosystem II D2 protein

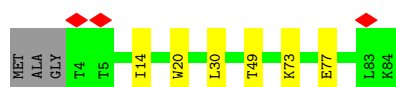
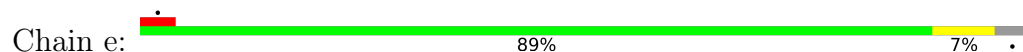
Chain d: 82% 14% .



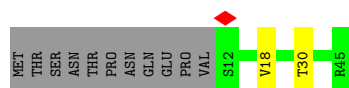
- Molecule 5: Cytochrome b559 subunit alpha



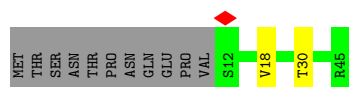
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



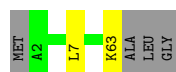
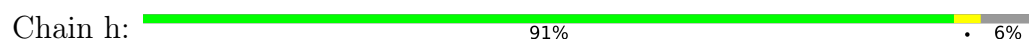
- Molecule 6: Cytochrome b559 subunit beta



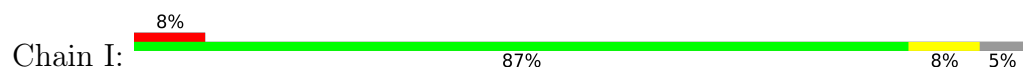
- Molecule 7: Photosystem II reaction center protein H

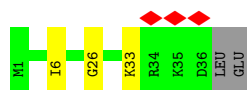


- Molecule 7: Photosystem II reaction center protein H

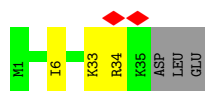
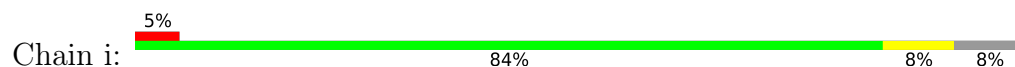


- Molecule 8: Photosystem II reaction center protein I

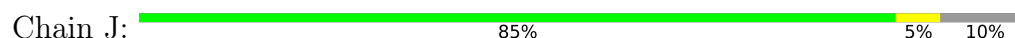




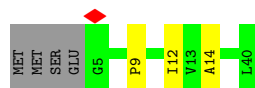
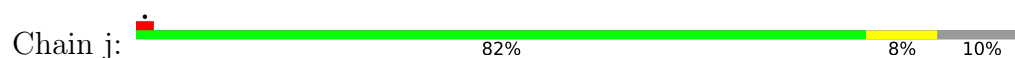
- Molecule 8: Photosystem II reaction center protein I



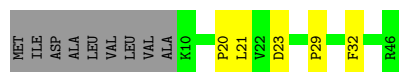
- Molecule 9: Photosystem II reaction center protein J



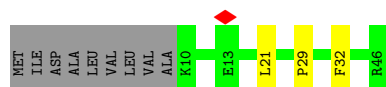
- Molecule 9: Photosystem II reaction center protein J



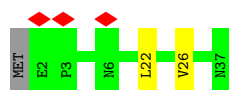
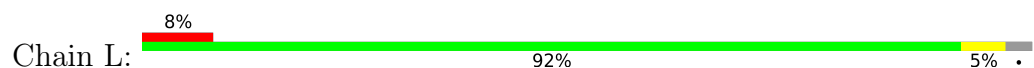
- Molecule 10: Photosystem II reaction center protein K



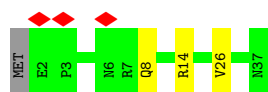
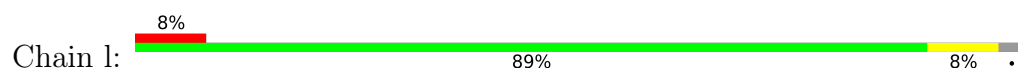
- Molecule 10: Photosystem II reaction center protein K



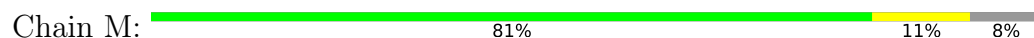
- Molecule 11: Photosystem II reaction center protein L



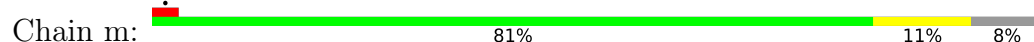
- Molecule 11: Photosystem II reaction center protein L



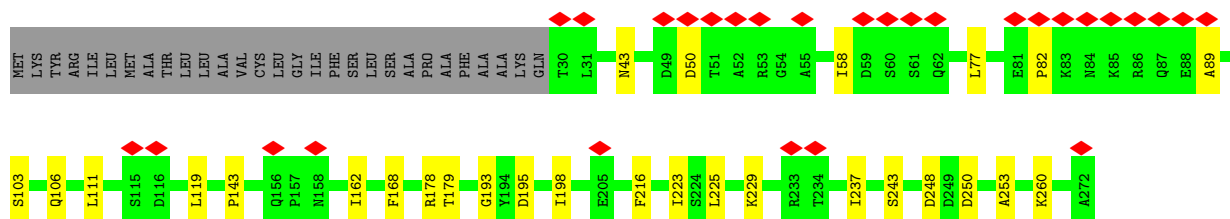
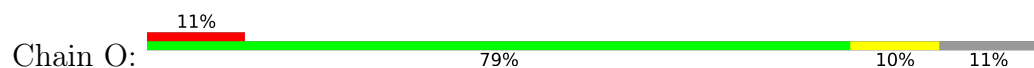
- Molecule 12: Photosystem II reaction center protein M



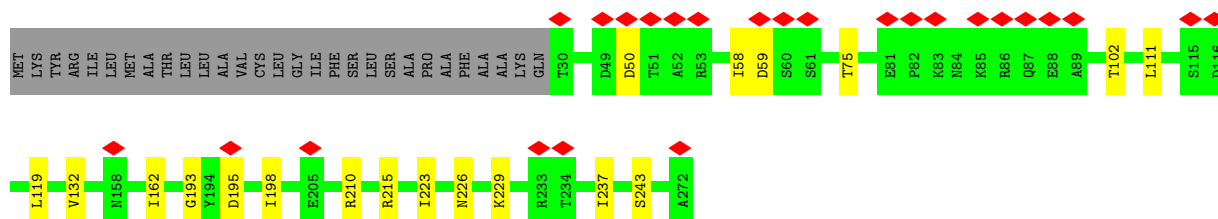
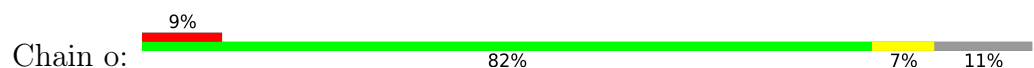
- Molecule 12: Photosystem II reaction center protein M



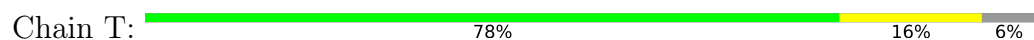
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T



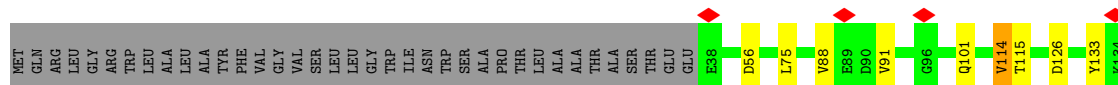
- Molecule 14: Photosystem II reaction center protein T

Chain t:  78% 16% 6%



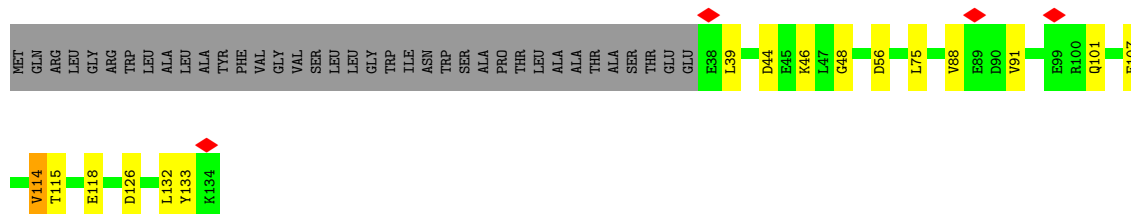
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  66% 6% 28%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  60% 11% 28%



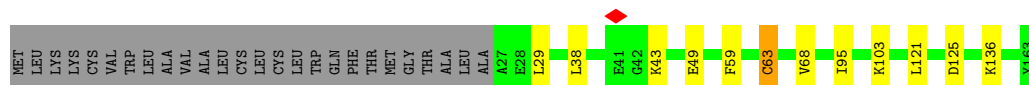
- Molecule 16: Cytochrome c-550

Chain V:  78% 6% 16%



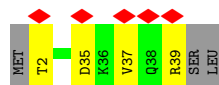
- Molecule 16: Cytochrome c-550

Chain v:  77% 7% 16%

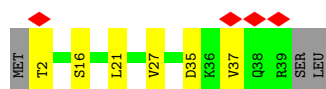
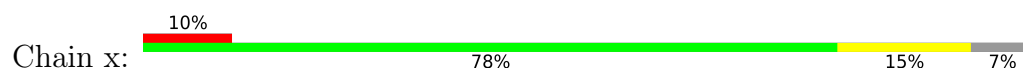


- Molecule 17: Photosystem II reaction center X protein

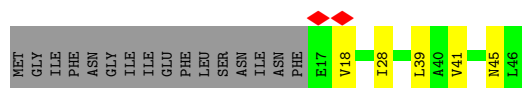
Chain X:  12% 83% 10% 7%



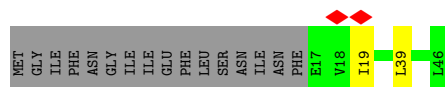
- Molecule 17: Photosystem II reaction center X protein



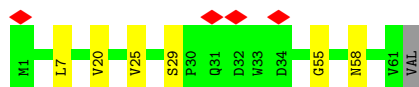
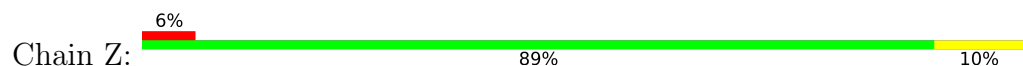
- Molecule 18: Photosystem II reaction center protein Ycf12



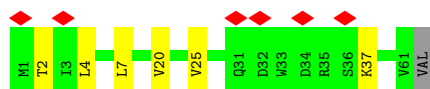
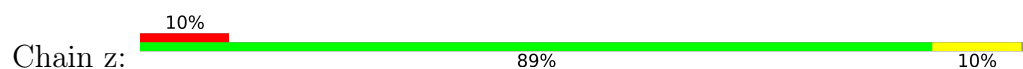
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C2                               | Depositor |
| Number of particles used             | 363811                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 80                                      | Depositor |
| Minimum defocus (nm)                 | 600                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | 81000                                   | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.369                                   | Depositor |
| Minimum map value                    | -0.147                                  | Depositor |
| Average map value                    | 0.004                                   | Depositor |
| Map value standard deviation         | 0.028                                   | Depositor |
| Recommended contour level            | 0.043                                   | Depositor |
| Map size (Å)                         | 135.5, 210.0, 118.0                     | wwPDB     |
| Map dimensions                       | 236, 420, 271                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.5, 0.5, 0.5                           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.21         | 0/2682  | 0.42        | 0/3661  |
| 1   | a     | 0.21         | 0/2682  | 0.43        | 0/3661  |
| 2   | B     | 0.18         | 0/4075  | 0.37        | 0/5558  |
| 2   | b     | 0.18         | 0/4069  | 0.37        | 0/5551  |
| 3   | C     | 0.18         | 0/3571  | 0.38        | 0/4864  |
| 3   | c     | 0.19         | 0/3574  | 0.39        | 0/4868  |
| 4   | D     | 0.21         | 0/2805  | 0.41        | 0/3823  |
| 4   | d     | 0.21         | 0/2805  | 0.42        | 0/3823  |
| 5   | E     | 0.19         | 0/669   | 0.41        | 0/914   |
| 5   | e     | 0.18         | 0/669   | 0.43        | 0/914   |
| 6   | F     | 0.20         | 0/284   | 0.42        | 0/387   |
| 6   | f     | 0.20         | 0/284   | 0.41        | 0/387   |
| 7   | H     | 0.19         | 0/502   | 0.43        | 0/686   |
| 7   | h     | 0.20         | 0/502   | 0.44        | 0/686   |
| 8   | I     | 0.19         | 0/290   | 0.46        | 0/392   |
| 8   | i     | 0.19         | 0/285   | 0.40        | 0/385   |
| 9   | J     | 0.16         | 0/263   | 0.39        | 0/356   |
| 9   | j     | 0.17         | 0/263   | 0.39        | 0/356   |
| 10  | K     | 0.28         | 0/299   | 0.55        | 0/412   |
| 10  | k     | 0.28         | 0/299   | 0.53        | 0/412   |
| 11  | L     | 0.13         | 0/293   | 0.32        | 0/400   |
| 11  | l     | 0.13         | 0/293   | 0.33        | 0/400   |
| 12  | M     | 0.29         | 0/257   | 0.52        | 0/351   |
| 12  | m     | 0.23         | 0/257   | 0.54        | 0/351   |
| 13  | O     | 0.16         | 0/1830  | 0.40        | 0/2492  |
| 13  | o     | 0.16         | 0/1825  | 0.39        | 0/2485  |
| 14  | T     | 0.17         | 0/255   | 0.34        | 0/346   |
| 14  | t     | 0.18         | 0/255   | 0.34        | 0/346   |
| 15  | U     | 0.16         | 0/769   | 0.37        | 0/1044  |
| 15  | u     | 0.16         | 0/769   | 0.38        | 0/1044  |
| 16  | V     | 0.14         | 0/1073  | 0.33        | 0/1459  |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 16  | v     | 0.16         | 0/1073  | 0.35        | 0/1459  |
| 17  | X     | 0.14         | 0/282   | 0.27        | 0/381   |
| 17  | x     | 0.14         | 0/278   | 0.30        | 0/376   |
| 18  | Y     | 0.29         | 0/215   | 0.59        | 0/291   |
| 18  | y     | 0.28         | 0/215   | 0.45        | 0/291   |
| 19  | Z     | 0.27         | 0/469   | 0.46        | 0/643   |
| 19  | z     | 0.17         | 0/469   | 0.35        | 0/643   |
| All | All   | 0.19         | 0/41749 | 0.40        | 0/56898 |

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     | 2597  | 0        | 2493     | 31      | 0            |
| 1   | a     | 2597  | 0        | 2493     | 30      | 0            |
| 2   | B     | 3935  | 0        | 3773     | 37      | 0            |
| 2   | b     | 3929  | 0        | 3762     | 37      | 0            |
| 3   | C     | 3458  | 0        | 3380     | 31      | 0            |
| 3   | c     | 3461  | 0        | 3382     | 26      | 0            |
| 4   | D     | 2710  | 0        | 2615     | 26      | 0            |
| 4   | d     | 2710  | 0        | 2615     | 38      | 0            |
| 5   | E     | 650   | 0        | 629      | 6       | 0            |
| 5   | e     | 650   | 0        | 629      | 5       | 0            |
| 6   | F     | 275   | 0        | 282      | 2       | 0            |
| 6   | f     | 275   | 0        | 282      | 2       | 0            |
| 7   | H     | 489   | 0        | 502      | 1       | 0            |
| 7   | h     | 489   | 0        | 502      | 1       | 0            |
| 8   | I     | 293   | 0        | 309      | 1       | 0            |
| 8   | i     | 288   | 0        | 307      | 1       | 0            |
| 9   | J     | 257   | 0        | 268      | 1       | 0            |
| 9   | j     | 257   | 0        | 268      | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | K     | 289   | 0        | 294      | 3       | 0            |
| 10  | k     | 289   | 0        | 294      | 2       | 0            |
| 11  | L     | 286   | 0        | 289      | 3       | 0            |
| 11  | l     | 286   | 0        | 289      | 3       | 0            |
| 12  | M     | 254   | 0        | 272      | 4       | 0            |
| 12  | m     | 254   | 0        | 272      | 4       | 0            |
| 13  | O     | 1799  | 0        | 1745     | 16      | 0            |
| 13  | o     | 1794  | 0        | 1736     | 11      | 0            |
| 14  | T     | 256   | 0        | 256      | 5       | 0            |
| 14  | t     | 256   | 0        | 256      | 5       | 0            |
| 15  | U     | 758   | 0        | 757      | 4       | 0            |
| 15  | u     | 758   | 0        | 757      | 7       | 0            |
| 16  | V     | 1052  | 0        | 1053     | 5       | 0            |
| 16  | v     | 1052  | 0        | 1053     | 6       | 0            |
| 17  | X     | 279   | 0        | 307      | 3       | 0            |
| 17  | x     | 275   | 0        | 301      | 4       | 0            |
| 18  | Y     | 214   | 0        | 234      | 4       | 0            |
| 18  | y     | 214   | 0        | 234      | 1       | 0            |
| 19  | Z     | 458   | 0        | 488      | 2       | 0            |
| 19  | z     | 458   | 0        | 488      | 1       | 0            |
| 20  | A     | 1     | 0        | 0        | 0       | 0            |
| 20  | a     | 1     | 0        | 0        | 0       | 0            |
| 21  | A     | 2     | 0        | 0        | 1       | 0            |
| 21  | a     | 2     | 0        | 0        | 1       | 0            |
| 22  | A     | 195   | 0        | 216      | 5       | 0            |
| 22  | B     | 1020  | 0        | 1113     | 23      | 0            |
| 22  | C     | 845   | 0        | 936      | 23      | 0            |
| 22  | D     | 195   | 0        | 216      | 3       | 0            |
| 22  | a     | 195   | 0        | 216      | 5       | 0            |
| 22  | b     | 1020  | 0        | 1113     | 27      | 0            |
| 22  | c     | 845   | 0        | 936      | 23      | 0            |
| 22  | d     | 195   | 0        | 216      | 5       | 0            |
| 23  | A     | 64    | 0        | 74       | 1       | 0            |
| 23  | D     | 64    | 0        | 74       | 1       | 0            |
| 23  | a     | 128   | 0        | 148      | 3       | 0            |
| 24  | A     | 40    | 0        | 56       | 1       | 0            |
| 24  | B     | 160   | 0        | 224      | 10      | 0            |
| 24  | C     | 80    | 0        | 112      | 6       | 0            |
| 24  | F     | 40    | 0        | 56       | 1       | 0            |
| 24  | K     | 40    | 0        | 56       | 1       | 0            |
| 24  | T     | 40    | 0        | 56       | 2       | 0            |
| 24  | Y     | 40    | 0        | 56       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | a     | 40    | 0        | 56       | 0       | 0            |
| 24  | b     | 120   | 0        | 168      | 10      | 0            |
| 24  | c     | 80    | 0        | 112      | 4       | 0            |
| 24  | f     | 40    | 0        | 56       | 0       | 0            |
| 24  | k     | 40    | 0        | 56       | 1       | 0            |
| 24  | y     | 40    | 0        | 56       | 1       | 0            |
| 25  | A     | 55    | 0        | 80       | 3       | 0            |
| 25  | D     | 55    | 0        | 80       | 4       | 0            |
| 25  | a     | 55    | 0        | 80       | 4       | 0            |
| 25  | d     | 55    | 0        | 80       | 4       | 0            |
| 26  | A     | 105   | 0        | 147      | 7       | 0            |
| 26  | D     | 45    | 0        | 57       | 2       | 0            |
| 26  | a     | 105   | 0        | 147      | 4       | 0            |
| 26  | b     | 54    | 0        | 78       | 2       | 0            |
| 26  | d     | 45    | 0        | 57       | 3       | 0            |
| 26  | l     | 54    | 0        | 78       | 3       | 0            |
| 27  | A     | 30    | 0        | 47       | 2       | 0            |
| 27  | B     | 79    | 0        | 124      | 5       | 0            |
| 27  | C     | 62    | 0        | 95       | 2       | 0            |
| 27  | D     | 31    | 0        | 49       | 1       | 0            |
| 27  | E     | 18    | 0        | 31       | 0       | 0            |
| 27  | F     | 14    | 0        | 20       | 0       | 0            |
| 27  | H     | 12    | 0        | 16       | 0       | 0            |
| 27  | L     | 18    | 0        | 31       | 1       | 0            |
| 27  | M     | 16    | 0        | 24       | 0       | 0            |
| 27  | X     | 17    | 0        | 26       | 0       | 0            |
| 27  | a     | 18    | 0        | 31       | 0       | 0            |
| 27  | b     | 65    | 0        | 104      | 1       | 0            |
| 27  | c     | 69    | 0        | 112      | 2       | 0            |
| 27  | d     | 12    | 0        | 16       | 0       | 0            |
| 27  | e     | 36    | 0        | 62       | 1       | 0            |
| 27  | j     | 35    | 0        | 57       | 1       | 0            |
| 27  | t     | 15    | 0        | 26       | 2       | 0            |
| 27  | x     | 18    | 0        | 31       | 2       | 0            |
| 28  | A     | 12    | 0        | 20       | 1       | 0            |
| 28  | B     | 28    | 0        | 43       | 3       | 0            |
| 28  | C     | 9     | 0        | 14       | 0       | 0            |
| 28  | E     | 20    | 0        | 42       | 2       | 0            |
| 28  | H     | 10    | 0        | 16       | 0       | 0            |
| 28  | I     | 39    | 0        | 75       | 2       | 0            |
| 28  | J     | 31    | 0        | 60       | 2       | 0            |
| 28  | T     | 17    | 0        | 33       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | a     | 25    | 0        | 38       | 0       | 0            |
| 28  | b     | 12    | 0        | 19       | 2       | 0            |
| 28  | d     | 27    | 0        | 49       | 0       | 0            |
| 28  | i     | 37    | 0        | 68       | 1       | 0            |
| 29  | A     | 10    | 0        | 0        | 0       | 0            |
| 29  | a     | 10    | 0        | 0        | 0       | 0            |
| 30  | A     | 4     | 0        | 0        | 0       | 0            |
| 30  | a     | 4     | 0        | 0        | 0       | 0            |
| 31  | A     | 46    | 0        | 65       | 1       | 0            |
| 31  | D     | 98    | 0        | 148      | 5       | 0            |
| 31  | E     | 40    | 0        | 53       | 0       | 0            |
| 31  | L     | 49    | 0        | 74       | 4       | 0            |
| 31  | a     | 95    | 0        | 139      | 5       | 0            |
| 31  | d     | 97    | 0        | 143      | 5       | 0            |
| 31  | l     | 49    | 0        | 74       | 3       | 0            |
| 32  | A     | 6     | 0        | 8        | 0       | 0            |
| 32  | a     | 6     | 0        | 8        | 1       | 0            |
| 33  | A     | 35    | 0        | 46       | 0       | 0            |
| 33  | B     | 129   | 0        | 173      | 5       | 0            |
| 33  | C     | 35    | 0        | 46       | 1       | 0            |
| 33  | J     | 24    | 0        | 35       | 2       | 0            |
| 33  | M     | 35    | 0        | 46       | 1       | 0            |
| 33  | T     | 59    | 0        | 81       | 1       | 0            |
| 33  | Z     | 35    | 0        | 46       | 0       | 0            |
| 33  | b     | 24    | 0        | 35       | 0       | 0            |
| 33  | f     | 35    | 0        | 46       | 0       | 0            |
| 33  | i     | 35    | 0        | 46       | 0       | 0            |
| 33  | j     | 24    | 0        | 35       | 0       | 0            |
| 33  | m     | 35    | 0        | 46       | 1       | 0            |
| 33  | z     | 35    | 0        | 46       | 1       | 0            |
| 34  | C     | 107   | 0        | 130      | 2       | 0            |
| 34  | D     | 44    | 0        | 57       | 2       | 0            |
| 34  | H     | 58    | 0        | 74       | 1       | 0            |
| 34  | J     | 61    | 0        | 83       | 3       | 0            |
| 34  | c     | 169   | 0        | 215      | 4       | 0            |
| 34  | d     | 47    | 0        | 59       | 1       | 0            |
| 34  | h     | 58    | 0        | 74       | 0       | 0            |
| 35  | C     | 102   | 0        | 144      | 1       | 0            |
| 35  | D     | 47    | 0        | 64       | 2       | 0            |
| 35  | M     | 51    | 0        | 72       | 5       | 0            |
| 35  | Y     | 51    | 0        | 72       | 2       | 0            |
| 35  | c     | 99    | 0        | 138      | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | d     | 47    | 0        | 64       | 2       | 0            |
| 35  | m     | 51    | 0        | 72       | 4       | 0            |
| 35  | y     | 51    | 0        | 72       | 1       | 0            |
| 36  | E     | 43    | 0        | 30       | 1       | 0            |
| 36  | V     | 43    | 0        | 30       | 1       | 0            |
| 36  | e     | 43    | 0        | 30       | 1       | 0            |
| 36  | v     | 43    | 0        | 30       | 1       | 0            |
| 37  | H     | 41    | 0        | 56       | 1       | 0            |
| 37  | h     | 41    | 0        | 56       | 1       | 0            |
| 38  | O     | 1     | 0        | 0        | 0       | 0            |
| 38  | o     | 1     | 0        | 0        | 0       | 0            |
| 39  | A     | 92    | 0        | 0        | 1       | 0            |
| 39  | B     | 133   | 0        | 0        | 0       | 0            |
| 39  | C     | 101   | 0        | 0        | 0       | 0            |
| 39  | D     | 91    | 0        | 0        | 1       | 0            |
| 39  | E     | 14    | 0        | 0        | 0       | 0            |
| 39  | F     | 3     | 0        | 0        | 0       | 0            |
| 39  | H     | 11    | 0        | 0        | 0       | 0            |
| 39  | I     | 1     | 0        | 0        | 0       | 0            |
| 39  | J     | 4     | 0        | 0        | 0       | 0            |
| 39  | K     | 1     | 0        | 0        | 0       | 0            |
| 39  | L     | 8     | 0        | 0        | 0       | 0            |
| 39  | M     | 3     | 0        | 0        | 0       | 0            |
| 39  | O     | 37    | 0        | 0        | 0       | 0            |
| 39  | T     | 4     | 0        | 0        | 0       | 0            |
| 39  | U     | 14    | 0        | 0        | 0       | 0            |
| 39  | V     | 26    | 0        | 0        | 0       | 0            |
| 39  | X     | 3     | 0        | 0        | 0       | 0            |
| 39  | a     | 94    | 0        | 0        | 1       | 0            |
| 39  | b     | 137   | 0        | 0        | 0       | 0            |
| 39  | c     | 104   | 0        | 0        | 0       | 0            |
| 39  | d     | 91    | 0        | 0        | 1       | 0            |
| 39  | e     | 15    | 0        | 0        | 0       | 0            |
| 39  | f     | 4     | 0        | 0        | 0       | 0            |
| 39  | h     | 11    | 0        | 0        | 0       | 0            |
| 39  | i     | 3     | 0        | 0        | 0       | 0            |
| 39  | j     | 4     | 0        | 0        | 0       | 0            |
| 39  | k     | 1     | 0        | 0        | 0       | 0            |
| 39  | l     | 10    | 0        | 0        | 0       | 0            |
| 39  | m     | 3     | 0        | 0        | 0       | 0            |
| 39  | o     | 39    | 0        | 0        | 1       | 0            |
| 39  | t     | 4     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 39  | u     | 13    | 0        | 0        | 0       | 0            |
| 39  | v     | 25    | 0        | 0        | 0       | 0            |
| 39  | x     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 51092 | 0        | 51568    | 465     | 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 (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:30:LEU:HD21   | 22:C:515:CLA:H2A  | 1.69                     | 0.74              |
| 3:c:30:LEU:HD21   | 22:c:516:CLA:H2A  | 1.71                     | 0.72              |
| 22:c:507:CLA:H61  | 22:c:517:CLA:H42  | 1.73                     | 0.70              |
| 5:E:8:ARG:HE      | 5:E:13:ILE:HG12   | 1.60                     | 0.66              |
| 3:C:303:MET:HE3   | 3:C:307:ILE:HD11  | 1.78                     | 0.65              |
| 1:A:192:ILE:HG13  | 1:A:293:MET:HE1   | 1.80                     | 0.64              |
| 4:D:192:THR:HG23  | 22:D:405:CLA:HBC2 | 1.80                     | 0.64              |
| 4:D:186:GLN:HB2   | 22:D:405:CLA:HBC1 | 1.79                     | 0.64              |
| 1:a:192:ILE:HG13  | 1:a:293:MET:HE1   | 1.79                     | 0.64              |
| 4:d:186:GLN:HB2   | 22:d:403:CLA:HBC1 | 1.80                     | 0.63              |
| 4:d:192:THR:HG23  | 22:d:403:CLA:HBC2 | 1.80                     | 0.63              |
| 4:D:23:LYS:HG2    | 4:D:135:LEU:HD21  | 1.80                     | 0.63              |
| 3:c:320:GLN:HE21  | 3:c:324:GLY:HA2   | 1.64                     | 0.62              |
| 27:B:625:PLM:H21  | 1:a:102:LEU:HD12  | 1.83                     | 0.61              |
| 21:A:402:CL:CL    | 39:D:584:HOH:O    | 2.53                     | 0.61              |
| 14:t:14:ILE:HG21  | 27:t:101:PLM:H82  | 1.83                     | 0.60              |
| 21:a:403:CL:CL    | 39:d:582:HOH:O    | 2.53                     | 0.60              |
| 4:D:24:ARG:NH2    | 17:X:35:ASP:OD2   | 2.34                     | 0.59              |
| 15:u:46:LYS:HE2   | 15:u:118:GLU:HB2  | 1.82                     | 0.59              |
| 2:B:12:LEU:HB2    | 22:B:612:CLA:HMC2 | 1.84                     | 0.58              |
| 4:d:54:PHE:O      | 5:e:49:THR:OG1    | 2.19                     | 0.58              |
| 2:b:12:LEU:HB2    | 22:b:614:CLA:HMC2 | 1.84                     | 0.58              |
| 3:C:14:ARG:NH2    | 18:Y:45:ASN:O     | 2.37                     | 0.58              |
| 3:c:306:LEU:HD12  | 3:c:328:TYR:HB3   | 1.86                     | 0.58              |
| 22:b:617:CLA:H161 | 7:h:7:LEU:HD21    | 1.86                     | 0.58              |
| 35:D:409:LMG:H121 | 34:J:102:DGD:HB51 | 1.84                     | 0.58              |
| 34:c:505:DGD:HB51 | 35:d:407:LMG:H121 | 1.85                     | 0.57              |
| 26:d:412:SQD:H241 | 6:f:18:VAL:HG22   | 1.85                     | 0.57              |
| 22:A:407:CLA:H152 | 22:C:510:CLA:H13  | 1.85                     | 0.57              |
| 28:A:412:LFA:H142 | 27:A:413:PLM:H31  | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:d:199:MET:HG2   | 25:d:402:PL9:H312 | 1.86                     | 0.57              |
| 2:B:352:GLU:OE1   | 2:B:378:LYS:NZ    | 2.38                     | 0.57              |
| 1:A:45:THR:HG21   | 26:A:410:SQD:H211 | 1.87                     | 0.57              |
| 22:B:615:CLA:H161 | 7:H:7:LEU:HD21    | 1.86                     | 0.57              |
| 31:a:415:LHG:H221 | 4:d:37:LEU:HD21   | 1.87                     | 0.57              |
| 4:D:199:MET:HG2   | 25:D:404:PL9:H312 | 1.86                     | 0.56              |
| 15:U:75:LEU:HD21  | 15:U:101:GLN:HB3  | 1.87                     | 0.56              |
| 2:b:352:GLU:OE1   | 2:b:378:LYS:NZ    | 2.38                     | 0.56              |
| 3:c:225:HIS:HA    | 3:c:228:ILE:HG22  | 1.87                     | 0.56              |
| 13:O:77:LEU:HD12  | 13:O:260:LYS:HD2  | 1.87                     | 0.56              |
| 1:a:215:HIS:ND1   | 25:a:410:PL9:O2   | 2.38                     | 0.56              |
| 15:U:88:VAL:HG23  | 15:U:114:VAL:HG22 | 1.87                     | 0.56              |
| 28:T:102:LFA:H51  | 24:b:602:BCR:H14C | 1.86                     | 0.56              |
| 1:A:188:ALA:HB2   | 1:A:328:MET:HB2   | 1.87                     | 0.56              |
| 28:B:626:LFA:H171 | 28:i:104:LFA:H141 | 1.87                     | 0.56              |
| 4:D:126:MET:HE3   | 4:D:150:ILE:HD12  | 1.86                     | 0.56              |
| 1:a:188:ALA:HB2   | 1:a:328:MET:HB2   | 1.88                     | 0.56              |
| 2:B:501:ASP:OD2   | 17:X:39:ARG:NH1   | 2.39                     | 0.55              |
| 15:u:88:VAL:HG23  | 15:u:114:VAL:HG22 | 1.89                     | 0.55              |
| 1:a:342:ASP:HB2   | 4:d:352:LEU:HD21  | 1.88                     | 0.55              |
| 4:D:54:PHE:O      | 5:E:49:THR:OG1    | 2.19                     | 0.55              |
| 23:a:420:PHO:HBC3 | 4:d:279:LEU:HD22  | 1.89                     | 0.55              |
| 2:b:18:ARG:NH2    | 26:b:601:SQD:O9   | 2.36                     | 0.55              |
| 4:d:126:MET:HE3   | 4:d:150:ILE:HD12  | 1.89                     | 0.54              |
| 1:A:121:LEU:HD11  | 22:C:509:CLA:H152 | 1.89                     | 0.54              |
| 3:C:311:LYS:NZ    | 3:C:377:GLU:OE1   | 2.40                     | 0.54              |
| 34:c:504:DGD:HA21 | 22:c:509:CLA:H42  | 1.88                     | 0.54              |
| 31:l:101:LHG:H322 | 12:m:18:PRO:HB3   | 1.88                     | 0.54              |
| 3:C:52:ALA:O      | 3:C:56:THR:OG1    | 2.25                     | 0.54              |
| 31:d:405:LHG:H351 | 31:d:405:LHG:H101 | 1.89                     | 0.54              |
| 15:u:75:LEU:HD21  | 15:u:101:GLN:HB3  | 1.89                     | 0.54              |
| 2:B:42:LEU:HD13   | 2:B:94:GLU:HG3    | 1.90                     | 0.54              |
| 2:B:116:VAL:HG21  | 24:B:619:BCR:H271 | 1.90                     | 0.54              |
| 4:D:279:LEU:HD22  | 23:D:403:PHO:HBC3 | 1.89                     | 0.54              |
| 1:a:82:VAL:HB     | 1:a:174:LEU:HB2   | 1.90                     | 0.54              |
| 4:d:23:LYS:HE3    | 4:d:135:LEU:HD11  | 1.90                     | 0.54              |
| 1:A:82:VAL:HB     | 1:A:174:LEU:HB2   | 1.90                     | 0.54              |
| 1:A:162:PRO:HB3   | 1:A:168:PHE:HA    | 1.90                     | 0.53              |
| 3:C:71:GLU:OE2    | 3:C:386:HIS:NE2   | 2.37                     | 0.53              |
| 1:a:165:GLN:NE2   | 39:a:510:HOH:O    | 2.40                     | 0.53              |
| 2:b:311:PHE:O     | 2:b:317:ASN:ND2   | 2.41                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:c:71:GLU:OE2    | 3:c:386:HIS:NE2   | 2.39                     | 0.53              |
| 13:o:111:LEU:HG   | 13:o:119:LEU:HD12 | 1.90                     | 0.53              |
| 1:A:267:ASN:HB3   | 1:A:270:SER:HB3   | 1.91                     | 0.53              |
| 4:D:302:GLU:OE1   | 4:D:315:TYR:OH    | 2.22                     | 0.53              |
| 1:A:215:HIS:ND1   | 25:A:409:PL9:O2   | 2.38                     | 0.53              |
| 1:A:283:VAL:HA    | 1:A:286:THR:HG22  | 1.91                     | 0.53              |
| 2:B:311:PHE:O     | 2:B:317:ASN:ND2   | 2.42                     | 0.52              |
| 24:B:632:BCR:HC7  | 14:t:18:PHE:HD1   | 1.74                     | 0.52              |
| 10:K:21:LEU:HD21  | 24:Y:102:BCR:HC31 | 1.90                     | 0.52              |
| 3:C:331:ARG:NH1   | 3:C:335:GLY:O     | 2.42                     | 0.52              |
| 1:a:162:PRO:HB3   | 1:a:168:PHE:HA    | 1.90                     | 0.52              |
| 3:c:331:ARG:NH1   | 3:c:335:GLY:O     | 2.42                     | 0.52              |
| 24:B:617:BCR:H402 | 26:l:102:SQD:H82  | 1.92                     | 0.52              |
| 15:U:56:ASP:OD2   | 15:U:115:THR:OG1  | 2.24                     | 0.52              |
| 3:c:285:TYR:O     | 3:c:411:ARG:NH2   | 2.42                     | 0.52              |
| 25:a:410:PL9:H221 | 23:a:420:PHO:HMA2 | 1.92                     | 0.52              |
| 15:u:56:ASP:OD2   | 15:u:115:THR:OG1  | 2.26                     | 0.52              |
| 22:a:408:CLA:H152 | 22:c:511:CLA:H13  | 1.91                     | 0.52              |
| 33:B:628:LMT:H102 | 27:B:629:PLM:HF1  | 1.91                     | 0.51              |
| 4:D:23:LYS:HE2    | 4:D:135:LEU:HD11  | 1.92                     | 0.51              |
| 13:O:195:ASP:OD1  | 13:O:195:ASP:N    | 2.43                     | 0.51              |
| 22:c:513:CLA:HBC3 | 22:c:515:CLA:H71  | 1.92                     | 0.51              |
| 1:A:84:PRO:HA     | 1:A:112:TYR:CG    | 2.46                     | 0.51              |
| 1:A:85:SER:HA     | 1:A:109:GLY:HA3   | 1.93                     | 0.51              |
| 4:D:172:SER:HB2   | 4:D:177:ALA:HB1   | 1.93                     | 0.51              |
| 1:A:46:ILE:HD13   | 26:A:410:SQD:H371 | 1.93                     | 0.51              |
| 3:C:285:TYR:O     | 3:C:411:ARG:NH2   | 2.41                     | 0.51              |
| 1:a:84:PRO:HA     | 1:a:112:TYR:CG    | 2.46                     | 0.51              |
| 1:a:283:VAL:HA    | 1:a:286:THR:HG22  | 1.92                     | 0.51              |
| 22:c:506:CLA:H203 | 22:c:512:CLA:H13  | 1.93                     | 0.51              |
| 1:A:165:GLN:NE2   | 39:A:511:HOH:O    | 2.43                     | 0.51              |
| 3:C:175:ASP:O     | 3:C:182:GLY:HA2   | 2.10                     | 0.51              |
| 1:a:85:SER:HA     | 1:a:109:GLY:HA3   | 1.92                     | 0.51              |
| 25:a:410:PL9:H422 | 26:d:412:SQD:H252 | 1.92                     | 0.51              |
| 2:b:256:MET:HA    | 2:b:263:THR:HG21  | 1.93                     | 0.51              |
| 22:C:512:CLA:HBC3 | 22:C:514:CLA:H71  | 1.91                     | 0.50              |
| 34:D:411:DGD:HD4  | 5:E:45:ASP:HB3    | 1.93                     | 0.50              |
| 14:T:18:PHE:HD1   | 24:b:602:BCR:HC7  | 1.76                     | 0.50              |
| 3:c:26:GLY:HA3    | 22:c:516:CLA:HMD2 | 1.93                     | 0.50              |
| 4:d:172:SER:HB2   | 4:d:177:ALA:HB1   | 1.93                     | 0.50              |
| 2:B:399:VAL:HG12  | 2:B:417:VAL:HG22  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:A:415:SQD:H262 | 31:A:417:LHG:H142 | 1.92                     | 0.50              |
| 13:O:58:ILE:HG21  | 13:O:119:LEU:HD21 | 1.93                     | 0.50              |
| 31:D:407:LHG:H101 | 31:D:407:LHG:H351 | 1.94                     | 0.50              |
| 3:C:213:VAL:HG13  | 3:C:277:PHE:HA    | 1.93                     | 0.50              |
| 10:k:21:LEU:HD21  | 24:y:102:BCR:HC31 | 1.92                     | 0.50              |
| 2:B:39:LEU:HD13   | 33:B:630:LMT:H81  | 1.94                     | 0.50              |
| 4:D:79:SER:HA     | 4:D:172:SER:HB3   | 1.94                     | 0.49              |
| 13:o:195:ASP:OD1  | 13:o:195:ASP:N    | 2.43                     | 0.49              |
| 13:O:223:ILE:HG13 | 13:O:243:SER:HB3  | 1.95                     | 0.49              |
| 22:b:609:CLA:H122 | 35:m:101:LMG:H241 | 1.93                     | 0.49              |
| 1:a:201:GLY:HA3   | 1:a:286:THR:HB    | 1.94                     | 0.49              |
| 18:y:39:LEU:HD21  | 19:z:25:VAL:HA    | 1.94                     | 0.49              |
| 22:C:507:CLA:H18  | 22:C:514:CLA:HBB2 | 1.95                     | 0.49              |
| 3:c:213:VAL:HG13  | 3:c:277:PHE:HA    | 1.94                     | 0.49              |
| 13:o:223:ILE:HG13 | 13:o:243:SER:HB3  | 1.95                     | 0.49              |
| 16:V:103:LYS:HG2  | 16:V:121:LEU:HD12 | 1.95                     | 0.49              |
| 2:b:42:LEU:HD13   | 2:b:94:GLU:HG3    | 1.95                     | 0.49              |
| 2:b:498:LYS:HE3   | 4:d:23:LYS:HE2    | 1.95                     | 0.49              |
| 4:d:296:TYR:OH    | 4:d:326:ARG:NH1   | 2.40                     | 0.49              |
| 31:a:415:LHG:HC42 | 27:e:102:PLM:H51  | 1.95                     | 0.49              |
| 2:b:7:ARG:O       | 2:b:10:THR:OG1    | 2.25                     | 0.49              |
| 12:m:14:PHE:HD2   | 35:m:101:LMG:H361 | 1.78                     | 0.49              |
| 2:B:247:PHE:HB2   | 22:B:608:CLA:HBC1 | 1.96                     | 0.48              |
| 13:O:111:LEU:HG   | 13:O:119:LEU:HD12 | 1.94                     | 0.48              |
| 3:c:49:VAL:HG13   | 3:c:106:HIS:HD2   | 1.78                     | 0.48              |
| 28:I:103:LFA:H121 | 28:b:623:LFA:H191 | 1.94                     | 0.48              |
| 26:b:601:SQD:H112 | 22:b:616:CLA:H43  | 1.95                     | 0.48              |
| 26:a:417:SQD:H302 | 22:c:513:CLA:H71  | 1.95                     | 0.48              |
| 2:b:498:LYS:HA    | 4:d:24:ARG:HA     | 1.95                     | 0.48              |
| 22:c:508:CLA:H18  | 22:c:515:CLA:HBB2 | 1.95                     | 0.48              |
| 16:v:125:ASP:OD1  | 16:v:125:ASP:N    | 2.45                     | 0.48              |
| 3:c:67:LYS:HE3    | 3:c:72:GLN:HG2    | 1.95                     | 0.48              |
| 1:A:201:GLY:HA3   | 1:A:286:THR:HB    | 1.95                     | 0.48              |
| 22:B:602:CLA:H101 | 22:B:609:CLA:H193 | 1.94                     | 0.48              |
| 28:B:620:LFA:H81  | 33:B:630:LMT:H121 | 1.94                     | 0.48              |
| 28:J:104:LFA:H62  | 18:Y:18:VAL:HG11  | 1.96                     | 0.48              |
| 12:M:4:ASN:ND2    | 35:M:101:LMG:O10  | 2.44                     | 0.48              |
| 11:l:26:VAL:HG21  | 31:l:101:LHG:H192 | 1.95                     | 0.48              |
| 22:B:604:CLA:H172 | 22:B:604:CLA:H13  | 1.75                     | 0.48              |
| 22:B:612:CLA:H171 | 22:B:613:CLA:HBB2 | 1.96                     | 0.48              |
| 22:b:614:CLA:H171 | 22:b:615:CLA:HBB2 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:d:93:TRP:HB3    | 27:x:101:PLM:H41  | 1.95                     | 0.48              |
| 31:d:406:LHG:H141 | 31:d:406:LHG:H292 | 1.95                     | 0.48              |
| 2:B:256:MET:HA    | 2:B:263:THR:HG21  | 1.95                     | 0.48              |
| 3:C:26:GLY:HA3    | 22:C:515:CLA:HMD2 | 1.95                     | 0.48              |
| 26:D:412:SQD:H241 | 6:F:18:VAL:HG22   | 1.95                     | 0.48              |
| 11:L:26:VAL:HG21  | 31:L:101:LHG:H192 | 1.95                     | 0.48              |
| 2:b:23:HIS:ND1    | 22:b:617:CLA:OBD  | 2.30                     | 0.48              |
| 1:A:38:ILE:HG23   | 26:A:410:SQD:H151 | 1.96                     | 0.48              |
| 1:A:340:PRO:HG3   | 15:U:133:TYR:CG   | 2.49                     | 0.48              |
| 2:B:25:MET:HG2    | 24:B:617:BCR:H23C | 1.96                     | 0.48              |
| 22:b:604:CLA:H101 | 22:b:611:CLA:H193 | 1.95                     | 0.48              |
| 3:c:306:LEU:HD21  | 3:c:368:ILE:HG23  | 1.96                     | 0.48              |
| 34:C:504:DGD:HA21 | 22:C:508:CLA:H42  | 1.96                     | 0.48              |
| 1:a:146:ALA:HB2   | 31:a:421:LHG:H261 | 1.95                     | 0.48              |
| 2:b:474:LEU:HD11  | 22:b:610:CLA:HAA2 | 1.96                     | 0.47              |
| 11:l:14:ARG:HH22  | 26:l:102:SQD:H3   | 1.79                     | 0.47              |
| 2:b:399:VAL:HG12  | 2:b:417:VAL:HG22  | 1.96                     | 0.47              |
| 2:B:498:LYS:HA    | 4:D:24:ARG:HA     | 1.96                     | 0.47              |
| 4:d:79:SER:HA     | 4:d:172:SER:HB3   | 1.96                     | 0.47              |
| 22:B:607:CLA:H2   | 35:M:101:LMG:H151 | 1.96                     | 0.47              |
| 3:C:197:ILE:HG23  | 24:C:502:BCR:H382 | 1.96                     | 0.47              |
| 1:a:77:ILE:HD11   | 14:t:6:TYR:HB3    | 1.97                     | 0.47              |
| 2:b:385:ARG:NH2   | 13:o:193:GLY:O    | 2.44                     | 0.47              |
| 22:c:507:CLA:HBB2 | 22:c:515:CLA:H151 | 1.96                     | 0.47              |
| 2:B:497:GLN:HG3   | 2:B:506:ARG:HD2   | 1.97                     | 0.47              |
| 33:B:630:LMT:H3O1 | 4:d:304:ARG:HH22  | 1.61                     | 0.47              |
| 3:C:226:ILE:HD13  | 27:C:524:PLM:H61  | 1.96                     | 0.47              |
| 22:C:506:CLA:HBB2 | 22:C:514:CLA:H151 | 1.97                     | 0.47              |
| 33:J:103:LMT:H102 | 33:J:103:LMT:H71  | 1.69                     | 0.47              |
| 14:T:7:VAL:HG12   | 33:T:101:LMT:H122 | 1.95                     | 0.47              |
| 2:b:116:VAL:HG21  | 24:b:620:BCR:H292 | 1.97                     | 0.47              |
| 2:b:247:PHE:HB2   | 22:b:610:CLA:HBC1 | 1.95                     | 0.47              |
| 1:a:103:ASP:OD1   | 32:a:401:GOL:O2   | 2.28                     | 0.47              |
| 2:B:109:LEU:HD13  | 26:a:411:SQD:H262 | 1.97                     | 0.47              |
| 22:B:607:CLA:H122 | 35:M:101:LMG:H241 | 1.95                     | 0.47              |
| 4:d:236:ASN:HB3   | 4:d:239:GLN:HB3   | 1.97                     | 0.47              |
| 5:e:30:LEU:HD11   | 36:e:103:HEM:HAB  | 1.97                     | 0.47              |
| 3:c:197:ILE:HG23  | 24:c:502:BCR:H382 | 1.97                     | 0.47              |
| 16:v:103:LYS:HG2  | 16:v:121:LEU:HD12 | 1.96                     | 0.46              |
| 1:A:77:ILE:HD11   | 14:T:6:TYR:HB3    | 1.96                     | 0.46              |
| 1:A:131:TRP:CH2   | 22:C:509:CLA:HAA2 | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:155:VAL:HG11  | 22:C:516:CLA:HBA2 | 1.97                     | 0.46              |
| 13:O:250:ASP:HB3  | 13:O:253:ALA:HB3  | 1.98                     | 0.46              |
| 1:a:131:TRP:CH2   | 22:c:510:CLA:HAA2 | 2.50                     | 0.46              |
| 3:C:49:VAL:HG13   | 3:C:106:HIS:HD2   | 1.79                     | 0.46              |
| 27:D:402:PLM:H41  | 27:D:410:PLM:H82  | 1.98                     | 0.46              |
| 2:b:158:LEU:HB3   | 2:b:199:VAL:HG22  | 1.96                     | 0.46              |
| 3:c:206:PHE:HZ    | 35:c:519:LMG:H161 | 1.81                     | 0.46              |
| 24:C:502:BCR:H16C | 22:C:511:CLA:H142 | 1.96                     | 0.46              |
| 1:a:140:ARG:HB2   | 4:d:220:ASN:HA    | 1.97                     | 0.46              |
| 1:a:214:MET:HB3   | 25:a:410:PL9:H103 | 1.97                     | 0.46              |
| 3:c:123:ARG:NH1   | 33:z:101:LMT:O3B  | 2.48                     | 0.46              |
| 2:b:379:ALA:HA    | 2:b:390:TYR:HB3   | 1.97                     | 0.46              |
| 22:b:609:CLA:H2   | 35:m:101:LMG:H151 | 1.98                     | 0.46              |
| 24:B:617:BCR:H341 | 24:B:632:BCR:H24C | 1.97                     | 0.46              |
| 3:C:60:LEU:HD11   | 3:C:96:THR:HB     | 1.98                     | 0.46              |
| 1:a:63:ILE:HB     | 3:c:323:THR:HG21  | 1.97                     | 0.46              |
| 1:a:267:ASN:HB3   | 1:a:270:SER:HB3   | 1.96                     | 0.46              |
| 1:a:340:PRO:HG3   | 15:u:133:TYR:CG   | 2.51                     | 0.46              |
| 10:k:29:PRO:O     | 10:k:32:PHE:HB2   | 2.16                     | 0.46              |
| 1:A:43:ALA:HB1    | 24:A:408:BCR:H362 | 1.97                     | 0.46              |
| 1:A:140:ARG:HB2   | 4:D:220:ASN:HA    | 1.97                     | 0.46              |
| 3:C:190:PRO:HD2   | 27:C:524:PLM:H22  | 1.98                     | 0.46              |
| 37:h:102:RRX:H3   | 17:x:2:THR:N      | 2.13                     | 0.46              |
| 2:B:23:HIS:ND1    | 22:B:615:CLA:OBD  | 2.29                     | 0.46              |
| 2:B:155:ALA:O     | 2:B:159:THR:OG1   | 2.28                     | 0.46              |
| 22:b:615:CLA:H18  | 31:d:405:LHG:H202 | 1.98                     | 0.46              |
| 22:A:404:CLA:H152 | 23:A:406:PHO:H52  | 1.98                     | 0.46              |
| 24:B:632:BCR:H351 | 26:l:102:SQD:H201 | 1.98                     | 0.46              |
| 5:E:30:LEU:HD11   | 36:E:104:HEM:HAB  | 1.97                     | 0.46              |
| 33:J:103:LMT:H92  | 35:Y:101:LMG:H332 | 1.98                     | 0.46              |
| 22:c:518:CLA:HBA2 | 27:c:520:PLM:H61  | 1.98                     | 0.46              |
| 4:d:148:ALA:HB2   | 4:d:276:VAL:HG13  | 1.98                     | 0.46              |
| 2:B:7:ARG:O       | 2:B:10:THR:OG1    | 2.26                     | 0.45              |
| 2:B:33:TRP:CD1    | 24:B:632:BCR:H381 | 2.51                     | 0.45              |
| 18:Y:39:LEU:HD21  | 19:Z:25:VAL:HA    | 1.98                     | 0.45              |
| 22:a:406:CLA:HED1 | 34:c:505:DGD:HBW2 | 1.98                     | 0.45              |
| 31:a:421:LHG:H151 | 31:a:421:LHG:H331 | 1.98                     | 0.45              |
| 9:J:9:PRO:HD2     | 9:J:12:ILE:HD12   | 1.99                     | 0.45              |
| 2:b:33:TRP:CD1    | 24:b:602:BCR:H381 | 2.51                     | 0.45              |
| 22:b:615:CLA:H193 | 24:b:619:BCR:HC32 | 1.99                     | 0.45              |
| 1:A:63:ILE:HB     | 3:C:323:THR:HG21  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:c:390:GLY:HA3   | 3:c:408:VAL:HG22  | 1.97                     | 0.45              |
| 15:u:44:ASP:OD1   | 15:u:44:ASP:N     | 2.49                     | 0.45              |
| 2:B:158:LEU:HB3   | 2:B:199:VAL:HG22  | 1.99                     | 0.45              |
| 17:x:16:SER:HB3   | 27:x:101:PLM:HA1  | 1.98                     | 0.45              |
| 33:C:518:LMT:H6'2 | 8:I:26:GLY:HA3    | 1.99                     | 0.45              |
| 12:M:14:PHE:HD2   | 35:M:101:LMG:H361 | 1.80                     | 0.45              |
| 24:T:103:BCR:H23C | 2:b:25:MET:HG2    | 1.98                     | 0.45              |
| 26:A:415:SQD:O7   | 3:C:16:GLN:NE2    | 2.42                     | 0.45              |
| 2:B:497:GLN:HB2   | 2:B:504:THR:HB    | 1.98                     | 0.45              |
| 10:K:29:PRO:O     | 10:K:32:PHE:HB2   | 2.16                     | 0.45              |
| 22:c:518:CLA:HBD  | 27:c:520:PLM:H32  | 1.98                     | 0.45              |
| 2:B:70:GLY:HA2    | 2:B:178:VAL:HG21  | 1.98                     | 0.45              |
| 12:M:31:SER:OG    | 12:m:31:SER:OG    | 2.34                     | 0.45              |
| 2:B:383:PHE:CZ    | 13:O:193:GLY:HA2  | 2.52                     | 0.45              |
| 3:C:452:GLU:OE2   | 4:D:245:SER:OG    | 2.32                     | 0.45              |
| 24:T:103:BCR:H341 | 24:b:602:BCR:H24C | 1.99                     | 0.45              |
| 2:B:74:SER:OG     | 2:B:94:GLU:OE2    | 2.32                     | 0.45              |
| 2:B:474:LEU:O     | 4:D:134:ARG:NH1   | 2.50                     | 0.45              |
| 22:B:613:CLA:H193 | 24:B:618:BCR:HC32 | 1.99                     | 0.45              |
| 27:B:622:PLM:H52  | 27:B:622:PLM:H82  | 1.77                     | 0.45              |
| 34:C:504:DGD:HA42 | 35:Y:101:LMG:H391 | 1.98                     | 0.45              |
| 4:d:103:ARG:HG3   | 5:e:73:LYS:HG3    | 1.99                     | 0.45              |
| 13:o:58:ILE:HG21  | 13:o:119:LEU:HD21 | 1.98                     | 0.45              |
| 25:A:409:PL9:H251 | 25:A:409:PL9:H271 | 1.59                     | 0.44              |
| 22:C:505:CLA:C2D  | 22:C:507:CLA:H2   | 2.47                     | 0.44              |
| 24:c:502:BCR:H16C | 22:c:512:CLA:H142 | 1.99                     | 0.44              |
| 22:B:615:CLA:H2   | 22:B:616:CLA:CBB  | 2.47                     | 0.44              |
| 13:O:143:PRO:HG2  | 13:O:248:ASP:HB3  | 1.99                     | 0.44              |
| 1:a:102:LEU:HD23  | 1:a:102:LEU:HA    | 1.84                     | 0.44              |
| 4:d:12:ARG:NH1    | 4:d:20:ASP:OD2    | 2.51                     | 0.44              |
| 28:I:103:LFA:H102 | 28:b:623:LFA:H171 | 1.99                     | 0.44              |
| 31:a:415:LHG:H241 | 31:a:415:LHG:HC61 | 1.74                     | 0.44              |
| 16:v:38:LEU:HD12  | 16:v:95:ILE:HB    | 1.99                     | 0.44              |
| 2:B:91:TRP:HE1    | 27:B:621:PLM:H42  | 1.82                     | 0.44              |
| 3:C:150:GLY:HA2   | 3:C:236:GLY:HA2   | 1.98                     | 0.44              |
| 4:D:148:ALA:HB2   | 4:D:276:VAL:HG13  | 1.99                     | 0.44              |
| 2:b:474:LEU:O     | 4:d:134:ARG:NH1   | 2.50                     | 0.44              |
| 24:b:619:BCR:H24C | 24:b:619:BCR:H371 | 1.87                     | 0.44              |
| 9:j:9:PRO:HD2     | 9:j:12:ILE:HD12   | 1.99                     | 0.44              |
| 13:o:210:ARG:HG3  | 13:o:215:ARG:HH12 | 1.81                     | 0.44              |
| 2:b:70:GLY:HA2    | 2:b:178:VAL:HG21  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:498:LYS:HD2   | 4:d:20:ASP:HA     | 2.00                     | 0.44              |
| 3:c:123:ARG:HD2   | 3:c:123:ARG:HA    | 1.80                     | 0.44              |
| 22:d:401:CLA:H52  | 25:d:402:PL9:H151 | 2.00                     | 0.44              |
| 14:t:11:ALA:HA    | 27:t:101:PLM:H52  | 2.00                     | 0.44              |
| 5:E:10:PHE:HB3    | 28:E:102:LFA:H132 | 1.99                     | 0.44              |
| 22:b:612:CLA:H192 | 22:b:617:CLA:HMD3 | 1.99                     | 0.44              |
| 34:c:504:DGD:HBT2 | 22:c:513:CLA:H192 | 1.99                     | 0.44              |
| 4:d:159:ILE:HG21  | 4:d:287:VAL:HG22  | 1.99                     | 0.44              |
| 37:H:102:RRX:H3   | 17:X:2:THR:N      | 2.16                     | 0.44              |
| 1:a:250:ALA:HA    | 2:b:491:VAL:HG11  | 2.00                     | 0.44              |
| 22:c:506:CLA:C2D  | 22:c:508:CLA:H2   | 2.48                     | 0.43              |
| 4:d:141:TYR:OH    | 31:d:405:LHG:O4   | 2.32                     | 0.43              |
| 2:B:278:SER:HB3   | 2:B:281:GLN:HE21  | 1.82                     | 0.43              |
| 2:B:383:PHE:N     | 4:D:344:GLU:O     | 2.44                     | 0.43              |
| 22:B:610:CLA:H192 | 22:B:615:CLA:HMD3 | 2.00                     | 0.43              |
| 22:C:514:CLA:HBC3 | 22:C:514:CLA:H192 | 2.00                     | 0.43              |
| 4:D:160:TYR:HA    | 4:D:290:ALA:HB2   | 2.00                     | 0.43              |
| 4:d:103:ARG:HH21  | 5:e:77:GLU:HG2    | 1.83                     | 0.43              |
| 22:B:611:CLA:H112 | 22:B:611:CLA:H72  | 1.81                     | 0.43              |
| 33:M:102:LMT:H112 | 12:m:17:VAL:HG13  | 1.99                     | 0.43              |
| 22:d:404:CLA:H202 | 22:d:404:CLA:H161 | 1.81                     | 0.43              |
| 26:a:411:SQD:H161 | 26:a:411:SQD:H192 | 1.44                     | 0.43              |
| 2:b:383:PHE:CZ    | 13:o:193:GLY:HA2  | 2.53                     | 0.43              |
| 22:b:607:CLA:H41  | 22:b:607:CLA:H62  | 1.74                     | 0.43              |
| 22:b:610:CLA:H3A  | 22:b:610:CLA:HBA2 | 1.84                     | 0.43              |
| 22:b:617:CLA:H2   | 22:b:618:CLA:CBB  | 2.48                     | 0.43              |
| 22:B:606:CLA:H61  | 22:B:606:CLA:H102 | 1.81                     | 0.43              |
| 3:C:206:PHE:HZ    | 35:C:519:LMG:H161 | 1.82                     | 0.43              |
| 1:a:93:PHE:HZ     | 22:a:408:CLA:HAA1 | 1.84                     | 0.43              |
| 3:c:150:GLY:HA2   | 3:c:236:GLY:HA2   | 1.99                     | 0.43              |
| 4:d:160:TYR:HA    | 4:d:290:ALA:HB2   | 2.01                     | 0.43              |
| 2:B:464:PHE:HD2   | 22:B:611:CLA:HAC2 | 1.83                     | 0.43              |
| 22:c:506:CLA:C3D  | 22:c:508:CLA:H2   | 2.49                     | 0.43              |
| 4:d:51:GLY:HA3    | 4:d:78:VAL:HG22   | 2.01                     | 0.43              |
| 35:m:101:LMG:H171 | 35:m:101:LMG:H142 | 1.90                     | 0.43              |
| 16:v:59:PHE:HA    | 16:v:63:CYS:SG    | 2.59                     | 0.43              |
| 4:D:51:GLY:HA3    | 4:D:78:VAL:HG22   | 2.01                     | 0.43              |
| 2:b:384:ARG:NH2   | 4:d:349:GLY:O     | 2.48                     | 0.43              |
| 9:j:14:ALA:HB2    | 27:j:103:PLM:H82  | 1.99                     | 0.43              |
| 13:o:50:ASP:HA    | 13:o:229:LYS:HE2  | 2.00                     | 0.43              |
| 3:C:403:ASN:OD1   | 34:J:102:DGD:O4D  | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:17:VAL:HG13  | 33:m:102:LMT:H112 | 2.01                     | 0.43              |
| 1:a:65:GLU:OE2    | 1:a:334:ARG:NH2   | 2.51                     | 0.43              |
| 27:B:625:PLM:H52  | 28:B:626:LFA:H192 | 2.01                     | 0.43              |
| 22:C:505:CLA:C3D  | 22:C:507:CLA:H2   | 2.48                     | 0.43              |
| 4:D:159:ILE:HG21  | 4:D:287:VAL:HG22  | 2.01                     | 0.43              |
| 4:D:161:PRO:HB3   | 4:D:170:ALA:HB2   | 2.01                     | 0.43              |
| 25:A:409:PL9:H371 | 25:A:409:PL9:H351 | 1.75                     | 0.43              |
| 22:B:604:CLA:H12  | 22:B:605:CLA:ND   | 2.34                     | 0.43              |
| 3:C:394:SER:HA    | 3:C:408:VAL:HG23  | 2.00                     | 0.43              |
| 4:D:141:TYR:OH    | 31:D:407:LHG:O4   | 2.31                     | 0.43              |
| 13:O:50:ASP:HA    | 13:O:229:LYS:HE2  | 2.01                     | 0.43              |
| 19:Z:55:GLY:O     | 19:Z:58:ASN:HB3   | 2.18                     | 0.43              |
| 26:a:417:SQD:O7   | 3:c:16:GLN:NE2    | 2.41                     | 0.42              |
| 2:b:464:PHE:HD2   | 22:b:613:CLA:HAC2 | 1.83                     | 0.42              |
| 22:D:401:CLA:H52  | 25:D:404:PL9:H151 | 2.00                     | 0.42              |
| 31:D:408:LHG:H182 | 14:T:17:PHE:HZ    | 1.85                     | 0.42              |
| 24:c:502:BCR:H341 | 22:c:510:CLA:HBC2 | 2.01                     | 0.42              |
| 34:d:410:DGD:HA51 | 34:d:410:DGD:HA22 | 1.81                     | 0.42              |
| 26:d:412:SQD:H281 | 17:x:27:VAL:HG11  | 2.01                     | 0.42              |
| 16:v:29:LEU:HD23  | 16:v:49:GLU:HG3   | 2.00                     | 0.42              |
| 27:L:102:PLM:H41  | 27:L:102:PLM:H71  | 1.83                     | 0.42              |
| 13:O:82:PRO:HG3   | 13:O:89:ALA:HB2   | 2.02                     | 0.42              |
| 1:a:308:ASP:OD1   | 1:a:312:ASN:N     | 2.52                     | 0.42              |
| 13:o:102:THR:HG22 | 13:o:132:VAL:HG22 | 2.01                     | 0.42              |
| 22:C:505:CLA:H151 | 22:C:511:CLA:H52  | 2.00                     | 0.42              |
| 36:V:201:HEM:HMB1 | 36:V:201:HEM:HBB2 | 2.02                     | 0.42              |
| 22:b:606:CLA:H12  | 22:b:607:CLA:ND   | 2.34                     | 0.42              |
| 3:c:270:MET:HG2   | 22:c:506:CLA:H61  | 2.02                     | 0.42              |
| 22:c:515:CLA:H192 | 22:c:515:CLA:HBC3 | 2.00                     | 0.42              |
| 4:d:24:ARG:NH2    | 17:x:35:ASP:OD2   | 2.50                     | 0.42              |
| 4:d:302:GLU:OE2   | 4:d:315:TYR:OH    | 2.27                     | 0.42              |
| 13:o:226:ASN:ND2  | 39:o:408:HOH:O    | 2.51                     | 0.42              |
| 22:B:615:CLA:H2   | 22:B:616:CLA:HBB2 | 2.01                     | 0.42              |
| 13:O:43:ASN:O     | 13:O:103:SER:OG   | 2.34                     | 0.42              |
| 1:A:65:GLU:OE2    | 1:A:334:ARG:NH2   | 2.52                     | 0.42              |
| 22:A:405:CLA:HED1 | 34:J:102:DGD:HBW2 | 2.00                     | 0.42              |
| 26:A:415:SQD:H461 | 26:A:415:SQD:H241 | 1.78                     | 0.42              |
| 22:C:516:CLA:H91  | 22:C:516:CLA:H111 | 1.80                     | 0.42              |
| 35:D:409:LMG:H412 | 6:F:30:THR:HG21   | 2.01                     | 0.42              |
| 24:F:101:BCR:H20C | 24:F:101:BCR:H361 | 1.94                     | 0.42              |
| 2:b:497:GLN:HB2   | 2:b:504:THR:HB    | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:d:402:PL9:H43  | 25:d:402:PL9:H472 | 1.88                     | 0.42              |
| 2:B:450:TRP:NE1   | 22:B:607:CLA:HBA1 | 2.35                     | 0.42              |
| 22:C:505:CLA:HBB2 | 22:C:511:CLA:H61  | 2.02                     | 0.42              |
| 25:D:404:PL9:H201 | 31:L:101:LHG:H202 | 2.02                     | 0.42              |
| 22:c:511:CLA:H18  | 22:c:511:CLA:H122 | 2.00                     | 0.42              |
| 25:d:402:PL9:H201 | 31:l:101:LHG:H202 | 2.01                     | 0.42              |
| 24:C:502:BCR:H352 | 22:C:510:CLA:H143 | 2.01                     | 0.42              |
| 5:E:14:ILE:O      | 5:E:20:TRP:NE1    | 2.52                     | 0.42              |
| 3:c:305:PHE:HE2   | 3:c:384:MET:HE1   | 1.85                     | 0.42              |
| 35:d:407:LMG:H412 | 6:f:30:THR:HG21   | 2.01                     | 0.42              |
| 27:A:413:PLM:H71  | 27:A:413:PLM:H42  | 1.73                     | 0.42              |
| 35:M:101:LMG:H171 | 35:M:101:LMG:H142 | 1.89                     | 0.42              |
| 22:a:405:CLA:H152 | 23:a:407:PHO:H52  | 2.01                     | 0.42              |
| 1:A:183:MET:HB3   | 22:A:404:CLA:HBC2 | 2.02                     | 0.42              |
| 1:A:277:ALA:HB1   | 26:A:415:SQD:H152 | 2.01                     | 0.42              |
| 3:C:228:ILE:HD13  | 3:C:228:ILE:HA    | 1.91                     | 0.42              |
| 28:E:102:LFA:H51  | 28:J:101:LFA:H42  | 2.01                     | 0.42              |
| 10:K:20:PRO:O     | 10:K:23:ASP:HB2   | 2.19                     | 0.42              |
| 11:L:22:LEU:HG    | 31:L:101:LHG:H181 | 2.02                     | 0.42              |
| 35:c:524:LMG:HC8  | 35:c:524:LMG:HC1  | 1.83                     | 0.42              |
| 2:B:422:ARG:NH1   | 13:O:195:ASP:OD2  | 2.53                     | 0.41              |
| 26:D:412:SQD:H282 | 26:D:412:SQD:H311 | 1.84                     | 0.41              |
| 2:b:393:GLU:HB3   | 15:u:48:GLY:HA2   | 2.01                     | 0.41              |
| 13:o:162:ILE:HG21 | 13:o:237:ILE:HG21 | 2.02                     | 0.41              |
| 1:A:308:ASP:OD1   | 1:A:312:ASN:N     | 2.53                     | 0.41              |
| 2:B:33:TRP:HD1    | 24:B:632:BCR:H381 | 1.85                     | 0.41              |
| 2:B:78:TRP:HZ3    | 2:B:80:ILE:HG23   | 1.85                     | 0.41              |
| 3:C:67:LYS:HE3    | 3:C:72:GLN:HG2    | 2.01                     | 0.41              |
| 16:V:125:ASP:OD1  | 16:V:125:ASP:N    | 2.49                     | 0.41              |
| 35:c:524:LMG:H332 | 35:c:524:LMG:H361 | 1.83                     | 0.41              |
| 4:d:161:PRO:HB3   | 4:d:170:ALA:HB2   | 2.02                     | 0.41              |
| 31:d:406:LHG:H182 | 14:t:17:PHE:HZ    | 1.86                     | 0.41              |
| 1:A:93:PHE:HZ     | 22:A:407:CLA:HAA1 | 1.85                     | 0.41              |
| 3:C:82:THR:HG22   | 22:C:505:CLA:HED1 | 2.03                     | 0.41              |
| 22:C:505:CLA:HBC1 | 22:C:516:CLA:H43  | 2.01                     | 0.41              |
| 13:O:168:PHE:HB2  | 13:O:225:LEU:HB2  | 2.02                     | 0.41              |
| 3:c:175:ASP:O     | 3:c:182:GLY:HA2   | 2.20                     | 0.41              |
| 22:B:615:CLA:H91  | 22:B:615:CLA:H112 | 1.92                     | 0.41              |
| 4:D:78:VAL:HG11   | 4:D:114:ILE:HD12  | 2.02                     | 0.41              |
| 24:K:101:BCR:H20C | 24:K:101:BCR:H361 | 1.87                     | 0.41              |
| 13:O:162:ILE:HG21 | 13:O:237:ILE:HG21 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:450:TRP:NE1   | 22:b:609:CLA:HBA1 | 2.36                     | 0.41              |
| 2:b:458:PHE:HB3   | 22:b:606:CLA:HBC2 | 2.03                     | 0.41              |
| 22:b:605:CLA:H62  | 22:b:605:CLA:H41  | 1.92                     | 0.41              |
| 2:B:30:VAL:HG12   | 22:B:605:CLA:HHD  | 2.02                     | 0.41              |
| 2:B:458:PHE:HB3   | 22:B:604:CLA:HBC2 | 2.02                     | 0.41              |
| 3:c:394:SER:HA    | 3:c:408:VAL:HG23  | 2.01                     | 0.41              |
| 1:A:279:PRO:HG2   | 4:D:212:ALA:HB2   | 2.02                     | 0.41              |
| 1:A:304:HIS:CE1   | 16:V:155:LYS:HD2  | 2.56                     | 0.41              |
| 31:D:407:LHG:H201 | 31:L:101:LHG:H322 | 2.01                     | 0.41              |
| 18:Y:28:ILE:HG23  | 24:Y:102:BCR:H10C | 2.02                     | 0.41              |
| 24:b:620:BCR:H20C | 24:b:620:BCR:H361 | 1.94                     | 0.41              |
| 4:d:155:SER:HA    | 4:d:159:ILE:HB    | 2.03                     | 0.41              |
| 1:A:102:LEU:HD23  | 1:A:102:LEU:HA    | 1.87                     | 0.41              |
| 1:a:183:MET:HB3   | 22:a:405:CLA:HBC2 | 2.03                     | 0.41              |
| 1:a:279:PRO:HG2   | 4:d:212:ALA:HB2   | 2.02                     | 0.41              |
| 2:b:160:GLY:HA3   | 2:b:180:PRO:HB3   | 2.02                     | 0.41              |
| 22:b:606:CLA:H172 | 22:b:606:CLA:H13  | 1.76                     | 0.41              |
| 22:b:617:CLA:H2   | 22:b:618:CLA:HBB2 | 2.03                     | 0.41              |
| 24:b:619:BCR:H20C | 24:b:619:BCR:H361 | 1.89                     | 0.41              |
| 4:d:314:PHE:HA    | 4:d:317:LYS:HD3   | 2.03                     | 0.41              |
| 33:B:633:LMT:H122 | 33:B:633:LMT:H91  | 1.82                     | 0.41              |
| 16:V:38:LEU:HD12  | 16:V:95:ILE:HB    | 2.02                     | 0.41              |
| 2:b:75:TRP:CE2    | 27:b:622:PLM:H41  | 2.55                     | 0.41              |
| 22:b:608:CLA:H102 | 22:b:608:CLA:H61  | 1.77                     | 0.41              |
| 36:v:201:HEM:HMB1 | 36:v:201:HEM:HBB2 | 2.01                     | 0.41              |
| 1:A:217:SER:HA    | 4:D:272:LEU:HD12  | 2.03                     | 0.41              |
| 2:B:112:CYS:HA    | 24:B:617:BCR:H282 | 2.03                     | 0.41              |
| 2:B:201:HIS:HB2   | 22:B:602:CLA:CHB  | 2.51                     | 0.41              |
| 2:B:379:ALA:HA    | 2:B:390:TYR:HB3   | 2.03                     | 0.41              |
| 3:C:130:GLU:H     | 3:C:130:GLU:HG2   | 1.62                     | 0.41              |
| 24:C:501:BCR:H20C | 24:C:501:BCR:H361 | 1.93                     | 0.41              |
| 22:b:617:CLA:H61  | 22:b:617:CLA:H92  | 1.87                     | 0.41              |
| 22:c:513:CLA:H151 | 35:y:101:LMG:H391 | 2.03                     | 0.41              |
| 4:d:78:VAL:HG11   | 4:d:114:ILE:HD12  | 2.01                     | 0.41              |
| 5:e:14:ILE:O      | 5:e:20:TRP:NE1    | 2.50                     | 0.41              |
| 1:A:96:ILE:HG12   | 1:A:105:TRP:CE2   | 2.56                     | 0.41              |
| 3:C:323:THR:O     | 13:O:178:ARG:NH1  | 2.52                     | 0.41              |
| 3:C:390:GLY:HA3   | 3:C:408:VAL:HG22  | 2.03                     | 0.41              |
| 31:D:408:LHG:H142 | 11:L:22:LEU:HD21  | 2.03                     | 0.41              |
| 2:b:11:VAL:HG12   | 11:l:8:GLN:HG3    | 2.03                     | 0.41              |
| 4:d:295:SER:O     | 4:d:295:SER:OG    | 2.39                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:c:443:PHE:HD2   | 8:i:33:LYS:HD3    | 1.86                     | 0.40              |
| 24:c:501:BCR:H20C | 24:c:501:BCR:H361 | 1.93                     | 0.40              |
| 3:C:152:HIS:ND1   | 22:C:511:CLA:OBD  | 2.39                     | 0.40              |
| 34:D:411:DGD:HA61 | 34:D:411:DGD:HB32 | 2.02                     | 0.40              |
| 2:b:30:VAL:HG12   | 22:b:607:CLA:HHD  | 2.02                     | 0.40              |
| 2:b:383:PHE:N     | 4:d:344:GLU:O     | 2.45                     | 0.40              |
| 16:v:38:LEU:N     | 16:v:43:LYS:O     | 2.49                     | 0.40              |
| 24:C:502:BCR:H343 | 22:C:509:CLA:HMD1 | 2.02                     | 0.40              |
| 13:O:179:THR:HA   | 13:O:216:PHE:HE2  | 1.85                     | 0.40              |
| 16:V:59:PHE:HA    | 16:V:63:CYS:SG    | 2.61                     | 0.40              |
| 1:a:60:ILE:HD12   | 1:a:84:PRO:HD2    | 2.04                     | 0.40              |
| 1:a:96:ILE:HG12   | 1:a:105:TRP:CE2   | 2.56                     | 0.40              |
| 22:b:606:CLA:H93  | 22:b:607:CLA:HAB  | 2.03                     | 0.40              |
| 25:D:404:PL9:H421 | 25:D:404:PL9:H401 | 1.89                     | 0.40              |
| 34:H:101:DGD:HB32 | 34:H:101:DGD:HB61 | 1.66                     | 0.40              |
| 14:T:14:ILE:HG21  | 28:T:102:LFA:H61  | 2.03                     | 0.40              |
| 2:b:334:ASP:OD1   | 2:b:334:ASP:N     | 2.55                     | 0.40              |
| 3:c:173:LEU:HB2   | 3:c:218:LEU:HD13  | 2.03                     | 0.40              |
| 24:k:101:BCR:H20C | 24:k:101:BCR:H361 | 1.95                     | 0.40              |
| 22:B:604:CLA:H93  | 22:B:605:CLA:HAB  | 2.03                     | 0.40              |
| 24:C:501:BCR:H24C | 24:C:501:BCR:H371 | 1.71                     | 0.40              |
| 22:C:513:CLA:H111 | 22:C:513:CLA:H91  | 1.92                     | 0.40              |
| 2:b:33:TRP:HD1    | 24:b:602:BCR:H381 | 1.85                     | 0.40              |
| 22:c:506:CLA:H111 | 22:c:506:CLA:H72  | 1.97                     | 0.40              |
| 22:d:404:CLA:H121 | 22:d:404:CLA:H162 | 1.76                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 331/360 (92%) | 326 (98%) | 5 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | a     | 331/360 (92%) | 327 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 2   | B     | 503/510 (99%) | 499 (99%) | 4 (1%)  | 0        | 100         | 100 |
| 2   | b     | 503/510 (99%) | 498 (99%) | 5 (1%)  | 0        | 100         | 100 |
| 3   | C     | 448/461 (97%) | 442 (99%) | 6 (1%)  | 0        | 100         | 100 |
| 3   | c     | 448/461 (97%) | 442 (99%) | 6 (1%)  | 0        | 100         | 100 |
| 4   | D     | 339/352 (96%) | 332 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 4   | d     | 339/352 (96%) | 334 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 5   | E     | 79/84 (94%)   | 78 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 5   | e     | 79/84 (94%)   | 78 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 6   | F     | 32/45 (71%)   | 32 (100%) | 0       | 0        | 100         | 100 |
| 6   | f     | 32/45 (71%)   | 32 (100%) | 0       | 0        | 100         | 100 |
| 7   | H     | 60/66 (91%)   | 58 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 7   | h     | 60/66 (91%)   | 60 (100%) | 0       | 0        | 100         | 100 |
| 8   | I     | 34/38 (90%)   | 33 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 8   | i     | 33/38 (87%)   | 32 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 9   | J     | 34/40 (85%)   | 33 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 9   | j     | 34/40 (85%)   | 34 (100%) | 0       | 0        | 100         | 100 |
| 10  | K     | 35/46 (76%)   | 35 (100%) | 0       | 0        | 100         | 100 |
| 10  | k     | 35/46 (76%)   | 35 (100%) | 0       | 0        | 100         | 100 |
| 11  | L     | 34/37 (92%)   | 34 (100%) | 0       | 0        | 100         | 100 |
| 11  | l     | 34/37 (92%)   | 34 (100%) | 0       | 0        | 100         | 100 |
| 12  | M     | 31/36 (86%)   | 30 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 12  | m     | 31/36 (86%)   | 30 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 13  | O     | 241/272 (89%) | 234 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 13  | o     | 241/272 (89%) | 234 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 14  | T     | 28/32 (88%)   | 28 (100%) | 0       | 0        | 100         | 100 |
| 14  | t     | 28/32 (88%)   | 28 (100%) | 0       | 0        | 100         | 100 |
| 15  | U     | 95/134 (71%)  | 93 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 15  | u     | 95/134 (71%)  | 93 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 16  | V     | 135/163 (83%) | 134 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 16  | v     | 135/163 (83%) | 133 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 17  | X     | 36/41 (88%)     | 36 (100%)  | 0       | 0        | 100         | 100 |
| 17  | x     | 36/41 (88%)     | 36 (100%)  | 0       | 0        | 100         | 100 |
| 18  | Y     | 28/46 (61%)     | 28 (100%)  | 0       | 0        | 100         | 100 |
| 18  | y     | 28/46 (61%)     | 28 (100%)  | 0       | 0        | 100         | 100 |
| 19  | Z     | 59/62 (95%)     | 59 (100%)  | 0       | 0        | 100         | 100 |
| 19  | z     | 59/62 (95%)     | 58 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| All | All   | 5163/5650 (91%) | 5090 (99%) | 73 (1%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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     | 264/291 (91%) | 262 (99%) | 2 (1%)   | 73          | 85  |
| 1   | a     | 264/291 (91%) | 261 (99%) | 3 (1%)   | 65          | 79  |
| 2   | B     | 391/407 (96%) | 385 (98%) | 6 (2%)   | 57          | 73  |
| 2   | b     | 390/407 (96%) | 383 (98%) | 7 (2%)   | 51          | 68  |
| 3   | C     | 346/362 (96%) | 340 (98%) | 6 (2%)   | 53          | 69  |
| 3   | c     | 347/362 (96%) | 343 (99%) | 4 (1%)   | 63          | 78  |
| 4   | D     | 274/283 (97%) | 271 (99%) | 3 (1%)   | 65          | 79  |
| 4   | d     | 274/283 (97%) | 269 (98%) | 5 (2%)   | 51          | 68  |
| 5   | E     | 69/73 (94%)   | 67 (97%)  | 2 (3%)   | 37          | 51  |
| 5   | e     | 69/73 (94%)   | 69 (100%) | 0        | 100         | 100 |
| 6   | F     | 28/39 (72%)   | 28 (100%) | 0        | 100         | 100 |
| 6   | f     | 28/39 (72%)   | 28 (100%) | 0        | 100         | 100 |
| 7   | H     | 52/55 (94%)   | 51 (98%)  | 1 (2%)   | 50          | 66  |
| 7   | h     | 52/55 (94%)   | 51 (98%)  | 1 (2%)   | 50          | 66  |
| 8   | I     | 31/34 (91%)   | 29 (94%)  | 2 (6%)   | 15          | 18  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 8   | i     | 31/34 (91%)     | 29 (94%)   | 2 (6%)   | 15          | 18  |
| 9   | J     | 24/28 (86%)     | 24 (100%)  | 0        | 100         | 100 |
| 9   | j     | 24/28 (86%)     | 24 (100%)  | 0        | 100         | 100 |
| 10  | K     | 29/37 (78%)     | 29 (100%)  | 0        | 100         | 100 |
| 10  | k     | 29/37 (78%)     | 29 (100%)  | 0        | 100         | 100 |
| 11  | L     | 32/35 (91%)     | 32 (100%)  | 0        | 100         | 100 |
| 11  | l     | 32/35 (91%)     | 32 (100%)  | 0        | 100         | 100 |
| 12  | M     | 29/33 (88%)     | 29 (100%)  | 0        | 100         | 100 |
| 12  | m     | 29/33 (88%)     | 29 (100%)  | 0        | 100         | 100 |
| 13  | O     | 190/228 (83%)   | 188 (99%)  | 2 (1%)   | 65          | 79  |
| 13  | o     | 189/228 (83%)   | 186 (98%)  | 3 (2%)   | 55          | 71  |
| 14  | T     | 25/28 (89%)     | 25 (100%)  | 0        | 100         | 100 |
| 14  | t     | 25/28 (89%)     | 25 (100%)  | 0        | 100         | 100 |
| 15  | U     | 80/112 (71%)    | 77 (96%)   | 3 (4%)   | 29          | 40  |
| 15  | u     | 80/112 (71%)    | 74 (92%)   | 6 (8%)   | 12          | 14  |
| 16  | V     | 114/138 (83%)   | 111 (97%)  | 3 (3%)   | 40          | 55  |
| 16  | v     | 114/138 (83%)   | 111 (97%)  | 3 (3%)   | 40          | 55  |
| 17  | X     | 30/34 (88%)     | 29 (97%)   | 1 (3%)   | 33          | 45  |
| 17  | x     | 29/34 (85%)     | 27 (93%)   | 2 (7%)   | 14          | 16  |
| 18  | Y     | 21/37 (57%)     | 20 (95%)   | 1 (5%)   | 23          | 30  |
| 18  | y     | 21/37 (57%)     | 20 (95%)   | 1 (5%)   | 23          | 30  |
| 19  | Z     | 48/52 (92%)     | 45 (94%)   | 3 (6%)   | 16          | 19  |
| 19  | z     | 48/52 (92%)     | 43 (90%)   | 5 (10%)  | 7           | 7   |
| All | All   | 4152/4612 (90%) | 4075 (98%) | 77 (2%)  | 49          | 66  |

All (77) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 35  | VAL  |
| 1   | A     | 244 | GLU  |
| 2   | B     | 80  | ILE  |
| 2   | B     | 84  | THR  |
| 2   | B     | 236 | THR  |
| 2   | B     | 245 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 350 | GLU  |
| 2   | B     | 362 | PHE  |
| 3   | C     | 130 | GLU  |
| 3   | C     | 144 | LYS  |
| 3   | C     | 228 | ILE  |
| 3   | C     | 243 | THR  |
| 3   | C     | 277 | PHE  |
| 3   | C     | 460 | LEU  |
| 4   | D     | 43  | LEU  |
| 4   | D     | 150 | ILE  |
| 4   | D     | 345 | VAL  |
| 5   | E     | 5   | THR  |
| 5   | E     | 80  | LEU  |
| 7   | H     | 63  | LYS  |
| 8   | I     | 6   | ILE  |
| 8   | I     | 33  | LYS  |
| 13  | O     | 106 | GLN  |
| 13  | O     | 198 | ILE  |
| 15  | U     | 91  | VAL  |
| 15  | U     | 114 | VAL  |
| 15  | U     | 126 | ASP  |
| 16  | V     | 63  | CYS  |
| 16  | V     | 68  | VAL  |
| 16  | V     | 71  | ILE  |
| 17  | X     | 37  | VAL  |
| 18  | Y     | 41  | VAL  |
| 19  | Z     | 7   | LEU  |
| 19  | Z     | 20  | VAL  |
| 19  | Z     | 29  | SER  |
| 1   | a     | 35  | VAL  |
| 1   | a     | 230 | THR  |
| 1   | a     | 329 | GLU  |
| 2   | b     | 80  | ILE  |
| 2   | b     | 84  | THR  |
| 2   | b     | 236 | THR  |
| 2   | b     | 245 | VAL  |
| 2   | b     | 362 | PHE  |
| 2   | b     | 479 | PHE  |
| 2   | b     | 491 | VAL  |
| 3   | c     | 96  | THR  |
| 3   | c     | 277 | PHE  |
| 3   | c     | 303 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | c     | 461 | ASP  |
| 4   | d     | 150 | ILE  |
| 4   | d     | 213 | ILE  |
| 4   | d     | 227 | GLU  |
| 4   | d     | 259 | ILE  |
| 4   | d     | 345 | VAL  |
| 7   | h     | 63  | LYS  |
| 8   | i     | 6   | ILE  |
| 8   | i     | 34  | ARG  |
| 13  | o     | 59  | ASP  |
| 13  | o     | 75  | THR  |
| 13  | o     | 198 | ILE  |
| 15  | u     | 39  | LEU  |
| 15  | u     | 91  | VAL  |
| 15  | u     | 107 | GLU  |
| 15  | u     | 114 | VAL  |
| 15  | u     | 126 | ASP  |
| 15  | u     | 132 | LEU  |
| 16  | v     | 63  | CYS  |
| 16  | v     | 68  | VAL  |
| 16  | v     | 136 | LYS  |
| 17  | x     | 21  | LEU  |
| 17  | x     | 37  | VAL  |
| 18  | y     | 19  | ILE  |
| 19  | z     | 2   | THR  |
| 19  | z     | 4   | LEU  |
| 19  | z     | 7   | LEU  |
| 19  | z     | 20  | VAL  |
| 19  | z     | 37  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ASN  |
| 1   | A     | 19  | ASN  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 303 | ASN  |
| 2   | B     | 281 | GLN  |
| 2   | B     | 282 | GLN  |
| 2   | B     | 394 | GLN  |
| 2   | B     | 438 | ASN  |
| 3   | C     | 16  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 370 | ASN  |
| 4   | D     | 255 | GLN  |
| 5   | E     | 74  | GLN  |
| 6   | F     | 44  | GLN  |
| 13  | O     | 72  | GLN  |
| 13  | O     | 150 | ASN  |
| 13  | O     | 156 | GLN  |
| 13  | O     | 158 | ASN  |
| 13  | O     | 173 | ASN  |
| 13  | O     | 202 | GLN  |
| 15  | U     | 111 | HIS  |
| 16  | V     | 132 | ASN  |
| 18  | Y     | 21  | GLN  |
| 19  | Z     | 38  | GLN  |
| 1   | a     | 165 | GLN  |
| 2   | b     | 438 | ASN  |
| 2   | b     | 497 | GLN  |
| 3   | c     | 16  | GLN  |
| 3   | c     | 299 | GLN  |
| 3   | c     | 320 | GLN  |
| 4   | d     | 255 | GLN  |
| 5   | e     | 74  | GLN  |
| 6   | f     | 44  | GLN  |
| 12  | m     | 5   | GLN  |
| 13  | o     | 62  | GLN  |
| 13  | o     | 84  | ASN  |
| 13  | o     | 150 | ASN  |
| 13  | o     | 173 | ASN  |
| 13  | o     | 202 | GLN  |
| 13  | o     | 222 | GLN  |
| 15  | u     | 67  | GLN  |
| 16  | v     | 132 | ASN  |
| 19  | z     | 38  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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       | 0.38 | 0           | 7,9,11      | 0.90 | 0           |
| 8   | FME  | i     | 1   | 8    | 8,9,10       | 0.38 | 0           | 7,9,11      | 0.85 | 0           |
| 14  | FME  | t     | 1   | 14   | 8,9,10       | 0.39 | 0           | 7,9,11      | 0.98 | 0           |
| 8   | FME  | I     | 1   | 8    | 8,9,10       | 0.36 | 0           | 7,9,11      | 0.84 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 14  | FME  | T     | 1   | 14   | -       | 4/7/9/11 | -     |
| 8   | FME  | i     | 1   | 8    | -       | 0/7/9/11 | -     |
| 14  | FME  | t     | 1   | 14   | -       | 3/7/9/11 | -     |
| 8   | FME  | I     | 1   | 8    | -       | 0/7/9/11 | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 14  | T     | 1   | FME  | C-CA-CB-CG  |
| 14  | t     | 1   | FME  | C-CA-CB-CG  |
| 14  | T     | 1   | FME  | N-CA-CB-CG  |
| 14  | t     | 1   | FME  | N-CA-CB-CG  |
| 14  | T     | 1   | FME  | CB-CG-SD-CE |
| 14  | t     | 1   | FME  | CB-CG-SD-CE |
| 14  | T     | 1   | FME  | CB-CA-N-CN  |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 8 are monoatomic - leaving 224 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link   | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|--------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |        | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 22  | CLA  | c     | 508 | 3      | 69,73,73     | 1.26 | 8 (11%)     | 83,113,113  | 1.31 | 9 (10%)     |
| 28  | LFA  | B     | 624 | -      | 6,6,19       | 0.25 | 0           | 5,5,18      | 0.19 | 0           |
| 34  | DGD  | C     | 504 | -      | 55,55,67     | 0.59 | 0           | 69,69,81    | 0.92 | 4 (5%)      |
| 33  | LMT  | m     | 102 | -      | 36,36,36     | 0.55 | 0           | 47,47,47    | 0.78 | 1 (2%)      |
| 26  | SQD  | a     | 411 | -      | 53,54,54     | 1.57 | 8 (15%)     | 62,65,65    | 1.42 | 9 (14%)     |
| 22  | CLA  | B     | 611 | 2      | 69,73,73     | 1.24 | 8 (11%)     | 83,113,113  | 1.36 | 9 (10%)     |
| 22  | CLA  | C     | 514 | 3      | 69,73,73     | 1.24 | 9 (13%)     | 83,113,113  | 1.28 | 6 (7%)      |
| 22  | CLA  | D     | 406 | 4      | 69,73,73     | 1.25 | 7 (10%)     | 83,113,113  | 1.33 | 8 (9%)      |
| 24  | BCR  | b     | 620 | -      | 41,41,41     | 0.33 | 0           | 56,56,56    | 0.91 | 2 (3%)      |
| 25  | PL9  | A     | 409 | -      | 55,55,55     | 1.09 | 4 (7%)      | 68,69,69    | 1.57 | 14 (20%)    |
| 22  | CLA  | b     | 613 | 2      | 69,73,73     | 1.24 | 8 (11%)     | 83,113,113  | 1.36 | 8 (9%)      |
| 24  | BCR  | K     | 101 | -      | 41,41,41     | 0.31 | 0           | 56,56,56    | 0.59 | 0           |
| 28  | LFA  | J     | 104 | -      | 10,10,19     | 0.23 | 0           | 9,9,18      | 0.28 | 0           |
| 33  | LMT  | T     | 101 | -      | 24,24,36     | 0.50 | 0           | 29,29,47    | 0.73 | 0           |
| 28  | LFA  | I     | 102 | -      | 10,10,19     | 0.23 | 0           | 9,9,18      | 0.24 | 0           |
| 37  | RRX  | h     | 102 | -      | 42,42,42     | 0.21 | 0           | 57,58,58    | 0.49 | 0           |
| 24  | BCR  | B     | 619 | -      | 41,41,41     | 0.32 | 0           | 56,56,56    | 1.04 | 2 (3%)      |
| 29  | OEX  | a     | 416 | 3,39,1 | 0,14,14      | -    | -           | -           | -    | -           |
| 34  | DGD  | c     | 505 | -      | 62,62,67     | 0.58 | 0           | 76,76,81    | 0.70 | 1 (1%)      |
| 31  | LHG  | d     | 405 | -      | 48,48,48     | 0.50 | 0           | 51,54,54    | 0.56 | 0           |
| 22  | CLA  | C     | 508 | 39     | 69,73,73     | 1.25 | 9 (13%)     | 83,113,113  | 1.34 | 6 (7%)      |
| 22  | CLA  | b     | 604 | 2      | 69,73,73     | 1.24 | 9 (13%)     | 83,113,113  | 1.30 | 7 (8%)      |
| 31  | LHG  | D     | 408 | -      | 48,48,48     | 0.51 | 0           | 51,54,54    | 0.53 | 0           |
| 27  | PLM  | M     | 103 | -      | 15,15,17     | 0.67 | 0           | 15,15,17    | 0.68 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | LHG  | l     | 101 | -    | 48,48,48     | 0.51 | 0        | 51,54,54    | 0.52 | 0        |
| 22  | CLA  | b     | 616 | 2    | 69,73,73     | 1.22 | 8 (11%)  | 83,113,113  | 1.34 | 6 (7%)   |
| 25  | PL9  | D     | 404 | -    | 55,55,55     | 1.14 | 4 (7%)   | 68,69,69    | 1.50 | 13 (19%) |
| 26  | SQD  | b     | 601 | -    | 53,54,54     | 1.52 | 9 (16%)  | 62,65,65    | 1.71 | 10 (16%) |
| 34  | DGD  | h     | 101 | -    | 59,59,67     | 0.57 | 0        | 73,73,81    | 0.76 | 0        |
| 22  | CLA  | b     | 603 | -    | 69,73,73     | 1.27 | 7 (10%)  | 83,113,113  | 1.25 | 5 (6%)   |
| 22  | CLA  | b     | 607 | 2    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.33 | 5 (6%)   |
| 22  | CLA  | c     | 510 | 3    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.32 | 5 (6%)   |
| 27  | PLM  | b     | 621 | -    | 17,17,17     | 0.65 | 0        | 17,17,17    | 0.58 | 0        |
| 22  | CLA  | C     | 512 | 3    | 69,73,73     | 1.24 | 8 (11%)  | 83,113,113  | 1.38 | 10 (12%) |
| 22  | CLA  | a     | 406 | 39   | 69,73,73     | 1.24 | 8 (11%)  | 83,113,113  | 1.38 | 8 (9%)   |
| 27  | PLM  | b     | 622 | -    | 12,12,17     | 0.79 | 0        | 12,12,17    | 0.69 | 0        |
| 33  | LMT  | B     | 628 | -    | 24,24,36     | 0.50 | 0        | 29,29,47    | 0.78 | 0        |
| 28  | LFA  | B     | 631 | -    | 4,4,19       | 0.29 | 0        | 3,3,18      | 0.24 | 0        |
| 27  | PLM  | C     | 520 | -    | 14,14,17     | 0.72 | 0        | 14,14,17    | 0.70 | 0        |
| 22  | CLA  | b     | 608 | 2    | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.36 | 6 (7%)   |
| 27  | PLM  | B     | 627 | -    | 16,16,17     | 0.67 | 0        | 16,16,17    | 0.63 | 0        |
| 27  | PLM  | e     | 102 | -    | 17,17,17     | 0.62 | 0        | 17,17,17    | 0.63 | 0        |
| 33  | LMT  | B     | 630 | -    | 36,36,36     | 0.54 | 0        | 47,47,47    | 0.70 | 0        |
| 22  | CLA  | a     | 408 | 1    | 69,73,73     | 1.22 | 9 (13%)  | 83,113,113  | 1.32 | 7 (8%)   |
| 27  | PLM  | c     | 521 | -    | 15,15,17     | 0.71 | 0        | 15,15,17    | 0.64 | 0        |
| 22  | CLA  | B     | 605 | 2    | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.34 | 6 (7%)   |
| 27  | PLM  | e     | 101 | -    | 17,17,17     | 0.68 | 0        | 17,17,17    | 0.58 | 0        |
| 28  | LFA  | a     | 413 | -    | 6,6,19       | 0.25 | 0        | 5,5,18      | 0.18 | 0        |
| 22  | CLA  | A     | 404 | 1    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.33 | 7 (8%)   |
| 26  | SQD  | A     | 415 | -    | 50,51,54     | 1.55 | 7 (14%)  | 59,62,65    | 1.57 | 10 (16%) |
| 33  | LMT  | Z     | 101 | -    | 36,36,36     | 0.54 | 0        | 47,47,47    | 0.94 | 3 (6%)   |
| 31  | LHG  | d     | 406 | -    | 47,47,48     | 0.51 | 0        | 50,53,54    | 0.53 | 0        |
| 22  | CLA  | C     | 505 | 3    | 69,73,73     | 1.26 | 6 (8%)   | 83,113,113  | 1.29 | 5 (6%)   |
| 35  | LMG  | M     | 101 | -    | 51,51,55     | 0.49 | 0        | 59,59,63    | 0.59 | 0        |
| 24  | BCR  | B     | 617 | -    | 41,41,41     | 0.34 | 0        | 56,56,56    | 0.73 | 0        |
| 27  | PLM  | L     | 102 | -    | 17,17,17     | 0.66 | 0        | 17,17,17    | 0.60 | 0        |
| 28  | LFA  | b     | 623 | -    | 7,7,19       | 0.25 | 0        | 6,6,18      | 0.22 | 0        |
| 22  | CLA  | B     | 609 | 2    | 69,73,73     | 1.23 | 7 (10%)  | 83,113,113  | 1.30 | 6 (7%)   |
| 28  | LFA  | H     | 103 | -    | 9,9,19       | 0.25 | 0        | 8,8,18      | 0.18 | 0        |
| 26  | SQD  | a     | 417 | -    | 50,51,54     | 1.54 | 6 (12%)  | 59,62,65    | 1.55 | 9 (15%)  |
| 27  | PLM  | c     | 520 | -    | 17,17,17     | 0.68 | 0        | 17,17,17    | 0.59 | 0        |
| 33  | LMT  | f     | 102 | -    | 36,36,36     | 0.48 | 0        | 47,47,47    | 0.87 | 2 (4%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 30  | BCT  | a     | 419 | 20   | 2,3,3        | 0.88 | 0        | 2,3,3       | 3.27 | 2 (100%) |
| 27  | PLM  | X     | 101 | -    | 16,16,17     | 0.71 | 0        | 16,16,17    | 0.59 | 0        |
| 35  | LMG  | C     | 525 | -    | 51,51,55     | 0.50 | 0        | 59,59,63    | 0.87 | 3 (5%)   |
| 28  | LFA  | d     | 408 | -    | 12,12,19     | 0.23 | 0        | 11,11,18    | 0.20 | 0        |
| 35  | LMG  | c     | 519 | -    | 51,51,55     | 0.52 | 0        | 59,59,63    | 0.64 | 0        |
| 22  | CLA  | c     | 509 | 39   | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.35 | 6 (7%)   |
| 27  | PLM  | d     | 411 | -    | 11,11,17     | 0.80 | 0        | 11,11,17    | 0.77 | 0        |
| 24  | BCR  | c     | 502 | -    | 41,41,41     | 0.35 | 0        | 56,56,56    | 0.83 | 2 (3%)   |
| 28  | LFA  | T     | 102 | -    | 16,16,19     | 0.22 | 0        | 15,15,18    | 0.21 | 0        |
| 33  | LMT  | B     | 633 | -    | 36,36,36     | 0.51 | 0        | 47,47,47    | 0.77 | 0        |
| 27  | PLM  | A     | 413 | -    | 11,11,17     | 0.80 | 0        | 11,11,17    | 0.76 | 0        |
| 27  | PLM  | H     | 104 | -    | 11,11,17     | 0.80 | 0        | 11,11,17    | 0.73 | 0        |
| 33  | LMT  | M     | 102 | -    | 36,36,36     | 0.54 | 0        | 47,47,47    | 0.77 | 0        |
| 22  | CLA  | c     | 518 | 3    | 69,73,73     | 1.23 | 8 (11%)  | 83,113,113  | 1.39 | 8 (9%)   |
| 22  | CLA  | b     | 618 | 2    | 49,53,73     | 1.48 | 8 (16%)  | 59,89,113   | 1.57 | 6 (10%)  |
| 25  | PL9  | a     | 410 | -    | 55,55,55     | 1.10 | 4 (7%)   | 68,69,69    | 1.56 | 12 (17%) |
| 22  | CLA  | B     | 603 | 2    | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.30 | 8 (9%)   |
| 26  | SQD  | A     | 410 | -    | 53,54,54     | 1.52 | 7 (13%)  | 62,65,65    | 1.35 | 6 (9%)   |
| 27  | PLM  | c     | 523 | -    | 16,16,17     | 0.68 | 0        | 16,16,17    | 0.59 | 0        |
| 22  | CLA  | B     | 607 | 39   | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.32 | 7 (8%)   |
| 22  | CLA  | c     | 515 | 3    | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.28 | 6 (7%)   |
| 22  | CLA  | B     | 604 | 2    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.49 | 10 (12%) |
| 22  | CLA  | c     | 516 | 3    | 69,73,73     | 1.25 | 7 (10%)  | 83,113,113  | 1.36 | 8 (9%)   |
| 22  | CLA  | c     | 517 | 3    | 69,73,73     | 1.23 | 8 (11%)  | 83,113,113  | 1.37 | 6 (7%)   |
| 24  | BCR  | C     | 501 | -    | 41,41,41     | 0.35 | 0        | 56,56,56    | 1.04 | 1 (1%)   |
| 34  | DGD  | d     | 410 | -    | 47,47,67     | 0.53 | 0        | 54,55,81    | 0.63 | 0        |
| 35  | LMG  | Y     | 101 | -    | 51,51,55     | 0.49 | 0        | 59,59,63    | 0.65 | 0        |
| 27  | PLM  | B     | 621 | -    | 17,17,17     | 0.63 | 0        | 17,17,17    | 0.64 | 0        |
| 27  | PLM  | F     | 102 | -    | 13,13,17     | 0.73 | 0        | 13,13,17    | 0.67 | 0        |
| 28  | LFA  | I     | 101 | -    | 19,19,19     | 0.24 | 0        | 18,18,18    | 0.16 | 0        |
| 27  | PLM  | D     | 410 | -    | 17,17,17     | 0.65 | 0        | 17,17,17    | 0.66 | 0        |
| 34  | DGD  | c     | 504 | -    | 56,56,67     | 0.58 | 0        | 70,70,81    | 0.87 | 2 (2%)   |
| 22  | CLA  | c     | 507 | 3    | 69,73,73     | 1.23 | 8 (11%)  | 83,113,113  | 1.34 | 4 (4%)   |
| 26  | SQD  | l     | 102 | -    | 53,54,54     | 1.56 | 9 (16%)  | 62,65,65    | 1.47 | 7 (11%)  |
| 31  | LHG  | A     | 417 | -    | 45,45,48     | 0.53 | 0        | 48,51,54    | 0.53 | 0        |
| 22  | CLA  | B     | 610 | 39   | 69,73,73     | 1.27 | 7 (10%)  | 83,113,113  | 1.34 | 7 (8%)   |
| 33  | LMT  | C     | 518 | -    | 36,36,36     | 0.49 | 0        | 47,47,47    | 1.19 | 4 (8%)   |
| 24  | BCR  | A     | 408 | -    | 41,41,41     | 0.30 | 0        | 56,56,56    | 0.63 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | B     | 615 | 2    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.28 | 7 (8%)   |
| 22  | CLA  | C     | 511 | 39   | 69,73,73     | 1.24 | 7 (10%)  | 83,113,113  | 1.37 | 8 (9%)   |
| 34  | DGD  | C     | 503 | -    | 54,54,67     | 0.65 | 0        | 68,68,81    | 0.72 | 1 (1%)   |
| 34  | DGD  | c     | 503 | -    | 54,54,67     | 0.64 | 0        | 68,68,81    | 0.73 | 1 (1%)   |
| 28  | LFA  | I     | 103 | -    | 7,7,19       | 0.25 | 0        | 6,6,18      | 0.21 | 0        |
| 31  | LHG  | a     | 415 | -    | 48,48,48     | 0.51 | 0        | 51,54,54    | 0.52 | 0        |
| 22  | CLA  | B     | 608 | 2    | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.37 | 10 (12%) |
| 28  | LFA  | i     | 101 | -    | 19,19,19     | 0.24 | 0        | 18,18,18    | 0.18 | 0        |
| 27  | PLM  | c     | 522 | -    | 17,17,17     | 0.65 | 0        | 17,17,17    | 0.60 | 0        |
| 33  | LMT  | b     | 626 | -    | 24,24,36     | 0.48 | 0        | 29,29,47    | 0.70 | 0        |
| 22  | CLA  | C     | 515 | 3    | 69,73,73     | 1.25 | 7 (10%)  | 83,113,113  | 1.38 | 8 (9%)   |
| 28  | LFA  | C     | 521 | -    | 8,8,19       | 0.22 | 0        | 7,7,18      | 0.29 | 0        |
| 22  | CLA  | B     | 606 | 2    | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.38 | 9 (10%)  |
| 22  | CLA  | a     | 405 | 1    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.33 | 7 (8%)   |
| 33  | LMT  | B     | 623 | -    | 36,36,36     | 0.52 | 0        | 47,47,47    | 0.70 | 0        |
| 27  | PLM  | x     | 101 | -    | 17,17,17     | 0.67 | 0        | 17,17,17    | 0.59 | 0        |
| 28  | LFA  | b     | 624 | -    | 3,3,19       | 0.38 | 0        | 2,2,18      | 0.51 | 0        |
| 24  | BCR  | T     | 103 | -    | 41,41,41     | 0.34 | 0        | 56,56,56    | 0.76 | 0        |
| 28  | LFA  | A     | 412 | -    | 11,11,19     | 0.24 | 0        | 10,10,18    | 0.20 | 0        |
| 27  | PLM  | B     | 629 | -    | 17,17,17     | 0.66 | 0        | 17,17,17    | 0.64 | 0        |
| 28  | LFA  | E     | 102 | -    | 19,19,19     | 0.24 | 0        | 18,18,18    | 0.20 | 0        |
| 22  | CLA  | b     | 609 | 39   | 69,73,73     | 1.24 | 10 (14%) | 83,113,113  | 1.32 | 5 (6%)   |
| 22  | CLA  | c     | 512 | 39   | 69,73,73     | 1.23 | 7 (10%)  | 83,113,113  | 1.38 | 7 (8%)   |
| 33  | LMT  | i     | 102 | -    | 36,36,36     | 0.49 | 0        | 47,47,47    | 1.17 | 5 (10%)  |
| 34  | DGD  | D     | 411 | -    | 44,44,67     | 0.54 | 0        | 52,52,81    | 0.74 | 1 (1%)   |
| 24  | BCR  | c     | 501 | -    | 41,41,41     | 0.36 | 0        | 56,56,56    | 1.08 | 2 (3%)   |
| 28  | LFA  | a     | 414 | -    | 10,10,19     | 0.25 | 0        | 9,9,18      | 0.19 | 0        |
| 22  | CLA  | B     | 602 | 2    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.30 | 7 (8%)   |
| 22  | CLA  | C     | 507 | 3    | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.31 | 9 (10%)  |
| 32  | GOL  | a     | 401 | -    | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.39 | 0        |
| 27  | PLM  | D     | 402 | -    | 12,12,17     | 0.73 | 0        | 12,12,17    | 0.76 | 1 (8%)   |
| 33  | LMT  | z     | 101 | -    | 36,36,36     | 0.53 | 0        | 47,47,47    | 0.86 | 3 (6%)   |
| 22  | CLA  | B     | 616 | 2    | 49,53,73     | 1.48 | 8 (16%)  | 59,89,113   | 1.59 | 5 (8%)   |
| 22  | CLA  | b     | 610 | 2    | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.37 | 10 (12%) |
| 27  | PLM  | A     | 411 | -    | 17,17,17     | 0.68 | 0        | 17,17,17    | 0.60 | 0        |
| 34  | DGD  | J     | 102 | -    | 62,62,67     | 0.57 | 0        | 76,76,81    | 1.29 | 4 (5%)   |
| 28  | LFA  | i     | 103 | -    | 8,8,19       | 0.23 | 0        | 7,7,18      | 0.21 | 0        |
| 22  | CLA  | d     | 404 | -    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.33 | 8 (9%)   |

| Mol | Type | Chain | Res | Link   | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |        | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | d     | 401 | 39     | 69,73,73     | 1.23 | 8 (11%)  | 83,113,113  | 1.41 | 6 (7%)   |
| 22  | CLA  | C     | 506 | 3      | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.34 | 4 (4%)   |
| 22  | CLA  | A     | 405 | 39     | 69,73,73     | 1.24 | 8 (11%)  | 83,113,113  | 1.37 | 8 (9%)   |
| 24  | BCR  | y     | 102 | -      | 41,41,41     | 0.35 | 0        | 56,56,56    | 0.93 | 1 (1%)   |
| 31  | LHG  | a     | 421 | -      | 45,45,48     | 0.52 | 0        | 48,51,54    | 0.55 | 0        |
| 24  | BCR  | b     | 619 | -      | 41,41,41     | 0.33 | 0        | 56,56,56    | 0.81 | 1 (1%)   |
| 24  | BCR  | B     | 618 | -      | 41,41,41     | 0.33 | 0        | 56,56,56    | 0.80 | 0        |
| 28  | LFA  | B     | 626 | -      | 7,7,19       | 0.26 | 0        | 6,6,18      | 0.18 | 0        |
| 36  | HEM  | e     | 103 | 5,6    | 50,50,50     | 1.45 | 7 (14%)  | 66,82,82    | 1.30 | 8 (12%)  |
| 24  | BCR  | a     | 409 | -      | 41,41,41     | 0.30 | 0        | 56,56,56    | 0.65 | 0        |
| 22  | CLA  | B     | 613 | 2      | 69,73,73     | 1.23 | 8 (11%)  | 83,113,113  | 1.30 | 7 (8%)   |
| 23  | PHO  | A     | 406 | -      | 58,69,69     | 1.22 | 4 (6%)   | 56,99,99    | 1.60 | 7 (12%)  |
| 22  | CLA  | B     | 601 | -      | 69,73,73     | 1.27 | 7 (10%)  | 83,113,113  | 1.25 | 5 (6%)   |
| 24  | BCR  | F     | 101 | -      | 41,41,41     | 0.36 | 0        | 56,56,56    | 0.85 | 2 (3%)   |
| 26  | SQD  | D     | 412 | -      | 44,45,54     | 1.64 | 9 (20%)  | 53,56,65    | 1.58 | 10 (18%) |
| 28  | LFA  | i     | 104 | -      | 7,7,19       | 0.24 | 0        | 6,6,18      | 0.20 | 0        |
| 30  | BCT  | A     | 416 | 20     | 2,3,3        | 0.87 | 0        | 2,3,3       | 3.26 | 2 (100%) |
| 33  | LMT  | j     | 101 | -      | 24,24,36     | 0.52 | 0        | 29,29,47    | 0.83 | 0        |
| 35  | LMG  | d     | 407 | -      | 47,47,55     | 0.51 | 0        | 55,55,63    | 0.67 | 0        |
| 22  | CLA  | c     | 506 | 3      | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.31 | 7 (8%)   |
| 27  | PLM  | B     | 622 | -      | 13,13,17     | 0.73 | 0        | 13,13,17    | 0.68 | 0        |
| 22  | CLA  | D     | 405 | 4      | 69,73,73     | 1.24 | 8 (11%)  | 83,113,113  | 1.27 | 4 (4%)   |
| 22  | CLA  | A     | 407 | 1      | 69,73,73     | 1.22 | 9 (13%)  | 83,113,113  | 1.32 | 7 (8%)   |
| 22  | CLA  | d     | 403 | 4      | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.26 | 4 (4%)   |
| 22  | CLA  | c     | 514 | 3      | 69,73,73     | 1.24 | 7 (10%)  | 83,113,113  | 1.39 | 9 (10%)  |
| 24  | BCR  | b     | 602 | -      | 41,41,41     | 0.36 | 0        | 56,56,56    | 1.52 | 6 (10%)  |
| 22  | CLA  | b     | 615 | 2      | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.30 | 7 (8%)   |
| 36  | HEM  | E     | 104 | 5,6    | 50,50,50     | 1.46 | 7 (14%)  | 66,82,82    | 1.32 | 10 (15%) |
| 35  | LMG  | c     | 524 | -      | 48,48,55     | 0.49 | 0        | 56,56,63    | 0.69 | 0        |
| 31  | LHG  | D     | 407 | -      | 48,48,48     | 0.51 | 0        | 51,54,54    | 0.57 | 0        |
| 29  | OEX  | A     | 414 | 3,39,1 | 0,14,14      | -    | -        | -           | -    | -        |
| 27  | PLM  | C     | 524 | -      | 12,12,17     | 0.76 | 0        | 12,12,17    | 0.70 | 0        |
| 27  | PLM  | C     | 522 | -      | 17,17,17     | 0.65 | 0        | 17,17,17    | 0.73 | 1 (5%)   |
| 22  | CLA  | C     | 516 | 3      | 69,73,73     | 1.23 | 8 (11%)  | 83,113,113  | 1.37 | 5 (6%)   |
| 37  | RRX  | H     | 102 | -      | 42,42,42     | 0.22 | 0        | 57,58,58    | 0.48 | 0        |
| 27  | PLM  | C     | 523 | -      | 15,15,17     | 0.69 | 0        | 15,15,17    | 0.64 | 0        |
| 24  | BCR  | B     | 632 | -      | 41,41,41     | 0.36 | 0        | 56,56,56    | 1.52 | 7 (12%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | D     | 401 | 39   | 69,73,73     | 1.23 | 8 (11%)  | 83,113,113  | 1.41 | 8 (9%)   |
| 36  | HEM  | V     | 201 | 16   | 50,50,50     | 1.40 | 7 (14%)  | 66,82,82    | 1.30 | 10 (15%) |
| 36  | HEM  | v     | 201 | 16   | 50,50,50     | 1.41 | 7 (14%)  | 66,82,82    | 1.31 | 10 (15%) |
| 23  | PHO  | a     | 407 | -    | 58,69,69     | 1.22 | 4 (6%)   | 56,99,99    | 1.61 | 7 (12%)  |
| 28  | LFA  | B     | 620 | -    | 7,7,19       | 0.23 | 0        | 6,6,18      | 0.22 | 0        |
| 28  | LFA  | d     | 409 | -    | 13,13,19     | 0.23 | 0        | 12,12,18    | 0.25 | 0        |
| 31  | LHG  | E     | 101 | -    | 39,39,48     | 0.57 | 0        | 42,45,54    | 0.51 | 0        |
| 22  | CLA  | C     | 510 | 3    | 69,73,73     | 1.26 | 10 (14%) | 83,113,113  | 1.37 | 10 (12%) |
| 27  | PLM  | b     | 627 | -    | 17,17,17     | 0.67 | 0        | 17,17,17    | 0.63 | 0        |
| 22  | CLA  | C     | 513 | 3    | 69,73,73     | 1.24 | 7 (10%)  | 83,113,113  | 1.37 | 7 (8%)   |
| 22  | CLA  | b     | 605 | 2    | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.31 | 7 (8%)   |
| 27  | PLM  | j     | 102 | -    | 16,16,17     | 0.69 | 0        | 16,16,17    | 0.69 | 0        |
| 22  | CLA  | c     | 511 | 3    | 69,73,73     | 1.27 | 10 (14%) | 83,113,113  | 1.37 | 10 (12%) |
| 24  | BCR  | C     | 502 | -    | 41,41,41     | 0.35 | 0        | 56,56,56    | 0.82 | 2 (3%)   |
| 22  | CLA  | b     | 611 | 2    | 69,73,73     | 1.24 | 7 (10%)  | 83,113,113  | 1.30 | 6 (7%)   |
| 24  | BCR  | Y     | 102 | -    | 41,41,41     | 0.35 | 0        | 56,56,56    | 0.94 | 1 (1%)   |
| 27  | PLM  | b     | 625 | -    | 15,15,17     | 0.68 | 0        | 15,15,17    | 0.64 | 0        |
| 27  | PLM  | t     | 101 | -    | 14,14,17     | 0.23 | 0        | 13,13,17    | 0.23 | 0        |
| 26  | SQD  | d     | 412 | -    | 44,45,54     | 1.64 | 9 (20%)  | 53,56,65    | 1.59 | 10 (18%) |
| 32  | GOL  | A     | 418 | -    | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.38 | 0        |
| 22  | CLA  | b     | 617 | 2    | 69,73,73     | 1.23 | 7 (10%)  | 83,113,113  | 1.29 | 7 (8%)   |
| 23  | PHO  | a     | 420 | -    | 58,69,69     | 1.19 | 4 (6%)   | 56,99,99    | 1.59 | 8 (14%)  |
| 27  | PLM  | j     | 103 | -    | 17,17,17     | 0.66 | 0        | 17,17,17    | 0.57 | 0        |
| 31  | LHG  | L     | 101 | -    | 48,48,48     | 0.50 | 0        | 51,54,54    | 0.56 | 0        |
| 28  | LFA  | J     | 101 | -    | 19,19,19     | 0.24 | 0        | 18,18,18    | 0.22 | 0        |
| 33  | LMT  | T     | 104 | -    | 36,36,36     | 0.51 | 0        | 47,47,47    | 0.72 | 0        |
| 35  | LMG  | y     | 101 | -    | 51,51,55     | 0.51 | 0        | 59,59,63    | 0.97 | 4 (6%)   |
| 35  | LMG  | D     | 409 | -    | 47,47,55     | 0.52 | 0        | 55,55,63    | 0.68 | 0        |
| 22  | CLA  | b     | 614 | 2    | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.36 | 8 (9%)   |
| 23  | PHO  | D     | 403 | -    | 58,69,69     | 1.19 | 4 (6%)   | 56,99,99    | 1.56 | 8 (14%)  |
| 27  | PLM  | E     | 103 | -    | 17,17,17     | 0.66 | 0        | 17,17,17    | 0.56 | 0        |
| 27  | PLM  | B     | 625 | -    | 11,11,17     | 0.82 | 0        | 11,11,17    | 0.79 | 0        |
| 22  | CLA  | c     | 513 | 3    | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.40 | 10 (12%) |
| 35  | LMG  | C     | 519 | -    | 51,51,55     | 0.51 | 0        | 59,59,63    | 0.65 | 0        |
| 22  | CLA  | C     | 509 | 3    | 69,73,73     | 1.24 | 8 (11%)  | 83,113,113  | 1.31 | 5 (6%)   |
| 22  | CLA  | b     | 606 | 2    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.48 | 10 (12%) |
| 24  | BCR  | k     | 101 | -    | 41,41,41     | 0.36 | 0        | 56,56,56    | 0.71 | 1 (1%)   |
| 33  | LMT  | A     | 419 | -    | 36,36,36     | 0.55 | 0        | 47,47,47    | 0.87 | 1 (2%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | B     | 614 | 2    | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.34 | 7 (8%)   |
| 28  | LFA  | a     | 418 | -    | 6,6,19       | 0.25 | 0        | 5,5,18      | 0.18 | 0        |
| 33  | LMT  | J     | 103 | -    | 24,24,36     | 0.50 | 0        | 29,29,47    | 0.91 | 1 (3%)   |
| 34  | DGD  | H     | 101 | -    | 59,59,67     | 0.56 | 0        | 73,73,81    | 0.78 | 0        |
| 35  | LMG  | m     | 101 | -    | 51,51,55     | 0.50 | 0        | 59,59,63    | 0.57 | 0        |
| 22  | CLA  | C     | 517 | 3    | 69,73,73     | 1.22 | 8 (11%)  | 83,113,113  | 1.39 | 9 (10%)  |
| 22  | CLA  | b     | 612 | 39   | 69,73,73     | 1.27 | 8 (11%)  | 83,113,113  | 1.34 | 7 (8%)   |
| 25  | PL9  | d     | 402 | -    | 55,55,55     | 1.14 | 3 (5%)   | 68,69,69    | 1.51 | 13 (19%) |
| 27  | PLM  | a     | 412 | -    | 17,17,17     | 0.67 | 0        | 17,17,17    | 0.67 | 0        |
| 22  | CLA  | B     | 612 | 2    | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.36 | 8 (9%)   |
| 24  | BCR  | f     | 101 | -    | 41,41,41     | 0.35 | 0        | 56,56,56    | 0.93 | 3 (5%)   |

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   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 22  | CLA  | c     | 508 | 3    | -       | 6/39/115/115  | -       |
| 28  | LFA  | B     | 624 | -    | -       | 1/4/4/17      | -       |
| 34  | DGD  | C     | 504 | -    | -       | 25/43/83/95   | 0/2/2/2 |
| 33  | LMT  | m     | 102 | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 26  | SQD  | a     | 411 | -    | -       | 25/49/69/69   | 0/1/1/1 |
| 22  | CLA  | B     | 611 | 2    | -       | 8/39/115/115  | -       |
| 22  | CLA  | C     | 514 | 3    | -       | 5/39/115/115  | -       |
| 22  | CLA  | D     | 406 | 4    | -       | 11/39/115/115 | -       |
| 24  | BCR  | b     | 620 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 25  | PL9  | A     | 409 | -    | -       | 28/53/73/73   | 0/1/1/1 |
| 22  | CLA  | b     | 613 | 2    | -       | 8/39/115/115  | -       |
| 24  | BCR  | K     | 101 | -    | -       | 5/29/63/63    | 0/2/2/2 |
| 28  | LFA  | J     | 104 | -    | -       | 3/8/8/17      | -       |
| 33  | LMT  | T     | 101 | -    | -       | 8/15/35/61    | 0/1/1/2 |
| 28  | LFA  | I     | 102 | -    | -       | 5/8/8/17      | -       |
| 37  | RRX  | h     | 102 | -    | -       | 3/29/65/65    | 0/2/2/2 |
| 24  | BCR  | B     | 619 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 34  | DGD  | c     | 505 | -    | -       | 19/50/90/95   | 0/2/2/2 |
| 31  | LHG  | d     | 405 | -    | -       | 18/53/53/53   | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 22  | CLA  | C     | 508 | 39   | -       | 9/39/115/115  | -       |
| 22  | CLA  | b     | 604 | 2    | -       | 5/39/115/115  | -       |
| 31  | LHG  | D     | 408 | -    | -       | 17/53/53/53   | -       |
| 27  | PLM  | M     | 103 | -    | -       | 11/13/13/15   | -       |
| 31  | LHG  | l     | 101 | -    | -       | 20/53/53/53   | -       |
| 22  | CLA  | b     | 616 | 2    | -       | 18/39/115/115 | -       |
| 25  | PL9  | D     | 404 | -    | -       | 19/53/73/73   | 0/1/1/1 |
| 26  | SQD  | b     | 601 | -    | -       | 28/49/69/69   | 0/1/1/1 |
| 34  | DGD  | h     | 101 | -    | -       | 7/47/87/95    | 0/2/2/2 |
| 22  | CLA  | b     | 603 | -    | -       | 14/39/115/115 | -       |
| 22  | CLA  | b     | 607 | 2    | -       | 5/39/115/115  | -       |
| 22  | CLA  | c     | 510 | 3    | -       | 11/39/115/115 | -       |
| 27  | PLM  | b     | 621 | -    | -       | 7/15/15/15    | -       |
| 22  | CLA  | C     | 512 | 3    | -       | 6/39/115/115  | -       |
| 22  | CLA  | a     | 406 | 39   | -       | 9/39/115/115  | -       |
| 27  | PLM  | b     | 622 | -    | -       | 4/10/10/15    | -       |
| 33  | LMT  | B     | 628 | -    | -       | 2/15/35/61    | 0/1/1/2 |
| 28  | LFA  | B     | 631 | -    | -       | 0/2/2/17      | -       |
| 27  | PLM  | C     | 520 | -    | -       | 8/12/12/15    | -       |
| 22  | CLA  | b     | 608 | 2    | -       | 9/39/115/115  | -       |
| 27  | PLM  | B     | 627 | -    | -       | 5/14/14/15    | -       |
| 27  | PLM  | e     | 102 | -    | -       | 8/15/15/15    | -       |
| 33  | LMT  | B     | 630 | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 22  | CLA  | a     | 408 | 1    | -       | 12/39/115/115 | -       |
| 27  | PLM  | c     | 521 | -    | -       | 4/13/13/15    | -       |
| 22  | CLA  | B     | 605 | 2    | -       | 5/39/115/115  | -       |
| 27  | PLM  | e     | 101 | -    | -       | 7/15/15/15    | -       |
| 28  | LFA  | a     | 413 | -    | -       | 3/4/4/17      | -       |
| 22  | CLA  | A     | 404 | 1    | -       | 7/39/115/115  | -       |
| 26  | SQD  | A     | 415 | -    | -       | 15/46/66/69   | 0/1/1/1 |
| 33  | LMT  | Z     | 101 | -    | -       | 11/21/61/61   | 0/2/2/2 |
| 31  | LHG  | d     | 406 | -    | -       | 21/52/52/53   | -       |
| 22  | CLA  | C     | 505 | 3    | -       | 10/39/115/115 | -       |
| 35  | LMG  | M     | 101 | -    | -       | 20/46/66/70   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 24  | BCR  | B     | 617 | -    | -       | 7/29/63/63    | 0/2/2/2 |
| 27  | PLM  | L     | 102 | -    | -       | 9/15/15/15    | -       |
| 28  | LFA  | b     | 623 | -    | -       | 0/5/5/17      | -       |
| 22  | CLA  | B     | 609 | 2    | -       | 12/39/115/115 | -       |
| 28  | LFA  | H     | 103 | -    | -       | 4/7/7/17      | -       |
| 26  | SQD  | a     | 417 | -    | -       | 24/46/66/69   | 0/1/1/1 |
| 27  | PLM  | c     | 520 | -    | -       | 9/15/15/15    | -       |
| 33  | LMT  | f     | 102 | -    | -       | 11/21/61/61   | 0/2/2/2 |
| 27  | PLM  | X     | 101 | -    | -       | 8/14/14/15    | -       |
| 35  | LMG  | C     | 525 | -    | -       | 19/46/66/70   | 0/1/1/1 |
| 28  | LFA  | d     | 408 | -    | -       | 7/10/10/17    | -       |
| 35  | LMG  | c     | 519 | -    | -       | 27/46/66/70   | 0/1/1/1 |
| 22  | CLA  | c     | 509 | 39   | -       | 9/39/115/115  | -       |
| 27  | PLM  | d     | 411 | -    | -       | 5/9/9/15      | -       |
| 24  | BCR  | c     | 502 | -    | -       | 10/29/63/63   | 0/2/2/2 |
| 28  | LFA  | T     | 102 | -    | -       | 9/14/14/17    | -       |
| 33  | LMT  | B     | 633 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 27  | PLM  | A     | 413 | -    | -       | 7/9/9/15      | -       |
| 27  | PLM  | H     | 104 | -    | -       | 1/9/9/15      | -       |
| 33  | LMT  | M     | 102 | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 22  | CLA  | c     | 518 | 3    | -       | 6/39/115/115  | -       |
| 22  | CLA  | b     | 618 | 2    | -       | 1/15/91/115   | -       |
| 25  | PL9  | a     | 410 | -    | -       | 28/53/73/73   | 0/1/1/1 |
| 22  | CLA  | B     | 603 | 2    | -       | 15/39/115/115 | -       |
| 26  | SQD  | A     | 410 | -    | -       | 21/49/69/69   | 0/1/1/1 |
| 27  | PLM  | c     | 523 | -    | -       | 9/14/14/15    | -       |
| 22  | CLA  | B     | 607 | 39   | -       | 6/39/115/115  | -       |
| 22  | CLA  | c     | 515 | 3    | -       | 4/39/115/115  | -       |
| 22  | CLA  | B     | 604 | 2    | -       | 14/39/115/115 | -       |
| 22  | CLA  | c     | 516 | 3    | -       | 4/39/115/115  | -       |
| 22  | CLA  | c     | 517 | 3    | -       | 18/39/115/115 | -       |
| 24  | BCR  | C     | 501 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 34  | DGD  | d     | 410 | -    | -       | 15/41/62/95   | 0/1/1/2 |
| 35  | LMG  | Y     | 101 | -    | -       | 10/46/66/70   | 0/1/1/1 |
| 27  | PLM  | B     | 621 | -    | -       | 8/15/15/15    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 27  | PLM  | F     | 102 | -    | -       | 2/11/11/15    | -       |
| 28  | LFA  | I     | 101 | -    | -       | 7/17/17/17    | -       |
| 27  | PLM  | D     | 410 | -    | -       | 8/15/15/15    | -       |
| 34  | DGD  | c     | 504 | -    | -       | 26/44/84/95   | 0/2/2/2 |
| 22  | CLA  | c     | 507 | 3    | -       | 12/39/115/115 | -       |
| 26  | SQD  | l     | 102 | -    | -       | 23/49/69/69   | 0/1/1/1 |
| 31  | LHG  | A     | 417 | -    | -       | 15/50/50/53   | -       |
| 22  | CLA  | B     | 610 | 39   | -       | 10/39/115/115 | -       |
| 33  | LMT  | C     | 518 | -    | -       | 10/21/61/61   | 0/2/2/2 |
| 24  | BCR  | A     | 408 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 615 | 2    | -       | 8/39/115/115  | -       |
| 22  | CLA  | C     | 511 | 39   | -       | 6/39/115/115  | -       |
| 34  | DGD  | C     | 503 | -    | -       | 21/42/82/95   | 0/2/2/2 |
| 34  | DGD  | c     | 503 | -    | -       | 22/42/82/95   | 0/2/2/2 |
| 28  | LFA  | I     | 103 | -    | -       | 2/5/5/17      | -       |
| 31  | LHG  | a     | 415 | -    | -       | 24/53/53/53   | -       |
| 22  | CLA  | B     | 608 | 2    | -       | 5/39/115/115  | -       |
| 28  | LFA  | i     | 101 | -    | -       | 12/17/17/17   | -       |
| 27  | PLM  | c     | 522 | -    | -       | 2/15/15/15    | -       |
| 33  | LMT  | b     | 626 | -    | -       | 6/15/35/61    | 0/1/1/2 |
| 22  | CLA  | C     | 515 | 3    | -       | 6/39/115/115  | -       |
| 28  | LFA  | C     | 521 | -    | -       | 5/6/6/17      | -       |
| 22  | CLA  | B     | 606 | 2    | -       | 8/39/115/115  | -       |
| 22  | CLA  | a     | 405 | 1    | -       | 7/39/115/115  | -       |
| 33  | LMT  | B     | 623 | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 27  | PLM  | x     | 101 | -    | -       | 10/15/15/15   | -       |
| 28  | LFA  | b     | 624 | -    | -       | 0/1/1/17      | -       |
| 24  | BCR  | T     | 103 | -    | -       | 5/29/63/63    | 0/2/2/2 |
| 28  | LFA  | A     | 412 | -    | -       | 1/9/9/17      | -       |
| 27  | PLM  | B     | 629 | -    | -       | 3/15/15/15    | -       |
| 28  | LFA  | E     | 102 | -    | -       | 4/17/17/17    | -       |
| 22  | CLA  | b     | 609 | 39   | -       | 6/39/115/115  | -       |
| 22  | CLA  | c     | 512 | 39   | -       | 6/39/115/115  | -       |
| 33  | LMT  | i     | 102 | -    | -       | 10/21/61/61   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 34  | DGD  | D     | 411 | -    | -       | 14/38/58/95   | 0/1/1/2 |
| 24  | BCR  | c     | 501 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 28  | LFA  | a     | 414 | -    | -       | 5/8/8/17      | -       |
| 22  | CLA  | B     | 602 | 2    | -       | 6/39/115/115  | -       |
| 22  | CLA  | C     | 507 | 3    | -       | 3/39/115/115  | -       |
| 32  | GOL  | a     | 401 | -    | -       | 4/4/4/4       | -       |
| 27  | PLM  | D     | 402 | -    | -       | 2/10/10/15    | -       |
| 33  | LMT  | z     | 101 | -    | -       | 11/21/61/61   | 0/2/2/2 |
| 22  | CLA  | B     | 616 | 2    | -       | 1/15/91/115   | -       |
| 22  | CLA  | b     | 610 | 2    | -       | 5/39/115/115  | -       |
| 27  | PLM  | A     | 411 | -    | -       | 7/15/15/15    | -       |
| 34  | DGD  | J     | 102 | -    | -       | 17/50/90/95   | 0/2/2/2 |
| 28  | LFA  | i     | 103 | -    | -       | 4/6/6/17      | -       |
| 22  | CLA  | d     | 404 | -    | -       | 10/39/115/115 | -       |
| 22  | CLA  | d     | 401 | 39   | -       | 5/39/115/115  | -       |
| 22  | CLA  | C     | 506 | 3    | -       | 14/39/115/115 | -       |
| 22  | CLA  | A     | 405 | 39   | -       | 8/39/115/115  | -       |
| 24  | BCR  | y     | 102 | -    | -       | 10/29/63/63   | 0/2/2/2 |
| 31  | LHG  | a     | 421 | -    | -       | 16/50/50/53   | -       |
| 24  | BCR  | b     | 619 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 24  | BCR  | B     | 618 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 28  | LFA  | B     | 626 | -    | -       | 0/5/5/17      | -       |
| 36  | HEM  | e     | 103 | 5,6  | -       | 2/14/54/54    | -       |
| 24  | BCR  | a     | 409 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 613 | 2    | -       | 6/39/115/115  | -       |
| 23  | PHO  | A     | 406 | -    | -       | 3/37/103/103  | 0/5/6/6 |
| 22  | CLA  | B     | 601 | -    | -       | 14/39/115/115 | -       |
| 24  | BCR  | F     | 101 | -    | -       | 8/29/63/63    | 0/2/2/2 |
| 26  | SQD  | D     | 412 | -    | -       | 13/40/60/69   | 0/1/1/1 |
| 28  | LFA  | i     | 104 | -    | -       | 2/5/5/17      | -       |
| 33  | LMT  | j     | 101 | -    | -       | 14/15/35/61   | 0/1/1/2 |
| 35  | LMG  | d     | 407 | -    | -       | 11/42/62/70   | 0/1/1/1 |
| 22  | CLA  | c     | 506 | 3    | -       | 6/39/115/115  | -       |
| 27  | PLM  | B     | 622 | -    | -       | 4/11/11/15    | -       |
| 22  | CLA  | D     | 405 | 4    | -       | 5/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 22  | CLA  | A     | 407 | 1    | -       | 10/39/115/115 | -       |
| 22  | CLA  | d     | 403 | 4    | -       | 5/39/115/115  | -       |
| 22  | CLA  | c     | 514 | 3    | -       | 5/39/115/115  | -       |
| 24  | BCR  | b     | 602 | -    | -       | 9/29/63/63    | 0/2/2/2 |
| 22  | CLA  | b     | 615 | 2    | -       | 6/39/115/115  | -       |
| 36  | HEM  | E     | 104 | 5,6  | -       | 2/14/54/54    | -       |
| 35  | LMG  | c     | 524 | -    | -       | 16/43/63/70   | 0/1/1/1 |
| 31  | LHG  | D     | 407 | -    | -       | 19/53/53/53   | -       |
| 27  | PLM  | C     | 524 | -    | -       | 2/10/10/15    | -       |
| 27  | PLM  | C     | 522 | -    | -       | 10/15/15/15   | -       |
| 22  | CLA  | C     | 516 | 3    | -       | 14/39/115/115 | -       |
| 37  | RRX  | H     | 102 | -    | -       | 3/29/65/65    | 0/2/2/2 |
| 27  | PLM  | C     | 523 | -    | -       | 2/13/13/15    | -       |
| 24  | BCR  | B     | 632 | -    | -       | 10/29/63/63   | 0/2/2/2 |
| 22  | CLA  | D     | 401 | 39   | -       | 5/39/115/115  | -       |
| 36  | HEM  | V     | 201 | 16   | -       | 2/14/54/54    | -       |
| 36  | HEM  | v     | 201 | 16   | -       | 2/14/54/54    | -       |
| 23  | PHO  | a     | 407 | -    | -       | 2/37/103/103  | 0/5/6/6 |
| 28  | LFA  | B     | 620 | -    | -       | 5/5/5/17      | -       |
| 28  | LFA  | d     | 409 | -    | -       | 2/11/11/17    | -       |
| 31  | LHG  | E     | 101 | -    | -       | 30/44/44/53   | -       |
| 22  | CLA  | C     | 510 | 3    | -       | 16/39/115/115 | -       |
| 27  | PLM  | b     | 627 | -    | -       | 3/15/15/15    | -       |
| 22  | CLA  | C     | 513 | 3    | -       | 8/39/115/115  | -       |
| 22  | CLA  | b     | 605 | 2    | -       | 14/39/115/115 | -       |
| 27  | PLM  | j     | 102 | -    | -       | 6/14/14/15    | -       |
| 22  | CLA  | c     | 511 | 3    | -       | 15/39/115/115 | -       |
| 24  | BCR  | C     | 502 | -    | -       | 11/29/63/63   | 0/2/2/2 |
| 22  | CLA  | b     | 611 | 2    | -       | 11/39/115/115 | -       |
| 24  | BCR  | Y     | 102 | -    | -       | 10/29/63/63   | 0/2/2/2 |
| 27  | PLM  | b     | 625 | -    | -       | 3/13/13/15    | -       |
| 27  | PLM  | t     | 101 | -    | -       | 6/12/12/15    | -       |
| 26  | SQD  | d     | 412 | -    | -       | 11/40/60/69   | 0/1/1/1 |
| 32  | GOL  | A     | 418 | -    | -       | 0/4/4/4       | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 22  | CLA  | b     | 617 | 2    | -       | 6/39/115/115  | -       |
| 23  | PHO  | a     | 420 | -    | -       | 5/37/103/103  | 0/5/6/6 |
| 27  | PLM  | j     | 103 | -    | -       | 7/15/15/15    | -       |
| 31  | LHG  | L     | 101 | -    | -       | 17/53/53/53   | -       |
| 28  | LFA  | J     | 101 | -    | -       | 4/17/17/17    | -       |
| 33  | LMT  | T     | 104 | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 35  | LMG  | y     | 101 | -    | -       | 14/46/66/70   | 0/1/1/1 |
| 35  | LMG  | D     | 409 | -    | -       | 10/42/62/70   | 0/1/1/1 |
| 22  | CLA  | b     | 614 | 2    | -       | 7/39/115/115  | -       |
| 23  | PHO  | D     | 403 | -    | -       | 7/37/103/103  | 0/5/6/6 |
| 27  | PLM  | E     | 103 | -    | -       | 3/15/15/15    | -       |
| 27  | PLM  | B     | 625 | -    | -       | 1/9/9/15      | -       |
| 22  | CLA  | c     | 513 | 3    | -       | 9/39/115/115  | -       |
| 35  | LMG  | C     | 519 | -    | -       | 25/46/66/70   | 0/1/1/1 |
| 22  | CLA  | C     | 509 | 3    | -       | 10/39/115/115 | -       |
| 22  | CLA  | b     | 606 | 2    | -       | 16/39/115/115 | -       |
| 24  | BCR  | k     | 101 | -    | -       | 8/29/63/63    | 0/2/2/2 |
| 33  | LMT  | A     | 419 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 22  | CLA  | B     | 614 | 2    | -       | 17/39/115/115 | -       |
| 28  | LFA  | a     | 418 | -    | -       | 2/4/4/17      | -       |
| 33  | LMT  | J     | 103 | -    | -       | 12/15/35/61   | 0/1/1/2 |
| 34  | DGD  | H     | 101 | -    | -       | 6/47/87/95    | 0/2/2/2 |
| 35  | LMG  | m     | 101 | -    | -       | 18/46/66/70   | 0/1/1/1 |
| 22  | CLA  | C     | 517 | 3    | -       | 5/39/115/115  | -       |
| 22  | CLA  | b     | 612 | 39   | -       | 11/39/115/115 | -       |
| 25  | PL9  | d     | 402 | -    | -       | 20/53/73/73   | 0/1/1/1 |
| 27  | PLM  | a     | 412 | -    | -       | 10/15/15/15   | -       |
| 22  | CLA  | B     | 612 | 2    | -       | 7/39/115/115  | -       |
| 24  | BCR  | f     | 101 | -    | -       | 9/29/63/63    | 0/2/2/2 |

All (699) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | a     | 407 | PHO  | C4D-ND  | -4.89 | 1.31        | 1.38     |
| 23  | A     | 406 | PHO  | C4D-ND  | -4.83 | 1.31        | 1.38     |
| 26  | A     | 410 | SQD  | O48-C23 | 4.66  | 1.47        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | a     | 417 | SQD  | O48-C23 | 4.66  | 1.47        | 1.33     |
| 26  | b     | 601 | SQD  | O48-C23 | 4.66  | 1.46        | 1.33     |
| 26  | a     | 411 | SQD  | O48-C23 | 4.65  | 1.46        | 1.33     |
| 23  | D     | 403 | PHO  | C4D-ND  | -4.65 | 1.32        | 1.38     |
| 26  | D     | 412 | SQD  | O48-C23 | 4.64  | 1.46        | 1.33     |
| 23  | a     | 420 | PHO  | C4D-ND  | -4.63 | 1.32        | 1.38     |
| 26  | A     | 415 | SQD  | O48-C23 | 4.62  | 1.46        | 1.33     |
| 26  | l     | 102 | SQD  | O48-C23 | 4.58  | 1.46        | 1.33     |
| 26  | d     | 412 | SQD  | O48-C23 | 4.57  | 1.46        | 1.33     |
| 23  | A     | 406 | PHO  | C1B-C2B | 4.45  | 1.44        | 1.39     |
| 23  | a     | 407 | PHO  | C1B-C2B | 4.41  | 1.44        | 1.39     |
| 25  | a     | 410 | PL9  | C7-C3   | -4.40 | 1.46        | 1.51     |
| 25  | A     | 409 | PL9  | C7-C3   | -4.12 | 1.47        | 1.51     |
| 23  | a     | 420 | PHO  | C1B-C2B | 4.09  | 1.44        | 1.39     |
| 23  | D     | 403 | PHO  | C1B-C2B | 3.97  | 1.44        | 1.39     |
| 22  | d     | 404 | CLA  | C1D-ND  | 3.94  | 1.42        | 1.37     |
| 22  | B     | 601 | CLA  | C1D-ND  | 3.92  | 1.42        | 1.37     |
| 22  | c     | 508 | CLA  | C1D-ND  | 3.91  | 1.42        | 1.37     |
| 36  | E     | 104 | HEM  | FE-NB   | 3.90  | 2.06        | 1.94     |
| 22  | b     | 603 | CLA  | C1D-ND  | 3.90  | 1.42        | 1.37     |
| 36  | E     | 104 | HEM  | FE-ND   | 3.88  | 2.06        | 1.94     |
| 22  | b     | 606 | CLA  | C1D-ND  | 3.87  | 1.42        | 1.37     |
| 22  | C     | 508 | CLA  | C1D-ND  | 3.85  | 1.42        | 1.37     |
| 22  | D     | 406 | CLA  | C1D-ND  | 3.85  | 1.42        | 1.37     |
| 22  | C     | 507 | CLA  | C1D-ND  | 3.85  | 1.42        | 1.37     |
| 22  | b     | 608 | CLA  | C1D-ND  | 3.84  | 1.42        | 1.37     |
| 22  | b     | 611 | CLA  | C1D-ND  | 3.84  | 1.42        | 1.37     |
| 36  | e     | 103 | HEM  | FE-NB   | 3.82  | 2.06        | 1.94     |
| 36  | e     | 103 | HEM  | FE-ND   | 3.81  | 2.06        | 1.94     |
| 22  | B     | 606 | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 26  | d     | 412 | SQD  | O5-C1   | 3.80  | 1.51        | 1.41     |
| 22  | a     | 406 | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 26  | D     | 412 | SQD  | O5-C1   | 3.78  | 1.51        | 1.41     |
| 23  | D     | 403 | PHO  | C3B-C4B | 3.78  | 1.45        | 1.41     |
| 22  | c     | 506 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 22  | C     | 510 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 22  | c     | 511 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 26  | a     | 411 | SQD  | O5-C1   | 3.77  | 1.51        | 1.41     |
| 22  | C     | 515 | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 22  | A     | 405 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 22  | C     | 505 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 22  | B     | 616 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | C     | 511 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 22  | C     | 512 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 22  | B     | 604 | CLA  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 23  | a     | 420 | PHO  | C3B-C4B | 3.74  | 1.45        | 1.41     |
| 22  | B     | 614 | CLA  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 22  | c     | 516 | CLA  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 22  | B     | 609 | CLA  | C1D-ND  | 3.73  | 1.42        | 1.37     |
| 22  | b     | 612 | CLA  | C1D-ND  | 3.73  | 1.42        | 1.37     |
| 22  | B     | 610 | CLA  | C1D-ND  | 3.72  | 1.42        | 1.37     |
| 22  | B     | 607 | CLA  | C1D-ND  | 3.71  | 1.42        | 1.37     |
| 22  | c     | 513 | CLA  | C1D-ND  | 3.71  | 1.42        | 1.37     |
| 22  | d     | 401 | CLA  | C1D-ND  | 3.71  | 1.42        | 1.37     |
| 22  | b     | 618 | CLA  | C1D-ND  | 3.71  | 1.42        | 1.37     |
| 25  | D     | 404 | PL9  | C7-C3   | -3.70 | 1.47        | 1.51     |
| 22  | c     | 509 | CLA  | C1D-ND  | 3.70  | 1.42        | 1.37     |
| 22  | c     | 512 | CLA  | C1D-ND  | 3.69  | 1.42        | 1.37     |
| 25  | d     | 402 | PL9  | C7-C3   | -3.69 | 1.47        | 1.51     |
| 22  | b     | 613 | CLA  | C1D-ND  | 3.69  | 1.42        | 1.37     |
| 22  | a     | 405 | CLA  | C1D-ND  | 3.69  | 1.42        | 1.37     |
| 22  | D     | 401 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 22  | b     | 609 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 22  | B     | 611 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 22  | A     | 404 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 22  | B     | 605 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 22  | b     | 607 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 22  | b     | 616 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 22  | c     | 518 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 22  | C     | 517 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 22  | A     | 407 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 22  | a     | 408 | CLA  | C1D-ND  | 3.63  | 1.42        | 1.37     |
| 22  | B     | 615 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 22  | b     | 610 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 22  | B     | 613 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 22  | b     | 615 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |
| 22  | B     | 602 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 22  | c     | 515 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 22  | b     | 604 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 22  | B     | 608 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 22  | C     | 506 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 22  | c     | 514 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 22  | b     | 617 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 22  | C     | 513 | CLA  | C1D-ND  | 3.54  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | C     | 514 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 26  | A     | 410 | SQD  | O47-C45 | -3.49 | 1.37        | 1.46     |
| 26  | a     | 417 | SQD  | O47-C45 | -3.48 | 1.37        | 1.46     |
| 22  | b     | 605 | CLA  | C1D-ND  | 3.48  | 1.42        | 1.37     |
| 22  | B     | 601 | CLA  | C4B-NB  | 3.47  | 1.42        | 1.37     |
| 22  | c     | 507 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 26  | a     | 411 | SQD  | O47-C45 | -3.45 | 1.38        | 1.46     |
| 26  | b     | 601 | SQD  | O47-C45 | -3.45 | 1.38        | 1.46     |
| 23  | A     | 406 | PHO  | C3B-C4B | 3.44  | 1.45        | 1.41     |
| 26  | l     | 102 | SQD  | O47-C7  | 3.44  | 1.44        | 1.34     |
| 22  | C     | 509 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 26  | D     | 412 | SQD  | O47-C45 | -3.44 | 1.38        | 1.46     |
| 22  | B     | 603 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 23  | a     | 407 | PHO  | C3B-C4B | 3.43  | 1.45        | 1.41     |
| 22  | d     | 401 | CLA  | C4D-ND  | -3.41 | 1.33        | 1.37     |
| 26  | d     | 412 | SQD  | O47-C45 | -3.41 | 1.38        | 1.46     |
| 22  | D     | 401 | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 22  | c     | 510 | CLA  | C1D-ND  | 3.39  | 1.41        | 1.37     |
| 25  | d     | 402 | PL9  | C3-C4   | -3.38 | 1.44        | 1.49     |
| 22  | C     | 505 | CLA  | C4B-NB  | 3.37  | 1.41        | 1.37     |
| 22  | c     | 509 | CLA  | C4D-ND  | -3.37 | 1.33        | 1.37     |
| 26  | A     | 410 | SQD  | O5-C1   | 3.36  | 1.50        | 1.41     |
| 22  | b     | 603 | CLA  | C4B-NB  | 3.36  | 1.41        | 1.37     |
| 25  | D     | 404 | PL9  | C3-C4   | -3.36 | 1.44        | 1.49     |
| 26  | l     | 102 | SQD  | O47-C45 | -3.33 | 1.38        | 1.46     |
| 22  | C     | 508 | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 22  | B     | 616 | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 22  | c     | 513 | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 22  | d     | 403 | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 36  | V     | 201 | HEM  | FE-NA   | 3.32  | 2.06        | 1.95     |
| 26  | A     | 415 | SQD  | O47-C45 | -3.31 | 1.38        | 1.46     |
| 26  | a     | 417 | SQD  | O47-C7  | 3.31  | 1.43        | 1.34     |
| 26  | l     | 102 | SQD  | O5-C1   | 3.30  | 1.50        | 1.41     |
| 26  | a     | 411 | SQD  | O47-C7  | 3.30  | 1.43        | 1.34     |
| 26  | b     | 601 | SQD  | O47-C7  | 3.30  | 1.43        | 1.34     |
| 26  | D     | 412 | SQD  | O47-C7  | 3.29  | 1.43        | 1.34     |
| 22  | C     | 512 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 22  | B     | 610 | CLA  | C4B-NB  | 3.29  | 1.41        | 1.37     |
| 36  | v     | 201 | HEM  | FE-NA   | 3.28  | 2.06        | 1.95     |
| 26  | A     | 415 | SQD  | O47-C7  | 3.28  | 1.43        | 1.34     |
| 26  | d     | 412 | SQD  | O47-C7  | 3.27  | 1.43        | 1.34     |
| 36  | v     | 201 | HEM  | FE-ND   | 3.26  | 2.04        | 1.94     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 618 | CLA  | C4D-ND  | -3.26 | 1.33        | 1.37     |
| 26  | A     | 410 | SQD  | O47-C7  | 3.26  | 1.43        | 1.34     |
| 22  | D     | 405 | CLA  | C4D-ND  | -3.25 | 1.33        | 1.37     |
| 22  | C     | 507 | CLA  | C4B-NB  | 3.25  | 1.41        | 1.37     |
| 22  | b     | 612 | CLA  | C4B-NB  | 3.24  | 1.41        | 1.37     |
| 22  | a     | 406 | CLA  | C4D-ND  | -3.24 | 1.33        | 1.37     |
| 22  | c     | 511 | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 22  | A     | 405 | CLA  | C4D-ND  | -3.23 | 1.33        | 1.37     |
| 22  | d     | 403 | CLA  | C1D-ND  | 3.22  | 1.41        | 1.37     |
| 36  | V     | 201 | HEM  | FE-ND   | 3.22  | 2.04        | 1.94     |
| 22  | C     | 510 | CLA  | C4B-NB  | 3.22  | 1.41        | 1.37     |
| 22  | c     | 511 | CLA  | C4B-NB  | 3.22  | 1.41        | 1.37     |
| 22  | B     | 614 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 22  | C     | 510 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 22  | B     | 611 | CLA  | C4D-ND  | -3.21 | 1.33        | 1.37     |
| 22  | D     | 405 | CLA  | C1D-ND  | 3.20  | 1.41        | 1.37     |
| 22  | B     | 607 | CLA  | C4D-ND  | -3.20 | 1.33        | 1.37     |
| 22  | c     | 517 | CLA  | C1D-ND  | 3.20  | 1.41        | 1.37     |
| 22  | b     | 612 | CLA  | C3B-C4B | 3.19  | 1.50        | 1.42     |
| 22  | c     | 506 | CLA  | C4B-NB  | 3.19  | 1.41        | 1.37     |
| 22  | B     | 602 | CLA  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 22  | B     | 606 | CLA  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 22  | a     | 405 | CLA  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 22  | B     | 605 | CLA  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 22  | b     | 611 | CLA  | C4B-NB  | 3.18  | 1.41        | 1.37     |
| 22  | c     | 517 | CLA  | C4B-NB  | 3.18  | 1.41        | 1.37     |
| 22  | b     | 604 | CLA  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 22  | b     | 613 | CLA  | C4D-ND  | -3.17 | 1.33        | 1.37     |
| 36  | E     | 104 | HEM  | CAC-C3C | 3.17  | 1.56        | 1.47     |
| 22  | c     | 510 | CLA  | C4B-NB  | 3.17  | 1.41        | 1.37     |
| 22  | B     | 604 | CLA  | C4B-NB  | 3.17  | 1.41        | 1.37     |
| 22  | C     | 509 | CLA  | C4B-NB  | 3.17  | 1.41        | 1.37     |
| 22  | B     | 615 | CLA  | C4B-NB  | 3.16  | 1.41        | 1.37     |
| 22  | b     | 607 | CLA  | C4D-ND  | -3.16 | 1.33        | 1.37     |
| 22  | c     | 517 | CLA  | C4D-ND  | -3.16 | 1.33        | 1.37     |
| 36  | E     | 104 | HEM  | CAB-C3B | 3.15  | 1.56        | 1.47     |
| 36  | v     | 201 | HEM  | CAB-C3B | 3.15  | 1.56        | 1.47     |
| 22  | C     | 517 | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 22  | c     | 509 | CLA  | C4B-NB  | 3.15  | 1.41        | 1.37     |
| 36  | e     | 103 | HEM  | CAB-C3B | 3.15  | 1.56        | 1.47     |
| 22  | b     | 609 | CLA  | C4D-ND  | -3.15 | 1.33        | 1.37     |
| 22  | b     | 606 | CLA  | C4B-NB  | 3.15  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | A     | 415 | SQD  | O5-C1   | 3.15  | 1.49        | 1.41     |
| 26  | a     | 417 | SQD  | O5-C1   | 3.15  | 1.49        | 1.41     |
| 36  | e     | 103 | HEM  | CAC-C3C | 3.14  | 1.56        | 1.47     |
| 22  | d     | 404 | CLA  | C4B-NB  | 3.14  | 1.41        | 1.37     |
| 22  | A     | 404 | CLA  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 22  | b     | 608 | CLA  | C4B-NB  | 3.14  | 1.41        | 1.37     |
| 22  | C     | 516 | CLA  | C1D-ND  | 3.14  | 1.41        | 1.37     |
| 22  | D     | 406 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 22  | B     | 606 | CLA  | C4B-NB  | 3.13  | 1.41        | 1.37     |
| 22  | c     | 518 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 22  | B     | 610 | CLA  | C3B-C4B | 3.13  | 1.50        | 1.42     |
| 22  | B     | 602 | CLA  | C4B-NB  | 3.13  | 1.41        | 1.37     |
| 22  | B     | 609 | CLA  | C4B-NB  | 3.13  | 1.41        | 1.37     |
| 22  | C     | 516 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 22  | B     | 612 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 36  | V     | 201 | HEM  | CAB-C3B | 3.12  | 1.55        | 1.47     |
| 22  | b     | 605 | CLA  | C4B-NB  | 3.12  | 1.41        | 1.37     |
| 22  | b     | 616 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 22  | b     | 614 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 36  | v     | 201 | HEM  | CAC-C3C | 3.11  | 1.55        | 1.47     |
| 22  | b     | 604 | CLA  | C4B-NB  | 3.10  | 1.41        | 1.37     |
| 22  | c     | 515 | CLA  | C4B-NB  | 3.10  | 1.41        | 1.37     |
| 22  | D     | 405 | CLA  | C4B-NB  | 3.10  | 1.41        | 1.37     |
| 22  | b     | 609 | CLA  | C4B-NB  | 3.10  | 1.41        | 1.37     |
| 22  | B     | 605 | CLA  | C4B-NB  | 3.10  | 1.41        | 1.37     |
| 22  | B     | 608 | CLA  | C4B-NB  | 3.10  | 1.41        | 1.37     |
| 22  | C     | 514 | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 22  | C     | 511 | CLA  | C4B-NB  | 3.10  | 1.41        | 1.37     |
| 26  | l     | 102 | SQD  | C24-C23 | 3.10  | 1.59        | 1.50     |
| 22  | B     | 611 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 22  | B     | 607 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 22  | C     | 516 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 22  | b     | 612 | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 36  | V     | 201 | HEM  | CAC-C3C | 3.09  | 1.55        | 1.47     |
| 26  | a     | 411 | SQD  | C24-C23 | 3.08  | 1.59        | 1.50     |
| 22  | b     | 613 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 22  | d     | 403 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 22  | c     | 510 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 22  | B     | 603 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 22  | C     | 506 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 22  | B     | 610 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 22  | c     | 515 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 615 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 22  | c     | 507 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 22  | C     | 515 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 22  | c     | 516 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 22  | B     | 601 | CLA  | C3B-C4B | 3.06  | 1.49        | 1.42     |
| 22  | C     | 515 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 22  | b     | 617 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 22  | c     | 516 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 22  | b     | 603 | CLA  | C3B-C4B | 3.05  | 1.49        | 1.42     |
| 22  | b     | 607 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 22  | A     | 407 | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |
| 22  | b     | 614 | CLA  | C1D-ND  | 3.05  | 1.41        | 1.37     |
| 22  | c     | 514 | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |
| 22  | b     | 610 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 22  | C     | 507 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 22  | C     | 513 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 22  | d     | 404 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 22  | b     | 605 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 22  | b     | 608 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 22  | c     | 506 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 22  | C     | 508 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 22  | c     | 508 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 26  | A     | 410 | SQD  | C24-C23 | 3.03  | 1.59        | 1.50     |
| 22  | a     | 408 | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 36  | v     | 201 | HEM  | FE-NB   | 3.03  | 2.04        | 1.94     |
| 22  | c     | 508 | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 22  | D     | 406 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 22  | c     | 512 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 22  | B     | 603 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 22  | C     | 511 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 22  | C     | 505 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 22  | B     | 602 | CLA  | C3B-C4B | 3.01  | 1.49        | 1.42     |
| 22  | B     | 613 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 22  | c     | 507 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 22  | C     | 506 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 26  | a     | 417 | SQD  | C24-C23 | 3.00  | 1.59        | 1.50     |
| 26  | d     | 412 | SQD  | C24-C23 | 3.00  | 1.59        | 1.50     |
| 22  | C     | 514 | CLA  | C4B-NB  | 3.00  | 1.41        | 1.37     |
| 22  | b     | 617 | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 26  | A     | 415 | SQD  | C24-C23 | 3.00  | 1.59        | 1.50     |
| 26  | D     | 412 | SQD  | C24-C23 | 2.99  | 1.59        | 1.50     |
| 22  | b     | 603 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 604 | CLA  | C3B-C4B | 2.98  | 1.49        | 1.42     |
| 22  | c     | 512 | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 22  | C     | 509 | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 22  | B     | 614 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |
| 22  | B     | 612 | CLA  | C1D-ND  | 2.97  | 1.41        | 1.37     |
| 22  | b     | 615 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 22  | b     | 611 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 22  | c     | 516 | CLA  | C3B-C4B | 2.96  | 1.49        | 1.42     |
| 22  | B     | 609 | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 22  | C     | 512 | CLA  | C3B-C4B | 2.96  | 1.49        | 1.42     |
| 22  | A     | 407 | CLA  | C4B-NB  | 2.96  | 1.41        | 1.37     |
| 22  | C     | 505 | CLA  | C3B-C4B | 2.96  | 1.49        | 1.42     |
| 22  | a     | 408 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 22  | b     | 613 | CLA  | C3B-C4B | 2.94  | 1.49        | 1.42     |
| 22  | B     | 608 | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 26  | b     | 601 | SQD  | C24-C23 | 2.94  | 1.59        | 1.50     |
| 22  | d     | 404 | CLA  | C3B-C4B | 2.94  | 1.49        | 1.42     |
| 22  | C     | 513 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 22  | d     | 401 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 22  | C     | 513 | CLA  | C3B-C4B | 2.94  | 1.49        | 1.42     |
| 22  | c     | 514 | CLA  | C3B-C4B | 2.93  | 1.49        | 1.42     |
| 22  | b     | 606 | CLA  | C4D-ND  | -2.93 | 1.33        | 1.37     |
| 26  | b     | 601 | SQD  | O5-C1   | 2.93  | 1.49        | 1.41     |
| 22  | c     | 514 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 22  | c     | 518 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 22  | b     | 610 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 22  | b     | 616 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 36  | V     | 201 | HEM  | FE-NB   | 2.92  | 2.03        | 1.94     |
| 22  | b     | 615 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 22  | A     | 404 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 22  | B     | 601 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 22  | B     | 604 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 22  | c     | 513 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 22  | B     | 611 | CLA  | C3B-C4B | 2.90  | 1.49        | 1.42     |
| 22  | A     | 405 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 22  | C     | 512 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 22  | b     | 618 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 22  | D     | 401 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 22  | c     | 513 | CLA  | C3B-C4B | 2.89  | 1.49        | 1.42     |
| 22  | b     | 614 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 22  | a     | 406 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 22  | C     | 517 | CLA  | C3B-C4B | 2.89  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | C     | 515 | CLA  | C3B-C4B | 2.89  | 1.49        | 1.42     |
| 22  | a     | 405 | CLA  | C3B-C4B | 2.89  | 1.49        | 1.42     |
| 22  | B     | 612 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 22  | A     | 404 | CLA  | C3B-C4B | 2.88  | 1.49        | 1.42     |
| 22  | c     | 508 | CLA  | C3B-C4B | 2.88  | 1.49        | 1.42     |
| 22  | c     | 518 | CLA  | C3B-C4B | 2.88  | 1.49        | 1.42     |
| 25  | a     | 410 | PL9  | C3-C4   | -2.87 | 1.44        | 1.49     |
| 25  | A     | 409 | PL9  | C3-C4   | -2.87 | 1.44        | 1.49     |
| 22  | c     | 511 | CLA  | C3B-C4B | 2.87  | 1.49        | 1.42     |
| 22  | b     | 606 | CLA  | C1B-C2B | 2.86  | 1.50        | 1.43     |
| 22  | B     | 613 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 22  | b     | 610 | CLA  | C3B-C4B | 2.85  | 1.49        | 1.42     |
| 22  | b     | 608 | CLA  | C3B-C4B | 2.85  | 1.49        | 1.42     |
| 22  | C     | 507 | CLA  | C3B-C4B | 2.85  | 1.49        | 1.42     |
| 22  | d     | 403 | CLA  | C3B-C4B | 2.84  | 1.49        | 1.42     |
| 22  | D     | 405 | CLA  | C3B-C4B | 2.84  | 1.49        | 1.42     |
| 22  | B     | 604 | CLA  | C1B-C2B | 2.84  | 1.50        | 1.43     |
| 22  | B     | 616 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 22  | C     | 510 | CLA  | C3B-C4B | 2.83  | 1.49        | 1.42     |
| 22  | B     | 608 | CLA  | C3B-C4B | 2.83  | 1.49        | 1.42     |
| 22  | D     | 406 | CLA  | C3B-C4B | 2.83  | 1.49        | 1.42     |
| 22  | c     | 509 | CLA  | C3B-C4B | 2.83  | 1.49        | 1.42     |
| 22  | a     | 405 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 22  | B     | 614 | CLA  | C3B-C4B | 2.82  | 1.49        | 1.42     |
| 22  | b     | 607 | CLA  | C3B-C4B | 2.82  | 1.49        | 1.42     |
| 22  | C     | 508 | CLA  | C3B-C4B | 2.81  | 1.49        | 1.42     |
| 22  | B     | 605 | CLA  | C3B-C4B | 2.81  | 1.49        | 1.42     |
| 22  | D     | 401 | CLA  | C3B-C4B | 2.80  | 1.49        | 1.42     |
| 22  | C     | 505 | CLA  | C1B-C2B | 2.80  | 1.49        | 1.43     |
| 36  | E     | 104 | HEM  | FE-NC   | 2.79  | 2.04        | 1.95     |
| 22  | c     | 517 | CLA  | C3B-C4B | 2.79  | 1.49        | 1.42     |
| 22  | b     | 616 | CLA  | C3B-C4B | 2.79  | 1.49        | 1.42     |
| 22  | d     | 401 | CLA  | C3B-C4B | 2.78  | 1.49        | 1.42     |
| 22  | C     | 517 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 22  | C     | 516 | CLA  | C3B-C4B | 2.76  | 1.49        | 1.42     |
| 22  | c     | 510 | CLA  | C3B-C4B | 2.76  | 1.49        | 1.42     |
| 22  | c     | 506 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 22  | C     | 511 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 36  | e     | 103 | HEM  | FE-NA   | 2.75  | 2.04        | 1.95     |
| 22  | b     | 617 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 22  | b     | 614 | CLA  | C3B-C4B | 2.74  | 1.49        | 1.42     |
| 22  | B     | 615 | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | C     | 516 | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 22  | c     | 507 | CLA  | C3B-C4B | 2.74  | 1.49        | 1.42     |
| 22  | C     | 506 | CLA  | C3B-C4B | 2.74  | 1.49        | 1.42     |
| 22  | B     | 607 | CLA  | C3B-C4B | 2.73  | 1.49        | 1.42     |
| 22  | D     | 406 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 22  | b     | 609 | CLA  | C3B-C4B | 2.73  | 1.49        | 1.42     |
| 22  | B     | 606 | CLA  | C3B-C4B | 2.72  | 1.49        | 1.42     |
| 36  | e     | 103 | HEM  | FE-NC   | 2.72  | 2.04        | 1.95     |
| 22  | C     | 509 | CLA  | C3B-C4B | 2.72  | 1.49        | 1.42     |
| 22  | b     | 617 | CLA  | C3B-C4B | 2.72  | 1.49        | 1.42     |
| 22  | a     | 406 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 22  | b     | 615 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 22  | c     | 517 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | C     | 514 | CLA  | C3B-C4B | 2.71  | 1.49        | 1.42     |
| 22  | c     | 512 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | A     | 407 | CLA  | C3B-C4B | 2.71  | 1.49        | 1.42     |
| 22  | a     | 408 | CLA  | C3B-C4B | 2.71  | 1.49        | 1.42     |
| 22  | d     | 404 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 22  | b     | 615 | CLA  | C3B-C4B | 2.70  | 1.49        | 1.42     |
| 22  | c     | 515 | CLA  | C3B-C4B | 2.70  | 1.49        | 1.42     |
| 22  | B     | 612 | CLA  | C3B-C4B | 2.69  | 1.49        | 1.42     |
| 22  | c     | 515 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 22  | A     | 405 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 22  | D     | 405 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 22  | B     | 613 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 22  | c     | 512 | CLA  | C3B-C4B | 2.69  | 1.49        | 1.42     |
| 22  | b     | 618 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 22  | B     | 616 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 22  | B     | 613 | CLA  | C3B-C4B | 2.68  | 1.49        | 1.42     |
| 22  | d     | 403 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 22  | B     | 615 | CLA  | C3B-C4B | 2.67  | 1.49        | 1.42     |
| 22  | c     | 506 | CLA  | C3B-C4B | 2.66  | 1.49        | 1.42     |
| 22  | B     | 609 | CLA  | C3B-C4B | 2.65  | 1.49        | 1.42     |
| 22  | C     | 514 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 22  | b     | 611 | CLA  | C3B-C4B | 2.64  | 1.48        | 1.42     |
| 25  | A     | 409 | PL9  | C6-C1   | -2.63 | 1.43        | 1.48     |
| 22  | c     | 509 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | c     | 507 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | B     | 601 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 22  | A     | 405 | CLA  | C3B-C4B | 2.63  | 1.48        | 1.42     |
| 22  | c     | 514 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 22  | C     | 511 | CLA  | C3B-C4B | 2.62  | 1.48        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | E     | 104 | HEM  | FE-NA   | 2.61  | 2.04        | 1.95     |
| 22  | b     | 603 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | B     | 605 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | B     | 602 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | C     | 515 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | b     | 607 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | b     | 605 | CLA  | C3B-C4B | 2.61  | 1.48        | 1.42     |
| 22  | C     | 506 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 22  | a     | 406 | CLA  | C3B-C4B | 2.61  | 1.48        | 1.42     |
| 22  | B     | 612 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 22  | b     | 604 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 22  | c     | 516 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 22  | C     | 513 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 22  | b     | 606 | CLA  | C3B-C4B | 2.59  | 1.48        | 1.42     |
| 22  | C     | 508 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 22  | c     | 510 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 22  | B     | 612 | CLA  | CMD-C2D | -2.58 | 1.45        | 1.50     |
| 22  | b     | 614 | CLA  | CMD-C2D | -2.58 | 1.45        | 1.50     |
| 22  | B     | 603 | CLA  | C3B-C4B | 2.58  | 1.48        | 1.42     |
| 22  | b     | 614 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 25  | D     | 404 | PL9  | C6-C1   | -2.57 | 1.44        | 1.48     |
| 22  | B     | 607 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 22  | b     | 613 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 22  | D     | 401 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 22  | d     | 401 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 22  | C     | 509 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 22  | C     | 507 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 22  | B     | 611 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 22  | c     | 510 | CLA  | CMD-C2D | -2.54 | 1.45        | 1.50     |
| 22  | c     | 508 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 22  | A     | 404 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 22  | b     | 608 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 22  | b     | 605 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 22  | b     | 609 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 22  | B     | 616 | CLA  | C3B-C4B | 2.53  | 1.48        | 1.42     |
| 22  | C     | 509 | CLA  | CMD-C2D | -2.53 | 1.45        | 1.50     |
| 25  | d     | 402 | PL9  | C6-C1   | -2.52 | 1.44        | 1.48     |
| 22  | B     | 616 | CLA  | CMC-C2C | -2.51 | 1.45        | 1.50     |
| 22  | b     | 618 | CLA  | CMC-C2C | -2.51 | 1.45        | 1.50     |
| 22  | a     | 405 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 22  | B     | 609 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 22  | b     | 611 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | a     | 410 | PL9  | C6-C1   | -2.50 | 1.44        | 1.48     |
| 22  | B     | 614 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 22  | b     | 618 | CLA  | C3B-C4B | 2.49  | 1.48        | 1.42     |
| 22  | b     | 616 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 22  | B     | 604 | CLA  | C3B-C4B | 2.48  | 1.48        | 1.42     |
| 22  | B     | 603 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 22  | a     | 408 | CLA  | C1B-C2B | 2.46  | 1.49        | 1.43     |
| 22  | B     | 608 | CLA  | C1B-C2B | 2.46  | 1.49        | 1.43     |
| 22  | b     | 610 | CLA  | C1B-C2B | 2.46  | 1.49        | 1.43     |
| 22  | C     | 517 | CLA  | C1B-C2B | 2.44  | 1.49        | 1.43     |
| 23  | a     | 407 | PHO  | C1D-C2D | 2.44  | 1.42        | 1.39     |
| 22  | B     | 606 | CLA  | C1B-C2B | 2.43  | 1.49        | 1.43     |
| 22  | b     | 605 | CLA  | CMB-C2B | -2.43 | 1.45        | 1.50     |
| 22  | B     | 603 | CLA  | CMD-C2D | -2.42 | 1.45        | 1.50     |
| 36  | v     | 201 | HEM  | FE-NC   | 2.41  | 2.03        | 1.95     |
| 22  | B     | 603 | CLA  | CMB-C2B | -2.41 | 1.45        | 1.50     |
| 22  | C     | 512 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 22  | A     | 404 | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 22  | c     | 513 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 22  | c     | 511 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 22  | B     | 610 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 22  | C     | 510 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 22  | A     | 407 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 22  | c     | 515 | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 22  | b     | 605 | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 22  | c     | 514 | CLA  | CHC-C1C | 2.37  | 1.43        | 1.38     |
| 22  | C     | 514 | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 22  | d     | 403 | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 22  | a     | 405 | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 22  | c     | 518 | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 22  | D     | 405 | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 22  | b     | 612 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 22  | C     | 513 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 22  | B     | 604 | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 22  | b     | 605 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 36  | V     | 201 | HEM  | FE-NC   | 2.32  | 2.03        | 1.95     |
| 22  | B     | 603 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 22  | B     | 602 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 22  | b     | 606 | CLA  | CMD-C2D | -2.30 | 1.45        | 1.50     |
| 22  | b     | 614 | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 22  | c     | 511 | CLA  | CMB-C2B | -2.30 | 1.45        | 1.50     |
| 22  | B     | 604 | CLA  | CMB-C2B | -2.29 | 1.45        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | A     | 406 | PHO  | C1D-C2D | 2.28  | 1.42        | 1.39     |
| 22  | b     | 606 | CLA  | CMB-C2B | -2.28 | 1.46        | 1.50     |
| 22  | b     | 604 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 22  | C     | 510 | CLA  | CMB-C2B | -2.28 | 1.46        | 1.50     |
| 22  | c     | 518 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 22  | C     | 516 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 26  | D     | 412 | SQD  | O5-C5   | 2.26  | 1.49        | 1.44     |
| 23  | a     | 420 | PHO  | C1D-C2D | 2.25  | 1.42        | 1.39     |
| 22  | c     | 517 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 22  | C     | 512 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 26  | a     | 411 | SQD  | O5-C5   | 2.24  | 1.49        | 1.44     |
| 22  | c     | 513 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 22  | b     | 612 | CLA  | CHC-C1C | 2.22  | 1.43        | 1.38     |
| 22  | B     | 605 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 23  | D     | 403 | PHO  | C1D-C2D | 2.22  | 1.42        | 1.39     |
| 22  | B     | 612 | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 22  | C     | 517 | CLA  | CHC-C1C | 2.22  | 1.43        | 1.38     |
| 22  | B     | 611 | CLA  | CHC-C1C | 2.21  | 1.43        | 1.38     |
| 22  | B     | 606 | CLA  | CMC-C2C | -2.21 | 1.46        | 1.50     |
| 26  | d     | 412 | SQD  | O5-C5   | 2.21  | 1.49        | 1.44     |
| 22  | b     | 618 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 22  | a     | 408 | CLA  | CHC-C1C | 2.20  | 1.43        | 1.38     |
| 22  | C     | 516 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 25  | a     | 410 | PL9  | C53-C6  | -2.20 | 1.46        | 1.50     |
| 22  | B     | 616 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 22  | B     | 610 | CLA  | CHC-C1C | 2.20  | 1.43        | 1.38     |
| 22  | b     | 613 | CLA  | CHC-C1C | 2.19  | 1.43        | 1.38     |
| 22  | c     | 510 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 22  | c     | 510 | CLA  | CHC-C1C | 2.18  | 1.43        | 1.38     |
| 22  | c     | 516 | CLA  | CHC-C1C | 2.18  | 1.43        | 1.38     |
| 22  | B     | 608 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 22  | b     | 616 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 22  | b     | 607 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 22  | b     | 613 | CLA  | CMC-C2C | -2.18 | 1.46        | 1.50     |
| 22  | b     | 610 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 22  | B     | 608 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 22  | b     | 614 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 22  | D     | 406 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 22  | C     | 509 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 22  | B     | 614 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 22  | B     | 612 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 22  | B     | 601 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | A     | 407 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 26  | D     | 412 | SQD  | O7-S    | 2.16  | 1.51        | 1.45     |
| 22  | A     | 407 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 26  | l     | 102 | SQD  | O7-S    | 2.16  | 1.51        | 1.45     |
| 22  | c     | 513 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 26  | l     | 102 | SQD  | O9-S    | 2.15  | 1.51        | 1.45     |
| 22  | a     | 405 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 25  | A     | 409 | PL9  | C53-C6  | -2.15 | 1.46        | 1.50     |
| 22  | C     | 512 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 22  | d     | 404 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 26  | b     | 601 | SQD  | C46-C45 | 2.15  | 1.57        | 1.50     |
| 22  | B     | 609 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 22  | d     | 403 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 26  | d     | 412 | SQD  | O9-S    | 2.15  | 1.51        | 1.45     |
| 26  | b     | 601 | SQD  | O7-S    | 2.15  | 1.51        | 1.45     |
| 26  | a     | 411 | SQD  | O9-S    | 2.15  | 1.51        | 1.45     |
| 36  | V     | 201 | HEM  | CMC-C2C | 2.15  | 1.55        | 1.50     |
| 22  | D     | 405 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 22  | b     | 607 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 22  | c     | 517 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 22  | C     | 515 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 26  | l     | 102 | SQD  | C8-C7   | 2.13  | 1.56        | 1.50     |
| 22  | b     | 610 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 22  | a     | 408 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 26  | d     | 412 | SQD  | O7-S    | 2.13  | 1.51        | 1.45     |
| 22  | B     | 606 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 26  | b     | 601 | SQD  | O9-S    | 2.13  | 1.51        | 1.45     |
| 22  | c     | 508 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 22  | B     | 611 | CLA  | CMC-C2C | -2.13 | 1.46        | 1.50     |
| 22  | A     | 404 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 22  | C     | 506 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 26  | A     | 415 | SQD  | O9-S    | 2.12  | 1.51        | 1.45     |
| 26  | D     | 412 | SQD  | O9-S    | 2.12  | 1.51        | 1.45     |
| 22  | C     | 509 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 22  | b     | 604 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 22  | a     | 408 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 22  | c     | 507 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 22  | c     | 518 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 22  | C     | 508 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 22  | B     | 608 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 22  | a     | 406 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 22  | b     | 610 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 603 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 22  | C     | 510 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 22  | B     | 608 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 26  | A     | 410 | SQD  | O9-S    | 2.11  | 1.51        | 1.45     |
| 22  | B     | 602 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 22  | C     | 514 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 22  | B     | 605 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 22  | B     | 615 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 22  | b     | 611 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 22  | c     | 506 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 22  | C     | 506 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 36  | v     | 201 | HEM  | CMC-C2C | 2.11  | 1.55        | 1.50     |
| 22  | B     | 612 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 22  | c     | 507 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 22  | d     | 403 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 22  | D     | 405 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 22  | c     | 514 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 22  | C     | 505 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 22  | b     | 608 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 22  | c     | 509 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 22  | A     | 407 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 22  | a     | 406 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 22  | b     | 617 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | B     | 606 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 22  | c     | 511 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 22  | c     | 515 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 22  | B     | 610 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 22  | C     | 513 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 36  | E     | 104 | HEM  | CMB-C2B | 2.09  | 1.55        | 1.50     |
| 22  | A     | 404 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 22  | b     | 614 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 22  | c     | 513 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 22  | c     | 511 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 22  | c     | 516 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 22  | D     | 401 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 22  | b     | 610 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 22  | A     | 405 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 22  | A     | 405 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | b     | 608 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 22  | b     | 608 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 26  | a     | 417 | SQD  | O9-S    | 2.07  | 1.51        | 1.45     |
| 22  | c     | 515 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | C     | 510 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 22  | a     | 405 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 22  | b     | 612 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 22  | b     | 615 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 22  | B     | 614 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 22  | B     | 609 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 26  | d     | 412 | SQD  | C8-C7   | 2.07  | 1.56        | 1.50     |
| 26  | A     | 410 | SQD  | O7-S    | 2.07  | 1.51        | 1.45     |
| 22  | B     | 606 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 22  | c     | 508 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 22  | C     | 510 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 22  | b     | 603 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 26  | l     | 102 | SQD  | C46-C45 | 2.06  | 1.57        | 1.50     |
| 22  | c     | 517 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 22  | c     | 512 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 22  | B     | 613 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 22  | C     | 511 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 22  | B     | 616 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 22  | a     | 408 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 22  | C     | 512 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 22  | B     | 607 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 22  | c     | 508 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 22  | c     | 506 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 22  | C     | 507 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 22  | b     | 615 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 22  | b     | 614 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 22  | b     | 611 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 22  | A     | 405 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 22  | b     | 607 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 22  | C     | 515 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 22  | D     | 401 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 36  | e     | 103 | HEM  | CMB-C2B | 2.05  | 1.55        | 1.50     |
| 22  | c     | 511 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 22  | a     | 406 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 22  | b     | 609 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | c     | 506 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 22  | b     | 616 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | B     | 607 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | C     | 517 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 22  | c     | 515 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 22  | b     | 613 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | c     | 509 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 609 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 22  | C     | 514 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 22  | C     | 508 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 22  | B     | 607 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 22  | b     | 609 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 22  | B     | 612 | CLA  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 22  | D     | 406 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 22  | c     | 507 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 22  | C     | 508 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 22  | C     | 507 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | b     | 605 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 22  | B     | 615 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 26  | A     | 415 | SQD  | C8-C7   | 2.03  | 1.56        | 1.50     |
| 22  | C     | 507 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 22  | C     | 507 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 22  | C     | 516 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 22  | C     | 511 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | B     | 615 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 22  | B     | 607 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | b     | 609 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | c     | 511 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | B     | 613 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 22  | d     | 404 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 22  | A     | 407 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | d     | 401 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | B     | 605 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 22  | b     | 604 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 26  | a     | 411 | SQD  | O7-S    | 2.03  | 1.51        | 1.45     |
| 22  | C     | 506 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | C     | 517 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 22  | b     | 608 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 22  | b     | 609 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 22  | C     | 514 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 22  | B     | 602 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 26  | b     | 601 | SQD  | C44-C45 | 2.02  | 1.56        | 1.50     |
| 22  | B     | 604 | CLA  | MG-NB   | -2.02 | 2.01        | 2.05     |
| 22  | c     | 510 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 22  | C     | 506 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | c     | 512 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 25  | D     | 404 | PL9  | C53-C6  | -2.02 | 1.46        | 1.50     |
| 22  | B     | 614 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | d     | 403 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | d     | 404 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | C     | 508 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 22  | c     | 509 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 22  | C     | 510 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | b     | 615 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | b     | 615 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | B     | 614 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | b     | 604 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | b     | 616 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 22  | b     | 612 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 26  | D     | 412 | SQD  | C8-C7   | 2.01  | 1.56        | 1.50     |
| 22  | d     | 401 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | b     | 617 | CLA  | CHC-C1C | 2.01  | 1.42        | 1.38     |
| 22  | D     | 401 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | d     | 401 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 22  | B     | 611 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | B     | 605 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 22  | B     | 613 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | b     | 618 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 22  | c     | 510 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 22  | c     | 518 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 22  | B     | 603 | CLA  | CHC-C1C | 2.00  | 1.42        | 1.38     |
| 22  | B     | 601 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 22  | c     | 513 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |

All (768) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | a     | 407 | PHO  | C4D-CHA-CBD | -8.25 | 104.79      | 108.52   |
| 23  | A     | 406 | PHO  | C4D-CHA-CBD | -8.04 | 104.88      | 108.52   |
| 22  | b     | 606 | CLA  | C4A-NA-C1A  | 7.94  | 110.28      | 106.71   |
| 22  | C     | 516 | CLA  | C4A-NA-C1A  | 7.92  | 110.27      | 106.71   |
| 22  | B     | 604 | CLA  | C4A-NA-C1A  | 7.80  | 110.21      | 106.71   |
| 23  | a     | 420 | PHO  | C4D-CHA-CBD | -7.63 | 105.07      | 108.52   |
| 22  | C     | 511 | CLA  | C4A-NA-C1A  | 7.58  | 110.11      | 106.71   |
| 22  | c     | 517 | CLA  | C4A-NA-C1A  | 7.51  | 110.08      | 106.71   |
| 22  | c     | 509 | CLA  | C4A-NA-C1A  | 7.51  | 110.08      | 106.71   |
| 22  | b     | 608 | CLA  | C4A-NA-C1A  | 7.39  | 110.03      | 106.71   |
| 23  | D     | 403 | PHO  | C4D-CHA-CBD | -7.39 | 105.17      | 108.52   |
| 22  | c     | 512 | CLA  | C4A-NA-C1A  | 7.37  | 110.02      | 106.71   |
| 22  | b     | 609 | CLA  | C4A-NA-C1A  | 7.36  | 110.01      | 106.71   |
| 22  | B     | 606 | CLA  | C4A-NA-C1A  | 7.34  | 110.01      | 106.71   |

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| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 22  | b     | 614 | CLA  | C4A-NA-C1A | 7.34 | 110.01      | 106.71   |
| 22  | C     | 508 | CLA  | C4A-NA-C1A | 7.32 | 110.00      | 106.71   |
| 22  | c     | 507 | CLA  | C4A-NA-C1A | 7.32 | 110.00      | 106.71   |
| 22  | B     | 612 | CLA  | C4A-NA-C1A | 7.30 | 109.99      | 106.71   |
| 22  | B     | 607 | CLA  | C4A-NA-C1A | 7.28 | 109.98      | 106.71   |
| 22  | B     | 616 | CLA  | C4A-NA-C1A | 7.26 | 109.97      | 106.71   |
| 22  | c     | 511 | CLA  | C4A-NA-C1A | 7.26 | 109.97      | 106.71   |
| 22  | C     | 506 | CLA  | C4A-NA-C1A | 7.25 | 109.96      | 106.71   |
| 22  | C     | 515 | CLA  | C4A-NA-C1A | 7.21 | 109.95      | 106.71   |
| 22  | d     | 401 | CLA  | C4A-NA-C1A | 7.16 | 109.92      | 106.71   |
| 22  | b     | 618 | CLA  | C4A-NA-C1A | 7.15 | 109.92      | 106.71   |
| 22  | C     | 509 | CLA  | C4A-NA-C1A | 7.15 | 109.92      | 106.71   |
| 22  | c     | 510 | CLA  | C4A-NA-C1A | 7.14 | 109.92      | 106.71   |
| 22  | D     | 401 | CLA  | C4A-NA-C1A | 7.12 | 109.91      | 106.71   |
| 22  | b     | 616 | CLA  | C4A-NA-C1A | 7.10 | 109.90      | 106.71   |
| 22  | C     | 510 | CLA  | C4A-NA-C1A | 7.10 | 109.90      | 106.71   |
| 22  | C     | 513 | CLA  | C4A-NA-C1A | 7.08 | 109.89      | 106.71   |
| 22  | B     | 614 | CLA  | C4A-NA-C1A | 7.05 | 109.87      | 106.71   |
| 22  | c     | 514 | CLA  | C4A-NA-C1A | 7.05 | 109.87      | 106.71   |
| 22  | B     | 605 | CLA  | C4A-NA-C1A | 7.04 | 109.87      | 106.71   |
| 22  | c     | 513 | CLA  | C4A-NA-C1A | 7.04 | 109.87      | 106.71   |
| 22  | b     | 607 | CLA  | C4A-NA-C1A | 7.02 | 109.86      | 106.71   |
| 22  | a     | 406 | CLA  | C4A-NA-C1A | 7.02 | 109.86      | 106.71   |
| 22  | c     | 516 | CLA  | C4A-NA-C1A | 7.00 | 109.86      | 106.71   |
| 22  | b     | 613 | CLA  | C4A-NA-C1A | 6.99 | 109.85      | 106.71   |
| 22  | A     | 405 | CLA  | C4A-NA-C1A | 6.98 | 109.84      | 106.71   |
| 22  | D     | 406 | CLA  | C4A-NA-C1A | 6.95 | 109.83      | 106.71   |
| 22  | b     | 615 | CLA  | C4A-NA-C1A | 6.94 | 109.83      | 106.71   |
| 22  | B     | 611 | CLA  | C4A-NA-C1A | 6.93 | 109.82      | 106.71   |
| 22  | B     | 613 | CLA  | C4A-NA-C1A | 6.88 | 109.80      | 106.71   |
| 22  | b     | 603 | CLA  | C4A-NA-C1A | 6.88 | 109.80      | 106.71   |
| 22  | C     | 512 | CLA  | C4A-NA-C1A | 6.88 | 109.80      | 106.71   |
| 22  | c     | 515 | CLA  | C4A-NA-C1A | 6.87 | 109.80      | 106.71   |
| 22  | B     | 601 | CLA  | C4A-NA-C1A | 6.82 | 109.77      | 106.71   |
| 22  | D     | 405 | CLA  | C4A-NA-C1A | 6.81 | 109.77      | 106.71   |
| 22  | c     | 518 | CLA  | C4A-NA-C1A | 6.80 | 109.76      | 106.71   |
| 22  | B     | 609 | CLA  | C4A-NA-C1A | 6.80 | 109.76      | 106.71   |
| 22  | C     | 517 | CLA  | C4A-NA-C1A | 6.79 | 109.76      | 106.71   |
| 22  | b     | 617 | CLA  | C4A-NA-C1A | 6.79 | 109.76      | 106.71   |
| 22  | C     | 505 | CLA  | C4A-NA-C1A | 6.78 | 109.76      | 106.71   |
| 22  | C     | 514 | CLA  | C4A-NA-C1A | 6.78 | 109.75      | 106.71   |
| 22  | d     | 403 | CLA  | C4A-NA-C1A | 6.78 | 109.75      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 507 | CLA  | C4A-NA-C1A  | 6.74  | 109.73      | 106.71   |
| 22  | b     | 605 | CLA  | C4A-NA-C1A  | 6.74  | 109.73      | 106.71   |
| 22  | B     | 608 | CLA  | C4A-NA-C1A  | 6.71  | 109.72      | 106.71   |
| 22  | b     | 611 | CLA  | C4A-NA-C1A  | 6.70  | 109.72      | 106.71   |
| 22  | b     | 610 | CLA  | C4A-NA-C1A  | 6.67  | 109.71      | 106.71   |
| 22  | d     | 404 | CLA  | C4A-NA-C1A  | 6.67  | 109.71      | 106.71   |
| 22  | c     | 506 | CLA  | C4A-NA-C1A  | 6.62  | 109.68      | 106.71   |
| 22  | B     | 615 | CLA  | C4A-NA-C1A  | 6.61  | 109.68      | 106.71   |
| 22  | B     | 603 | CLA  | C4A-NA-C1A  | 6.54  | 109.64      | 106.71   |
| 22  | a     | 408 | CLA  | C4A-NA-C1A  | 6.53  | 109.64      | 106.71   |
| 22  | A     | 407 | CLA  | C4A-NA-C1A  | 6.47  | 109.61      | 106.71   |
| 22  | a     | 405 | CLA  | C4A-NA-C1A  | 6.43  | 109.60      | 106.71   |
| 22  | A     | 404 | CLA  | C4A-NA-C1A  | 6.39  | 109.58      | 106.71   |
| 22  | c     | 508 | CLA  | C4A-NA-C1A  | 6.33  | 109.55      | 106.71   |
| 22  | b     | 612 | CLA  | C4A-NA-C1A  | 6.28  | 109.53      | 106.71   |
| 24  | b     | 602 | BCR  | C15-C14-C13 | 6.28  | 136.27      | 127.31   |
| 22  | B     | 610 | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 22  | B     | 602 | CLA  | C4A-NA-C1A  | 6.14  | 109.47      | 106.71   |
| 22  | b     | 604 | CLA  | C4A-NA-C1A  | 6.09  | 109.44      | 106.71   |
| 24  | B     | 632 | BCR  | C15-C14-C13 | 6.08  | 135.98      | 127.31   |
| 34  | J     | 102 | DGD  | O5D-C1E-C2E | 5.99  | 117.65      | 108.30   |
| 34  | J     | 102 | DGD  | C6D-O5D-C1E | 5.60  | 124.68      | 113.74   |
| 25  | a     | 410 | PL9  | C7-C3-C4    | 5.18  | 121.09      | 116.88   |
| 25  | A     | 409 | PL9  | C7-C3-C4    | 5.10  | 121.03      | 116.88   |
| 26  | b     | 601 | SQD  | O6-C1-C2    | 5.10  | 116.26      | 108.30   |
| 26  | l     | 102 | SQD  | O7-S-C6     | 4.99  | 112.88      | 106.94   |
| 26  | b     | 601 | SQD  | O7-S-C6     | 4.91  | 112.78      | 106.94   |
| 25  | d     | 402 | PL9  | C7-C3-C4    | 4.72  | 120.72      | 116.88   |
| 25  | D     | 404 | PL9  | C7-C3-C4    | 4.72  | 120.71      | 116.88   |
| 26  | l     | 102 | SQD  | O47-C7-C8   | 4.66  | 121.56      | 111.50   |
| 23  | a     | 407 | PHO  | C2B-C1B-NB  | -4.33 | 106.53      | 109.53   |
| 26  | d     | 412 | SQD  | O47-C7-C8   | 4.32  | 120.81      | 111.50   |
| 23  | A     | 406 | PHO  | C2B-C1B-NB  | -4.30 | 106.56      | 109.53   |
| 34  | J     | 102 | DGD  | O5D-C6D-C5D | 4.17  | 116.76      | 109.05   |
| 24  | B     | 632 | BCR  | C16-C15-C14 | 4.16  | 131.99      | 123.47   |
| 26  | b     | 601 | SQD  | C1-O5-C5    | -4.07 | 105.69      | 113.69   |
| 26  | a     | 411 | SQD  | O9-S-C6     | 4.05  | 111.75      | 106.94   |
| 26  | D     | 412 | SQD  | O47-C7-C8   | 4.04  | 120.21      | 111.50   |
| 26  | b     | 601 | SQD  | O47-C7-C8   | 4.01  | 120.15      | 111.50   |
| 30  | a     | 419 | BCT  | O2-C-O1     | 3.98  | 129.86      | 119.55   |
| 30  | A     | 416 | BCT  | O2-C-O1     | 3.97  | 129.85      | 119.55   |
| 26  | A     | 415 | SQD  | O47-C7-C8   | 3.96  | 120.04      | 111.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | d     | 412 | SQD  | O9-S-C6     | 3.96  | 111.65      | 106.94   |
| 33  | i     | 102 | LMT  | C1B-O5B-C5B | 3.95  | 121.44      | 113.69   |
| 26  | a     | 417 | SQD  | O9-S-C6     | 3.95  | 111.63      | 106.94   |
| 26  | A     | 415 | SQD  | O9-S-C6     | 3.91  | 111.58      | 106.94   |
| 26  | A     | 410 | SQD  | O47-C7-C8   | 3.89  | 119.88      | 111.50   |
| 23  | a     | 420 | PHO  | C2B-C1B-NB  | -3.83 | 106.88      | 109.53   |
| 26  | A     | 415 | SQD  | O6-C1-C2    | 3.80  | 114.24      | 108.30   |
| 26  | a     | 411 | SQD  | O47-C7-C8   | 3.77  | 119.62      | 111.50   |
| 26  | D     | 412 | SQD  | O5-C5-C4    | 3.74  | 116.48      | 109.69   |
| 26  | a     | 417 | SQD  | O47-C7-C8   | 3.72  | 119.51      | 111.50   |
| 24  | B     | 632 | BCR  | C15-C16-C17 | -3.70 | 115.90      | 123.47   |
| 26  | b     | 601 | SQD  | O9-S-O7     | -3.68 | 101.20      | 113.95   |
| 34  | C     | 504 | DGD  | C6D-O5D-C1E | 3.67  | 120.91      | 113.74   |
| 26  | a     | 417 | SQD  | O6-C1-C2    | 3.65  | 114.01      | 108.30   |
| 26  | a     | 417 | SQD  | O9-S-O7     | -3.65 | 101.31      | 113.95   |
| 26  | a     | 411 | SQD  | O9-S-O7     | -3.65 | 101.33      | 113.95   |
| 23  | D     | 403 | PHO  | C2B-C1B-NB  | -3.63 | 107.02      | 109.53   |
| 26  | d     | 412 | SQD  | O7-S-C6     | 3.63  | 111.25      | 106.94   |
| 24  | b     | 602 | BCR  | C16-C15-C14 | 3.63  | 130.91      | 123.47   |
| 23  | a     | 420 | PHO  | C2D-C1D-ND  | -3.63 | 107.02      | 109.53   |
| 26  | A     | 415 | SQD  | O7-S-C6     | 3.62  | 111.25      | 106.94   |
| 33  | C     | 518 | LMT  | C1B-O5B-C5B | 3.59  | 120.73      | 113.69   |
| 34  | c     | 504 | DGD  | C6D-O5D-C1E | 3.58  | 120.73      | 113.74   |
| 25  | a     | 410 | PL9  | C7-C3-C2    | -3.57 | 118.60      | 123.30   |
| 26  | a     | 417 | SQD  | O7-S-C6     | 3.57  | 111.18      | 106.94   |
| 24  | b     | 602 | BCR  | C15-C16-C17 | -3.56 | 116.17      | 123.47   |
| 23  | D     | 403 | PHO  | C2D-C1D-ND  | -3.56 | 107.07      | 109.53   |
| 26  | A     | 410 | SQD  | O9-S-O7     | -3.55 | 101.68      | 113.95   |
| 26  | A     | 410 | SQD  | O9-S-C6     | 3.54  | 111.15      | 106.94   |
| 26  | A     | 415 | SQD  | O9-S-O7     | -3.54 | 101.70      | 113.95   |
| 25  | A     | 409 | PL9  | C7-C3-C2    | -3.49 | 118.70      | 123.30   |
| 26  | D     | 412 | SQD  | O9-S-O7     | -3.49 | 101.88      | 113.95   |
| 26  | D     | 412 | SQD  | O7-S-C6     | 3.47  | 111.07      | 106.94   |
| 26  | d     | 412 | SQD  | O9-S-O7     | -3.47 | 101.96      | 113.95   |
| 26  | l     | 102 | SQD  | O9-S-O7     | -3.43 | 102.08      | 113.95   |
| 22  | b     | 604 | CLA  | O2D-CGD-O1D | -3.41 | 117.17      | 123.84   |
| 35  | C     | 525 | LMG  | C4-C3-C2    | 3.40  | 116.75      | 110.82   |
| 22  | B     | 602 | CLA  | O2D-CGD-O1D | -3.39 | 117.22      | 123.84   |
| 22  | c     | 512 | CLA  | O2D-CGD-O1D | -3.37 | 117.25      | 123.84   |
| 26  | l     | 102 | SQD  | O9-S-C6     | 3.36  | 110.93      | 106.94   |
| 26  | d     | 412 | SQD  | O5-C5-C4    | 3.36  | 115.80      | 109.69   |
| 22  | C     | 511 | CLA  | O2D-CGD-O1D | -3.29 | 117.40      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 517 | CLA  | O2D-CGD-O1D | -3.28 | 117.42      | 123.84   |
| 22  | C     | 516 | CLA  | O2D-CGD-O1D | -3.28 | 117.42      | 123.84   |
| 23  | a     | 420 | PHO  | CMB-C2B-C3B | 3.27  | 130.80      | 124.68   |
| 23  | D     | 403 | PHO  | CMB-C2B-C3B | 3.25  | 130.76      | 124.68   |
| 22  | A     | 407 | CLA  | O2D-CGD-O1D | -3.24 | 117.50      | 123.84   |
| 22  | d     | 404 | CLA  | O2D-CGD-O1D | -3.24 | 117.50      | 123.84   |
| 22  | C     | 512 | CLA  | CMB-C2B-C1B | -3.24 | 120.44      | 125.37   |
| 22  | a     | 408 | CLA  | O2D-CGD-O1D | -3.24 | 117.51      | 123.84   |
| 22  | B     | 614 | CLA  | O2D-CGD-O1D | -3.22 | 117.55      | 123.84   |
| 22  | c     | 518 | CLA  | CMB-C2B-C1B | -3.22 | 120.47      | 125.37   |
| 22  | C     | 517 | CLA  | CMB-C2B-C1B | -3.22 | 120.47      | 125.37   |
| 22  | c     | 513 | CLA  | CMB-C2B-C1B | -3.21 | 120.48      | 125.37   |
| 22  | B     | 612 | CLA  | O2D-CGD-O1D | -3.21 | 117.56      | 123.84   |
| 25  | a     | 410 | PL9  | C40-C39-C41 | 3.18  | 120.62      | 115.27   |
| 22  | b     | 614 | CLA  | O2D-CGD-O1D | -3.17 | 117.63      | 123.84   |
| 26  | A     | 410 | SQD  | O7-S-C6     | 3.17  | 110.70      | 106.94   |
| 25  | d     | 402 | PL9  | C7-C3-C2    | -3.16 | 119.14      | 123.30   |
| 22  | b     | 616 | CLA  | O2D-CGD-O1D | -3.15 | 117.67      | 123.84   |
| 22  | C     | 512 | CLA  | O2D-CGD-O1D | -3.15 | 117.68      | 123.84   |
| 25  | D     | 404 | PL9  | C7-C3-C2    | -3.14 | 119.17      | 123.30   |
| 22  | B     | 606 | CLA  | O2D-CGD-O1D | -3.13 | 117.71      | 123.84   |
| 22  | c     | 513 | CLA  | O2D-CGD-O1D | -3.13 | 117.73      | 123.84   |
| 22  | c     | 511 | CLA  | CMB-C2B-C1B | -3.12 | 120.62      | 125.37   |
| 22  | D     | 406 | CLA  | O2D-CGD-O1D | -3.12 | 117.74      | 123.84   |
| 23  | A     | 406 | PHO  | C2D-C1D-ND  | -3.11 | 107.38      | 109.53   |
| 22  | d     | 404 | CLA  | C3B-C4B-NB  | -3.11 | 107.63      | 110.52   |
| 22  | b     | 618 | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 22  | B     | 616 | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 22  | c     | 518 | CLA  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 23  | a     | 407 | PHO  | C2D-C1D-ND  | -3.11 | 107.38      | 109.53   |
| 24  | b     | 602 | BCR  | C12-C13-C14 | -3.09 | 114.20      | 118.94   |
| 33  | A     | 419 | LMT  | C2'-C3'-C4' | 3.09  | 116.73      | 109.68   |
| 22  | D     | 401 | CLA  | CMB-C2B-C1B | -3.08 | 120.69      | 125.37   |
| 22  | d     | 401 | CLA  | CMB-C2B-C1B | -3.07 | 120.69      | 125.37   |
| 22  | C     | 517 | CLA  | O2D-CGD-O1D | -3.06 | 117.86      | 123.84   |
| 35  | C     | 525 | LMG  | O6-C5-C4    | 3.04  | 115.22      | 109.69   |
| 35  | y     | 101 | LMG  | O6-C5-C4    | 3.04  | 115.21      | 109.69   |
| 22  | C     | 513 | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 22  | B     | 611 | CLA  | O2D-CGD-O1D | -3.02 | 117.92      | 123.84   |
| 24  | c     | 501 | BCR  | C7-C8-C9    | -3.02 | 121.67      | 126.23   |
| 22  | b     | 608 | CLA  | O2D-CGD-O1D | -3.01 | 117.95      | 123.84   |
| 22  | C     | 510 | CLA  | CMB-C2B-C1B | -3.01 | 120.78      | 125.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 514 | CLA  | CHB-C4A-NA  | 3.00  | 128.66      | 124.51   |
| 26  | b     | 601 | SQD  | O9-S-C6     | 3.00  | 110.50      | 106.94   |
| 23  | A     | 406 | PHO  | C1C-C2C-C3C | -2.99 | 106.12      | 108.61   |
| 23  | a     | 407 | PHO  | C1C-C2C-C3C | -2.99 | 106.12      | 108.61   |
| 36  | v     | 201 | HEM  | C1B-NB-C4B  | 2.99  | 108.16      | 105.07   |
| 22  | b     | 614 | CLA  | CMB-C2B-C1B | -2.98 | 120.84      | 125.37   |
| 36  | e     | 103 | HEM  | C4D-ND-C1D  | 2.97  | 108.14      | 105.07   |
| 26  | a     | 411 | SQD  | O5-C5-C4    | 2.97  | 115.08      | 109.69   |
| 22  | c     | 514 | CLA  | O2D-CGD-O1D | -2.97 | 118.04      | 123.84   |
| 22  | a     | 406 | CLA  | O2D-CGD-O1D | -2.96 | 118.04      | 123.84   |
| 22  | D     | 401 | CLA  | O2D-CGD-O1D | -2.96 | 118.05      | 123.84   |
| 22  | A     | 404 | CLA  | CMB-C2B-C1B | -2.96 | 120.86      | 125.37   |
| 34  | D     | 411 | DGD  | C3G-O3G-C1D | 2.95  | 119.50      | 113.74   |
| 36  | E     | 104 | HEM  | C4D-ND-C1D  | 2.95  | 108.12      | 105.07   |
| 22  | A     | 405 | CLA  | O2D-CGD-O1D | -2.94 | 118.08      | 123.84   |
| 36  | V     | 201 | HEM  | C4A-NA-C1A  | 2.94  | 108.23      | 105.35   |
| 22  | C     | 513 | CLA  | CHB-C4A-NA  | 2.94  | 128.58      | 124.51   |
| 36  | E     | 104 | HEM  | CBD-CAD-C3D | -2.94 | 104.46      | 112.63   |
| 36  | e     | 103 | HEM  | CBD-CAD-C3D | -2.93 | 104.50      | 112.63   |
| 22  | a     | 405 | CLA  | CMB-C2B-C1B | -2.92 | 120.93      | 125.37   |
| 22  | b     | 603 | CLA  | O2D-CGD-O1D | -2.92 | 118.14      | 123.84   |
| 25  | A     | 409 | PL9  | C40-C39-C41 | 2.91  | 120.17      | 115.27   |
| 22  | C     | 513 | CLA  | CMB-C2B-C1B | -2.91 | 120.93      | 125.37   |
| 22  | B     | 612 | CLA  | CMB-C2B-C1B | -2.91 | 120.94      | 125.37   |
| 24  | B     | 632 | BCR  | C12-C13-C14 | -2.91 | 114.47      | 118.94   |
| 22  | B     | 603 | CLA  | O2D-CGD-O1D | -2.91 | 118.15      | 123.84   |
| 24  | C     | 501 | BCR  | C7-C8-C9    | -2.90 | 121.85      | 126.23   |
| 25  | d     | 402 | PL9  | C40-C39-C41 | 2.90  | 120.16      | 115.27   |
| 22  | b     | 612 | CLA  | O2D-CGD-O1D | -2.90 | 118.16      | 123.84   |
| 36  | V     | 201 | HEM  | C1B-NB-C4B  | 2.90  | 108.07      | 105.07   |
| 22  | b     | 613 | CLA  | CMB-C2B-C1B | -2.90 | 120.95      | 125.37   |
| 22  | c     | 514 | CLA  | CMB-C2B-C1B | -2.90 | 120.95      | 125.37   |
| 22  | c     | 507 | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 22  | B     | 601 | CLA  | O2D-CGD-O1D | -2.90 | 118.18      | 123.84   |
| 22  | d     | 401 | CLA  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |
| 22  | C     | 506 | CLA  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |
| 22  | B     | 611 | CLA  | CMB-C2B-C1B | -2.89 | 120.96      | 125.37   |
| 26  | A     | 415 | SQD  | O48-C23-C24 | 2.89  | 120.98      | 111.91   |
| 22  | c     | 508 | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 22  | b     | 605 | CLA  | O2D-CGD-O1D | -2.88 | 118.21      | 123.84   |
| 22  | B     | 608 | CLA  | O2D-CGD-O1D | -2.88 | 118.21      | 123.84   |
| 22  | C     | 505 | CLA  | C3B-C4B-NB  | -2.87 | 107.85      | 110.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | v     | 201 | HEM  | C4A-NA-C1A  | 2.87  | 108.16      | 105.35   |
| 22  | B     | 610 | CLA  | C3B-C4B-NB  | -2.87 | 107.85      | 110.52   |
| 22  | b     | 613 | CLA  | O2D-CGD-O1D | -2.87 | 118.23      | 123.84   |
| 22  | C     | 515 | CLA  | CHB-C4A-NA  | 2.87  | 128.48      | 124.51   |
| 22  | C     | 505 | CLA  | O2D-CGD-O1D | -2.87 | 118.23      | 123.84   |
| 26  | D     | 412 | SQD  | O8-S-C6     | 2.86  | 110.30      | 105.74   |
| 22  | B     | 610 | CLA  | O2D-CGD-O1D | -2.86 | 118.24      | 123.84   |
| 22  | C     | 511 | CLA  | CHB-C4A-NA  | 2.86  | 128.47      | 124.51   |
| 26  | a     | 411 | SQD  | O8-S-C6     | 2.86  | 110.30      | 105.74   |
| 22  | b     | 608 | CLA  | CHB-C4A-NA  | 2.86  | 128.46      | 124.51   |
| 22  | C     | 516 | CLA  | CHB-C4A-NA  | 2.86  | 128.46      | 124.51   |
| 26  | D     | 412 | SQD  | O9-S-C6     | 2.85  | 110.33      | 106.94   |
| 24  | B     | 619 | BCR  | C23-C22-C21 | -2.85 | 114.56      | 118.94   |
| 22  | c     | 516 | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 25  | D     | 404 | PL9  | C40-C39-C41 | 2.85  | 120.06      | 115.27   |
| 22  | b     | 612 | CLA  | C3B-C4B-NB  | -2.85 | 107.87      | 110.52   |
| 22  | b     | 610 | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 26  | D     | 412 | SQD  | O48-C23-C24 | 2.85  | 120.84      | 111.91   |
| 26  | a     | 417 | SQD  | O8-S-C6     | 2.84  | 110.27      | 105.74   |
| 22  | c     | 510 | CLA  | O2D-CGD-O1D | -2.84 | 118.28      | 123.84   |
| 22  | C     | 516 | CLA  | C3B-C4B-NB  | -2.84 | 107.88      | 110.52   |
| 22  | c     | 516 | CLA  | CHB-C4A-NA  | 2.84  | 128.43      | 124.51   |
| 22  | C     | 509 | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 22  | c     | 508 | CLA  | CMB-C2B-C1B | -2.83 | 121.06      | 125.37   |
| 24  | b     | 620 | BCR  | C23-C22-C21 | -2.82 | 114.61      | 118.94   |
| 25  | d     | 402 | PL9  | C7-C8-C9    | -2.82 | 122.11      | 126.79   |
| 25  | D     | 404 | PL9  | C7-C8-C9    | -2.81 | 122.11      | 126.79   |
| 22  | c     | 506 | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 22  | c     | 512 | CLA  | CHB-C4A-NA  | 2.81  | 128.39      | 124.51   |
| 25  | A     | 409 | PL9  | C36-C34-C33 | -2.80 | 115.44      | 121.12   |
| 35  | y     | 101 | LMG  | C9-C8-C7    | 2.80  | 118.42      | 111.79   |
| 22  | c     | 517 | CLA  | C3B-C4B-NB  | -2.80 | 107.92      | 110.52   |
| 22  | b     | 609 | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 26  | A     | 410 | SQD  | O8-S-C6     | 2.79  | 110.19      | 105.74   |
| 22  | C     | 515 | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 22  | B     | 615 | CLA  | O2D-CGD-O1D | -2.79 | 118.39      | 123.84   |
| 22  | a     | 408 | CLA  | C3B-C4B-NB  | -2.78 | 107.93      | 110.52   |
| 36  | E     | 104 | HEM  | C4A-NA-C1A  | 2.78  | 108.07      | 105.35   |
| 26  | d     | 412 | SQD  | O48-C23-C24 | 2.77  | 120.61      | 111.91   |
| 22  | c     | 515 | CLA  | O2D-CGD-O1D | -2.77 | 118.42      | 123.84   |
| 22  | B     | 604 | CLA  | O2D-CGD-O1D | -2.76 | 118.44      | 123.84   |
| 22  | A     | 407 | CLA  | C3B-C4B-NB  | -2.76 | 107.96      | 110.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 506 | CLA  | C3B-C4B-NB  | -2.76 | 107.96      | 110.52   |
| 22  | b     | 606 | CLA  | CHB-C4A-NA  | 2.75  | 128.32      | 124.51   |
| 22  | C     | 514 | CLA  | O2D-CGD-O1D | -2.75 | 118.45      | 123.84   |
| 22  | C     | 517 | CLA  | CHB-C4A-NA  | 2.75  | 128.31      | 124.51   |
| 22  | D     | 406 | CLA  | C3B-C4B-NB  | -2.75 | 107.97      | 110.52   |
| 22  | c     | 518 | CLA  | CHB-C4A-NA  | 2.75  | 128.31      | 124.51   |
| 22  | b     | 617 | CLA  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 22  | c     | 518 | CLA  | CMB-C2B-C3B | 2.74  | 133.22      | 126.59   |
| 22  | C     | 517 | CLA  | CMB-C2B-C3B | 2.74  | 133.22      | 126.59   |
| 22  | B     | 607 | CLA  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 22  | A     | 407 | CLA  | CHB-C4A-NA  | 2.74  | 128.29      | 124.51   |
| 22  | B     | 613 | CLA  | O2D-CGD-O1D | -2.74 | 118.49      | 123.84   |
| 22  | B     | 604 | CLA  | C4-C3-C5    | 2.74  | 119.87      | 115.27   |
| 22  | B     | 610 | CLA  | CHB-C1B-NB  | 2.73  | 127.15      | 124.26   |
| 26  | a     | 411 | SQD  | O48-C23-C24 | 2.72  | 120.45      | 111.91   |
| 22  | C     | 507 | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 22  | B     | 606 | CLA  | CHB-C4A-NA  | 2.72  | 128.27      | 124.51   |
| 36  | v     | 201 | HEM  | CBD-CAD-C3D | -2.72 | 105.08      | 112.63   |
| 22  | B     | 604 | CLA  | CHB-C4A-NA  | 2.72  | 128.27      | 124.51   |
| 25  | a     | 410 | PL9  | C36-C34-C33 | -2.71 | 115.63      | 121.12   |
| 22  | c     | 509 | CLA  | O2D-CGD-O1D | -2.70 | 118.55      | 123.84   |
| 23  | a     | 420 | PHO  | C1C-C2C-C3C | -2.70 | 106.36      | 108.61   |
| 22  | B     | 610 | CLA  | CAA-CBA-CGA | -2.70 | 105.36      | 113.25   |
| 22  | b     | 612 | CLA  | CAA-CBA-CGA | -2.70 | 105.36      | 113.25   |
| 22  | B     | 616 | CLA  | CMB-C2B-C1B | -2.70 | 121.25      | 125.37   |
| 22  | c     | 517 | CLA  | CHB-C4A-NA  | 2.70  | 128.24      | 124.51   |
| 22  | b     | 616 | CLA  | CHB-C4A-NA  | 2.70  | 128.24      | 124.51   |
| 22  | d     | 403 | CLA  | C3B-C4B-NB  | -2.69 | 108.02      | 110.52   |
| 22  | b     | 618 | CLA  | CMB-C2B-C1B | -2.69 | 121.27      | 125.37   |
| 22  | D     | 401 | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 22  | B     | 615 | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 22  | b     | 615 | CLA  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 22  | d     | 401 | CLA  | CHB-C4A-NA  | 2.69  | 128.23      | 124.51   |
| 36  | V     | 201 | HEM  | CBD-CAD-C3D | -2.69 | 105.17      | 112.63   |
| 22  | b     | 617 | CLA  | CHB-C4A-NA  | 2.68  | 128.22      | 124.51   |
| 33  | f     | 102 | LMT  | C1B-O5B-C5B | 2.68  | 118.96      | 113.69   |
| 22  | b     | 612 | CLA  | CAA-C2A-C3A | -2.68 | 105.43      | 112.78   |
| 22  | C     | 508 | CLA  | O2D-CGD-O1D | -2.68 | 118.59      | 123.84   |
| 22  | B     | 610 | CLA  | CAA-C2A-C3A | -2.68 | 105.44      | 112.78   |
| 22  | b     | 606 | CLA  | C4-C3-C5    | 2.68  | 119.78      | 115.27   |
| 22  | D     | 405 | CLA  | C3B-C4B-NB  | -2.68 | 108.03      | 110.52   |
| 22  | D     | 405 | CLA  | O2D-CGD-O1D | -2.68 | 118.61      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 614 | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 22  | a     | 408 | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 22  | b     | 614 | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 22  | c     | 518 | CLA  | CHD-C1D-ND  | -2.67 | 122.00      | 124.45   |
| 22  | B     | 608 | CLA  | CHB-C4A-NA  | 2.67  | 128.20      | 124.51   |
| 36  | V     | 201 | HEM  | C4D-ND-C1D  | 2.67  | 107.83      | 105.07   |
| 22  | B     | 612 | CLA  | CHB-C4A-NA  | 2.67  | 128.20      | 124.51   |
| 36  | e     | 103 | HEM  | C4C-NC-C1C  | 2.66  | 107.95      | 105.35   |
| 26  | A     | 415 | SQD  | O8-S-C6     | 2.66  | 109.98      | 105.74   |
| 26  | a     | 411 | SQD  | O7-S-C6     | 2.66  | 110.10      | 106.94   |
| 25  | d     | 402 | PL9  | C27-C28-C29 | -2.66 | 121.26      | 127.66   |
| 26  | b     | 601 | SQD  | O8-S-C6     | 2.66  | 109.97      | 105.74   |
| 22  | b     | 606 | CLA  | O2D-CGD-O1D | -2.65 | 118.65      | 123.84   |
| 24  | b     | 620 | BCR  | C2-C1-C6    | 2.65  | 114.56      | 110.48   |
| 26  | A     | 410 | SQD  | O48-C23-C24 | 2.65  | 120.22      | 111.91   |
| 22  | C     | 507 | CLA  | C3B-C4B-NB  | -2.65 | 108.06      | 110.52   |
| 22  | D     | 406 | CLA  | CHB-C4A-NA  | 2.65  | 128.17      | 124.51   |
| 36  | e     | 103 | HEM  | C4A-NA-C1A  | 2.64  | 107.94      | 105.35   |
| 22  | c     | 507 | CLA  | CHB-C4A-NA  | 2.64  | 128.17      | 124.51   |
| 22  | b     | 612 | CLA  | CHB-C1B-NB  | 2.64  | 127.06      | 124.26   |
| 22  | b     | 610 | CLA  | CHB-C4A-NA  | 2.64  | 128.17      | 124.51   |
| 25  | D     | 404 | PL9  | C27-C28-C29 | -2.64 | 121.30      | 127.66   |
| 22  | c     | 511 | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 23  | D     | 403 | PHO  | C1C-C2C-C3C | -2.63 | 106.42      | 108.61   |
| 33  | C     | 518 | LMT  | C1'-O5'-C5' | 2.63  | 118.84      | 113.69   |
| 26  | a     | 417 | SQD  | O48-C23-C24 | 2.62  | 120.14      | 111.91   |
| 22  | d     | 404 | CLA  | CHB-C4A-NA  | 2.62  | 128.14      | 124.51   |
| 22  | C     | 517 | CLA  | CHD-C1D-ND  | -2.62 | 122.04      | 124.45   |
| 22  | B     | 602 | CLA  | C3B-C4B-NB  | -2.62 | 108.08      | 110.52   |
| 22  | C     | 508 | CLA  | CHB-C4A-NA  | 2.62  | 128.13      | 124.51   |
| 36  | E     | 104 | HEM  | C4C-NC-C1C  | 2.62  | 107.91      | 105.35   |
| 22  | c     | 510 | CLA  | C3B-C4B-NB  | -2.61 | 108.09      | 110.52   |
| 22  | c     | 509 | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 24  | B     | 619 | BCR  | C2-C1-C6    | 2.61  | 114.50      | 110.48   |
| 26  | A     | 415 | SQD  | O5-C5-C4    | 2.61  | 114.43      | 109.69   |
| 22  | C     | 509 | CLA  | C3B-C4B-NB  | -2.61 | 108.10      | 110.52   |
| 22  | d     | 403 | CLA  | O2D-CGD-O1D | -2.60 | 118.75      | 123.84   |
| 22  | b     | 604 | CLA  | C3B-C4B-NB  | -2.60 | 108.10      | 110.52   |
| 22  | C     | 506 | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 22  | C     | 510 | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 22  | B     | 607 | CLA  | CHB-C4A-NA  | 2.59  | 128.10      | 124.51   |
| 22  | B     | 605 | CLA  | CHB-C4A-NA  | 2.59  | 128.10      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 603 | CLA  | CHB-C4A-NA  | 2.59  | 128.09      | 124.51   |
| 25  | A     | 409 | PL9  | C7-C8-C9    | -2.59 | 122.49      | 126.79   |
| 22  | B     | 614 | CLA  | C3B-C4B-NB  | -2.59 | 108.12      | 110.52   |
| 22  | b     | 609 | CLA  | CHB-C4A-NA  | 2.58  | 128.09      | 124.51   |
| 22  | b     | 607 | CLA  | CHB-C4A-NA  | 2.58  | 128.08      | 124.51   |
| 22  | C     | 510 | CLA  | O2D-CGD-O1D | -2.58 | 118.79      | 123.84   |
| 22  | b     | 616 | CLA  | C3B-C4B-NB  | -2.58 | 108.12      | 110.52   |
| 22  | b     | 611 | CLA  | O2D-CGD-O1D | -2.58 | 118.80      | 123.84   |
| 22  | B     | 601 | CLA  | CHB-C4A-NA  | 2.58  | 128.07      | 124.51   |
| 22  | B     | 605 | CLA  | CHD-C1D-ND  | -2.57 | 122.09      | 124.45   |
| 36  | v     | 201 | HEM  | C4D-ND-C1D  | 2.57  | 107.73      | 105.07   |
| 22  | b     | 612 | CLA  | CHB-C4A-NA  | 2.57  | 128.07      | 124.51   |
| 25  | a     | 410 | PL9  | C7-C8-C9    | -2.57 | 122.52      | 126.79   |
| 22  | B     | 609 | CLA  | CHB-C4A-NA  | 2.56  | 128.05      | 124.51   |
| 35  | y     | 101 | LMG  | C7-O1-C1    | 2.56  | 118.74      | 113.74   |
| 22  | a     | 406 | CLA  | CHB-C4A-NA  | 2.56  | 128.05      | 124.51   |
| 22  | C     | 505 | CLA  | CHB-C4A-NA  | 2.56  | 128.05      | 124.51   |
| 22  | C     | 512 | CLA  | CMB-C2B-C3B | 2.56  | 132.78      | 126.59   |
| 22  | A     | 404 | CLA  | O2D-CGD-O1D | -2.56 | 118.84      | 123.84   |
| 22  | c     | 513 | CLA  | CMB-C2B-C3B | 2.55  | 132.77      | 126.59   |
| 33  | Z     | 101 | LMT  | C1'-O5'-C5' | 2.55  | 118.70      | 113.69   |
| 22  | a     | 405 | CLA  | O2D-CGD-O1D | -2.55 | 118.85      | 123.84   |
| 22  | b     | 611 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 22  | B     | 602 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 22  | B     | 610 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 22  | B     | 605 | CLA  | O2D-CGD-O1D | -2.54 | 118.86      | 123.84   |
| 22  | b     | 607 | CLA  | O2D-CGD-O1D | -2.54 | 118.88      | 123.84   |
| 26  | D     | 412 | SQD  | C1-O5-C5    | 2.54  | 118.67      | 113.69   |
| 22  | b     | 604 | CLA  | CHB-C4A-NA  | 2.53  | 128.02      | 124.51   |
| 22  | b     | 610 | CLA  | CMB-C2B-C1B | -2.53 | 121.51      | 125.37   |
| 22  | B     | 613 | CLA  | CMB-C2B-C1B | -2.53 | 121.51      | 125.37   |
| 22  | A     | 405 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 22  | b     | 613 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 22  | B     | 609 | CLA  | O2D-CGD-O1D | -2.53 | 118.89      | 123.84   |
| 25  | D     | 404 | PL9  | C22-C23-C24 | -2.52 | 121.58      | 127.66   |
| 22  | B     | 616 | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 22  | c     | 513 | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 22  | b     | 604 | CLA  | CMB-C2B-C1B | -2.52 | 121.53      | 125.37   |
| 22  | B     | 605 | CLA  | C3B-C4B-NB  | -2.52 | 108.18      | 110.52   |
| 22  | b     | 615 | CLA  | CMB-C2B-C1B | -2.52 | 121.53      | 125.37   |
| 22  | B     | 601 | CLA  | C3B-C4B-NB  | -2.52 | 108.18      | 110.52   |
| 22  | b     | 608 | CLA  | C3B-C4B-NB  | -2.51 | 108.18      | 110.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | d     | 402 | PL9  | C22-C23-C24 | -2.51 | 121.61      | 127.66   |
| 22  | B     | 606 | CLA  | C3B-C4B-NB  | -2.51 | 108.18      | 110.52   |
| 26  | a     | 417 | SQD  | O5-C5-C4    | 2.51  | 114.26      | 109.69   |
| 22  | b     | 607 | CLA  | CHD-C1D-ND  | -2.51 | 122.14      | 124.45   |
| 22  | C     | 508 | CLA  | CMB-C2B-C1B | -2.51 | 121.54      | 125.37   |
| 22  | c     | 509 | CLA  | CMB-C2B-C1B | -2.51 | 121.55      | 125.37   |
| 26  | b     | 601 | SQD  | O48-C23-C24 | 2.50  | 119.76      | 111.91   |
| 36  | e     | 103 | HEM  | CMC-C2C-C1C | -2.50 | 120.30      | 124.71   |
| 22  | A     | 405 | CLA  | CMB-C2B-C1B | -2.50 | 121.56      | 125.37   |
| 26  | d     | 412 | SQD  | O8-S-C6     | 2.50  | 109.72      | 105.74   |
| 36  | V     | 201 | HEM  | CMB-C2B-C1B | -2.50 | 121.24      | 125.04   |
| 22  | B     | 611 | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 22  | c     | 512 | CLA  | O2D-CGD-CBD | 2.49  | 115.70      | 111.27   |
| 22  | c     | 511 | CLA  | O2D-CGD-O1D | -2.49 | 118.97      | 123.84   |
| 25  | A     | 409 | PL9  | C22-C23-C24 | -2.49 | 121.67      | 127.66   |
| 24  | b     | 602 | BCR  | C19-C18-C17 | -2.49 | 115.12      | 118.94   |
| 22  | B     | 608 | CLA  | C3B-C4B-NB  | -2.49 | 108.21      | 110.52   |
| 22  | a     | 406 | CLA  | CMB-C2B-C1B | -2.49 | 121.58      | 125.37   |
| 26  | b     | 601 | SQD  | C4-C3-C2    | 2.49  | 115.17      | 110.82   |
| 26  | l     | 102 | SQD  | O48-C23-C24 | 2.49  | 119.71      | 111.91   |
| 36  | E     | 104 | HEM  | CMC-C2C-C1C | -2.48 | 120.33      | 124.71   |
| 22  | c     | 508 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 22  | C     | 507 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 22  | B     | 608 | CLA  | CMB-C2B-C1B | -2.48 | 121.59      | 125.37   |
| 24  | b     | 602 | BCR  | C16-C17-C18 | 2.48  | 130.85      | 127.31   |
| 22  | C     | 508 | CLA  | CHD-C1D-ND  | -2.48 | 122.18      | 124.45   |
| 33  | f     | 102 | LMT  | C1-O1'-C1'  | 2.48  | 117.94      | 113.84   |
| 36  | E     | 104 | HEM  | CHC-C1C-NC  | 2.47  | 127.12      | 124.44   |
| 22  | b     | 607 | CLA  | C3B-C4B-NB  | -2.47 | 108.22      | 110.52   |
| 34  | c     | 503 | DGD  | C6D-O5D-C1E | 2.47  | 118.56      | 113.74   |
| 36  | V     | 201 | HEM  | C4C-NC-C1C  | 2.47  | 107.76      | 105.35   |
| 22  | a     | 408 | CLA  | O2D-CGD-CBD | 2.46  | 115.65      | 111.27   |
| 22  | b     | 618 | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 22  | A     | 404 | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 22  | B     | 602 | CLA  | CMB-C2B-C1B | -2.46 | 121.62      | 125.37   |
| 22  | B     | 603 | CLA  | C3B-C4B-NB  | -2.46 | 108.23      | 110.52   |
| 25  | A     | 409 | PL9  | C27-C28-C29 | -2.46 | 121.73      | 127.66   |
| 26  | D     | 412 | SQD  | O5-C1-C2    | 2.46  | 115.56      | 110.35   |
| 22  | b     | 610 | CLA  | C3B-C4B-NB  | -2.46 | 108.23      | 110.52   |
| 33  | Z     | 101 | LMT  | C1'-C2'-C3' | -2.46 | 104.87      | 110.00   |
| 36  | v     | 201 | HEM  | C4C-NC-C1C  | 2.46  | 107.76      | 105.35   |
| 22  | d     | 404 | CLA  | O2D-CGD-CBD | 2.46  | 115.64      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 516 | CLA  | CMB-C2B-C1B | -2.45 | 121.63      | 125.37   |
| 22  | C     | 512 | CLA  | CHB-C4A-NA  | 2.45  | 127.91      | 124.51   |
| 22  | b     | 603 | CLA  | C3B-C4B-NB  | -2.45 | 108.24      | 110.52   |
| 22  | A     | 405 | CLA  | CAA-C2A-C3A | -2.45 | 106.07      | 112.78   |
| 22  | A     | 407 | CLA  | O2D-CGD-CBD | 2.45  | 115.62      | 111.27   |
| 22  | C     | 515 | CLA  | CMB-C2B-C1B | -2.45 | 121.64      | 125.37   |
| 35  | y     | 101 | LMG  | C4-C3-C2    | 2.45  | 115.09      | 110.82   |
| 22  | a     | 406 | CLA  | CAA-C2A-C3A | -2.44 | 106.09      | 112.78   |
| 26  | a     | 411 | SQD  | C1-O5-C5    | 2.44  | 118.47      | 113.69   |
| 22  | B     | 611 | CLA  | CHD-C1D-ND  | -2.44 | 122.21      | 124.45   |
| 25  | a     | 410 | PL9  | C22-C23-C24 | -2.44 | 121.79      | 127.66   |
| 22  | b     | 613 | CLA  | CHD-C1D-ND  | -2.43 | 122.22      | 124.45   |
| 23  | D     | 403 | PHO  | C4A-C3A-C2A | -2.43 | 100.53      | 102.84   |
| 26  | d     | 412 | SQD  | C1-O5-C5    | 2.43  | 118.46      | 113.69   |
| 22  | d     | 401 | CLA  | CMB-C2B-C3B | 2.43  | 132.47      | 126.59   |
| 22  | D     | 401 | CLA  | CMB-C2B-C3B | 2.43  | 132.47      | 126.59   |
| 22  | c     | 510 | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 34  | c     | 504 | DGD  | C3G-O3G-C1D | 2.43  | 118.48      | 113.74   |
| 22  | C     | 513 | CLA  | CMB-C2B-C3B | 2.43  | 132.46      | 126.59   |
| 22  | c     | 514 | CLA  | CMB-C2B-C3B | 2.42  | 132.46      | 126.59   |
| 22  | a     | 405 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 33  | z     | 101 | LMT  | C1'-O5'-C5' | 2.42  | 118.44      | 113.69   |
| 22  | c     | 506 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 24  | f     | 101 | BCR  | C23-C22-C21 | -2.42 | 115.23      | 118.94   |
| 22  | B     | 613 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 22  | b     | 615 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 36  | e     | 103 | HEM  | CHC-C1C-NC  | 2.42  | 127.05      | 124.44   |
| 34  | C     | 503 | DGD  | C6D-O5D-C1E | 2.41  | 118.46      | 113.74   |
| 22  | A     | 404 | CLA  | CMB-C2B-C3B | 2.41  | 132.44      | 126.59   |
| 25  | D     | 404 | PL9  | O1-C4-C3    | -2.41 | 118.06      | 120.72   |
| 22  | C     | 512 | CLA  | O2D-CGD-CBD | 2.41  | 115.56      | 111.27   |
| 25  | d     | 402 | PL9  | O1-C4-C3    | -2.41 | 118.06      | 120.72   |
| 22  | C     | 506 | CLA  | C3B-C4B-NB  | -2.41 | 108.28      | 110.52   |
| 26  | D     | 412 | SQD  | C3-C4-C5    | 2.41  | 114.54      | 110.24   |
| 22  | C     | 511 | CLA  | O2D-CGD-CBD | 2.41  | 115.55      | 111.27   |
| 22  | c     | 507 | CLA  | C3B-C4B-NB  | -2.41 | 108.28      | 110.52   |
| 22  | a     | 405 | CLA  | CMB-C2B-C3B | 2.41  | 132.41      | 126.59   |
| 22  | B     | 614 | CLA  | CHD-C1D-ND  | -2.40 | 122.25      | 124.45   |
| 26  | b     | 601 | SQD  | C3-C4-C5    | 2.40  | 114.51      | 110.24   |
| 22  | D     | 401 | CLA  | CHD-C1D-ND  | -2.40 | 122.25      | 124.45   |
| 24  | B     | 632 | BCR  | C19-C18-C17 | -2.39 | 115.27      | 118.94   |
| 22  | C     | 507 | CLA  | CMB-C2B-C1B | -2.39 | 121.73      | 125.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 509 | CLA  | CHB-C4A-NA  | 2.39  | 127.82      | 124.51   |
| 22  | b     | 616 | CLA  | CHD-C1D-ND  | -2.39 | 122.26      | 124.45   |
| 22  | c     | 509 | CLA  | CHD-C1D-ND  | -2.38 | 122.26      | 124.45   |
| 22  | c     | 514 | CLA  | C16-C15-C13 | -2.38 | 108.22      | 115.92   |
| 36  | v     | 201 | HEM  | CMB-C2B-C1B | -2.38 | 121.41      | 125.04   |
| 22  | A     | 405 | CLA  | O2D-CGD-CBD | 2.38  | 115.50      | 111.27   |
| 22  | B     | 604 | CLA  | C1-C2-C3    | -2.38 | 121.93      | 126.04   |
| 22  | c     | 513 | CLA  | O2D-CGD-CBD | 2.37  | 115.49      | 111.27   |
| 22  | c     | 518 | CLA  | C3B-C4B-NB  | -2.37 | 108.31      | 110.52   |
| 24  | C     | 502 | BCR  | C7-C8-C9    | -2.37 | 122.65      | 126.23   |
| 22  | b     | 605 | CLA  | C3B-C4B-NB  | -2.37 | 108.31      | 110.52   |
| 36  | E     | 104 | HEM  | C1B-NB-C4B  | 2.37  | 107.52      | 105.07   |
| 24  | c     | 502 | BCR  | C7-C8-C9    | -2.36 | 122.67      | 126.23   |
| 36  | e     | 103 | HEM  | C1B-NB-C4B  | 2.36  | 107.51      | 105.07   |
| 30  | a     | 419 | BCT  | O3-C-O1     | -2.35 | 113.44      | 119.55   |
| 24  | k     | 101 | BCR  | C11-C10-C9  | 2.35  | 130.67      | 127.31   |
| 23  | a     | 420 | PHO  | C4A-C3A-C2A | -2.35 | 100.60      | 102.84   |
| 36  | V     | 201 | HEM  | C3B-C2B-C1B | 2.35  | 108.23      | 106.49   |
| 22  | a     | 406 | CLA  | O2D-CGD-CBD | 2.35  | 115.44      | 111.27   |
| 25  | A     | 409 | PL9  | C37-C38-C39 | -2.35 | 122.01      | 127.66   |
| 22  | b     | 611 | CLA  | C3B-C4B-NB  | -2.34 | 108.34      | 110.52   |
| 30  | A     | 416 | BCT  | O3-C-O1     | -2.34 | 113.47      | 119.55   |
| 22  | c     | 506 | CLA  | CHC-C4B-NB  | 2.34  | 126.73      | 124.26   |
| 22  | B     | 613 | CLA  | O1D-CGD-CBD | 2.34  | 129.26      | 124.48   |
| 22  | C     | 515 | CLA  | C3B-C4B-NB  | -2.34 | 108.35      | 110.52   |
| 26  | l     | 102 | SQD  | C3-C4-C5    | 2.34  | 114.41      | 110.24   |
| 22  | B     | 611 | CLA  | CMB-C2B-C3B | 2.33  | 132.24      | 126.59   |
| 22  | d     | 401 | CLA  | CHD-C1D-ND  | -2.33 | 122.31      | 124.45   |
| 22  | C     | 517 | CLA  | C3B-C4B-NB  | -2.33 | 108.35      | 110.52   |
| 22  | c     | 508 | CLA  | CMB-C2B-C3B | 2.33  | 132.23      | 126.59   |
| 22  | c     | 515 | CLA  | CHB-C4A-NA  | 2.33  | 127.73      | 124.51   |
| 22  | b     | 614 | CLA  | CMB-C2B-C3B | 2.33  | 132.22      | 126.59   |
| 25  | d     | 402 | PL9  | C20-C19-C21 | 2.33  | 119.18      | 115.27   |
| 36  | V     | 201 | HEM  | C3D-C4D-ND  | -2.32 | 107.58      | 110.17   |
| 22  | c     | 512 | CLA  | CMB-C2B-C1B | -2.32 | 121.83      | 125.37   |
| 22  | A     | 404 | CLA  | C3B-C4B-NB  | -2.32 | 108.36      | 110.52   |
| 22  | d     | 404 | CLA  | CHD-C1D-ND  | -2.32 | 122.32      | 124.45   |
| 33  | C     | 518 | LMT  | C1-O1'-C1'  | 2.32  | 117.68      | 113.84   |
| 22  | C     | 514 | CLA  | CHB-C4A-NA  | 2.32  | 127.72      | 124.51   |
| 22  | B     | 611 | CLA  | C3B-C4B-NB  | -2.32 | 108.37      | 110.52   |
| 25  | a     | 410 | PL9  | C27-C28-C29 | -2.31 | 122.09      | 127.66   |
| 22  | c     | 508 | CLA  | C3B-C4B-NB  | -2.31 | 108.37      | 110.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 615 | CLA  | C3B-C4B-NB  | -2.31 | 108.37      | 110.52   |
| 22  | c     | 513 | CLA  | CHB-C1B-NB  | 2.31  | 126.70      | 124.26   |
| 22  | B     | 608 | CLA  | O2A-CGA-O1A | -2.31 | 117.77      | 123.59   |
| 36  | v     | 201 | HEM  | C3D-C4D-ND  | -2.31 | 107.60      | 110.17   |
| 22  | c     | 506 | CLA  | CHD-C1D-ND  | -2.31 | 122.33      | 124.45   |
| 22  | b     | 615 | CLA  | O1D-CGD-CBD | 2.31  | 129.20      | 124.48   |
| 22  | b     | 613 | CLA  | CMB-C2B-C3B | 2.31  | 132.17      | 126.59   |
| 24  | F     | 101 | BCR  | C24-C23-C22 | -2.30 | 122.75      | 126.23   |
| 22  | B     | 606 | CLA  | O2D-CGD-CBD | 2.30  | 115.36      | 111.27   |
| 26  | d     | 412 | SQD  | O5-C1-C2    | 2.30  | 115.21      | 110.35   |
| 22  | b     | 609 | CLA  | CHD-C1D-ND  | -2.30 | 122.34      | 124.45   |
| 22  | C     | 512 | CLA  | CHB-C1B-NB  | 2.30  | 126.69      | 124.26   |
| 22  | B     | 609 | CLA  | C3B-C4B-NB  | -2.29 | 108.39      | 110.52   |
| 22  | b     | 613 | CLA  | C3B-C4B-NB  | -2.29 | 108.39      | 110.52   |
| 22  | B     | 607 | CLA  | CHD-C1D-ND  | -2.29 | 122.35      | 124.45   |
| 22  | a     | 405 | CLA  | C3B-C4B-NB  | -2.29 | 108.39      | 110.52   |
| 25  | D     | 404 | PL9  | C20-C19-C21 | 2.29  | 119.12      | 115.27   |
| 26  | l     | 102 | SQD  | C1-O5-C5    | -2.28 | 109.21      | 113.69   |
| 24  | c     | 501 | BCR  | C24-C23-C22 | -2.28 | 122.79      | 126.23   |
| 22  | D     | 406 | CLA  | O2D-CGD-CBD | 2.28  | 115.32      | 111.27   |
| 22  | B     | 612 | CLA  | CMB-C2B-C3B | 2.28  | 132.10      | 126.59   |
| 33  | i     | 102 | LMT  | C1'-O5'-C5' | 2.28  | 118.16      | 113.69   |
| 22  | d     | 403 | CLA  | CHB-C4A-NA  | 2.28  | 127.66      | 124.51   |
| 22  | b     | 604 | CLA  | O2D-CGD-CBD | 2.27  | 115.31      | 111.27   |
| 33  | Z     | 101 | LMT  | C3'-C4'-C5' | -2.27 | 105.72      | 110.93   |
| 22  | C     | 510 | CLA  | CHB-C1B-NB  | 2.27  | 126.66      | 124.26   |
| 22  | D     | 405 | CLA  | CHB-C4A-NA  | 2.27  | 127.65      | 124.51   |
| 22  | B     | 607 | CLA  | C3B-C4B-NB  | -2.27 | 108.41      | 110.52   |
| 22  | C     | 505 | CLA  | CHD-C1D-ND  | -2.27 | 122.37      | 124.45   |
| 22  | B     | 602 | CLA  | O2D-CGD-CBD | 2.26  | 115.29      | 111.27   |
| 22  | C     | 512 | CLA  | C3B-C4B-NB  | -2.26 | 108.42      | 110.52   |
| 22  | b     | 610 | CLA  | CHD-C1D-ND  | -2.26 | 122.38      | 124.45   |
| 33  | J     | 103 | LMT  | C1'-O5'-C5' | 2.25  | 118.11      | 113.69   |
| 22  | b     | 605 | CLA  | CHB-C4A-NA  | 2.25  | 127.62      | 124.51   |
| 22  | B     | 603 | CLA  | O2A-CGA-O1A | -2.25 | 117.92      | 123.59   |
| 22  | c     | 513 | CLA  | CHD-C1D-ND  | -2.25 | 122.39      | 124.45   |
| 22  | B     | 603 | CLA  | CHB-C4A-NA  | 2.24  | 127.61      | 124.51   |
| 22  | c     | 511 | CLA  | CHB-C1B-NB  | 2.24  | 126.63      | 124.26   |
| 22  | D     | 406 | CLA  | C1-C2-C3    | -2.24 | 122.17      | 126.04   |
| 22  | B     | 609 | CLA  | CHC-C4B-NB  | 2.24  | 126.63      | 124.26   |
| 22  | c     | 516 | CLA  | C3B-C4B-NB  | -2.24 | 108.44      | 110.52   |
| 22  | b     | 605 | CLA  | O2A-CGA-O1A | -2.23 | 117.95      | 123.59   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 512 | CLA  | CHD-C1D-ND  | -2.23 | 122.40      | 124.45   |
| 35  | C     | 525 | LMG  | C1-O6-C5    | 2.23  | 118.07      | 113.69   |
| 34  | C     | 504 | DGD  | C3G-O3G-C1D | 2.23  | 118.10      | 113.74   |
| 22  | b     | 610 | CLA  | O2A-CGA-O1A | -2.23 | 117.96      | 123.59   |
| 22  | c     | 512 | CLA  | C2A-C1A-CHA | 2.23  | 127.76      | 123.86   |
| 26  | a     | 417 | SQD  | C3-C4-C5    | 2.23  | 114.21      | 110.24   |
| 22  | c     | 511 | CLA  | CMB-C2B-C3B | 2.23  | 131.98      | 126.59   |
| 22  | D     | 406 | CLA  | CHD-C1D-ND  | -2.23 | 122.41      | 124.45   |
| 22  | C     | 507 | CLA  | O2A-CGA-O1A | -2.22 | 117.98      | 123.59   |
| 22  | B     | 608 | CLA  | CHD-C1D-ND  | -2.22 | 122.41      | 124.45   |
| 36  | V     | 201 | HEM  | C2A-C1A-NA  | -2.22 | 107.67      | 110.15   |
| 22  | c     | 508 | CLA  | CHD-C1D-ND  | -2.22 | 122.42      | 124.45   |
| 22  | b     | 609 | CLA  | C3B-C4B-NB  | -2.22 | 108.46      | 110.52   |
| 22  | C     | 507 | CLA  | CHD-C1D-ND  | -2.22 | 122.42      | 124.45   |
| 26  | A     | 415 | SQD  | C3-C4-C5    | 2.22  | 114.19      | 110.24   |
| 34  | J     | 102 | DGD  | O2E-C2E-C1E | 2.22  | 115.43      | 110.05   |
| 22  | b     | 618 | CLA  | CMB-C2B-C3B | 2.22  | 131.95      | 126.59   |
| 25  | a     | 410 | PL9  | C37-C38-C39 | -2.21 | 122.33      | 127.66   |
| 22  | b     | 605 | CLA  | CHC-C4B-NB  | 2.21  | 126.60      | 124.26   |
| 22  | B     | 603 | CLA  | CHC-C4B-NB  | 2.21  | 126.59      | 124.26   |
| 23  | a     | 407 | PHO  | C4B-NB-C1B  | 2.21  | 112.24      | 108.83   |
| 23  | a     | 420 | PHO  | C4D-ND-C1D  | 2.21  | 111.07      | 108.83   |
| 22  | c     | 513 | CLA  | C3B-C4B-NB  | -2.21 | 108.47      | 110.52   |
| 22  | B     | 606 | CLA  | O2A-CGA-O1A | -2.20 | 118.03      | 123.59   |
| 22  | B     | 616 | CLA  | CMB-C2B-C3B | 2.20  | 131.92      | 126.59   |
| 36  | v     | 201 | HEM  | C2A-C1A-NA  | -2.20 | 107.69      | 110.15   |
| 27  | C     | 522 | PLM  | O2-C1-C2    | -2.20 | 116.02      | 123.08   |
| 22  | C     | 517 | CLA  | CAA-C2A-C3A | -2.20 | 106.77      | 112.78   |
| 22  | d     | 404 | CLA  | CHC-C4B-NB  | 2.19  | 126.58      | 124.26   |
| 26  | d     | 412 | SQD  | C3-C4-C5    | 2.19  | 114.15      | 110.24   |
| 22  | B     | 606 | CLA  | CHB-C1B-NB  | 2.19  | 126.58      | 124.26   |
| 22  | b     | 604 | CLA  | CMB-C2B-C3B | 2.19  | 131.89      | 126.59   |
| 22  | B     | 604 | CLA  | CAA-C2A-C3A | -2.19 | 106.79      | 112.78   |
| 24  | f     | 101 | BCR  | C29-C30-C25 | 2.18  | 113.84      | 110.48   |
| 23  | A     | 406 | PHO  | CMB-C2B-C3B | 2.18  | 128.76      | 124.68   |
| 22  | C     | 510 | CLA  | CMB-C2B-C3B | 2.18  | 131.87      | 126.59   |
| 22  | C     | 511 | CLA  | CMB-C2B-C1B | -2.18 | 122.06      | 125.37   |
| 22  | B     | 611 | CLA  | O2D-CGD-CBD | 2.17  | 115.13      | 111.27   |
| 23  | a     | 407 | PHO  | CMB-C2B-C3B | 2.17  | 128.74      | 124.68   |
| 34  | c     | 505 | DGD  | C6D-O5D-C1E | 2.17  | 117.98      | 113.74   |
| 23  | A     | 406 | PHO  | C4B-NB-C1B  | 2.17  | 112.19      | 108.83   |
| 23  | D     | 403 | PHO  | C4D-ND-C1D  | 2.17  | 111.04      | 108.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | a     | 411 | SQD  | O5-C1-C2    | 2.17  | 114.94      | 110.35   |
| 24  | b     | 619 | BCR  | C29-C30-C25 | 2.17  | 113.82      | 110.48   |
| 22  | b     | 606 | CLA  | CAA-C2A-C3A | -2.17 | 106.85      | 112.78   |
| 22  | A     | 404 | CLA  | C2D-C1D-ND  | -2.16 | 108.51      | 110.10   |
| 25  | d     | 402 | PL9  | C32-C33-C34 | -2.16 | 122.45      | 127.66   |
| 25  | A     | 409 | PL9  | C32-C33-C34 | -2.16 | 122.45      | 127.66   |
| 22  | C     | 511 | CLA  | C2A-C1A-CHA | 2.16  | 127.64      | 123.86   |
| 22  | B     | 614 | CLA  | CMB-C2B-C1B | -2.16 | 122.08      | 125.37   |
| 22  | c     | 514 | CLA  | C11-C12-C13 | -2.16 | 108.93      | 115.92   |
| 22  | B     | 602 | CLA  | CMB-C2B-C3B | 2.16  | 131.82      | 126.59   |
| 22  | b     | 611 | CLA  | CHC-C4B-NB  | 2.16  | 126.54      | 124.26   |
| 33  | i     | 102 | LMT  | O1B-C4'-C3' | 2.16  | 113.02      | 107.28   |
| 22  | B     | 603 | CLA  | CHB-C1B-NB  | 2.16  | 126.54      | 124.26   |
| 36  | v     | 201 | HEM  | C3B-C2B-C1B | 2.16  | 108.08      | 106.49   |
| 22  | C     | 515 | CLA  | C2A-C1A-CHA | 2.15  | 127.63      | 123.86   |
| 22  | b     | 614 | CLA  | C3B-C4B-NB  | -2.15 | 108.52      | 110.52   |
| 25  | D     | 404 | PL9  | C32-C33-C34 | -2.15 | 122.48      | 127.66   |
| 33  | i     | 102 | LMT  | C1B-C2B-C3B | 2.15  | 114.47      | 110.00   |
| 22  | b     | 608 | CLA  | O2D-CGD-CBD | 2.15  | 115.09      | 111.27   |
| 22  | d     | 404 | CLA  | O2A-CGA-O1A | -2.15 | 118.17      | 123.59   |
| 22  | c     | 510 | CLA  | O2D-CGD-CBD | 2.14  | 115.08      | 111.27   |
| 24  | f     | 101 | BCR  | C20-C21-C22 | 2.14  | 130.37      | 127.31   |
| 22  | C     | 514 | CLA  | CMB-C2B-C1B | -2.14 | 122.11      | 125.37   |
| 22  | a     | 405 | CLA  | C2D-C1D-ND  | -2.14 | 108.53      | 110.10   |
| 22  | C     | 510 | CLA  | C1-C2-C3    | -2.14 | 122.34      | 126.04   |
| 22  | A     | 407 | CLA  | O2A-CGA-O1A | -2.14 | 118.19      | 123.59   |
| 22  | c     | 515 | CLA  | CMB-C2B-C1B | -2.14 | 122.11      | 125.37   |
| 22  | A     | 407 | CLA  | CHD-C1D-ND  | -2.14 | 122.49      | 124.45   |
| 22  | c     | 517 | CLA  | C11-C12-C13 | -2.14 | 109.02      | 115.92   |
| 23  | a     | 420 | PHO  | C4B-NB-C1B  | 2.13  | 112.13      | 108.83   |
| 22  | c     | 508 | CLA  | O2A-CGA-O1A | -2.13 | 118.20      | 123.59   |
| 22  | B     | 606 | CLA  | CMB-C2B-C1B | -2.13 | 122.12      | 125.37   |
| 24  | c     | 502 | BCR  | C38-C26-C27 | -2.13 | 109.52      | 113.62   |
| 22  | C     | 510 | CLA  | CHD-C1D-ND  | -2.13 | 122.50      | 124.45   |
| 22  | c     | 512 | CLA  | CMB-C2B-C3B | 2.13  | 131.75      | 126.59   |
| 36  | v     | 201 | HEM  | CAC-C3C-C4C | -2.13 | 119.75      | 124.90   |
| 22  | B     | 615 | CLA  | CHC-C4B-NB  | 2.13  | 126.51      | 124.26   |
| 24  | C     | 502 | BCR  | C38-C26-C27 | -2.13 | 109.53      | 113.62   |
| 22  | b     | 606 | CLA  | CHC-C4B-NB  | 2.12  | 126.51      | 124.26   |
| 22  | C     | 514 | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 24  | Y     | 102 | BCR  | C20-C21-C22 | 2.12  | 130.34      | 127.31   |
| 22  | b     | 605 | CLA  | CHB-C1B-NB  | 2.12  | 126.50      | 124.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 606 | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 22  | a     | 408 | CLA  | O2A-CGA-O1A | -2.12 | 118.25      | 123.59   |
| 25  | D     | 404 | PL9  | O2-C1-C2    | -2.12 | 116.93      | 121.78   |
| 22  | b     | 616 | CLA  | CMB-C2B-C1B | -2.12 | 122.15      | 125.37   |
| 25  | A     | 409 | PL9  | C25-C24-C26 | 2.11  | 118.83      | 115.27   |
| 22  | C     | 517 | CLA  | CHB-C1B-NB  | 2.11  | 126.50      | 124.26   |
| 22  | B     | 613 | CLA  | CHD-C1D-ND  | -2.11 | 122.51      | 124.45   |
| 22  | A     | 405 | CLA  | CHD-C1D-ND  | -2.11 | 122.51      | 124.45   |
| 22  | b     | 606 | CLA  | C1-C2-C3    | -2.11 | 122.39      | 126.04   |
| 22  | D     | 406 | CLA  | O2A-CGA-O1A | -2.11 | 118.26      | 123.59   |
| 22  | C     | 509 | CLA  | O2D-CGD-CBD | 2.11  | 115.02      | 111.27   |
| 22  | b     | 610 | CLA  | CMB-C2B-C3B | 2.11  | 131.69      | 126.59   |
| 22  | b     | 606 | CLA  | O2A-CGA-O1A | -2.11 | 118.28      | 123.59   |
| 22  | a     | 406 | CLA  | CHD-C1D-ND  | -2.11 | 122.52      | 124.45   |
| 22  | c     | 511 | CLA  | O2A-CGA-O1A | -2.10 | 118.28      | 123.59   |
| 22  | C     | 513 | CLA  | C3B-C4B-NB  | -2.10 | 108.56      | 110.52   |
| 25  | A     | 409 | PL9  | O1-C4-C3    | -2.10 | 118.40      | 120.72   |
| 22  | a     | 408 | CLA  | CHD-C1D-ND  | -2.10 | 122.52      | 124.45   |
| 22  | B     | 611 | CLA  | O2A-CGA-O1A | -2.10 | 118.29      | 123.59   |
| 22  | B     | 614 | CLA  | CHB-C1B-NB  | 2.10  | 126.48      | 124.26   |
| 33  | m     | 102 | LMT  | C1-O1'-C1'  | 2.10  | 117.32      | 113.84   |
| 22  | C     | 515 | CLA  | CMB-C2B-C3B | 2.10  | 131.67      | 126.59   |
| 25  | d     | 402 | PL9  | O2-C1-C2    | -2.10 | 116.97      | 121.78   |
| 22  | c     | 515 | CLA  | C3B-C4B-NB  | -2.10 | 108.57      | 110.52   |
| 36  | E     | 104 | HEM  | CBA-CAA-C2A | -2.10 | 106.80      | 112.63   |
| 22  | c     | 516 | CLA  | CHD-C1D-ND  | -2.10 | 122.53      | 124.45   |
| 22  | c     | 516 | CLA  | CMB-C2B-C3B | 2.09  | 131.66      | 126.59   |
| 22  | c     | 517 | CLA  | O2D-CGD-CBD | 2.09  | 114.99      | 111.27   |
| 22  | b     | 608 | CLA  | O2A-CGA-O1A | -2.09 | 118.31      | 123.59   |
| 22  | b     | 615 | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 22  | c     | 508 | CLA  | CHB-C1B-NB  | 2.09  | 126.47      | 124.26   |
| 22  | b     | 613 | CLA  | O2A-CGA-O1A | -2.09 | 118.32      | 123.59   |
| 22  | C     | 516 | CLA  | O2D-CGD-CBD | 2.09  | 114.98      | 111.27   |
| 22  | B     | 608 | CLA  | CMB-C2B-C3B | 2.09  | 131.64      | 126.59   |
| 22  | B     | 609 | CLA  | CHD-C1D-ND  | -2.08 | 122.54      | 124.45   |
| 25  | a     | 410 | PL9  | C26-C24-C23 | -2.08 | 116.90      | 121.12   |
| 25  | d     | 402 | PL9  | C36-C34-C33 | -2.08 | 116.90      | 121.12   |
| 22  | C     | 514 | CLA  | C3B-C4B-NB  | -2.08 | 108.58      | 110.52   |
| 22  | b     | 611 | CLA  | CHD-C1D-ND  | -2.08 | 122.54      | 124.45   |
| 22  | B     | 604 | CLA  | CHC-C4B-NB  | 2.08  | 126.46      | 124.26   |
| 22  | D     | 401 | CLA  | O2D-CGD-CBD | 2.08  | 114.96      | 111.27   |
| 22  | B     | 604 | CLA  | O2A-CGA-O1A | -2.08 | 118.35      | 123.59   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 606 | CLA  | C16-C15-C13 | -2.07 | 109.21      | 115.92   |
| 33  | C     | 518 | LMT  | O1B-C4'-C3' | 2.07  | 112.80      | 107.28   |
| 22  | c     | 514 | CLA  | C3B-C4B-NB  | -2.07 | 108.59      | 110.52   |
| 22  | a     | 406 | CLA  | CMB-C2B-C3B | 2.07  | 131.61      | 126.59   |
| 22  | b     | 615 | CLA  | CMB-C2B-C3B | 2.07  | 131.61      | 126.59   |
| 25  | D     | 404 | PL9  | C37-C38-C39 | -2.07 | 122.67      | 127.66   |
| 25  | D     | 404 | PL9  | O2-C1-C6    | 2.07  | 124.17      | 120.59   |
| 22  | B     | 612 | CLA  | O2D-CGD-CBD | 2.07  | 114.94      | 111.27   |
| 25  | d     | 402 | PL9  | O2-C1-C6    | 2.07  | 124.17      | 120.59   |
| 22  | c     | 518 | CLA  | CHB-C1B-NB  | 2.07  | 126.44      | 124.26   |
| 22  | C     | 512 | CLA  | O2A-CGA-O1A | -2.07 | 118.38      | 123.59   |
| 22  | A     | 405 | CLA  | CMB-C2B-C3B | 2.06  | 131.59      | 126.59   |
| 24  | B     | 632 | BCR  | C16-C17-C18 | 2.06  | 130.25      | 127.31   |
| 22  | b     | 614 | CLA  | O2A-CGA-O1A | -2.06 | 118.39      | 123.59   |
| 22  | C     | 515 | CLA  | CHD-C1D-ND  | -2.06 | 122.56      | 124.45   |
| 22  | c     | 506 | CLA  | C1-C2-C3    | -2.06 | 122.48      | 126.04   |
| 24  | y     | 102 | BCR  | C20-C21-C22 | 2.06  | 130.25      | 127.31   |
| 25  | d     | 402 | PL9  | C37-C38-C39 | -2.06 | 122.70      | 127.66   |
| 22  | c     | 515 | CLA  | CHD-C1D-ND  | -2.06 | 122.56      | 124.45   |
| 36  | E     | 104 | HEM  | CMB-C2B-C1B | -2.06 | 121.90      | 125.04   |
| 22  | C     | 507 | CLA  | CHB-C1B-NB  | 2.06  | 126.44      | 124.26   |
| 25  | A     | 409 | PL9  | C26-C24-C23 | -2.06 | 116.95      | 121.12   |
| 25  | a     | 410 | PL9  | O1-C4-C3    | -2.06 | 118.45      | 120.72   |
| 36  | e     | 103 | HEM  | CMB-C2B-C1B | -2.06 | 121.91      | 125.04   |
| 22  | c     | 516 | CLA  | C2A-C1A-CHA | 2.06  | 127.46      | 123.86   |
| 33  | i     | 102 | LMT  | O5B-C5B-C4B | 2.06  | 113.43      | 109.69   |
| 22  | B     | 604 | CLA  | C16-C15-C13 | -2.05 | 109.28      | 115.92   |
| 22  | B     | 613 | CLA  | CMB-C2B-C3B | 2.05  | 131.56      | 126.59   |
| 22  | C     | 510 | CLA  | O2A-CGA-O1A | -2.05 | 118.41      | 123.59   |
| 22  | C     | 507 | CLA  | CMB-C2B-C3B | 2.05  | 131.56      | 126.59   |
| 25  | a     | 410 | PL9  | O2-C1-C2    | -2.05 | 117.08      | 121.78   |
| 22  | B     | 607 | CLA  | CHB-C1B-NB  | 2.05  | 126.43      | 124.26   |
| 22  | c     | 511 | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 22  | B     | 612 | CLA  | O2A-CGA-O1A | -2.05 | 118.43      | 123.59   |
| 33  | z     | 101 | LMT  | C1'-C2'-C3' | -2.04 | 105.74      | 110.00   |
| 22  | B     | 603 | CLA  | C2D-C1D-ND  | -2.04 | 108.60      | 110.10   |
| 34  | C     | 504 | DGD  | C4D-C3D-C2D | 2.04  | 114.38      | 110.82   |
| 25  | a     | 410 | PL9  | C20-C19-C21 | 2.04  | 118.70      | 115.27   |
| 22  | b     | 606 | CLA  | C11-C12-C13 | -2.04 | 109.33      | 115.92   |
| 22  | b     | 610 | CLA  | CHB-C1B-NB  | 2.04  | 126.42      | 124.26   |
| 22  | C     | 511 | CLA  | CMB-C2B-C3B | 2.04  | 131.52      | 126.59   |
| 22  | b     | 617 | CLA  | CHC-C4B-NB  | 2.04  | 126.41      | 124.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | D     | 403 | PHO  | C4B-NB-C1B  | 2.04  | 111.98      | 108.83   |
| 22  | B     | 615 | CLA  | C2A-C1A-CHA | 2.03  | 127.42      | 123.86   |
| 25  | A     | 409 | PL9  | C31-C32-C33 | -2.03 | 105.20      | 111.88   |
| 36  | V     | 201 | HEM  | CAC-C3C-C4C | -2.03 | 119.99      | 124.90   |
| 22  | B     | 615 | CLA  | O2A-CGA-O1A | -2.03 | 118.46      | 123.59   |
| 22  | B     | 604 | CLA  | C2A-C1A-CHA | 2.03  | 127.41      | 123.86   |
| 36  | E     | 104 | HEM  | C2A-C1A-NA  | -2.03 | 107.88      | 110.15   |
| 22  | c     | 514 | CLA  | CHD-C1D-ND  | -2.03 | 122.59      | 124.45   |
| 22  | B     | 608 | CLA  | O2D-CGD-CBD | 2.03  | 114.88      | 111.27   |
| 22  | B     | 612 | CLA  | C3B-C4B-NB  | -2.03 | 108.63      | 110.52   |
| 26  | A     | 415 | SQD  | C44-O6-C1   | -2.03 | 109.77      | 113.74   |
| 22  | c     | 513 | CLA  | O2A-CGA-O1A | -2.03 | 118.48      | 123.59   |
| 22  | C     | 508 | CLA  | CMB-C2B-C3B | 2.03  | 131.50      | 126.59   |
| 34  | C     | 504 | DGD  | O6E-C1E-O5D | 2.03  | 114.77      | 109.97   |
| 23  | a     | 407 | PHO  | C4D-ND-C1D  | 2.02  | 110.89      | 108.83   |
| 24  | B     | 632 | BCR  | C2-C3-C4    | 2.02  | 115.90      | 111.38   |
| 22  | C     | 510 | CLA  | O1D-CGD-CBD | 2.02  | 128.62      | 124.48   |
| 33  | z     | 101 | LMT  | C3'-C4'-C5' | -2.02 | 106.29      | 110.93   |
| 24  | F     | 101 | BCR  | C23-C22-C21 | -2.02 | 115.84      | 118.94   |
| 22  | c     | 511 | CLA  | C1-C2-C3    | -2.02 | 122.55      | 126.04   |
| 22  | b     | 614 | CLA  | O2D-CGD-CBD | 2.02  | 114.86      | 111.27   |
| 22  | B     | 607 | CLA  | CHC-C4B-NB  | 2.02  | 126.39      | 124.26   |
| 22  | C     | 511 | CLA  | C3B-C4B-NB  | -2.02 | 108.64      | 110.52   |
| 22  | B     | 605 | CLA  | CMB-C2B-C1B | -2.02 | 122.30      | 125.37   |
| 22  | b     | 603 | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 22  | b     | 617 | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 22  | c     | 511 | CLA  | O1D-CGD-CBD | 2.02  | 128.61      | 124.48   |
| 22  | b     | 617 | CLA  | C2A-C1A-CHA | 2.01  | 127.38      | 123.86   |
| 23  | A     | 406 | PHO  | C4D-ND-C1D  | 2.01  | 110.88      | 108.83   |
| 22  | B     | 601 | CLA  | O2A-CGA-O1A | -2.01 | 118.51      | 123.59   |
| 27  | D     | 402 | PLM  | O2-C1-C2    | -2.01 | 116.62      | 123.08   |
| 25  | D     | 404 | PL9  | C36-C34-C33 | -2.01 | 117.05      | 121.12   |
| 22  | D     | 401 | CLA  | CAA-C2A-C3A | -2.01 | 107.27      | 112.78   |
| 22  | b     | 610 | CLA  | O2D-CGD-CBD | 2.01  | 114.84      | 111.27   |
| 22  | b     | 618 | CLA  | O2A-CGA-O1A | -2.01 | 118.30      | 123.30   |
| 22  | B     | 608 | CLA  | CHB-C1B-NB  | 2.01  | 126.38      | 124.26   |
| 22  | c     | 509 | CLA  | CMB-C2B-C3B | 2.00  | 131.44      | 126.59   |
| 22  | b     | 617 | CLA  | C3B-C4B-NB  | -2.00 | 108.66      | 110.52   |
| 22  | C     | 513 | CLA  | CHD-C1D-ND  | -2.00 | 122.61      | 124.45   |
| 25  | A     | 409 | PL9  | O2-C1-C2    | -2.00 | 117.20      | 121.78   |

There are no chirality outliers.

All (1964) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 404 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 405 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 601 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 601 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 603 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 603 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 604 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 614 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 512 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 512 | CLA  | CHA-CBD-CGD-O2D |
| 22  | D     | 401 | CLA  | CHA-CBD-CGD-O1D |
| 22  | D     | 401 | CLA  | CHA-CBD-CGD-O2D |
| 22  | a     | 405 | CLA  | CBD-CGD-O2D-CED |
| 22  | a     | 406 | CLA  | CHA-CBD-CGD-O1D |
| 22  | a     | 406 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 604 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 605 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 605 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 606 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 607 | CLA  | C2-C3-C5-C6     |
| 22  | b     | 607 | CLA  | C4-C3-C5-C6     |
| 22  | b     | 616 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 616 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 616 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 616 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 508 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 513 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 513 | CLA  | CHA-CBD-CGD-O2D |
| 22  | d     | 401 | CLA  | CHA-CBD-CGD-O1D |
| 22  | d     | 401 | CLA  | CHA-CBD-CGD-O2D |
| 24  | B     | 617 | BCR  | C1-C6-C7-C8     |
| 24  | B     | 619 | BCR  | C37-C22-C23-C24 |
| 24  | C     | 501 | BCR  | C7-C8-C9-C10    |
| 24  | C     | 501 | BCR  | C7-C8-C9-C34    |
| 24  | C     | 502 | BCR  | C7-C8-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | C     | 502 | BCR  | C7-C8-C9-C34    |
| 24  | C     | 502 | BCR  | C23-C24-C25-C26 |
| 24  | F     | 101 | BCR  | C1-C6-C7-C8     |
| 24  | F     | 101 | BCR  | C7-C8-C9-C10    |
| 24  | F     | 101 | BCR  | C7-C8-C9-C34    |
| 24  | F     | 101 | BCR  | C23-C24-C25-C26 |
| 24  | T     | 103 | BCR  | C1-C6-C7-C8     |
| 24  | Y     | 102 | BCR  | C5-C6-C7-C8     |
| 24  | Y     | 102 | BCR  | C17-C18-C19-C20 |
| 24  | Y     | 102 | BCR  | C36-C18-C19-C20 |
| 24  | Y     | 102 | BCR  | C21-C22-C23-C24 |
| 24  | Y     | 102 | BCR  | C37-C22-C23-C24 |
| 24  | b     | 602 | BCR  | C13-C14-C15-C16 |
| 24  | b     | 620 | BCR  | C21-C22-C23-C24 |
| 24  | b     | 620 | BCR  | C37-C22-C23-C24 |
| 24  | c     | 501 | BCR  | C7-C8-C9-C10    |
| 24  | c     | 501 | BCR  | C7-C8-C9-C34    |
| 24  | c     | 502 | BCR  | C7-C8-C9-C10    |
| 24  | c     | 502 | BCR  | C7-C8-C9-C34    |
| 24  | c     | 502 | BCR  | C23-C24-C25-C26 |
| 24  | f     | 101 | BCR  | C1-C6-C7-C8     |
| 24  | f     | 101 | BCR  | C7-C8-C9-C10    |
| 24  | f     | 101 | BCR  | C7-C8-C9-C34    |
| 24  | f     | 101 | BCR  | C23-C24-C25-C26 |
| 24  | k     | 101 | BCR  | C9-C10-C11-C12  |
| 24  | k     | 101 | BCR  | C11-C12-C13-C14 |
| 24  | k     | 101 | BCR  | C11-C12-C13-C35 |
| 24  | k     | 101 | BCR  | C21-C22-C23-C24 |
| 24  | k     | 101 | BCR  | C37-C22-C23-C24 |
| 24  | y     | 102 | BCR  | C5-C6-C7-C8     |
| 24  | y     | 102 | BCR  | C17-C18-C19-C20 |
| 24  | y     | 102 | BCR  | C36-C18-C19-C20 |
| 24  | y     | 102 | BCR  | C21-C22-C23-C24 |
| 24  | y     | 102 | BCR  | C37-C22-C23-C24 |
| 25  | A     | 409 | PL9  | C7-C8-C9-C10    |
| 25  | A     | 409 | PL9  | C7-C8-C9-C11    |
| 25  | A     | 409 | PL9  | C17-C18-C19-C20 |
| 25  | A     | 409 | PL9  | C32-C33-C34-C35 |
| 25  | A     | 409 | PL9  | C33-C34-C36-C37 |
| 25  | A     | 409 | PL9  | C34-C36-C37-C38 |
| 25  | A     | 409 | PL9  | C37-C38-C39-C41 |
| 25  | D     | 404 | PL9  | C24-C26-C27-C28 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | D     | 404 | PL9  | C27-C28-C29-C30 |
| 25  | D     | 404 | PL9  | C27-C28-C29-C31 |
| 25  | D     | 404 | PL9  | C32-C33-C34-C35 |
| 25  | D     | 404 | PL9  | C44-C46-C47-C48 |
| 25  | a     | 410 | PL9  | C7-C8-C9-C10    |
| 25  | a     | 410 | PL9  | C7-C8-C9-C11    |
| 25  | a     | 410 | PL9  | C12-C13-C14-C15 |
| 25  | a     | 410 | PL9  | C12-C13-C14-C16 |
| 25  | a     | 410 | PL9  | C17-C18-C19-C20 |
| 25  | a     | 410 | PL9  | C25-C24-C26-C27 |
| 25  | a     | 410 | PL9  | C24-C26-C27-C28 |
| 25  | a     | 410 | PL9  | C32-C33-C34-C35 |
| 25  | a     | 410 | PL9  | C37-C38-C39-C41 |
| 25  | d     | 402 | PL9  | C24-C26-C27-C28 |
| 25  | d     | 402 | PL9  | C27-C28-C29-C30 |
| 25  | d     | 402 | PL9  | C27-C28-C29-C31 |
| 25  | d     | 402 | PL9  | C32-C33-C34-C35 |
| 25  | d     | 402 | PL9  | C44-C46-C47-C48 |
| 26  | A     | 410 | SQD  | C5-C6-S-O7      |
| 26  | A     | 410 | SQD  | C5-C6-S-O8      |
| 26  | A     | 415 | SQD  | O6-C44-C45-O47  |
| 26  | A     | 415 | SQD  | O10-C23-O48-C46 |
| 26  | A     | 415 | SQD  | C24-C23-O48-C46 |
| 26  | D     | 412 | SQD  | O6-C44-C45-O47  |
| 26  | a     | 417 | SQD  | O10-C23-O48-C46 |
| 26  | a     | 417 | SQD  | C24-C23-O48-C46 |
| 26  | b     | 601 | SQD  | O49-C7-O47-C45  |
| 26  | b     | 601 | SQD  | C5-C6-S-O7      |
| 26  | b     | 601 | SQD  | C5-C6-S-O8      |
| 26  | d     | 412 | SQD  | O6-C44-C45-O47  |
| 26  | l     | 102 | SQD  | O49-C7-O47-C45  |
| 26  | l     | 102 | SQD  | C8-C7-O47-C45   |
| 26  | l     | 102 | SQD  | O5-C5-C6-S      |
| 31  | D     | 407 | LHG  | C1-C2-C3-O3     |
| 31  | D     | 407 | LHG  | O2-C2-C3-O3     |
| 31  | D     | 407 | LHG  | C8-C7-O7-C5     |
| 31  | D     | 408 | LHG  | O1-C1-C2-C3     |
| 31  | D     | 408 | LHG  | C4-O6-P-O4      |
| 31  | E     | 101 | LHG  | C3-O3-P-O4      |
| 31  | E     | 101 | LHG  | C4-O6-P-O4      |
| 31  | E     | 101 | LHG  | C4-O6-P-O5      |
| 31  | L     | 101 | LHG  | C3-O3-P-O4      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | L     | 101 | LHG  | C4-O6-P-O4      |
| 31  | a     | 415 | LHG  | C3-O3-P-O4      |
| 31  | a     | 415 | LHG  | C3-O3-P-O5      |
| 31  | a     | 415 | LHG  | C4-O6-P-O3      |
| 31  | d     | 405 | LHG  | C1-C2-C3-O3     |
| 31  | d     | 405 | LHG  | O2-C2-C3-O3     |
| 31  | d     | 405 | LHG  | C8-C7-O7-C5     |
| 31  | d     | 406 | LHG  | O1-C1-C2-C3     |
| 31  | d     | 406 | LHG  | C4-O6-P-O4      |
| 31  | l     | 101 | LHG  | C3-O3-P-O4      |
| 31  | l     | 101 | LHG  | C4-O6-P-O4      |
| 32  | a     | 401 | GOL  | O1-C1-C2-C3     |
| 33  | B     | 633 | LMT  | C2'-C1'-O1'-C1  |
| 33  | B     | 633 | LMT  | O5'-C1'-O1'-C1  |
| 33  | J     | 103 | LMT  | C2'-C1'-O1'-C1  |
| 33  | J     | 103 | LMT  | O5'-C1'-O1'-C1  |
| 33  | J     | 103 | LMT  | C2-C1-O1'-C1'   |
| 33  | M     | 102 | LMT  | C2-C1-O1'-C1'   |
| 33  | T     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 33  | T     | 104 | LMT  | O5'-C1'-O1'-C1  |
| 33  | Z     | 101 | LMT  | C2'-C1'-O1'-C1  |
| 33  | Z     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 33  | Z     | 101 | LMT  | C2-C1-O1'-C1'   |
| 33  | b     | 626 | LMT  | O5'-C1'-O1'-C1  |
| 33  | b     | 626 | LMT  | C2-C1-O1'-C1'   |
| 33  | j     | 101 | LMT  | C2'-C1'-O1'-C1  |
| 33  | j     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 33  | z     | 101 | LMT  | C2'-C1'-O1'-C1  |
| 33  | z     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 33  | z     | 101 | LMT  | C2-C1-O1'-C1'   |
| 34  | C     | 503 | DGD  | O2G-C2G-C3G-O3G |
| 34  | C     | 504 | DGD  | C2D-C1D-O3G-C3G |
| 34  | C     | 504 | DGD  | O6D-C1D-O3G-C3G |
| 34  | C     | 504 | DGD  | C2E-C1E-O5D-C6D |
| 34  | C     | 504 | DGD  | O6E-C1E-O5D-C6D |
| 34  | D     | 411 | DGD  | C2B-C1B-O2G-C2G |
| 34  | D     | 411 | DGD  | O1G-C1G-C2G-O2G |
| 34  | D     | 411 | DGD  | O6D-C1D-O3G-C3G |
| 34  | J     | 102 | DGD  | O2G-C2G-C3G-O3G |
| 34  | c     | 503 | DGD  | O2G-C2G-C3G-O3G |
| 34  | c     | 504 | DGD  | O1G-C1G-C2G-O2G |
| 34  | c     | 504 | DGD  | O6D-C1D-O3G-C3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | c     | 504 | DGD  | C2E-C1E-O5D-C6D |
| 34  | c     | 504 | DGD  | O6E-C1E-O5D-C6D |
| 34  | d     | 410 | DGD  | C2B-C1B-O2G-C2G |
| 35  | Y     | 101 | LMG  | O6-C1-O1-C7     |
| 35  | c     | 524 | LMG  | O6-C1-O1-C7     |
| 22  | c     | 508 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 415 | LHG  | O10-C23-O8-C6   |
| 22  | C     | 515 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 516 | CLA  | CBD-CGD-O2D-CED |
| 26  | b     | 601 | SQD  | O10-C23-O48-C46 |
| 34  | J     | 102 | DGD  | O1A-C1A-O1G-C1G |
| 35  | C     | 525 | LMG  | O10-C28-O8-C9   |
| 35  | c     | 519 | LMG  | O10-C28-O8-C9   |
| 22  | A     | 404 | CLA  | O1D-CGD-O2D-CED |
| 22  | a     | 405 | CLA  | O1D-CGD-O2D-CED |
| 34  | C     | 504 | DGD  | O6D-C5D-C6D-O5D |
| 22  | B     | 610 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 614 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 616 | CLA  | CBD-CGD-O2D-CED |
| 31  | D     | 407 | LHG  | O9-C7-O7-C5     |
| 31  | d     | 405 | LHG  | O9-C7-O7-C5     |
| 34  | D     | 411 | DGD  | O1B-C1B-O2G-C2G |
| 34  | d     | 410 | DGD  | O1B-C1B-O2G-C2G |
| 22  | B     | 614 | CLA  | C3-C5-C6-C7     |
| 22  | b     | 616 | CLA  | C3-C5-C6-C7     |
| 31  | a     | 415 | LHG  | C24-C23-O8-C6   |
| 34  | J     | 102 | DGD  | C2A-C1A-O1G-C1G |
| 35  | C     | 519 | LMG  | C29-C28-O8-C9   |
| 35  | C     | 525 | LMG  | C29-C28-O8-C9   |
| 33  | i     | 102 | LMT  | O5B-C5B-C6B-O6B |
| 26  | b     | 601 | SQD  | C8-C7-O47-C45   |
| 25  | a     | 410 | PL9  | C47-C48-C49-C50 |
| 22  | b     | 611 | CLA  | CBD-CGD-O2D-CED |
| 34  | c     | 504 | DGD  | O6D-C5D-C6D-O5D |
| 33  | C     | 518 | LMT  | O5B-C5B-C6B-O6B |
| 34  | C     | 504 | DGD  | O6E-C5E-C6E-O5E |
| 34  | C     | 504 | DGD  | C4D-C5D-C6D-O5D |
| 34  | c     | 504 | DGD  | C4D-C5D-C6D-O5D |
| 22  | B     | 605 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 604 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 605 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 606 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 517 | CLA  | O1A-CGA-O2A-C1  |
| 22  | b     | 603 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 517 | CLA  | CBA-CGA-O2A-C1  |
| 26  | b     | 601 | SQD  | C24-C23-O48-C46 |
| 35  | c     | 519 | LMG  | C29-C28-O8-C9   |
| 34  | c     | 504 | DGD  | O6E-C5E-C6E-O5E |
| 25  | A     | 409 | PL9  | C37-C38-C39-C40 |
| 25  | a     | 410 | PL9  | C37-C38-C39-C40 |
| 22  | B     | 609 | CLA  | CBD-CGD-O2D-CED |
| 33  | T     | 101 | LMT  | C7-C8-C9-C10    |
| 33  | j     | 101 | LMT  | C3-C4-C5-C6     |
| 26  | d     | 412 | SQD  | O49-C7-O47-C45  |
| 25  | A     | 409 | PL9  | C12-C13-C14-C16 |
| 25  | A     | 409 | PL9  | C17-C18-C19-C21 |
| 25  | A     | 409 | PL9  | C32-C33-C34-C36 |
| 25  | D     | 404 | PL9  | C32-C33-C34-C36 |
| 25  | a     | 410 | PL9  | C17-C18-C19-C21 |
| 25  | a     | 410 | PL9  | C27-C28-C29-C31 |
| 25  | a     | 410 | PL9  | C32-C33-C34-C36 |
| 25  | d     | 402 | PL9  | C32-C33-C34-C36 |
| 35  | C     | 519 | LMG  | O10-C28-O8-C9   |
| 24  | B     | 632 | BCR  | C13-C14-C15-C16 |
| 35  | Y     | 101 | LMG  | O6-C5-C6-O5     |
| 22  | B     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 609 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 601 | CLA  | C3-C5-C6-C7     |
| 33  | i     | 102 | LMT  | C4B-C5B-C6B-O6B |
| 26  | d     | 412 | SQD  | C8-C7-O47-C45   |
| 22  | B     | 607 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 506 | CLA  | CBD-CGD-O2D-CED |
| 22  | b     | 605 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 507 | CLA  | CBD-CGD-O2D-CED |
| 33  | M     | 102 | LMT  | O5'-C5'-C6'-O6' |
| 27  | a     | 412 | PLM  | C8-C9-CA-CB     |
| 26  | A     | 410 | SQD  | C16-C17-C18-C19 |
| 26  | a     | 411 | SQD  | C16-C17-C18-C19 |
| 33  | b     | 626 | LMT  | C5-C6-C7-C8     |
| 33  | i     | 102 | LMT  | C3'-C4'-O1B-C1B |
| 34  | C     | 503 | DGD  | C4A-C5A-C6A-C7A |
| 33  | C     | 518 | LMT  | C3'-C4'-O1B-C1B |
| 22  | B     | 604 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 606 | CLA  | C3-C5-C6-C7     |
| 33  | B     | 628 | LMT  | O5'-C5'-C6'-O6' |
| 33  | m     | 102 | LMT  | O5'-C5'-C6'-O6' |
| 35  | y     | 101 | LMG  | O6-C5-C6-O5     |
| 33  | C     | 518 | LMT  | C4B-C5B-C6B-O6B |
| 27  | L     | 102 | PLM  | C4-C5-C6-C7     |
| 28  | a     | 414 | LFA  | C9-C10-C11-C12  |
| 25  | A     | 409 | PL9  | C47-C48-C49-C50 |
| 33  | f     | 102 | LMT  | O5'-C5'-C6'-O6' |
| 33  | j     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 25  | A     | 409 | PL9  | C15-C14-C16-C17 |
| 25  | A     | 409 | PL9  | C25-C24-C26-C27 |
| 34  | C     | 504 | DGD  | C4E-C5E-C6E-O5E |
| 25  | A     | 409 | PL9  | C13-C14-C16-C17 |
| 25  | A     | 409 | PL9  | C23-C24-C26-C27 |
| 25  | a     | 410 | PL9  | C23-C24-C26-C27 |
| 22  | B     | 606 | CLA  | C2A-CAA-CBA-CGA |
| 22  | C     | 511 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 608 | CLA  | C2A-CAA-CBA-CGA |
| 22  | c     | 512 | CLA  | C2A-CAA-CBA-CGA |
| 26  | D     | 412 | SQD  | O5-C1-O6-C44    |
| 26  | l     | 102 | SQD  | O5-C1-O6-C44    |
| 25  | A     | 409 | PL9  | C44-C46-C47-C48 |
| 25  | a     | 410 | PL9  | C9-C11-C12-C13  |
| 25  | a     | 410 | PL9  | C19-C21-C22-C23 |
| 25  | a     | 410 | PL9  | C44-C46-C47-C48 |
| 31  | E     | 101 | LHG  | C13-C14-C15-C16 |
| 33  | T     | 104 | LMT  | O5B-C5B-C6B-O6B |
| 33  | M     | 102 | LMT  | C4'-C5'-C6'-O6' |
| 34  | C     | 504 | DGD  | C2B-C1B-O2G-C2G |
| 34  | c     | 504 | DGD  | C2B-C1B-O2G-C2G |
| 33  | m     | 102 | LMT  | C4'-C5'-C6'-O6' |
| 25  | A     | 409 | PL9  | C12-C13-C14-C15 |
| 22  | c     | 516 | CLA  | O1D-CGD-O2D-CED |
| 34  | d     | 410 | DGD  | C4A-C5A-C6A-C7A |
| 25  | A     | 409 | PL9  | C27-C28-C29-C31 |
| 33  | C     | 518 | LMT  | C4'-C5'-C6'-O6' |
| 33  | f     | 102 | LMT  | C4'-C5'-C6'-O6' |
| 34  | c     | 504 | DGD  | C4E-C5E-C6E-O5E |
| 22  | C     | 516 | CLA  | CBA-CGA-O2A-C1  |
| 22  | D     | 406 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 510 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | d     | 404 | CLA  | CBA-CGA-O2A-C1  |
| 26  | l     | 102 | SQD  | C24-C23-O48-C46 |
| 35  | y     | 101 | LMG  | C29-C28-O8-C9   |
| 33  | J     | 103 | LMT  | C7-C8-C9-C10    |
| 35  | y     | 101 | LMG  | O10-C28-O8-C9   |
| 33  | j     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 31  | E     | 101 | LHG  | O6-C4-C5-O7     |
| 34  | D     | 411 | DGD  | C9B-CAB-CBB-CCB |
| 34  | J     | 102 | DGD  | O6D-C5D-C6D-O5D |
| 22  | B     | 613 | CLA  | C15-C16-C17-C18 |
| 31  | E     | 101 | LHG  | C23-C24-C25-C26 |
| 35  | c     | 524 | LMG  | C2-C1-O1-C7     |
| 35  | y     | 101 | LMG  | C2-C1-O1-C7     |
| 26  | a     | 417 | SQD  | O6-C44-C45-O47  |
| 26  | l     | 102 | SQD  | O47-C45-C46-O48 |
| 22  | B     | 601 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 601 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 506 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 513 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 603 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 603 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 514 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 517 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 407 | CLA  | C15-C16-C17-C18 |
| 24  | B     | 617 | BCR  | C36-C18-C19-C20 |
| 24  | B     | 632 | BCR  | C7-C8-C9-C34    |
| 24  | B     | 632 | BCR  | C37-C22-C23-C24 |
| 24  | C     | 502 | BCR  | C11-C12-C13-C35 |
| 24  | C     | 502 | BCR  | C36-C18-C19-C20 |
| 24  | T     | 103 | BCR  | C36-C18-C19-C20 |
| 24  | b     | 602 | BCR  | C7-C8-C9-C34    |
| 24  | c     | 502 | BCR  | C36-C18-C19-C20 |
| 24  | B     | 619 | BCR  | C21-C22-C23-C24 |
| 24  | B     | 632 | BCR  | C7-C8-C9-C10    |
| 24  | b     | 602 | BCR  | C7-C8-C9-C10    |
| 33  | Z     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 33  | Z     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 33  | z     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 34  | C     | 503 | DGD  | C2B-C1B-O2G-C2G |
| 34  | c     | 503 | DGD  | C2B-C1B-O2G-C2G |
| 34  | H     | 101 | DGD  | C3B-C4B-C5B-C6B |
| 22  | C     | 516 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | a     | 405 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 516 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 515 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 602 | CLA  | C3-C5-C6-C7     |
| 22  | C     | 509 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 404 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 602 | CLA  | C13-C15-C16-C17 |
| 22  | d     | 404 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 612 | CLA  | O1D-CGD-O2D-CED |
| 33  | b     | 626 | LMT  | C7-C8-C9-C10    |
| 22  | C     | 517 | CLA  | C10-C11-C12-C13 |
| 22  | b     | 615 | CLA  | C15-C16-C17-C18 |
| 22  | c     | 517 | CLA  | C10-C11-C12-C13 |
| 22  | c     | 517 | CLA  | C15-C16-C17-C18 |
| 22  | D     | 406 | CLA  | O1A-CGA-O2A-C1  |
| 26  | D     | 412 | SQD  | C23-C24-C25-C26 |
| 26  | a     | 417 | SQD  | C7-C8-C9-C10    |
| 27  | b     | 621 | PLM  | C1-C2-C3-C4     |
| 31  | E     | 101 | LHG  | C7-C8-C9-C10    |
| 34  | D     | 411 | DGD  | C1B-C2B-C3B-C4B |
| 35  | C     | 519 | LMG  | C28-C29-C30-C31 |
| 35  | Y     | 101 | LMG  | C10-C11-C12-C13 |
| 22  | B     | 614 | CLA  | C5-C6-C7-C8     |
| 34  | C     | 504 | DGD  | O1B-C1B-O2G-C2G |
| 34  | c     | 504 | DGD  | O1B-C1B-O2G-C2G |
| 22  | B     | 611 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 513 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 604 | CLA  | C13-C15-C16-C17 |
| 26  | A     | 415 | SQD  | C7-C8-C9-C10    |
| 27  | L     | 102 | PLM  | C1-C2-C3-C4     |
| 34  | c     | 505 | DGD  | C1A-C2A-C3A-C4A |
| 22  | b     | 616 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 610 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 515 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 516 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 515 | CLA  | C6-C7-C8-C10    |
| 22  | d     | 404 | CLA  | O1A-CGA-O2A-C1  |
| 26  | l     | 102 | SQD  | O10-C23-O48-C46 |
| 34  | J     | 102 | DGD  | C4D-C5D-C6D-O5D |
| 22  | A     | 404 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 516 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 613 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | z     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 22  | c     | 510 | CLA  | O1A-CGA-O2A-C1  |
| 35  | Y     | 101 | LMG  | C4-C5-C6-O5     |
| 35  | y     | 101 | LMG  | C4-C5-C6-O5     |
| 22  | B     | 614 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 616 | CLA  | O1D-CGD-O2D-CED |
| 25  | A     | 409 | PL9  | C24-C26-C27-C28 |
| 27  | B     | 621 | PLM  | C1-C2-C3-C4     |
| 33  | f     | 102 | LMT  | O5B-C5B-C6B-O6B |
| 22  | B     | 601 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 603 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 510 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 603 | CLA  | C8-C10-C11-C12  |
| 33  | J     | 103 | LMT  | O1'-C1-C2-C3    |
| 33  | f     | 102 | LMT  | C4B-C5B-C6B-O6B |
| 22  | B     | 610 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 612 | CLA  | C15-C16-C17-C18 |
| 31  | A     | 417 | LHG  | C29-C30-C31-C32 |
| 22  | b     | 611 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 509 | CLA  | O1A-CGA-O2A-C1  |
| 27  | c     | 521 | PLM  | C5-C6-C7-C8     |
| 22  | a     | 405 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 511 | CLA  | C5-C6-C7-C8     |
| 31  | E     | 101 | LHG  | C3-O3-P-O6      |
| 31  | E     | 101 | LHG  | C4-O6-P-O3      |
| 31  | L     | 101 | LHG  | C4-O6-P-O3      |
| 31  | a     | 415 | LHG  | C3-O3-P-O6      |
| 31  | l     | 101 | LHG  | C4-O6-P-O3      |
| 34  | c     | 505 | DGD  | C9B-CAB-CBB-CCB |
| 22  | A     | 407 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 511 | CLA  | CBA-CGA-O2A-C1  |
| 35  | c     | 524 | LMG  | C29-C28-O8-C9   |
| 22  | C     | 507 | CLA  | CBD-CGD-O2D-CED |
| 33  | T     | 104 | LMT  | C4B-C5B-C6B-O6B |
| 33  | z     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 27  | C     | 522 | PLM  | C1-C2-C3-C4     |
| 34  | c     | 503 | DGD  | C1B-C2B-C3B-C4B |
| 35  | c     | 519 | LMG  | C28-C29-C30-C31 |
| 34  | C     | 503 | DGD  | O1B-C1B-O2G-C2G |
| 34  | c     | 503 | DGD  | O1B-C1B-O2G-C2G |
| 25  | a     | 410 | PL9  | C28-C29-C31-C32 |
| 33  | i     | 102 | LMT  | O1'-C1-C2-C3    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 517 | CLA  | C2A-CAA-CBA-CGA |
| 33  | T     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 22  | C     | 510 | CLA  | CBA-CGA-O2A-C1  |
| 31  | E     | 101 | LHG  | C24-C23-O8-C6   |
| 22  | b     | 605 | CLA  | C5-C6-C7-C8     |
| 27  | e     | 102 | PLM  | CC-CD-CE-CF     |
| 31  | d     | 406 | LHG  | C11-C10-C9-C8   |
| 31  | l     | 101 | LHG  | C13-C14-C15-C16 |
| 33  | B     | 630 | LMT  | C7-C8-C9-C10    |
| 35  | M     | 101 | LMG  | C36-C37-C38-C39 |
| 22  | C     | 510 | CLA  | CBD-CGD-O2D-CED |
| 22  | C     | 511 | CLA  | CBD-CGD-O2D-CED |
| 26  | D     | 412 | SQD  | C8-C7-O47-C45   |
| 26  | A     | 410 | SQD  | C29-C30-C31-C32 |
| 26  | a     | 411 | SQD  | C14-C15-C16-C17 |
| 27  | L     | 102 | PLM  | C6-C7-C8-C9     |
| 27  | M     | 103 | PLM  | C7-C8-C9-CA     |
| 27  | c     | 520 | PLM  | C5-C6-C7-C8     |
| 27  | c     | 523 | PLM  | C5-C6-C7-C8     |
| 27  | x     | 101 | PLM  | CB-CC-CD-CE     |
| 28  | I     | 101 | LFA  | C3-C4-C5-C6     |
| 28  | T     | 102 | LFA  | C10-C11-C12-C13 |
| 28  | T     | 102 | LFA  | C13-C14-C15-C16 |
| 31  | A     | 417 | LHG  | C16-C17-C18-C19 |
| 31  | D     | 408 | LHG  | C11-C10-C9-C8   |
| 31  | l     | 101 | LHG  | C10-C11-C12-C13 |
| 33  | i     | 102 | LMT  | C4-C5-C6-C7     |
| 34  | C     | 503 | DGD  | C5B-C6B-C7B-C8B |
| 34  | D     | 411 | DGD  | C5B-C6B-C7B-C8B |
| 35  | C     | 525 | LMG  | C20-C21-C22-C23 |
| 35  | M     | 101 | LMG  | C31-C32-C33-C34 |
| 22  | C     | 508 | CLA  | CBA-CGA-O2A-C1  |
| 25  | a     | 410 | PL9  | C47-C48-C49-C51 |
| 26  | a     | 411 | SQD  | C33-C34-C35-C36 |
| 26  | b     | 601 | SQD  | C30-C31-C32-C33 |
| 27  | C     | 522 | PLM  | C3-C4-C5-C6     |
| 28  | J     | 104 | LFA  | C11-C12-C13-C14 |
| 28  | a     | 414 | LFA  | C10-C11-C12-C13 |
| 28  | d     | 408 | LFA  | C15-C16-C17-C18 |
| 28  | i     | 103 | LFA  | C9-C10-C11-C12  |
| 31  | L     | 101 | LHG  | C10-C11-C12-C13 |
| 31  | a     | 421 | LHG  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | B     | 630 | LMT  | C6-C7-C8-C9     |
| 33  | J     | 103 | LMT  | C11-C10-C9-C8   |
| 35  | C     | 519 | LMG  | C12-C13-C14-C15 |
| 35  | d     | 407 | LMG  | C15-C16-C17-C18 |
| 22  | B     | 609 | CLA  | O1D-CGD-O2D-CED |
| 26  | D     | 412 | SQD  | O49-C7-O47-C45  |
| 35  | M     | 101 | LMG  | C28-C29-C30-C31 |
| 22  | d     | 404 | CLA  | CBD-CGD-O2D-CED |
| 26  | a     | 411 | SQD  | C15-C16-C17-C18 |
| 26  | b     | 601 | SQD  | C9-C10-C11-C12  |
| 26  | b     | 601 | SQD  | C12-C13-C14-C15 |
| 26  | b     | 601 | SQD  | C14-C15-C16-C17 |
| 27  | M     | 103 | PLM  | C3-C4-C5-C6     |
| 31  | E     | 101 | LHG  | C11-C10-C9-C8   |
| 31  | E     | 101 | LHG  | C14-C15-C16-C17 |
| 31  | L     | 101 | LHG  | C32-C33-C34-C35 |
| 31  | d     | 405 | LHG  | C25-C26-C27-C28 |
| 34  | c     | 504 | DGD  | C7B-C8B-C9B-CAB |
| 35  | c     | 519 | LMG  | C17-C18-C19-C20 |
| 35  | c     | 519 | LMG  | C29-C30-C31-C32 |
| 35  | d     | 407 | LMG  | C12-C13-C14-C15 |
| 27  | e     | 102 | PLM  | C3-C4-C5-C6     |
| 27  | x     | 101 | PLM  | C2-C3-C4-C5     |
| 27  | x     | 101 | PLM  | C4-C5-C6-C7     |
| 28  | T     | 102 | LFA  | C11-C10-C9-C8   |
| 28  | a     | 414 | LFA  | C12-C13-C14-C15 |
| 31  | L     | 101 | LHG  | C34-C35-C36-C37 |
| 34  | C     | 504 | DGD  | C6B-C7B-C8B-C9B |
| 34  | J     | 102 | DGD  | C9B-CAB-CBB-CCB |
| 34  | c     | 504 | DGD  | C6B-C7B-C8B-C9B |
| 34  | h     | 101 | DGD  | C7B-C8B-C9B-CAB |
| 35  | c     | 519 | LMG  | C34-C35-C36-C37 |
| 35  | m     | 101 | LMG  | C31-C32-C33-C34 |
| 31  | D     | 408 | LHG  | O2-C2-C3-O3     |
| 27  | a     | 412 | PLM  | C7-C8-C9-CA     |
| 28  | E     | 102 | LFA  | C14-C15-C16-C17 |
| 31  | D     | 407 | LHG  | C25-C26-C27-C28 |
| 33  | f     | 102 | LMT  | C4-C5-C6-C7     |
| 34  | C     | 504 | DGD  | C9A-CAA-CBA-CCA |
| 35  | M     | 101 | LMG  | C33-C34-C35-C36 |
| 35  | Y     | 101 | LMG  | C11-C12-C13-C14 |
| 22  | b     | 604 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | b     | 601 | SQD  | C7-C8-C9-C10    |
| 33  | A     | 419 | LMT  | C2'-C1'-O1'-C1  |
| 33  | i     | 102 | LMT  | C2'-C1'-O1'-C1  |
| 34  | D     | 411 | DGD  | C2D-C1D-O3G-C3G |
| 34  | c     | 504 | DGD  | C2D-C1D-O3G-C3G |
| 35  | Y     | 101 | LMG  | C2-C1-O1-C7     |
| 26  | a     | 411 | SQD  | C9-C10-C11-C12  |
| 27  | L     | 102 | PLM  | CC-CD-CE-CF     |
| 27  | b     | 621 | PLM  | CC-CD-CE-CF     |
| 27  | c     | 520 | PLM  | C3-C4-C5-C6     |
| 28  | T     | 102 | LFA  | C3-C4-C5-C6     |
| 28  | T     | 102 | LFA  | C5-C6-C7-C8     |
| 31  | L     | 101 | LHG  | C13-C14-C15-C16 |
| 35  | m     | 101 | LMG  | C19-C20-C21-C22 |
| 25  | d     | 402 | PL9  | C15-C14-C16-C17 |
| 28  | H     | 103 | LFA  | C11-C10-C9-C8   |
| 31  | a     | 421 | LHG  | C24-C25-C26-C27 |
| 33  | Z     | 101 | LMT  | C7-C8-C9-C10    |
| 35  | M     | 101 | LMG  | C19-C20-C21-C22 |
| 25  | D     | 404 | PL9  | C23-C24-C26-C27 |
| 22  | B     | 606 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 510 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 516 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 609 | CLA  | O1D-CGD-O2D-CED |
| 26  | b     | 601 | SQD  | C17-C18-C19-C20 |
| 27  | e     | 101 | PLM  | CC-CD-CE-CF     |
| 28  | I     | 101 | LFA  | C7-C8-C9-C10    |
| 31  | A     | 417 | LHG  | C24-C25-C26-C27 |
| 31  | d     | 405 | LHG  | C11-C12-C13-C14 |
| 33  | J     | 103 | LMT  | C5-C6-C7-C8     |
| 34  | C     | 504 | DGD  | C4B-C5B-C6B-C7B |
| 34  | c     | 504 | DGD  | C2B-C3B-C4B-C5B |
| 34  | c     | 504 | DGD  | C4B-C5B-C6B-C7B |
| 35  | m     | 101 | LMG  | C30-C31-C32-C33 |
| 22  | B     | 607 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 609 | CLA  | C2A-CAA-CBA-CGA |
| 24  | B     | 617 | BCR  | C37-C22-C23-C24 |
| 24  | F     | 101 | BCR  | C37-C22-C23-C24 |
| 24  | K     | 101 | BCR  | C37-C22-C23-C24 |
| 24  | f     | 101 | BCR  | C37-C22-C23-C24 |
| 27  | C     | 522 | PLM  | C7-C8-C9-CA     |
| 27  | x     | 101 | PLM  | CC-CD-CE-CF     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | I     | 101 | LFA  | C4-C5-C6-C7     |
| 31  | a     | 415 | LHG  | C24-C25-C26-C27 |
| 34  | c     | 504 | DGD  | C2A-C3A-C4A-C5A |
| 35  | c     | 519 | LMG  | C31-C32-C33-C34 |
| 35  | m     | 101 | LMG  | C12-C13-C14-C15 |
| 35  | m     | 101 | LMG  | C33-C34-C35-C36 |
| 31  | A     | 417 | LHG  | O1-C1-C2-C3     |
| 31  | D     | 407 | LHG  | O1-C1-C2-C3     |
| 31  | a     | 421 | LHG  | O1-C1-C2-C3     |
| 31  | d     | 405 | LHG  | O1-C1-C2-C3     |
| 24  | F     | 101 | BCR  | C21-C22-C23-C24 |
| 24  | f     | 101 | BCR  | C21-C22-C23-C24 |
| 22  | d     | 404 | CLA  | C3-C5-C6-C7     |
| 34  | J     | 102 | DGD  | C2B-C1B-O2G-C2G |
| 26  | b     | 601 | SQD  | C29-C30-C31-C32 |
| 27  | X     | 101 | PLM  | C4-C5-C6-C7     |
| 27  | c     | 520 | PLM  | C4-C5-C6-C7     |
| 27  | x     | 101 | PLM  | C3-C4-C5-C6     |
| 28  | H     | 103 | LFA  | C11-C12-C13-C14 |
| 34  | c     | 503 | DGD  | C7A-C8A-C9A-CAA |
| 35  | M     | 101 | LMG  | C12-C13-C14-C15 |
| 35  | m     | 101 | LMG  | C28-C29-C30-C31 |
| 26  | a     | 411 | SQD  | C17-C18-C19-C20 |
| 26  | a     | 417 | SQD  | C25-C26-C27-C28 |
| 26  | b     | 601 | SQD  | C16-C17-C18-C19 |
| 27  | a     | 412 | PLM  | CA-CB-CC-CD     |
| 27  | j     | 103 | PLM  | C9-CA-CB-CC     |
| 28  | a     | 418 | LFA  | C7-C8-C9-C10    |
| 31  | a     | 415 | LHG  | C26-C27-C28-C29 |
| 31  | l     | 101 | LHG  | C29-C30-C31-C32 |
| 34  | h     | 101 | DGD  | C2B-C3B-C4B-C5B |
| 35  | C     | 519 | LMG  | C29-C30-C31-C32 |
| 35  | D     | 409 | LMG  | C12-C13-C14-C15 |
| 35  | D     | 409 | LMG  | C35-C36-C37-C38 |
| 35  | m     | 101 | LMG  | C39-C40-C41-C42 |
| 22  | C     | 509 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 516 | CLA  | C4B-C3B-CAB-CBB |
| 22  | D     | 406 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 506 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 510 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 517 | CLA  | C4B-C3B-CAB-CBB |
| 22  | d     | 404 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 615 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 617 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 617 | CLA  | C16-C17-C18-C20 |
| 33  | A     | 419 | LMT  | O5'-C1'-O1'-C1  |
| 23  | D     | 403 | PHO  | C8-C10-C11-C12  |
| 26  | A     | 415 | SQD  | C12-C13-C14-C15 |
| 26  | a     | 417 | SQD  | C9-C10-C11-C12  |
| 26  | a     | 417 | SQD  | C30-C31-C32-C33 |
| 27  | a     | 412 | PLM  | C6-C7-C8-C9     |
| 27  | b     | 621 | PLM  | C3-C4-C5-C6     |
| 27  | c     | 523 | PLM  | C3-C4-C5-C6     |
| 28  | i     | 103 | LFA  | C11-C12-C13-C14 |
| 31  | D     | 408 | LHG  | C32-C33-C34-C35 |
| 31  | E     | 101 | LHG  | C15-C16-C17-C18 |
| 31  | E     | 101 | LHG  | C17-C18-C19-C20 |
| 31  | E     | 101 | LHG  | C25-C26-C27-C28 |
| 33  | B     | 633 | LMT  | C11-C10-C9-C8   |
| 33  | J     | 103 | LMT  | C6-C7-C8-C9     |
| 33  | j     | 101 | LMT  | C11-C10-C9-C8   |
| 33  | z     | 101 | LMT  | C7-C8-C9-C10    |
| 34  | d     | 410 | DGD  | C6B-C7B-C8B-C9B |
| 35  | c     | 519 | LMG  | C12-C13-C14-C15 |
| 22  | B     | 611 | CLA  | CBD-CGD-O2D-CED |
| 26  | A     | 410 | SQD  | C17-C18-C19-C20 |
| 26  | a     | 417 | SQD  | C27-C28-C29-C30 |
| 27  | c     | 520 | PLM  | C7-C8-C9-CA     |
| 27  | e     | 102 | PLM  | C4-C5-C6-C7     |
| 28  | B     | 620 | LFA  | C11-C10-C9-C8   |
| 28  | T     | 102 | LFA  | C11-C12-C13-C14 |
| 33  | z     | 101 | LMT  | O1'-C1-C2-C3    |
| 34  | C     | 504 | DGD  | C3B-C4B-C5B-C6B |
| 35  | d     | 407 | LMG  | C35-C36-C37-C38 |
| 26  | A     | 415 | SQD  | C23-C24-C25-C26 |
| 34  | C     | 503 | DGD  | C1B-C2B-C3B-C4B |
| 22  | A     | 407 | CLA  | O1A-CGA-O2A-C1  |
| 31  | E     | 101 | LHG  | O10-C23-O8-C6   |
| 26  | A     | 410 | SQD  | C11-C12-C13-C14 |
| 27  | B     | 621 | PLM  | C5-C6-C7-C8     |
| 27  | D     | 410 | PLM  | CB-CC-CD-CE     |
| 35  | M     | 101 | LMG  | C39-C40-C41-C42 |
| 35  | c     | 519 | LMG  | C19-C20-C21-C22 |
| 22  | a     | 405 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | a     | 408 | CLA  | CBA-CGA-O2A-C1  |
| 33  | f     | 102 | LMT  | C6-C7-C8-C9     |
| 35  | c     | 519 | LMG  | C18-C19-C20-C21 |
| 35  | m     | 101 | LMG  | C18-C19-C20-C21 |
| 33  | T     | 104 | LMT  | C2-C1-O1'-C1'   |
| 33  | j     | 101 | LMT  | C2-C1-O1'-C1'   |
| 26  | a     | 417 | SQD  | C14-C15-C16-C17 |
| 27  | A     | 413 | PLM  | C4-C5-C6-C7     |
| 27  | D     | 410 | PLM  | C3-C4-C5-C6     |
| 27  | M     | 103 | PLM  | CA-CB-CC-CD     |
| 31  | d     | 406 | LHG  | C14-C15-C16-C17 |
| 34  | J     | 102 | DGD  | CCB-CDB-CEB-CFB |
| 34  | c     | 505 | DGD  | C4B-C5B-C6B-C7B |
| 34  | d     | 410 | DGD  | C4B-C5B-C6B-C7B |
| 35  | M     | 101 | LMG  | C18-C19-C20-C21 |
| 35  | c     | 519 | LMG  | C38-C39-C40-C41 |
| 22  | c     | 511 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 615 | CLA  | C16-C17-C18-C20 |
| 27  | B     | 622 | PLM  | C3-C4-C5-C6     |
| 28  | J     | 101 | LFA  | C5-C6-C7-C8     |
| 31  | D     | 407 | LHG  | C11-C12-C13-C14 |
| 34  | h     | 101 | DGD  | C4B-C5B-C6B-C7B |
| 35  | C     | 519 | LMG  | C18-C19-C20-C21 |
| 35  | C     | 525 | LMG  | C19-C20-C21-C22 |
| 22  | B     | 603 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 506 | CLA  | O1D-CGD-O2D-CED |
| 34  | c     | 503 | DGD  | C5B-C6B-C7B-C8B |
| 22  | A     | 404 | CLA  | C3-C5-C6-C7     |
| 34  | C     | 504 | DGD  | C1B-C2B-C3B-C4B |
| 34  | c     | 504 | DGD  | C1B-C2B-C3B-C4B |
| 27  | C     | 520 | PLM  | C9-CA-CB-CC     |
| 31  | a     | 421 | LHG  | C12-C13-C14-C15 |
| 23  | a     | 407 | PHO  | C4-C3-C5-C6     |
| 25  | a     | 410 | PL9  | C45-C44-C46-C47 |
| 22  | c     | 509 | CLA  | CBA-CGA-O2A-C1  |
| 34  | c     | 503 | DGD  | C2A-C1A-O1G-C1G |
| 23  | A     | 406 | PHO  | C2-C3-C5-C6     |
| 23  | a     | 407 | PHO  | C2-C3-C5-C6     |
| 25  | d     | 402 | PL9  | C23-C24-C26-C27 |
| 22  | c     | 507 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 516 | CLA  | C2A-CAA-CBA-CGA |
| 32  | a     | 401 | GOL  | O1-C1-C2-O2     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | b     | 601 | SQD  | C24-C25-C26-C27 |
| 31  | D     | 407 | LHG  | C11-C10-C9-C8   |
| 31  | L     | 101 | LHG  | C33-C34-C35-C36 |
| 31  | a     | 415 | LHG  | C14-C15-C16-C17 |
| 34  | C     | 504 | DGD  | C2B-C3B-C4B-C5B |
| 34  | c     | 503 | DGD  | C4A-C5A-C6A-C7A |
| 35  | C     | 519 | LMG  | C38-C39-C40-C41 |
| 35  | c     | 524 | LMG  | O10-C28-O8-C9   |
| 22  | C     | 509 | CLA  | C2B-C3B-CAB-CBB |
| 22  | C     | 516 | CLA  | C2B-C3B-CAB-CBB |
| 22  | D     | 406 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 506 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 510 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 517 | CLA  | C2B-C3B-CAB-CBB |
| 22  | d     | 404 | CLA  | C2B-C3B-CAB-CBB |
| 31  | d     | 406 | LHG  | O2-C2-C3-O3     |
| 23  | a     | 420 | PHO  | C8-C10-C11-C12  |
| 33  | j     | 101 | LMT  | C4-C5-C6-C7     |
| 33  | B     | 628 | LMT  | C4'-C5'-C6'-O6' |
| 27  | c     | 520 | PLM  | C6-C7-C8-C9     |
| 27  | j     | 102 | PLM  | CB-CC-CD-CE     |
| 31  | a     | 421 | LHG  | C14-C15-C16-C17 |
| 31  | l     | 101 | LHG  | C30-C31-C32-C33 |
| 33  | J     | 103 | LMT  | C4-C5-C6-C7     |
| 35  | M     | 101 | LMG  | C30-C31-C32-C33 |
| 35  | c     | 519 | LMG  | C30-C31-C32-C33 |
| 22  | C     | 510 | CLA  | O1A-CGA-O2A-C1  |
| 27  | t     | 101 | PLM  | C8-C9-CA-CB     |
| 34  | C     | 504 | DGD  | C5B-C6B-C7B-C8B |
| 34  | J     | 102 | DGD  | O1B-C1B-O2G-C2G |
| 34  | C     | 503 | DGD  | O6D-C5D-C6D-O5D |
| 34  | c     | 503 | DGD  | O6D-C5D-C6D-O5D |
| 27  | A     | 411 | PLM  | C3-C4-C5-C6     |
| 27  | c     | 523 | PLM  | CB-CC-CD-CE     |
| 35  | D     | 409 | LMG  | C15-C16-C17-C18 |
| 35  | y     | 101 | LMG  | C29-C30-C31-C32 |
| 22  | C     | 508 | CLA  | C13-C15-C16-C17 |
| 22  | a     | 408 | CLA  | C15-C16-C17-C18 |
| 22  | C     | 508 | CLA  | O1A-CGA-O2A-C1  |
| 33  | T     | 101 | LMT  | C1-C2-C3-C4     |
| 33  | j     | 101 | LMT  | C1-C2-C3-C4     |
| 26  | A     | 410 | SQD  | C27-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | a     | 417 | SQD  | C31-C32-C33-C34 |
| 26  | b     | 601 | SQD  | C25-C26-C27-C28 |
| 28  | I     | 101 | LFA  | C13-C14-C15-C16 |
| 31  | l     | 101 | LHG  | C31-C32-C33-C34 |
| 34  | c     | 505 | DGD  | CCB-CDB-CEB-CFB |
| 26  | d     | 412 | SQD  | C23-C24-C25-C26 |
| 24  | A     | 408 | BCR  | C23-C24-C25-C26 |
| 24  | B     | 617 | BCR  | C5-C6-C7-C8     |
| 24  | B     | 632 | BCR  | C1-C6-C7-C8     |
| 24  | B     | 632 | BCR  | C5-C6-C7-C8     |
| 24  | C     | 502 | BCR  | C5-C6-C7-C8     |
| 24  | C     | 502 | BCR  | C23-C24-C25-C30 |
| 24  | F     | 101 | BCR  | C5-C6-C7-C8     |
| 24  | F     | 101 | BCR  | C23-C24-C25-C30 |
| 24  | T     | 103 | BCR  | C5-C6-C7-C8     |
| 24  | Y     | 102 | BCR  | C1-C6-C7-C8     |
| 24  | a     | 409 | BCR  | C23-C24-C25-C26 |
| 24  | b     | 602 | BCR  | C1-C6-C7-C8     |
| 24  | b     | 602 | BCR  | C5-C6-C7-C8     |
| 24  | c     | 502 | BCR  | C5-C6-C7-C8     |
| 24  | c     | 502 | BCR  | C23-C24-C25-C30 |
| 24  | f     | 101 | BCR  | C5-C6-C7-C8     |
| 24  | f     | 101 | BCR  | C23-C24-C25-C30 |
| 24  | k     | 101 | BCR  | C23-C24-C25-C26 |
| 24  | k     | 101 | BCR  | C23-C24-C25-C30 |
| 24  | y     | 102 | BCR  | C1-C6-C7-C8     |
| 34  | J     | 102 | DGD  | C4B-C5B-C6B-C7B |
| 35  | C     | 519 | LMG  | C16-C17-C18-C19 |
| 35  | C     | 525 | LMG  | C21-C22-C23-C24 |
| 34  | C     | 503 | DGD  | C2A-C1A-O1G-C1G |
| 28  | i     | 101 | LFA  | C9-C10-C11-C12  |
| 31  | D     | 407 | LHG  | C24-C25-C26-C27 |
| 22  | a     | 408 | CLA  | O1A-CGA-O2A-C1  |
| 26  | l     | 102 | SQD  | C23-C24-C25-C26 |
| 31  | a     | 415 | LHG  | C23-C24-C25-C26 |
| 33  | Z     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 28  | i     | 101 | LFA  | C14-C15-C16-C17 |
| 25  | D     | 404 | PL9  | C47-C48-C49-C51 |
| 25  | d     | 402 | PL9  | C47-C48-C49-C51 |
| 26  | A     | 410 | SQD  | C11-C10-C9-C8   |
| 26  | D     | 412 | SQD  | C32-C33-C34-C35 |
| 22  | b     | 616 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | A     | 406 | PHO  | C4-C3-C5-C6     |
| 25  | D     | 404 | PL9  | C15-C14-C16-C17 |
| 25  | D     | 404 | PL9  | C35-C34-C36-C37 |
| 25  | D     | 404 | PL9  | C45-C44-C46-C47 |
| 25  | d     | 402 | PL9  | C35-C34-C36-C37 |
| 25  | d     | 402 | PL9  | C45-C44-C46-C47 |
| 22  | C     | 514 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 510 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 516 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 517 | CLA  | C6-C7-C8-C10    |
| 22  | D     | 406 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 509 | CLA  | O1A-CGA-O2A-C1  |
| 34  | c     | 503 | DGD  | O1A-C1A-O1G-C1G |
| 34  | c     | 504 | DGD  | C5B-C6B-C7B-C8B |
| 24  | B     | 632 | BCR  | C15-C16-C17-C18 |
| 34  | d     | 410 | DGD  | C2A-C1A-O1G-C1G |
| 26  | A     | 410 | SQD  | C9-C10-C11-C12  |
| 27  | E     | 103 | PLM  | CB-CC-CD-CE     |
| 31  | L     | 101 | LHG  | C31-C32-C33-C34 |
| 33  | b     | 626 | LMT  | O1'-C1-C2-C3    |
| 34  | H     | 101 | DGD  | C2B-C3B-C4B-C5B |
| 22  | B     | 607 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 617 | CLA  | C5-C6-C7-C8     |
| 27  | b     | 621 | PLM  | C7-C8-C9-CA     |
| 35  | m     | 101 | LMG  | C36-C37-C38-C39 |
| 25  | D     | 404 | PL9  | C47-C48-C49-C50 |
| 33  | f     | 102 | LMT  | C5-C6-C7-C8     |
| 26  | a     | 417 | SQD  | C23-C24-C25-C26 |
| 35  | C     | 519 | LMG  | C10-C11-C12-C13 |
| 27  | B     | 621 | PLM  | CC-CD-CE-CF     |
| 28  | B     | 620 | LFA  | C9-C10-C11-C12  |
| 28  | i     | 104 | LFA  | C11-C12-C13-C14 |
| 33  | T     | 104 | LMT  | C7-C8-C9-C10    |
| 28  | i     | 101 | LFA  | C7-C8-C9-C10    |
| 31  | d     | 405 | LHG  | C24-C25-C26-C27 |
| 35  | d     | 407 | LMG  | O6-C5-C6-O5     |
| 34  | c     | 505 | DGD  | C2A-C1A-O1G-C1G |
| 33  | i     | 102 | LMT  | O5'-C1'-O1'-C1  |
| 25  | A     | 409 | PL9  | C39-C41-C42-C43 |
| 27  | C     | 522 | PLM  | C2-C3-C4-C5     |
| 27  | L     | 102 | PLM  | CB-CC-CD-CE     |
| 27  | c     | 520 | PLM  | CB-CC-CD-CE     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | L     | 101 | LHG  | C11-C10-C9-C8   |
| 31  | l     | 101 | LHG  | C16-C17-C18-C19 |
| 35  | C     | 519 | LMG  | C11-C12-C13-C14 |
| 26  | A     | 410 | SQD  | C8-C7-O47-C45   |
| 31  | E     | 101 | LHG  | C8-C7-O7-C5     |
| 34  | c     | 505 | DGD  | C2B-C1B-O2G-C2G |
| 35  | c     | 524 | LMG  | C11-C10-O7-C8   |
| 27  | c     | 520 | PLM  | C2-C3-C4-C5     |
| 35  | c     | 524 | LMG  | C18-C19-C20-C21 |
| 22  | D     | 406 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 512 | CLA  | CBD-CGD-O2D-CED |
| 22  | c     | 517 | CLA  | CBD-CGD-O2D-CED |
| 28  | H     | 103 | LFA  | C9-C10-C11-C12  |
| 31  | E     | 101 | LHG  | O9-C7-O7-C5     |
| 33  | Z     | 101 | LMT  | C4B-C5B-C6B-O6B |
| 34  | J     | 102 | DGD  | C1B-C2B-C3B-C4B |
| 33  | T     | 101 | LMT  | C2'-C1'-O1'-C1  |
| 34  | J     | 102 | DGD  | C2E-C1E-O5D-C6D |
| 34  | C     | 504 | DGD  | O1G-C1G-C2G-O2G |
| 34  | d     | 410 | DGD  | O2G-C2G-C3G-O3G |
| 35  | y     | 101 | LMG  | O1-C7-C8-O7     |
| 35  | D     | 409 | LMG  | O6-C5-C6-O5     |
| 27  | B     | 621 | PLM  | C6-C7-C8-C9     |
| 33  | j     | 101 | LMT  | O1'-C1-C2-C3    |
| 35  | Y     | 101 | LMG  | C30-C31-C32-C33 |
| 27  | X     | 101 | PLM  | C3-C4-C5-C6     |
| 31  | D     | 407 | LHG  | C15-C16-C17-C18 |
| 31  | a     | 421 | LHG  | C30-C31-C32-C33 |
| 22  | B     | 604 | CLA  | C8-C10-C11-C12  |
| 27  | B     | 622 | PLM  | C1-C2-C3-C4     |
| 27  | c     | 523 | PLM  | C1-C2-C3-C4     |
| 33  | z     | 101 | LMT  | C1-C2-C3-C4     |
| 22  | B     | 603 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 614 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 512 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 514 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 515 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 605 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 616 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 515 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 605 | CLA  | O1D-CGD-O2D-CED |
| 26  | D     | 412 | SQD  | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | A     | 413 | PLM  | C3-C4-C5-C6     |
| 27  | L     | 102 | PLM  | C5-C6-C7-C8     |
| 28  | B     | 624 | LFA  | C6-C7-C8-C9     |
| 31  | d     | 406 | LHG  | C33-C34-C35-C36 |
| 31  | l     | 101 | LHG  | C33-C34-C35-C36 |
| 33  | B     | 633 | LMT  | C9-C10-C11-C12  |
| 22  | A     | 404 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 601 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 22  | a     | 405 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 612 | CLA  | C2A-CAA-CBA-CGA |
| 26  | A     | 415 | SQD  | C9-C10-C11-C12  |
| 26  | a     | 411 | SQD  | C26-C27-C28-C29 |
| 28  | I     | 101 | LFA  | C14-C15-C16-C17 |
| 35  | C     | 519 | LMG  | C17-C18-C19-C20 |
| 27  | b     | 622 | PLM  | C3-C4-C5-C6     |
| 31  | D     | 408 | LHG  | C17-C18-C19-C20 |
| 33  | T     | 104 | LMT  | C2-C3-C4-C5     |
| 34  | C     | 503 | DGD  | O1A-C1A-O1G-C1G |
| 22  | A     | 405 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 407 | CLA  | C1A-C2A-CAA-CBA |
| 22  | C     | 517 | CLA  | C1A-C2A-CAA-CBA |
| 22  | D     | 401 | CLA  | C1A-C2A-CAA-CBA |
| 22  | a     | 406 | CLA  | C1A-C2A-CAA-CBA |
| 22  | a     | 408 | CLA  | C1A-C2A-CAA-CBA |
| 22  | d     | 401 | CLA  | C1A-C2A-CAA-CBA |
| 33  | C     | 518 | LMT  | O5'-C5'-C6'-O6' |
| 26  | A     | 410 | SQD  | O49-C7-O47-C45  |
| 27  | C     | 522 | PLM  | C9-CA-CB-CC     |
| 31  | d     | 405 | LHG  | C11-C10-C9-C8   |
| 34  | C     | 504 | DGD  | C5A-C6A-C7A-C8A |
| 22  | B     | 615 | CLA  | C5-C6-C7-C8     |
| 22  | c     | 511 | CLA  | C13-C15-C16-C17 |
| 26  | b     | 601 | SQD  | C28-C29-C30-C31 |
| 28  | a     | 413 | LFA  | C9-C10-C11-C12  |
| 31  | A     | 417 | LHG  | C10-C11-C12-C13 |
| 26  | a     | 417 | SQD  | C10-C11-C12-C13 |
| 28  | i     | 101 | LFA  | C15-C16-C17-C18 |
| 35  | c     | 524 | LMG  | C17-C18-C19-C20 |
| 22  | c     | 509 | CLA  | C13-C15-C16-C17 |
| 33  | f     | 102 | LMT  | C11-C10-C9-C8   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | b     | 601 | SQD  | C23-C24-C25-C26 |
| 22  | B     | 611 | CLA  | C16-C17-C18-C20 |
| 27  | M     | 103 | PLM  | C2-C3-C4-C5     |
| 28  | I     | 102 | LFA  | C11-C12-C13-C14 |
| 31  | A     | 417 | LHG  | C25-C26-C27-C28 |
| 22  | b     | 606 | CLA  | C8-C10-C11-C12  |
| 26  | l     | 102 | SQD  | C11-C12-C13-C14 |
| 31  | D     | 408 | LHG  | C1-C2-C3-O3     |
| 31  | E     | 101 | LHG  | C1-C2-C3-O3     |
| 25  | D     | 404 | PL9  | C25-C24-C26-C27 |
| 25  | d     | 402 | PL9  | C25-C24-C26-C27 |
| 27  | B     | 627 | PLM  | C4-C5-C6-C7     |
| 27  | L     | 102 | PLM  | C7-C8-C9-CA     |
| 31  | a     | 421 | LHG  | C17-C18-C19-C20 |
| 35  | M     | 101 | LMG  | C17-C18-C19-C20 |
| 22  | C     | 513 | CLA  | C10-C11-C12-C13 |
| 26  | A     | 410 | SQD  | C12-C13-C14-C15 |
| 27  | c     | 523 | PLM  | CA-CB-CC-CD     |
| 27  | e     | 101 | PLM  | C5-C6-C7-C8     |
| 28  | i     | 104 | LFA  | C13-C14-C15-C16 |
| 35  | c     | 519 | LMG  | C33-C34-C35-C36 |
| 35  | m     | 101 | LMG  | C17-C18-C19-C20 |
| 28  | H     | 103 | LFA  | C7-C8-C9-C10    |
| 22  | b     | 613 | CLA  | C16-C17-C18-C20 |
| 26  | a     | 417 | SQD  | C44-C45-C46-O48 |
| 26  | d     | 412 | SQD  | O6-C44-C45-C46  |
| 26  | l     | 102 | SQD  | C44-C45-C46-O48 |
| 31  | E     | 101 | LHG  | C4-C5-C6-O8     |
| 31  | E     | 101 | LHG  | C19-C20-C21-C22 |
| 31  | a     | 415 | LHG  | C4-C5-C6-O8     |
| 33  | z     | 101 | LMT  | C4-C5-C6-C7     |
| 34  | C     | 503 | DGD  | C1G-C2G-C3G-O3G |
| 34  | J     | 102 | DGD  | C1G-C2G-C3G-O3G |
| 34  | c     | 503 | DGD  | C1G-C2G-C3G-O3G |
| 35  | C     | 519 | LMG  | C7-C8-C9-O8     |
| 35  | D     | 409 | LMG  | C16-C17-C18-C19 |
| 35  | Y     | 101 | LMG  | C7-C8-C9-O8     |
| 35  | c     | 519 | LMG  | C7-C8-C9-O8     |
| 35  | c     | 519 | LMG  | C11-C12-C13-C14 |
| 22  | c     | 508 | CLA  | C8-C10-C11-C12  |
| 27  | A     | 413 | PLM  | C5-C6-C7-C8     |
| 28  | B     | 620 | LFA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | C     | 521 | LFA  | C10-C11-C12-C13 |
| 31  | l     | 101 | LHG  | C11-C10-C9-C8   |
| 31  | D     | 407 | LHG  | C23-C24-C25-C26 |
| 26  | a     | 411 | SQD  | C45-C44-O6-C1   |
| 34  | C     | 504 | DGD  | C5D-C6D-O5D-C1E |
| 34  | J     | 102 | DGD  | C5D-C6D-O5D-C1E |
| 34  | c     | 504 | DGD  | C5D-C6D-O5D-C1E |
| 35  | c     | 524 | LMG  | C8-C7-O1-C1     |
| 35  | M     | 101 | LMG  | O6-C5-C6-O5     |
| 22  | C     | 516 | CLA  | O1D-CGD-O2D-CED |
| 26  | a     | 417 | SQD  | C32-C33-C34-C35 |
| 28  | a     | 413 | LFA  | C11-C12-C13-C14 |
| 33  | b     | 626 | LMT  | C11-C10-C9-C8   |
| 27  | D     | 402 | PLM  | C1-C2-C3-C4     |
| 26  | a     | 411 | SQD  | C19-C20-C21-C22 |
| 35  | y     | 101 | LMG  | O6-C1-O1-C7     |
| 31  | d     | 406 | LHG  | C17-C18-C19-C20 |
| 31  | D     | 408 | LHG  | O1-C1-C2-O2     |
| 31  | E     | 101 | LHG  | O1-C1-C2-O2     |
| 31  | d     | 406 | LHG  | O1-C1-C2-O2     |
| 26  | D     | 412 | SQD  | C10-C11-C12-C13 |
| 27  | M     | 103 | PLM  | CB-CC-CD-CE     |
| 33  | C     | 518 | LMT  | C5'-C4'-O1B-C1B |
| 34  | d     | 410 | DGD  | O1A-C1A-O1G-C1G |
| 34  | C     | 503 | DGD  | C4D-C5D-C6D-O5D |
| 34  | c     | 503 | DGD  | C4D-C5D-C6D-O5D |
| 35  | c     | 524 | LMG  | C29-C30-C31-C32 |
| 35  | c     | 519 | LMG  | C11-C10-O7-C8   |
| 34  | C     | 503 | DGD  | O6E-C5E-C6E-O5E |
| 34  | c     | 503 | DGD  | O6E-C5E-C6E-O5E |
| 35  | C     | 525 | LMG  | O6-C5-C6-O5     |
| 26  | a     | 417 | SQD  | C29-C30-C31-C32 |
| 28  | I     | 101 | LFA  | C11-C10-C9-C8   |
| 31  | a     | 415 | LHG  | C7-C8-C9-C10    |
| 31  | d     | 405 | LHG  | C23-C24-C25-C26 |
| 34  | c     | 504 | DGD  | C1A-C2A-C3A-C4A |
| 27  | c     | 520 | PLM  | CD-CE-CF-CG     |
| 33  | i     | 102 | LMT  | C5'-C4'-O1B-C1B |
| 26  | d     | 412 | SQD  | C10-C11-C12-C13 |
| 33  | j     | 101 | LMT  | C9-C10-C11-C12  |
| 28  | a     | 414 | LFA  | C13-C14-C15-C16 |
| 31  | d     | 406 | LHG  | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | C     | 507 | CLA  | C8-C10-C11-C12  |
| 22  | C     | 510 | CLA  | C13-C15-C16-C17 |
| 31  | d     | 405 | LHG  | C14-C15-C16-C17 |
| 34  | c     | 504 | DGD  | C3B-C4B-C5B-C6B |
| 34  | c     | 505 | DGD  | O1A-C1A-O1G-C1G |
| 22  | B     | 611 | CLA  | C16-C17-C18-C19 |
| 31  | d     | 406 | LHG  | C34-C35-C36-C37 |
| 34  | C     | 503 | DGD  | C2B-C3B-C4B-C5B |
| 34  | h     | 101 | DGD  | C7A-C8A-C9A-CAA |
| 34  | d     | 410 | DGD  | O6D-C5D-C6D-O5D |
| 35  | c     | 519 | LMG  | O6-C5-C6-O5     |
| 27  | A     | 413 | PLM  | C7-C8-C9-CA     |
| 33  | i     | 102 | LMT  | C4'-C5'-C6'-O6' |
| 22  | C     | 507 | CLA  | O1D-CGD-O2D-CED |
| 22  | C     | 510 | CLA  | O1D-CGD-O2D-CED |
| 28  | I     | 103 | LFA  | C10-C11-C12-C13 |
| 34  | H     | 101 | DGD  | C7A-C8A-C9A-CAA |
| 34  | c     | 504 | DGD  | C7A-C8A-C9A-CAA |
| 22  | C     | 516 | CLA  | C10-C11-C12-C13 |
| 28  | C     | 521 | LFA  | C6-C7-C8-C9     |
| 26  | A     | 415 | SQD  | O47-C7-C8-C9    |
| 34  | c     | 505 | DGD  | O2G-C2G-C3G-O3G |
| 35  | c     | 519 | LMG  | O1-C7-C8-O7     |
| 31  | a     | 415 | LHG  | C13-C14-C15-C16 |
| 31  | a     | 421 | LHG  | C32-C33-C34-C35 |
| 35  | C     | 525 | LMG  | C11-C12-C13-C14 |
| 34  | c     | 505 | DGD  | O1B-C1B-O2G-C2G |
| 22  | C     | 510 | CLA  | C10-C11-C12-C13 |
| 26  | b     | 601 | SQD  | C19-C20-C21-C22 |
| 27  | L     | 102 | PLM  | CD-CE-CF-CG     |
| 28  | d     | 408 | LFA  | C13-C14-C15-C16 |
| 31  | a     | 415 | LHG  | C25-C26-C27-C28 |
| 35  | d     | 407 | LMG  | C16-C17-C18-C19 |
| 35  | C     | 519 | LMG  | O6-C5-C6-O5     |
| 27  | c     | 521 | PLM  | C4-C5-C6-C7     |
| 27  | t     | 101 | PLM  | CC-CD-CE-CF     |
| 28  | d     | 408 | LFA  | C11-C10-C9-C8   |
| 34  | C     | 504 | DGD  | C7B-C8B-C9B-CAB |
| 22  | B     | 603 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 606 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 614 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 614 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 615 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 508 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 509 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 510 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 512 | CLA  | C11-C10-C8-C7   |
| 22  | a     | 408 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 605 | CLA  | C6-C7-C8-C10    |
| 22  | b     | 616 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 616 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 617 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 509 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 511 | CLA  | C11-C12-C13-C15 |
| 22  | c     | 513 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 514 | CLA  | C6-C7-C8-C10    |
| 22  | a     | 408 | CLA  | C3-C5-C6-C7     |
| 26  | a     | 411 | SQD  | C25-C26-C27-C28 |
| 22  | B     | 614 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 509 | CLA  | C11-C12-C13-C14 |
| 22  | C     | 516 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 517 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 616 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 507 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 513 | CLA  | C11-C10-C8-C9   |
| 26  | A     | 415 | SQD  | C17-C18-C19-C20 |
| 35  | m     | 101 | LMG  | C32-C33-C34-C35 |
| 35  | m     | 101 | LMG  | C34-C35-C36-C37 |
| 22  | C     | 506 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 507 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 510 | CLA  | C2A-CAA-CBA-CGA |
| 34  | D     | 411 | DGD  | CBB-CCB-CDB-CEB |
| 33  | Z     | 101 | LMT  | C1-C2-C3-C4     |
| 33  | i     | 102 | LMT  | C1-C2-C3-C4     |
| 24  | B     | 632 | BCR  | C21-C22-C23-C24 |
| 34  | c     | 503 | DGD  | C6A-C7A-C8A-C9A |
| 35  | c     | 519 | LMG  | C32-C33-C34-C35 |
| 27  | a     | 412 | PLM  | C3-C4-C5-C6     |
| 26  | A     | 410 | SQD  | C14-C15-C16-C17 |
| 31  | d     | 405 | LHG  | C15-C16-C17-C18 |
| 31  | a     | 421 | LHG  | C7-C8-C9-C10    |
| 22  | c     | 511 | CLA  | C10-C11-C12-C13 |
| 25  | d     | 402 | PL9  | C47-C48-C49-C50 |
| 27  | A     | 411 | PLM  | C2-C3-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | B     | 630 | LMT  | C11-C10-C9-C8   |
| 22  | B     | 603 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 606 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 609 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 506 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 605 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 608 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 611 | CLA  | C4B-C3B-CAB-CBB |
| 22  | c     | 507 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 613 | CLA  | C16-C17-C18-C19 |
| 31  | E     | 101 | LHG  | O6-C4-C5-C6     |
| 26  | A     | 410 | SQD  | C13-C14-C15-C16 |
| 28  | I     | 102 | LFA  | C12-C13-C14-C15 |
| 26  | d     | 412 | SQD  | C7-C8-C9-C10    |
| 27  | c     | 521 | PLM  | C7-C8-C9-CA     |
| 22  | B     | 614 | CLA  | C4-C3-C5-C6     |
| 25  | A     | 409 | PL9  | C12-C11-C9-C10  |
| 22  | b     | 616 | CLA  | C2-C3-C5-C6     |
| 27  | j     | 102 | PLM  | C1-C2-C3-C4     |
| 35  | c     | 524 | LMG  | O9-C10-O7-C8    |
| 26  | a     | 417 | SQD  | C11-C12-C13-C14 |
| 28  | i     | 101 | LFA  | C13-C14-C15-C16 |
| 31  | D     | 407 | LHG  | C14-C15-C16-C17 |
| 27  | e     | 102 | PLM  | C1-C2-C3-C4     |
| 27  | A     | 413 | PLM  | C2-C3-C4-C5     |
| 27  | X     | 101 | PLM  | C6-C7-C8-C9     |
| 33  | f     | 102 | LMT  | O1'-C1-C2-C3    |
| 35  | C     | 519 | LMG  | C19-C20-C21-C22 |
| 26  | a     | 411 | SQD  | C31-C32-C33-C34 |
| 28  | B     | 620 | LFA  | C6-C7-C8-C9     |
| 31  | L     | 101 | LHG  | C16-C17-C18-C19 |
| 33  | j     | 101 | LMT  | C2-C3-C4-C5     |
| 33  | j     | 101 | LMT  | C6-C7-C8-C9     |
| 34  | d     | 410 | DGD  | C3B-C4B-C5B-C6B |
| 35  | C     | 525 | LMG  | C32-C33-C34-C35 |
| 25  | A     | 409 | PL9  | C47-C48-C49-C51 |
| 33  | f     | 102 | LMT  | C2-C1-O1'-C1'   |
| 33  | m     | 102 | LMT  | C2-C1-O1'-C1'   |
| 26  | a     | 417 | SQD  | C12-C13-C14-C15 |
| 27  | F     | 102 | PLM  | C4-C5-C6-C7     |
| 27  | j     | 103 | PLM  | C3-C4-C5-C6     |
| 28  | I     | 102 | LFA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | M     | 101 | LMG  | C20-C21-C22-C23 |
| 22  | c     | 517 | CLA  | C3-C5-C6-C7     |
| 35  | m     | 101 | LMG  | C20-C21-C22-C23 |
| 22  | B     | 614 | CLA  | C10-C11-C12-C13 |
| 26  | A     | 415 | SQD  | O6-C44-C45-C46  |
| 26  | D     | 412 | SQD  | O6-C44-C45-C46  |
| 26  | a     | 411 | SQD  | O6-C44-C45-C46  |
| 26  | a     | 417 | SQD  | O6-C44-C45-C46  |
| 34  | C     | 504 | DGD  | O1G-C1G-C2G-C3G |
| 34  | D     | 411 | DGD  | O1G-C1G-C2G-C3G |
| 34  | d     | 410 | DGD  | C1G-C2G-C3G-O3G |
| 35  | y     | 101 | LMG  | O1-C7-C8-C9     |
| 27  | D     | 410 | PLM  | CD-CE-CF-CG     |
| 27  | X     | 101 | PLM  | C7-C8-C9-CA     |
| 28  | I     | 102 | LFA  | C13-C14-C15-C16 |
| 26  | l     | 102 | SQD  | C32-C33-C34-C35 |
| 27  | H     | 104 | PLM  | C7-C8-C9-CA     |
| 33  | T     | 104 | LMT  | C5-C6-C7-C8     |
| 22  | B     | 613 | CLA  | C10-C11-C12-C13 |
| 27  | D     | 410 | PLM  | C5-C6-C7-C8     |
| 31  | a     | 415 | LHG  | C17-C18-C19-C20 |
| 22  | d     | 404 | CLA  | O1D-CGD-O2D-CED |
| 35  | y     | 101 | LMG  | C10-C11-C12-C13 |
| 22  | c     | 507 | CLA  | O1A-CGA-O2A-C1  |
| 33  | f     | 102 | LMT  | C1-C2-C3-C4     |
| 22  | B     | 611 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 417 | LHG  | O1-C1-C2-O2     |
| 22  | b     | 614 | CLA  | C10-C11-C12-C13 |
| 27  | C     | 520 | PLM  | CA-CB-CC-CD     |
| 27  | d     | 411 | PLM  | C5-C6-C7-C8     |
| 28  | J     | 104 | LFA  | C12-C13-C14-C15 |
| 33  | Z     | 101 | LMT  | O1'-C1-C2-C3    |
| 22  | C     | 506 | CLA  | O1A-CGA-O2A-C1  |
| 27  | A     | 411 | PLM  | CD-CE-CF-CG     |
| 28  | i     | 101 | LFA  | C3-C4-C5-C6     |
| 22  | b     | 608 | CLA  | C2B-C3B-CAB-CBB |
| 31  | a     | 415 | LHG  | O2-C2-C3-O3     |
| 26  | a     | 411 | SQD  | C13-C14-C15-C16 |
| 33  | J     | 103 | LMT  | C3-C4-C5-C6     |
| 33  | C     | 518 | LMT  | C4-C5-C6-C7     |
| 26  | a     | 411 | SQD  | O6-C44-C45-O47  |
| 31  | E     | 101 | LHG  | O7-C5-C6-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | a     | 415 | LHG  | O7-C5-C6-O8     |
| 35  | c     | 519 | LMG  | O7-C8-C9-O8     |
| 22  | B     | 612 | CLA  | C10-C11-C12-C13 |
| 26  | a     | 417 | SQD  | C17-C18-C19-C20 |
| 31  | D     | 408 | LHG  | C14-C15-C16-C17 |
| 34  | c     | 504 | DGD  | C8B-C9B-CAB-CBB |
| 27  | b     | 622 | PLM  | C7-C8-C9-CA     |
| 28  | I     | 102 | LFA  | C14-C15-C16-C17 |
| 25  | A     | 409 | PL9  | C19-C21-C22-C23 |
| 31  | d     | 406 | LHG  | C1-C2-C3-O3     |
| 27  | A     | 411 | PLM  | C9-CA-CB-CC     |
| 27  | C     | 520 | PLM  | C6-C7-C8-C9     |
| 28  | T     | 102 | LFA  | C12-C13-C14-C15 |
| 22  | B     | 608 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 613 | CLA  | C2-C1-O2A-CGA   |
| 22  | b     | 610 | CLA  | C2-C1-O2A-CGA   |
| 22  | b     | 615 | CLA  | C2-C1-O2A-CGA   |
| 22  | C     | 509 | CLA  | C6-C7-C8-C9     |
| 22  | C     | 510 | CLA  | C11-C12-C13-C14 |
| 22  | c     | 507 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 511 | CLA  | C11-C12-C13-C14 |
| 27  | x     | 101 | PLM  | CA-CB-CC-CD     |
| 31  | A     | 417 | LHG  | C17-C18-C19-C20 |
| 22  | C     | 513 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 417 | LHG  | C2-C3-O3-P      |
| 31  | E     | 101 | LHG  | C2-C3-O3-P      |
| 26  | D     | 412 | SQD  | C25-C26-C27-C28 |
| 27  | C     | 523 | PLM  | C5-C6-C7-C8     |
| 22  | C     | 509 | CLA  | C2A-CAA-CBA-CGA |
| 24  | B     | 617 | BCR  | C23-C24-C25-C26 |
| 24  | K     | 101 | BCR  | C23-C24-C25-C26 |
| 24  | Y     | 102 | BCR  | C23-C24-C25-C26 |
| 24  | b     | 620 | BCR  | C23-C24-C25-C26 |
| 24  | c     | 502 | BCR  | C1-C6-C7-C8     |
| 24  | y     | 102 | BCR  | C23-C24-C25-C26 |
| 22  | B     | 613 | CLA  | C5-C6-C7-C8     |
| 22  | b     | 615 | CLA  | C5-C6-C7-C8     |
| 24  | C     | 502 | BCR  | C11-C12-C13-C14 |
| 22  | D     | 406 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 616 | CLA  | C10-C11-C12-C13 |
| 34  | C     | 504 | DGD  | C2A-C3A-C4A-C5A |
| 35  | c     | 519 | LMG  | O9-C10-O7-C8    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | M     | 103 | PLM  | C9-CA-CB-CC     |
| 28  | T     | 102 | LFA  | C7-C8-C9-C10    |
| 22  | c     | 513 | CLA  | C16-C17-C18-C19 |
| 26  | a     | 417 | SQD  | C24-C25-C26-C27 |
| 22  | c     | 517 | CLA  | O1D-CGD-O2D-CED |
| 26  | A     | 415 | SQD  | C13-C14-C15-C16 |
| 34  | C     | 503 | DGD  | C6A-C7A-C8A-C9A |
| 22  | A     | 405 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 601 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 604 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 509 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 513 | CLA  | C6-C7-C8-C10    |
| 22  | C     | 517 | CLA  | C12-C13-C15-C16 |
| 22  | D     | 405 | CLA  | C11-C12-C13-C15 |
| 22  | a     | 406 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 603 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 606 | CLA  | C6-C7-C8-C10    |
| 22  | d     | 403 | CLA  | C11-C12-C13-C15 |
| 22  | C     | 511 | CLA  | O1D-CGD-O2D-CED |
| 33  | B     | 623 | LMT  | C11-C10-C9-C8   |
| 35  | M     | 101 | LMG  | C13-C14-C15-C16 |
| 24  | C     | 501 | BCR  | C19-C20-C21-C22 |
| 24  | c     | 501 | BCR  | C19-C20-C21-C22 |
| 28  | i     | 101 | LFA  | C16-C17-C18-C19 |
| 34  | J     | 102 | DGD  | C6B-C7B-C8B-C9B |
| 35  | m     | 101 | LMG  | C13-C14-C15-C16 |
| 22  | b     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 22  | c     | 514 | CLA  | C10-C11-C12-C13 |
| 35  | c     | 519 | LMG  | C16-C17-C18-C19 |
| 34  | h     | 101 | DGD  | CCA-CDA-CEA-CFA |
| 35  | c     | 524 | LMG  | C12-C13-C14-C15 |
| 27  | B     | 627 | PLM  | C5-C6-C7-C8     |
| 27  | c     | 523 | PLM  | CC-CD-CE-CF     |
| 22  | B     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 31  | d     | 406 | LHG  | C12-C13-C14-C15 |
| 34  | H     | 101 | DGD  | CCA-CDA-CEA-CFA |
| 34  | c     | 505 | DGD  | C6B-C7B-C8B-C9B |
| 27  | B     | 622 | PLM  | C5-C6-C7-C8     |
| 22  | B     | 603 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 505 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 513 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 514 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 605 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 506 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 514 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 518 | CLA  | CAD-CBD-CGD-O2D |
| 27  | e     | 102 | PLM  | C8-C9-CA-CB     |
| 31  | l     | 101 | LHG  | C34-C35-C36-C37 |
| 35  | c     | 524 | LMG  | C15-C16-C17-C18 |
| 33  | T     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 26  | l     | 102 | SQD  | C14-C15-C16-C17 |
| 33  | C     | 518 | LMT  | O5'-C1'-O1'-C1  |
| 34  | C     | 503 | DGD  | O6E-C1E-O5D-C6D |
| 34  | c     | 503 | DGD  | O6E-C1E-O5D-C6D |
| 35  | c     | 519 | LMG  | C10-C11-C12-C13 |
| 31  | a     | 421 | LHG  | C2-C3-O3-P      |
| 34  | c     | 505 | DGD  | O1G-C1G-C2G-C3G |
| 34  | d     | 410 | DGD  | O1G-C1G-C2G-C3G |
| 27  | j     | 103 | PLM  | CA-CB-CC-CD     |
| 28  | a     | 414 | LFA  | C6-C7-C8-C9     |
| 22  | b     | 615 | CLA  | C10-C11-C12-C13 |
| 23  | D     | 403 | PHO  | C10-C11-C12-C13 |
| 27  | j     | 103 | PLM  | C6-C7-C8-C9     |
| 22  | c     | 506 | CLA  | C2A-CAA-CBA-CGA |
| 23  | a     | 420 | PHO  | C10-C11-C12-C13 |
| 31  | D     | 408 | LHG  | C9-C10-C11-C12  |
| 27  | F     | 102 | PLM  | C2-C3-C4-C5     |
| 31  | d     | 406 | LHG  | C9-C10-C11-C12  |
| 22  | A     | 405 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 606 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 606 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 609 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 614 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 506 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 506 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 510 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 606 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 608 | CLA  | CHA-CBD-CGD-O1D |
| 22  | b     | 608 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 611 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 507 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 507 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 508 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 508 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 509 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 512 | CLA  | CHA-CBD-CGD-O1D |
| 33  | C     | 518 | LMT  | C2'-C1'-O1'-C1  |
| 27  | C     | 522 | PLM  | C6-C7-C8-C9     |
| 26  | A     | 410 | SQD  | O47-C45-C46-O48 |
| 26  | a     | 417 | SQD  | O47-C45-C46-O48 |
| 34  | c     | 505 | DGD  | O6E-C5E-C6E-O5E |
| 22  | B     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 33  | j     | 101 | LMT  | C7-C8-C9-C10    |
| 31  | D     | 407 | LHG  | O1-C1-C2-O2     |
| 31  | a     | 421 | LHG  | O1-C1-C2-O2     |
| 31  | d     | 405 | LHG  | O1-C1-C2-O2     |
| 34  | C     | 503 | DGD  | C5A-C6A-C7A-C8A |
| 35  | C     | 525 | LMG  | C16-C17-C18-C19 |
| 25  | A     | 409 | PL9  | C4-C3-C7-C8     |
| 25  | a     | 410 | PL9  | C4-C3-C7-C8     |
| 22  | B     | 601 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 604 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 611 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 603 | CLA  | C11-C12-C13-C14 |
| 27  | D     | 410 | PLM  | CA-CB-CC-CD     |
| 34  | D     | 411 | DGD  | C4B-C5B-C6B-C7B |
| 22  | b     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 27  | d     | 411 | PLM  | C4-C5-C6-C7     |
| 22  | C     | 505 | CLA  | C2A-CAA-CBA-CGA |
| 27  | b     | 625 | PLM  | C9-CA-CB-CC     |
| 31  | D     | 407 | LHG  | C29-C30-C31-C32 |
| 27  | B     | 625 | PLM  | C4-C5-C6-C7     |
| 27  | e     | 102 | PLM  | C7-C8-C9-CA     |
| 24  | B     | 617 | BCR  | C17-C18-C19-C20 |
| 24  | C     | 502 | BCR  | C17-C18-C19-C20 |
| 24  | c     | 502 | BCR  | C17-C18-C19-C20 |
| 27  | x     | 101 | PLM  | C5-C6-C7-C8     |
| 22  | C     | 505 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 506 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 509 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 608 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 513 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 404 | CLA  | C2-C1-O2A-CGA   |
| 22  | a     | 405 | CLA  | C2-C1-O2A-CGA   |
| 24  | Y     | 102 | BCR  | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | L     | 101 | LHG  | C3-O3-P-O6      |
| 31  | d     | 406 | LHG  | C4-O6-P-O3      |
| 28  | d     | 408 | LFA  | C11-C12-C13-C14 |
| 22  | D     | 406 | CLA  | O1D-CGD-O2D-CED |
| 28  | i     | 101 | LFA  | C4-C5-C6-C7     |
| 22  | B     | 601 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 610 | CLA  | C4B-C3B-CAB-CBB |
| 22  | C     | 505 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 603 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 612 | CLA  | C4B-C3B-CAB-CBB |
| 31  | L     | 101 | LHG  | C4-O6-P-O5      |
| 31  | a     | 415 | LHG  | C4-O6-P-O4      |
| 31  | l     | 101 | LHG  | C4-O6-P-O5      |
| 22  | B     | 609 | CLA  | C16-C17-C18-C20 |
| 22  | a     | 408 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 511 | CLA  | C16-C17-C18-C19 |
| 22  | c     | 510 | CLA  | C13-C15-C16-C17 |
| 27  | A     | 411 | PLM  | CC-CD-CE-CF     |
| 28  | i     | 103 | LFA  | C10-C11-C12-C13 |
| 33  | z     | 101 | LMT  | C4B-C5B-C6B-O6B |
| 26  | A     | 415 | SQD  | C14-C15-C16-C17 |
| 27  | j     | 102 | PLM  | CA-CB-CC-CD     |
| 28  | J     | 101 | LFA  | C10-C11-C12-C13 |
| 34  | h     | 101 | DGD  | C3B-C4B-C5B-C6B |
| 22  | B     | 601 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 609 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 506 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 510 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 603 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 611 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 507 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 508 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 511 | CLA  | CAD-CBD-CGD-O1D |
| 26  | A     | 410 | SQD  | C5-C6-S-O9      |
| 26  | b     | 601 | SQD  | C5-C6-S-O9      |
| 26  | l     | 102 | SQD  | C5-C6-S-O7      |
| 22  | c     | 513 | CLA  | C5-C6-C7-C8     |
| 26  | a     | 411 | SQD  | C27-C28-C29-C30 |
| 33  | Z     | 101 | LMT  | C11-C10-C9-C8   |
| 34  | c     | 505 | DGD  | C1B-C2B-C3B-C4B |
| 26  | a     | 411 | SQD  | C32-C33-C34-C35 |
| 28  | I     | 103 | LFA  | C11-C10-C9-C8   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | H     | 101 | DGD  | C6B-C7B-C8B-C9B |
| 26  | a     | 411 | SQD  | C11-C12-C13-C14 |
| 31  | d     | 405 | LHG  | C29-C30-C31-C32 |
| 35  | C     | 525 | LMG  | C12-C13-C14-C15 |
| 35  | M     | 101 | LMG  | C16-C17-C18-C19 |
| 22  | C     | 512 | CLA  | C16-C17-C18-C19 |
| 25  | a     | 410 | PL9  | C15-C14-C16-C17 |
| 22  | A     | 407 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 601 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 604 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 609 | CLA  | C12-C13-C15-C16 |
| 22  | C     | 505 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 603 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 606 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 611 | CLA  | C12-C13-C15-C16 |
| 22  | c     | 511 | CLA  | C6-C7-C8-C10    |
| 22  | c     | 518 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 518 | CLA  | C12-C13-C15-C16 |
| 25  | D     | 404 | PL9  | C13-C14-C16-C17 |
| 25  | D     | 404 | PL9  | C33-C34-C36-C37 |
| 25  | d     | 402 | PL9  | C13-C14-C16-C17 |
| 31  | d     | 405 | LHG  | C19-C20-C21-C22 |
| 24  | y     | 102 | BCR  | C19-C20-C21-C22 |
| 27  | B     | 629 | PLM  | C6-C7-C8-C9     |
| 27  | b     | 627 | PLM  | C1-C2-C3-C4     |
| 22  | c     | 512 | CLA  | O1D-CGD-O2D-CED |
| 35  | C     | 525 | LMG  | C14-C15-C16-C17 |
| 35  | m     | 101 | LMG  | C16-C17-C18-C19 |
| 26  | D     | 412 | SQD  | C9-C10-C11-C12  |
| 27  | C     | 522 | PLM  | C4-C5-C6-C7     |
| 28  | d     | 408 | LFA  | C16-C17-C18-C19 |
| 26  | A     | 410 | SQD  | C44-C45-C46-O48 |
| 26  | l     | 102 | SQD  | O6-C44-C45-C46  |
| 28  | i     | 101 | LFA  | C10-C11-C12-C13 |
| 34  | c     | 504 | DGD  | O1G-C1G-C2G-C3G |
| 34  | c     | 505 | DGD  | C1G-C2G-C3G-O3G |
| 35  | C     | 519 | LMG  | O1-C7-C8-C9     |
| 35  | c     | 519 | LMG  | O1-C7-C8-C9     |
| 35  | c     | 519 | LMG  | C39-C40-C41-C42 |
| 26  | l     | 102 | SQD  | O6-C44-C45-O47  |
| 34  | c     | 505 | DGD  | O1G-C1G-C2G-O2G |
| 35  | C     | 519 | LMG  | O1-C7-C8-O7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | C     | 519 | LMG  | O7-C8-C9-O8     |
| 35  | Y     | 101 | LMG  | O7-C8-C9-O8     |
| 26  | b     | 601 | SQD  | C11-C12-C13-C14 |
| 33  | C     | 518 | LMT  | O1'-C1-C2-C3    |
| 35  | C     | 525 | LMG  | C15-C16-C17-C18 |
| 26  | a     | 417 | SQD  | C19-C20-C21-C22 |
| 27  | X     | 101 | PLM  | C5-C6-C7-C8     |
| 31  | l     | 101 | LHG  | C18-C19-C20-C21 |
| 35  | M     | 101 | LMG  | C34-C35-C36-C37 |
| 35  | C     | 525 | LMG  | C8-C7-O1-C1     |
| 26  | d     | 412 | SQD  | O47-C7-C8-C9    |
| 26  | b     | 601 | SQD  | C33-C34-C35-C36 |
| 26  | l     | 102 | SQD  | C13-C14-C15-C16 |
| 28  | d     | 408 | LFA  | C10-C11-C12-C13 |
| 22  | A     | 405 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 610 | CLA  | C11-C12-C13-C14 |
| 22  | a     | 406 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 606 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 608 | CLA  | C14-C13-C15-C16 |
| 22  | b     | 612 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 613 | CLA  | C14-C13-C15-C16 |
| 23  | D     | 403 | PHO  | C11-C10-C8-C9   |
| 23  | a     | 420 | PHO  | C11-C10-C8-C9   |
| 26  | a     | 417 | SQD  | C11-C10-C9-C8   |
| 27  | B     | 621 | PLM  | C8-C9-CA-CB     |
| 22  | B     | 608 | CLA  | C13-C15-C16-C17 |
| 27  | t     | 101 | PLM  | C1-C2-C3-C4     |
| 35  | C     | 519 | LMG  | C32-C33-C34-C35 |
| 28  | d     | 409 | LFA  | C12-C13-C14-C15 |
| 31  | a     | 421 | LHG  | C26-C27-C28-C29 |
| 28  | C     | 521 | LFA  | C11-C10-C9-C8   |
| 24  | B     | 617 | BCR  | C21-C22-C23-C24 |
| 24  | T     | 103 | BCR  | C17-C18-C19-C20 |
| 28  | E     | 102 | LFA  | C5-C6-C7-C8     |
| 22  | A     | 407 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 603 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 606 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 609 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 615 | CLA  | C2B-C3B-CAB-CBB |
| 22  | C     | 506 | CLA  | C2B-C3B-CAB-CBB |
| 22  | a     | 408 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 605 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 611 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 507 | CLA  | C2B-C3B-CAB-CBB |
| 35  | C     | 525 | LMG  | C17-C18-C19-C20 |
| 27  | C     | 522 | PLM  | C5-C6-C7-C8     |
| 31  | E     | 101 | LHG  | C10-C11-C12-C13 |
| 25  | D     | 404 | PL9  | C38-C39-C41-C42 |
| 34  | c     | 504 | DGD  | C3A-C4A-C5A-C6A |
| 22  | B     | 601 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 602 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 610 | CLA  | C13-C15-C16-C17 |
| 26  | l     | 102 | SQD  | C12-C13-C14-C15 |
| 33  | B     | 633 | LMT  | C5-C6-C7-C8     |
| 26  | l     | 102 | SQD  | O48-C23-C24-C25 |
| 31  | a     | 421 | LHG  | C9-C10-C11-C12  |
| 26  | b     | 601 | SQD  | C46-C45-O47-C7  |
| 33  | J     | 103 | LMT  | C1-C2-C3-C4     |
| 28  | a     | 418 | LFA  | C6-C7-C8-C9     |
| 22  | D     | 405 | CLA  | C2-C1-O2A-CGA   |
| 22  | d     | 403 | CLA  | C2-C1-O2A-CGA   |
| 27  | j     | 103 | PLM  | C2-C3-C4-C5     |
| 31  | L     | 101 | LHG  | C9-C10-C11-C12  |
| 35  | y     | 101 | LMG  | C16-C17-C18-C19 |
| 27  | C     | 523 | PLM  | C8-C9-CA-CB     |
| 35  | C     | 525 | LMG  | C13-C14-C15-C16 |
| 22  | C     | 505 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 603 | CLA  | C10-C11-C12-C13 |
| 31  | D     | 407 | LHG  | C12-C13-C14-C15 |
| 24  | B     | 632 | BCR  | C23-C24-C25-C30 |
| 24  | C     | 502 | BCR  | C1-C6-C7-C8     |
| 24  | K     | 101 | BCR  | C1-C6-C7-C8     |
| 37  | h     | 102 | RRX  | C23-C24-C25-C30 |
| 37  | h     | 102 | RRX  | C23-C24-C25-C26 |
| 25  | d     | 402 | PL9  | C33-C34-C36-C37 |
| 25  | d     | 402 | PL9  | C38-C39-C41-C42 |
| 33  | m     | 102 | LMT  | C4-C5-C6-C7     |
| 35  | c     | 519 | LMG  | C20-C21-C22-C23 |
| 22  | a     | 408 | CLA  | C16-C17-C18-C20 |
| 22  | c     | 511 | CLA  | C16-C17-C18-C20 |
| 28  | i     | 101 | LFA  | C2-C3-C4-C5     |
| 22  | a     | 406 | CLA  | C2A-CAA-CBA-CGA |
| 25  | a     | 410 | PL9  | C39-C41-C42-C43 |
| 34  | C     | 503 | DGD  | C2E-C1E-O5D-C6D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | c     | 503 | DGD  | C2E-C1E-O5D-C6D |
| 34  | d     | 410 | DGD  | O1G-C1G-C2G-O2G |
| 27  | C     | 520 | PLM  | C7-C8-C9-CA     |
| 22  | b     | 613 | CLA  | CBD-CGD-O2D-CED |
| 31  | D     | 408 | LHG  | C3-O3-P-O6      |
| 31  | D     | 408 | LHG  | C4-O6-P-O3      |
| 31  | d     | 406 | LHG  | C3-O3-P-O6      |
| 31  | l     | 101 | LHG  | C3-O3-P-O6      |
| 22  | B     | 606 | CLA  | C16-C17-C18-C19 |
| 28  | d     | 409 | LFA  | C9-C10-C11-C12  |
| 35  | D     | 409 | LMG  | C14-C15-C16-C17 |
| 31  | A     | 417 | LHG  | C4-C5-C6-O8     |
| 34  | D     | 411 | DGD  | C6B-C7B-C8B-C9B |
| 22  | B     | 611 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 614 | CLA  | C2-C3-C5-C6     |
| 22  | c     | 510 | CLA  | C6-C7-C8-C10    |
| 25  | a     | 410 | PL9  | C43-C44-C46-C47 |
| 22  | B     | 604 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 609 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 615 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 508 | CLA  | C14-C13-C15-C16 |
| 22  | D     | 405 | CLA  | C11-C12-C13-C14 |
| 22  | a     | 408 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 606 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 617 | CLA  | C14-C13-C15-C16 |
| 22  | c     | 509 | CLA  | C14-C13-C15-C16 |
| 22  | d     | 403 | CLA  | C11-C12-C13-C14 |
| 24  | c     | 502 | BCR  | C13-C14-C15-C16 |
| 22  | C     | 513 | CLA  | C16-C17-C18-C19 |
| 27  | c     | 523 | PLM  | C6-C7-C8-C9     |
| 28  | i     | 101 | LFA  | C5-C6-C7-C8     |
| 35  | D     | 409 | LMG  | C32-C33-C34-C35 |
| 22  | A     | 405 | CLA  | C2A-CAA-CBA-CGA |
| 35  | d     | 407 | LMG  | C10-C11-C12-C13 |
| 27  | M     | 103 | PLM  | C6-C7-C8-C9     |
| 31  | d     | 406 | LHG  | C25-C26-C27-C28 |
| 28  | B     | 620 | LFA  | C7-C8-C9-C10    |
| 31  | E     | 101 | LHG  | O1-C1-C2-C3     |
| 27  | t     | 101 | PLM  | CA-CB-CC-CD     |
| 35  | d     | 407 | LMG  | C34-C35-C36-C37 |
| 31  | E     | 101 | LHG  | C18-C19-C20-C21 |
| 25  | D     | 404 | PL9  | C37-C38-C39-C41 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 609 | CLA  | C16-C17-C18-C19 |
| 28  | J     | 101 | LFA  | C6-C7-C8-C9     |
| 31  | L     | 101 | LHG  | C35-C36-C37-C38 |
| 31  | l     | 101 | LHG  | C9-C10-C11-C12  |
| 33  | M     | 102 | LMT  | C4-C5-C6-C7     |
| 34  | C     | 504 | DGD  | C7A-C8A-C9A-CAA |
| 34  | d     | 410 | DGD  | C2A-C3A-C4A-C5A |
| 22  | A     | 407 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 615 | CLA  | C4B-C3B-CAB-CBB |
| 22  | a     | 408 | CLA  | C4B-C3B-CAB-CBB |
| 22  | b     | 606 | CLA  | C4B-C3B-CAB-CBB |
| 24  | C     | 502 | BCR  | C19-C20-C21-C22 |
| 24  | b     | 602 | BCR  | C15-C16-C17-C18 |
| 24  | c     | 502 | BCR  | C19-C20-C21-C22 |
| 26  | d     | 412 | SQD  | C32-C33-C34-C35 |
| 25  | a     | 410 | PL9  | C14-C16-C17-C18 |
| 31  | D     | 407 | LHG  | C19-C20-C21-C22 |
| 27  | a     | 412 | PLM  | O2-C1-C2-C3     |
| 31  | D     | 408 | LHG  | C15-C16-C17-C18 |
| 22  | b     | 611 | CLA  | C16-C17-C18-C20 |
| 25  | a     | 410 | PL9  | C40-C39-C41-C42 |
| 31  | A     | 417 | LHG  | C11-C12-C13-C14 |
| 33  | B     | 623 | LMT  | C1-C2-C3-C4     |
| 27  | b     | 625 | PLM  | O2-C1-C2-C3     |
| 36  | e     | 103 | HEM  | CAD-CBD-CGD-O1D |
| 22  | B     | 614 | CLA  | C2A-CAA-CBA-CGA |
| 35  | C     | 519 | LMG  | C20-C21-C22-C23 |
| 35  | C     | 525 | LMG  | C22-C23-C24-C25 |
| 22  | b     | 613 | CLA  | O1D-CGD-O2D-CED |
| 26  | b     | 601 | SQD  | C31-C32-C33-C34 |
| 22  | B     | 607 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 608 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 22  | b     | 610 | CLA  | C3A-C2A-CAA-CBA |
| 27  | c     | 522 | PLM  | O2-C1-C2-C3     |
| 35  | D     | 409 | LMG  | C34-C35-C36-C37 |
| 26  | d     | 412 | SQD  | C24-C25-C26-C27 |
| 31  | d     | 405 | LHG  | C12-C13-C14-C15 |
| 33  | T     | 101 | LMT  | C6-C7-C8-C9     |
| 34  | D     | 411 | DGD  | CCB-CDB-CEB-CFB |
| 36  | e     | 103 | HEM  | CAD-CBD-CGD-O2D |
| 35  | D     | 409 | LMG  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | d     | 407 | LMG  | C32-C33-C34-C35 |
| 22  | A     | 407 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 604 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 506 | CLA  | C6-C7-C8-C9     |
| 22  | D     | 401 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 606 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 510 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 518 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 518 | CLA  | C14-C13-C15-C16 |
| 22  | d     | 401 | CLA  | C11-C12-C13-C14 |
| 22  | d     | 404 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 417 | LHG  | C26-C27-C28-C29 |
| 35  | c     | 519 | LMG  | C40-C41-C42-C43 |
| 26  | a     | 411 | SQD  | C11-C10-C9-C8   |
| 28  | C     | 521 | LFA  | C7-C8-C9-C10    |
| 28  | J     | 104 | LFA  | C9-C10-C11-C12  |
| 26  | b     | 601 | SQD  | C35-C36-C37-C38 |
| 35  | y     | 101 | LMG  | C40-C41-C42-C43 |
| 36  | E     | 104 | HEM  | CAD-CBD-CGD-O2D |
| 27  | B     | 627 | PLM  | C2-C3-C4-C5     |
| 31  | A     | 417 | LHG  | C30-C31-C32-C33 |
| 22  | D     | 406 | CLA  | C16-C17-C18-C19 |
| 22  | C     | 515 | CLA  | CBA-CGA-O2A-C1  |
| 26  | l     | 102 | SQD  | C28-C29-C30-C31 |
| 27  | j     | 102 | PLM  | CC-CD-CE-CF     |
| 27  | j     | 102 | PLM  | O2-C1-C2-C3     |
| 27  | d     | 411 | PLM  | O2-C1-C2-C3     |
| 22  | C     | 508 | CLA  | C1A-C2A-CAA-CBA |
| 22  | c     | 518 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 603 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 604 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 612 | CLA  | C11-C10-C8-C7   |
| 22  | C     | 506 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 605 | CLA  | C11-C10-C8-C7   |
| 22  | b     | 606 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 608 | CLA  | C12-C13-C15-C16 |
| 22  | b     | 614 | CLA  | C11-C10-C8-C7   |
| 22  | c     | 517 | CLA  | C11-C12-C13-C15 |
| 31  | D     | 408 | LHG  | C25-C26-C27-C28 |
| 27  | C     | 522 | PLM  | O2-C1-C2-C3     |
| 27  | d     | 411 | PLM  | O1-C1-C2-C3     |
| 27  | t     | 101 | PLM  | CB-CC-CD-CE     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | y     | 102 | BCR  | C9-C10-C11-C12  |
| 26  | d     | 412 | SQD  | C28-C29-C30-C31 |
| 27  | b     | 625 | PLM  | O1-C1-C2-C3     |
| 36  | E     | 104 | HEM  | CAD-CBD-CGD-O1D |
| 28  | i     | 101 | LFA  | C17-C18-C19-C20 |
| 22  | A     | 407 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 605 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 607 | CLA  | C2A-CAA-CBA-CGA |
| 28  | I     | 101 | LFA  | C12-C13-C14-C15 |
| 34  | h     | 101 | DGD  | O2G-C1B-C2B-C3B |
| 26  | a     | 411 | SQD  | C30-C31-C32-C33 |
| 27  | e     | 101 | PLM  | C3-C4-C5-C6     |
| 27  | C     | 524 | PLM  | O2-C1-C2-C3     |
| 27  | j     | 102 | PLM  | O1-C1-C2-C3     |
| 22  | b     | 617 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 601 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 610 | CLA  | C2B-C3B-CAB-CBB |
| 22  | C     | 505 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 603 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 612 | CLA  | C2B-C3B-CAB-CBB |
| 31  | a     | 421 | LHG  | C28-C29-C30-C31 |
| 35  | C     | 519 | LMG  | C33-C34-C35-C36 |
| 28  | J     | 101 | LFA  | C2-C3-C4-C5     |
| 26  | a     | 411 | SQD  | O47-C45-C46-O48 |
| 31  | A     | 417 | LHG  | O7-C5-C6-O8     |
| 24  | Y     | 102 | BCR  | C9-C10-C11-C12  |
| 22  | B     | 610 | CLA  | C16-C17-C18-C19 |
| 27  | B     | 621 | PLM  | C7-C8-C9-CA     |
| 27  | D     | 410 | PLM  | O1-C1-C2-C3     |
| 27  | a     | 412 | PLM  | O1-C1-C2-C3     |
| 36  | V     | 201 | HEM  | CAD-CBD-CGD-O2D |
| 28  | T     | 102 | LFA  | C6-C7-C8-C9     |
| 22  | C     | 506 | CLA  | C2-C1-O2A-CGA   |
| 22  | c     | 507 | CLA  | C2-C1-O2A-CGA   |
| 28  | E     | 102 | LFA  | C13-C14-C15-C16 |
| 22  | D     | 406 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 611 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 515 | CLA  | O1A-CGA-O2A-C1  |
| 35  | C     | 519 | LMG  | C30-C31-C32-C33 |
| 31  | E     | 101 | LHG  | O2-C2-C3-O3     |
| 26  | D     | 412 | SQD  | C27-C28-C29-C30 |
| 22  | B     | 603 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 605 | CLA  | C2A-CAA-CBA-CGA |
| 22  | b     | 616 | CLA  | C2A-CAA-CBA-CGA |
| 27  | c     | 522 | PLM  | O1-C1-C2-C3     |
| 26  | A     | 415 | SQD  | O49-C7-C8-C9    |
| 24  | A     | 408 | BCR  | C23-C24-C25-C30 |
| 24  | Y     | 102 | BCR  | C23-C24-C25-C30 |
| 24  | a     | 409 | BCR  | C23-C24-C25-C30 |
| 24  | b     | 602 | BCR  | C23-C24-C25-C30 |
| 24  | k     | 101 | BCR  | C1-C6-C7-C8     |
| 24  | y     | 102 | BCR  | C23-C24-C25-C30 |
| 37  | H     | 102 | RRX  | C23-C24-C25-C30 |
| 37  | H     | 102 | RRX  | C23-C24-C25-C26 |
| 37  | H     | 102 | RRX  | C1-C6-C7-C8     |
| 37  | h     | 102 | RRX  | C1-C6-C7-C8     |
| 26  | D     | 412 | SQD  | O47-C7-C8-C9    |
| 26  | a     | 417 | SQD  | O47-C7-C8-C9    |
| 34  | H     | 101 | DGD  | O2G-C1B-C2B-C3B |
| 27  | D     | 410 | PLM  | C6-C7-C8-C9     |
| 33  | B     | 623 | LMT  | O1'-C1-C2-C3    |
| 34  | c     | 503 | DGD  | C9A-CAA-CBA-CCA |
| 27  | C     | 524 | PLM  | O1-C1-C2-C3     |
| 22  | C     | 512 | CLA  | C5-C6-C7-C8     |
| 32  | a     | 401 | GOL  | C1-C2-C3-O3     |
| 34  | C     | 504 | DGD  | C3A-C4A-C5A-C6A |
| 24  | b     | 602 | BCR  | C9-C10-C11-C12  |
| 24  | K     | 101 | BCR  | C21-C22-C23-C24 |
| 22  | b     | 612 | CLA  | C16-C17-C18-C19 |
| 27  | M     | 103 | PLM  | O1-C1-C2-C3     |
| 34  | c     | 505 | DGD  | C7A-C8A-C9A-CAA |
| 34  | C     | 503 | DGD  | C5D-C6D-O5D-C1E |
| 34  | c     | 503 | DGD  | C5D-C6D-O5D-C1E |
| 27  | b     | 621 | PLM  | C2-C3-C4-C5     |
| 33  | J     | 103 | LMT  | C2-C3-C4-C5     |
| 27  | B     | 629 | PLM  | O1-C1-C2-C3     |
| 27  | C     | 522 | PLM  | O1-C1-C2-C3     |
| 27  | D     | 410 | PLM  | O2-C1-C2-C3     |
| 22  | C     | 506 | CLA  | C15-C16-C17-C18 |
| 22  | b     | 604 | CLA  | C8-C10-C11-C12  |
| 22  | b     | 608 | CLA  | C10-C11-C12-C13 |
| 22  | D     | 405 | CLA  | C4B-C3B-CAB-CBB |
| 22  | d     | 403 | CLA  | C4B-C3B-CAB-CBB |
| 22  | d     | 404 | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | c     | 503 | DGD  | C8A-C9A-CAA-CBA |
| 22  | C     | 511 | CLA  | C5-C6-C7-C8     |
| 22  | C     | 510 | CLA  | C6-C7-C8-C10    |
| 22  | D     | 401 | CLA  | C11-C12-C13-C15 |
| 22  | b     | 613 | CLA  | C12-C13-C15-C16 |
| 22  | d     | 401 | CLA  | C11-C12-C13-C15 |
| 23  | D     | 403 | PHO  | C11-C10-C8-C7   |
| 23  | a     | 420 | PHO  | C11-C10-C8-C7   |
| 27  | e     | 101 | PLM  | O2-C1-C2-C3     |
| 32  | a     | 401 | GOL  | O2-C2-C3-O3     |
| 24  | C     | 501 | BCR  | C9-C10-C11-C12  |
| 27  | A     | 411 | PLM  | C5-C6-C7-C8     |
| 31  | a     | 421 | LHG  | C29-C30-C31-C32 |
| 27  | e     | 101 | PLM  | O1-C1-C2-C3     |
| 36  | V     | 201 | HEM  | CAD-CBD-CGD-O1D |
| 22  | B     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 615 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 609 | CLA  | C15-C16-C17-C18 |
| 27  | B     | 629 | PLM  | O2-C1-C2-C3     |
| 26  | b     | 601 | SQD  | C26-C27-C28-C29 |
| 22  | B     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 614 | CLA  | CAA-CBA-CGA-O2A |
| 26  | a     | 411 | SQD  | O48-C23-C24-C25 |
| 22  | C     | 508 | CLA  | C4-C3-C5-C6     |
| 25  | D     | 404 | PL9  | C30-C29-C31-C32 |
| 25  | a     | 410 | PL9  | C12-C11-C9-C10  |
| 25  | d     | 402 | PL9  | C30-C29-C31-C32 |
| 28  | A     | 412 | LFA  | C11-C10-C9-C8   |
| 25  | A     | 409 | PL9  | C28-C29-C31-C32 |
| 31  | d     | 406 | LHG  | C26-C27-C28-C29 |
| 22  | B     | 610 | CLA  | C16-C17-C18-C20 |
| 22  | C     | 510 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 612 | CLA  | C11-C10-C8-C9   |
| 22  | C     | 505 | CLA  | C11-C12-C13-C14 |
| 22  | b     | 614 | CLA  | C11-C10-C8-C9   |
| 22  | c     | 511 | CLA  | C6-C7-C8-C9     |
| 22  | c     | 517 | CLA  | C11-C12-C13-C14 |
| 27  | c     | 521 | PLM  | C3-C4-C5-C6     |
| 26  | A     | 415 | SQD  | C29-C30-C31-C32 |
| 33  | T     | 104 | LMT  | C6-C7-C8-C9     |
| 23  | D     | 403 | PHO  | C3A-C2A-CAA-CBA |
| 27  | a     | 412 | PLM  | C2-C3-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | a     | 415 | LHG  | O8-C23-C24-C25  |
| 35  | c     | 524 | LMG  | C34-C35-C36-C37 |
| 27  | C     | 520 | PLM  | O2-C1-C2-C3     |
| 22  | B     | 607 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 616 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 509 | CLA  | CAD-CBD-CGD-O2D |
| 22  | C     | 517 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 612 | CLA  | CAD-CBD-CGD-O2D |
| 22  | b     | 618 | CLA  | CAD-CBD-CGD-O2D |
| 22  | c     | 510 | CLA  | CAD-CBD-CGD-O2D |
| 22  | D     | 406 | CLA  | C16-C17-C18-C20 |
| 22  | b     | 611 | CLA  | C16-C17-C18-C19 |
| 22  | b     | 612 | CLA  | C16-C17-C18-C20 |
| 31  | D     | 407 | LHG  | C26-C27-C28-C29 |
| 35  | C     | 525 | LMG  | O9-C10-O7-C8    |
| 25  | d     | 402 | PL9  | C37-C38-C39-C41 |
| 31  | d     | 405 | LHG  | C26-C27-C28-C29 |
| 34  | c     | 504 | DGD  | C5A-C6A-C7A-C8A |
| 22  | c     | 517 | CLA  | C4-C3-C5-C6     |
| 25  | A     | 409 | PL9  | C35-C34-C36-C37 |
| 26  | b     | 601 | SQD  | O5-C1-O6-C44    |
| 25  | A     | 409 | PL9  | C12-C11-C9-C8   |
| 22  | C     | 514 | CLA  | CAA-CBA-CGA-O2A |
| 22  | c     | 515 | CLA  | CAA-CBA-CGA-O2A |
| 34  | C     | 503 | DGD  | O2G-C1B-C2B-C3B |
| 34  | c     | 503 | DGD  | O2G-C1B-C2B-C3B |
| 27  | B     | 621 | PLM  | C4-C5-C6-C7     |
| 27  | D     | 402 | PLM  | C4-C5-C6-C7     |
| 31  | a     | 415 | LHG  | C10-C11-C12-C13 |
| 26  | a     | 411 | SQD  | C44-C45-C46-O48 |
| 27  | e     | 102 | PLM  | O2-C1-C2-C3     |
| 27  | x     | 101 | PLM  | O2-C1-C2-C3     |
| 34  | c     | 505 | DGD  | O1G-C1A-C2A-C3A |
| 26  | b     | 601 | SQD  | C13-C14-C15-C16 |
| 35  | Y     | 101 | LMG  | C12-C13-C14-C15 |
| 35  | m     | 101 | LMG  | C10-C11-C12-C13 |
| 27  | M     | 103 | PLM  | O2-C1-C2-C3     |
| 27  | b     | 622 | PLM  | O1-C1-C2-C3     |
| 27  | b     | 627 | PLM  | O1-C1-C2-C3     |
| 27  | x     | 101 | PLM  | O1-C1-C2-C3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | v     | 201 | HEM  | CAD-CBD-CGD-O1D |
| 36  | v     | 201 | HEM  | CAD-CBD-CGD-O2D |
| 22  | C     | 513 | CLA  | O2A-C1-C2-C3    |
| 22  | C     | 516 | CLA  | O2A-C1-C2-C3    |
| 22  | c     | 514 | CLA  | O2A-C1-C2-C3    |
| 22  | c     | 517 | CLA  | O2A-C1-C2-C3    |
| 23  | A     | 406 | PHO  | O2A-C1-C2-C3    |
| 22  | A     | 407 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 511 | CLA  | C15-C16-C17-C18 |
| 27  | C     | 520 | PLM  | C8-C9-CA-CB     |
| 35  | d     | 407 | LMG  | C33-C34-C35-C36 |
| 26  | A     | 410 | SQD  | C10-C11-C12-C13 |
| 35  | m     | 101 | LMG  | O9-C10-O7-C8    |
| 22  | B     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 604 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 609 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 508 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 510 | CLA  | CHA-CBD-CGD-O2D |
| 22  | C     | 511 | CLA  | CHA-CBD-CGD-O1D |
| 22  | C     | 511 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 605 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 606 | CLA  | CHA-CBD-CGD-O2D |
| 22  | b     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 509 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 511 | CLA  | CHA-CBD-CGD-O1D |
| 22  | c     | 511 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 512 | CLA  | CHA-CBD-CGD-O2D |
| 24  | f     | 101 | BCR  | C13-C14-C15-C16 |
| 27  | b     | 622 | PLM  | O2-C1-C2-C3     |
| 27  | b     | 627 | PLM  | O2-C1-C2-C3     |
| 26  | l     | 102 | SQD  | O47-C7-C8-C9    |
| 31  | d     | 406 | LHG  | C15-C16-C17-C18 |
| 35  | C     | 519 | LMG  | C34-C35-C36-C37 |
| 35  | C     | 525 | LMG  | C29-C30-C31-C32 |
| 22  | c     | 517 | CLA  | C13-C15-C16-C17 |
| 35  | m     | 101 | LMG  | O8-C28-C29-C30  |
| 27  | b     | 621 | PLM  | CB-CC-CD-CE     |
| 22  | C     | 516 | CLA  | C13-C15-C16-C17 |
| 23  | D     | 403 | PHO  | CHA-CBD-CGD-O1D |
| 23  | D     | 403 | PHO  | CHA-CBD-CGD-O2D |
| 23  | a     | 420 | PHO  | CHA-CBD-CGD-O1D |
| 27  | a     | 412 | PLM  | C4-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | j     | 103 | PLM  | CD-CE-CF-CG     |
| 33  | A     | 419 | LMT  | C4-C5-C6-C7     |
| 27  | e     | 102 | PLM  | O1-C1-C2-C3     |
| 35  | C     | 519 | LMG  | C40-C41-C42-C43 |
| 35  | c     | 524 | LMG  | C28-C29-C30-C31 |
| 27  | C     | 520 | PLM  | C2-C3-C4-C5     |
| 27  | L     | 102 | PLM  | C8-C9-CA-CB     |
| 35  | M     | 101 | LMG  | O9-C10-O7-C8    |
| 35  | y     | 101 | LMG  | O9-C10-O7-C8    |
| 35  | C     | 519 | LMG  | O6-C1-O1-C7     |
| 22  | B     | 603 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 604 | CLA  | C14-C13-C15-C16 |
| 22  | C     | 510 | CLA  | C6-C7-C8-C9     |
| 22  | b     | 605 | CLA  | C11-C10-C8-C9   |
| 22  | b     | 606 | CLA  | C14-C13-C15-C16 |
| 27  | t     | 101 | PLM  | C5-C6-C7-C8     |
| 22  | D     | 405 | CLA  | C2B-C3B-CAB-CBB |
| 22  | b     | 606 | CLA  | C2B-C3B-CAB-CBB |
| 22  | c     | 513 | CLA  | C2B-C3B-CAB-CBB |
| 22  | d     | 403 | CLA  | C2B-C3B-CAB-CBB |
| 35  | d     | 407 | LMG  | C14-C15-C16-C17 |
| 31  | a     | 415 | LHG  | O7-C7-C8-C9     |
| 26  | a     | 411 | SQD  | C5-C6-S-O8      |
| 28  | i     | 103 | LFA  | C7-C8-C9-C10    |
| 27  | C     | 520 | PLM  | O1-C1-C2-C3     |
| 28  | d     | 408 | LFA  | C17-C18-C19-C20 |
| 31  | d     | 406 | LHG  | C28-C29-C30-C31 |
| 22  | B     | 608 | CLA  | CBA-CGA-O2A-C1  |
| 26  | l     | 102 | SQD  | C11-C10-C9-C8   |
| 27  | d     | 411 | PLM  | C1-C2-C3-C4     |
| 22  | B     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 22  | b     | 615 | CLA  | CAA-CBA-CGA-O1A |
| 34  | c     | 503 | DGD  | O1B-C1B-C2B-C3B |
| 31  | l     | 101 | LHG  | O1-C1-C2-C3     |
| 31  | D     | 407 | LHG  | C33-C34-C35-C36 |
| 35  | D     | 409 | LMG  | C37-C38-C39-C40 |
| 27  | X     | 101 | PLM  | O2-C1-C2-C3     |
| 22  | b     | 610 | CLA  | CBA-CGA-O2A-C1  |
| 27  | M     | 103 | PLM  | C8-C9-CA-CB     |
| 22  | B     | 607 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 608 | CLA  | C1A-C2A-CAA-CBA |
| 22  | b     | 609 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | b     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 421 | LHG  | C27-C28-C29-C30 |
| 22  | C     | 510 | CLA  | C16-C17-C18-C20 |
| 26  | l     | 102 | SQD  | O49-C7-C8-C9    |
| 22  | a     | 408 | CLA  | C8-C10-C11-C12  |
| 27  | x     | 101 | PLM  | C8-C9-CA-CB     |
| 27  | a     | 412 | PLM  | CB-CC-CD-CE     |
| 28  | a     | 413 | LFA  | C10-C11-C12-C13 |
| 22  | C     | 514 | CLA  | CAA-CBA-CGA-O1A |
| 22  | b     | 614 | CLA  | CAA-CBA-CGA-O1A |
| 22  | c     | 515 | CLA  | CAA-CBA-CGA-O1A |
| 26  | a     | 411 | SQD  | O10-C23-C24-C25 |
| 34  | C     | 503 | DGD  | O1B-C1B-C2B-C3B |
| 26  | a     | 411 | SQD  | C10-C11-C12-C13 |
| 34  | C     | 503 | DGD  | C8A-C9A-CAA-CBA |
| 26  | A     | 410 | SQD  | O48-C23-C24-C25 |
| 27  | B     | 622 | PLM  | C6-C7-C8-C9     |
| 28  | E     | 102 | LFA  | C6-C7-C8-C9     |
| 31  | D     | 408 | LHG  | C11-C12-C13-C14 |
| 27  | X     | 101 | PLM  | C1-C2-C3-C4     |
| 22  | B     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 34  | d     | 410 | DGD  | C8B-C9B-CAB-CBB |
| 27  | c     | 523 | PLM  | O1-C1-C2-C3     |
| 22  | B     | 602 | CLA  | C15-C16-C17-C18 |
| 31  | a     | 415 | LHG  | O10-C23-C24-C25 |
| 31  | E     | 101 | LHG  | C16-C17-C18-C19 |
| 35  | c     | 524 | LMG  | C14-C15-C16-C17 |
| 22  | a     | 406 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 417 | LHG  | C15-C16-C17-C18 |
| 31  | D     | 408 | LHG  | C3-O3-P-O5      |
| 31  | D     | 408 | LHG  | C4-O6-P-O5      |
| 31  | L     | 101 | LHG  | C3-O3-P-O5      |
| 31  | d     | 406 | LHG  | C3-O3-P-O5      |
| 31  | d     | 406 | LHG  | C4-O6-P-O5      |
| 26  | A     | 415 | SQD  | C30-C31-C32-C33 |
| 27  | b     | 621 | PLM  | C5-C6-C7-C8     |
| 33  | A     | 419 | LMT  | C6-C7-C8-C9     |
| 34  | c     | 503 | DGD  | C2B-C3B-C4B-C5B |
| 35  | c     | 524 | LMG  | C16-C17-C18-C19 |
| 24  | B     | 632 | BCR  | C23-C24-C25-C26 |
| 24  | K     | 101 | BCR  | C5-C6-C7-C8     |
| 24  | T     | 103 | BCR  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | A     | 410 | SQD  | C26-C27-C28-C29 |
| 27  | e     | 101 | PLM  | C9-CA-CB-CC     |
| 27  | B     | 627 | PLM  | O1-C1-C2-C3     |
| 26  | l     | 102 | SQD  | C27-C28-C29-C30 |
| 25  | D     | 404 | PL9  | C42-C43-C44-C46 |
| 31  | d     | 405 | LHG  | C33-C34-C35-C36 |
| 22  | B     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 605 | CLA  | CAD-CBD-CGD-O1D |
| 22  | C     | 508 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 606 | CLA  | CAD-CBD-CGD-O1D |
| 22  | b     | 607 | CLA  | CAD-CBD-CGD-O1D |
| 22  | c     | 509 | CLA  | CAD-CBD-CGD-O1D |
| 34  | c     | 505 | DGD  | O1A-C1A-C2A-C3A |
| 27  | j     | 103 | PLM  | C8-C9-CA-CB     |
| 35  | C     | 519 | LMG  | C31-C32-C33-C34 |
| 35  | y     | 101 | LMG  | C39-C40-C41-C42 |
| 34  | D     | 411 | DGD  | O2G-C1B-C2B-C3B |
| 22  | A     | 405 | CLA  | C6-C7-C8-C9     |
| 22  | a     | 406 | CLA  | C6-C7-C8-C9     |
| 27  | M     | 103 | PLM  | C5-C6-C7-C8     |
| 22  | c     | 513 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 506 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 605 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 607 | CLA  | C13-C15-C16-C17 |
| 22  | c     | 517 | CLA  | C8-C10-C11-C12  |
| 27  | X     | 101 | PLM  | O1-C1-C2-C3     |
| 35  | M     | 101 | LMG  | C10-C11-C12-C13 |
| 27  | A     | 411 | PLM  | C8-C9-CA-CB     |
| 28  | C     | 521 | LFA  | C11-C12-C13-C14 |
| 31  | l     | 101 | LHG  | C26-C27-C28-C29 |
| 34  | c     | 505 | DGD  | C8A-C9A-CAA-CBA |
| 22  | B     | 614 | CLA  | CAA-CBA-CGA-O2A |
| 22  | b     | 616 | CLA  | CAA-CBA-CGA-O2A |
| 31  | D     | 407 | LHG  | O7-C7-C8-C9     |
| 31  | l     | 101 | LHG  | O7-C7-C8-C9     |
| 22  | b     | 613 | CLA  | C8-C10-C11-C12  |
| 35  | M     | 101 | LMG  | C29-C30-C31-C32 |
| 35  | d     | 407 | LMG  | C37-C38-C39-C40 |
| 26  | A     | 410 | SQD  | O10-C23-C24-C25 |
| 22  | b     | 612 | CLA  | C13-C15-C16-C17 |
| 25  | d     | 402 | PL9  | C42-C43-C44-C46 |
| 22  | C     | 516 | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | a     | 406 | CLA  | C6-C7-C8-C10    |
| 25  | d     | 402 | PL9  | C43-C44-C46-C47 |
| 27  | A     | 413 | PLM  | O2-C1-C2-C3     |
| 27  | c     | 523 | PLM  | O2-C1-C2-C3     |
| 22  | C     | 505 | CLA  | CAA-CBA-CGA-O2A |
| 31  | L     | 101 | LHG  | O7-C7-C8-C9     |
| 35  | C     | 525 | LMG  | O8-C28-C29-C30  |
| 27  | B     | 621 | PLM  | C2-C3-C4-C5     |
| 34  | J     | 102 | DGD  | C7A-C8A-C9A-CAA |
| 24  | b     | 602 | BCR  | C21-C22-C23-C24 |
| 27  | E     | 103 | PLM  | O1-C1-C2-C3     |
| 27  | c     | 520 | PLM  | O2-C1-C2-C3     |
| 24  | a     | 409 | BCR  | C19-C20-C21-C22 |
| 27  | e     | 101 | PLM  | CA-CB-CC-CD     |
| 33  | A     | 419 | LMT  | C2-C1-O1'-C1'   |
| 33  | T     | 101 | LMT  | C2-C1-O1'-C1'   |
| 31  | l     | 101 | LHG  | O9-C7-C8-C9     |
| 27  | A     | 413 | PLM  | O1-C1-C2-C3     |
| 27  | E     | 103 | PLM  | C7-C8-C9-CA     |
| 22  | B     | 611 | CLA  | C8-C10-C11-C12  |
| 22  | c     | 512 | CLA  | C5-C6-C7-C8     |
| 34  | J     | 102 | DGD  | O6E-C5E-C6E-O5E |
| 22  | A     | 405 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 615 | CLA  | C10-C11-C12-C13 |
| 31  | a     | 415 | LHG  | O9-C7-C8-C9     |
| 22  | B     | 603 | CLA  | C13-C15-C16-C17 |
| 22  | C     | 505 | CLA  | C13-C15-C16-C17 |
| 22  | b     | 616 | CLA  | C8-C10-C11-C12  |
| 31  | a     | 415 | LHG  | C16-C17-C18-C19 |
| 35  | M     | 101 | LMG  | C14-C15-C16-C17 |
| 35  | M     | 101 | LMG  | O8-C28-C29-C30  |
| 27  | B     | 627 | PLM  | O2-C1-C2-C3     |

There are no ring outliers.

163 monomers are involved in 253 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | c     | 508 | CLA  | 3       | 0            |
| 34  | C     | 504 | DGD  | 2       | 0            |
| 33  | m     | 102 | LMT  | 1       | 0            |
| 26  | a     | 411 | SQD  | 2       | 0            |
| 22  | B     | 611 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | C     | 514 | CLA  | 4       | 0            |
| 24  | b     | 620 | BCR  | 2       | 0            |
| 25  | A     | 409 | PL9  | 3       | 0            |
| 22  | b     | 613 | CLA  | 1       | 0            |
| 24  | K     | 101 | BCR  | 1       | 0            |
| 28  | J     | 104 | LFA  | 1       | 0            |
| 33  | T     | 101 | LMT  | 1       | 0            |
| 37  | h     | 102 | RRX  | 1       | 0            |
| 24  | B     | 619 | BCR  | 1       | 0            |
| 34  | c     | 505 | DGD  | 2       | 0            |
| 31  | d     | 405 | LHG  | 3       | 0            |
| 22  | C     | 508 | CLA  | 1       | 0            |
| 22  | b     | 604 | CLA  | 1       | 0            |
| 31  | D     | 408 | LHG  | 2       | 0            |
| 31  | l     | 101 | LHG  | 3       | 0            |
| 22  | b     | 616 | CLA  | 1       | 0            |
| 25  | D     | 404 | PL9  | 4       | 0            |
| 26  | b     | 601 | SQD  | 2       | 0            |
| 22  | b     | 607 | CLA  | 4       | 0            |
| 22  | c     | 510 | CLA  | 2       | 0            |
| 22  | C     | 512 | CLA  | 1       | 0            |
| 22  | a     | 406 | CLA  | 1       | 0            |
| 27  | b     | 622 | PLM  | 1       | 0            |
| 33  | B     | 628 | LMT  | 1       | 0            |
| 22  | b     | 608 | CLA  | 1       | 0            |
| 27  | e     | 102 | PLM  | 1       | 0            |
| 33  | B     | 630 | LMT  | 3       | 0            |
| 22  | a     | 408 | CLA  | 2       | 0            |
| 22  | B     | 605 | CLA  | 3       | 0            |
| 22  | A     | 404 | CLA  | 2       | 0            |
| 26  | A     | 415 | SQD  | 4       | 0            |
| 31  | d     | 406 | LHG  | 2       | 0            |
| 22  | C     | 505 | CLA  | 6       | 0            |
| 35  | M     | 101 | LMG  | 5       | 0            |
| 24  | B     | 617 | BCR  | 4       | 0            |
| 27  | L     | 102 | PLM  | 1       | 0            |
| 28  | b     | 623 | LFA  | 2       | 0            |
| 22  | B     | 609 | CLA  | 1       | 0            |
| 26  | a     | 417 | SQD  | 2       | 0            |
| 27  | c     | 520 | PLM  | 2       | 0            |
| 35  | c     | 519 | LMG  | 1       | 0            |
| 22  | c     | 509 | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | c     | 502 | BCR  | 3       | 0            |
| 28  | T     | 102 | LFA  | 2       | 0            |
| 33  | B     | 633 | LMT  | 1       | 0            |
| 27  | A     | 413 | PLM  | 2       | 0            |
| 33  | M     | 102 | LMT  | 1       | 0            |
| 22  | c     | 518 | CLA  | 2       | 0            |
| 22  | b     | 618 | CLA  | 2       | 0            |
| 25  | a     | 410 | PL9  | 4       | 0            |
| 26  | A     | 410 | SQD  | 3       | 0            |
| 22  | B     | 607 | CLA  | 3       | 0            |
| 22  | c     | 515 | CLA  | 4       | 0            |
| 22  | B     | 604 | CLA  | 4       | 0            |
| 22  | c     | 516 | CLA  | 2       | 0            |
| 22  | c     | 517 | CLA  | 1       | 0            |
| 24  | C     | 501 | BCR  | 2       | 0            |
| 34  | d     | 410 | DGD  | 1       | 0            |
| 35  | Y     | 101 | LMG  | 2       | 0            |
| 27  | B     | 621 | PLM  | 1       | 0            |
| 27  | D     | 410 | PLM  | 1       | 0            |
| 34  | c     | 504 | DGD  | 2       | 0            |
| 22  | c     | 507 | CLA  | 2       | 0            |
| 26  | l     | 102 | SQD  | 3       | 0            |
| 31  | A     | 417 | LHG  | 1       | 0            |
| 22  | B     | 610 | CLA  | 1       | 0            |
| 33  | C     | 518 | LMT  | 1       | 0            |
| 24  | A     | 408 | BCR  | 1       | 0            |
| 22  | B     | 615 | CLA  | 6       | 0            |
| 22  | C     | 511 | CLA  | 4       | 0            |
| 28  | I     | 103 | LFA  | 2       | 0            |
| 31  | a     | 415 | LHG  | 3       | 0            |
| 22  | B     | 608 | CLA  | 1       | 0            |
| 22  | C     | 515 | CLA  | 2       | 0            |
| 22  | B     | 606 | CLA  | 1       | 0            |
| 22  | a     | 405 | CLA  | 2       | 0            |
| 27  | x     | 101 | PLM  | 2       | 0            |
| 24  | T     | 103 | BCR  | 2       | 0            |
| 28  | A     | 412 | LFA  | 1       | 0            |
| 27  | B     | 629 | PLM  | 1       | 0            |
| 28  | E     | 102 | LFA  | 2       | 0            |
| 22  | b     | 609 | CLA  | 3       | 0            |
| 22  | c     | 512 | CLA  | 2       | 0            |
| 34  | D     | 411 | DGD  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | c     | 501 | BCR  | 1       | 0            |
| 22  | B     | 602 | CLA  | 2       | 0            |
| 22  | C     | 507 | CLA  | 3       | 0            |
| 32  | a     | 401 | GOL  | 1       | 0            |
| 27  | D     | 402 | PLM  | 1       | 0            |
| 33  | z     | 101 | LMT  | 1       | 0            |
| 22  | B     | 616 | CLA  | 2       | 0            |
| 22  | b     | 610 | CLA  | 3       | 0            |
| 34  | J     | 102 | DGD  | 3       | 0            |
| 22  | d     | 404 | CLA  | 2       | 0            |
| 22  | d     | 401 | CLA  | 1       | 0            |
| 22  | C     | 506 | CLA  | 1       | 0            |
| 22  | A     | 405 | CLA  | 1       | 0            |
| 24  | y     | 102 | BCR  | 1       | 0            |
| 31  | a     | 421 | LHG  | 2       | 0            |
| 24  | b     | 619 | BCR  | 3       | 0            |
| 24  | B     | 618 | BCR  | 1       | 0            |
| 28  | B     | 626 | LFA  | 2       | 0            |
| 36  | e     | 103 | HEM  | 1       | 0            |
| 22  | B     | 613 | CLA  | 2       | 0            |
| 23  | A     | 406 | PHO  | 1       | 0            |
| 24  | F     | 101 | BCR  | 1       | 0            |
| 26  | D     | 412 | SQD  | 2       | 0            |
| 28  | i     | 104 | LFA  | 1       | 0            |
| 35  | d     | 407 | LMG  | 2       | 0            |
| 22  | c     | 506 | CLA  | 5       | 0            |
| 27  | B     | 622 | PLM  | 1       | 0            |
| 22  | D     | 405 | CLA  | 2       | 0            |
| 22  | A     | 407 | CLA  | 2       | 0            |
| 22  | d     | 403 | CLA  | 2       | 0            |
| 24  | b     | 602 | BCR  | 5       | 0            |
| 22  | b     | 615 | CLA  | 3       | 0            |
| 36  | E     | 104 | HEM  | 1       | 0            |
| 35  | c     | 524 | LMG  | 2       | 0            |
| 31  | D     | 407 | LHG  | 3       | 0            |
| 27  | C     | 524 | PLM  | 2       | 0            |
| 22  | C     | 516 | CLA  | 3       | 0            |
| 37  | H     | 102 | RRX  | 1       | 0            |
| 24  | B     | 632 | BCR  | 5       | 0            |
| 22  | D     | 401 | CLA  | 1       | 0            |
| 36  | V     | 201 | HEM  | 1       | 0            |
| 36  | v     | 201 | HEM  | 1       | 0            |

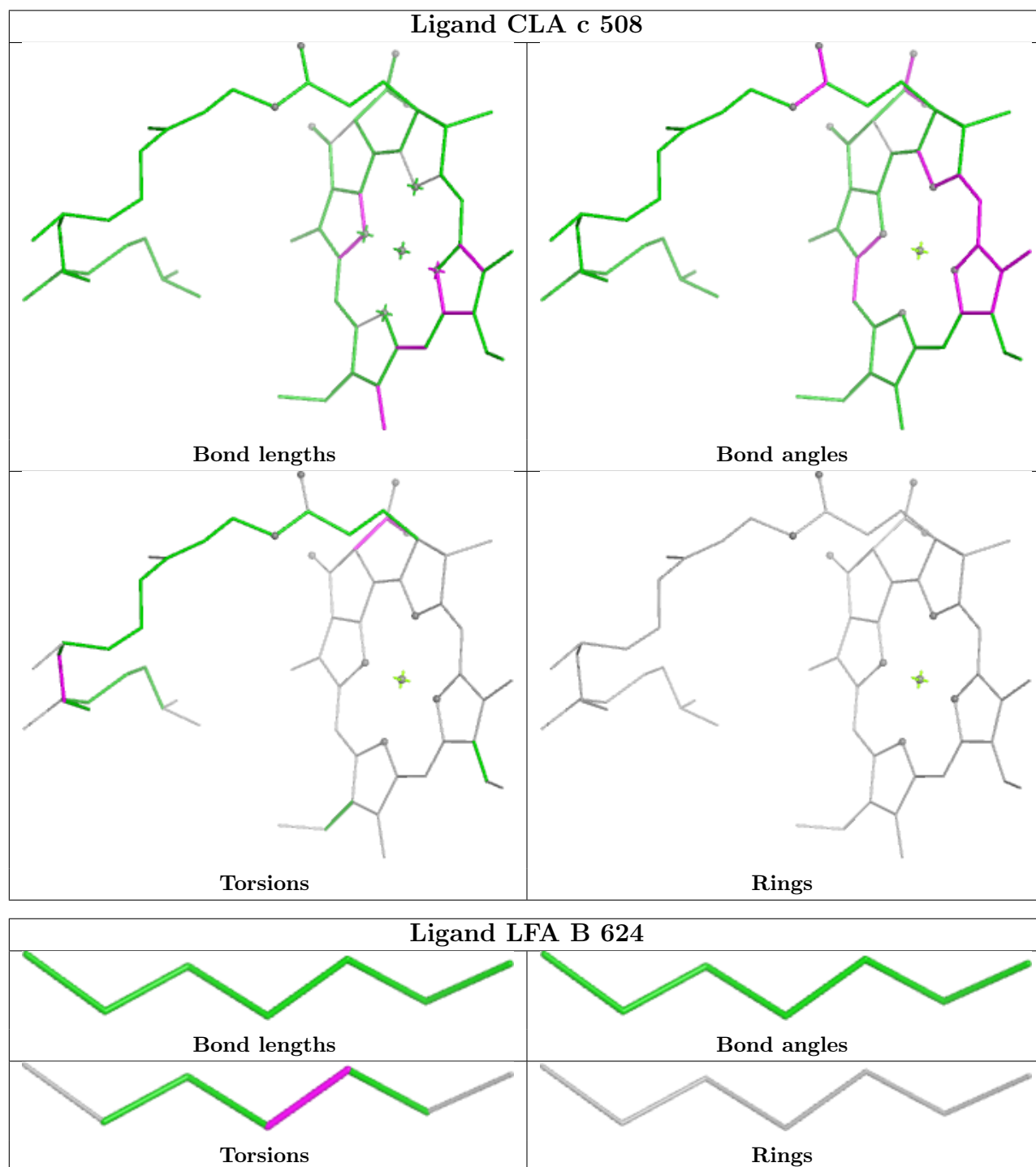
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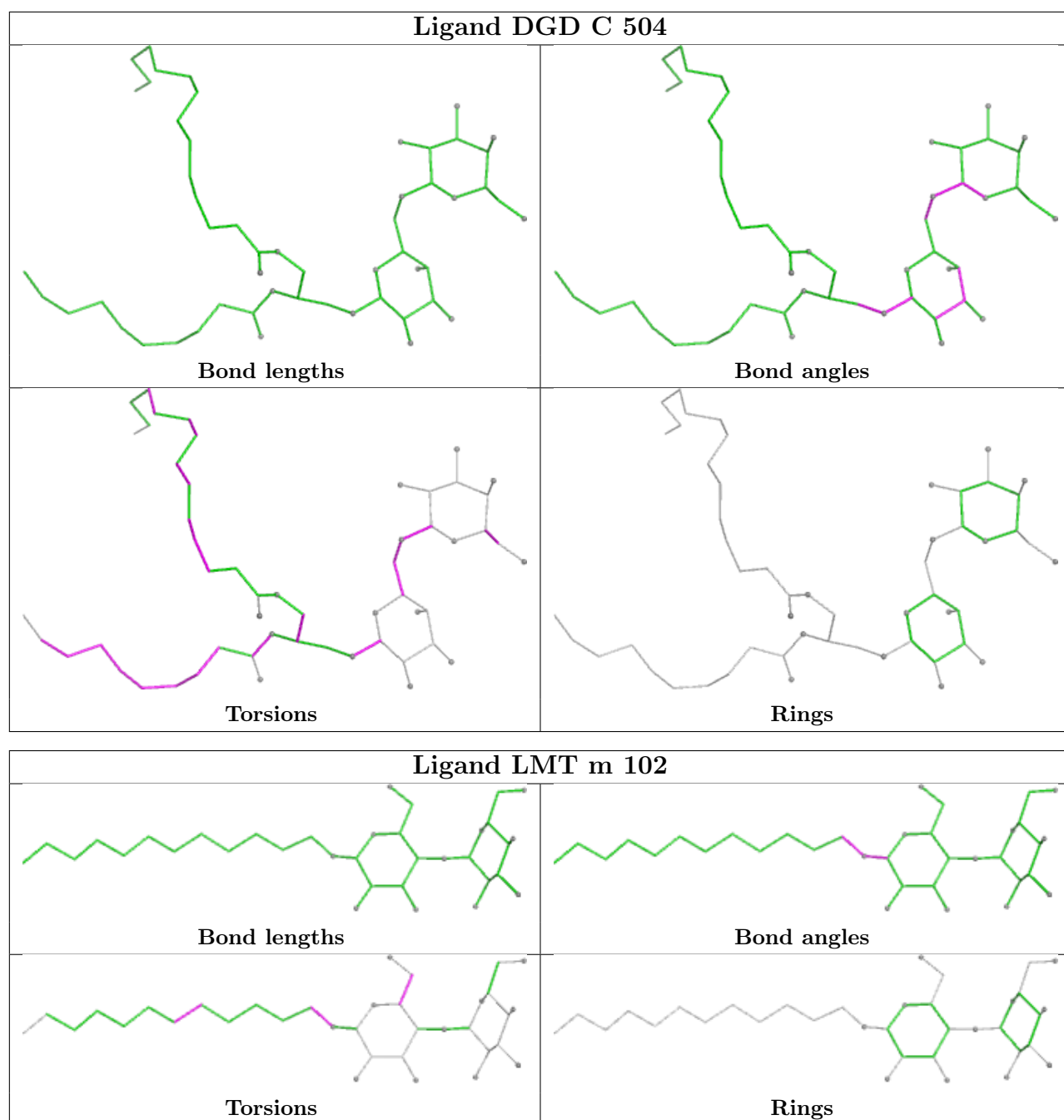
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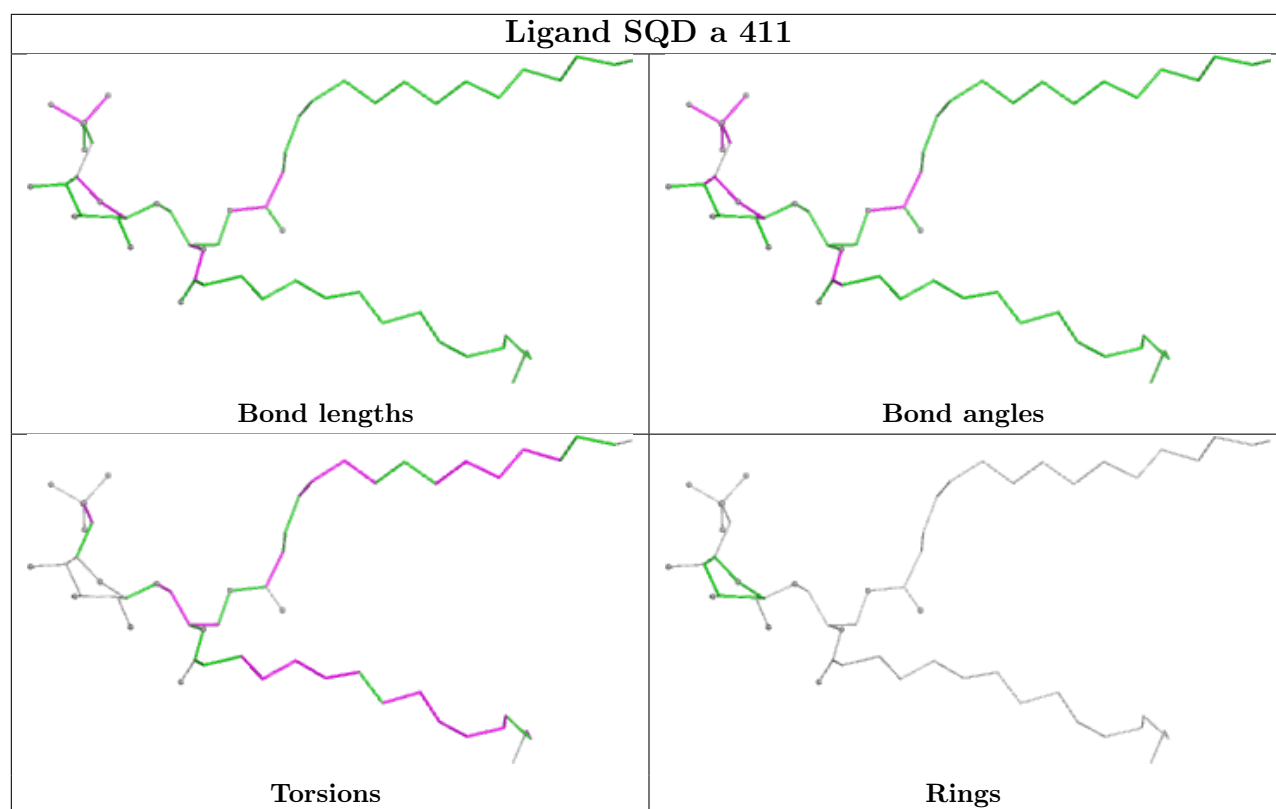
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | a     | 407 | PHO  | 1       | 0            |
| 28  | B     | 620 | LFA  | 1       | 0            |
| 22  | C     | 510 | CLA  | 2       | 0            |
| 22  | C     | 513 | CLA  | 1       | 0            |
| 22  | b     | 605 | CLA  | 1       | 0            |
| 22  | c     | 511 | CLA  | 2       | 0            |
| 24  | C     | 502 | BCR  | 4       | 0            |
| 22  | b     | 611 | CLA  | 1       | 0            |
| 24  | Y     | 102 | BCR  | 2       | 0            |
| 27  | t     | 101 | PLM  | 2       | 0            |
| 26  | d     | 412 | SQD  | 3       | 0            |
| 22  | b     | 617 | CLA  | 6       | 0            |
| 23  | a     | 420 | PHO  | 2       | 0            |
| 27  | j     | 103 | PLM  | 1       | 0            |
| 31  | L     | 101 | LHG  | 4       | 0            |
| 28  | J     | 101 | LFA  | 1       | 0            |
| 35  | y     | 101 | LMG  | 1       | 0            |
| 35  | D     | 409 | LMG  | 2       | 0            |
| 22  | b     | 614 | CLA  | 2       | 0            |
| 23  | D     | 403 | PHO  | 1       | 0            |
| 27  | B     | 625 | PLM  | 2       | 0            |
| 22  | c     | 513 | CLA  | 4       | 0            |
| 35  | C     | 519 | LMG  | 1       | 0            |
| 22  | C     | 509 | CLA  | 3       | 0            |
| 22  | b     | 606 | CLA  | 4       | 0            |
| 24  | k     | 101 | BCR  | 1       | 0            |
| 33  | J     | 103 | LMT  | 2       | 0            |
| 34  | H     | 101 | DGD  | 1       | 0            |
| 35  | m     | 101 | LMG  | 4       | 0            |
| 22  | b     | 612 | CLA  | 1       | 0            |
| 25  | d     | 402 | PL9  | 4       | 0            |
| 22  | B     | 612 | CLA  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

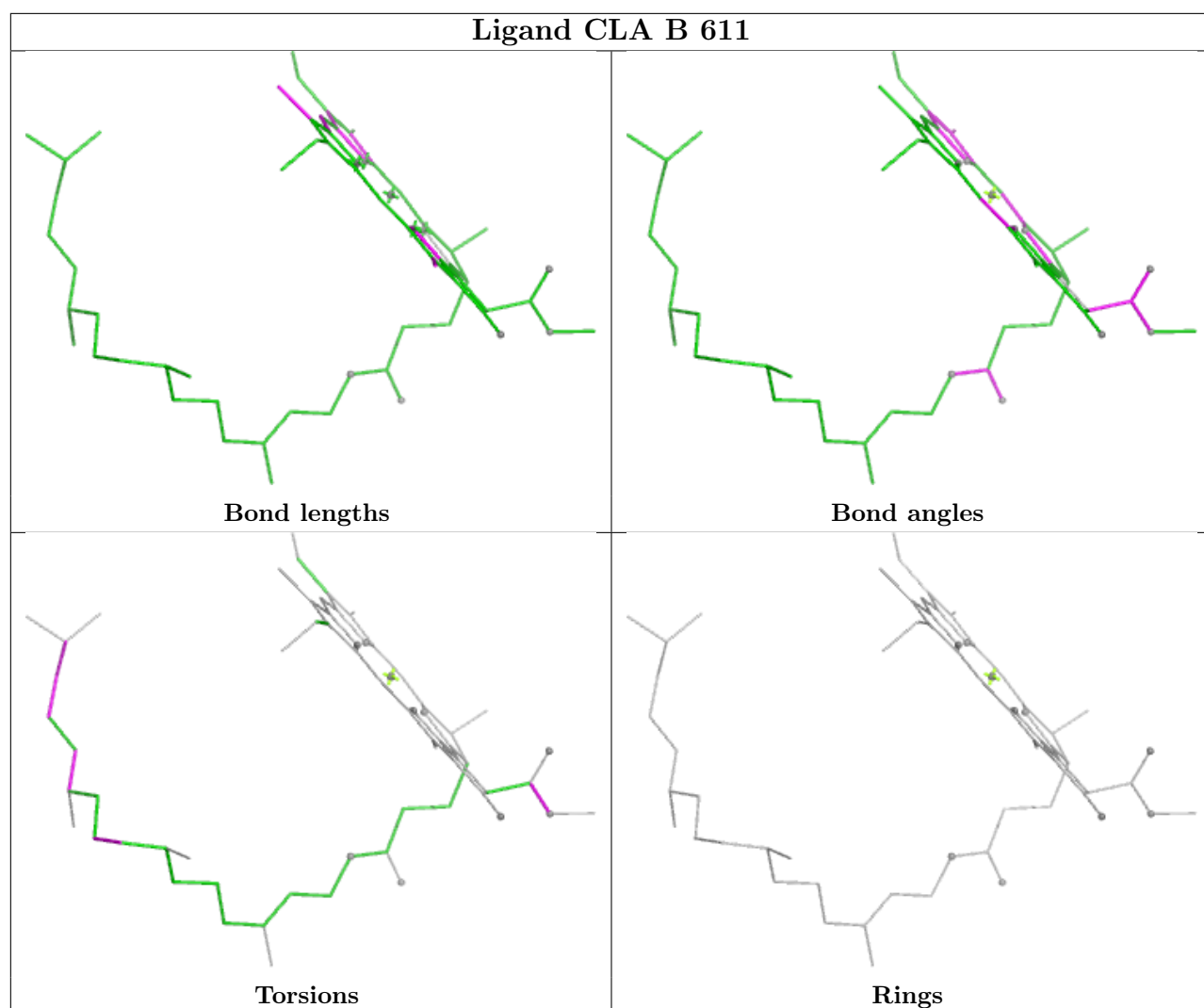
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



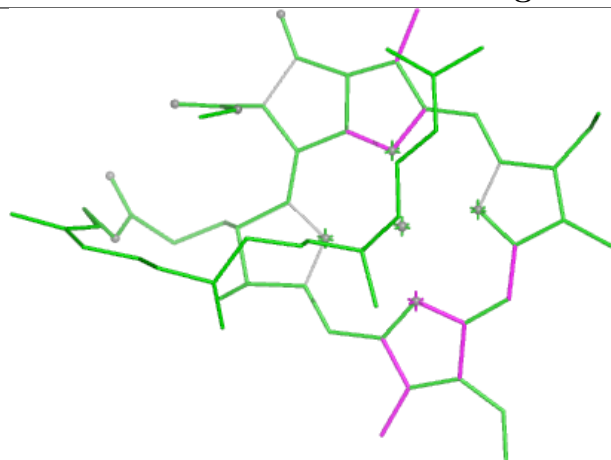




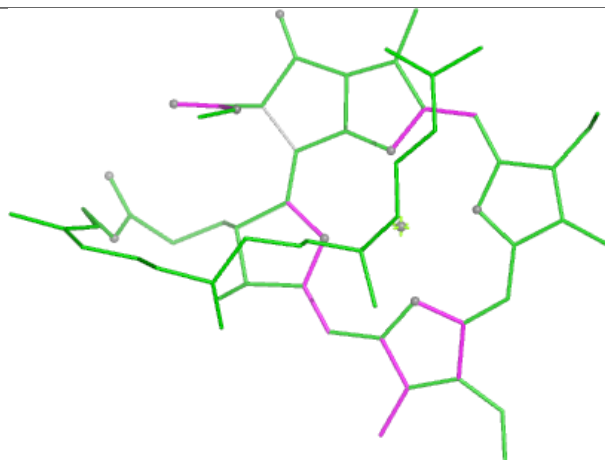




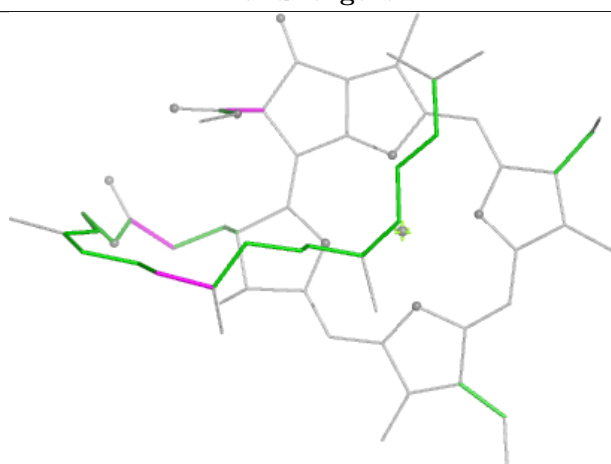
## Ligand CLA C 514



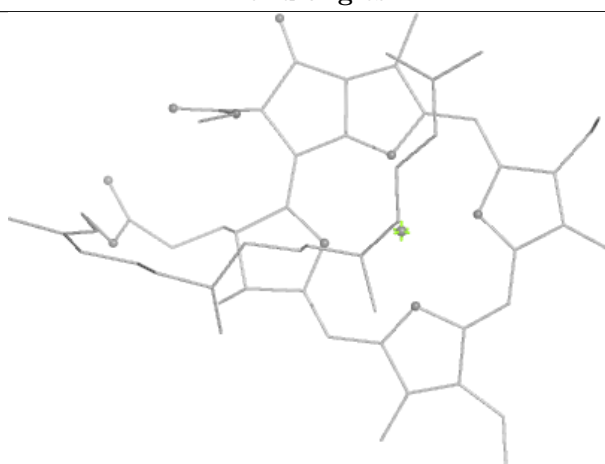
Bond lengths



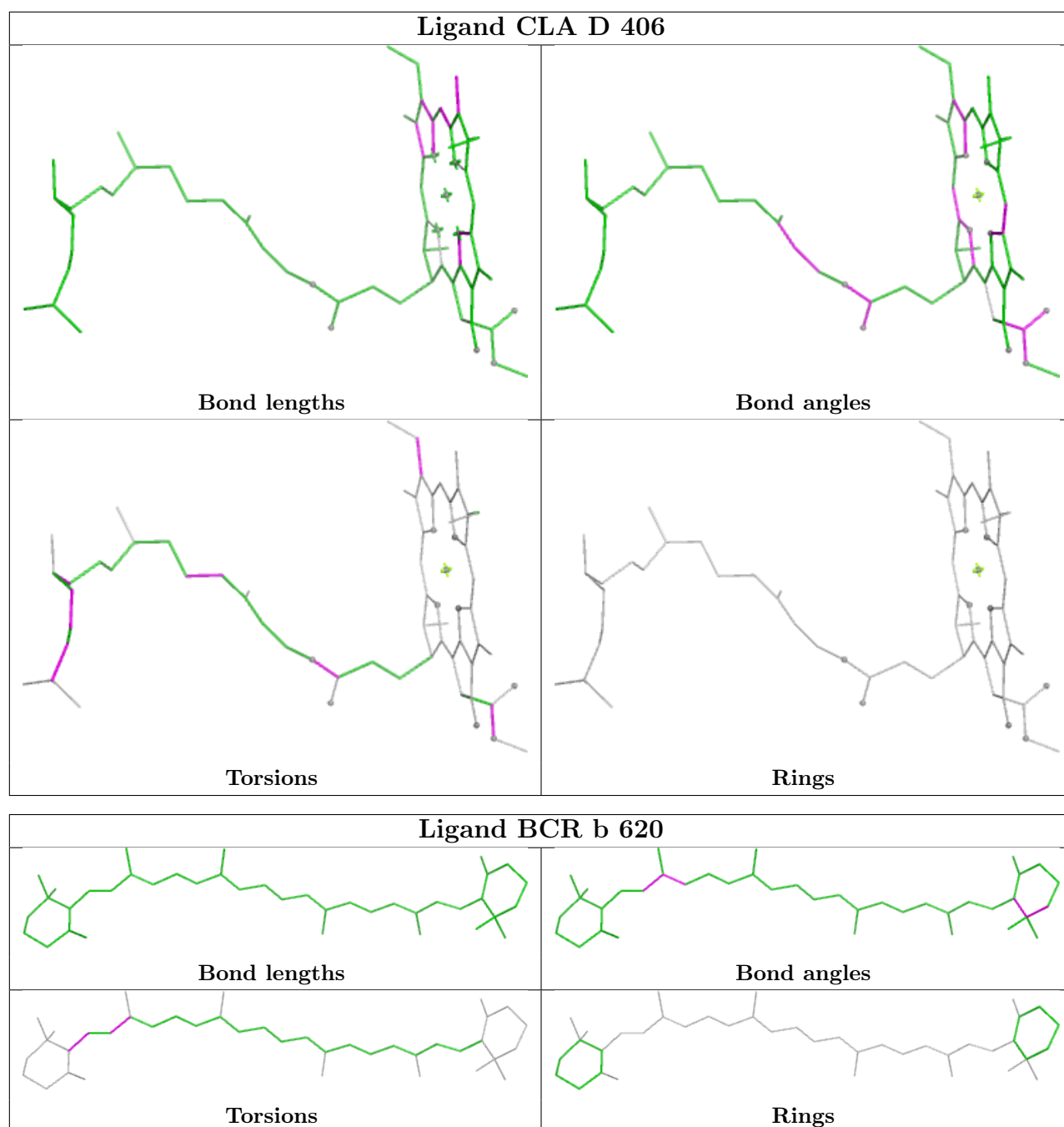
Bond angles

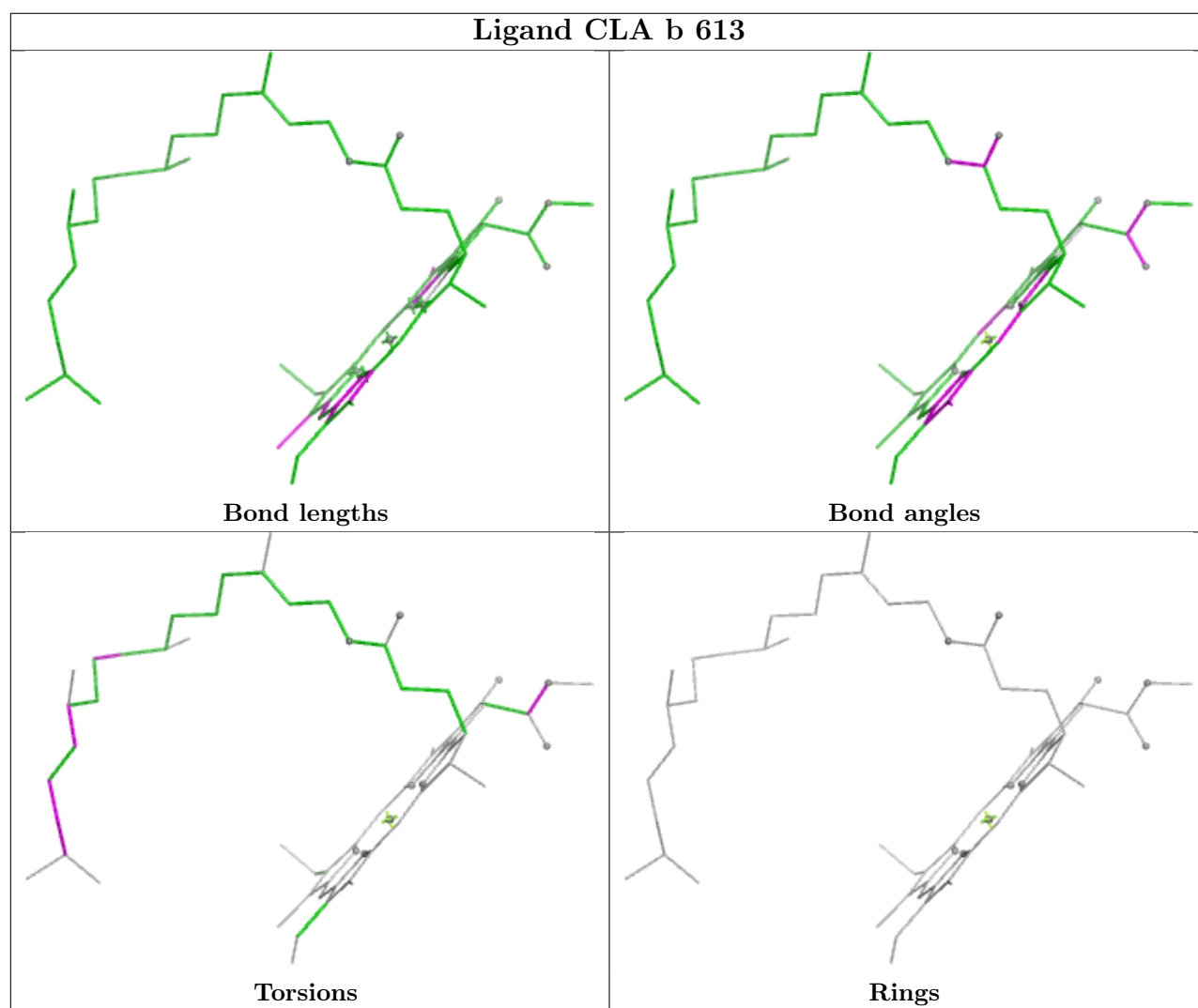
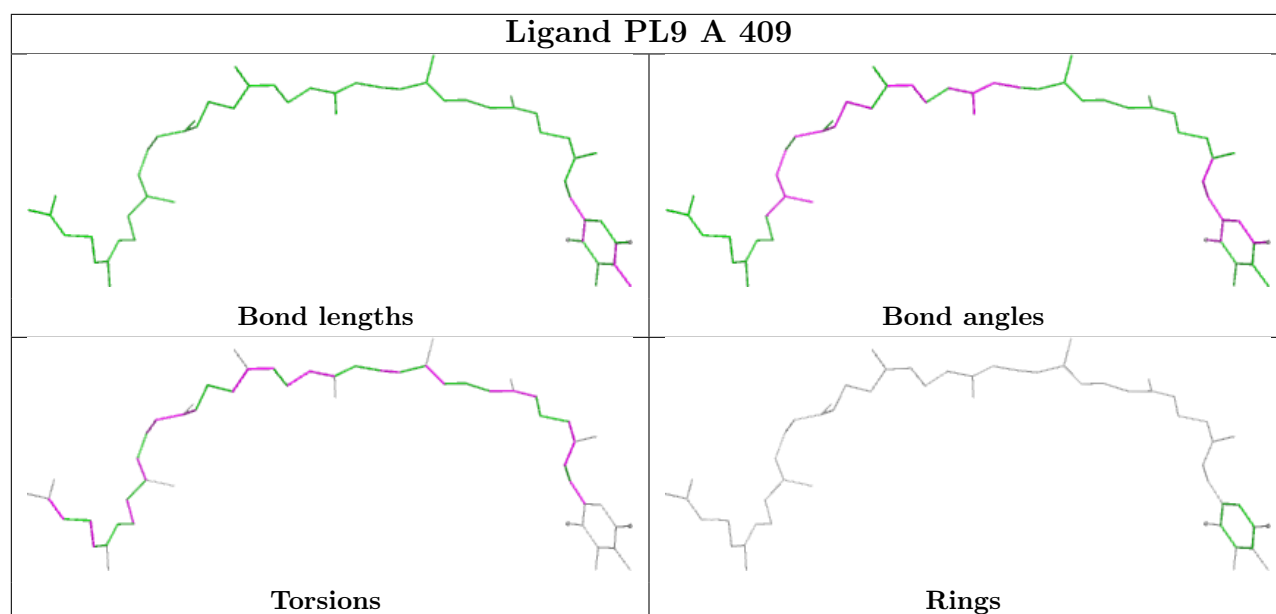


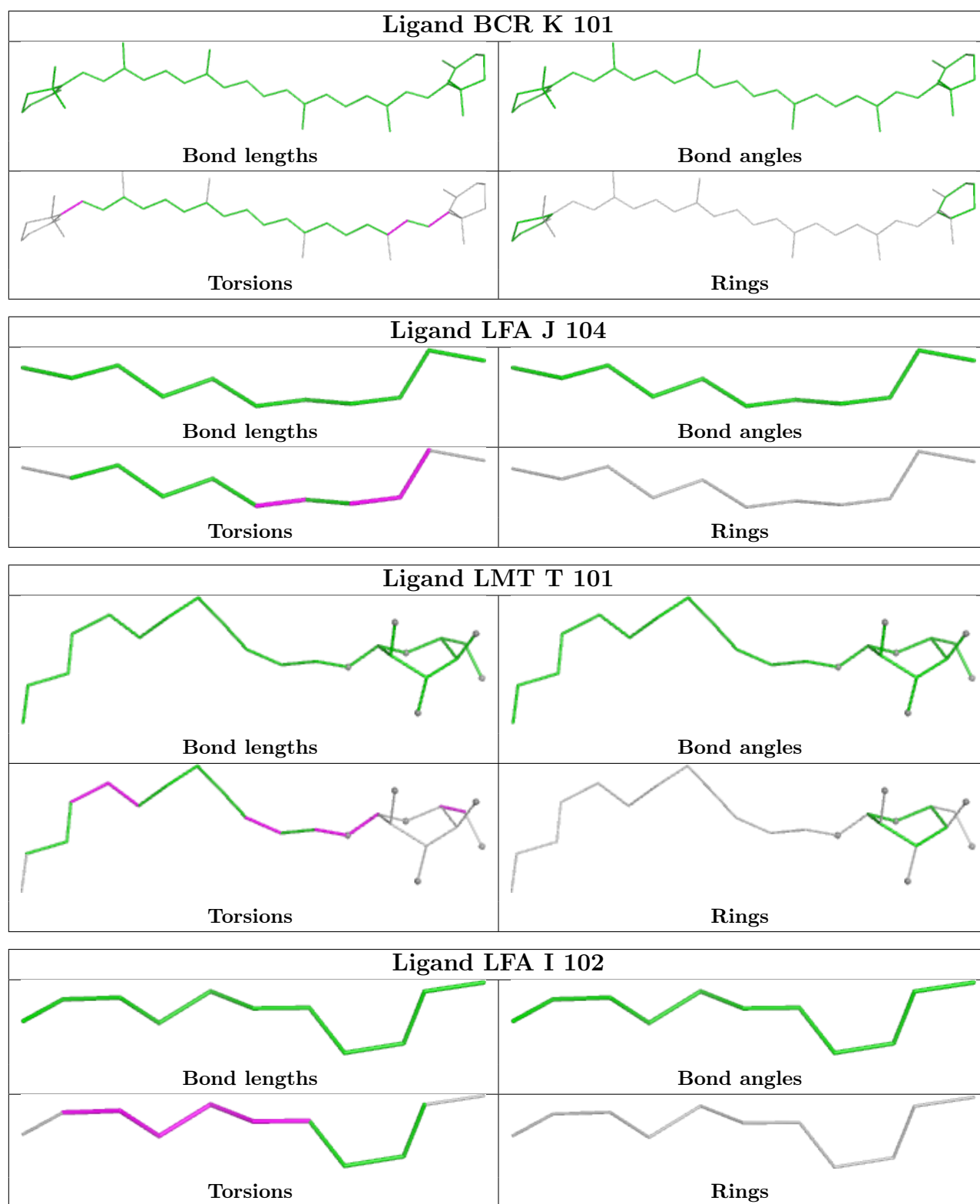
Torsions

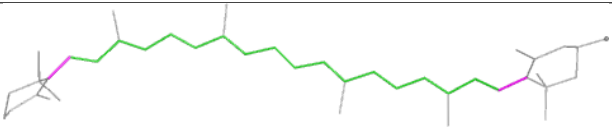
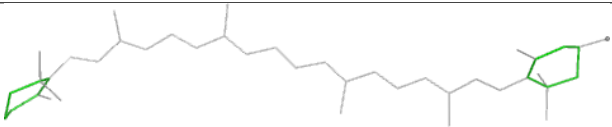
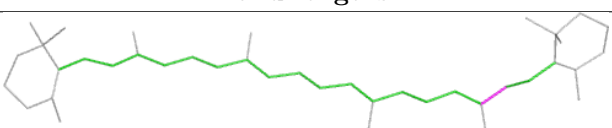
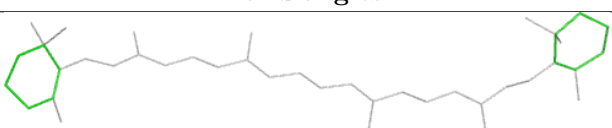
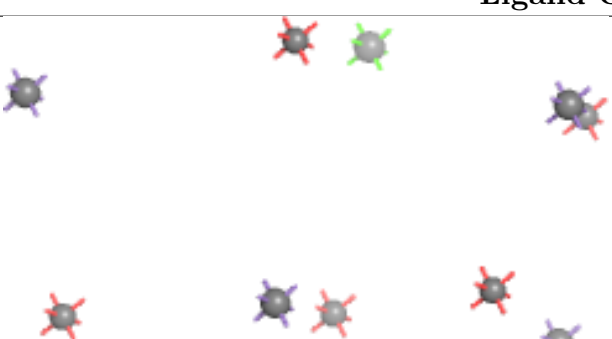
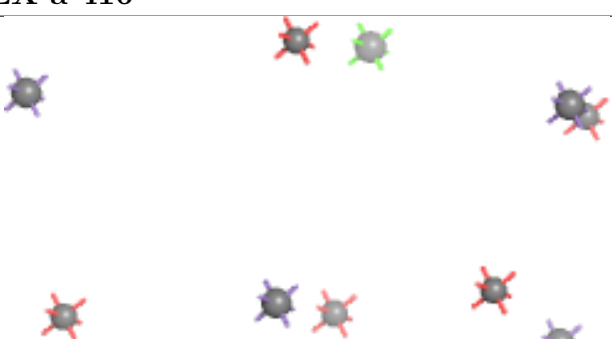
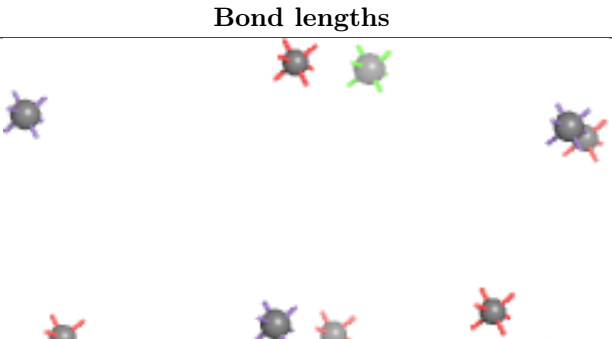
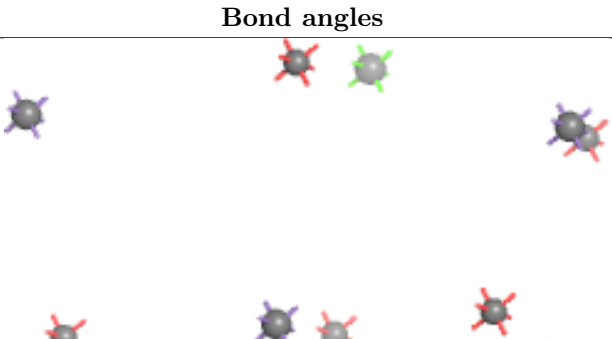


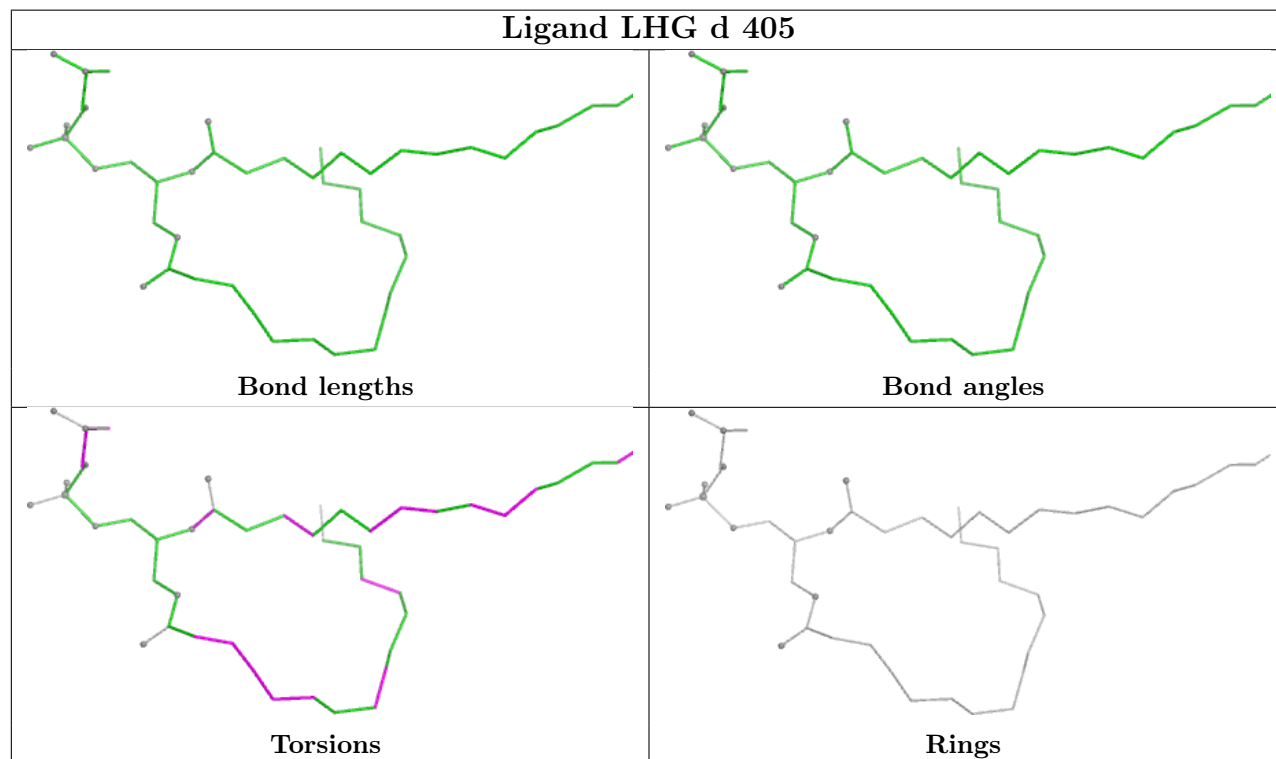
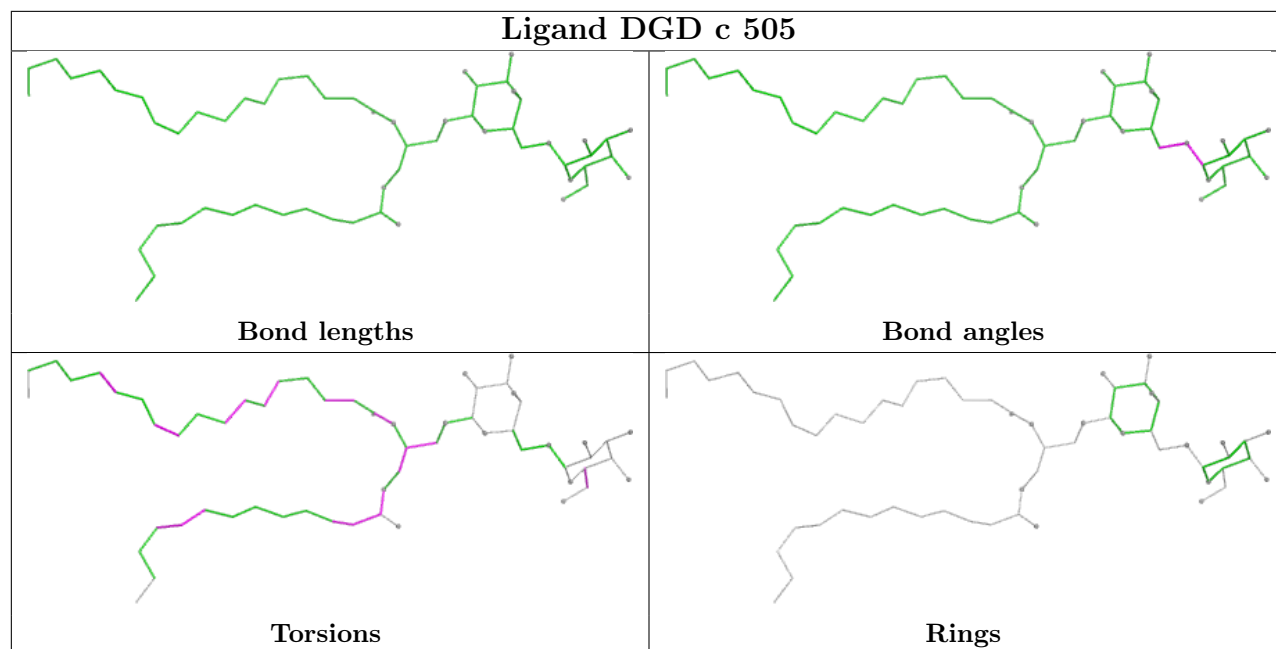
Rings

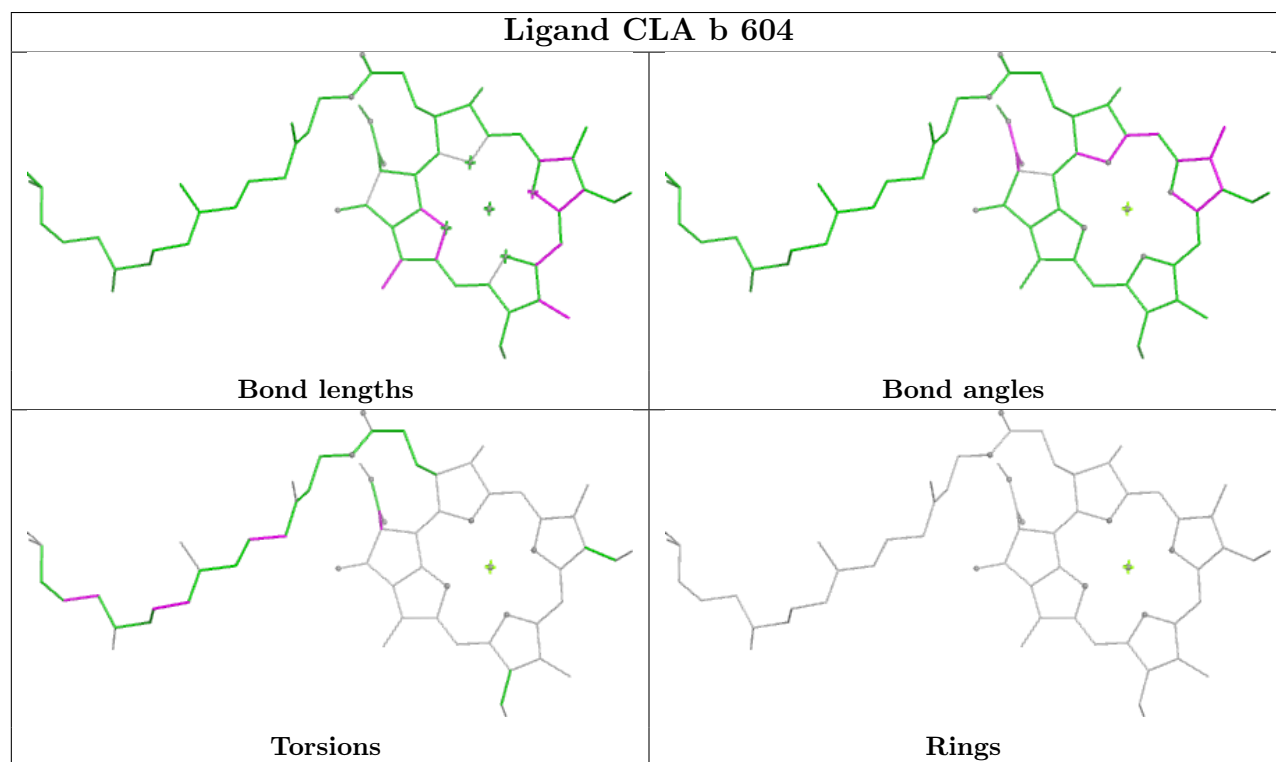
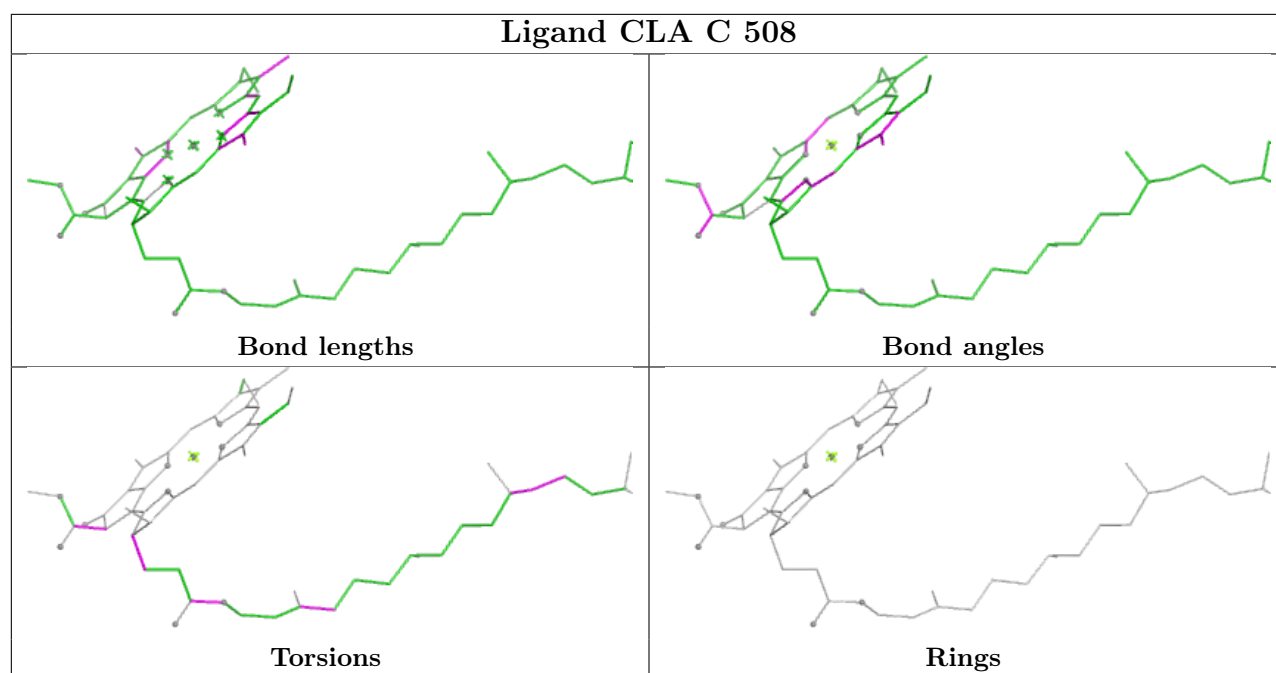




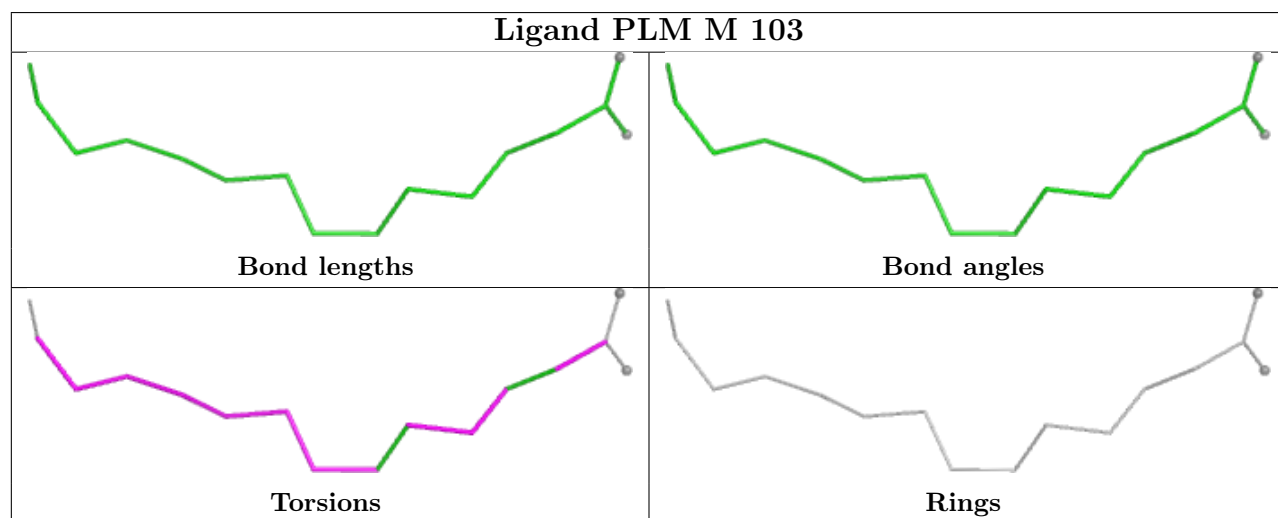
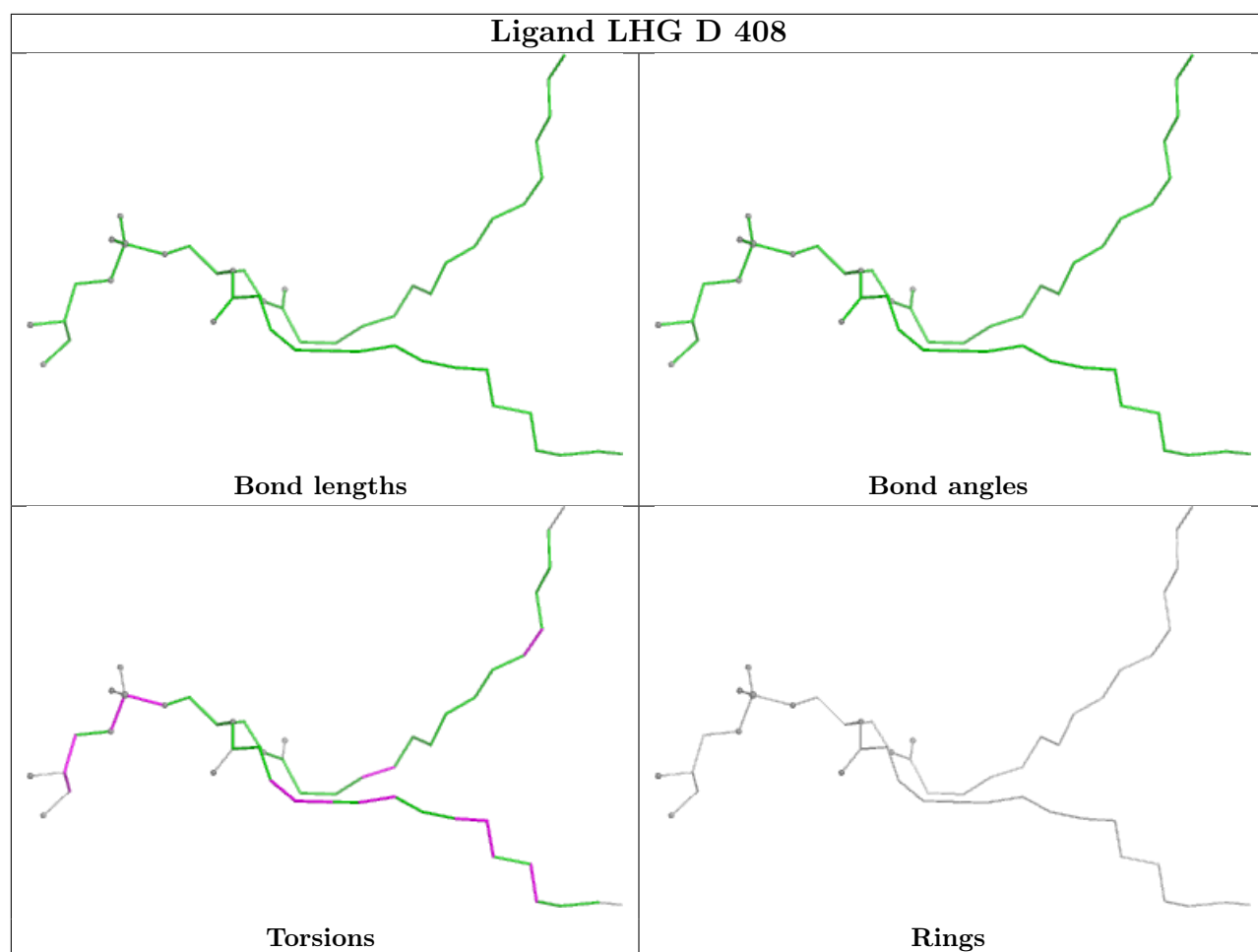


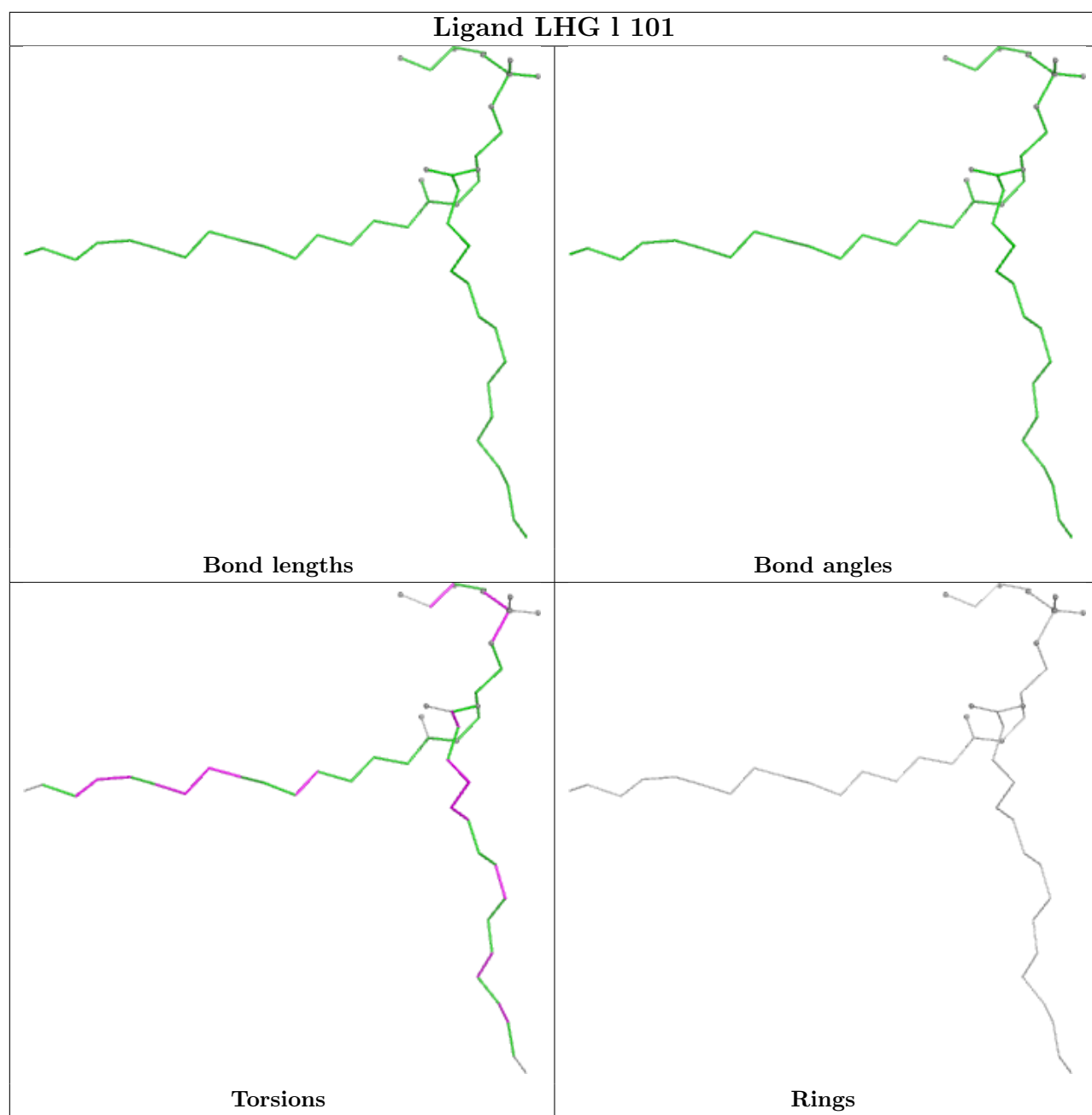
| Ligand RRX h 102                                                                                       |                                                                                                        |
|--------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand BCR B 619                                                                                       |                                                                                                        |
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand OEX a 416                                                                                       |                                                                                                        |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |

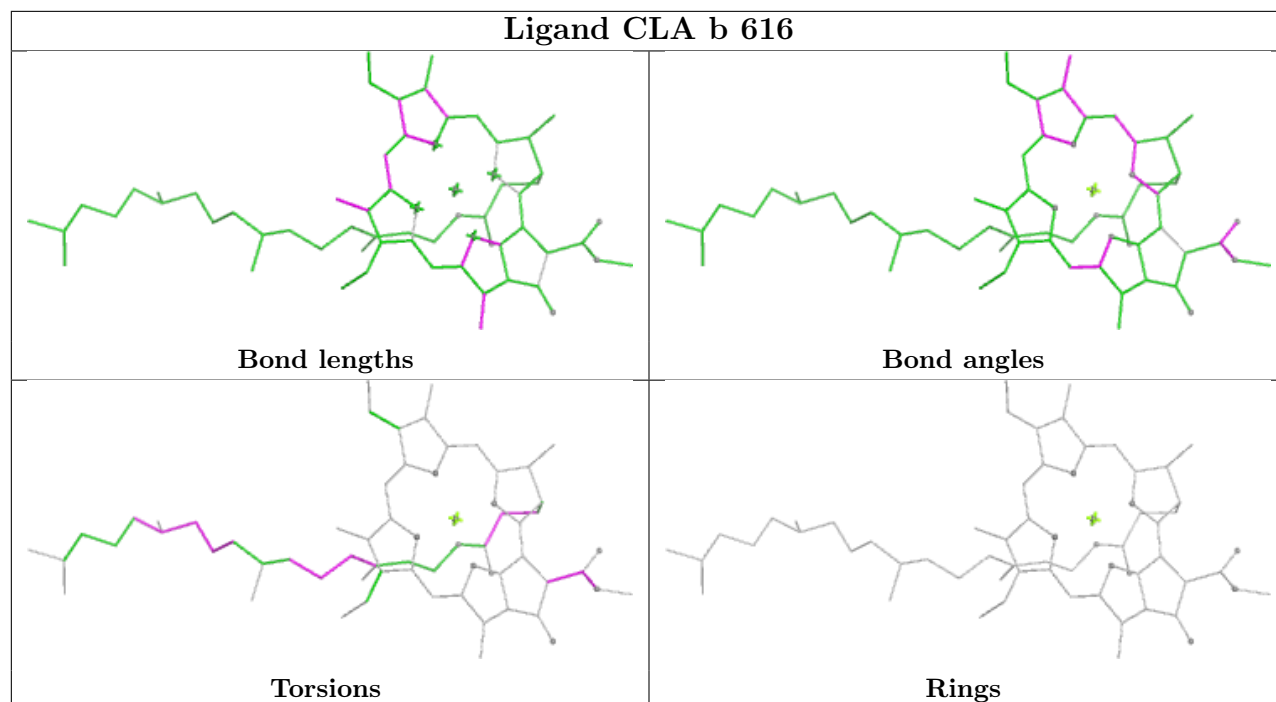
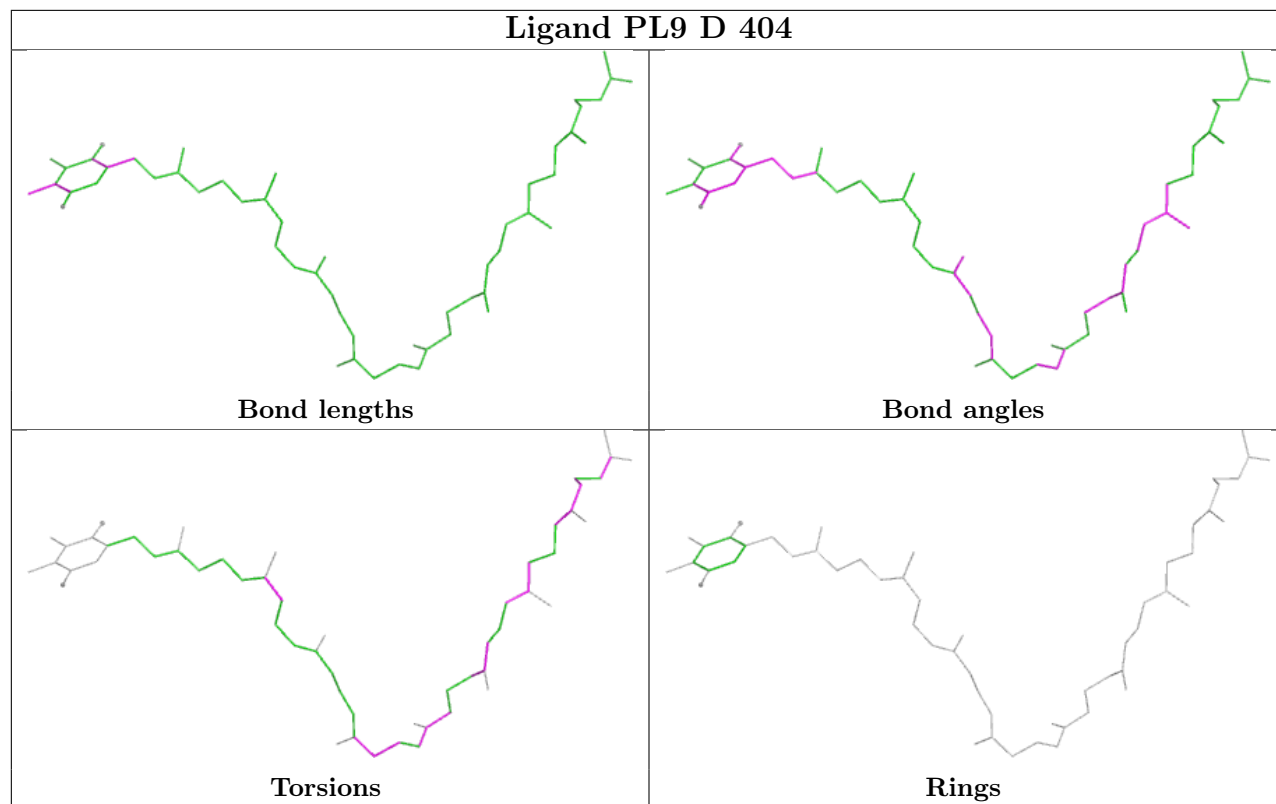


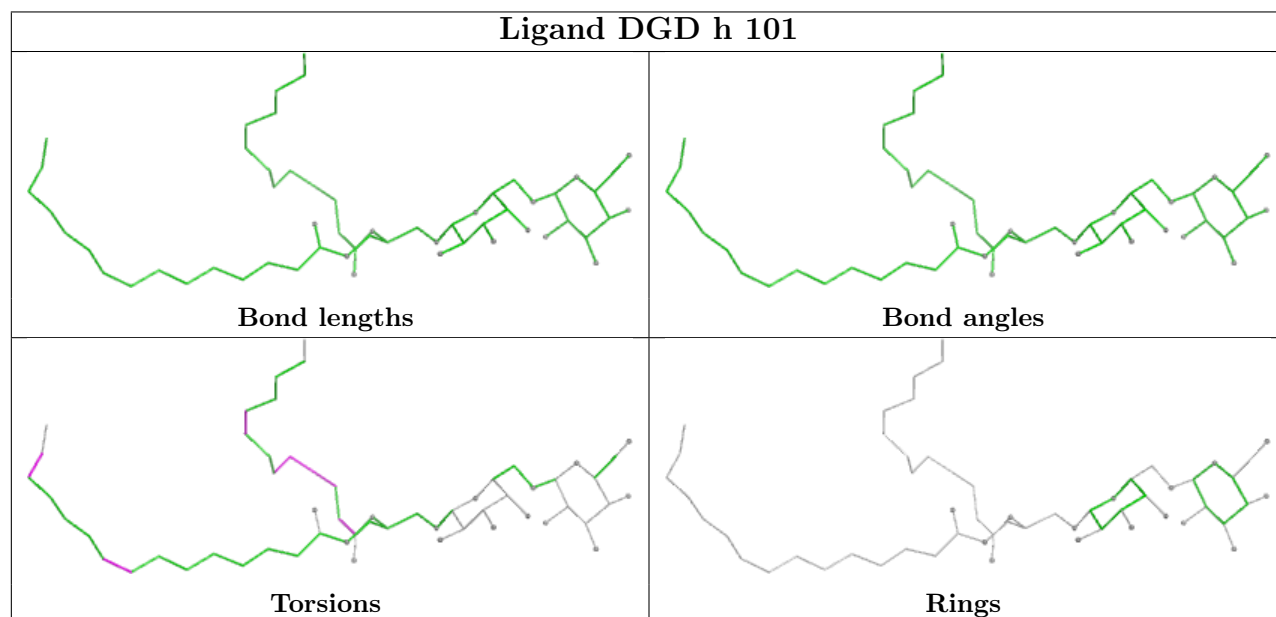
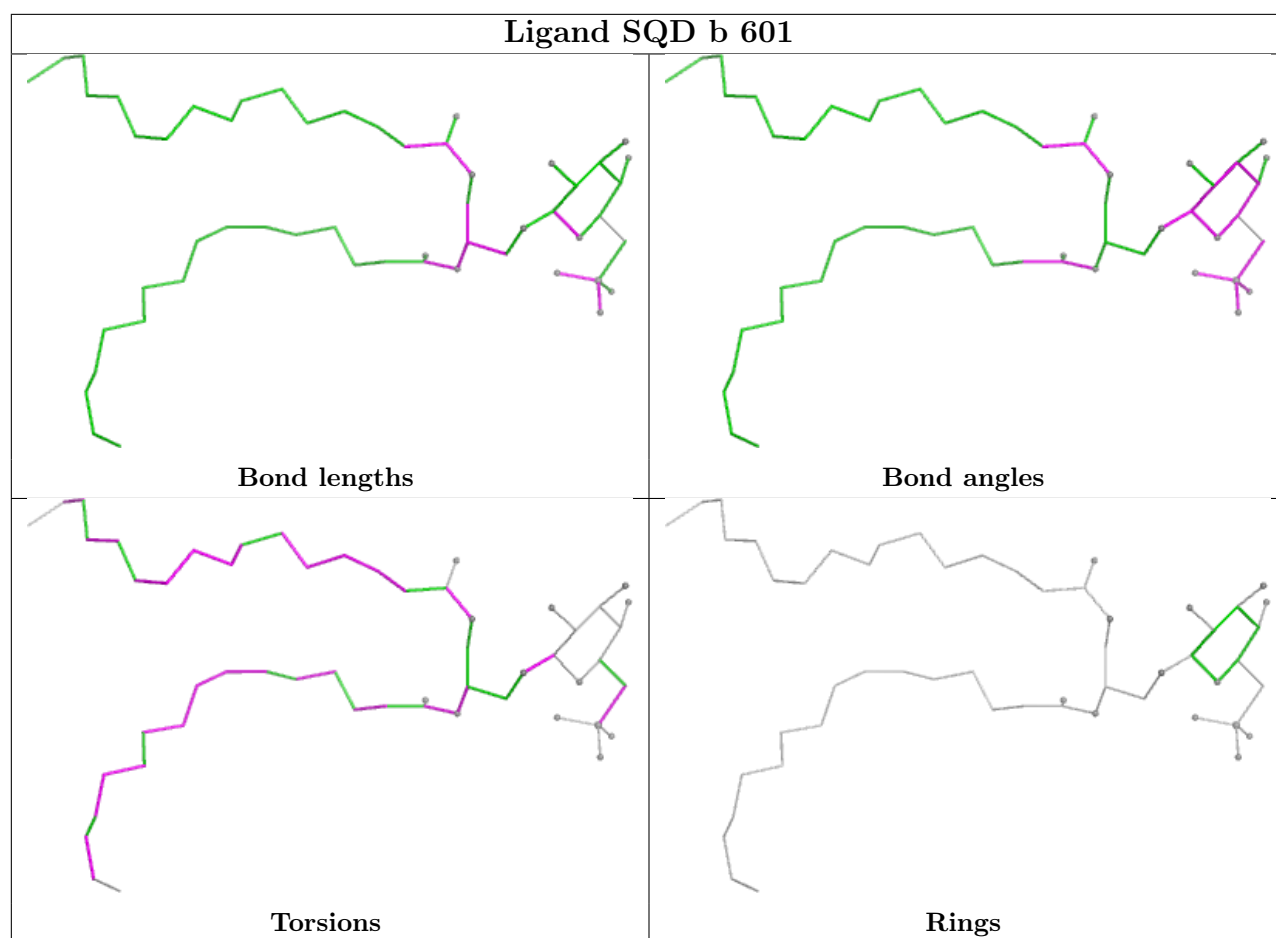




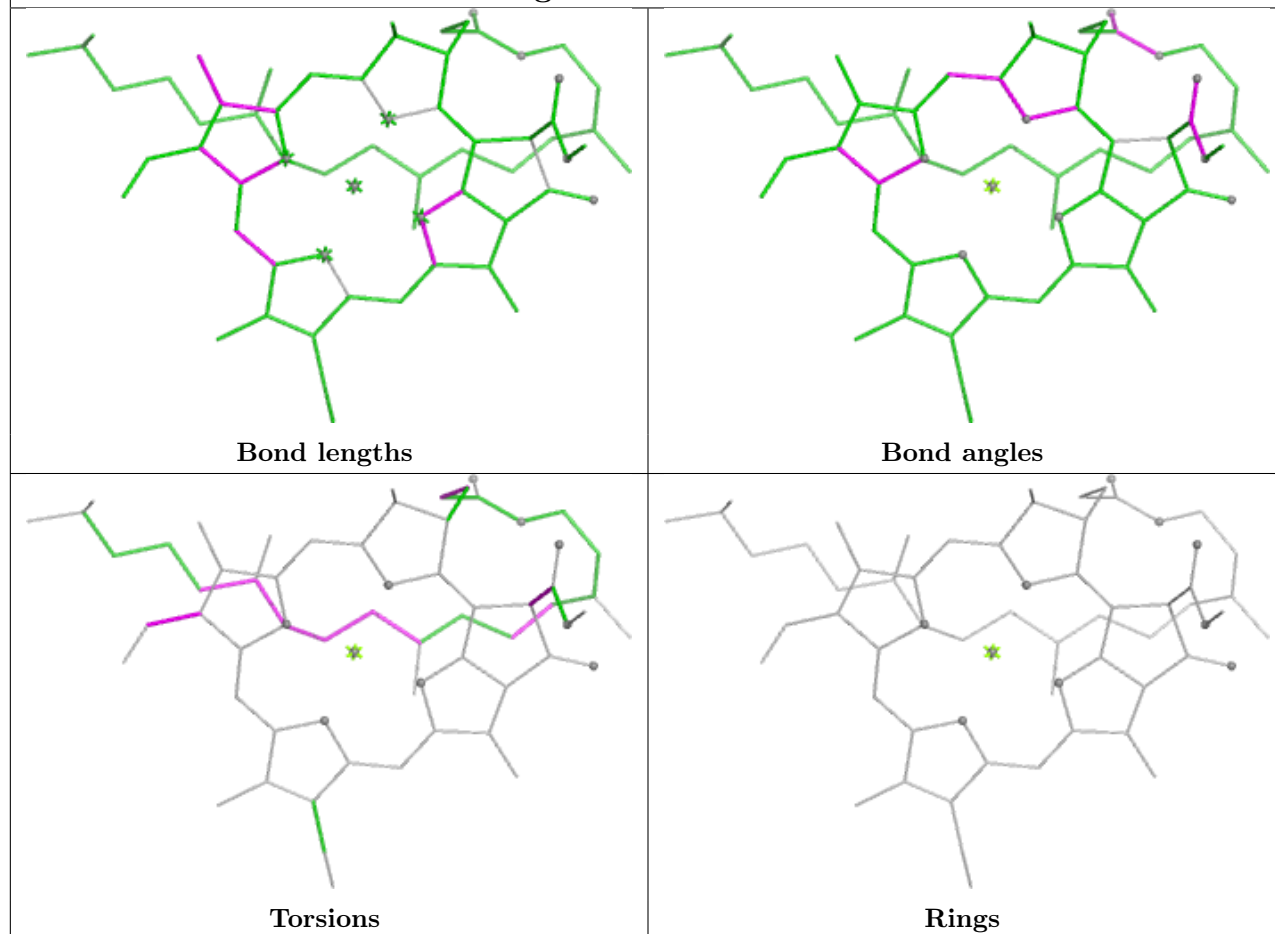




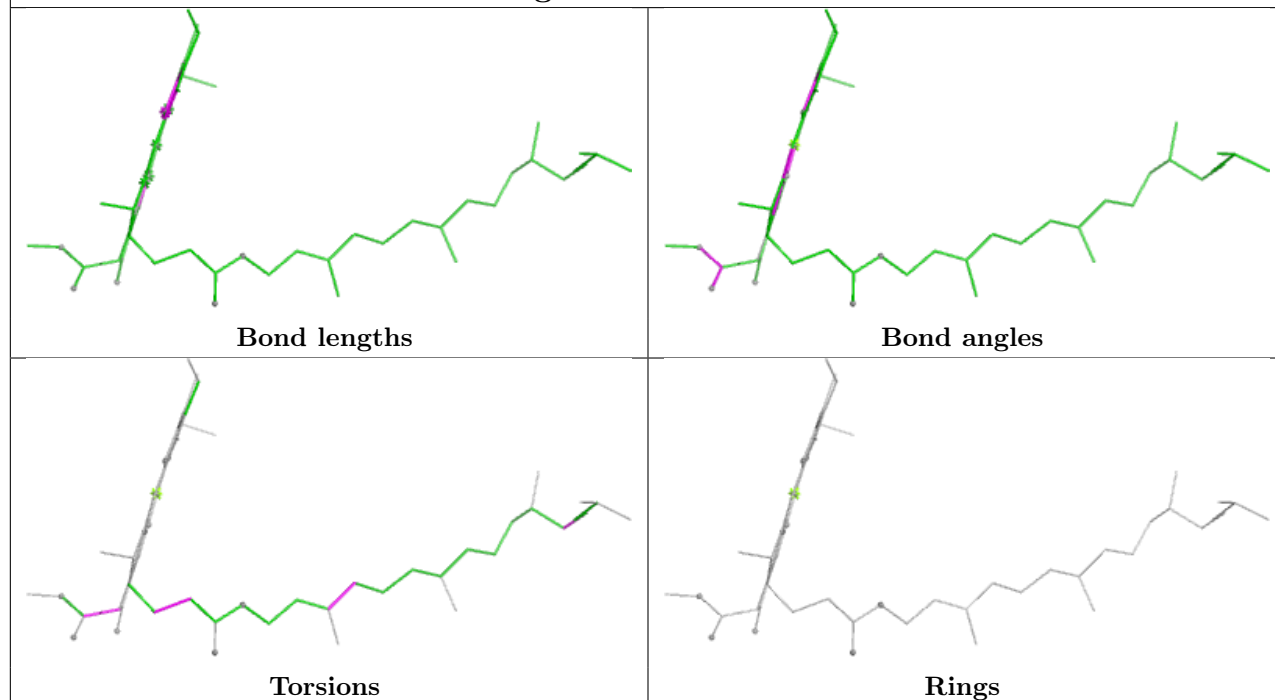
**Ligand CLA b 616****Ligand PL9 D 404**

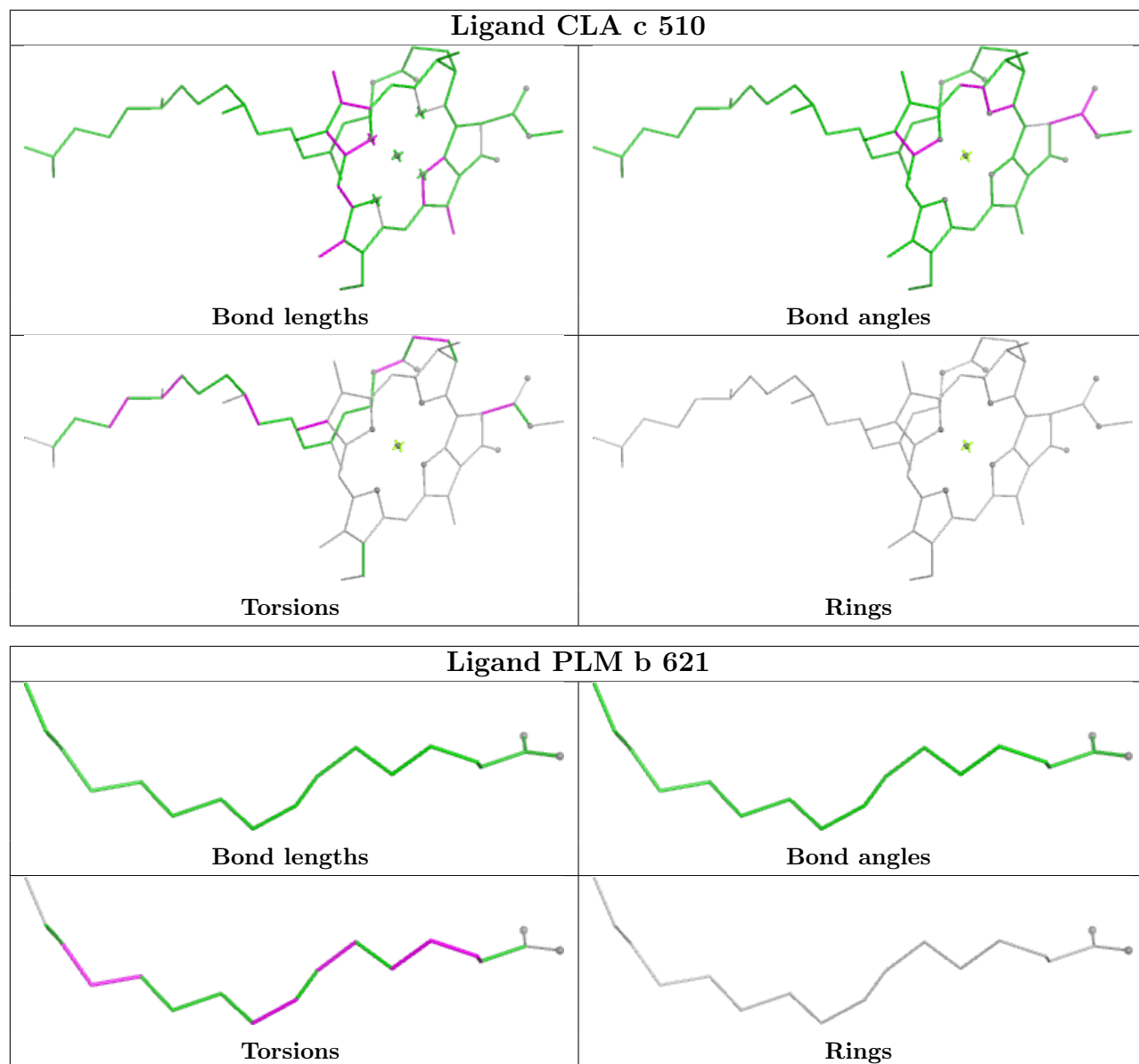


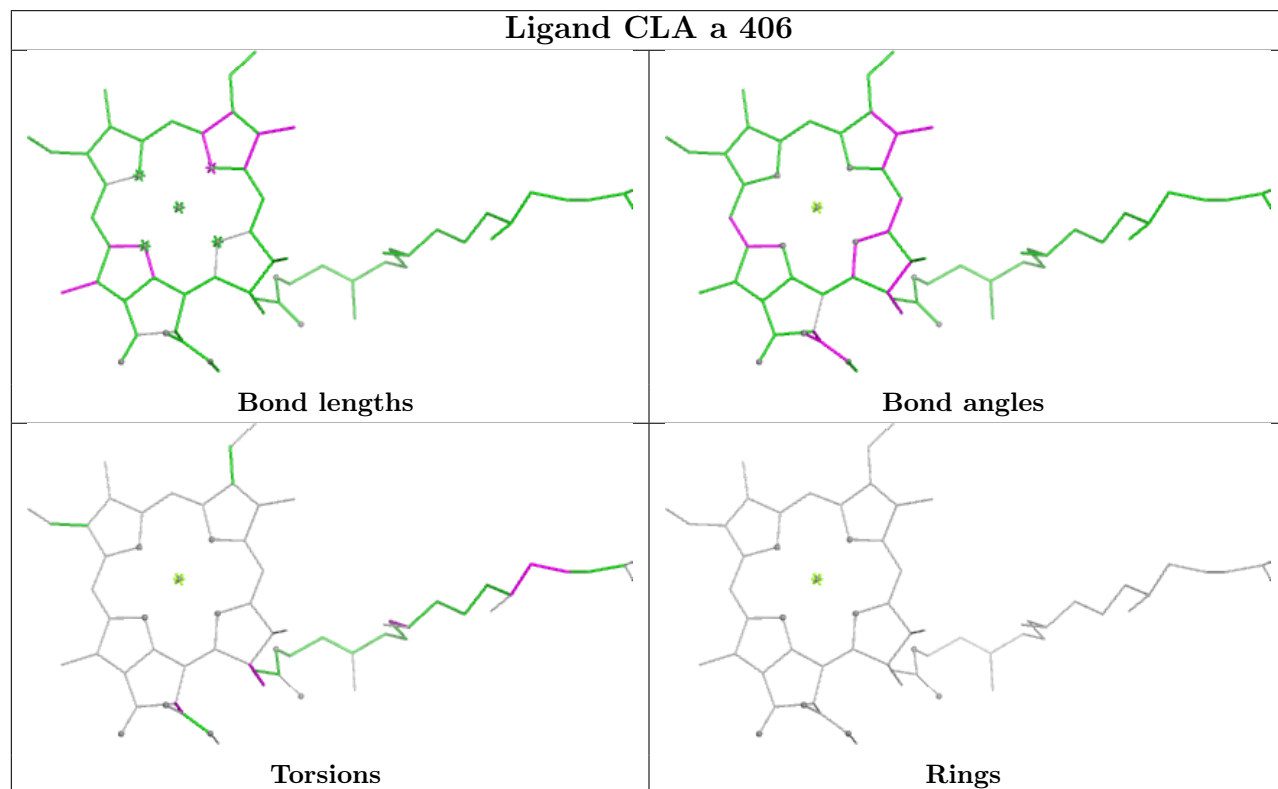
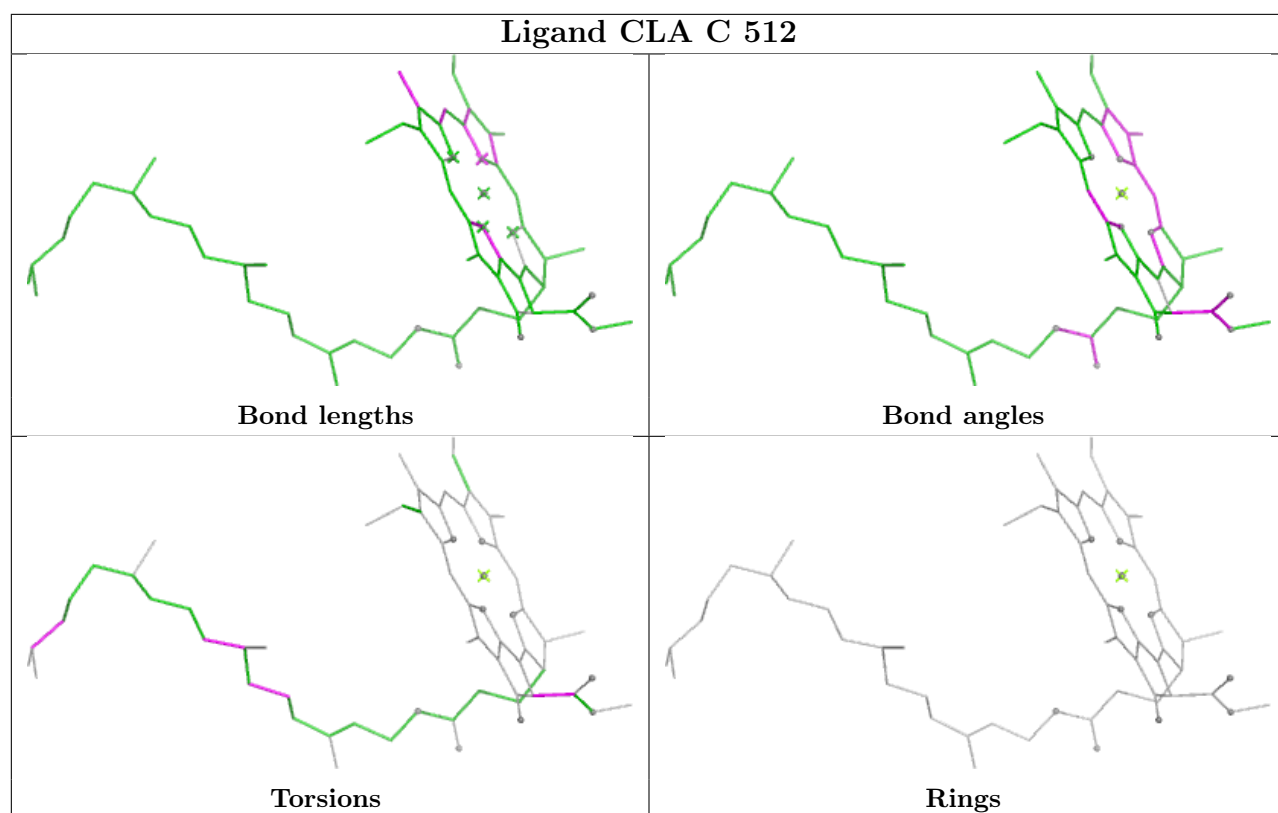
## Ligand CLA b 603

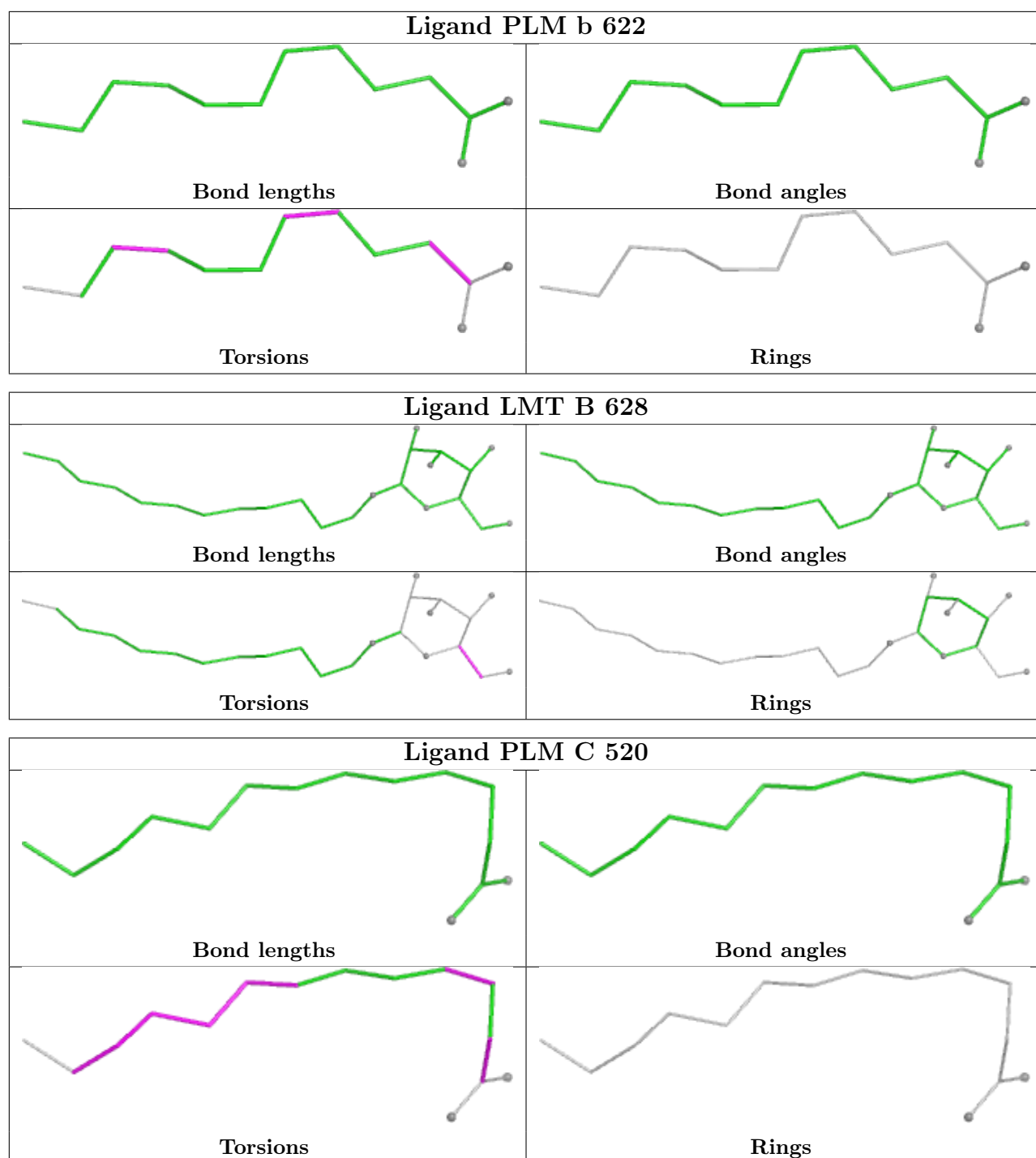


## Ligand CLA b 607

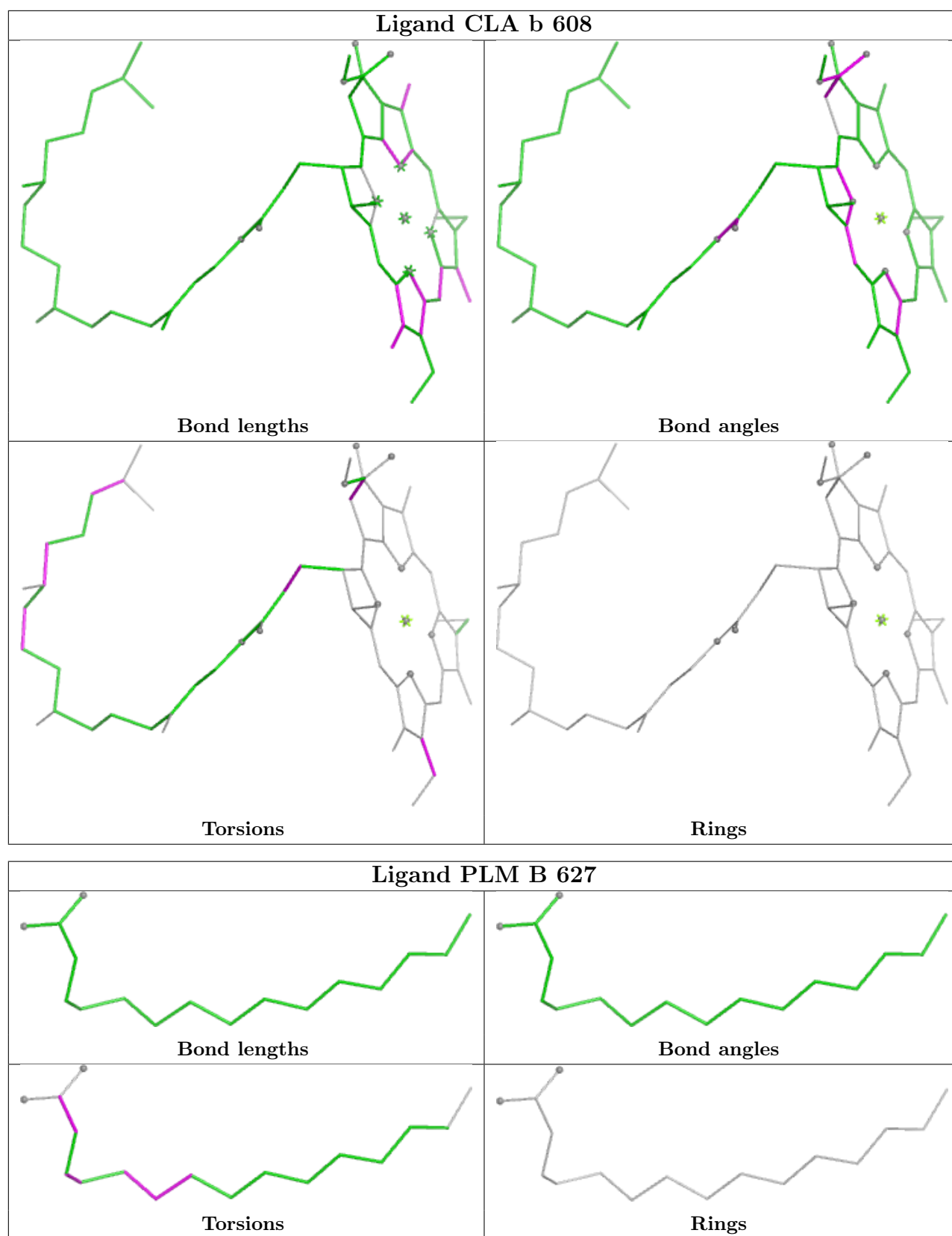


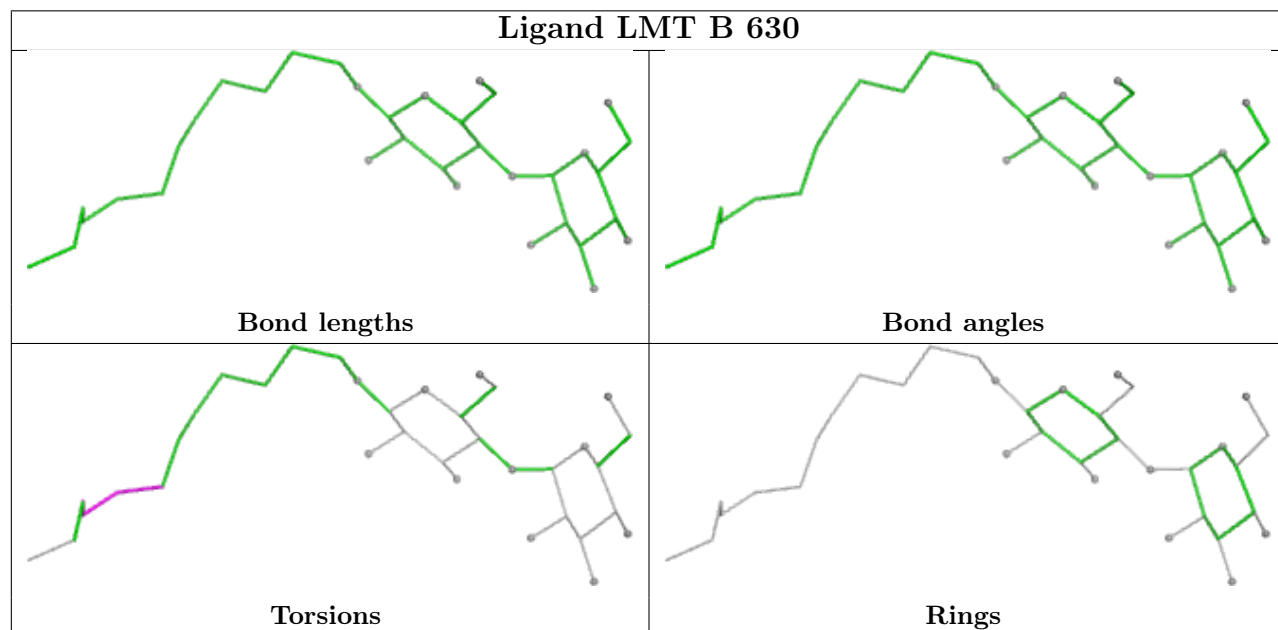
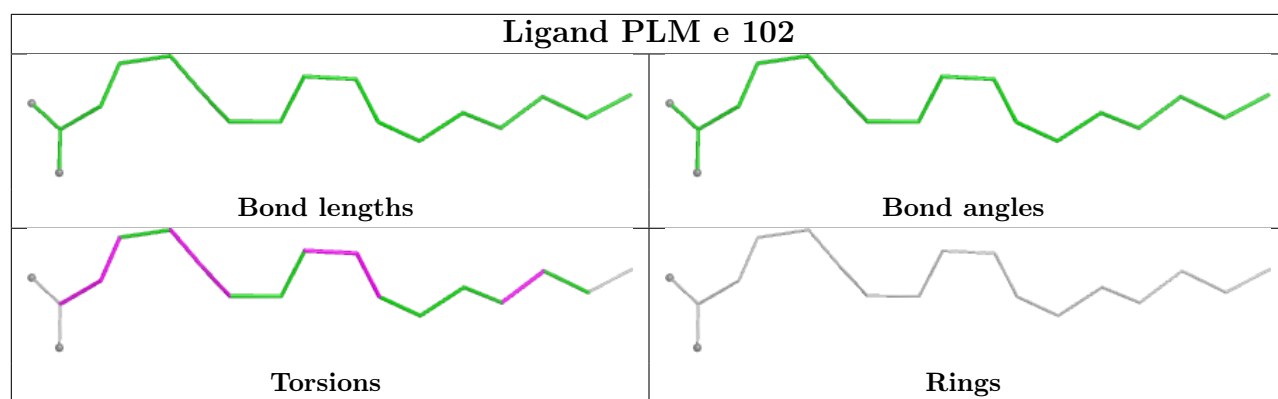


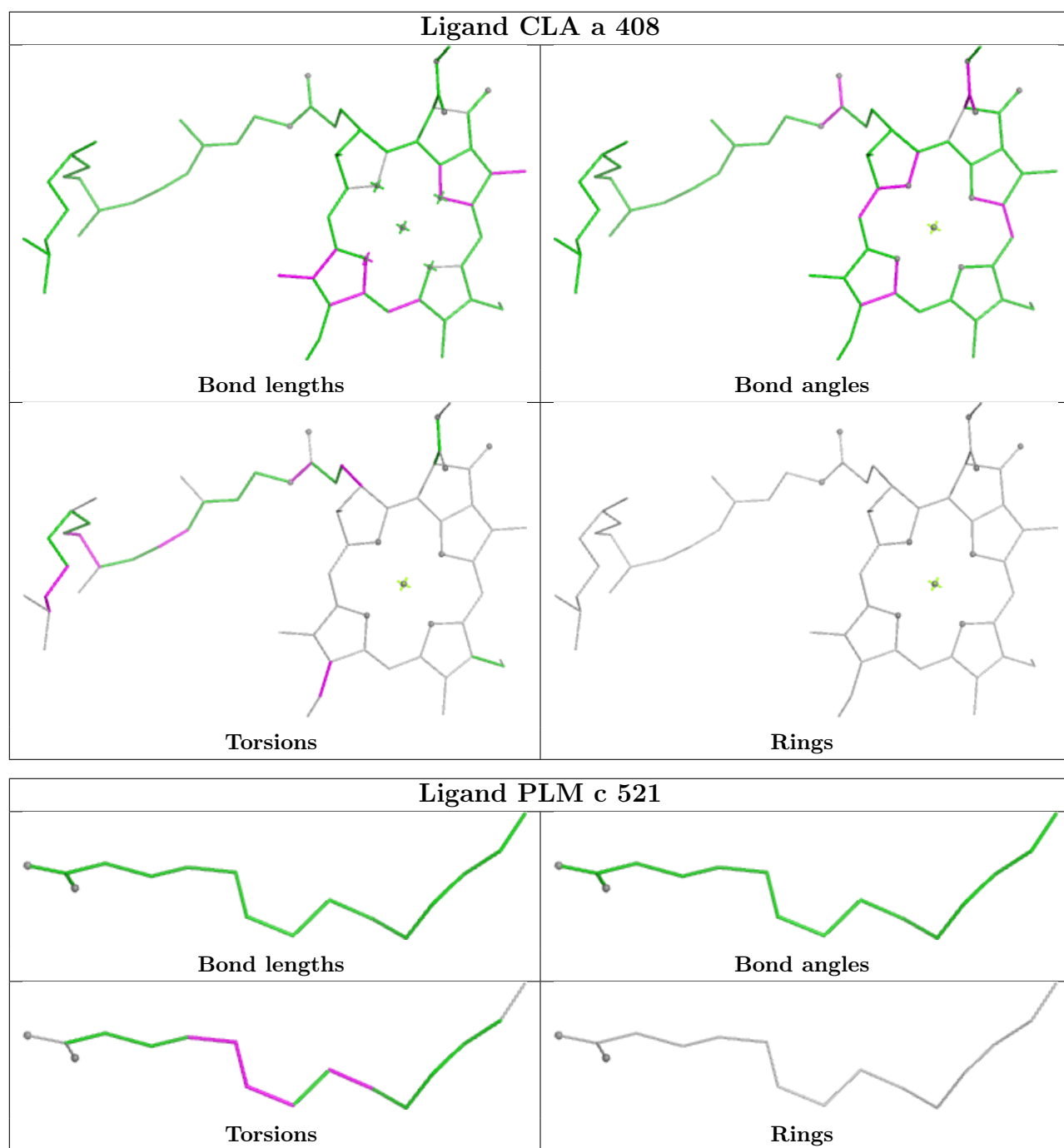


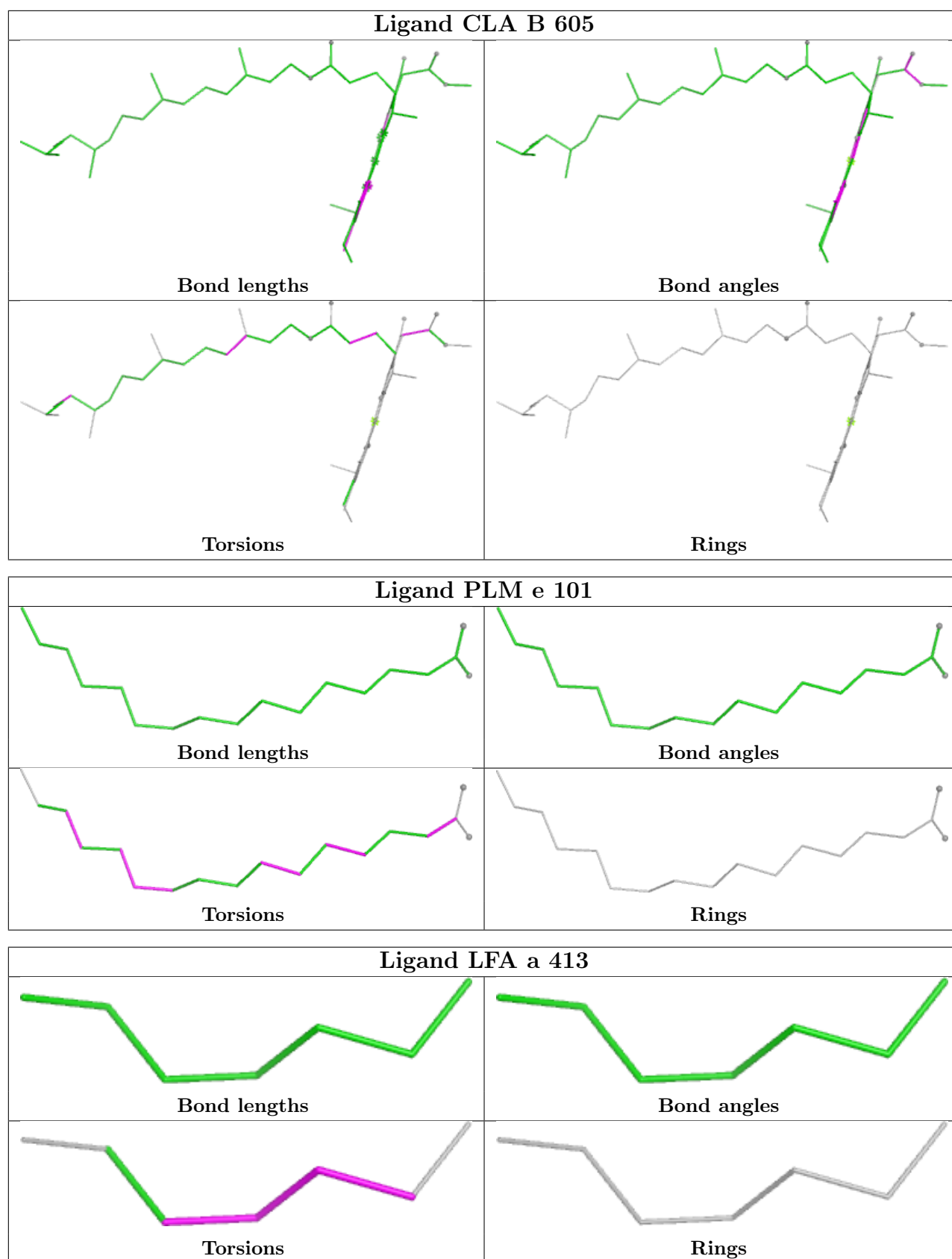


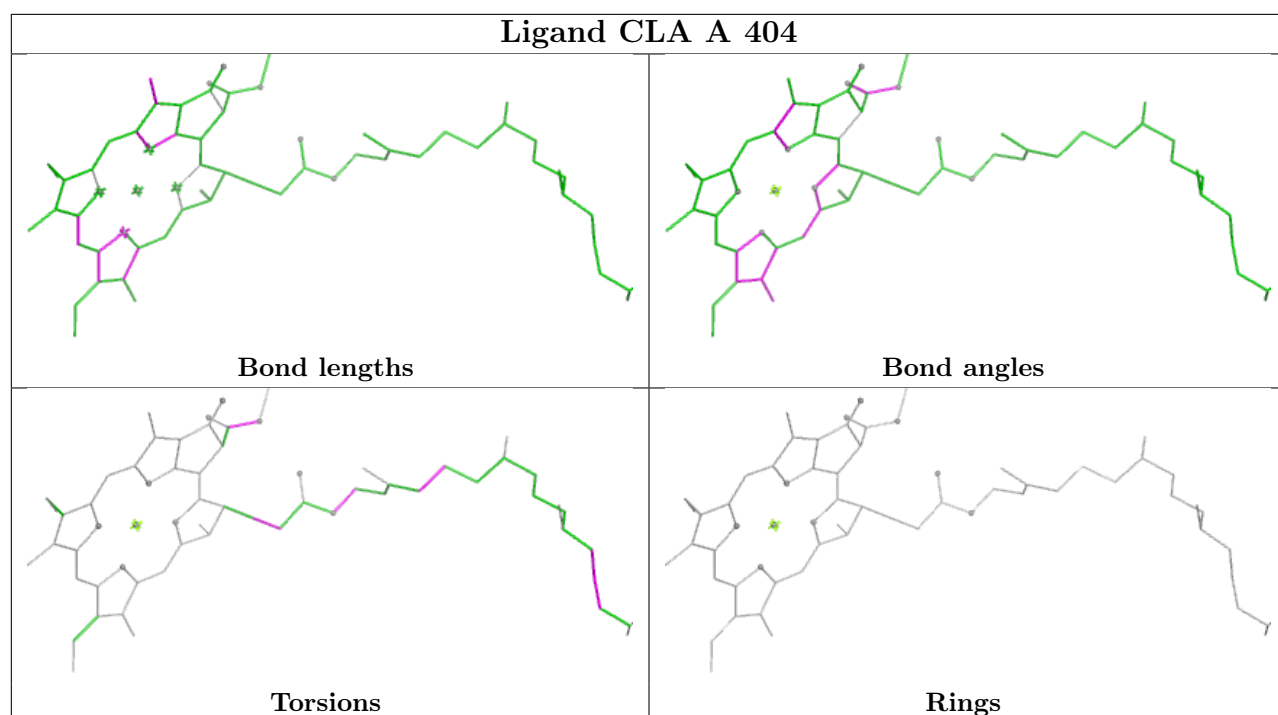


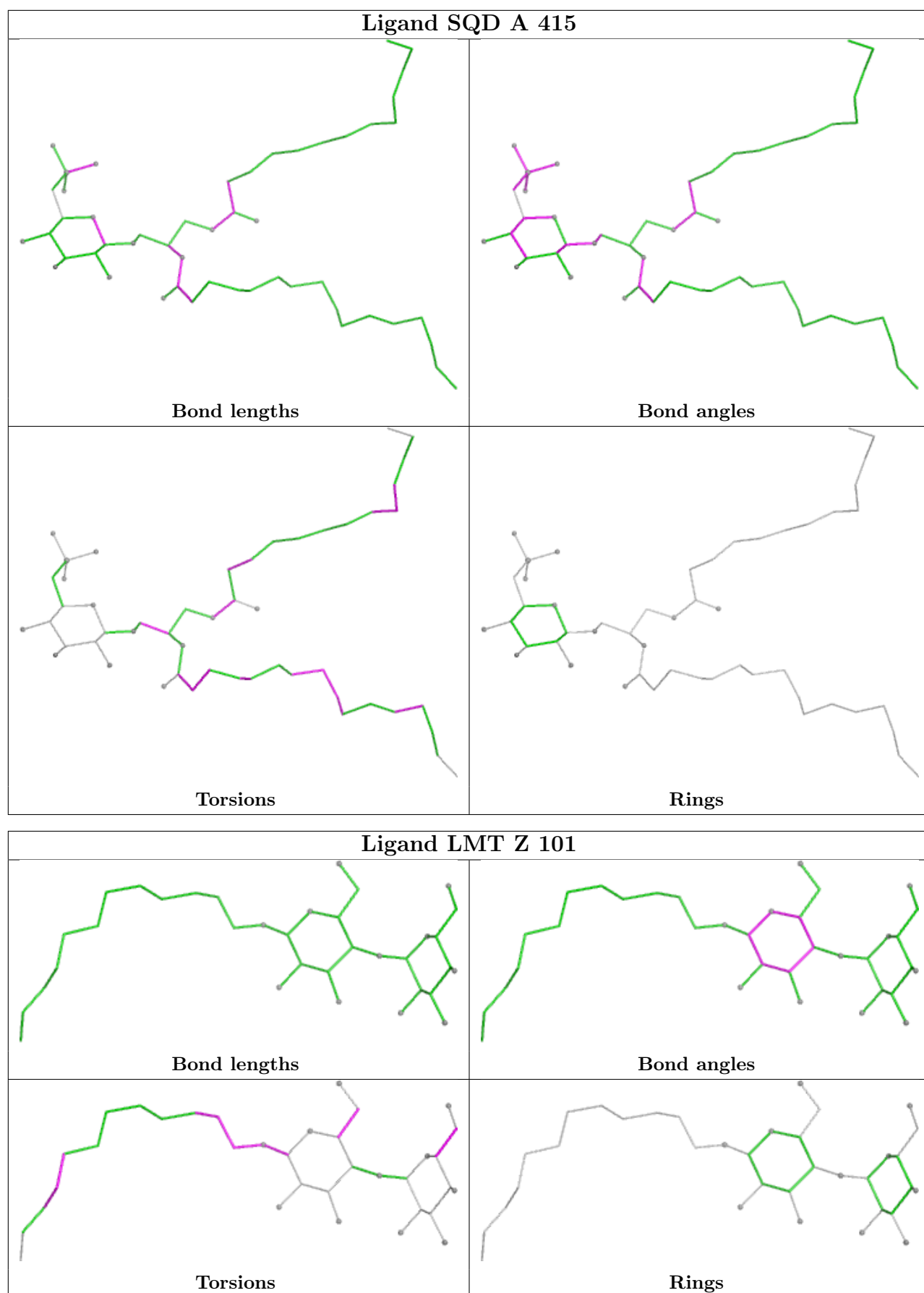


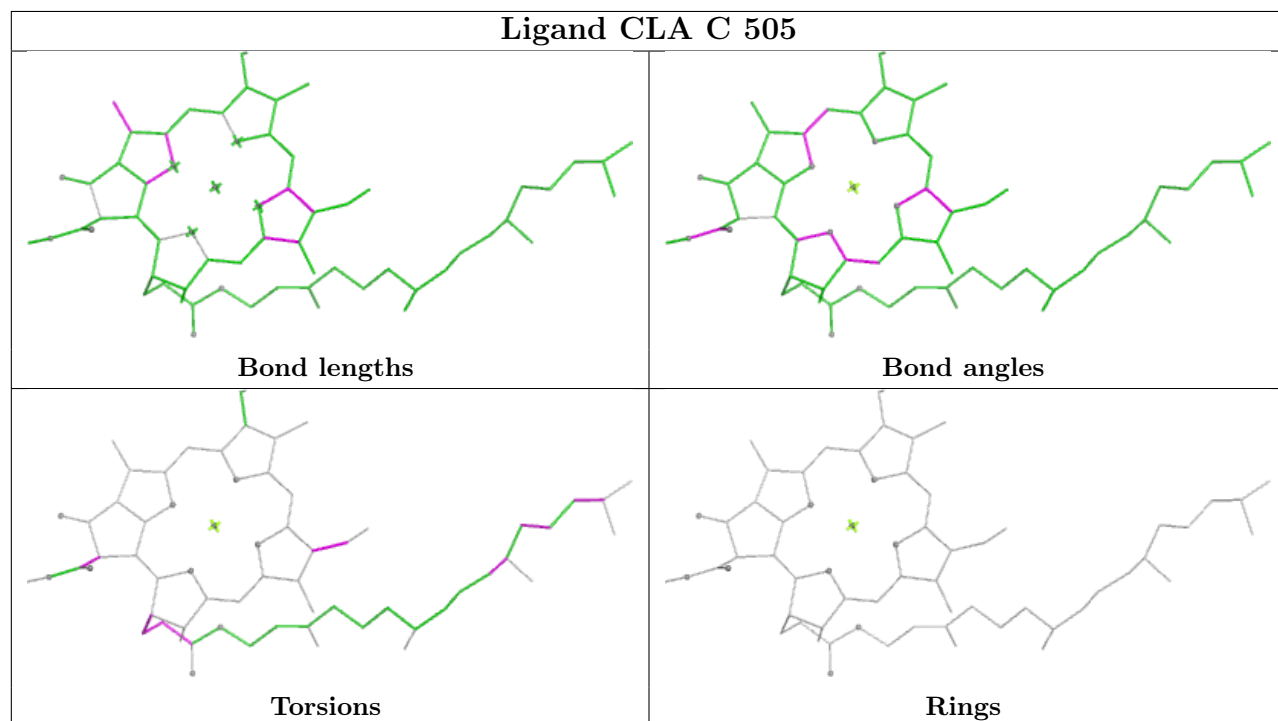
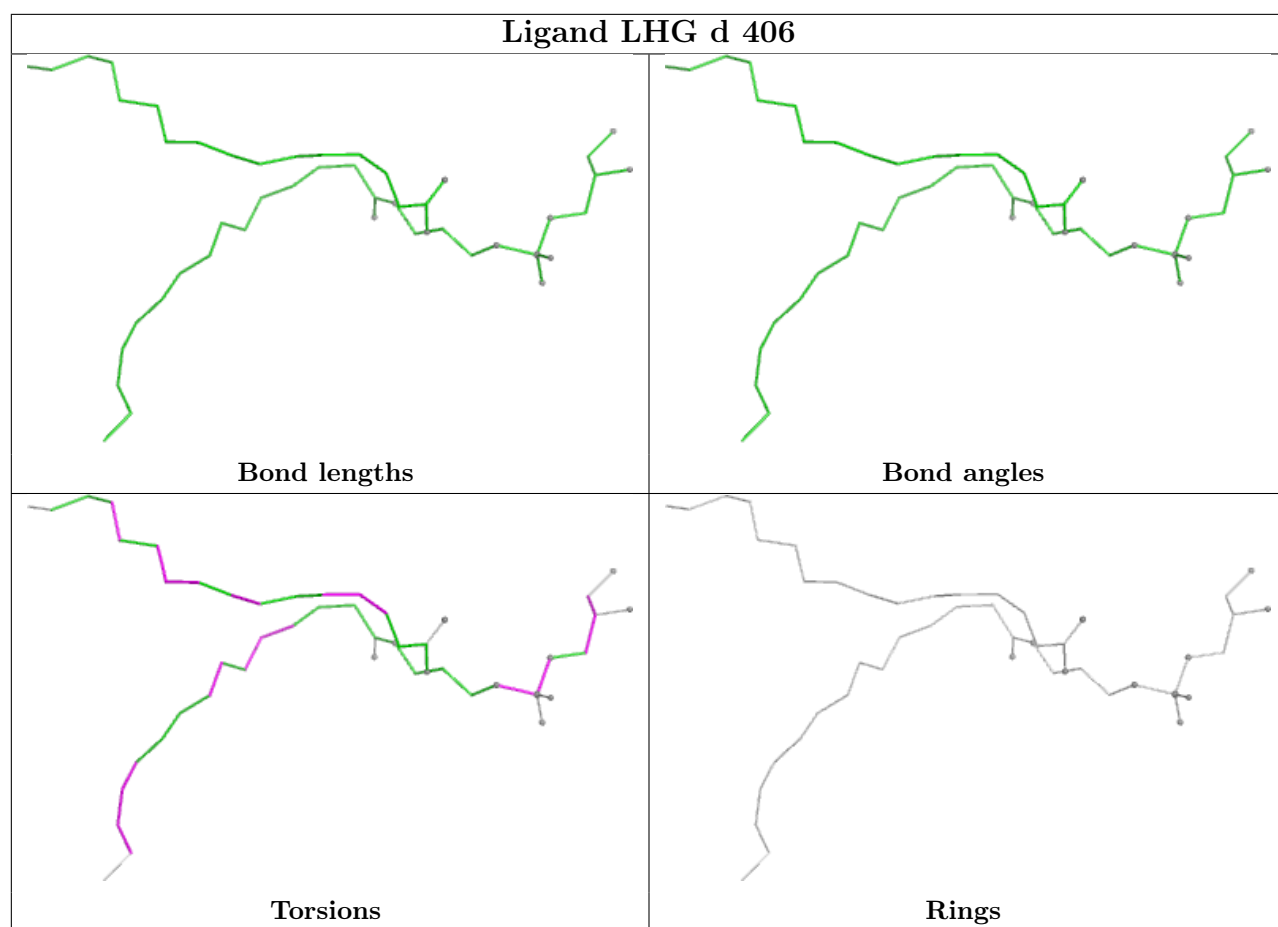


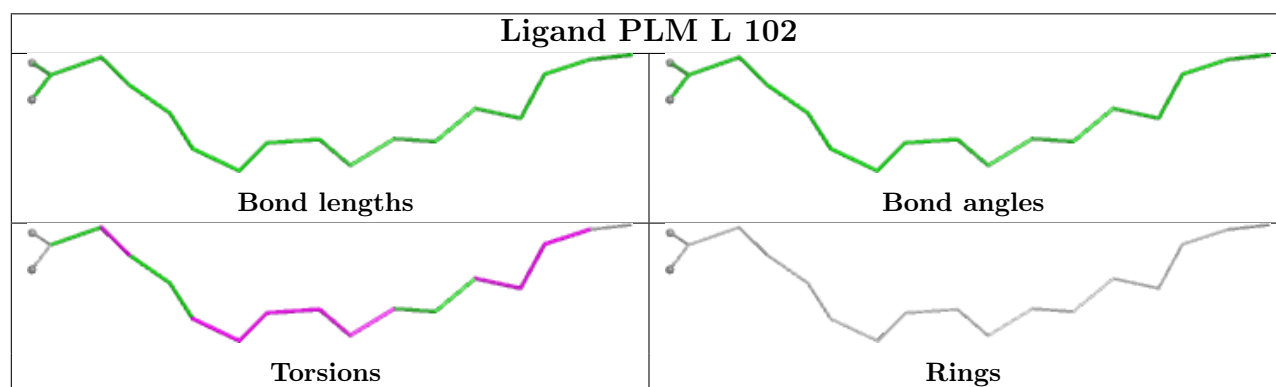
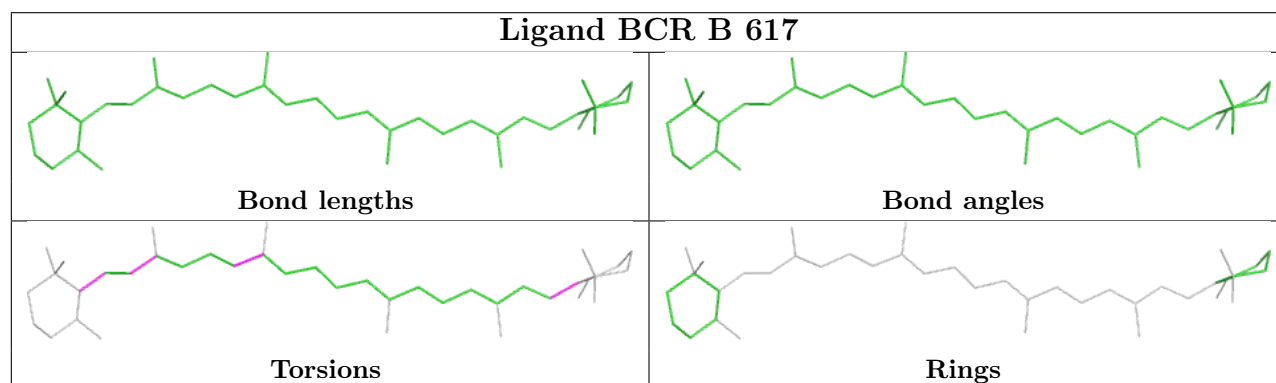
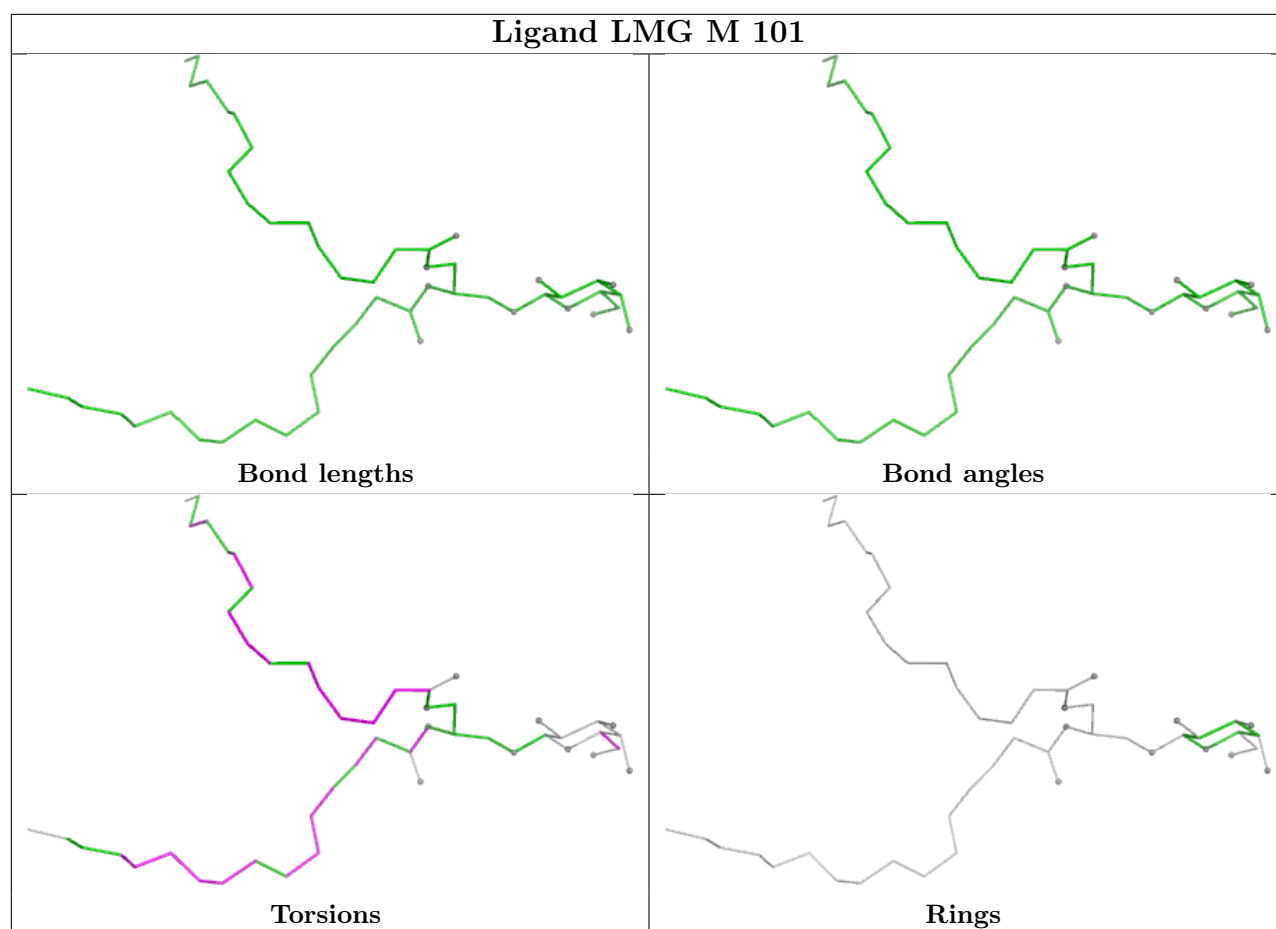




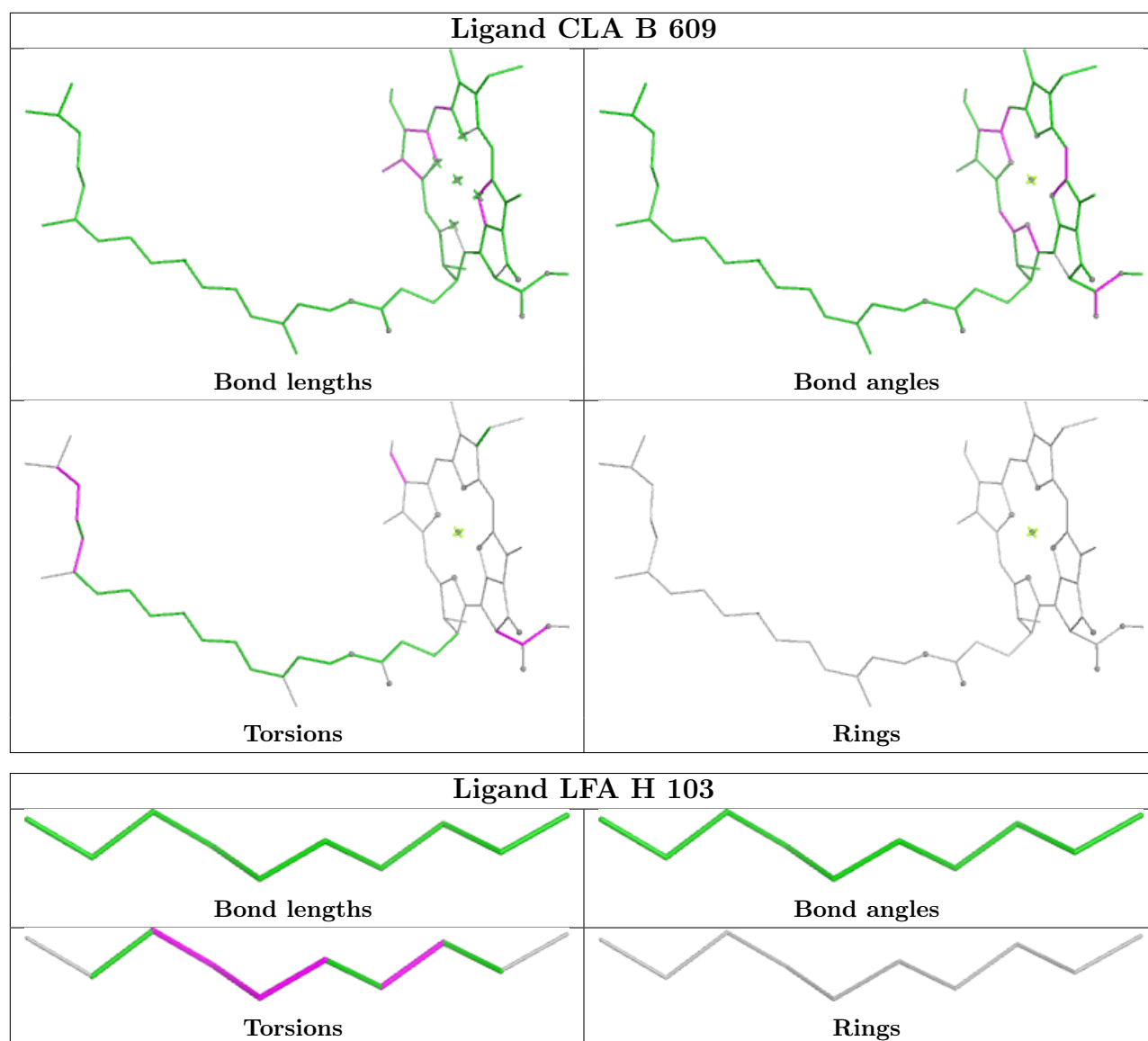


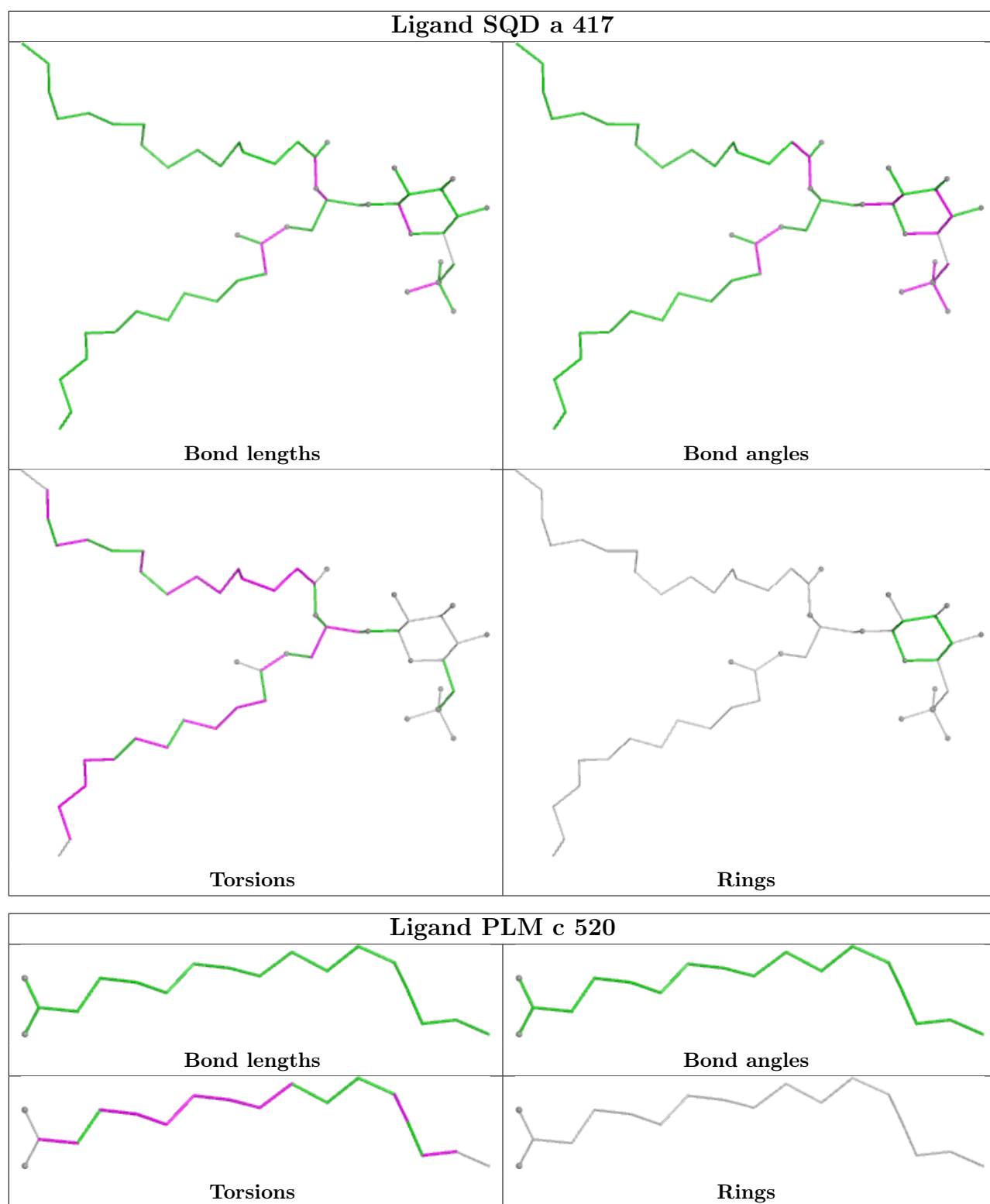


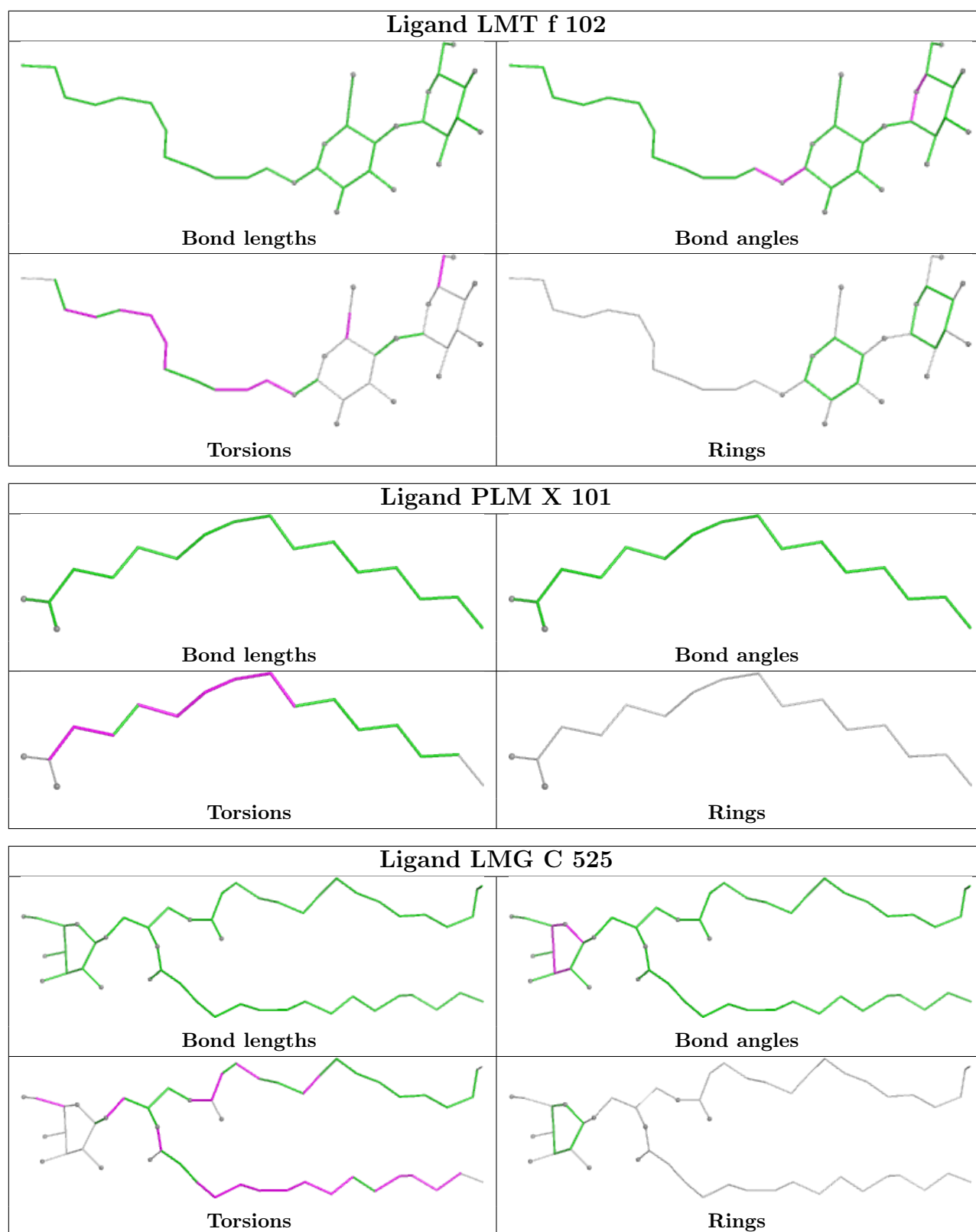


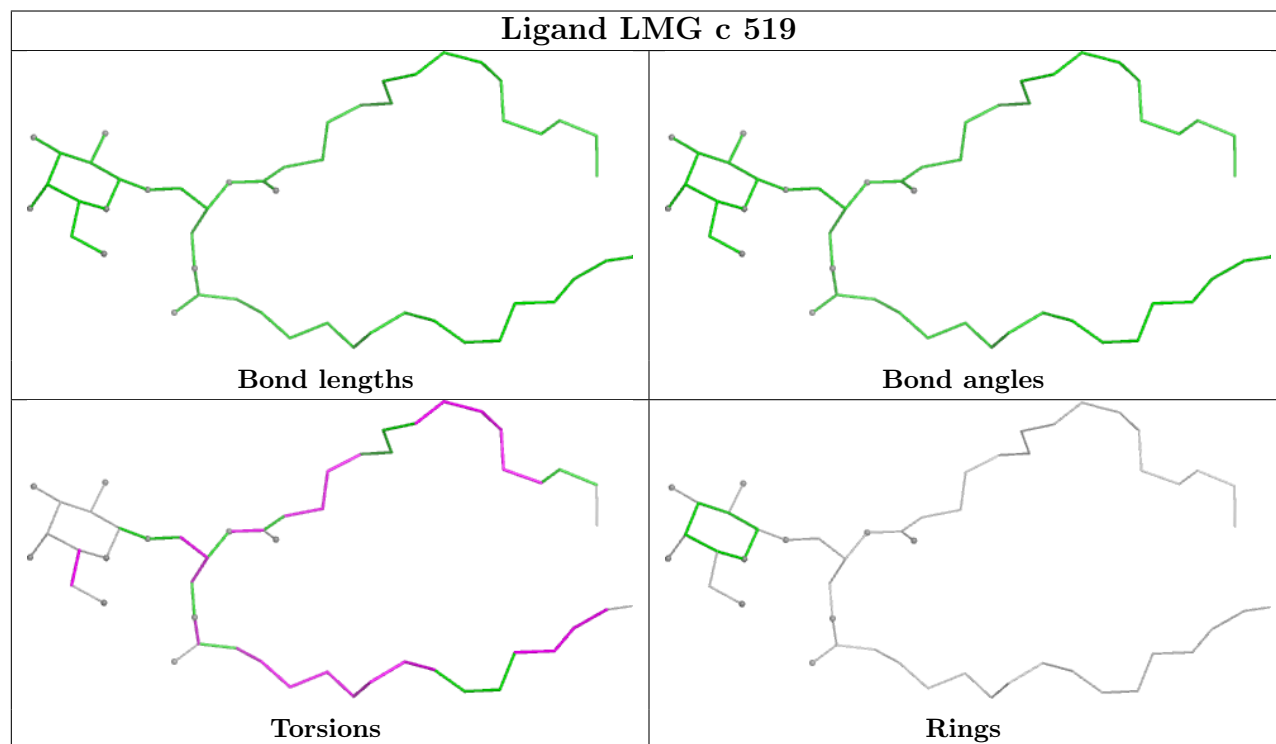
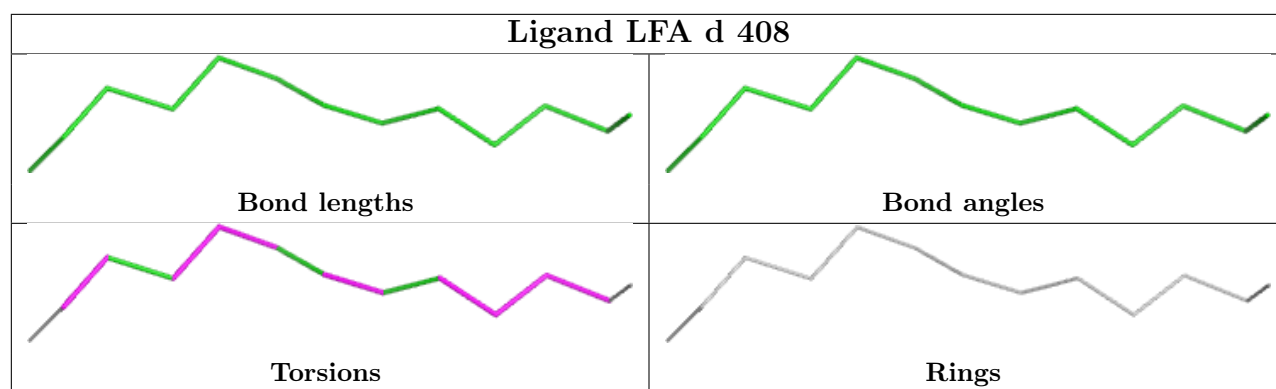


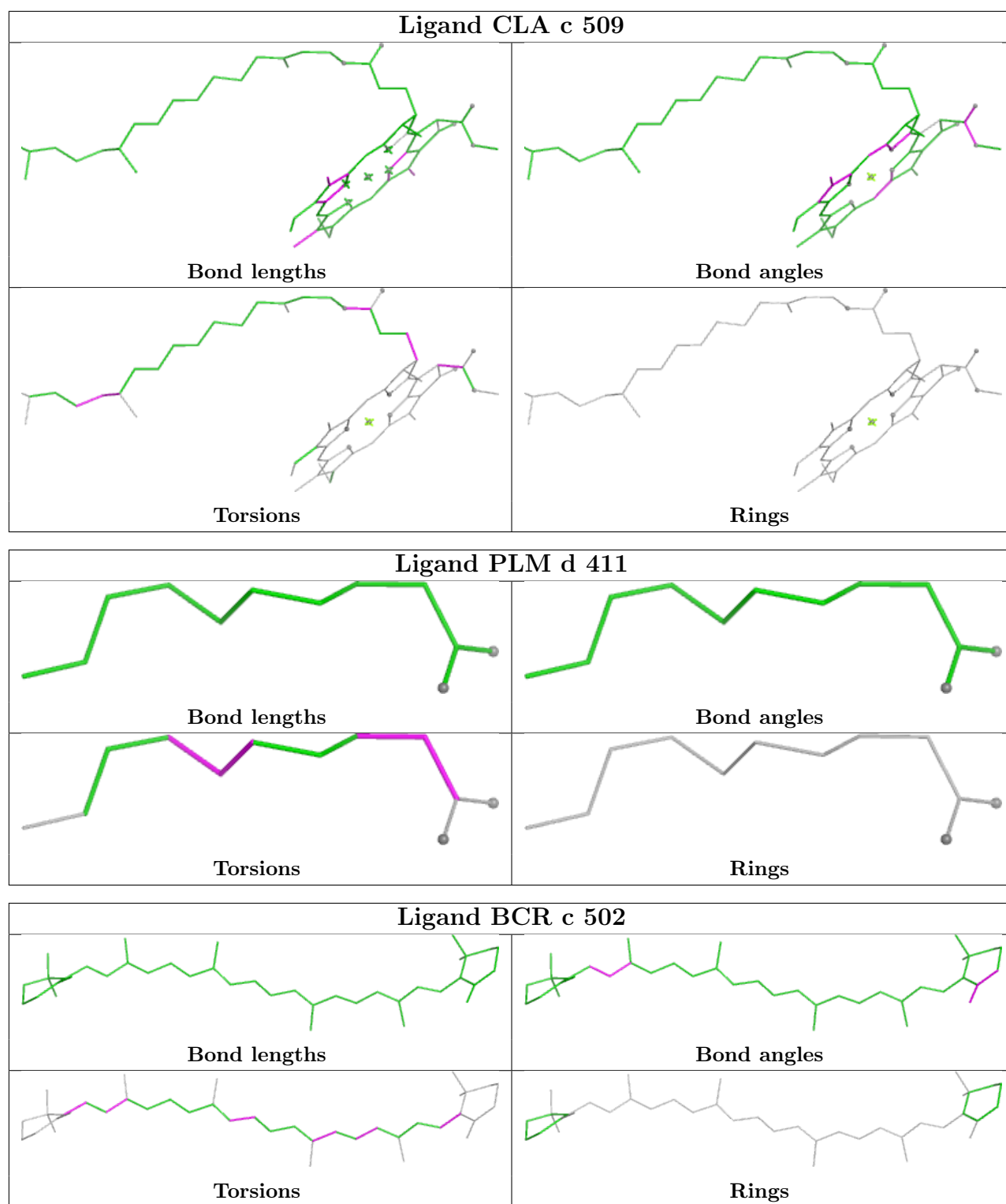


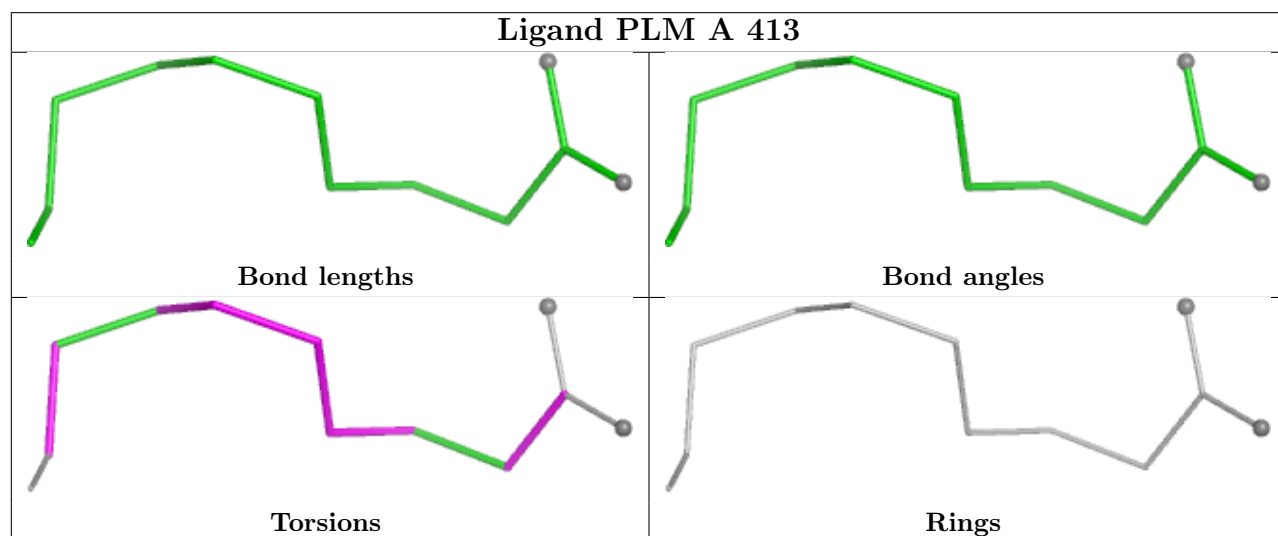
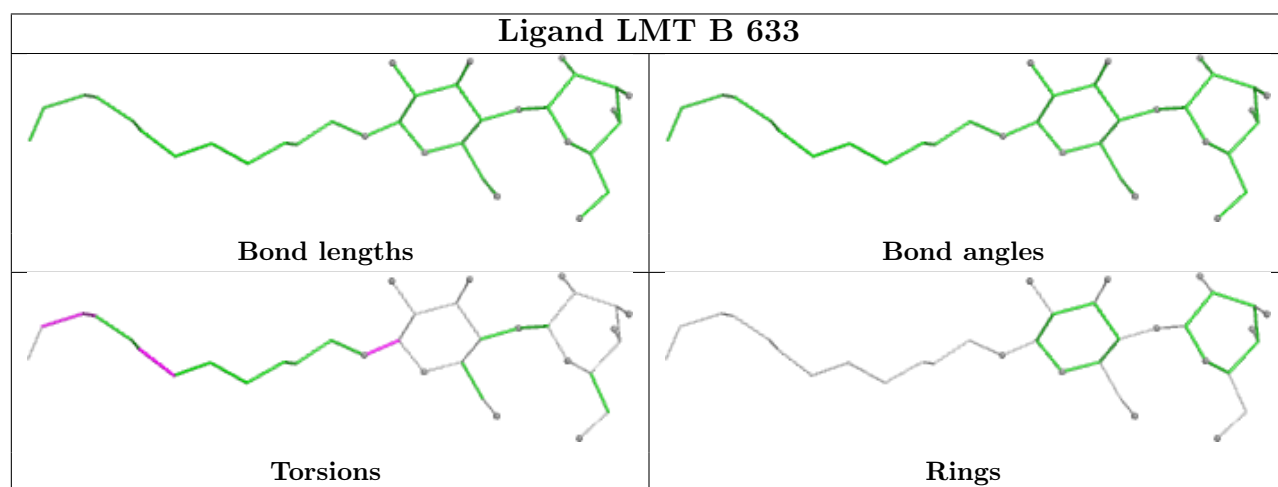
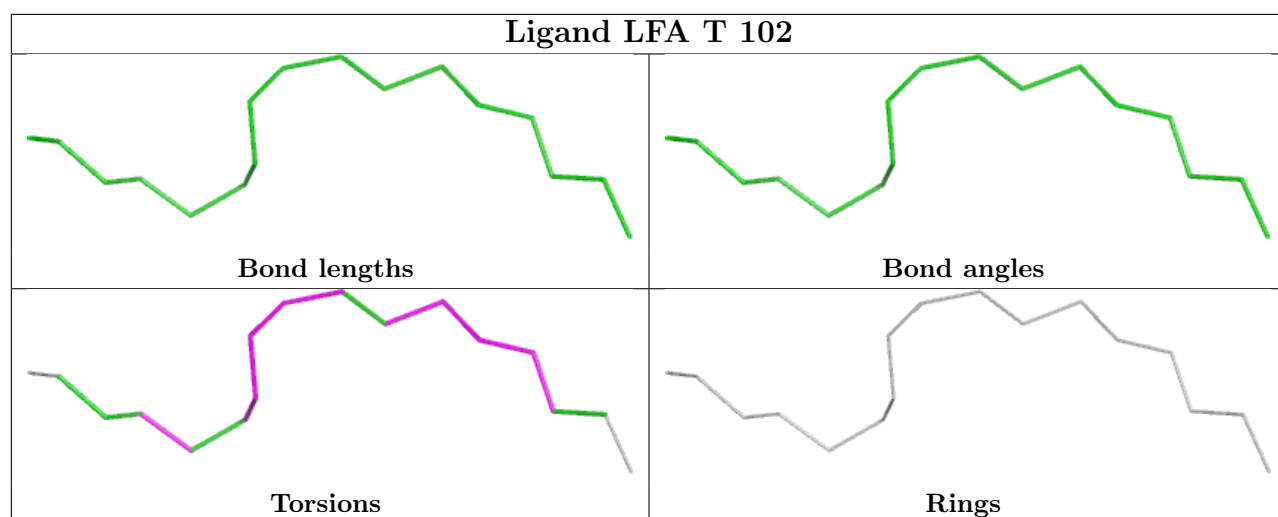


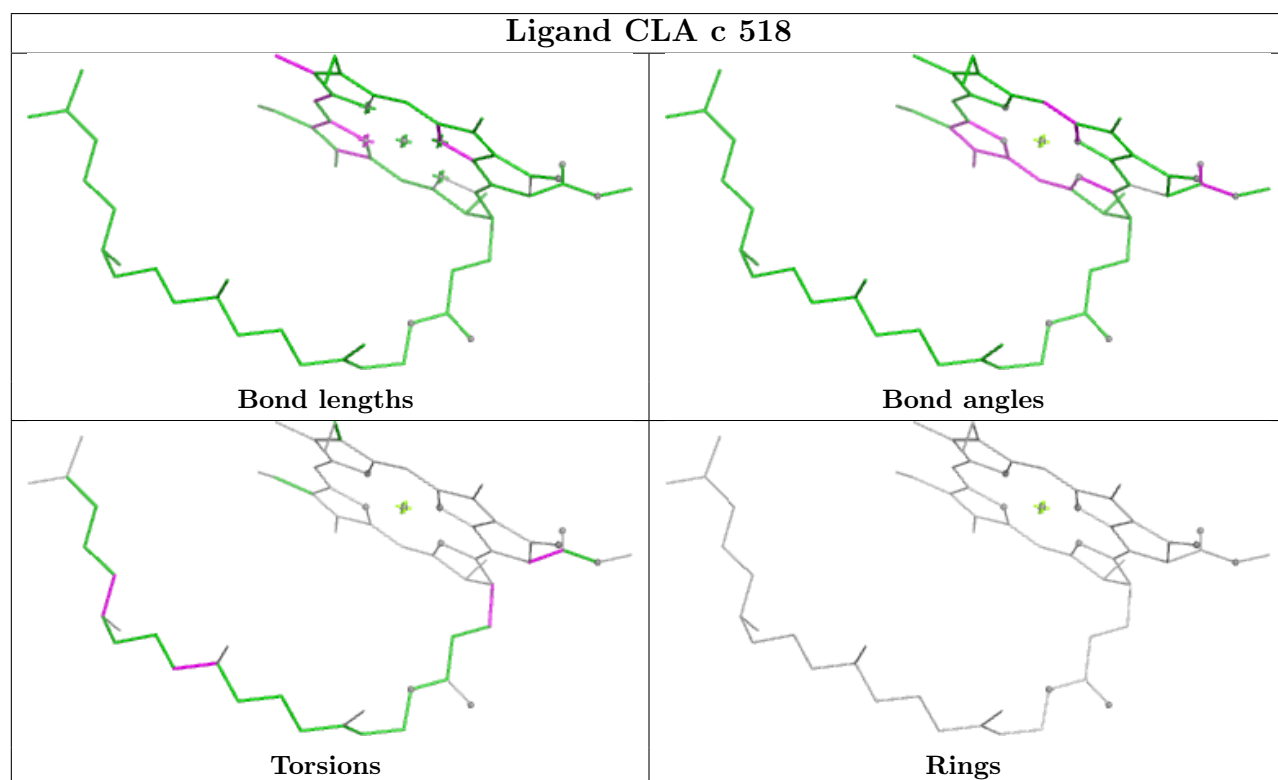
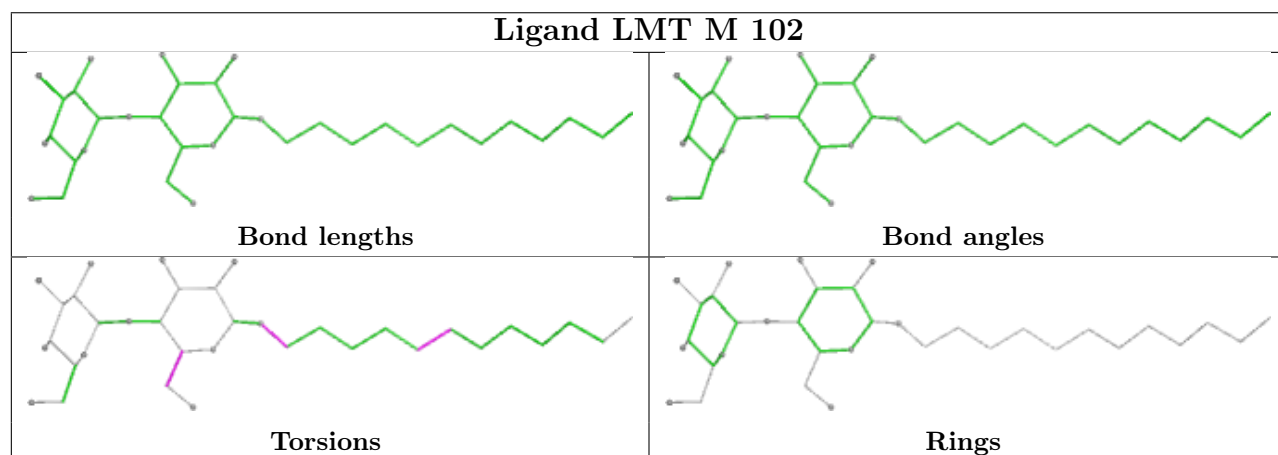
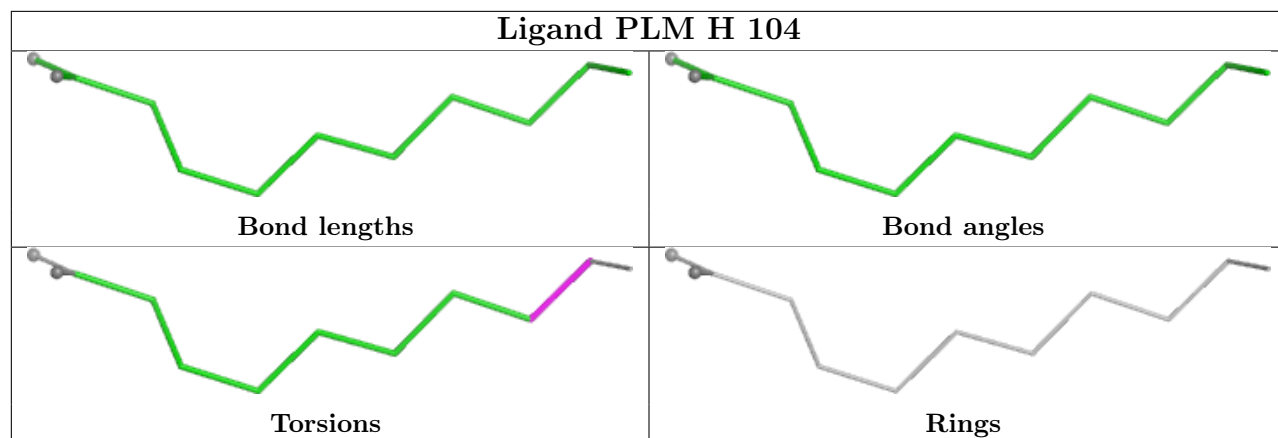




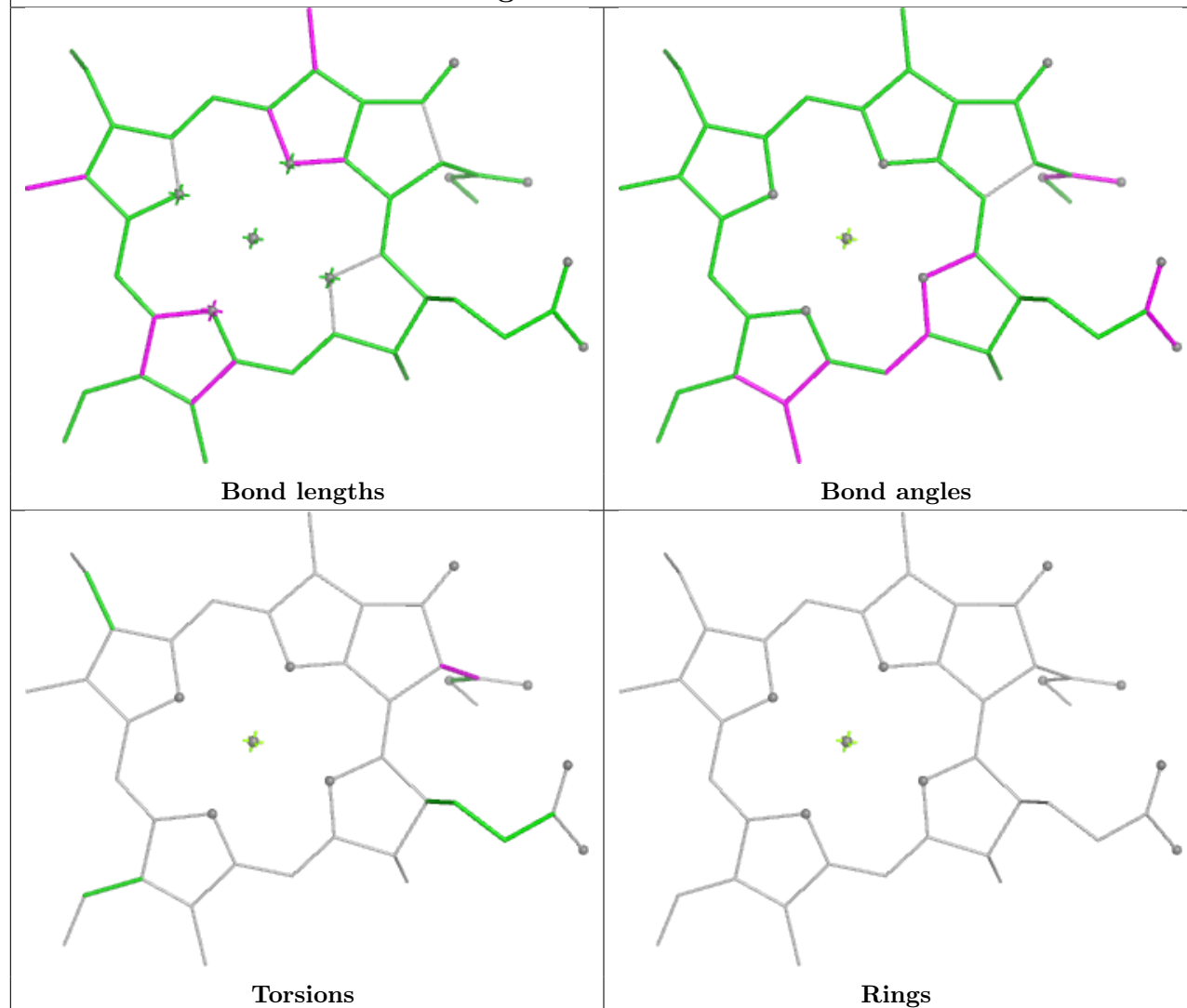




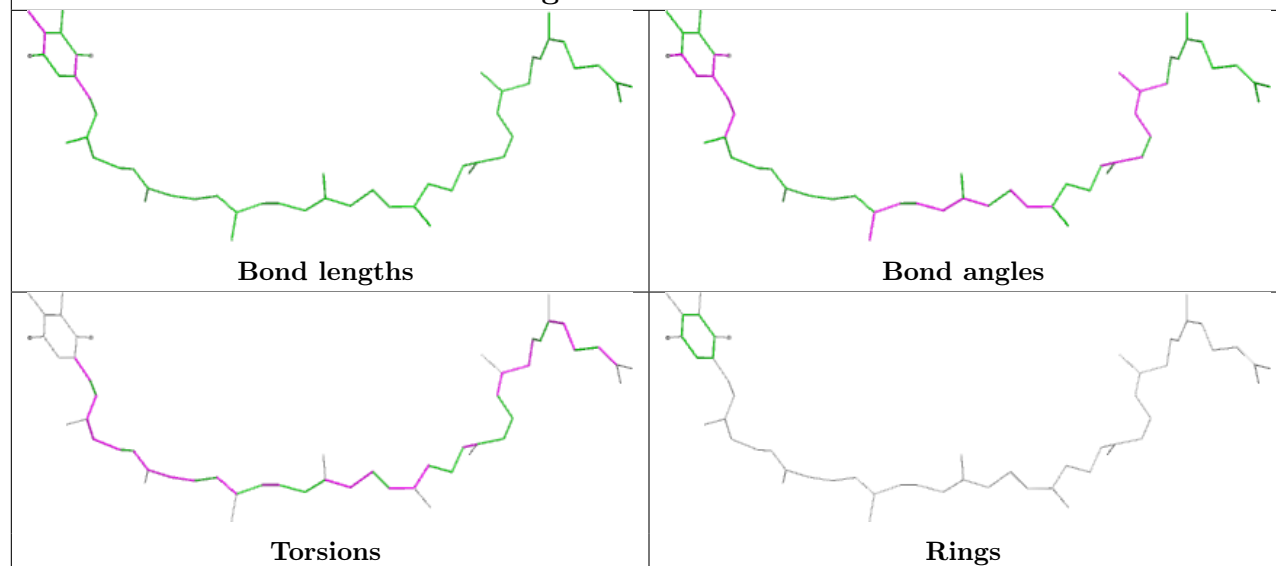




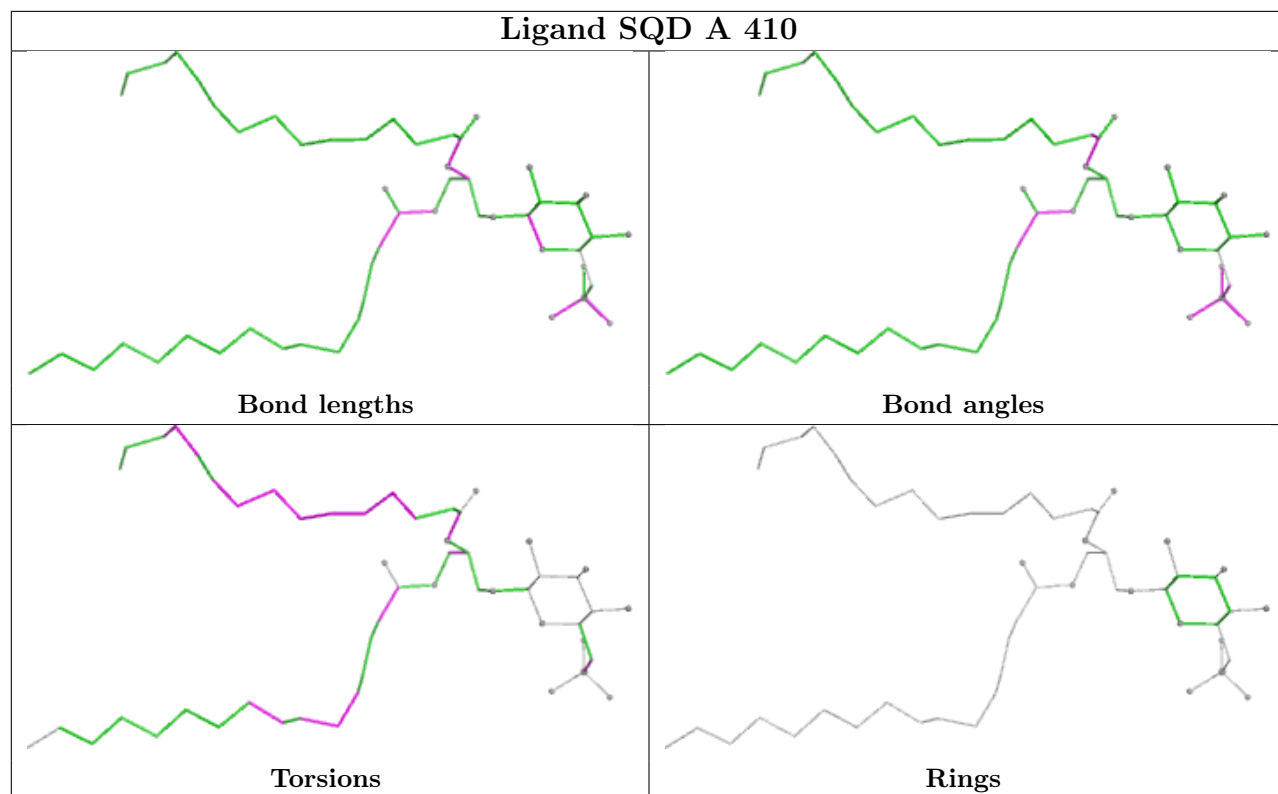
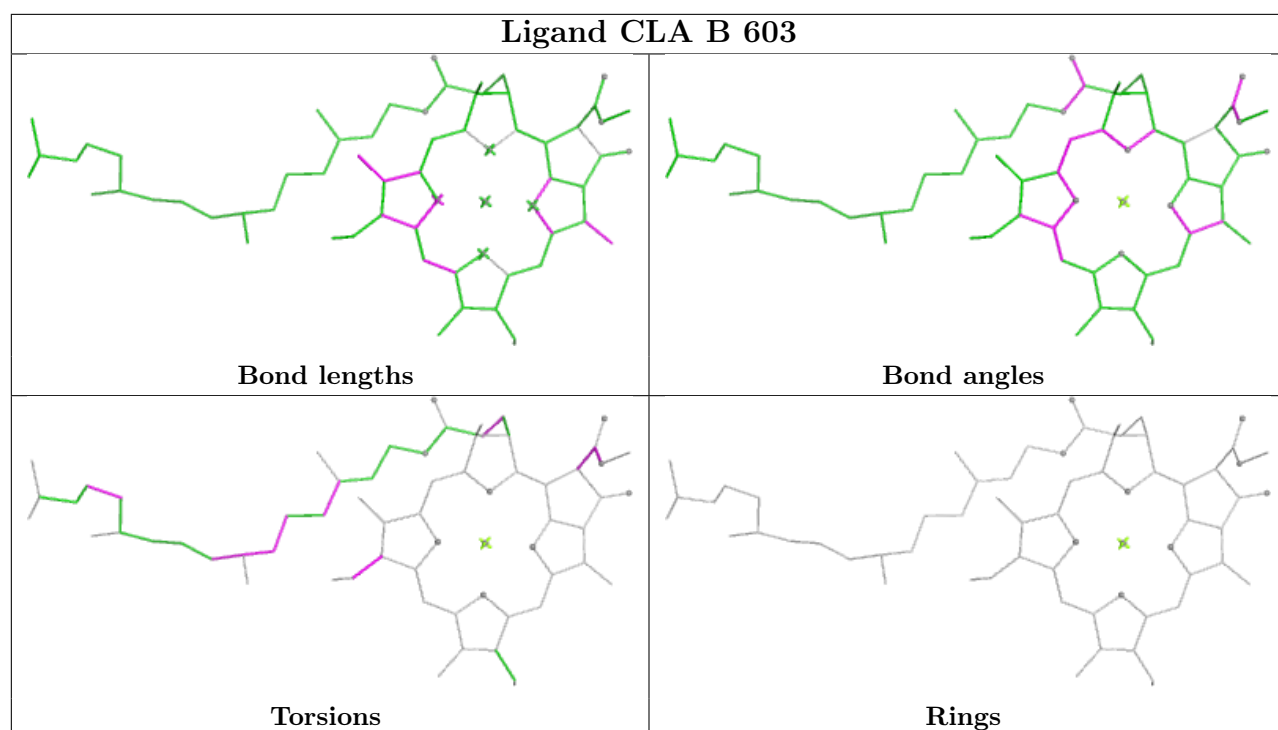
## Ligand CLA b 618

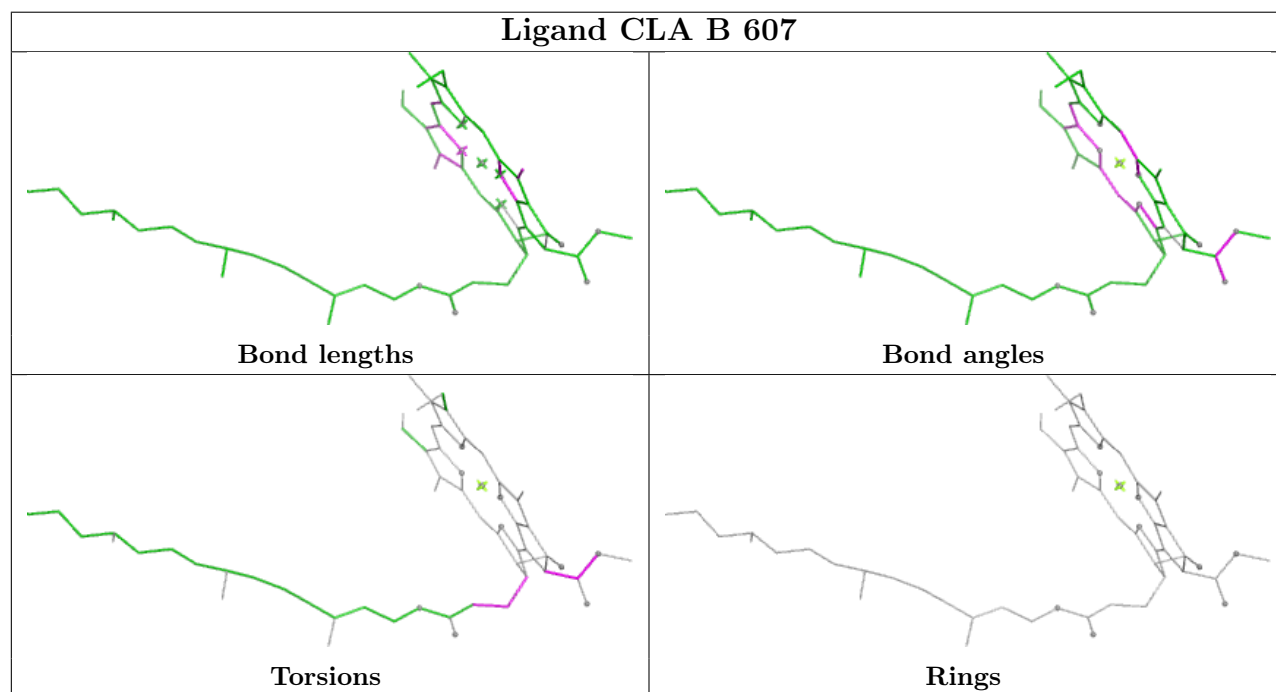
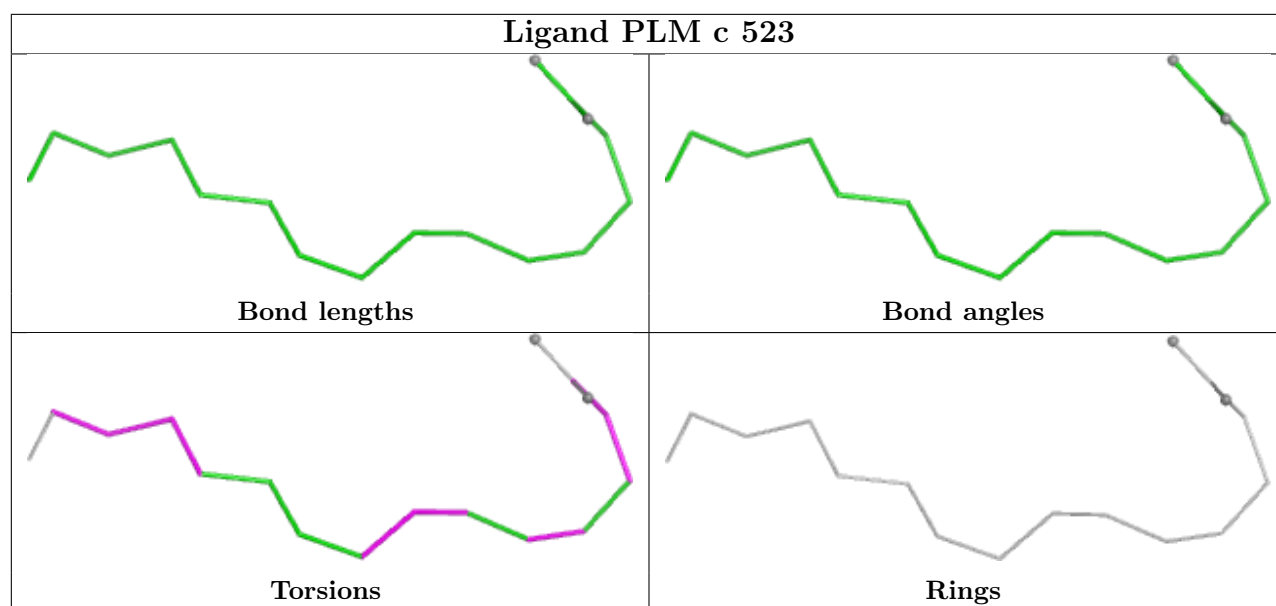


## Ligand PL9 a 410

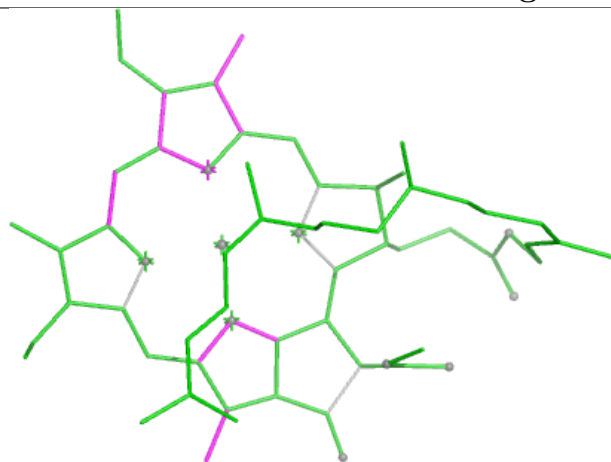




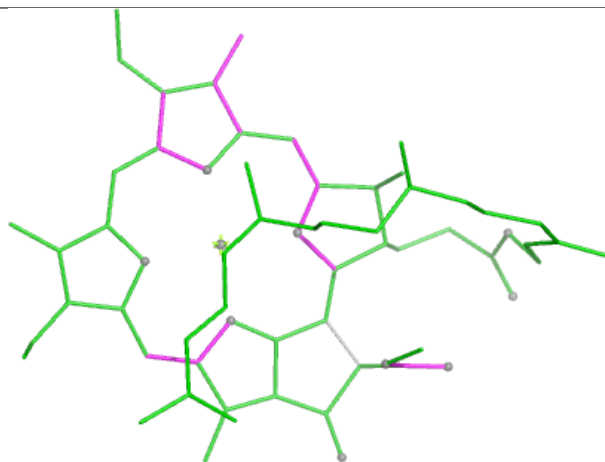




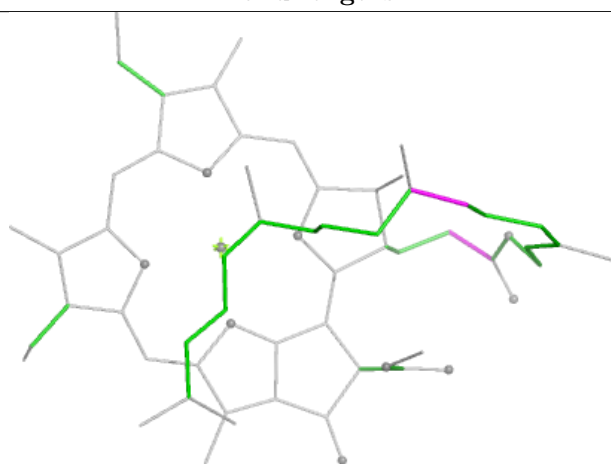
## Ligand CLA c 515



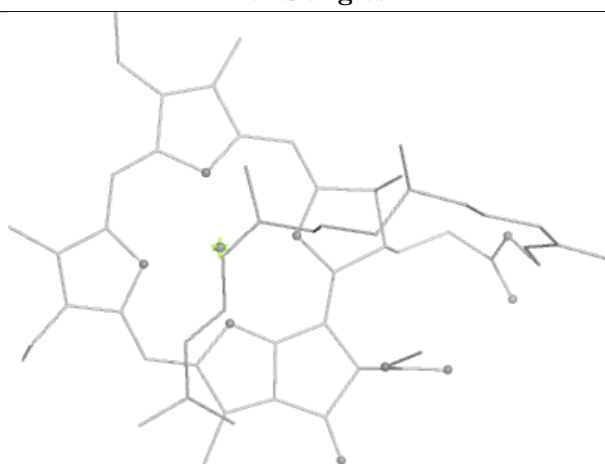
Bond lengths



Bond angles

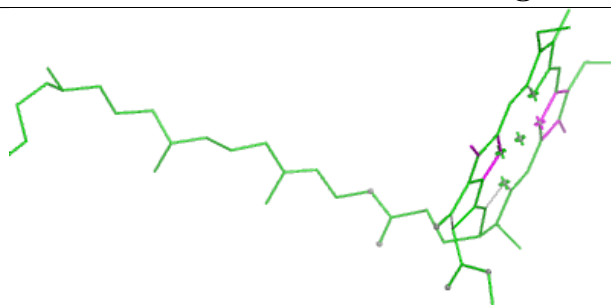


Torsions

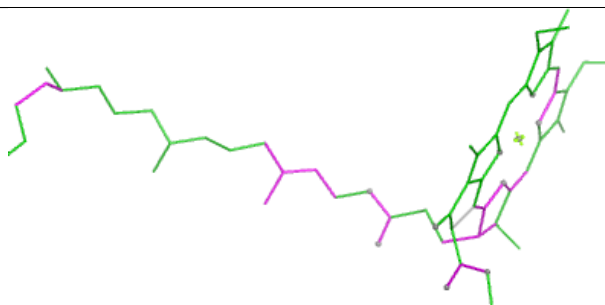


Rings

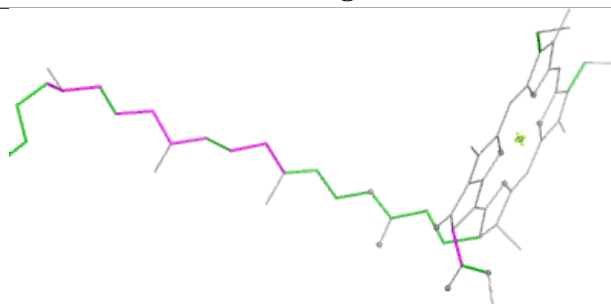
## Ligand CLA B 604



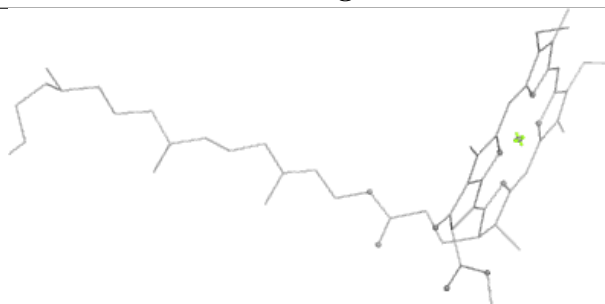
Bond lengths



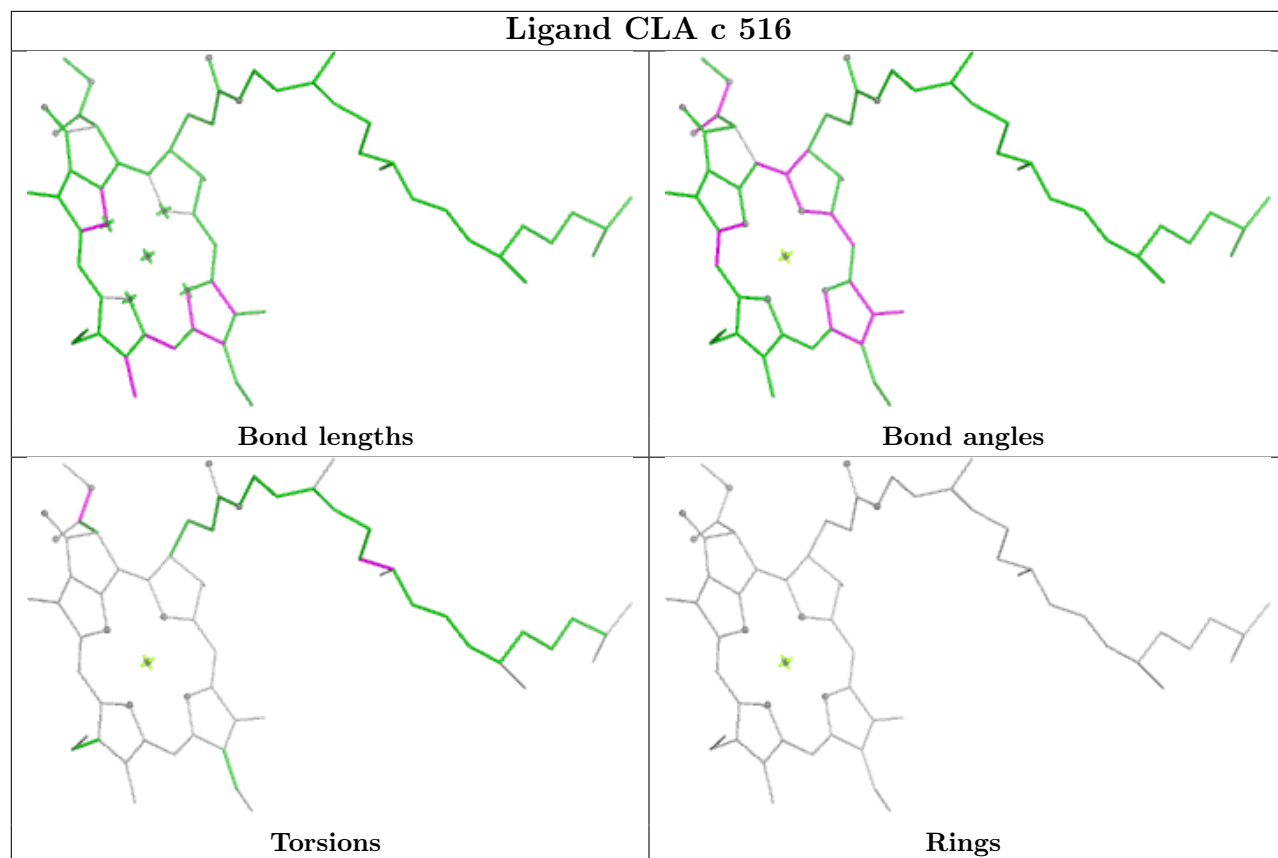
Bond angles



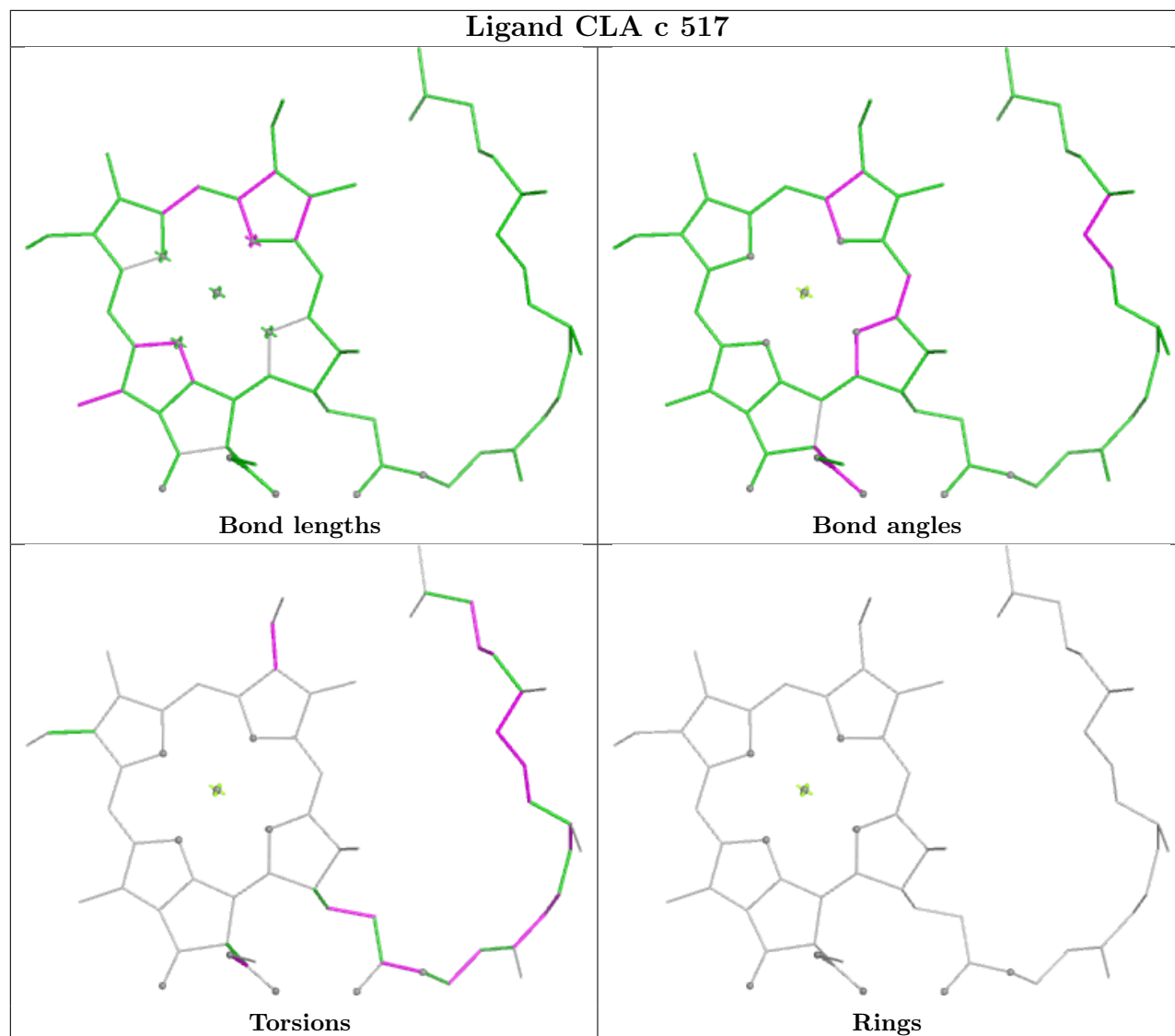
Torsions



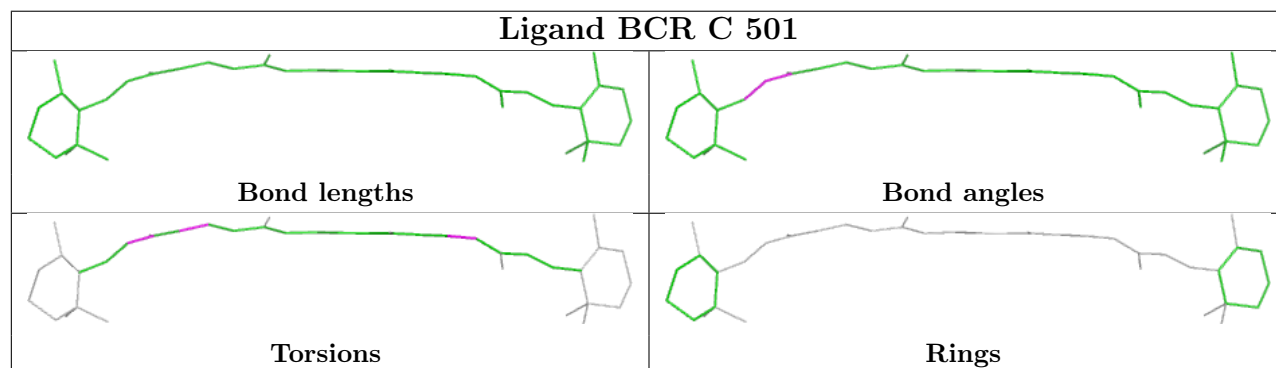
Rings

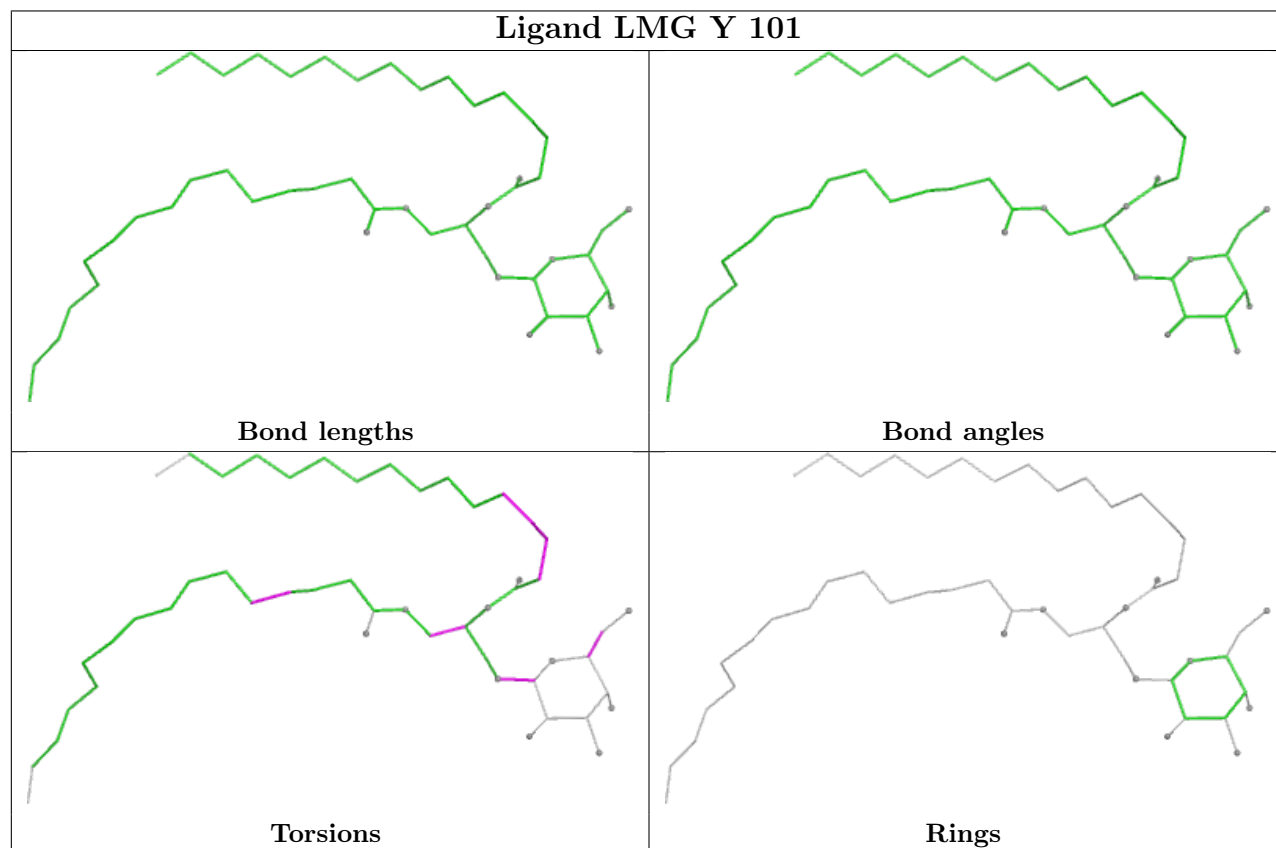
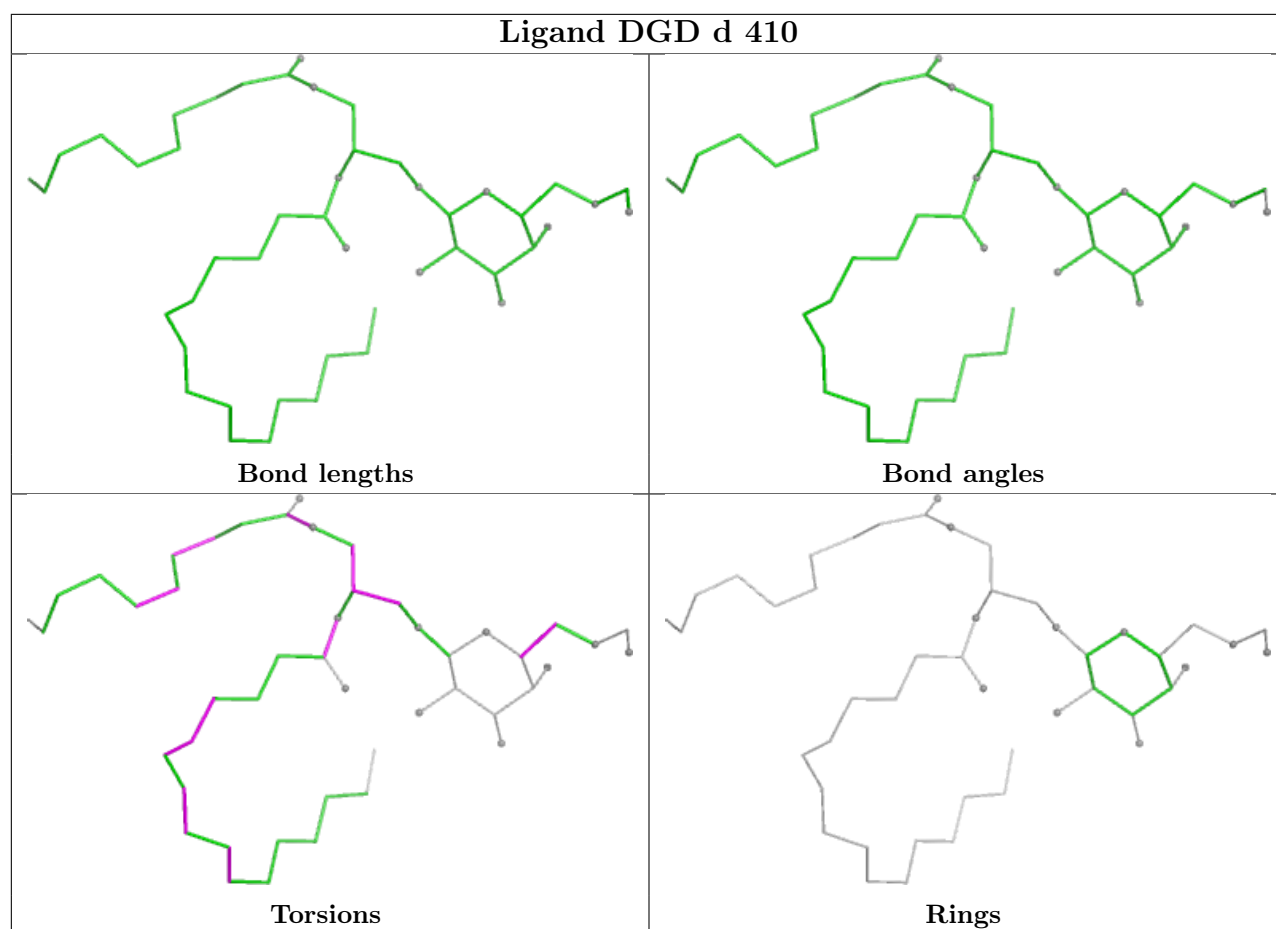


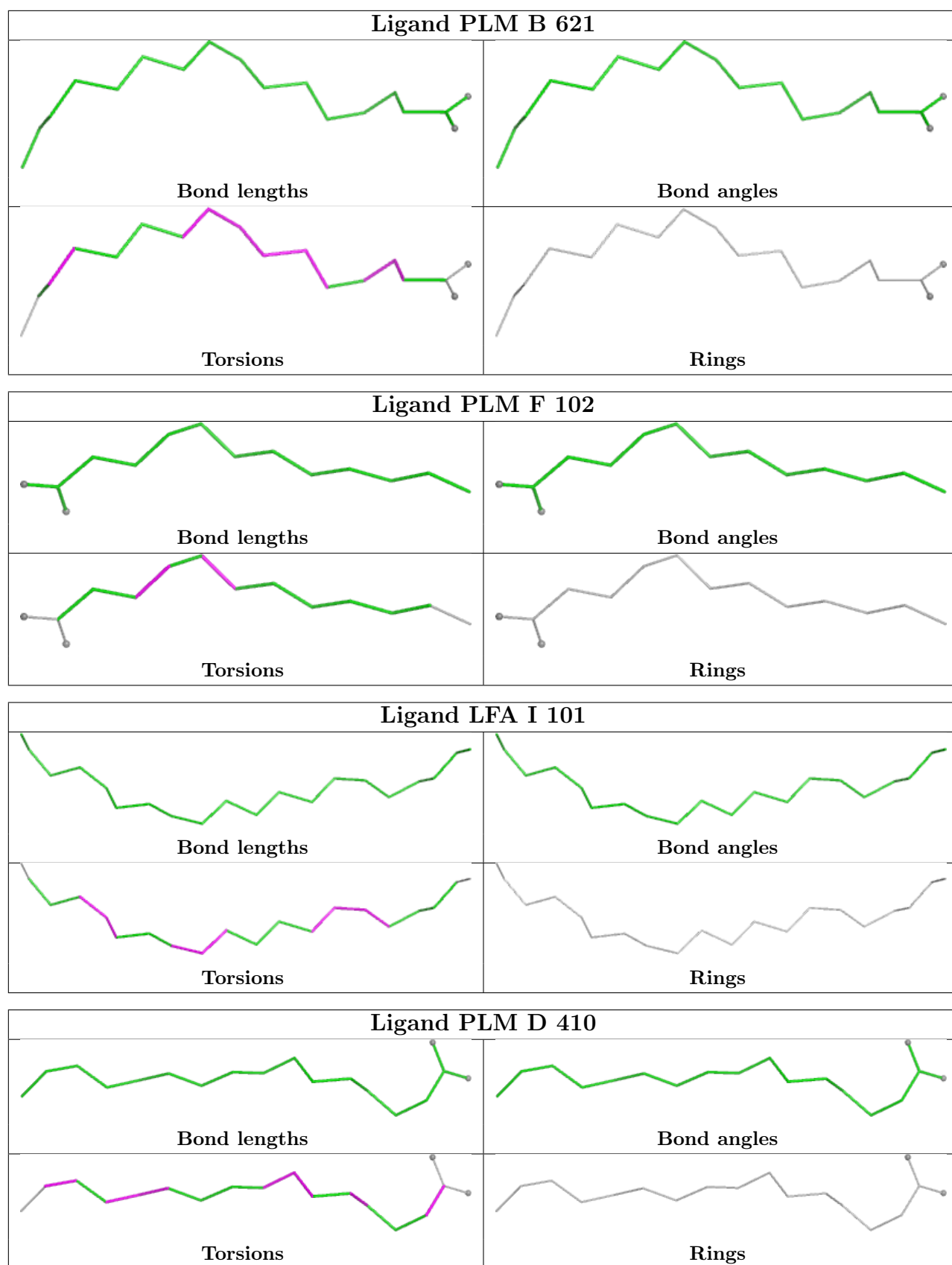
## Ligand CLA c 517

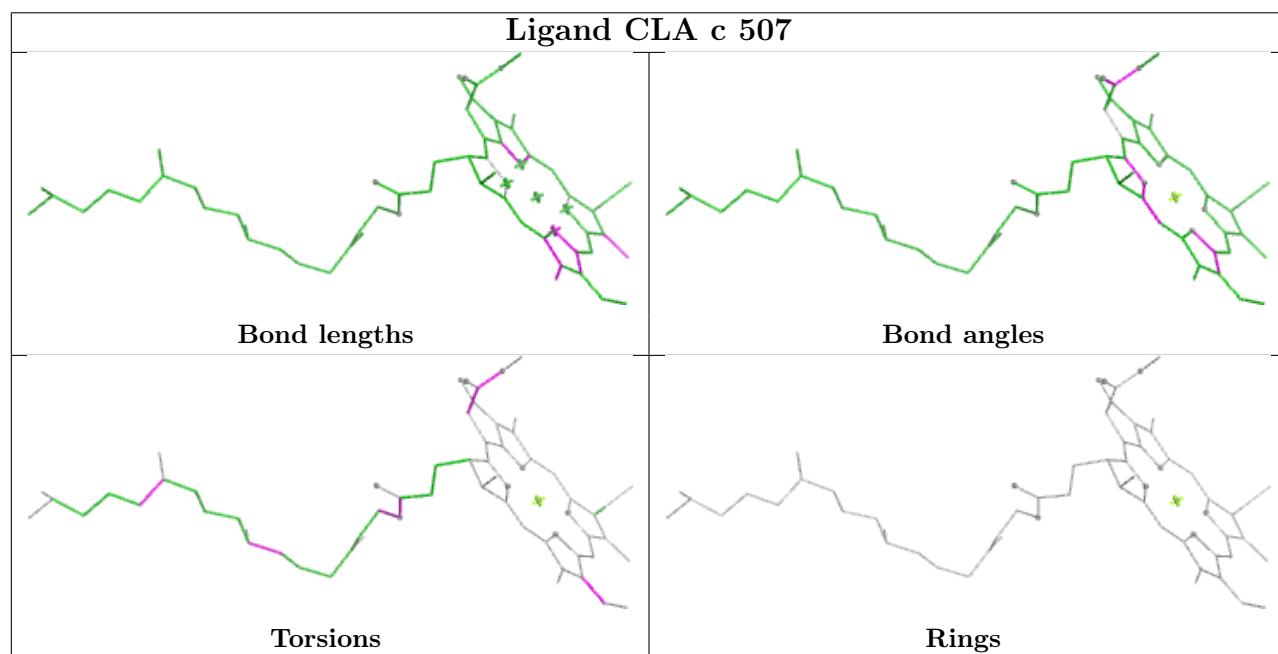
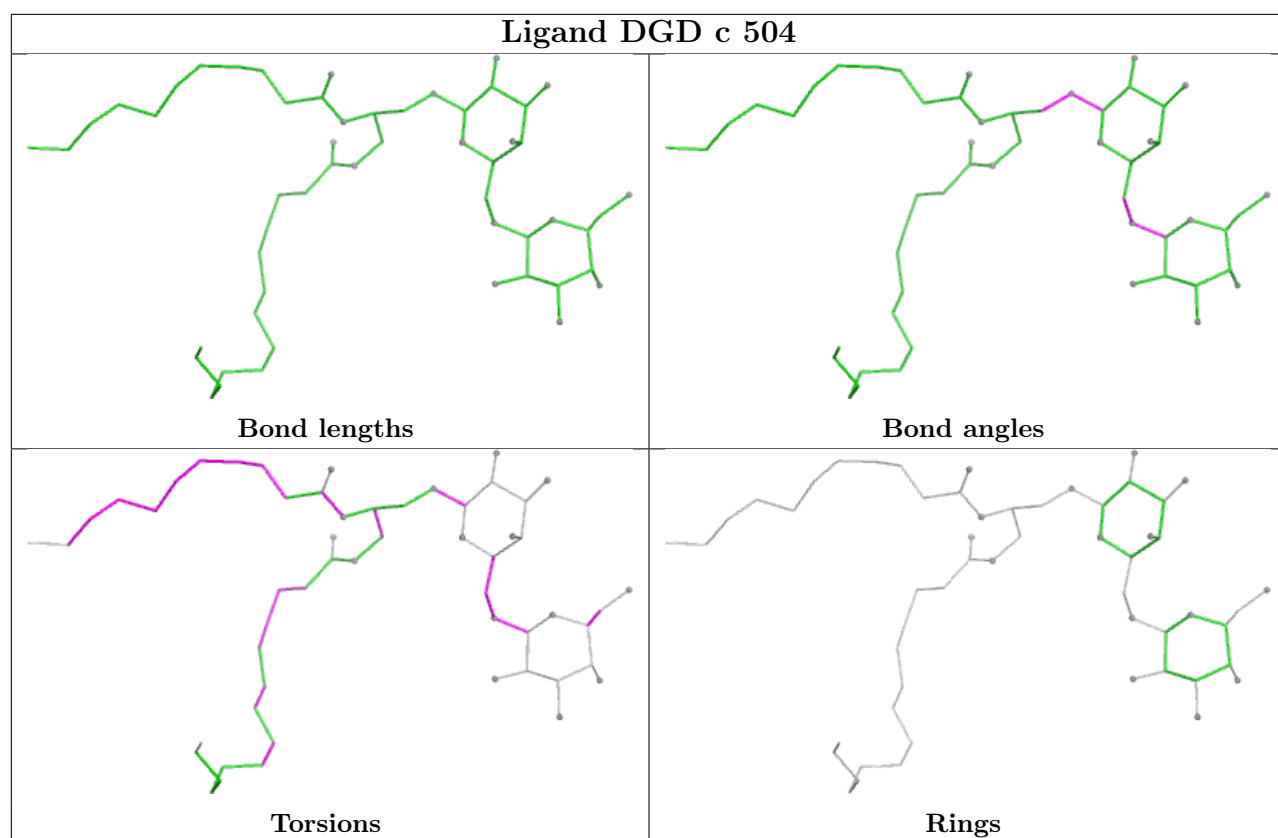


## Ligand BCR C 501

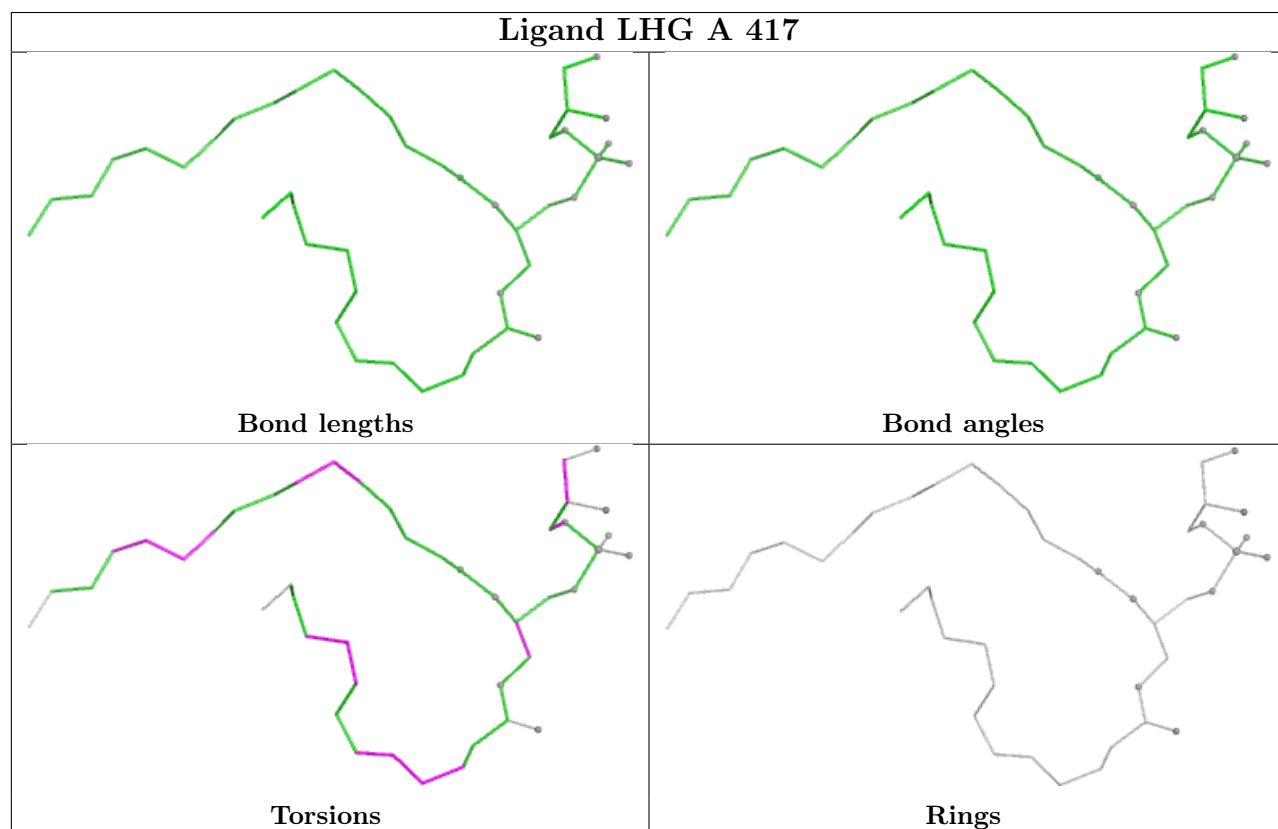
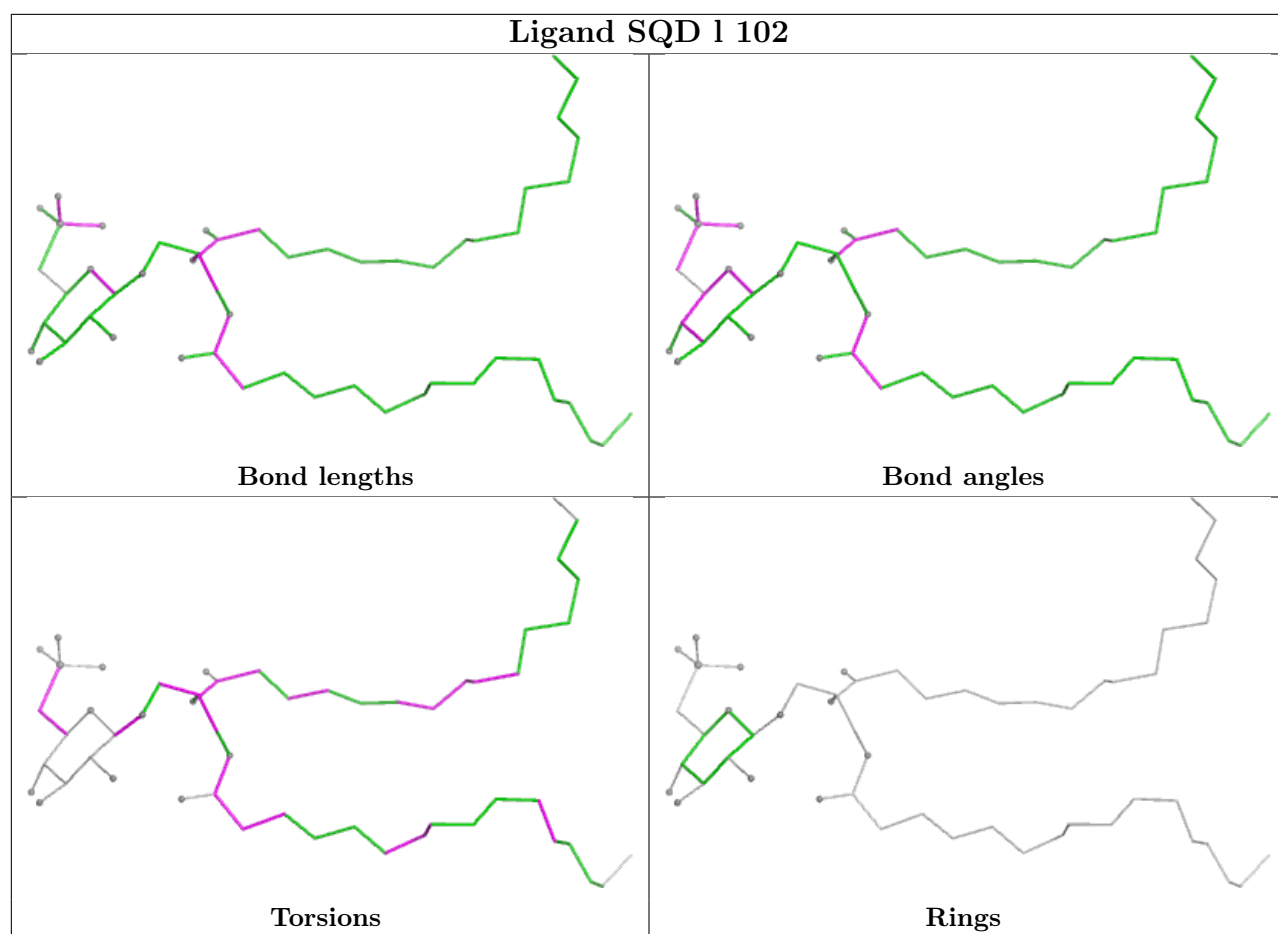




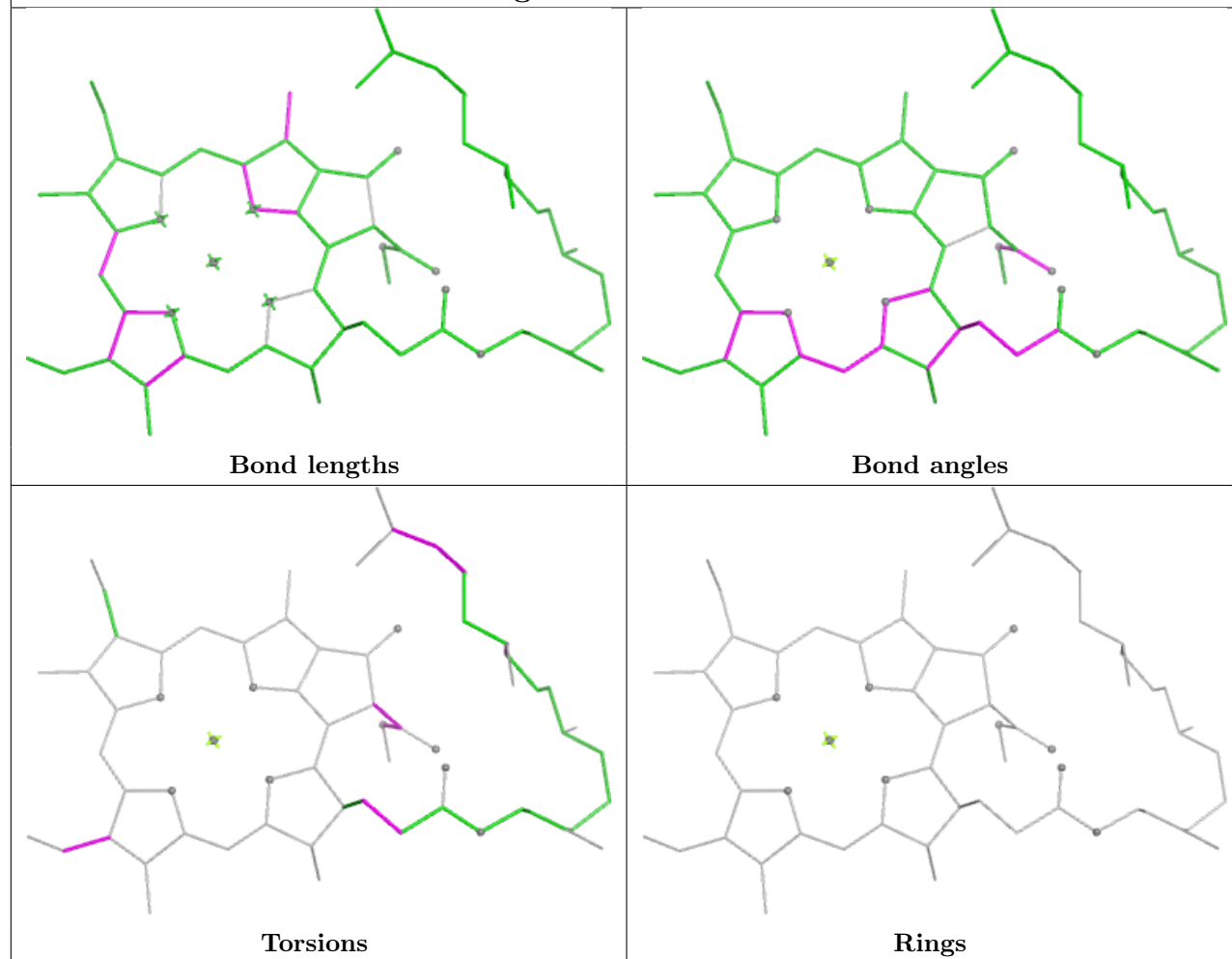




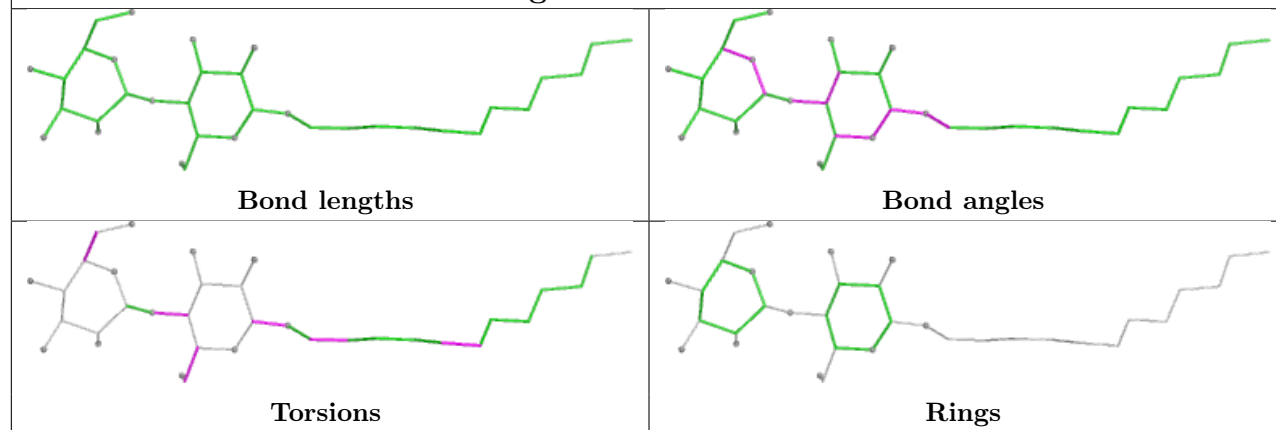


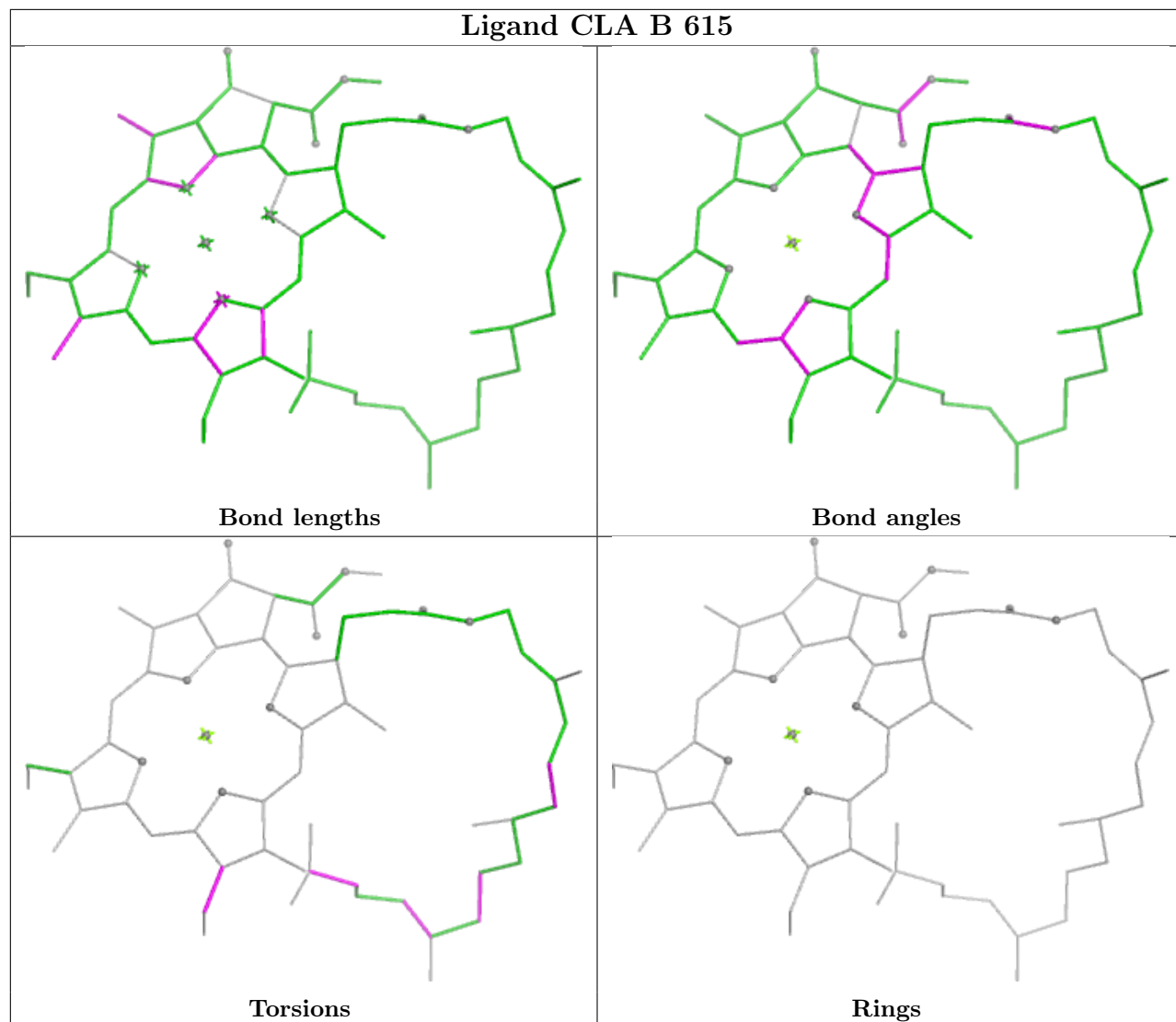
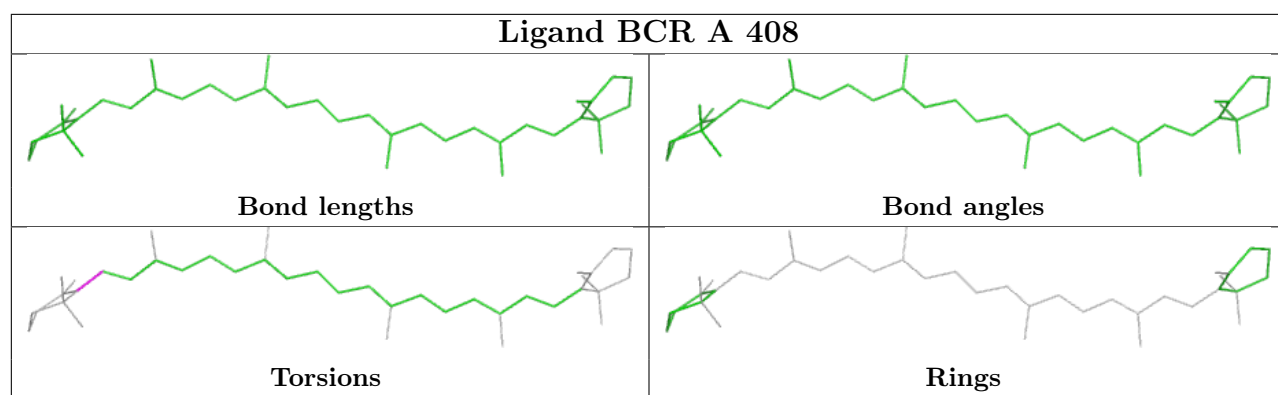


## Ligand CLA B 610

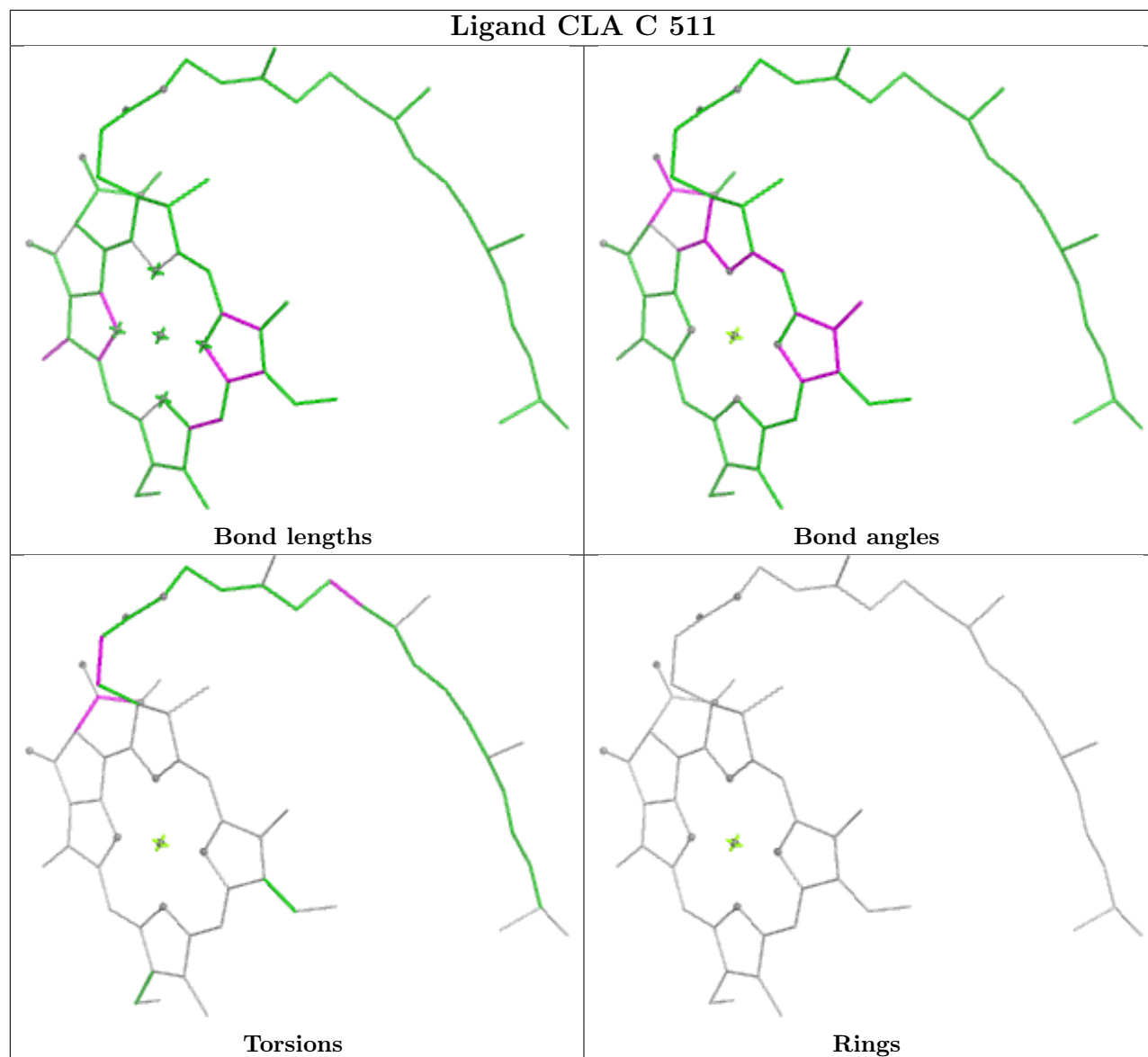


## Ligand LMT C 518

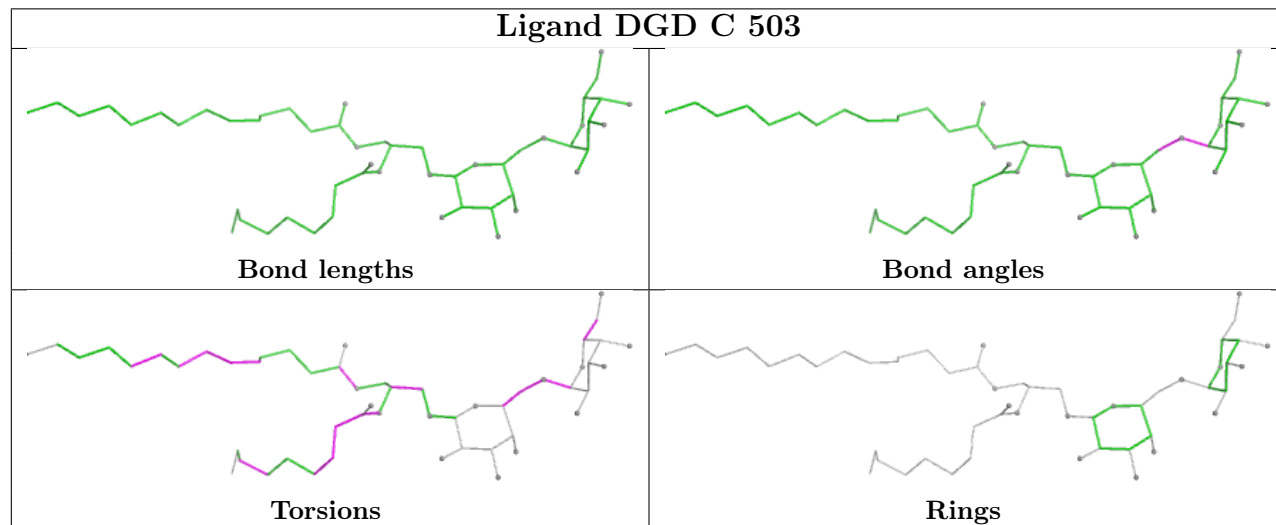


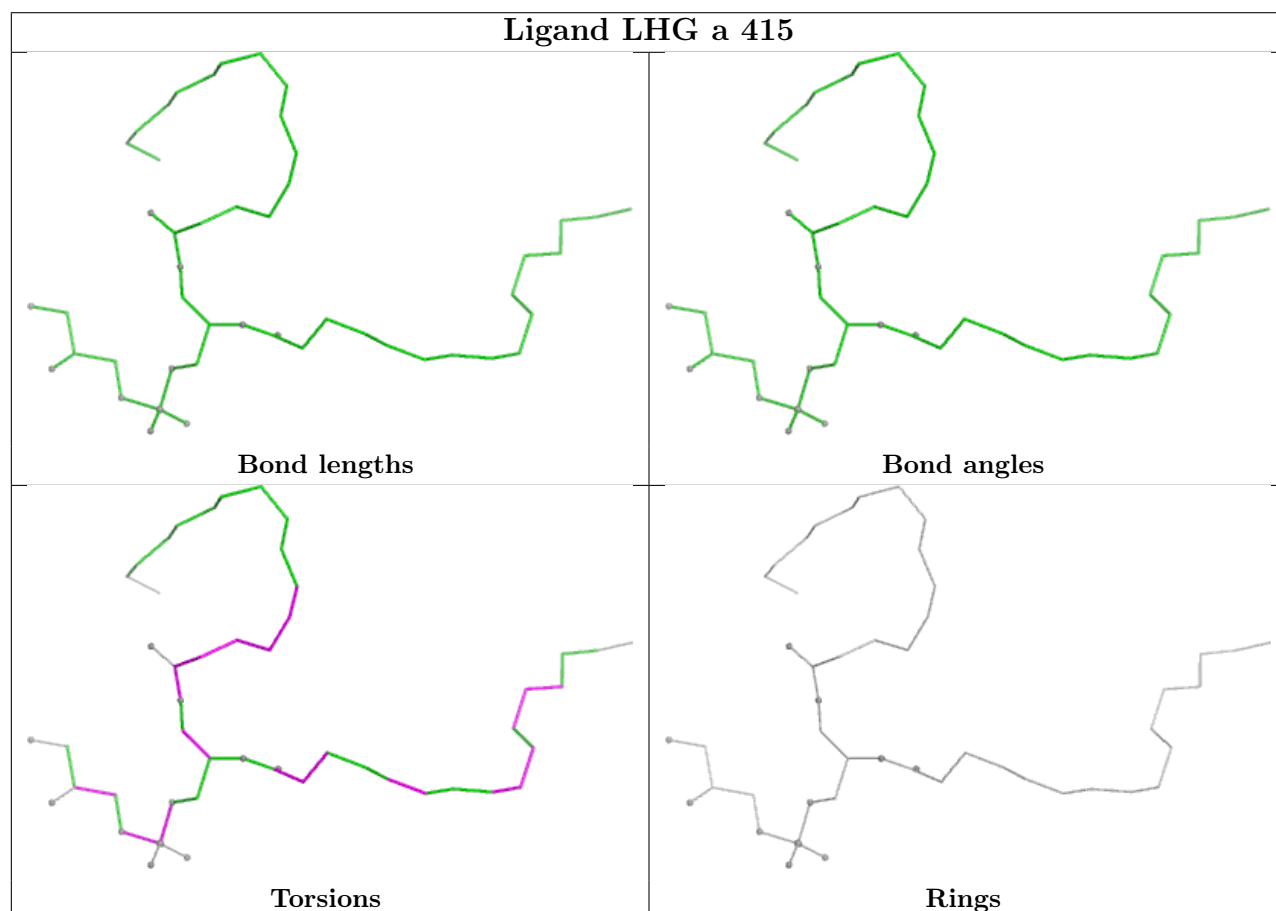
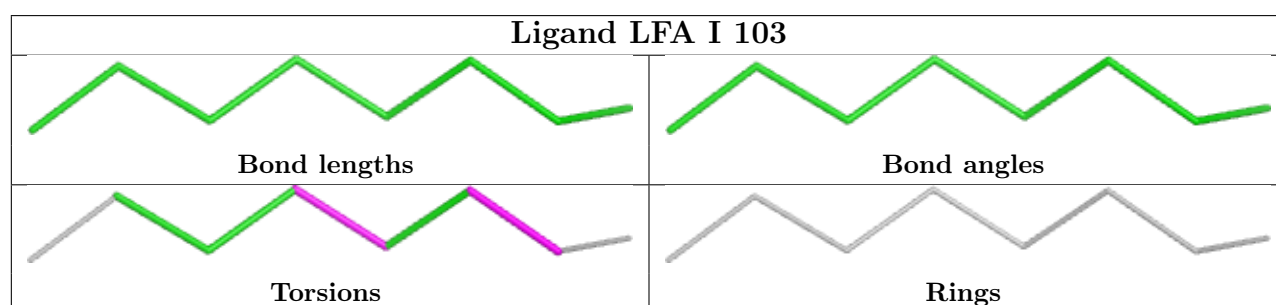
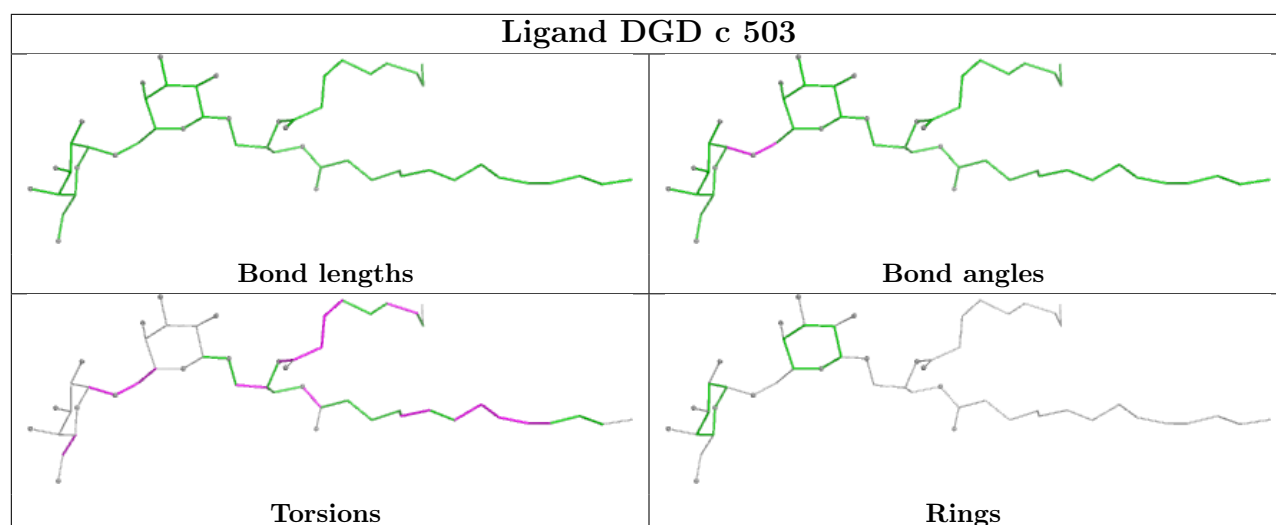


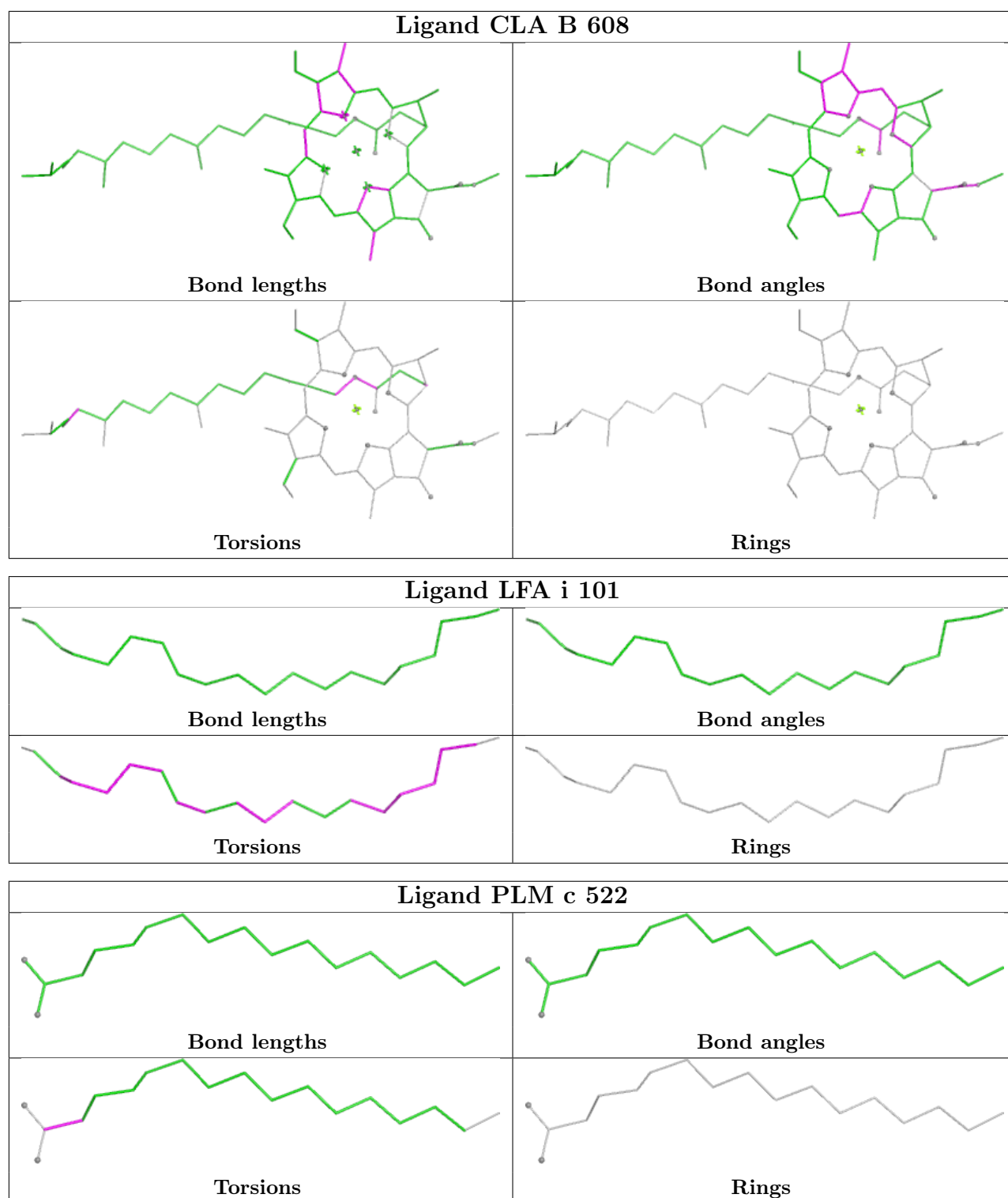
## Ligand CLA C 511

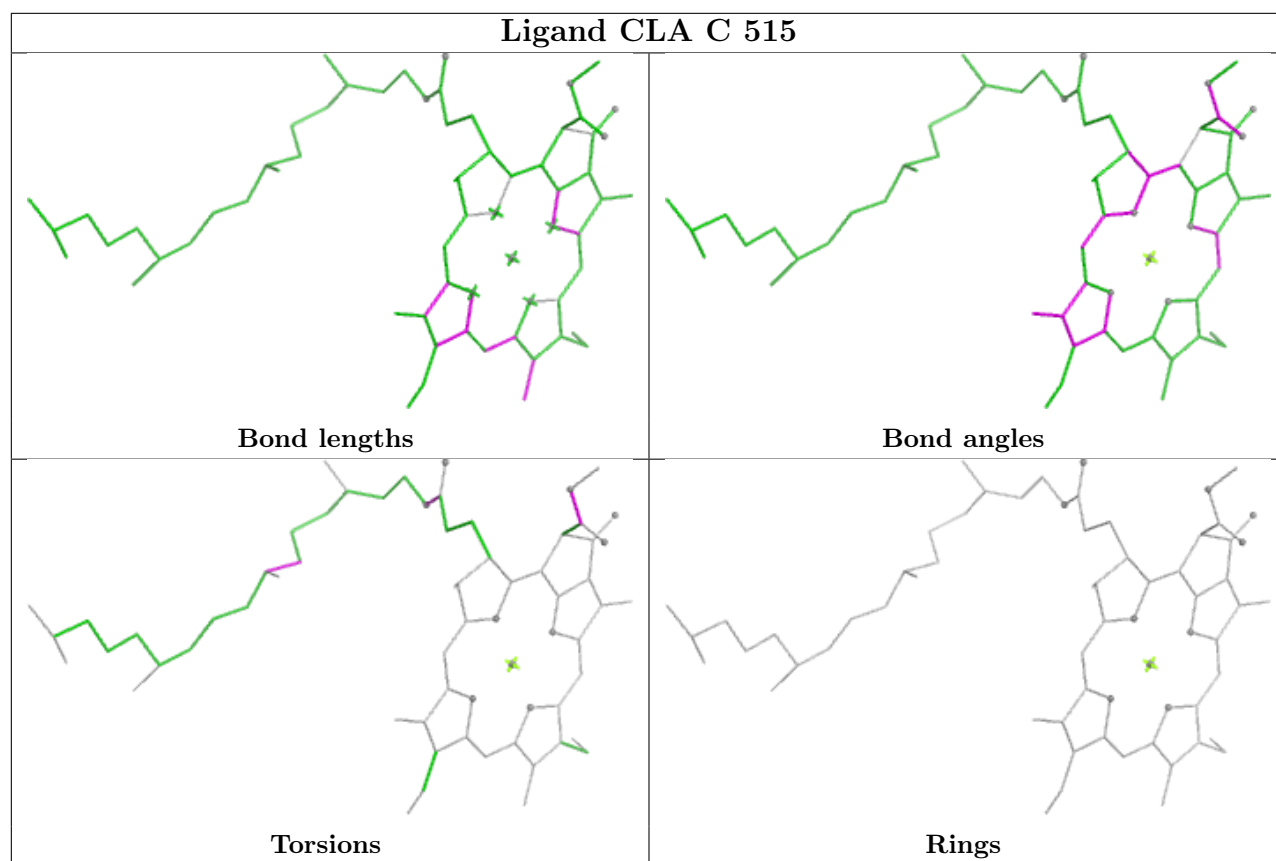
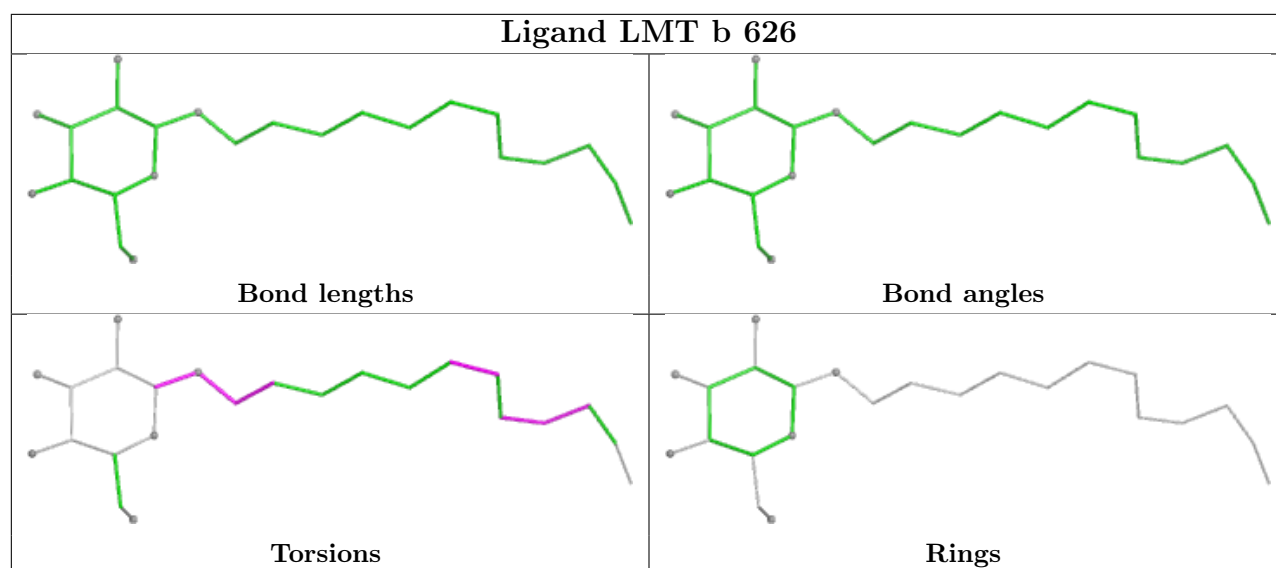


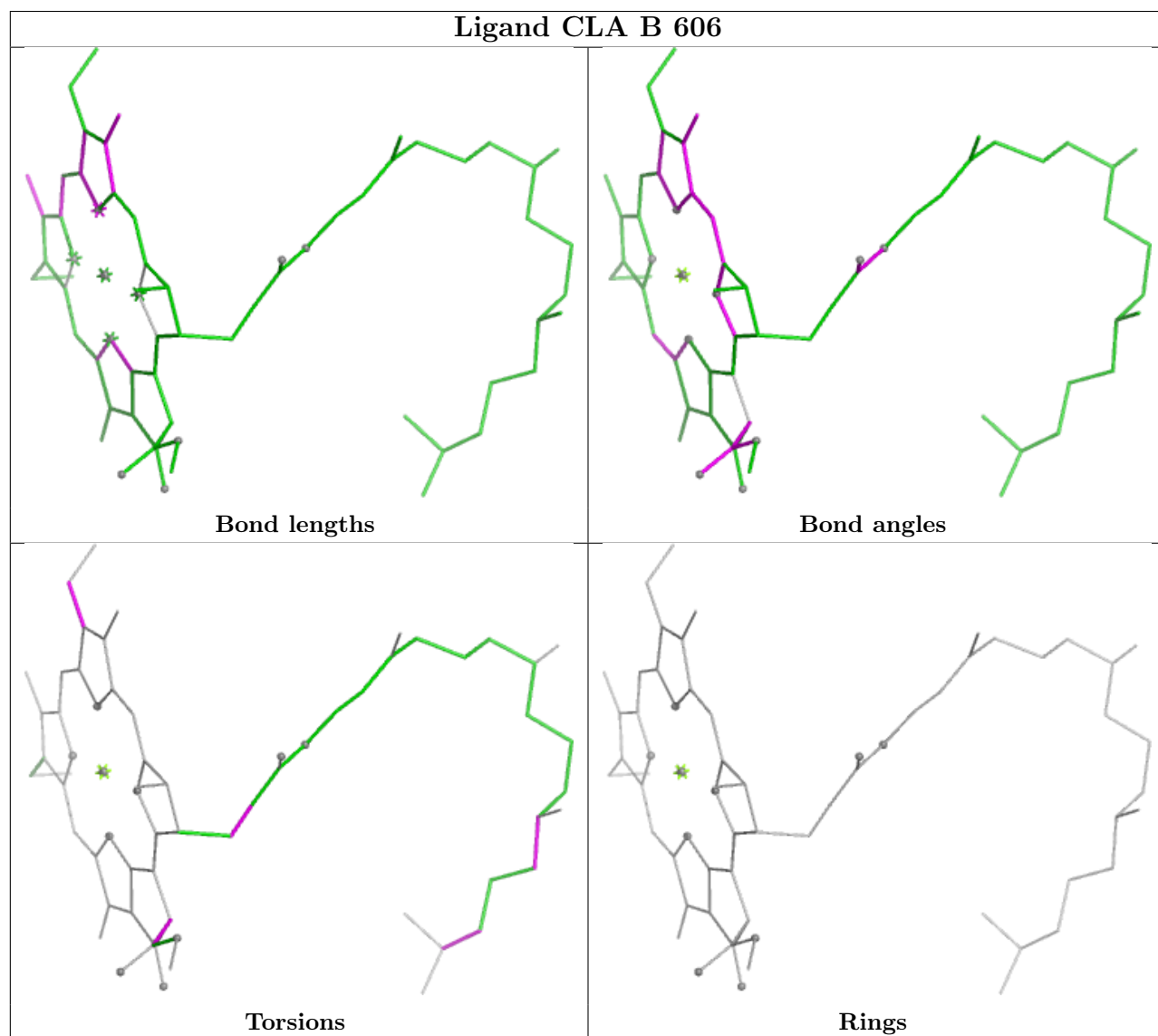
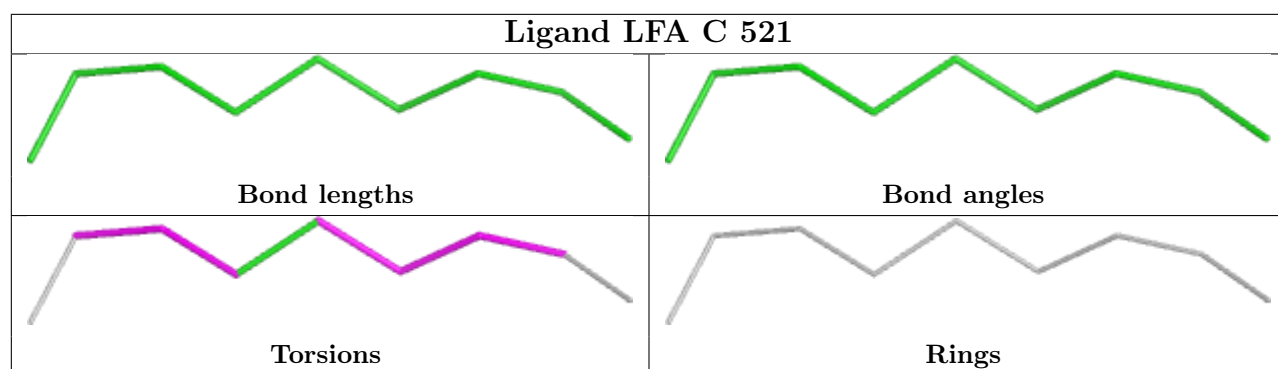
## Ligand DGD C 503



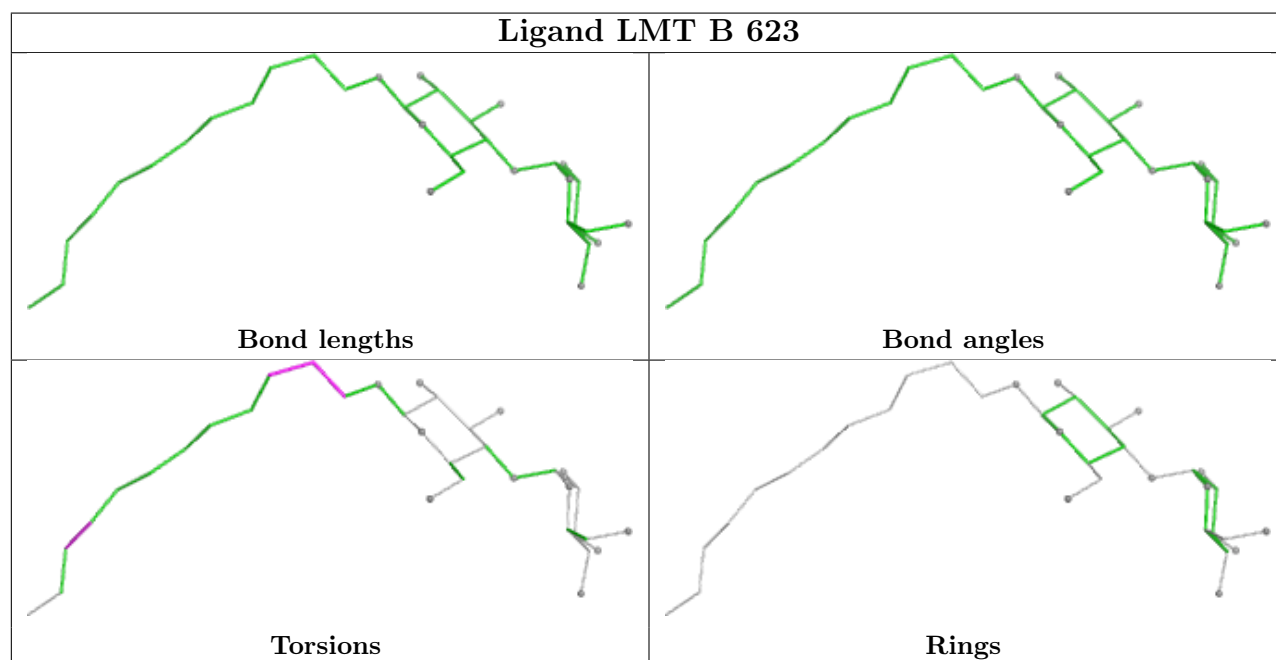
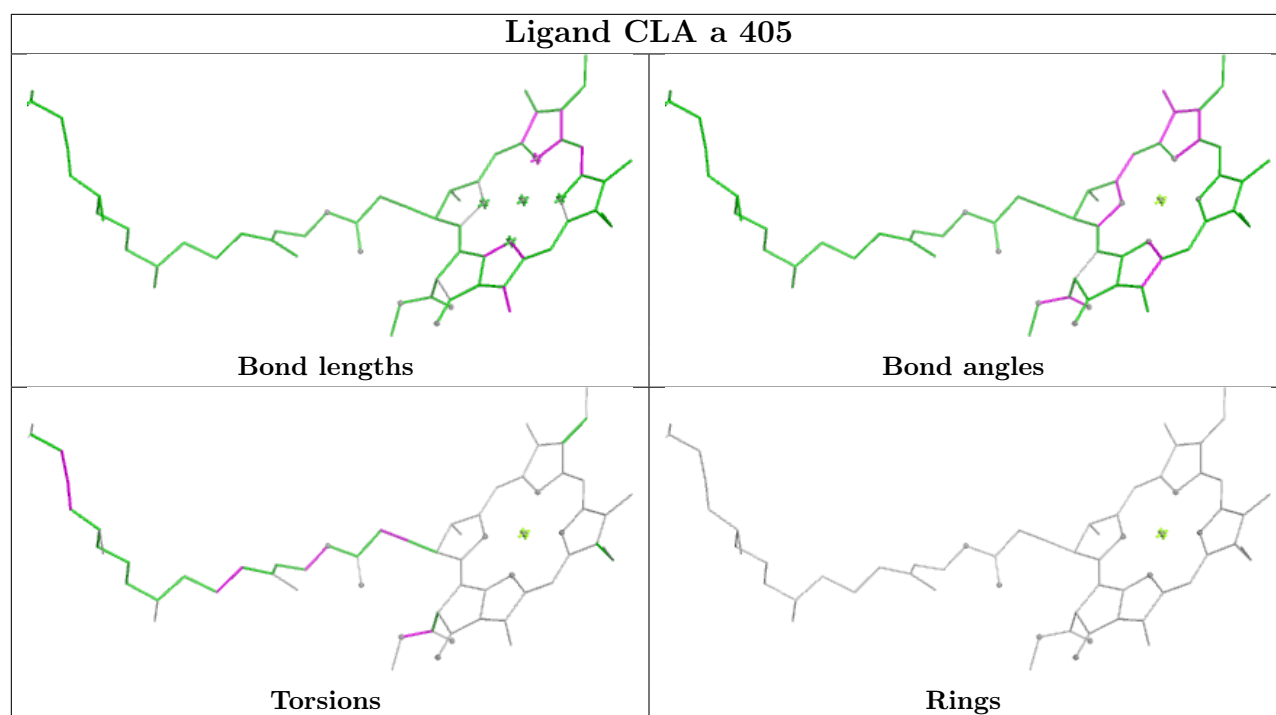


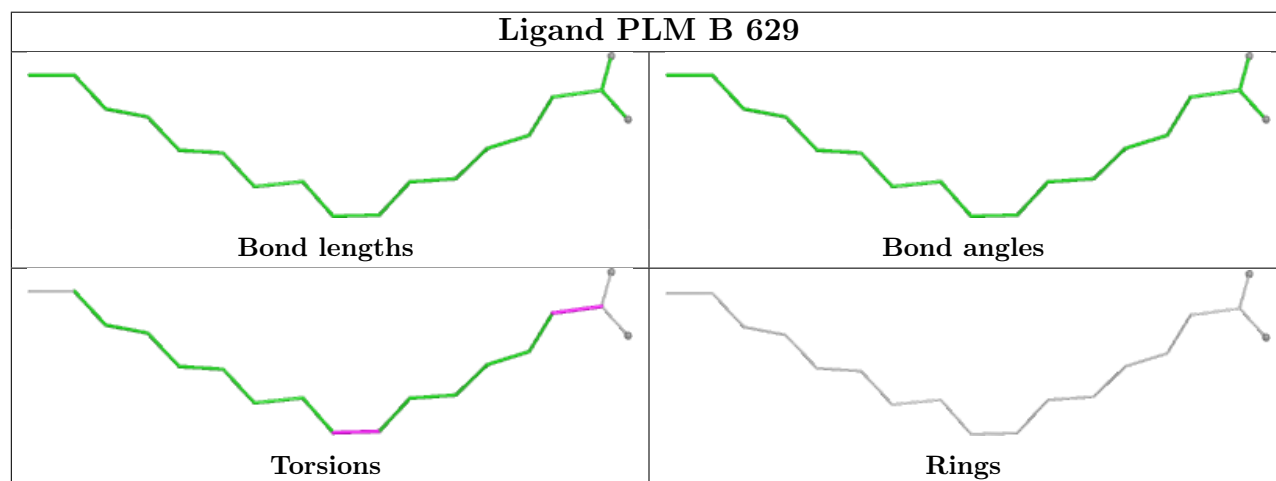
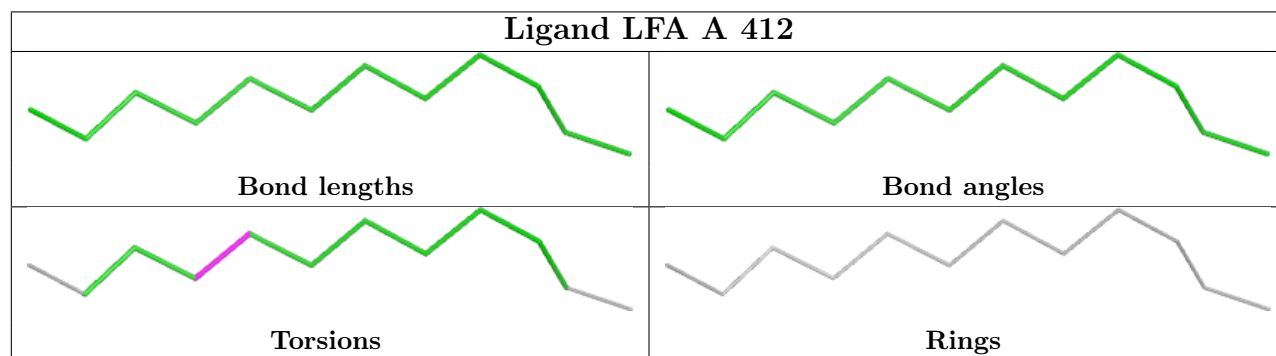
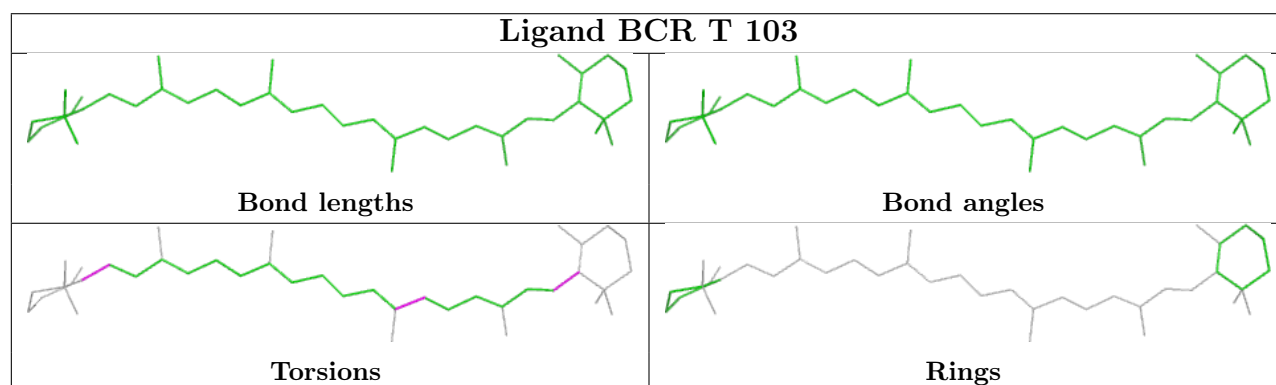
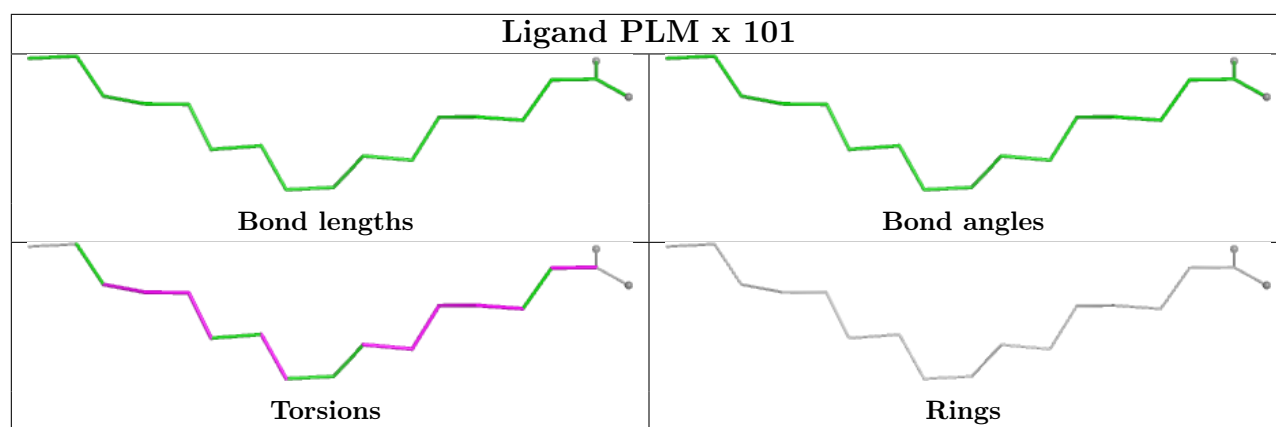


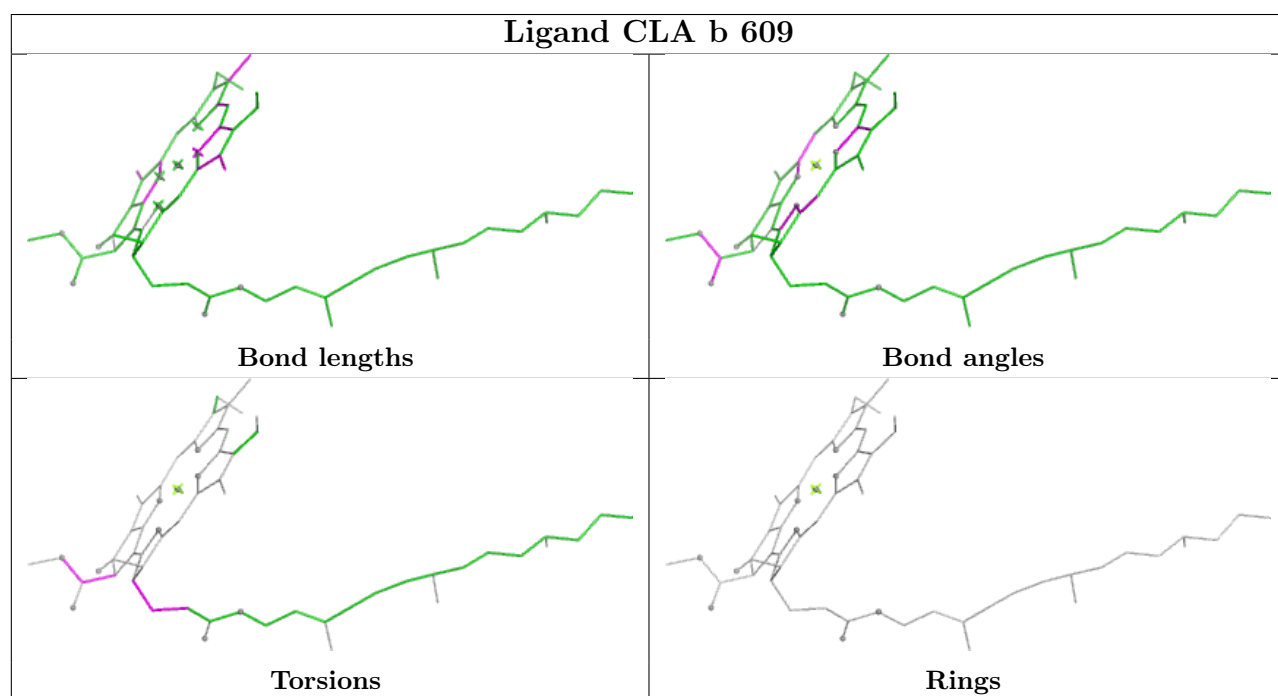
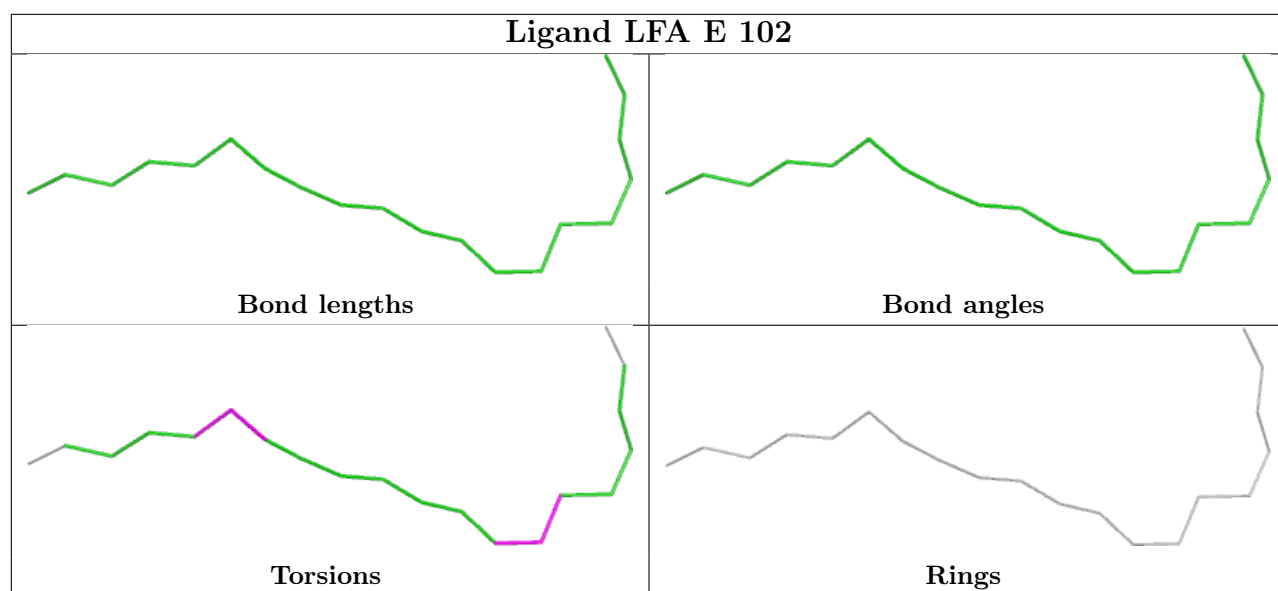




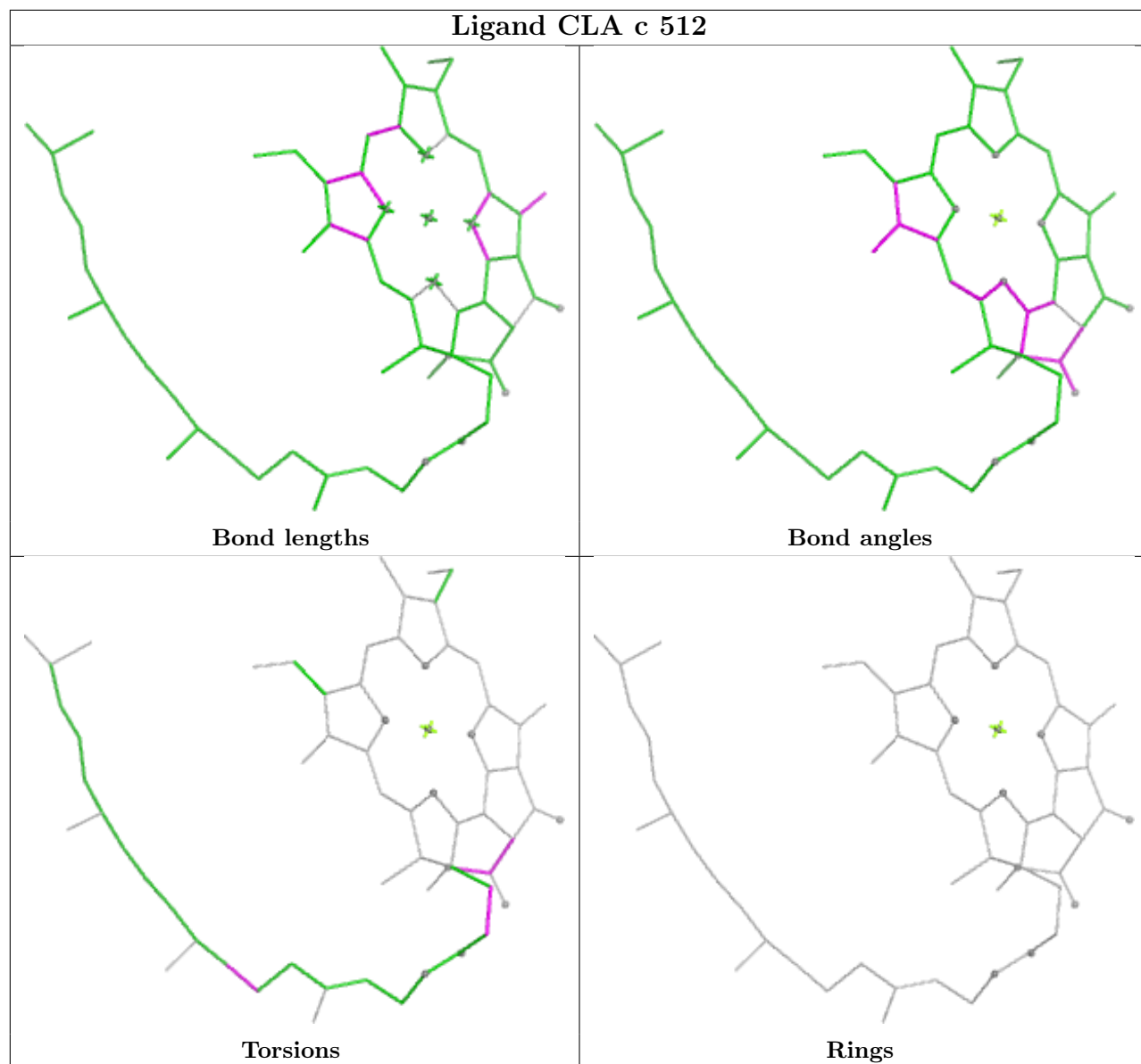




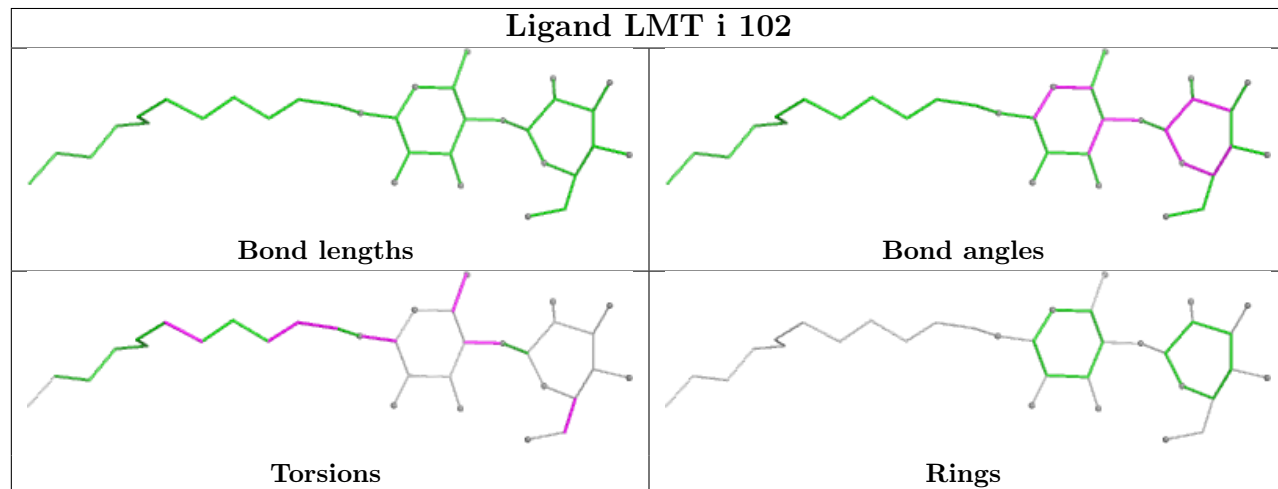


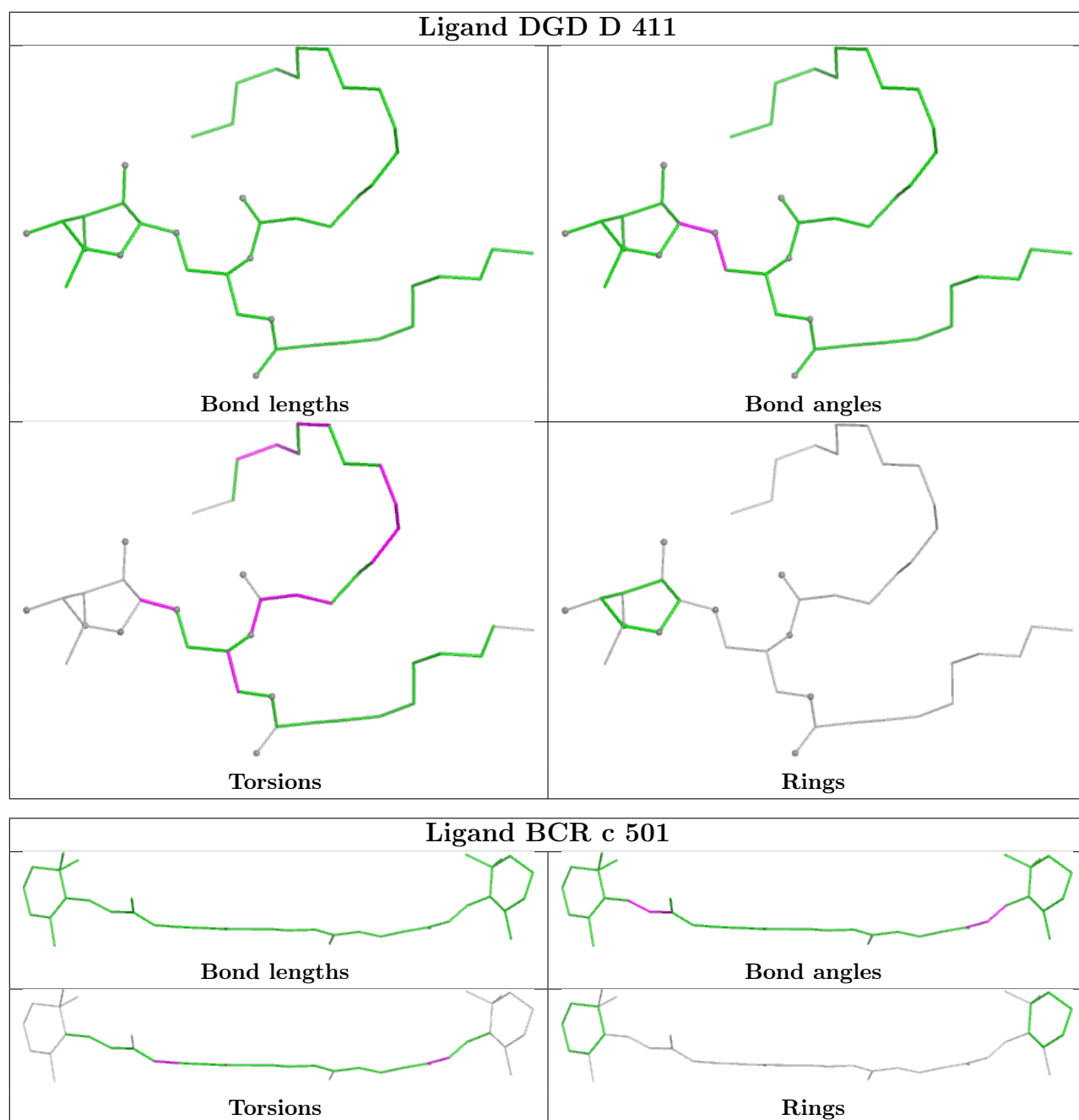


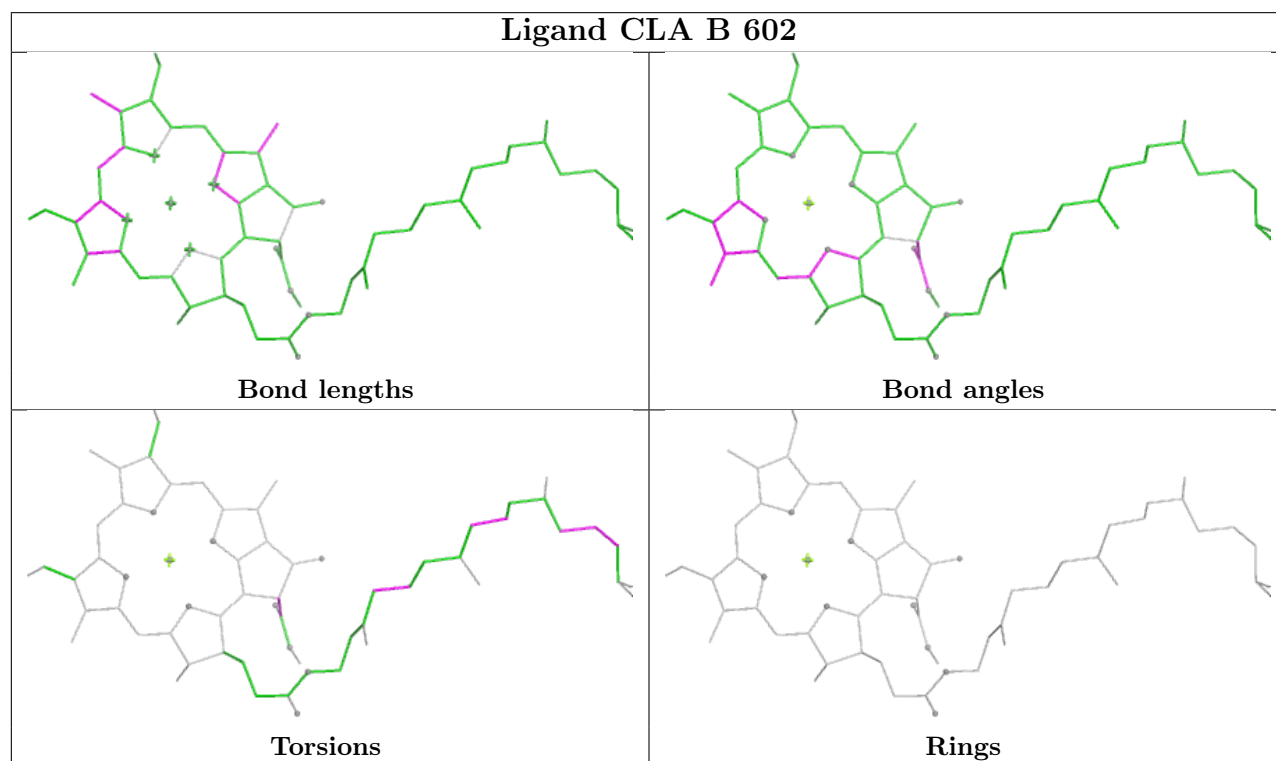
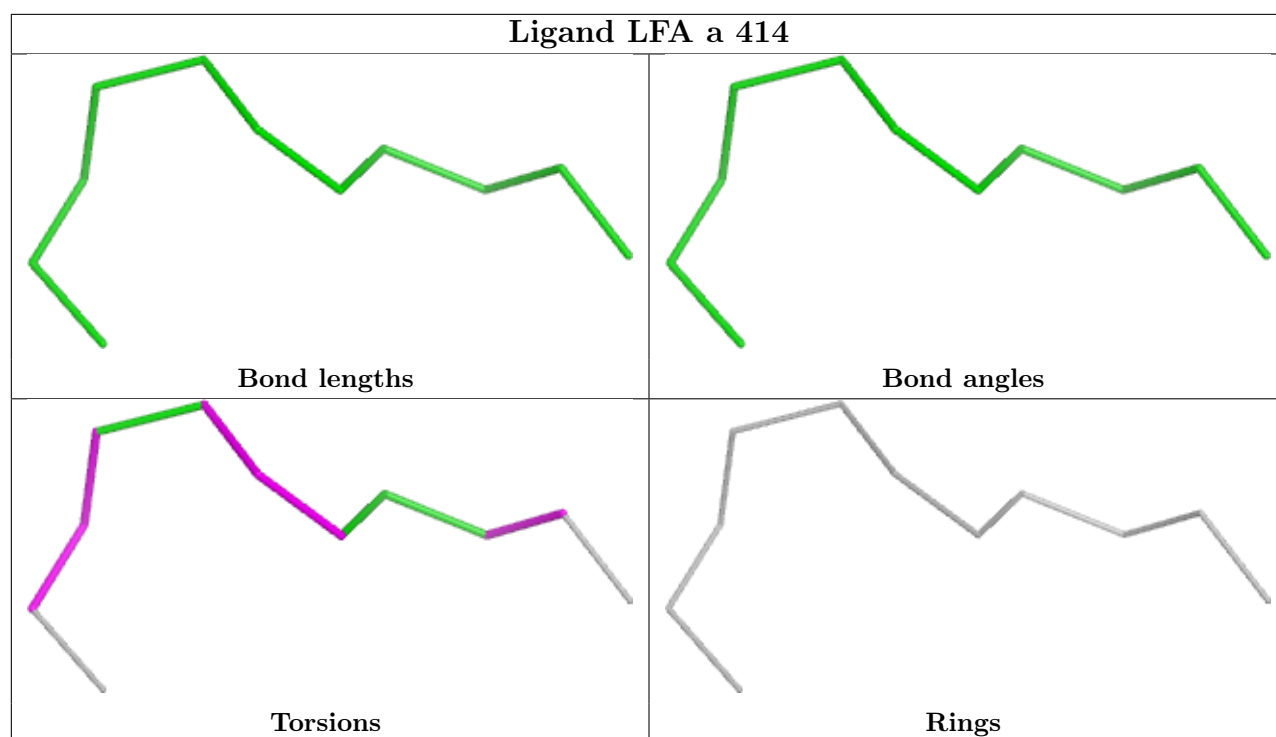
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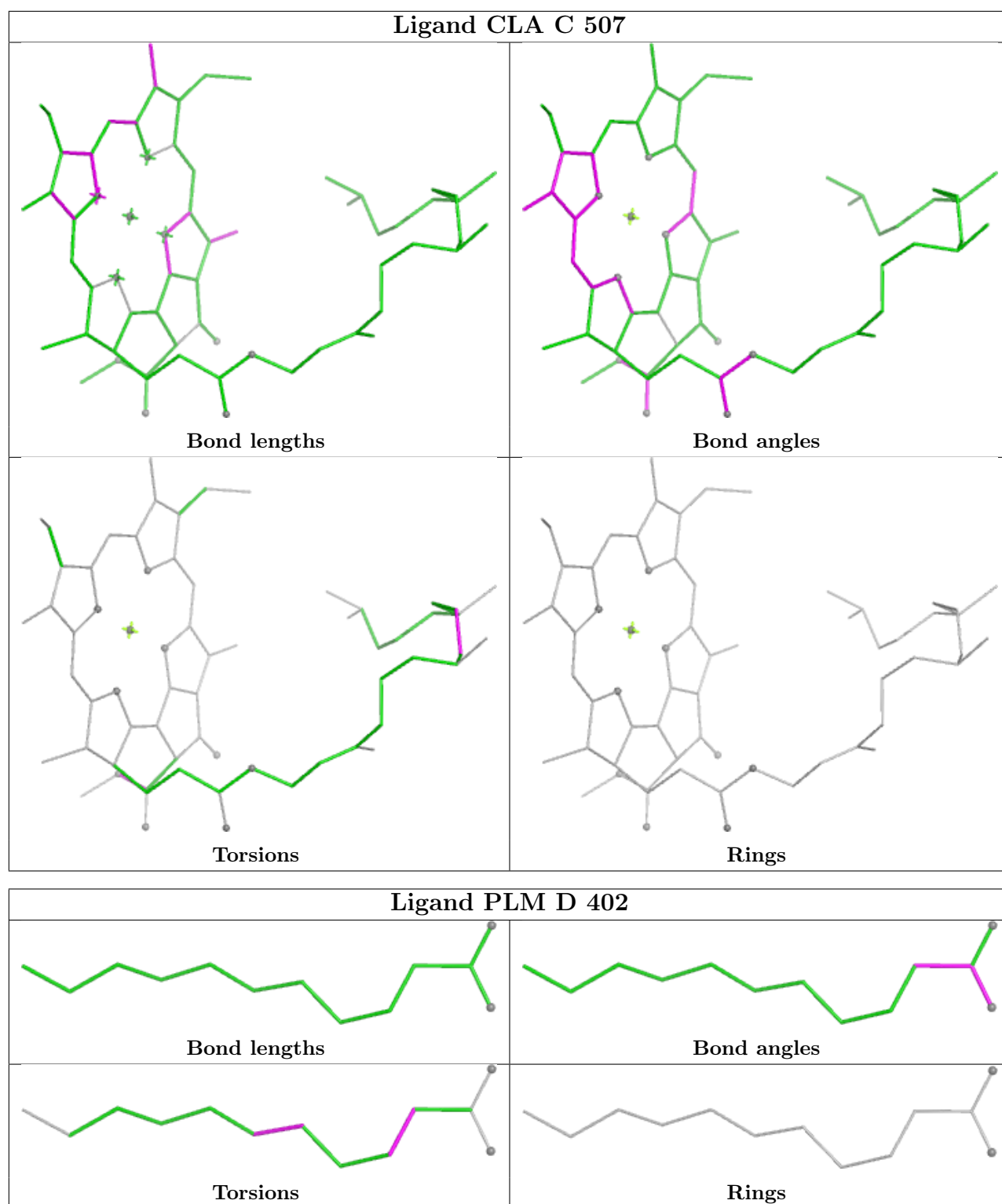


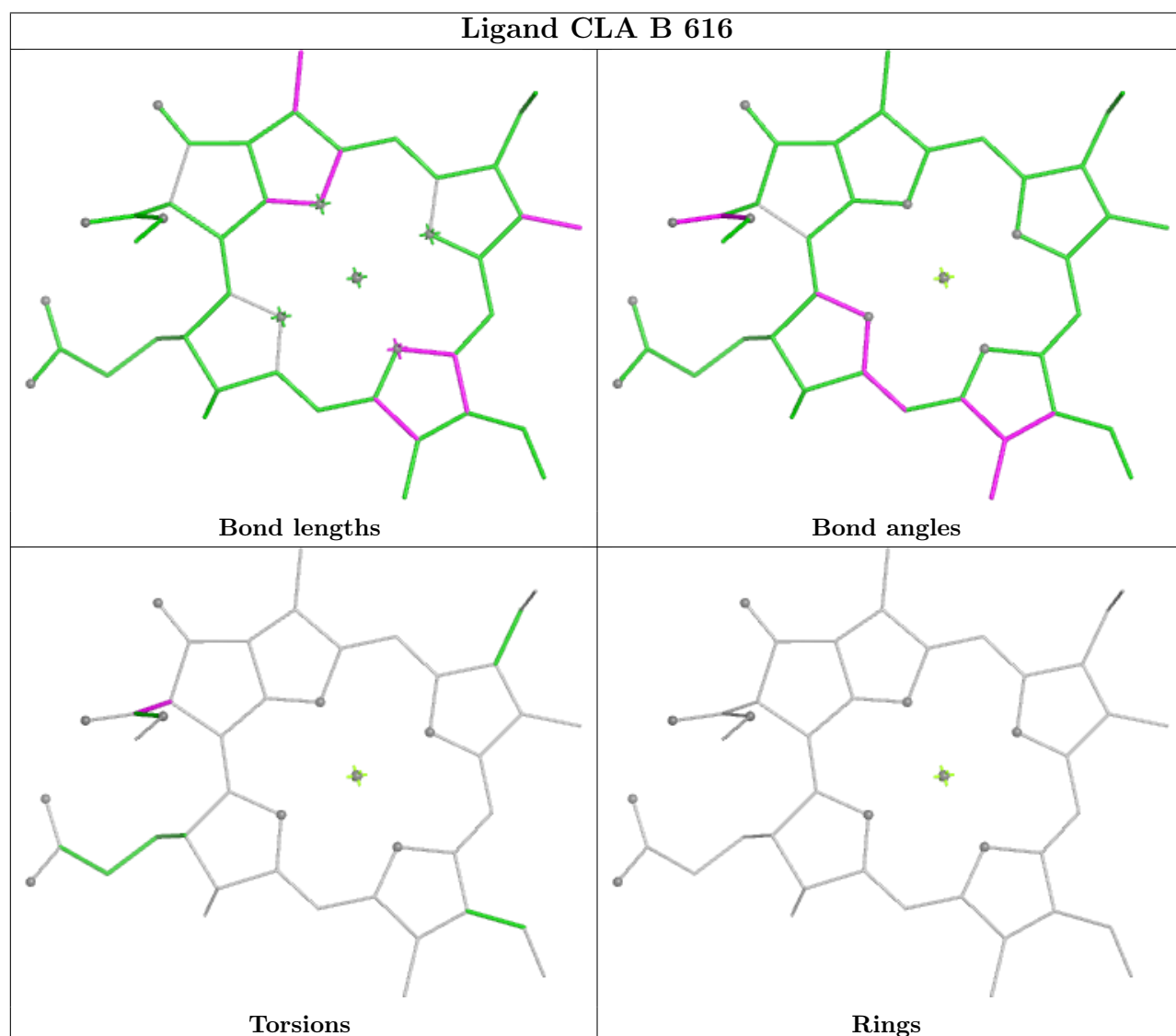
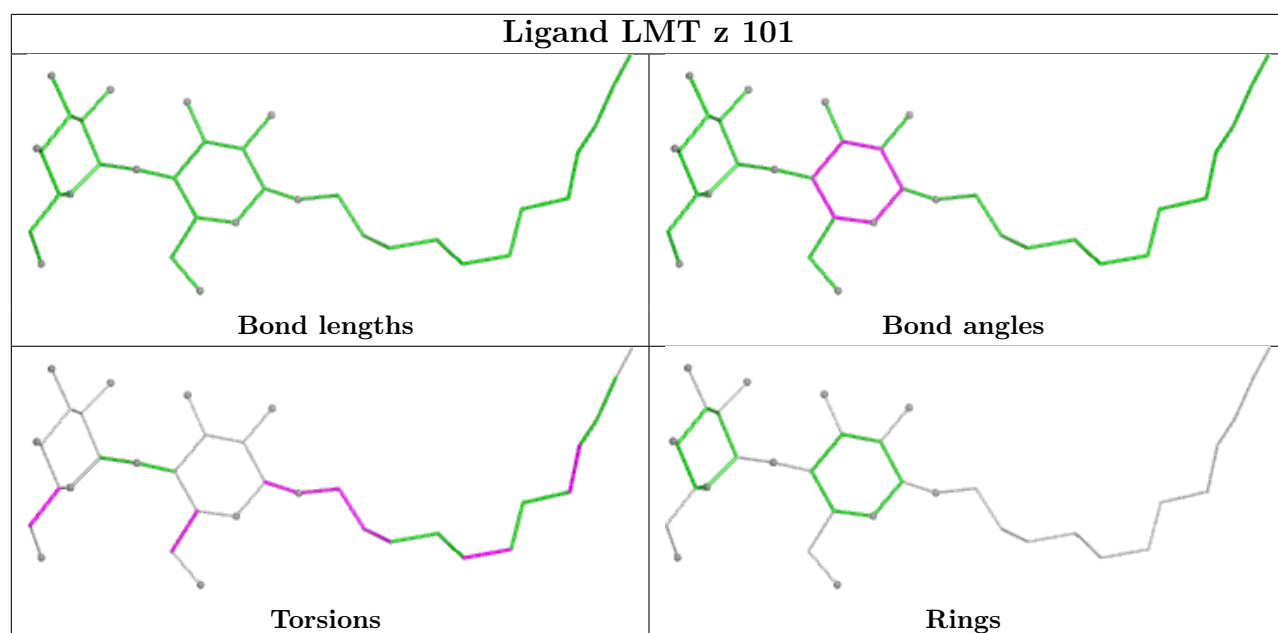
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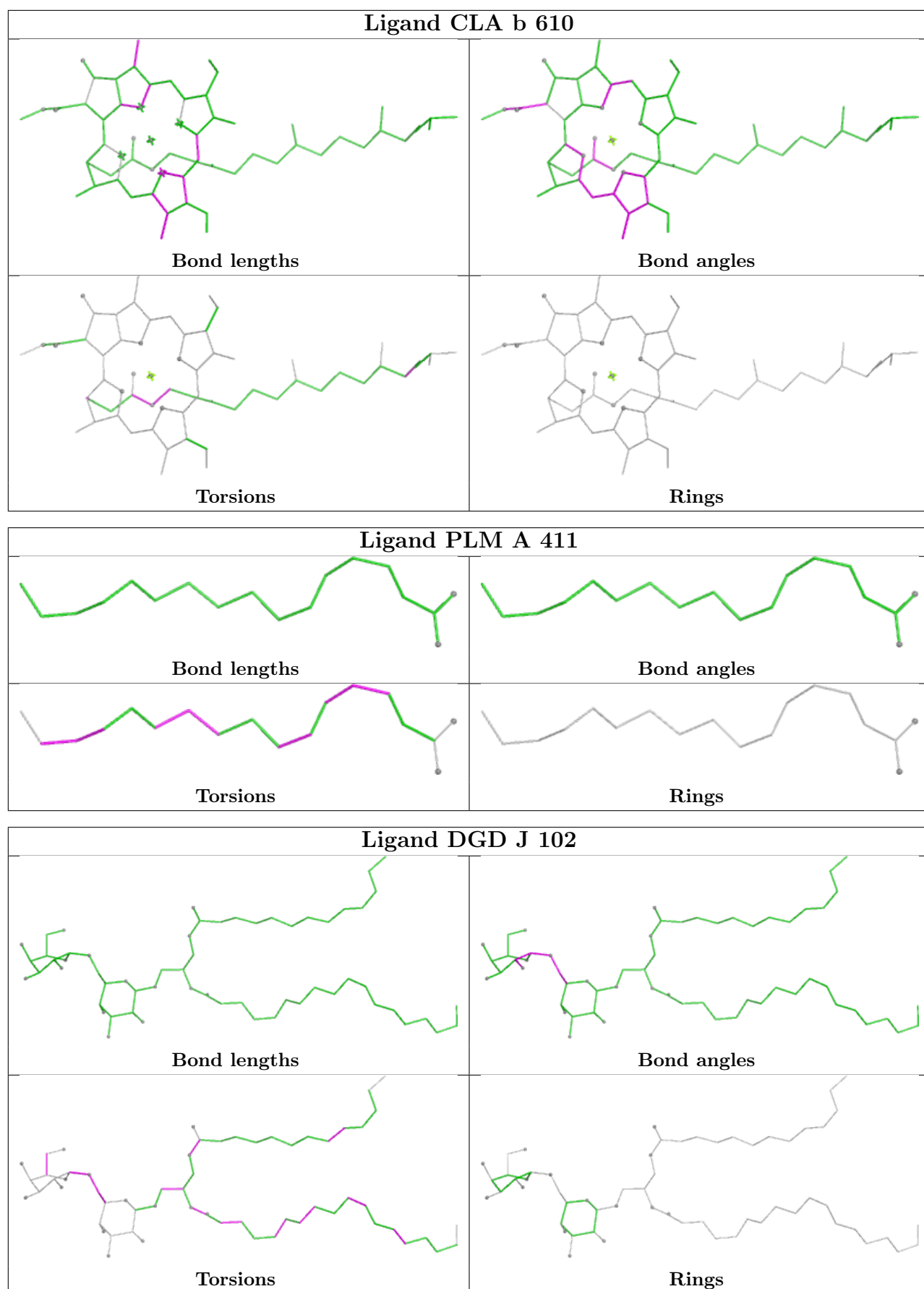


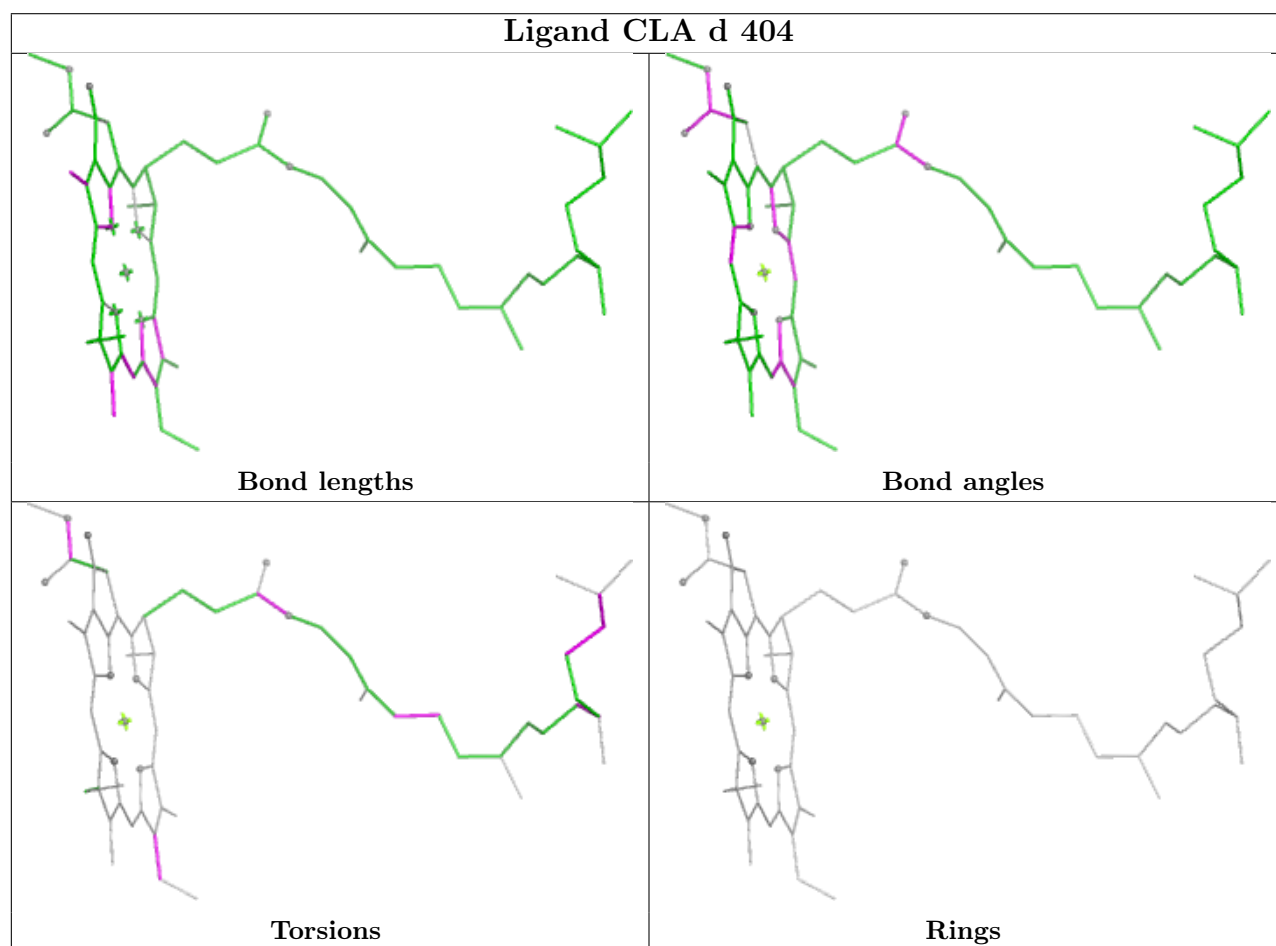
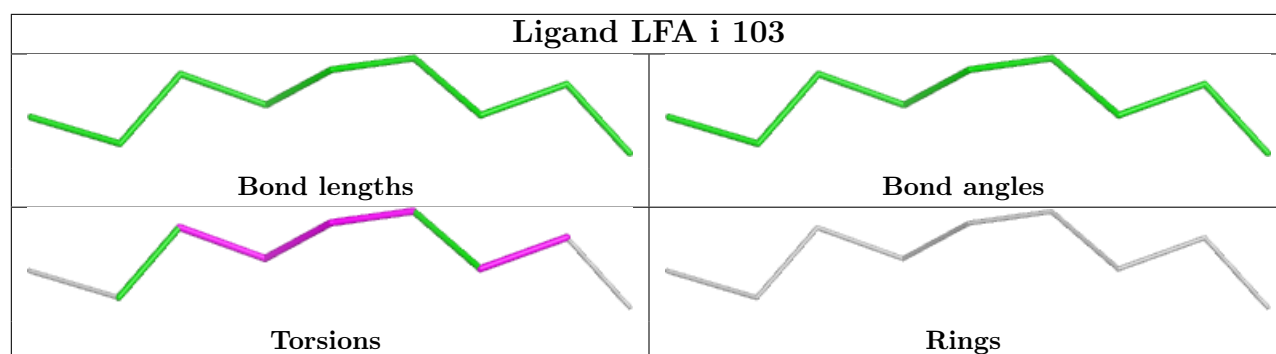




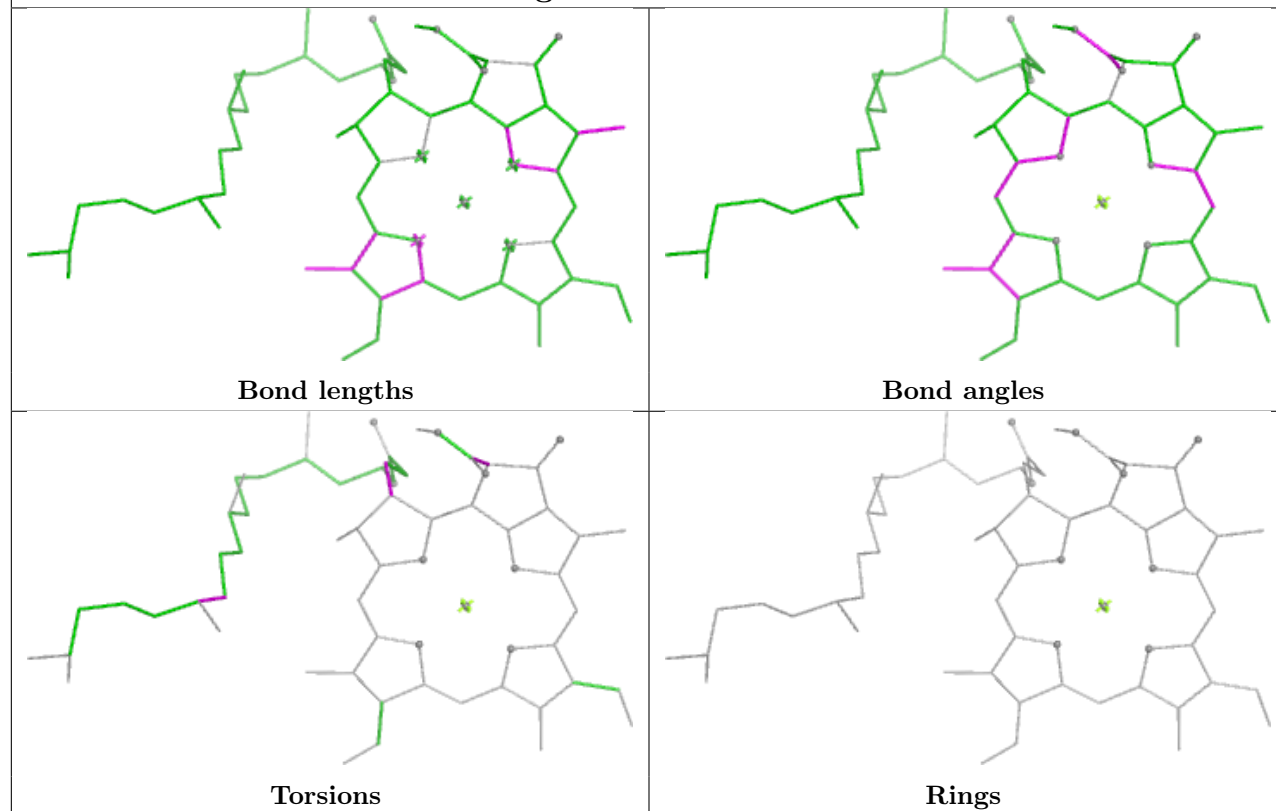




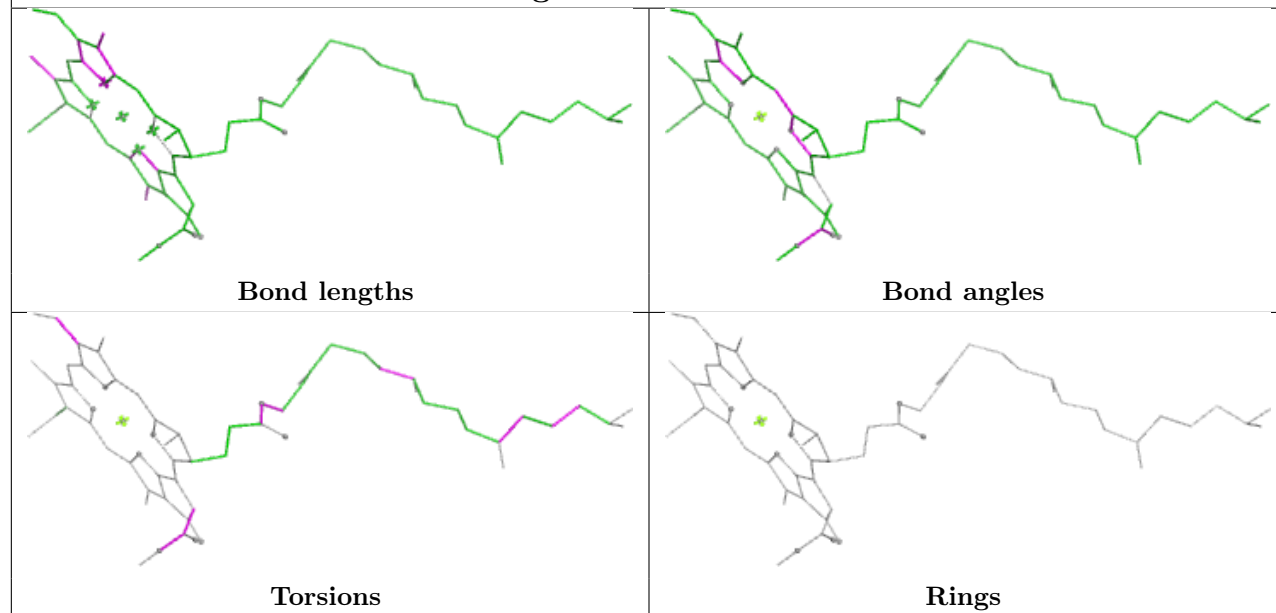


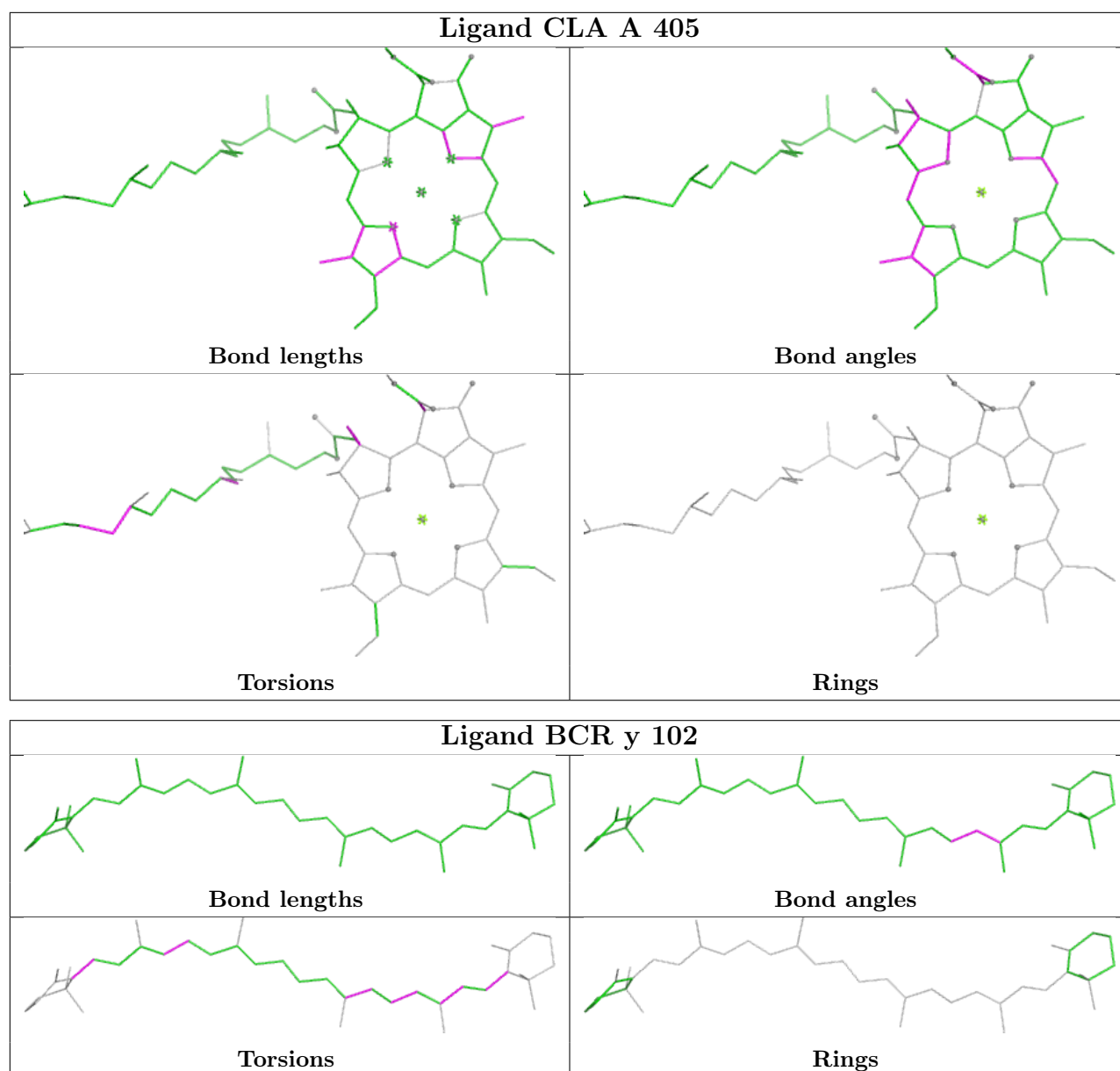


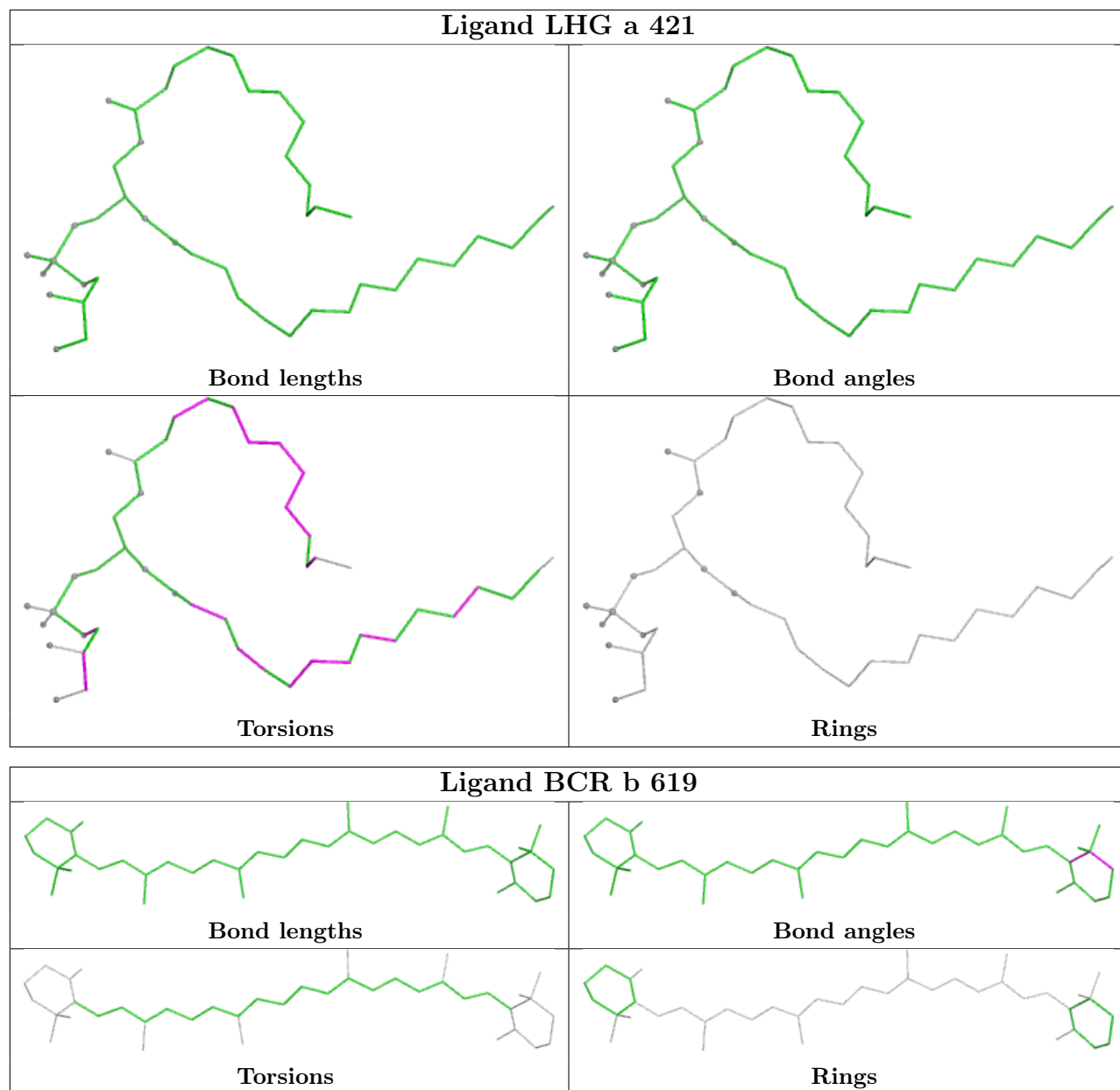
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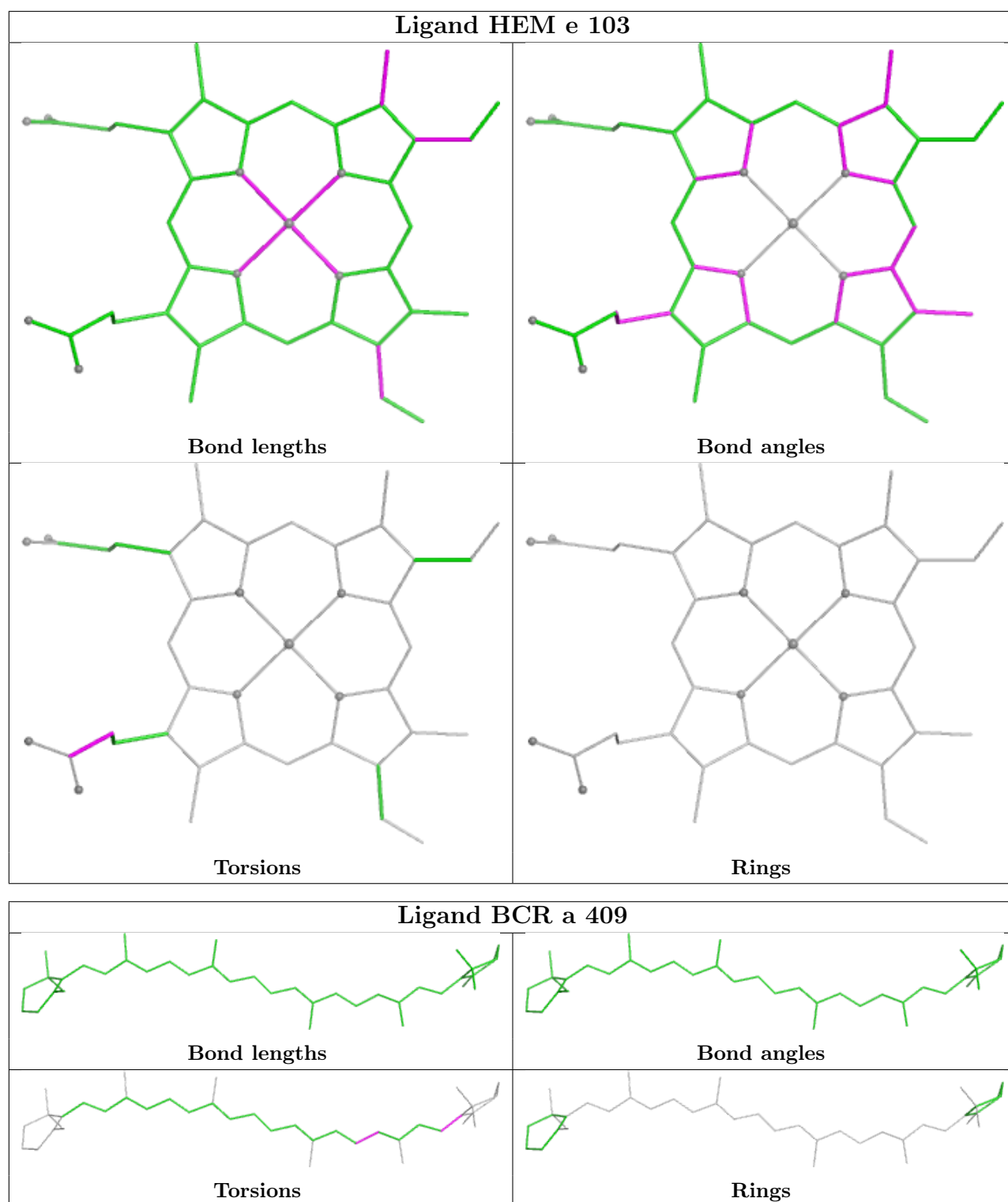


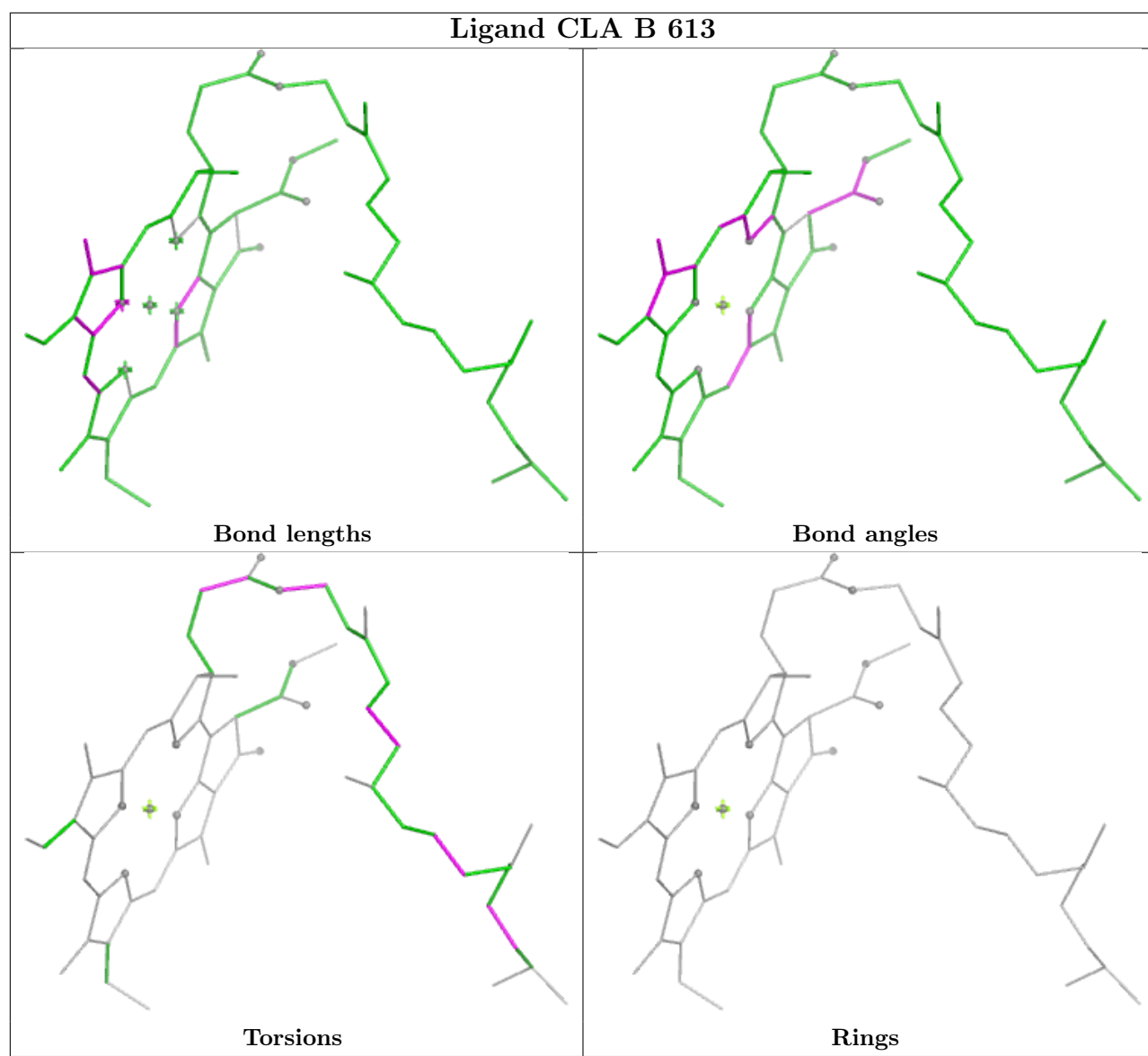
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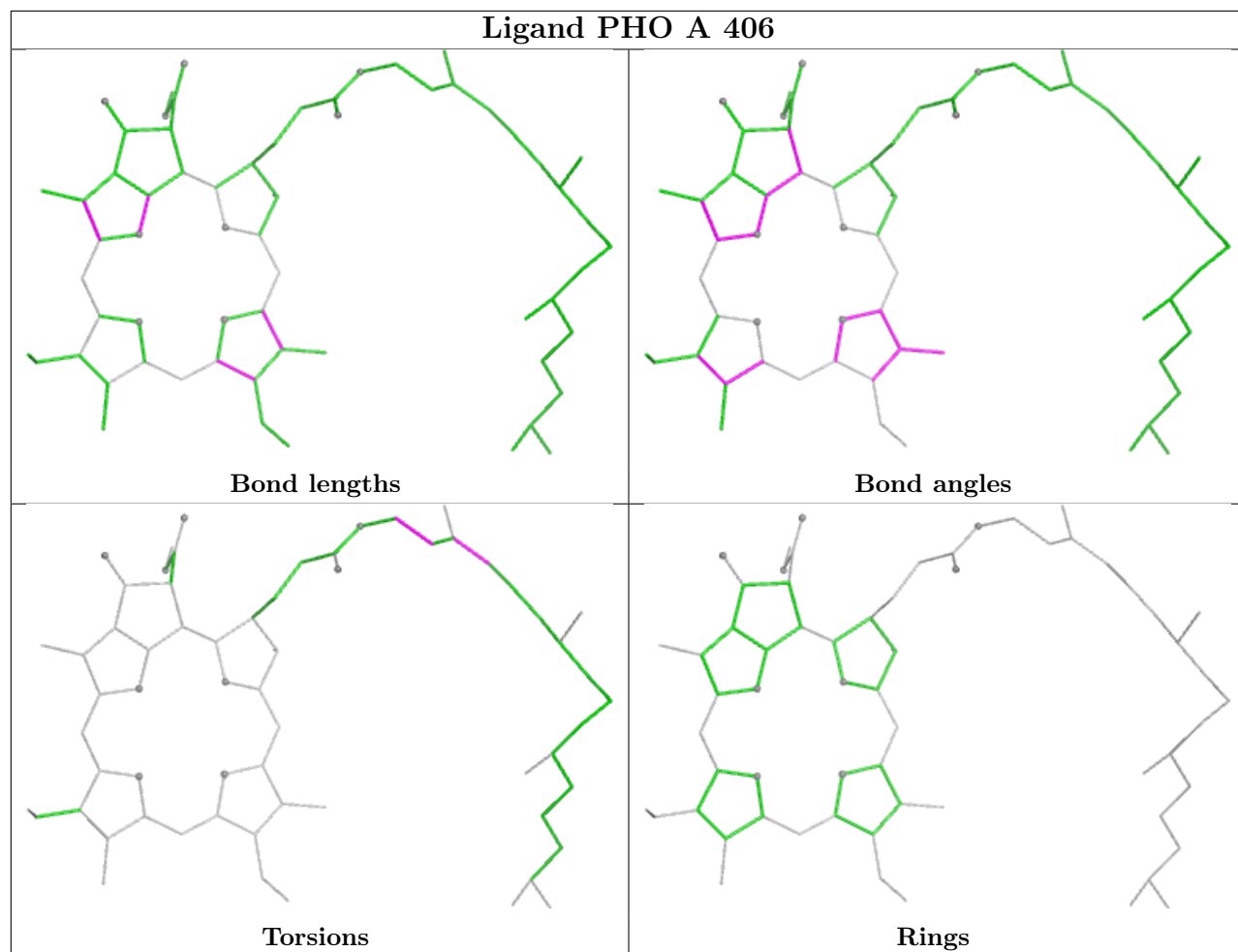




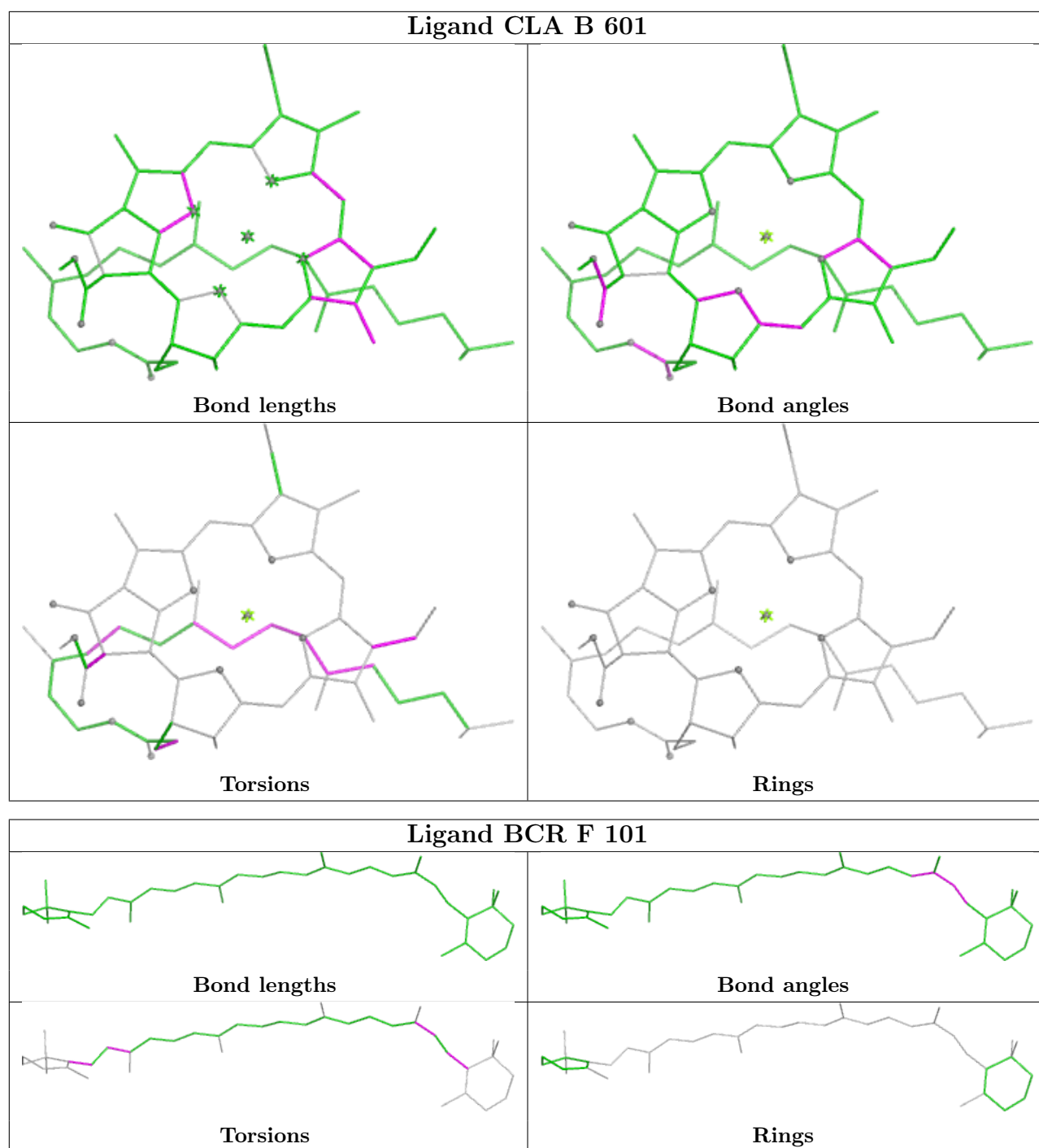


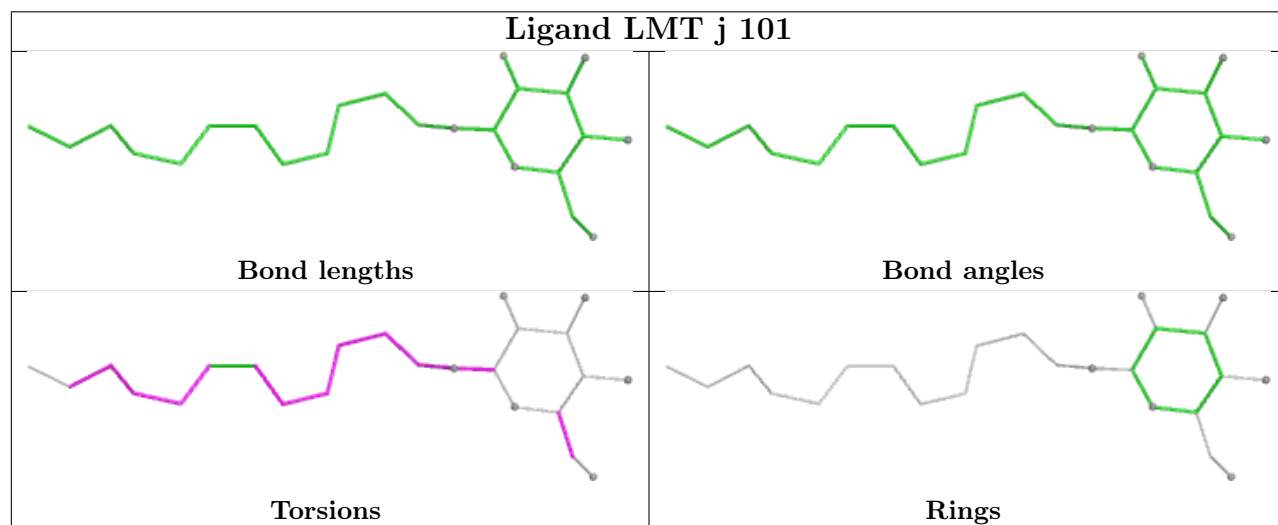
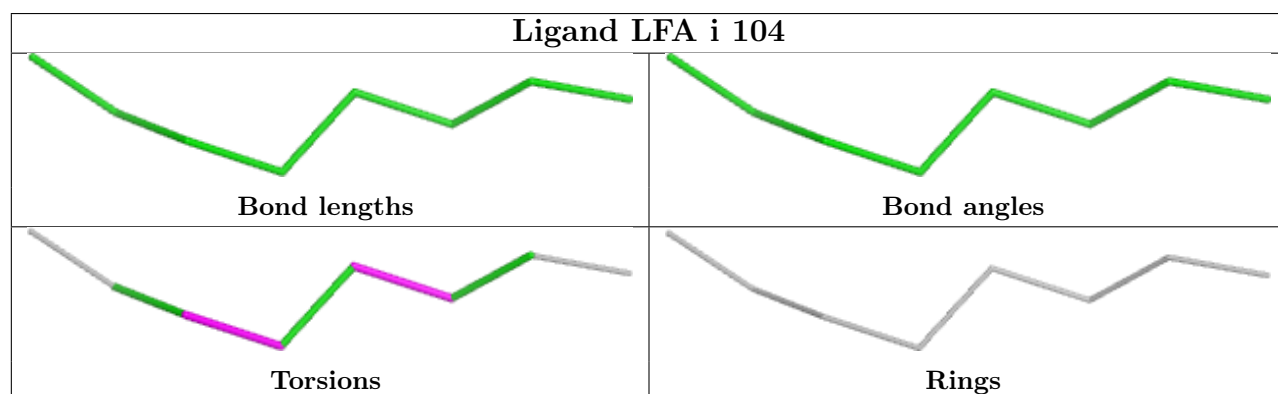
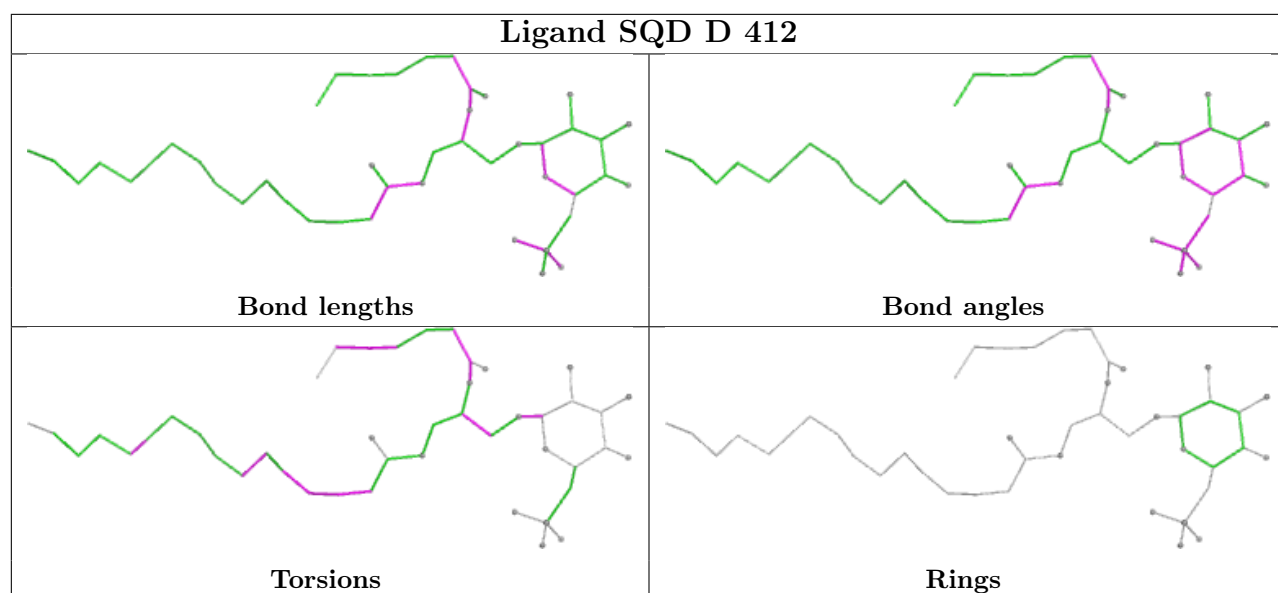


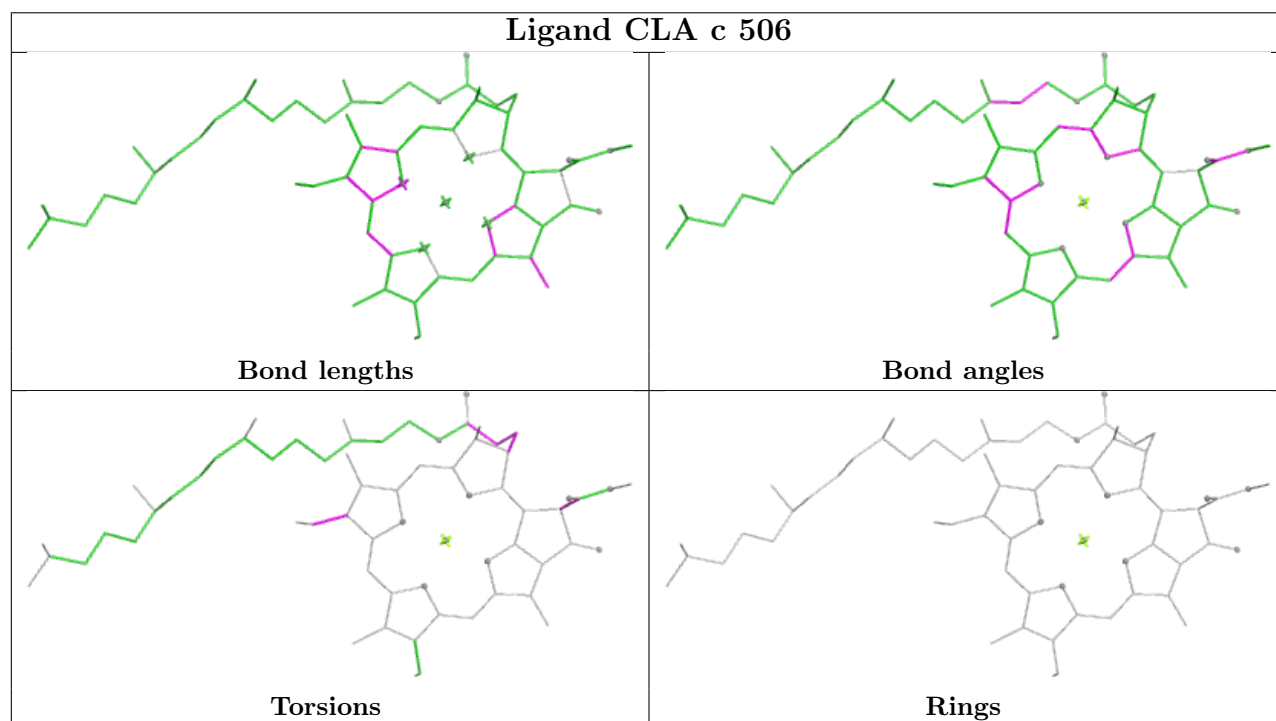
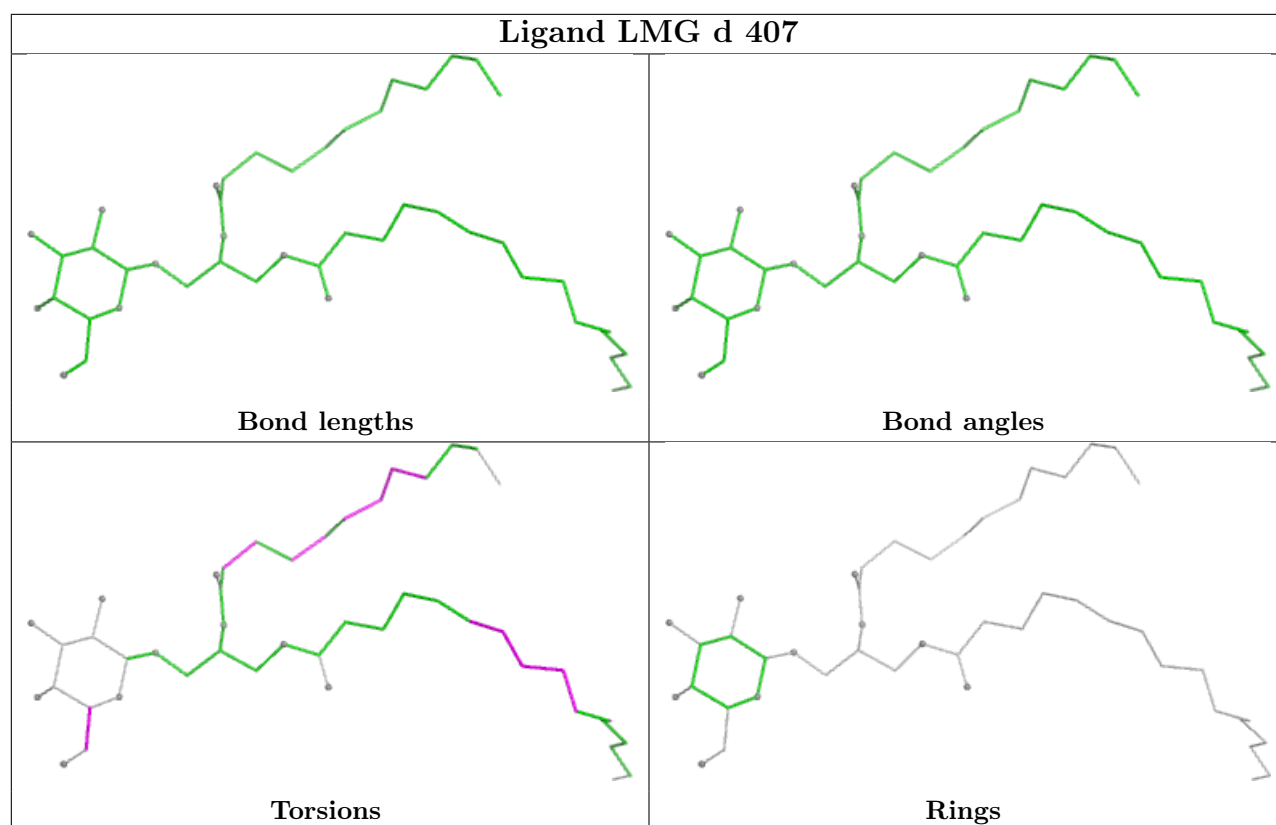


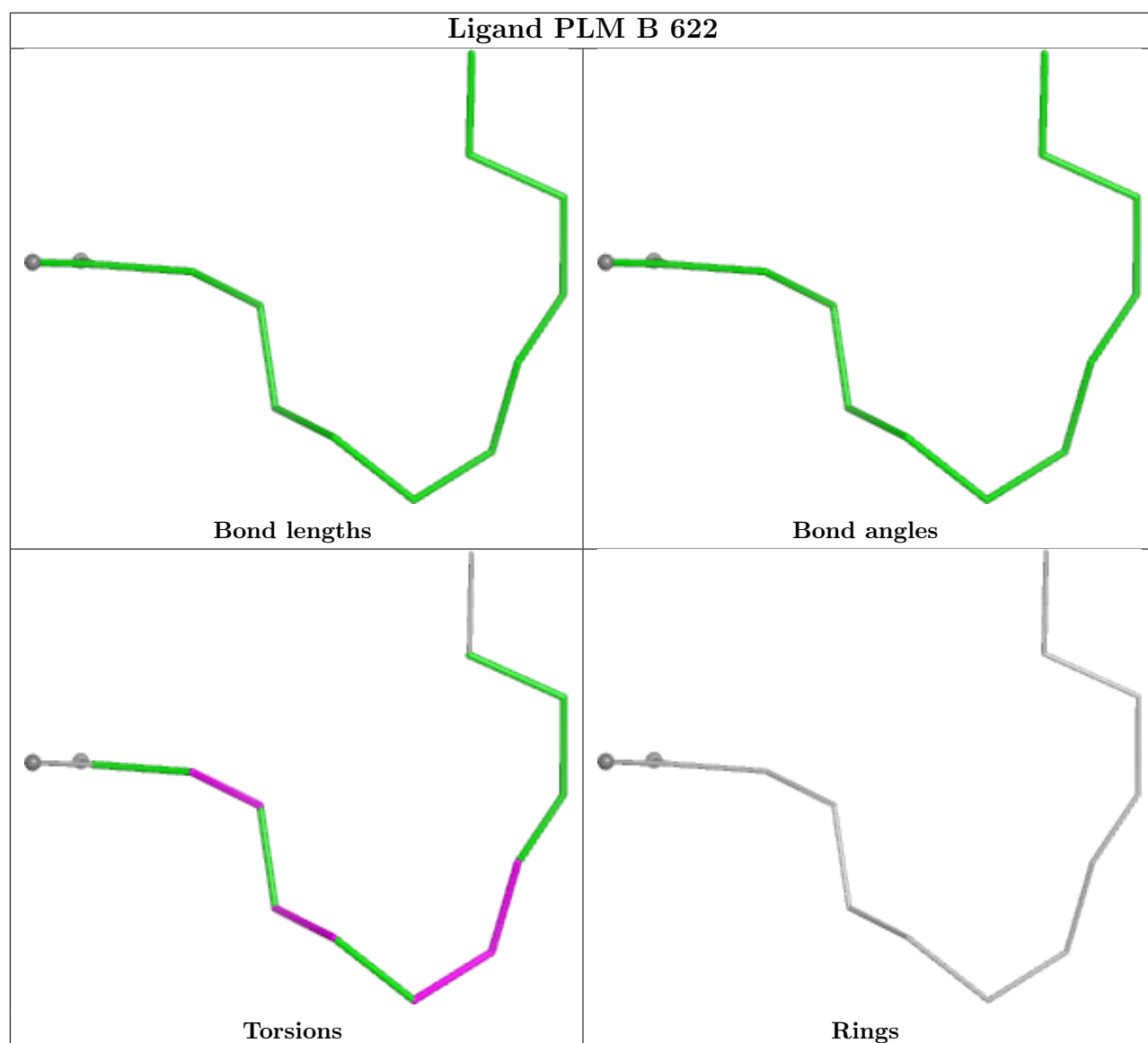


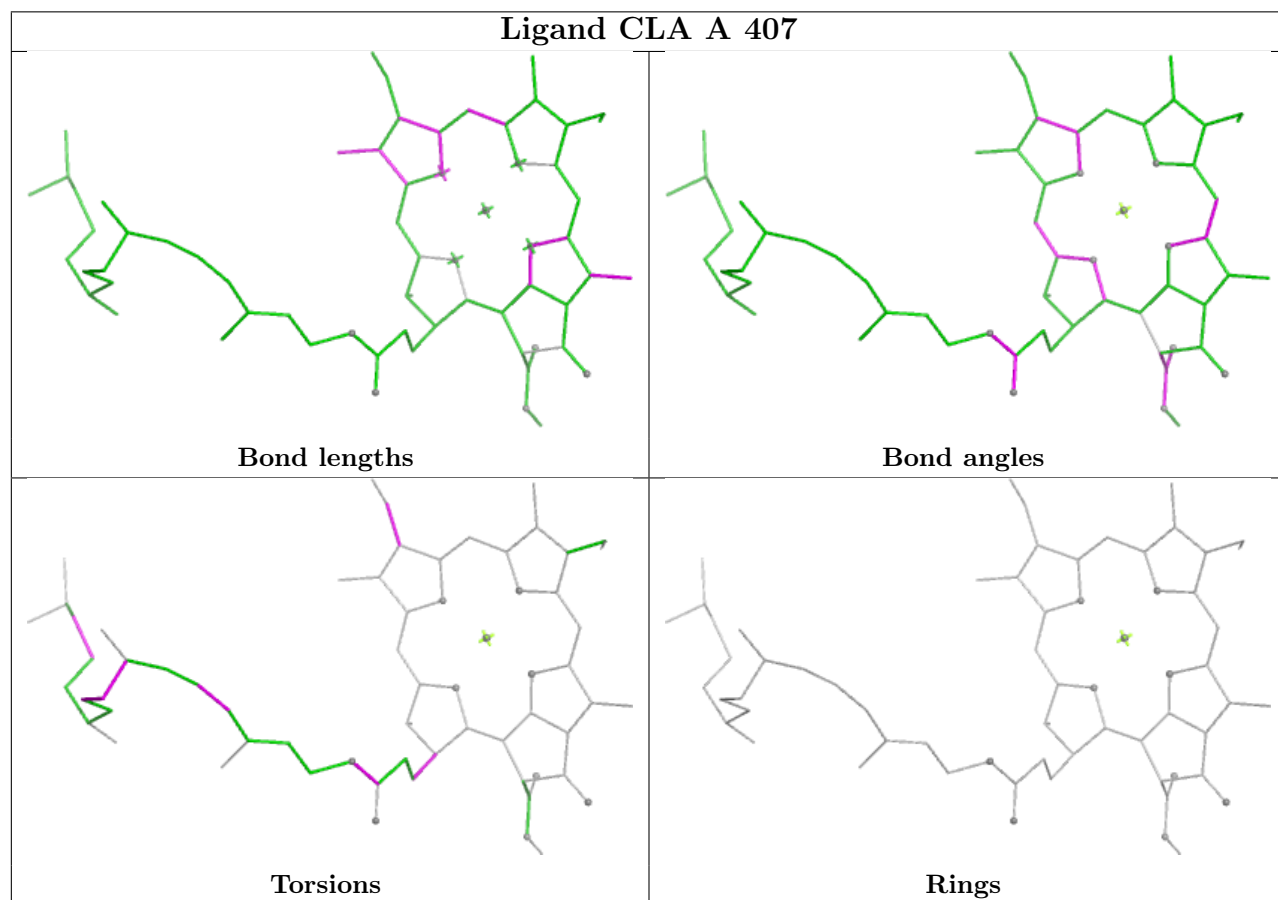
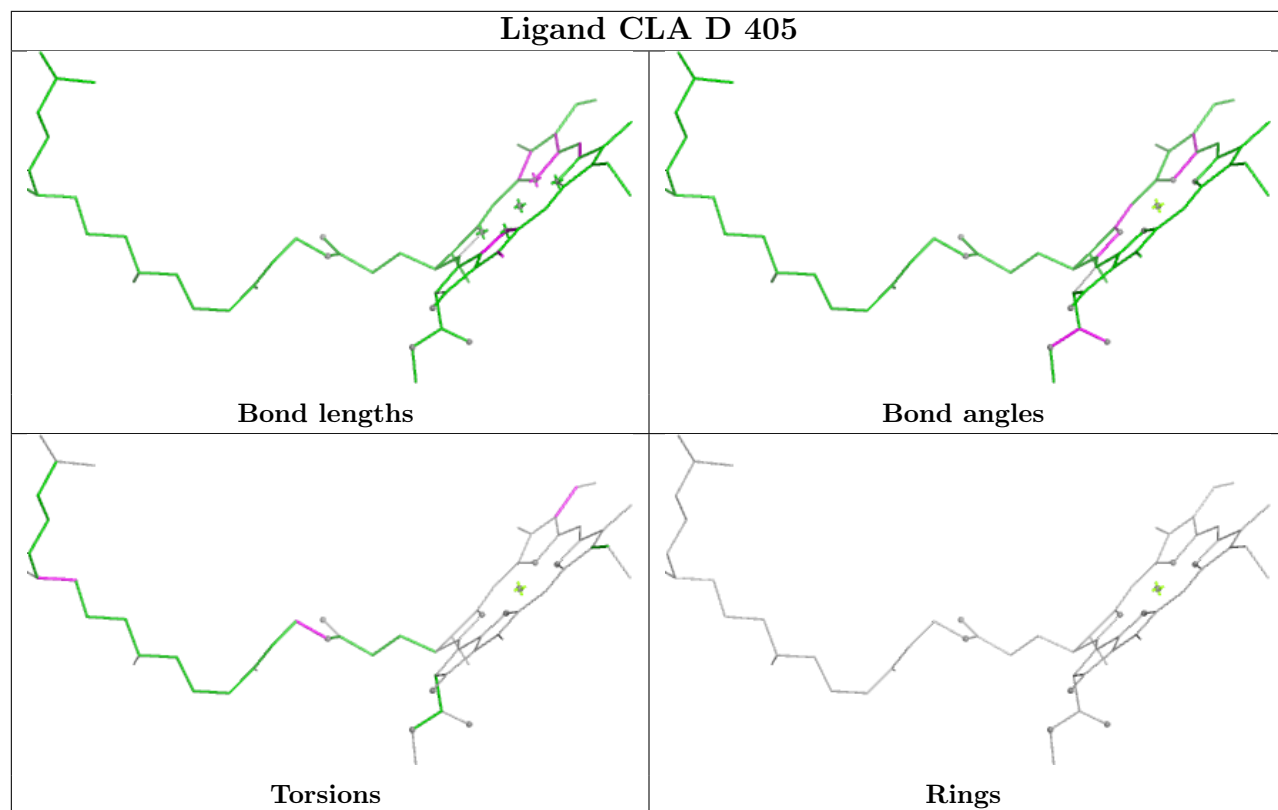


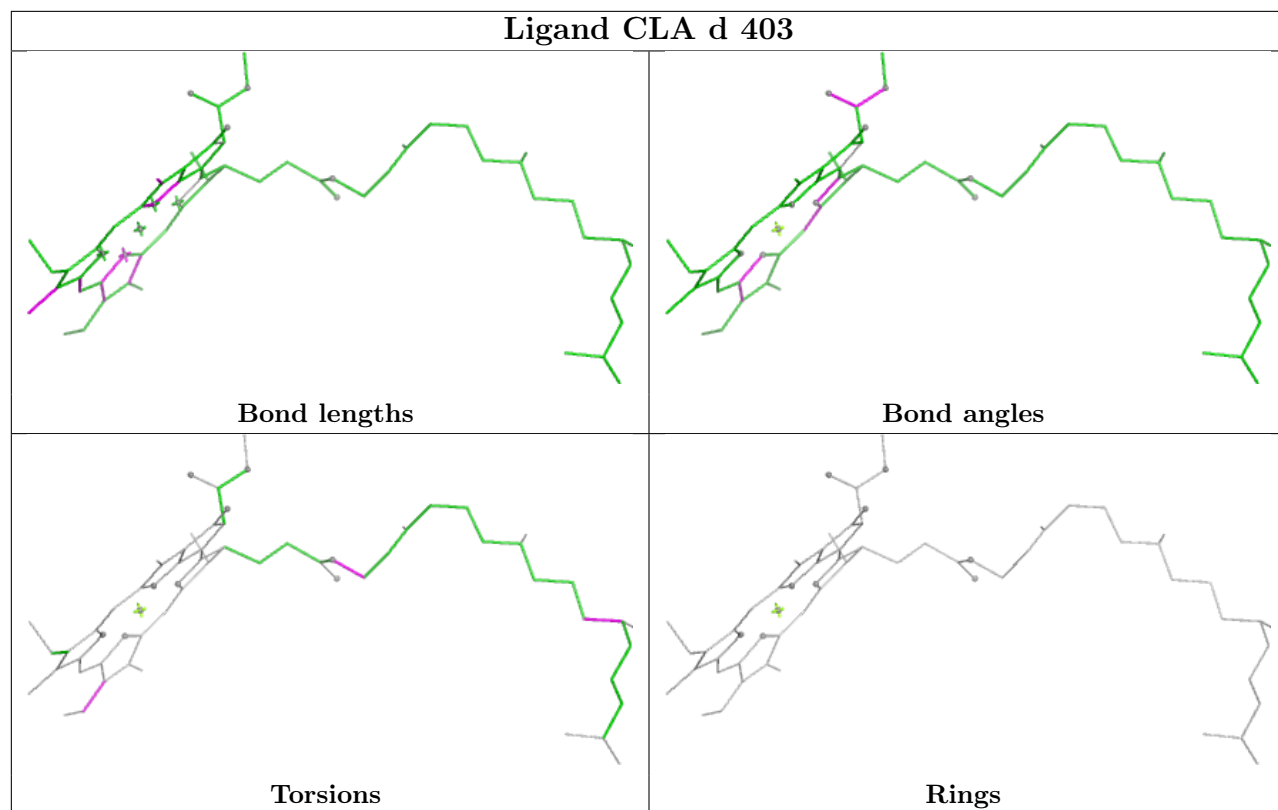




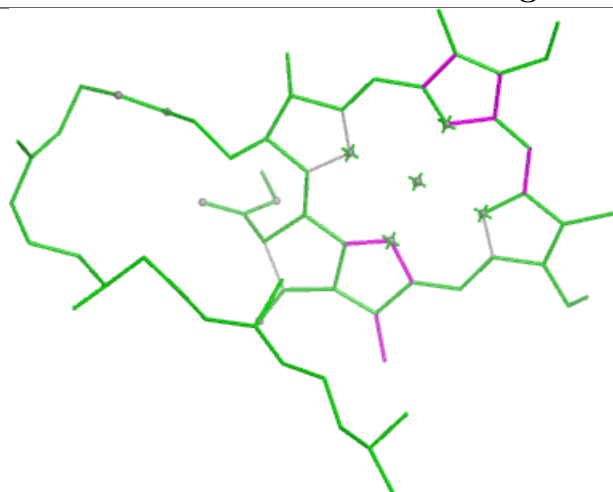




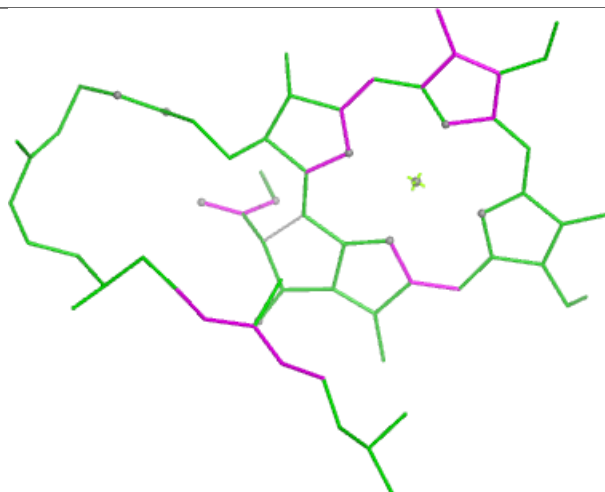




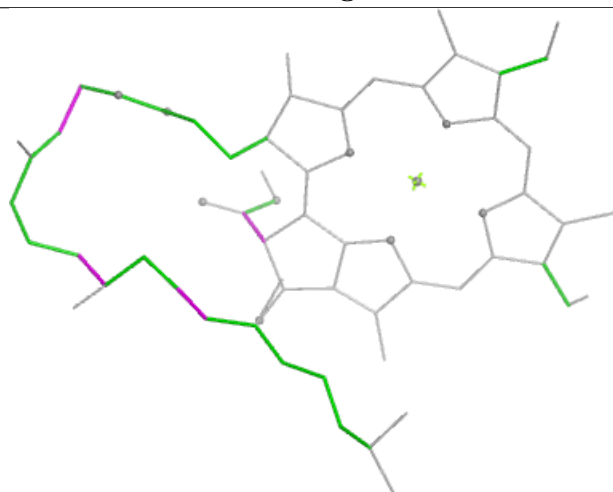
## Ligand CLA c 514



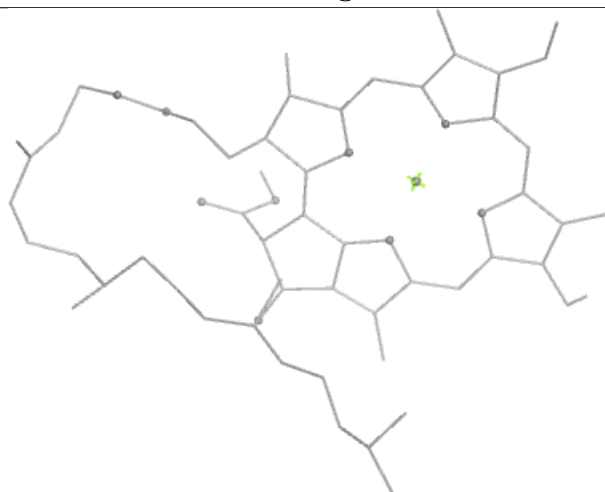
Bond lengths



Bond angles



Torsions

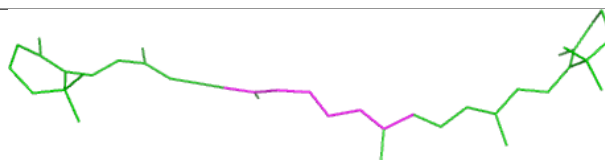


Rings

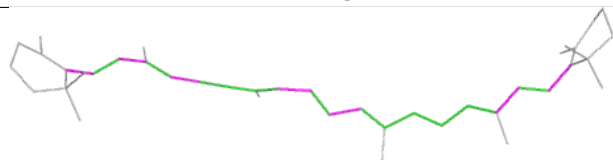
## Ligand BCR b 602



Bond lengths



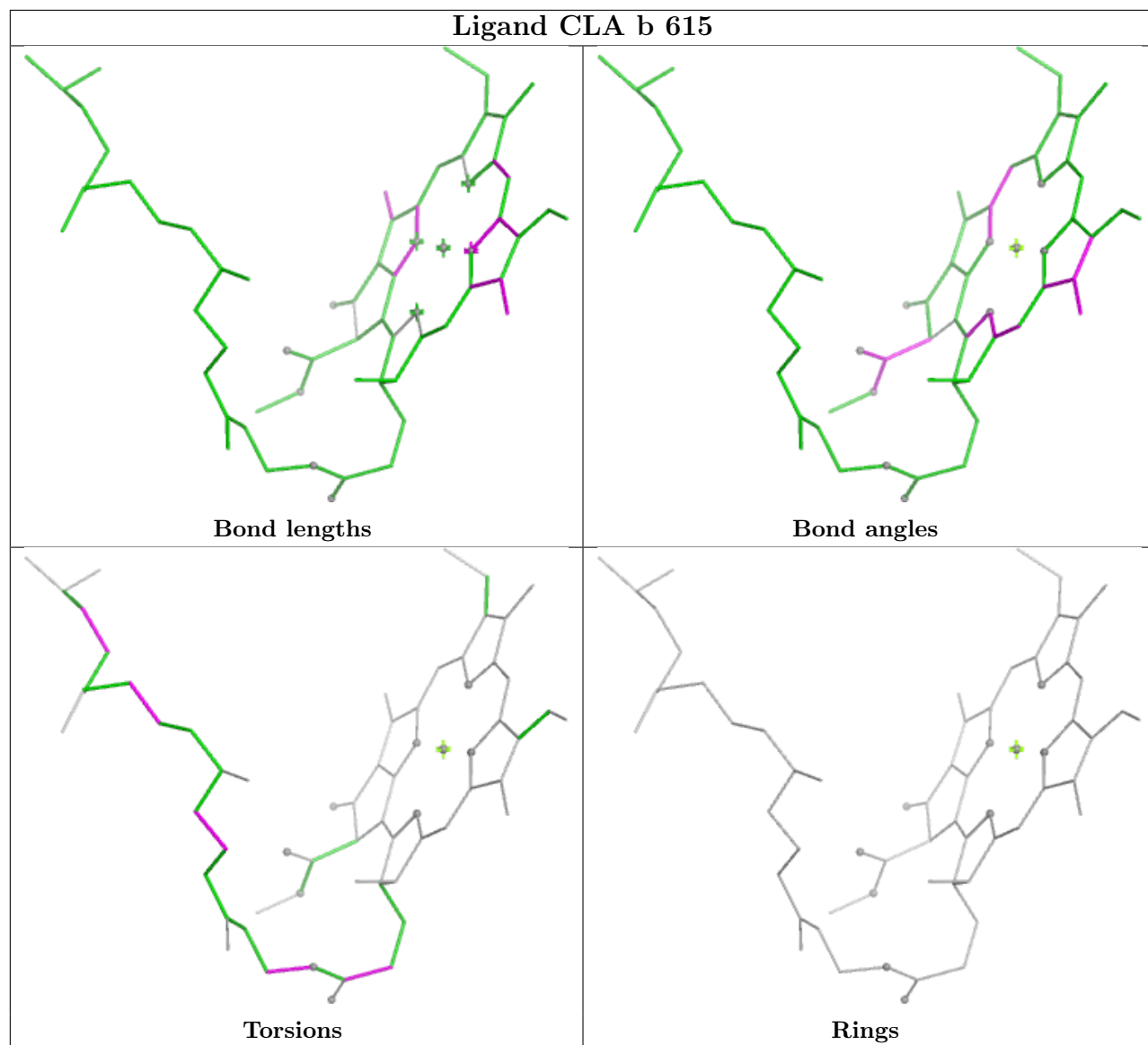
Bond angles



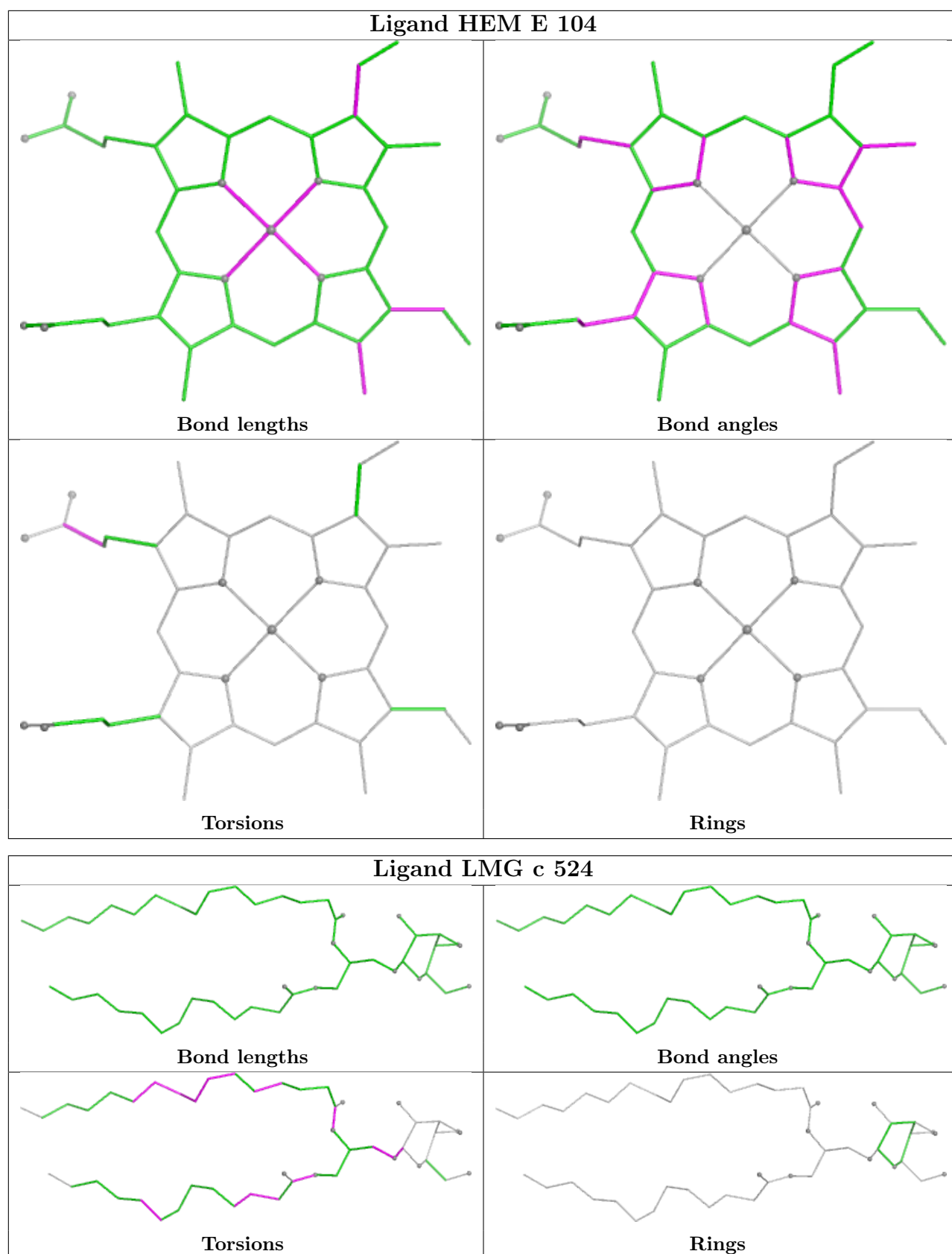
Torsions

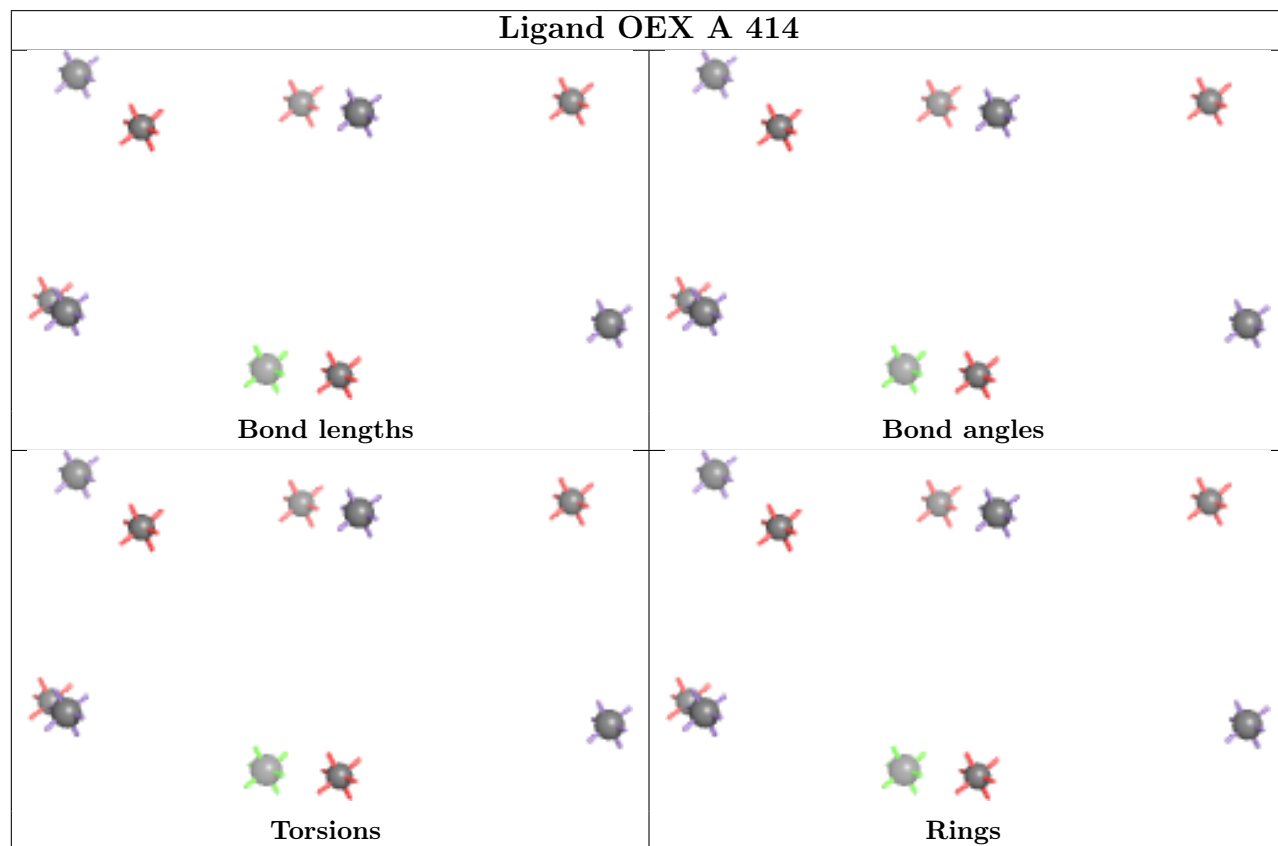
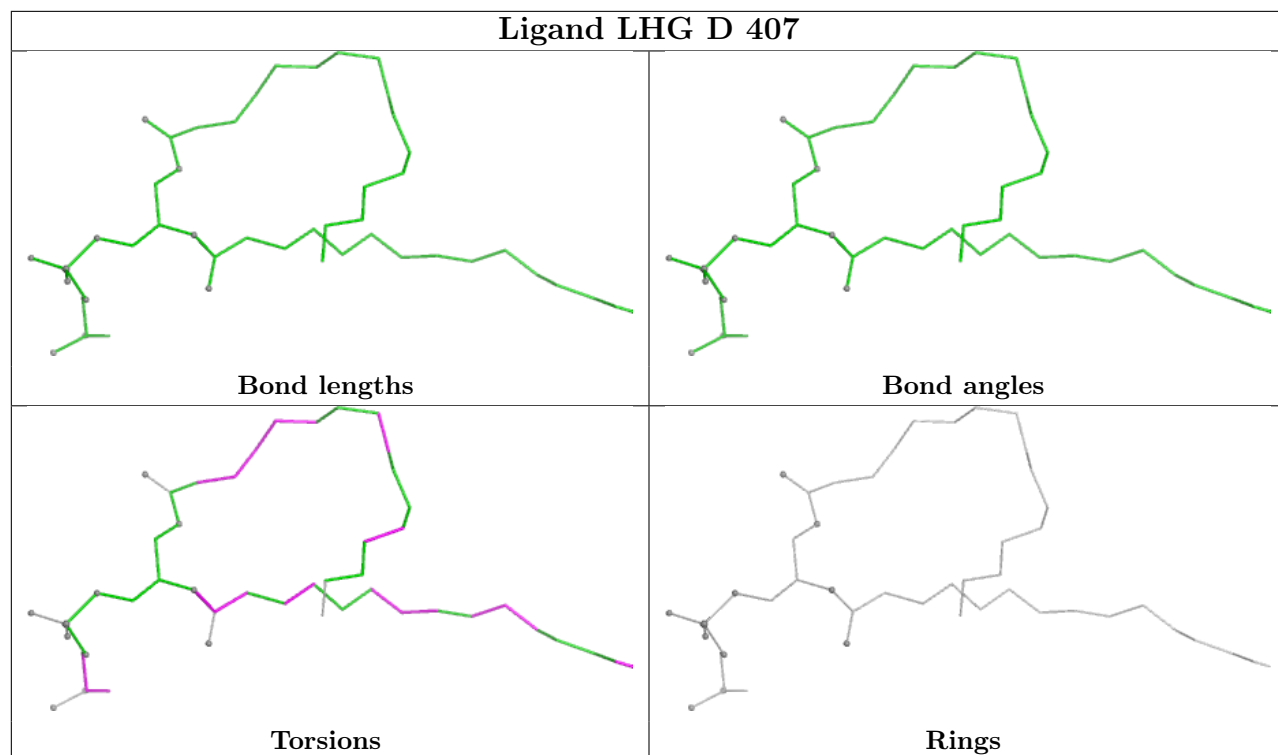


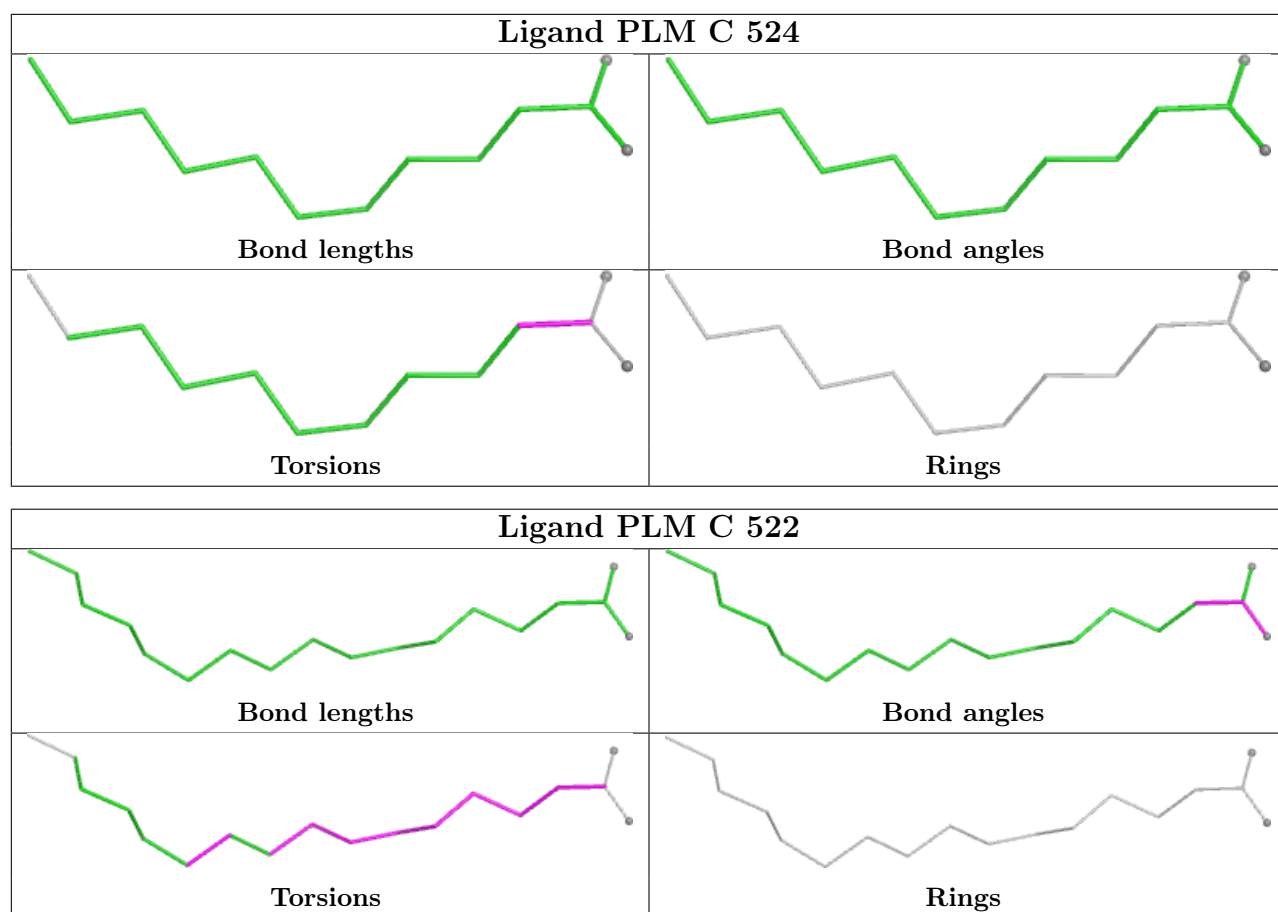
Rings

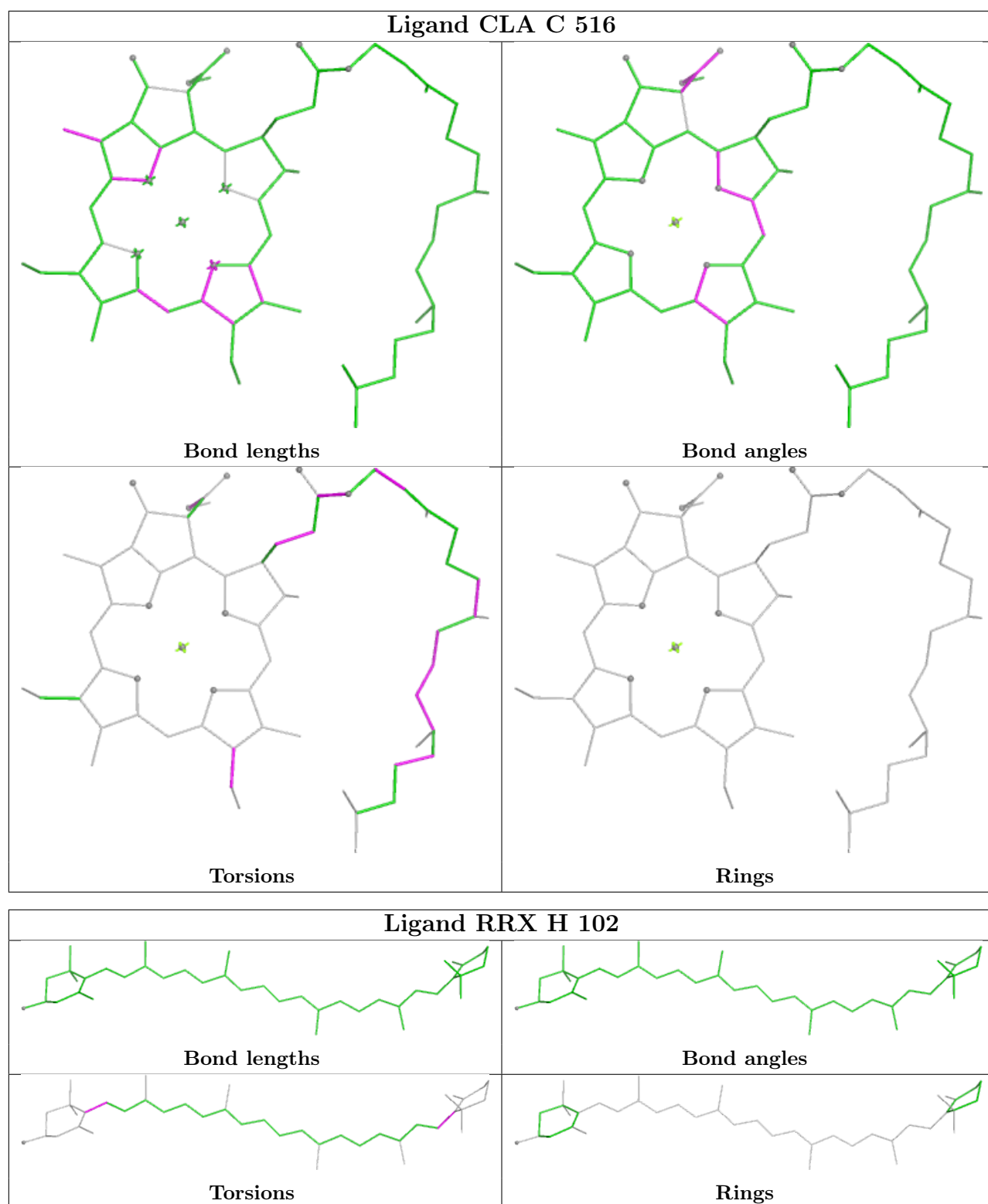


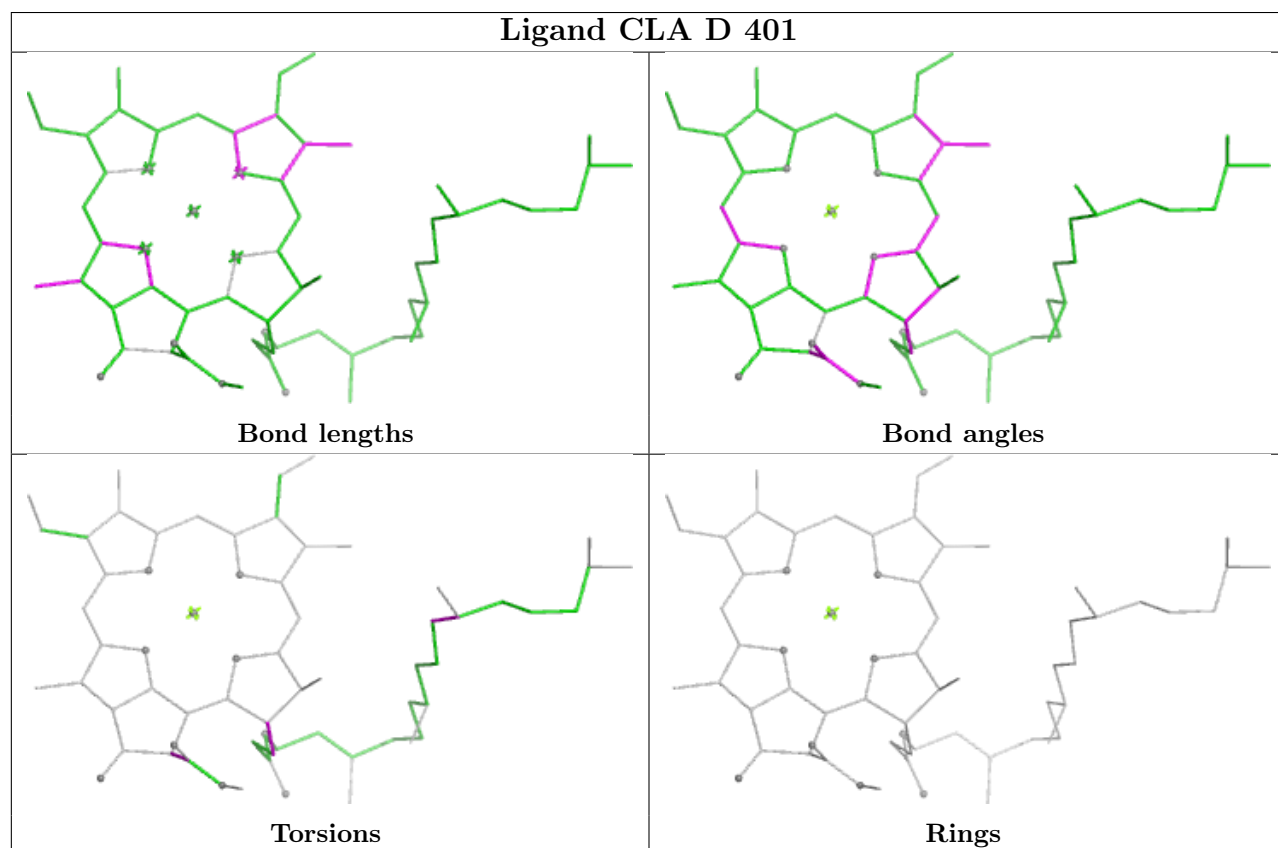
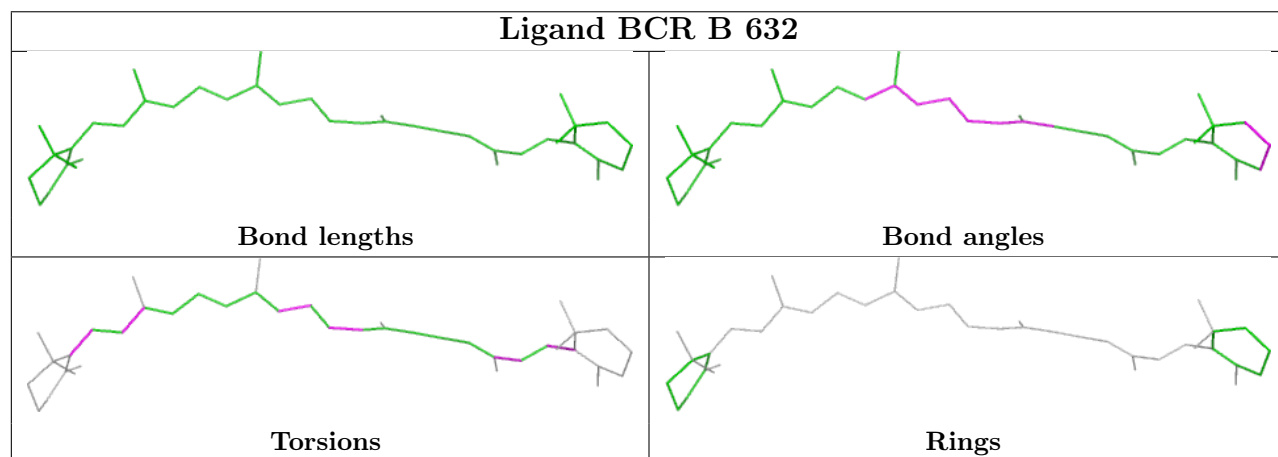
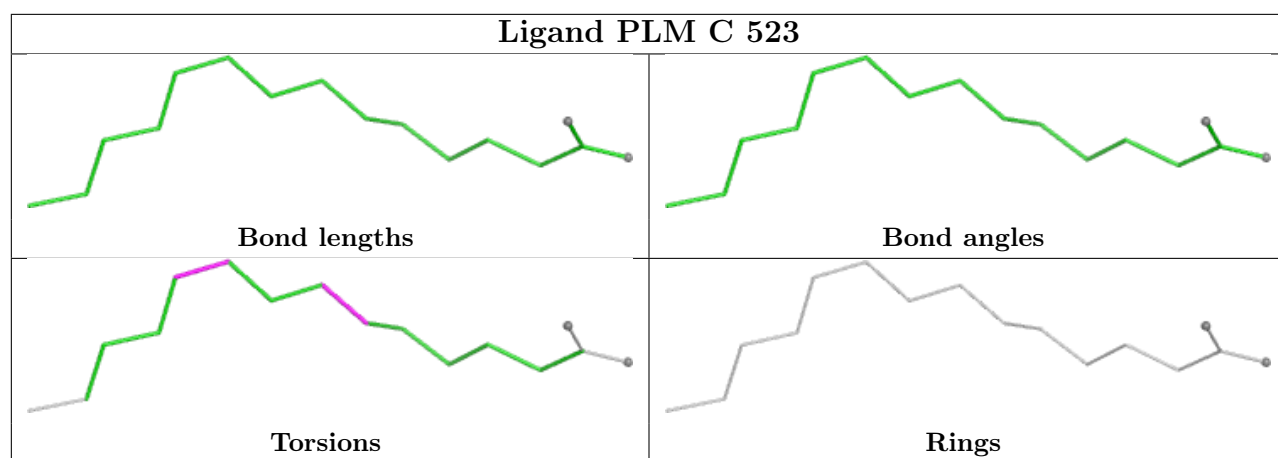


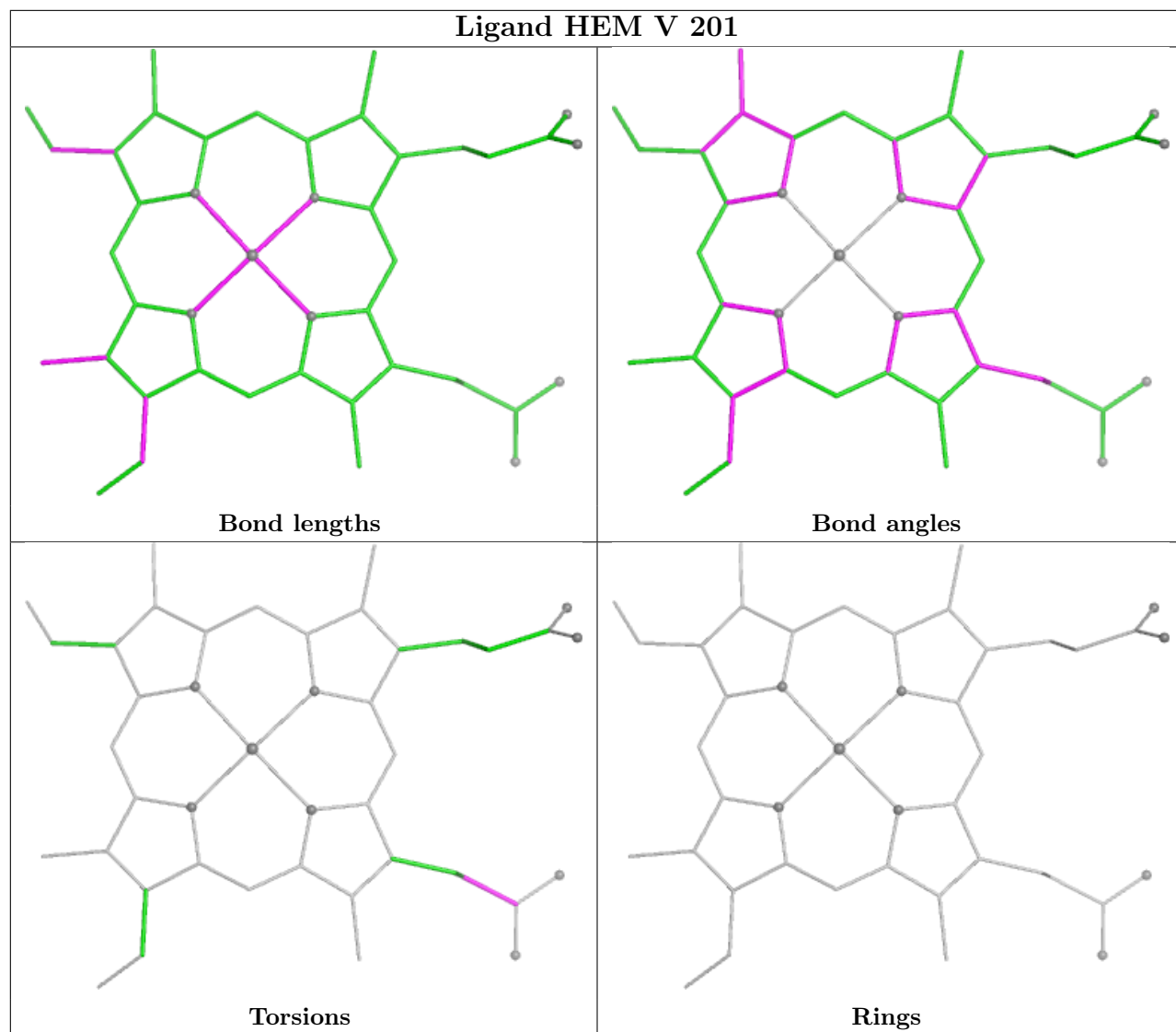


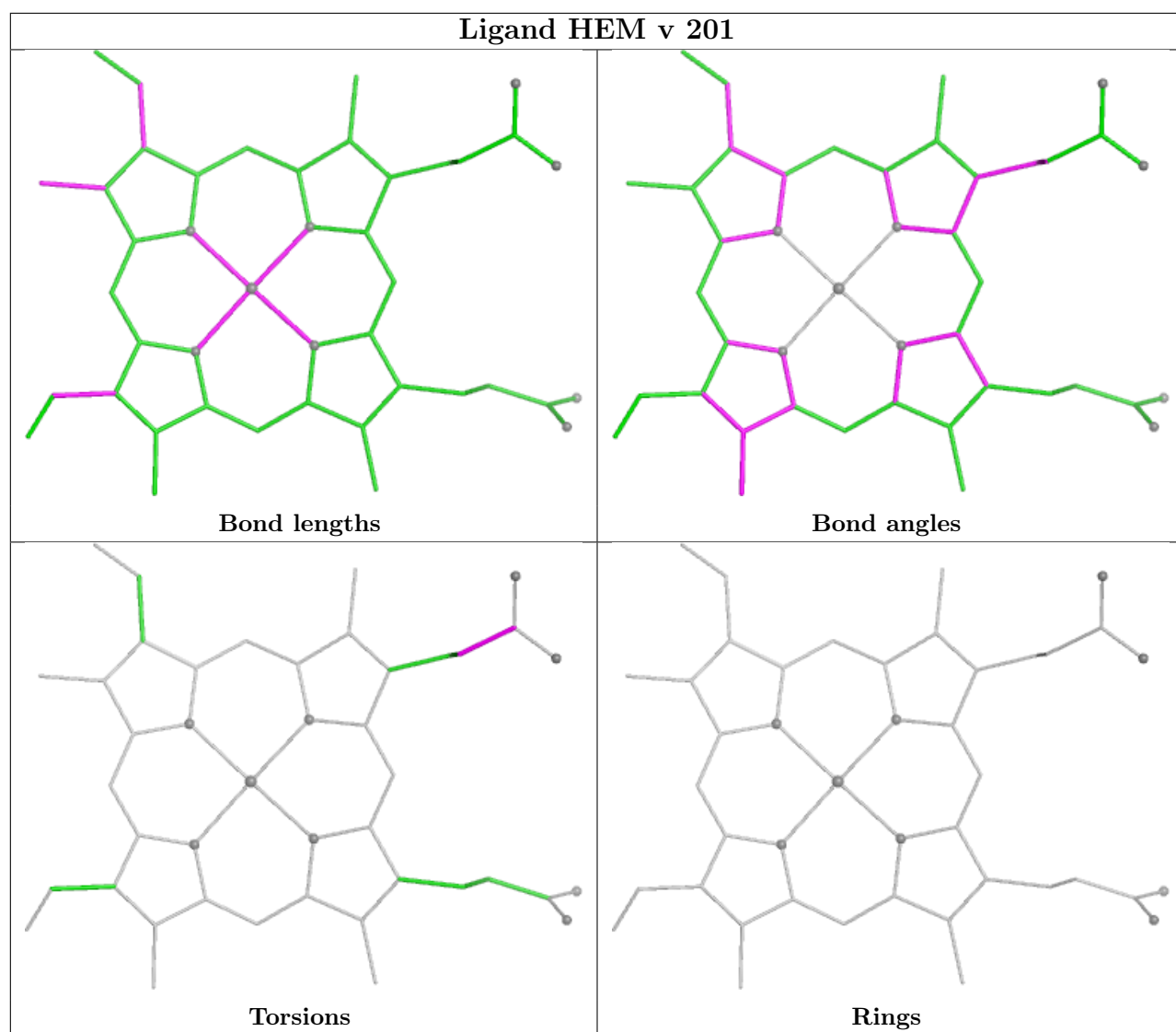


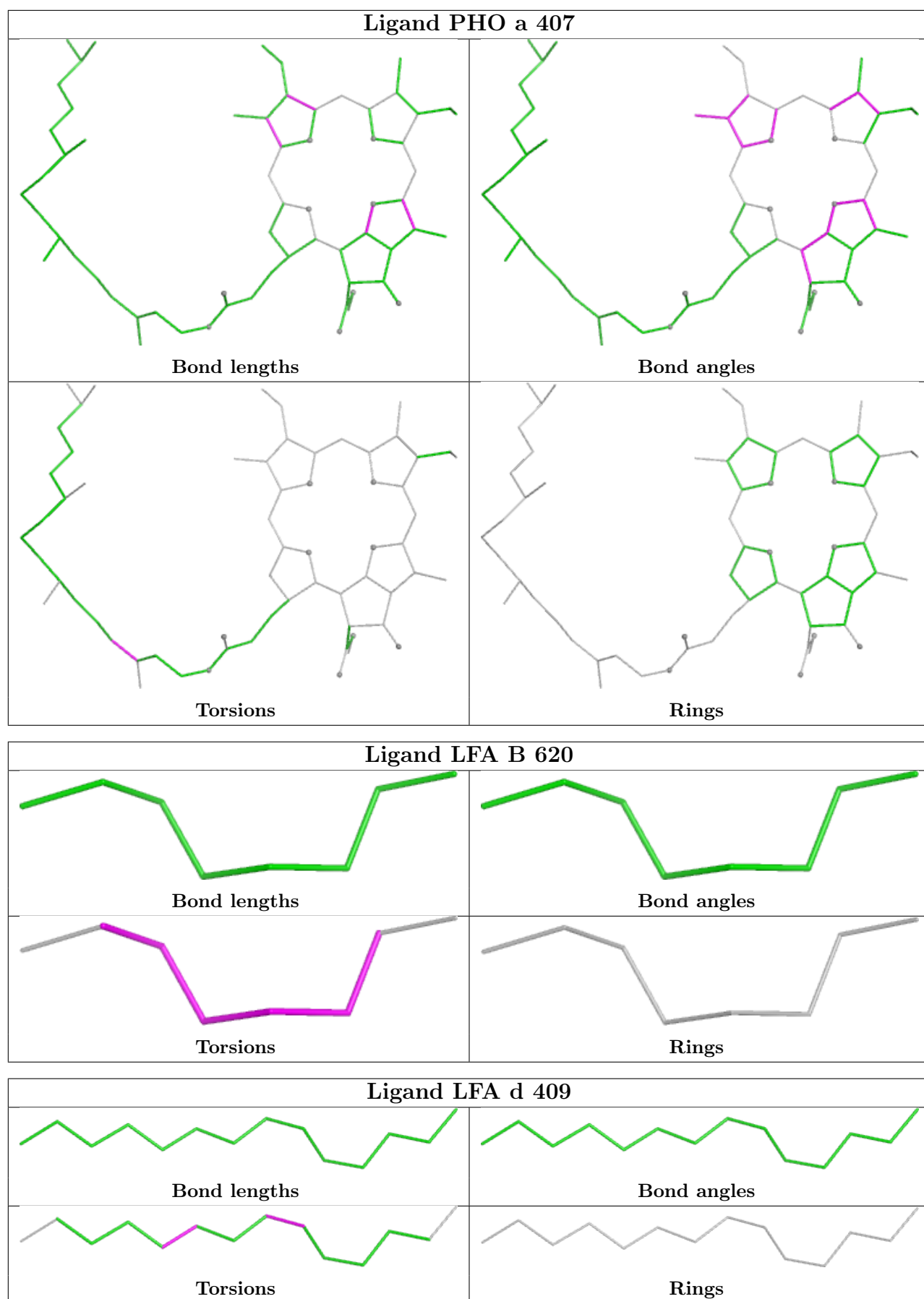




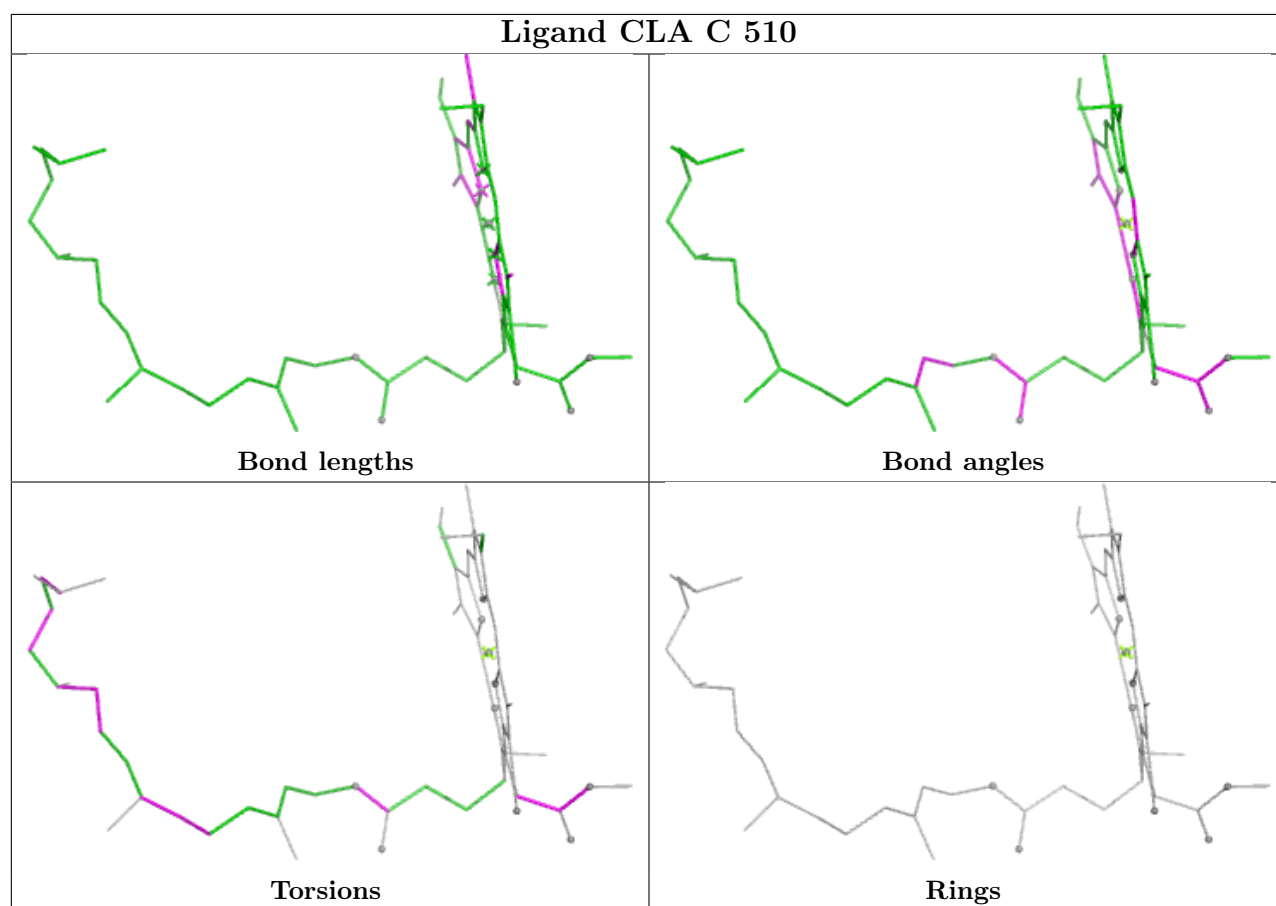
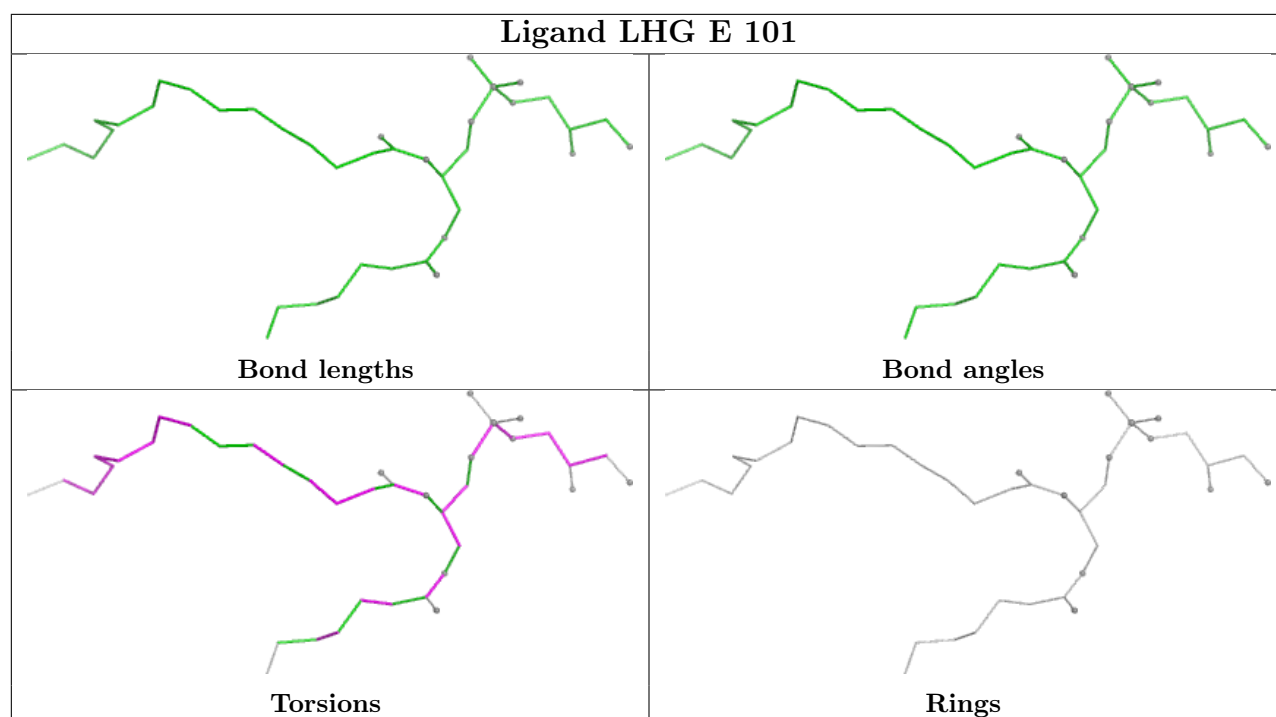


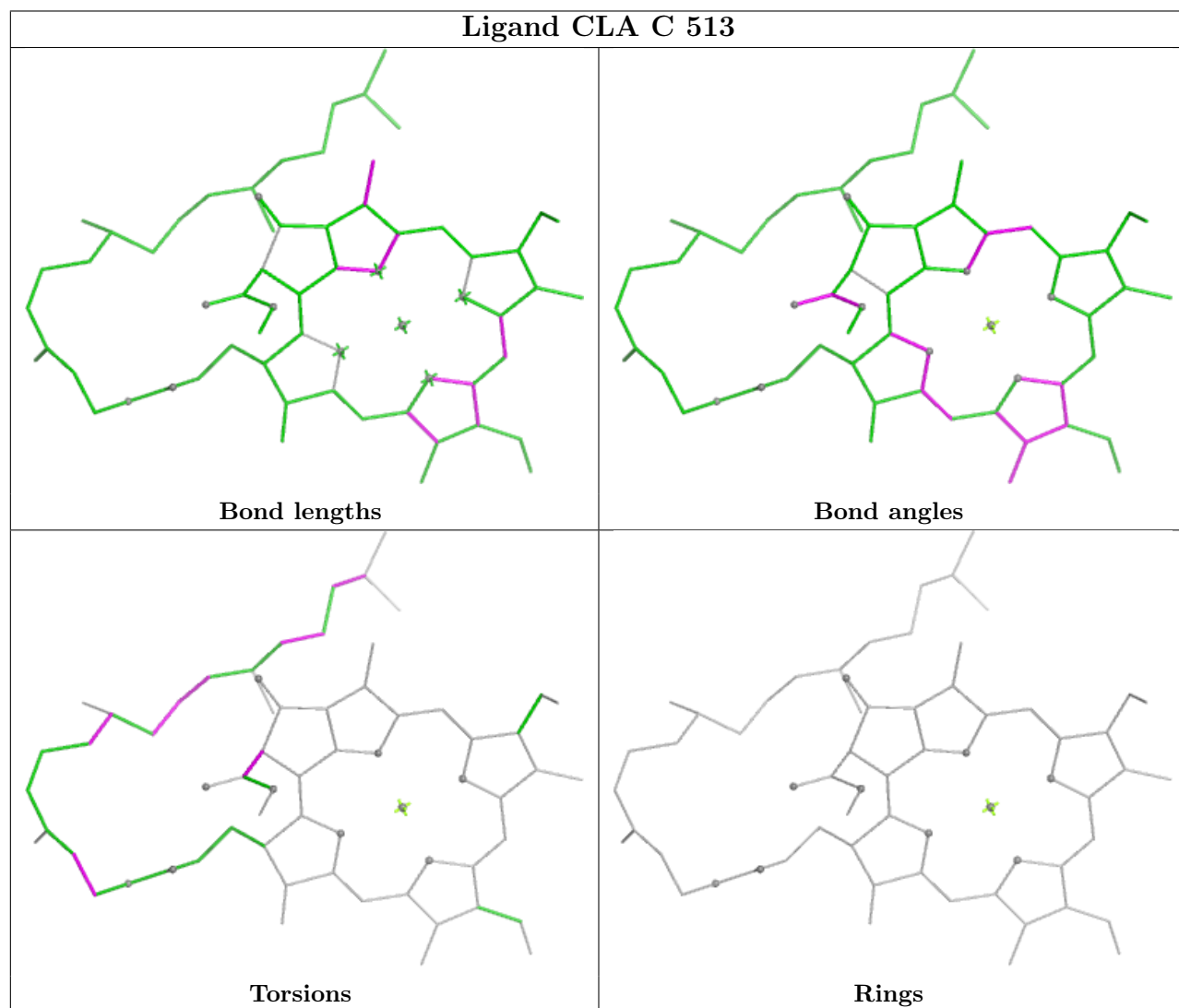
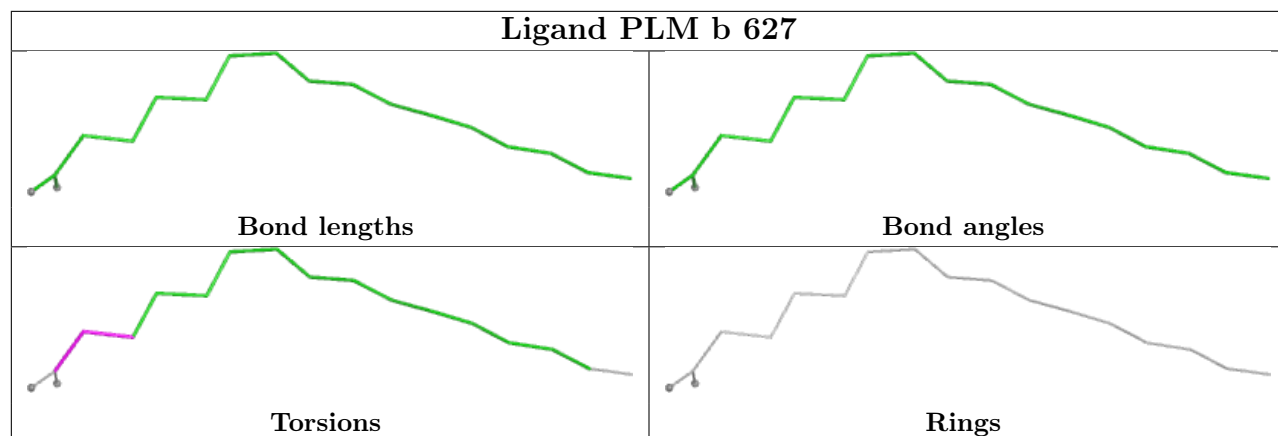


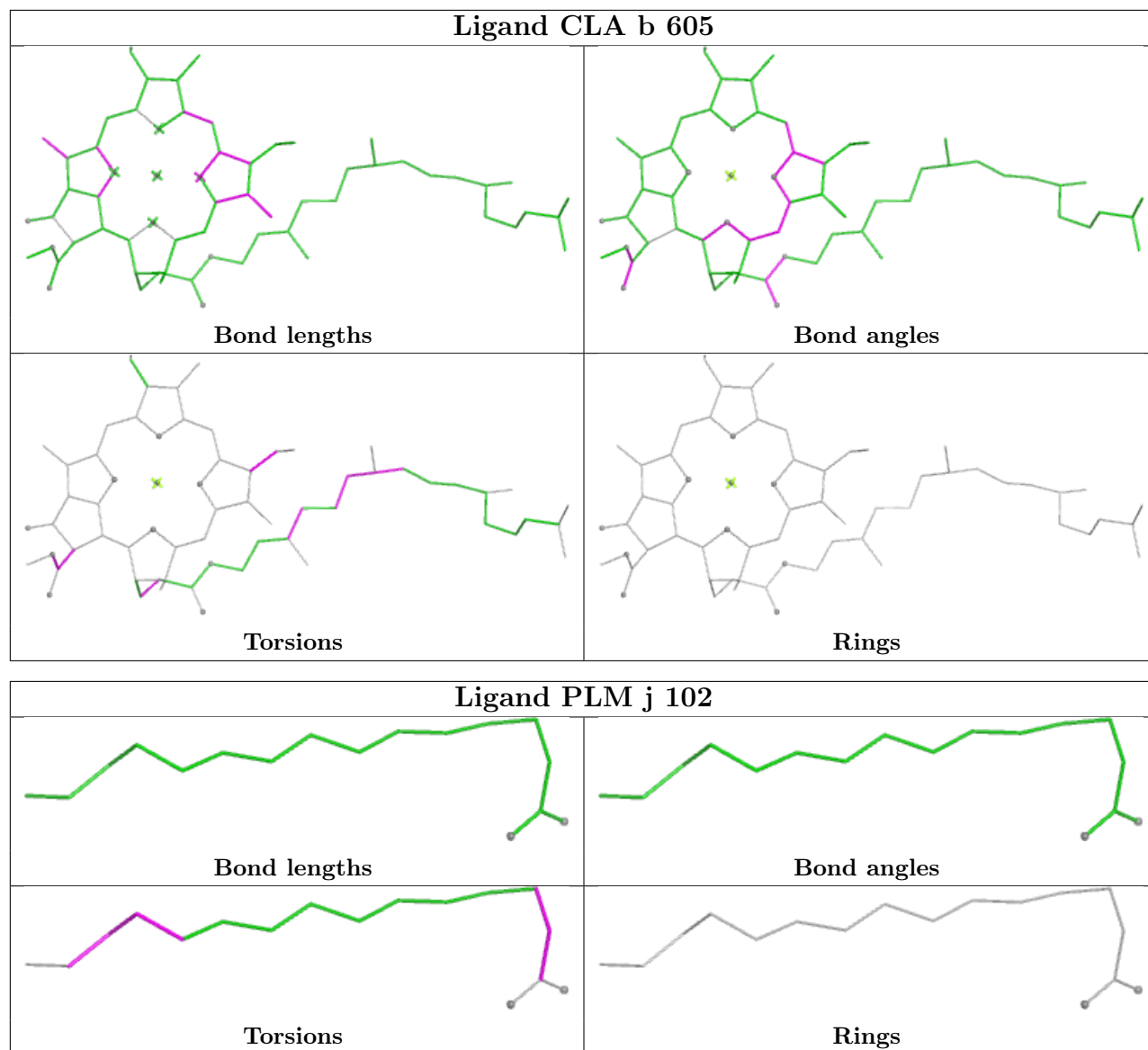


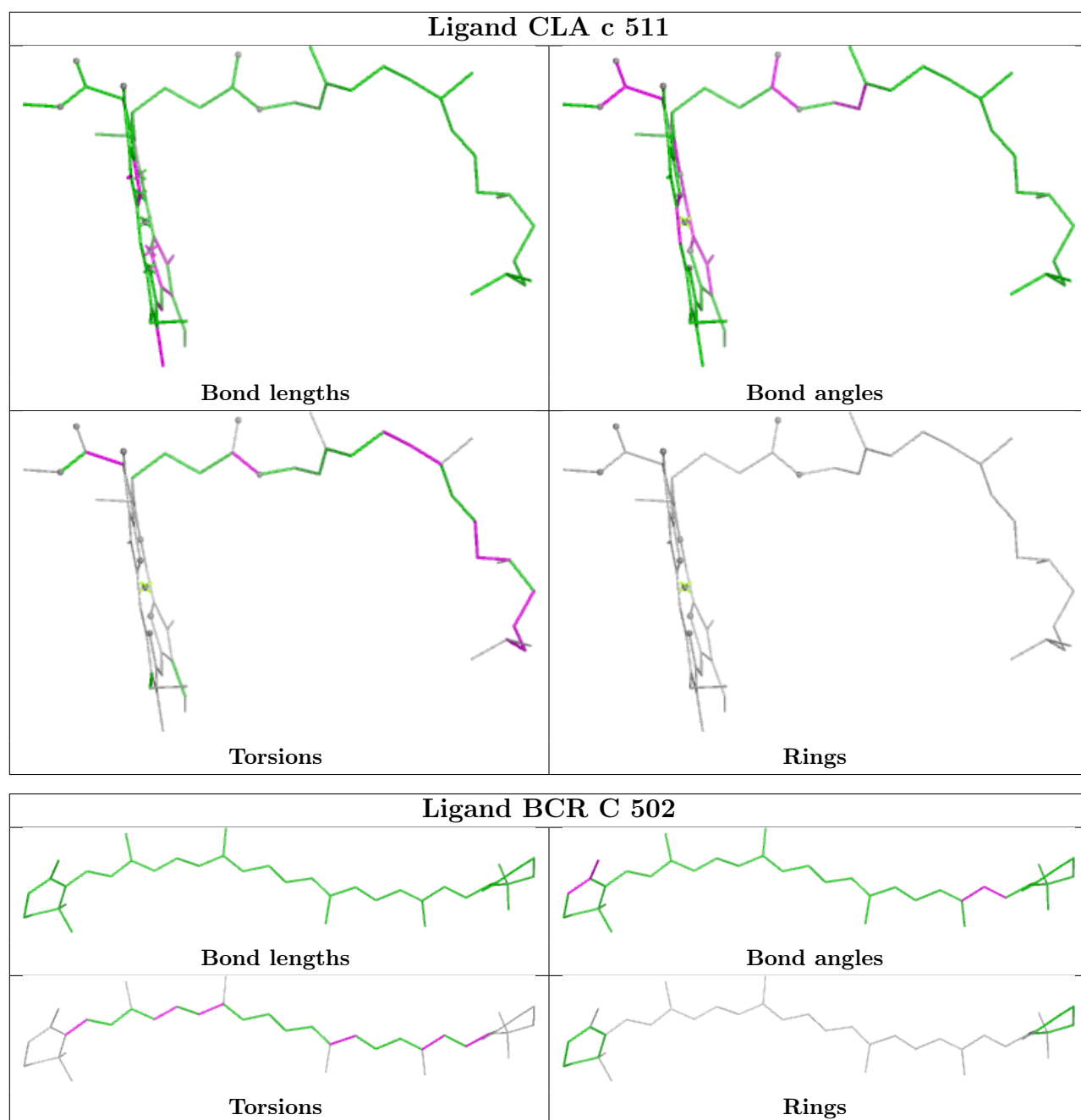


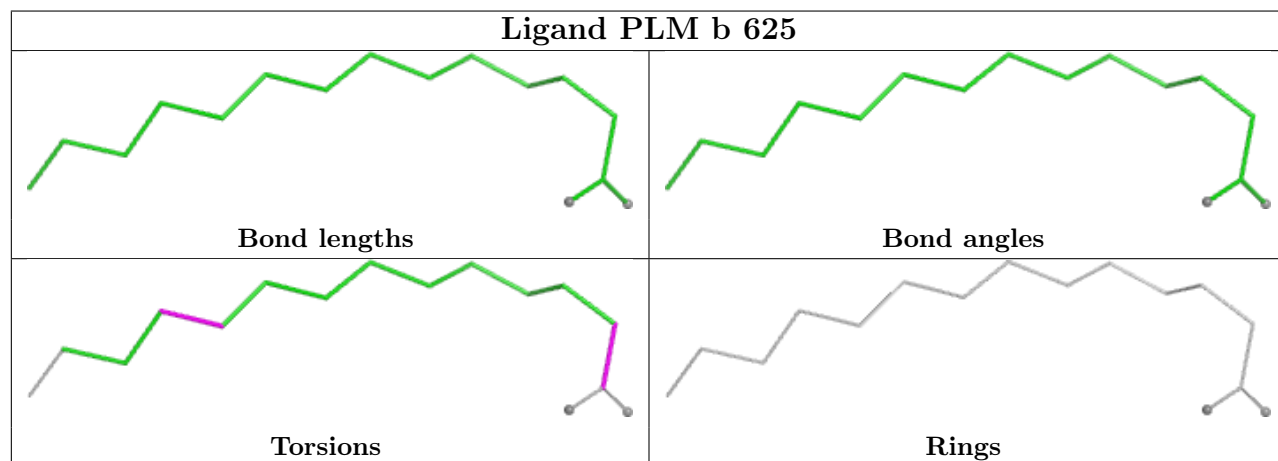
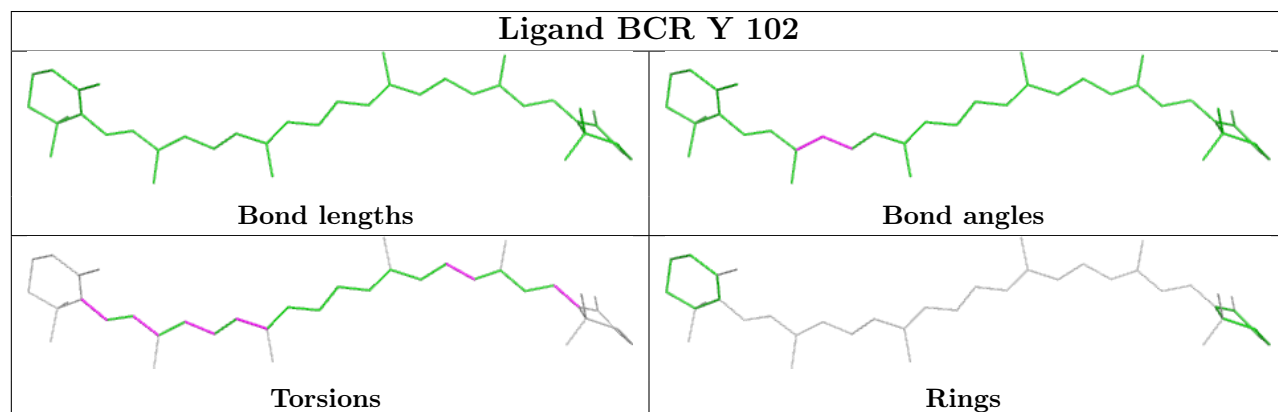
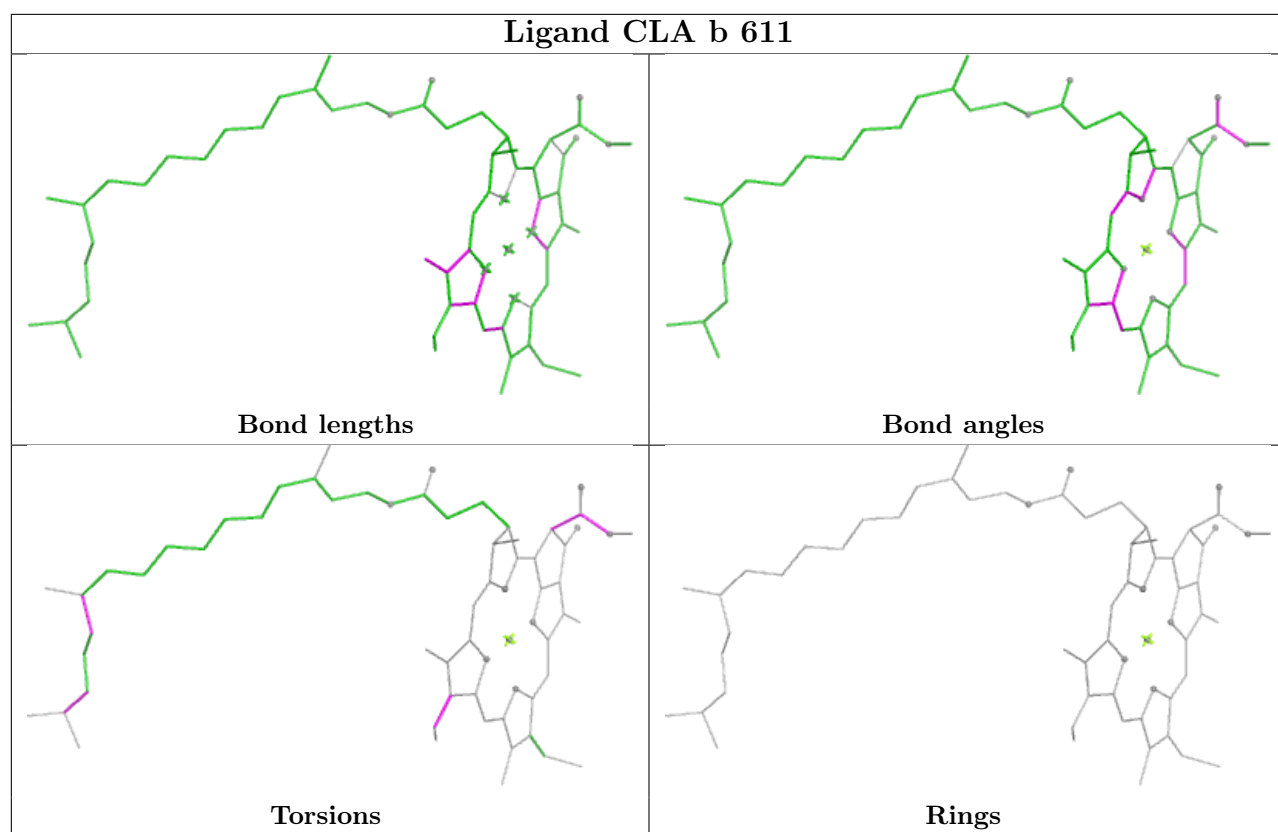


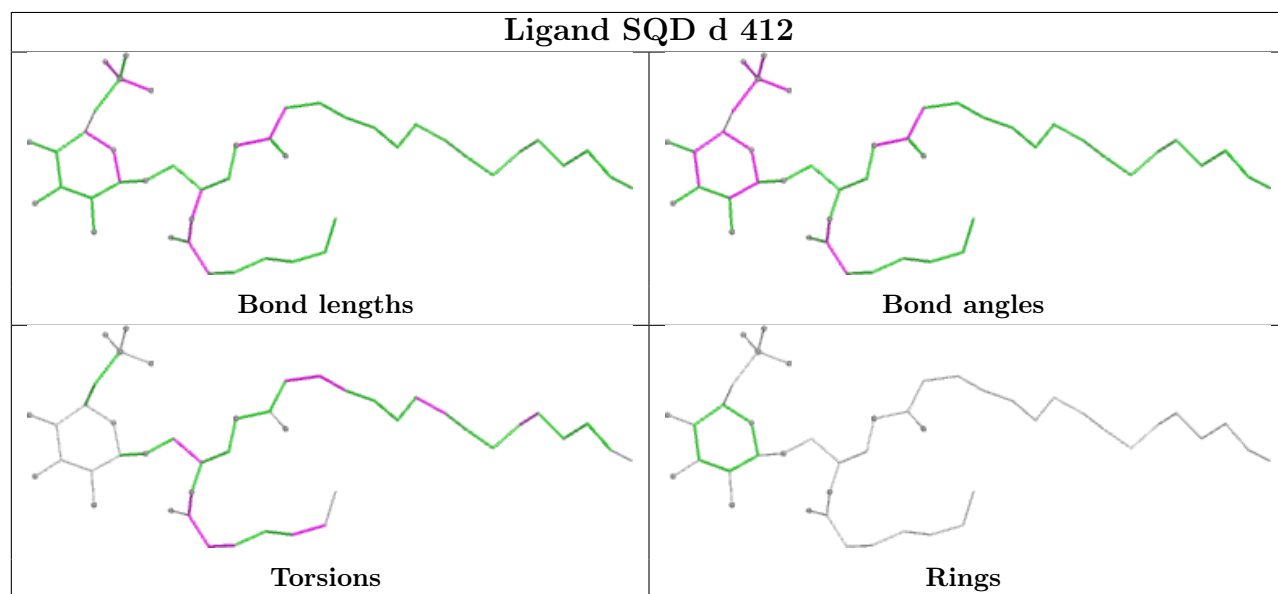
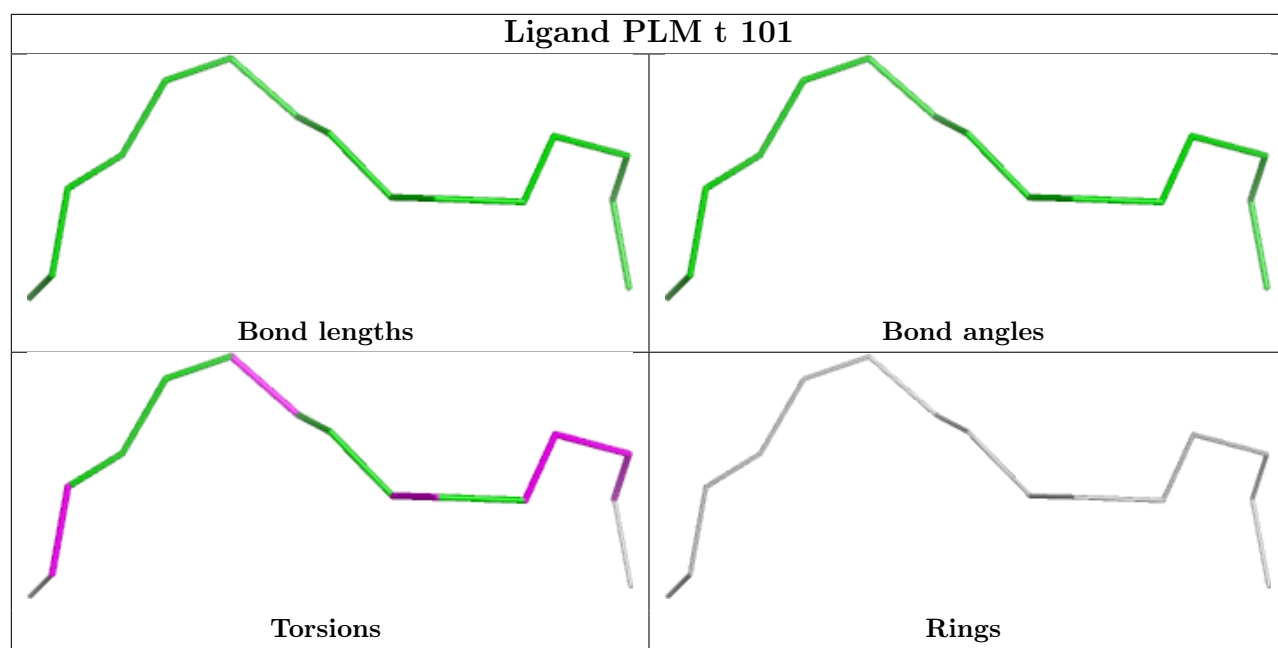




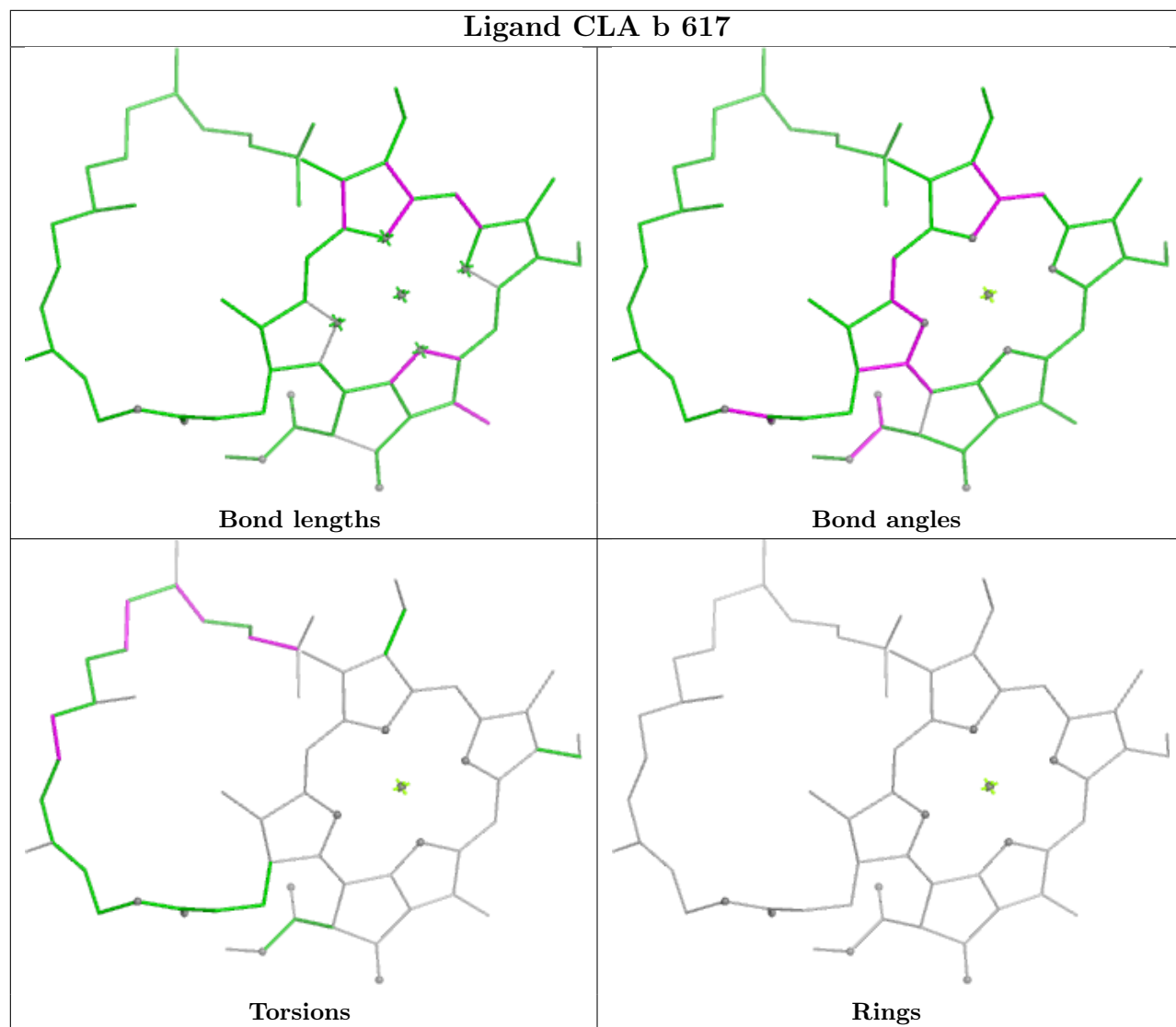


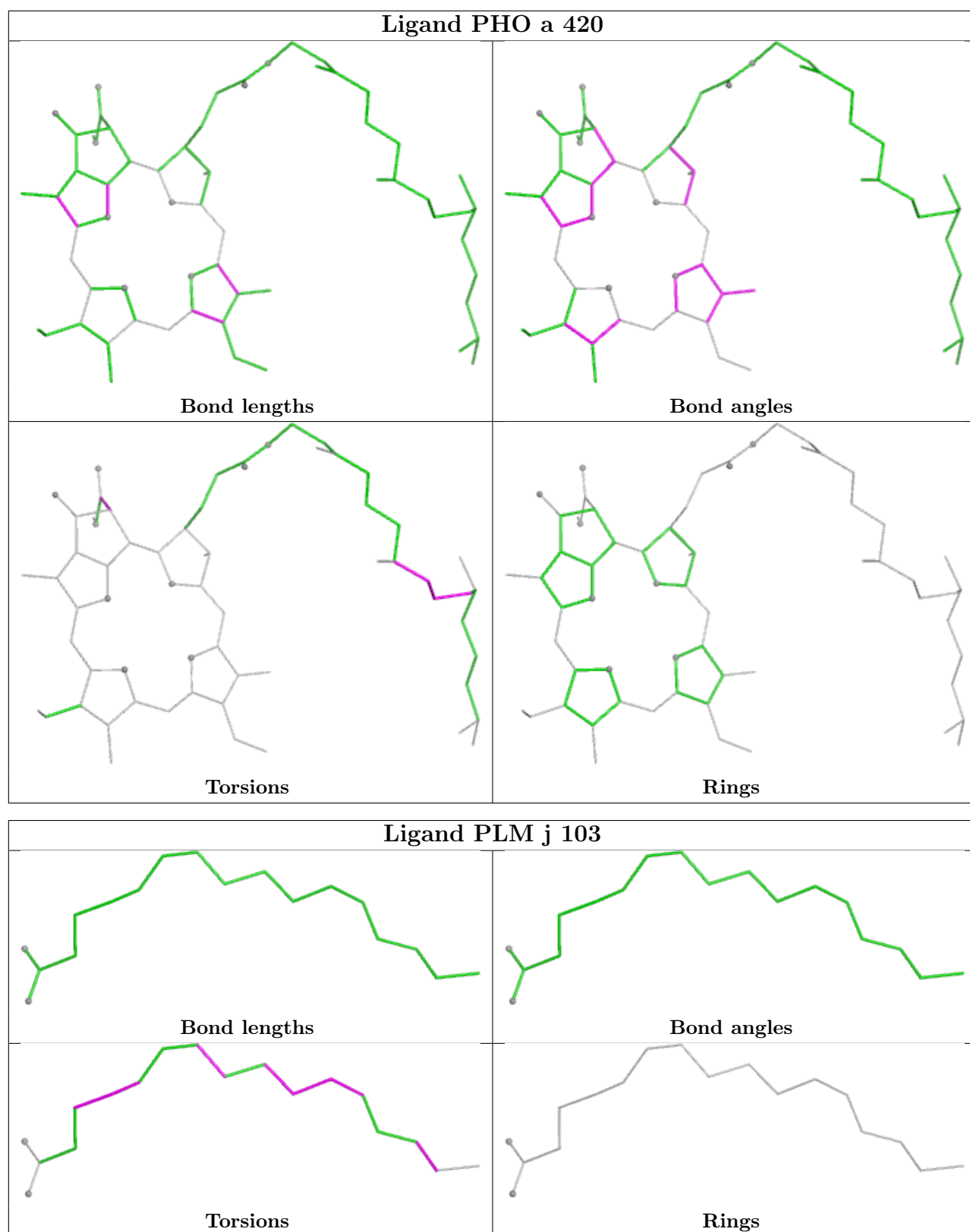




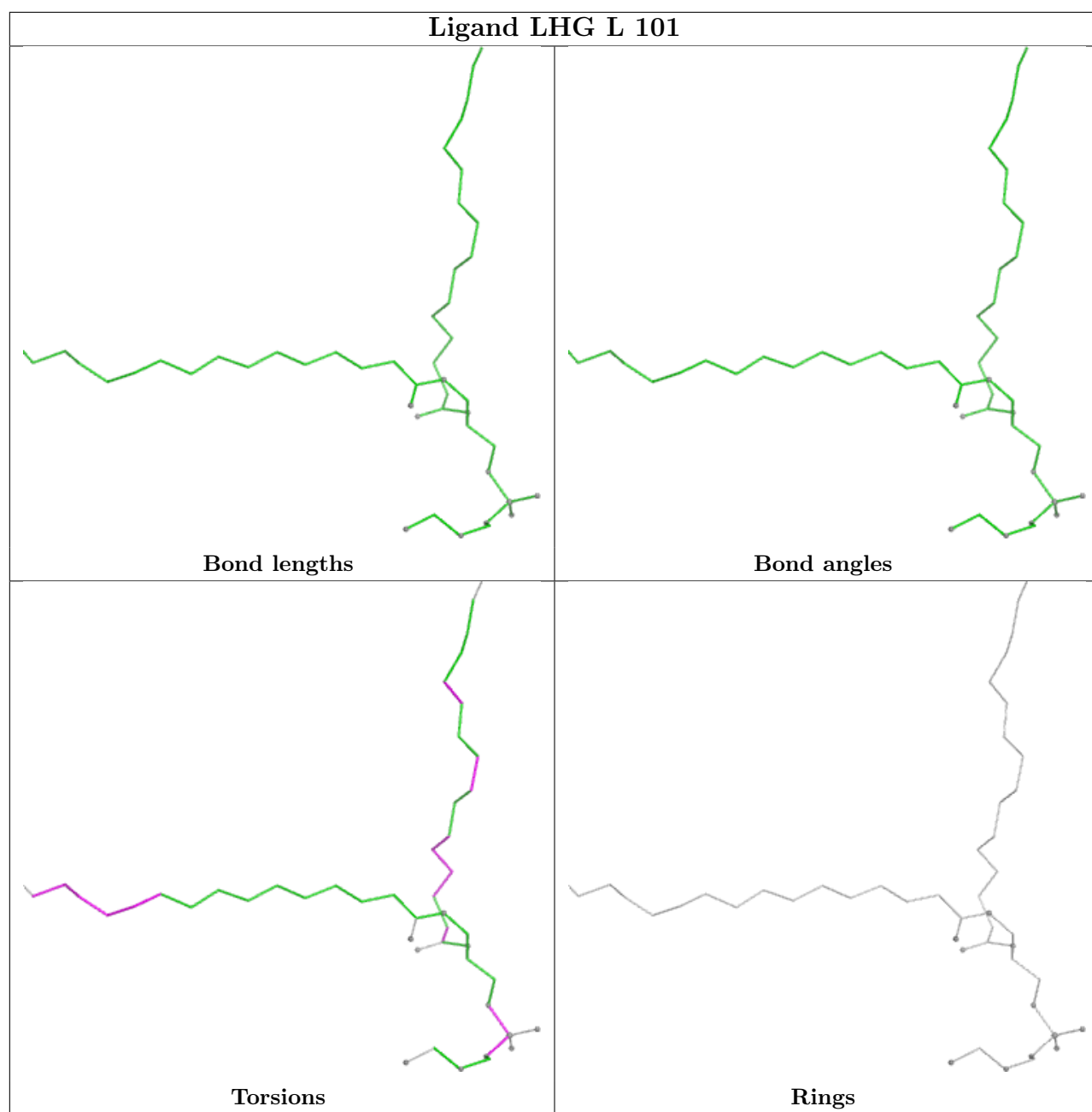


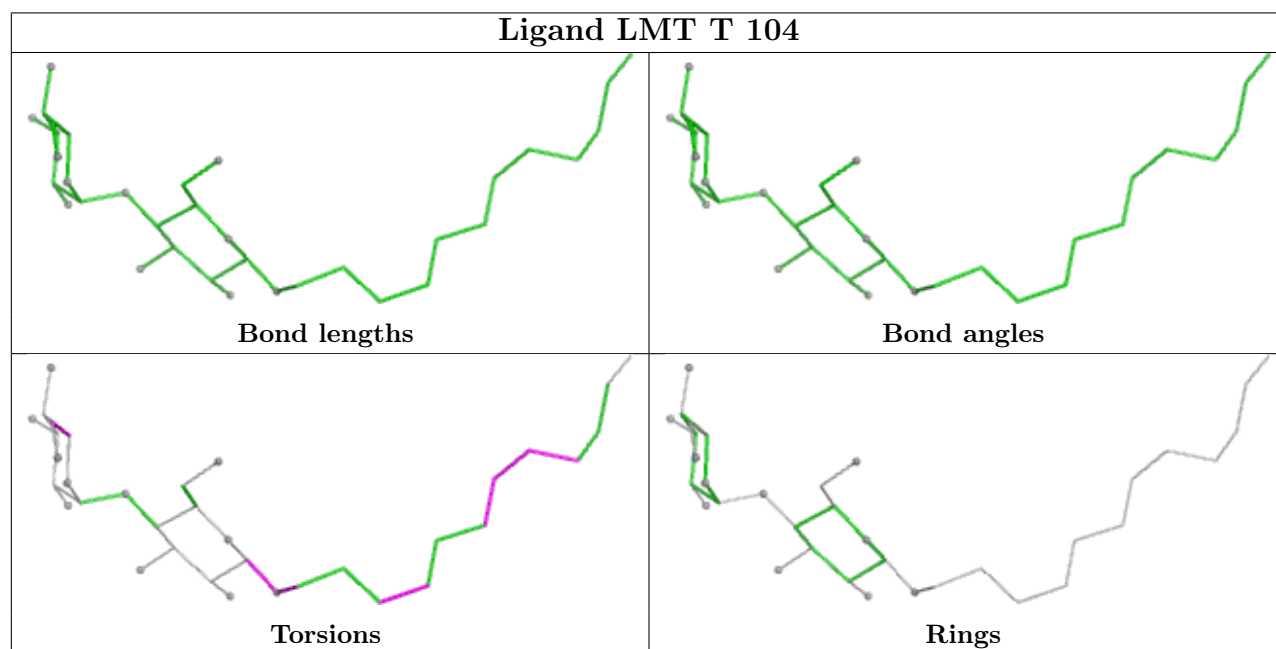
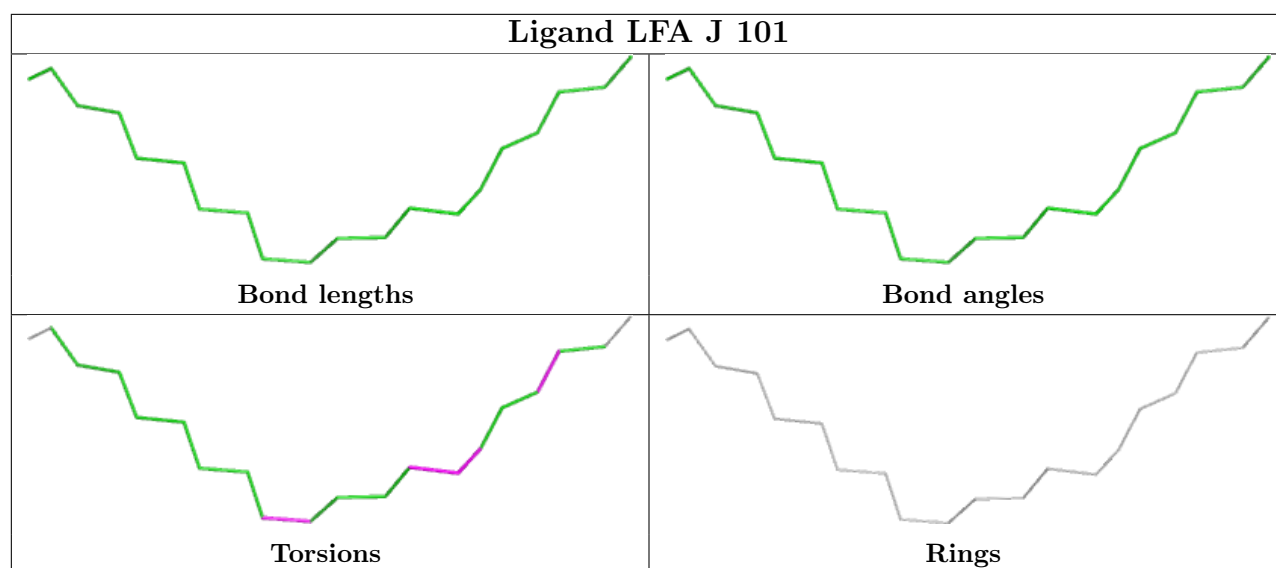
## Ligand CLA b 617

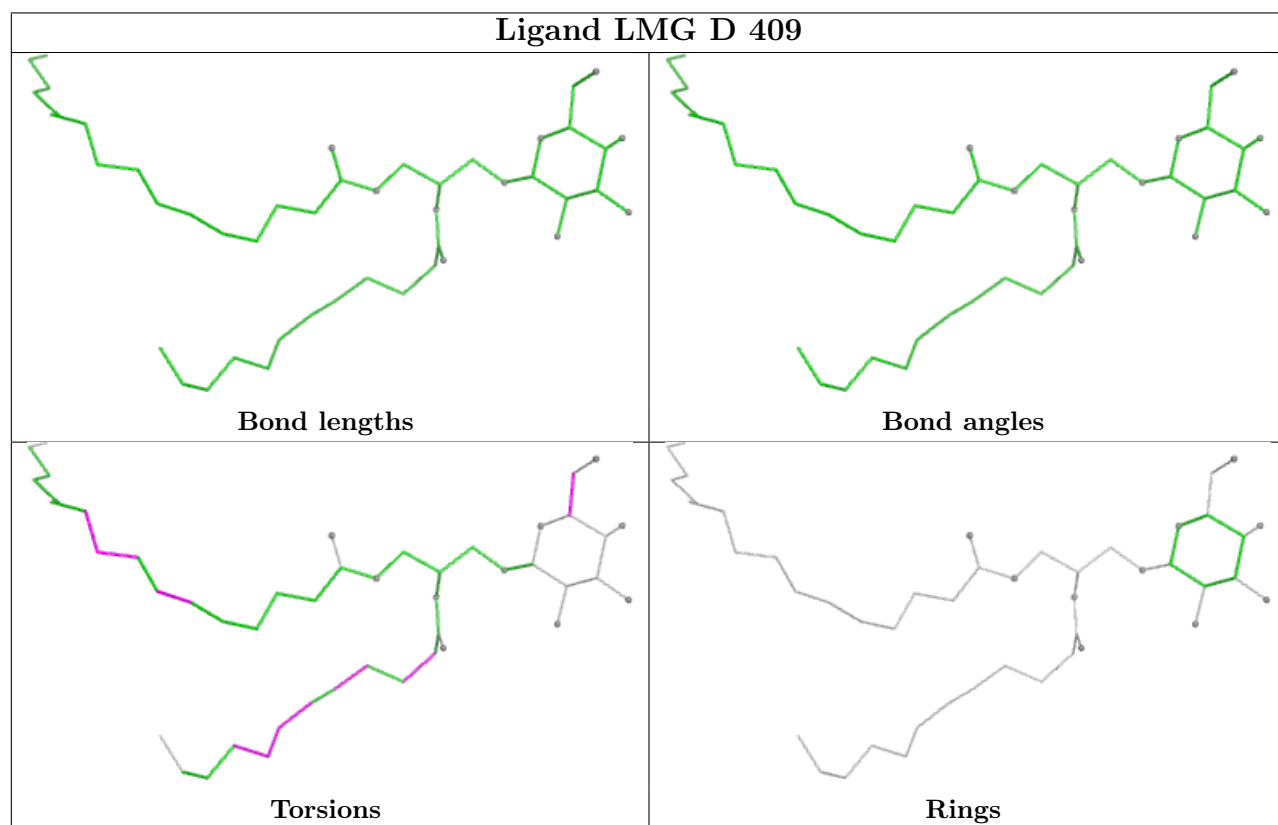
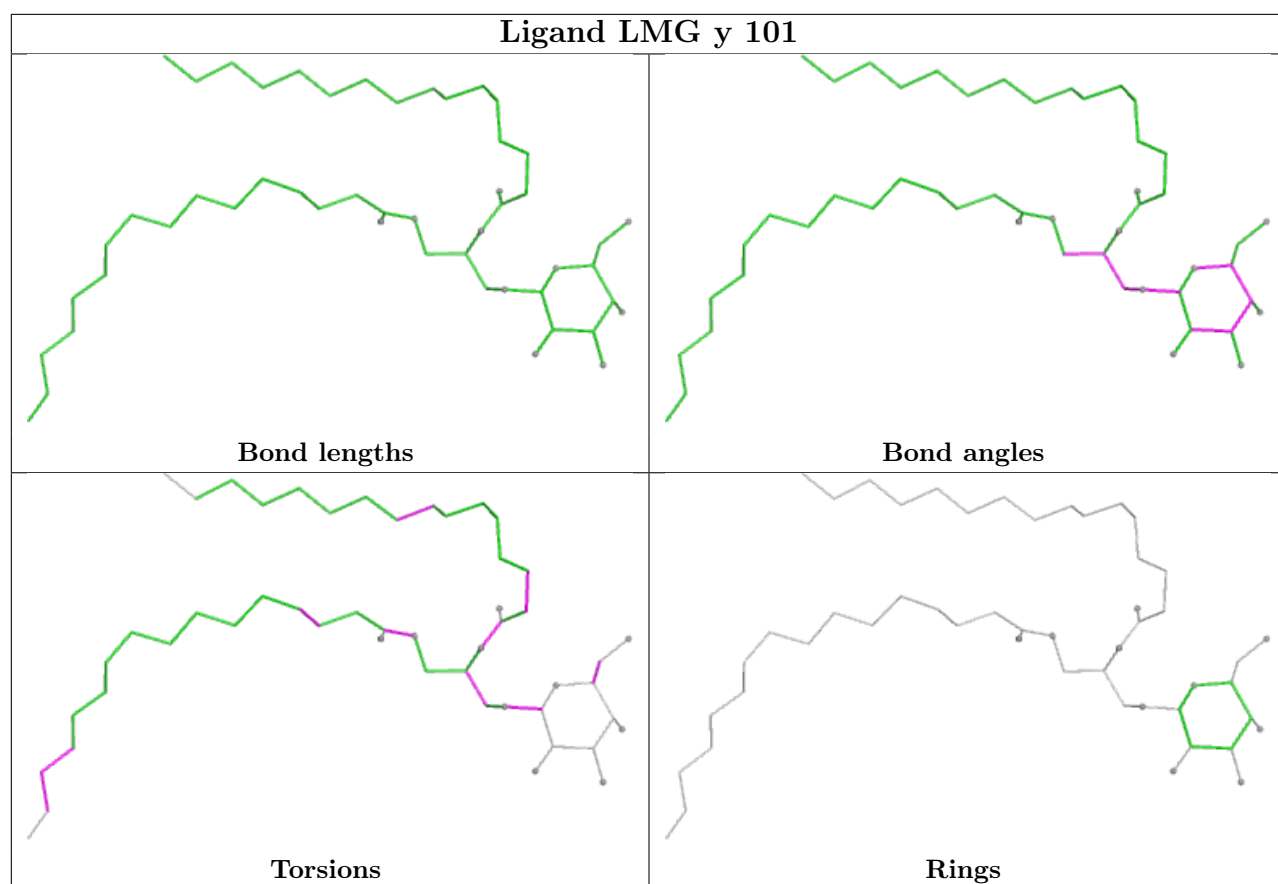


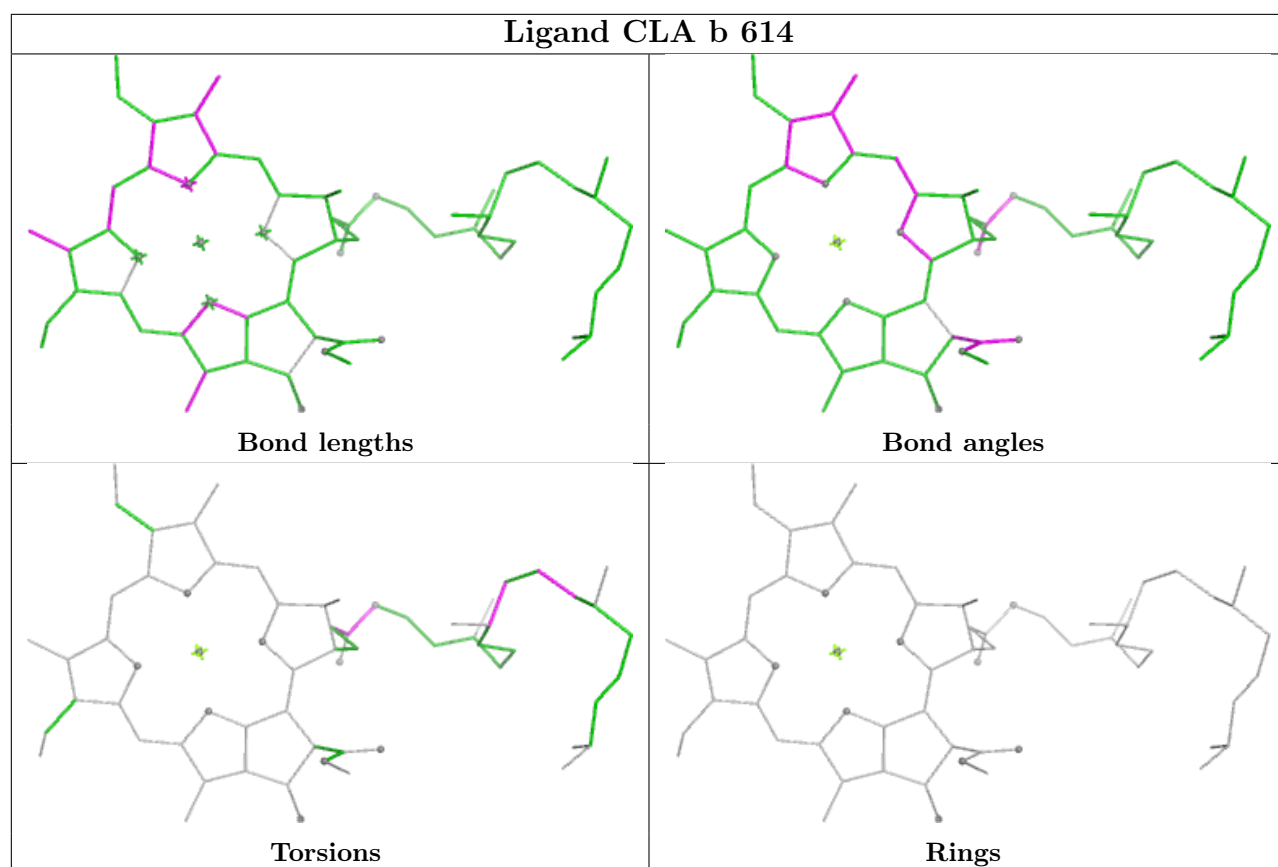


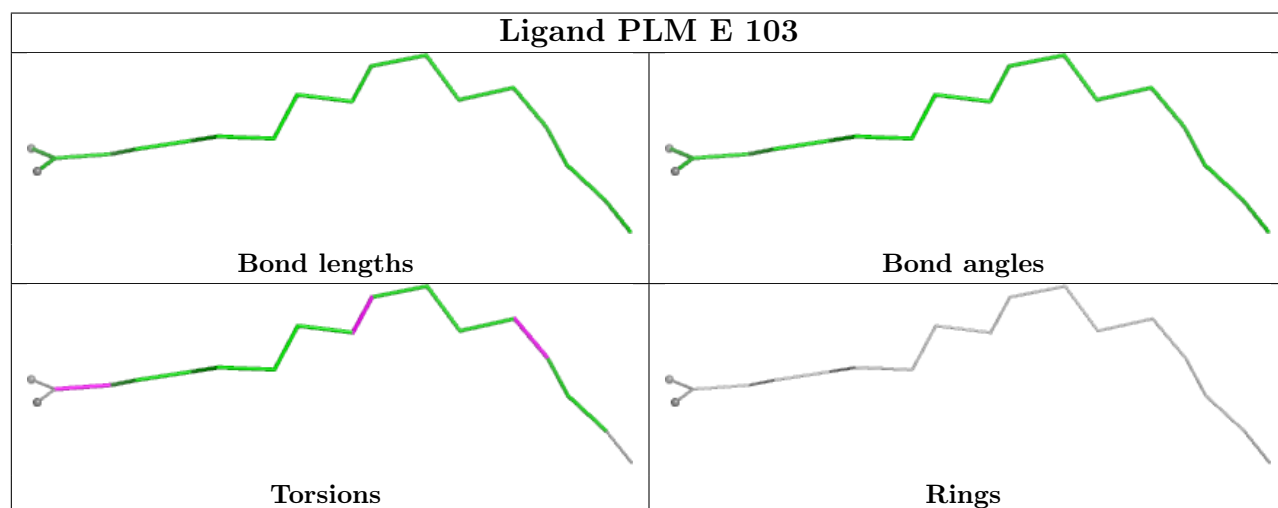
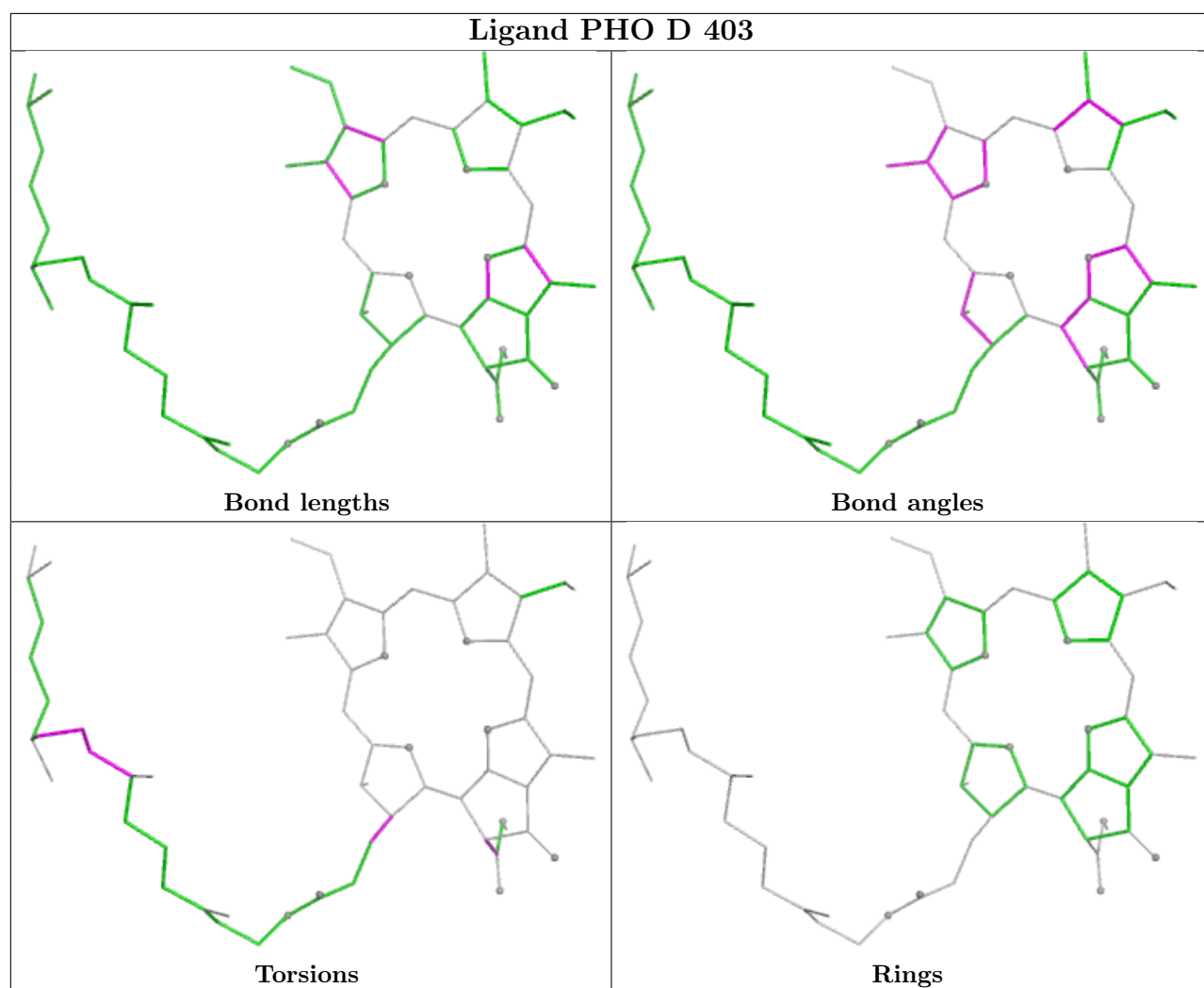


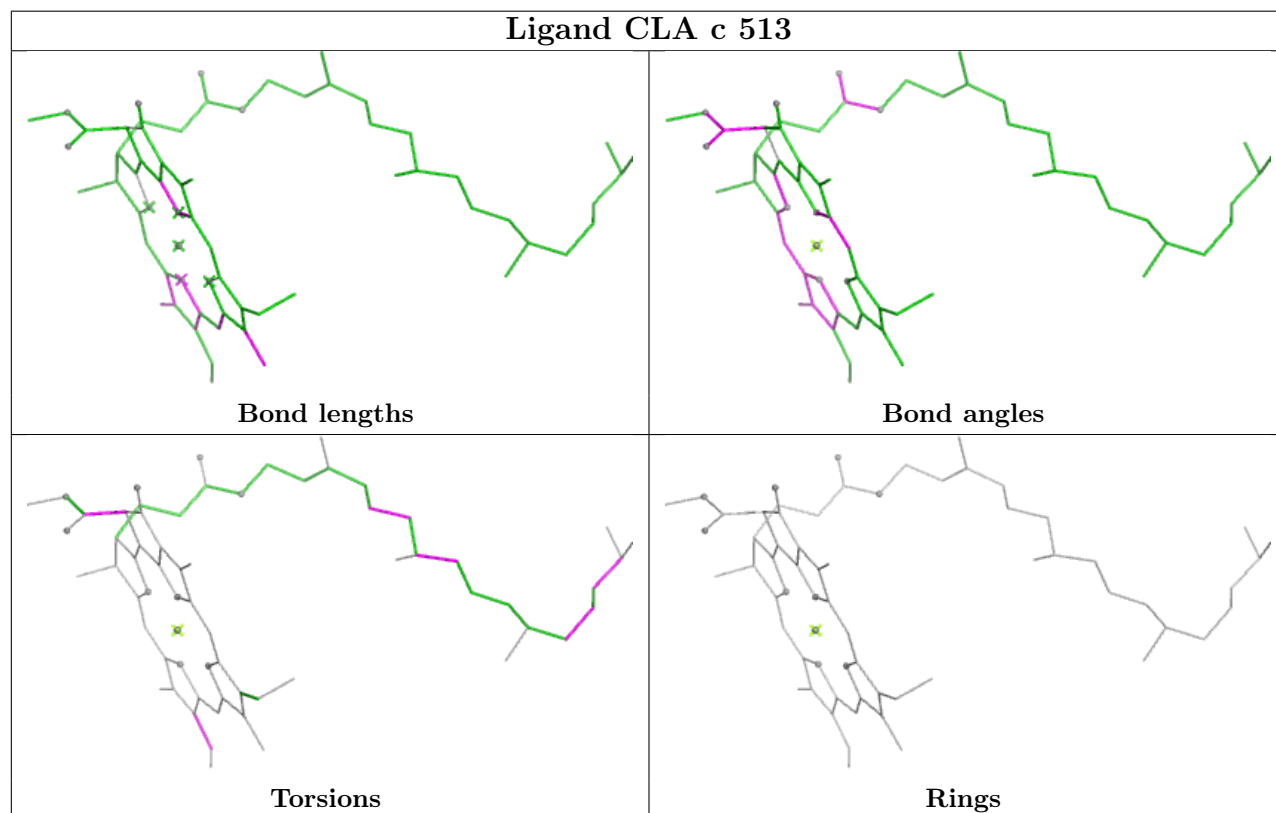
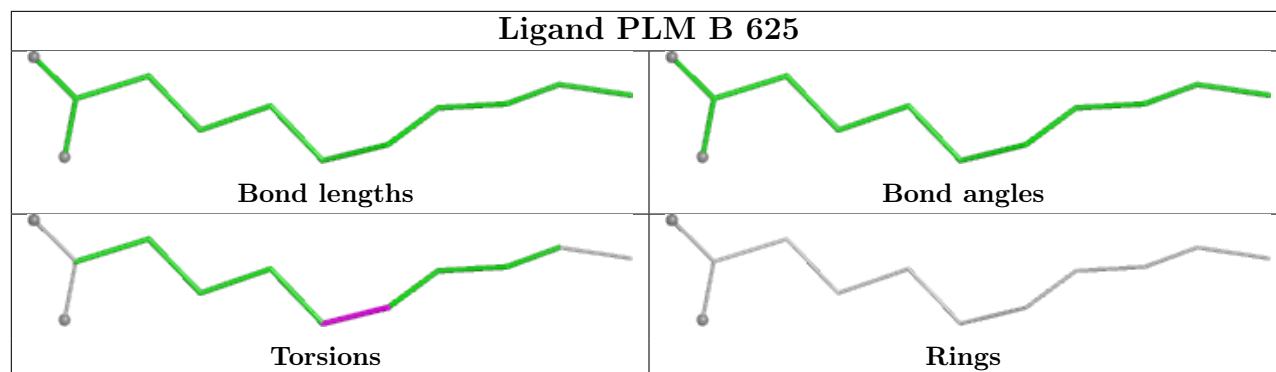


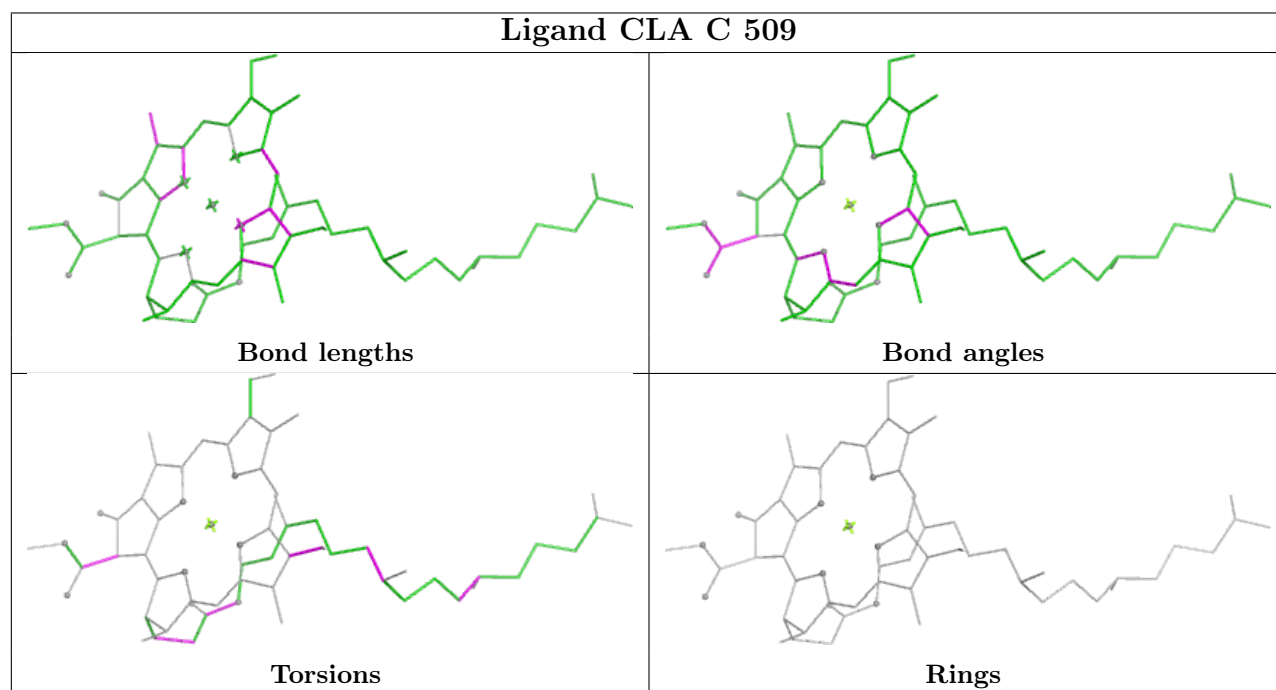
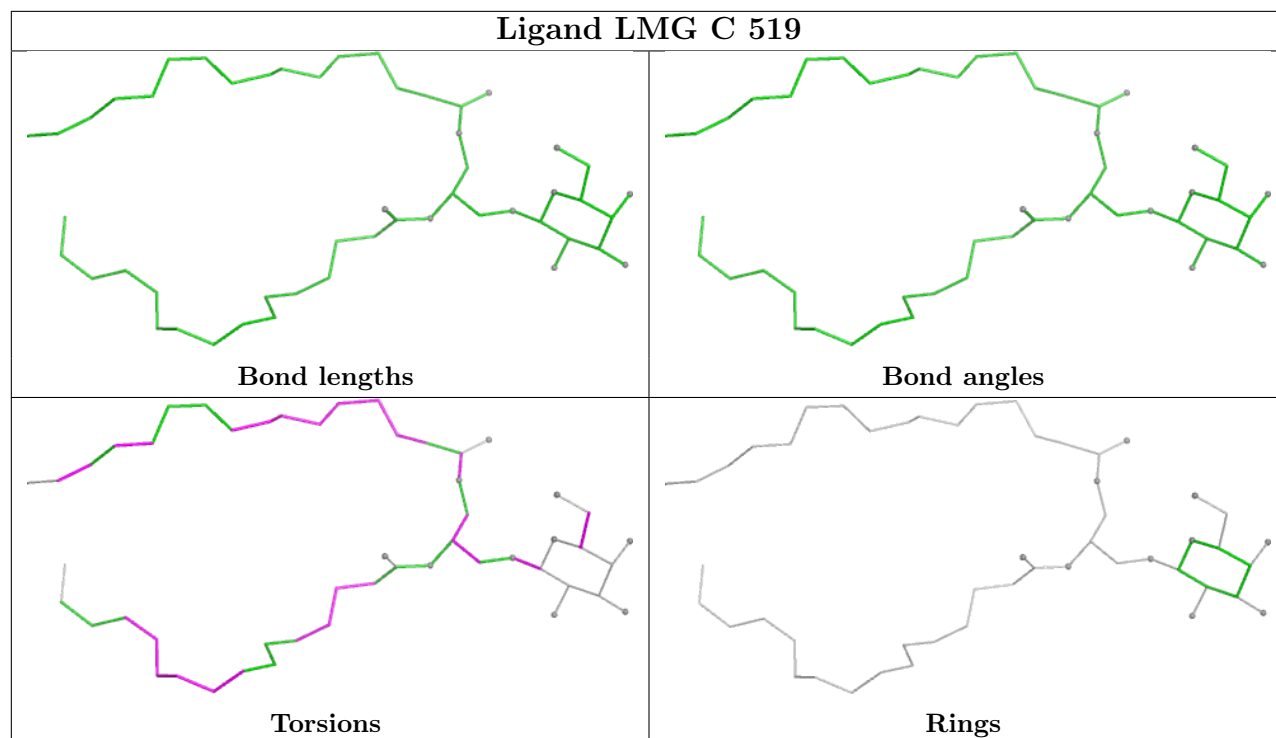


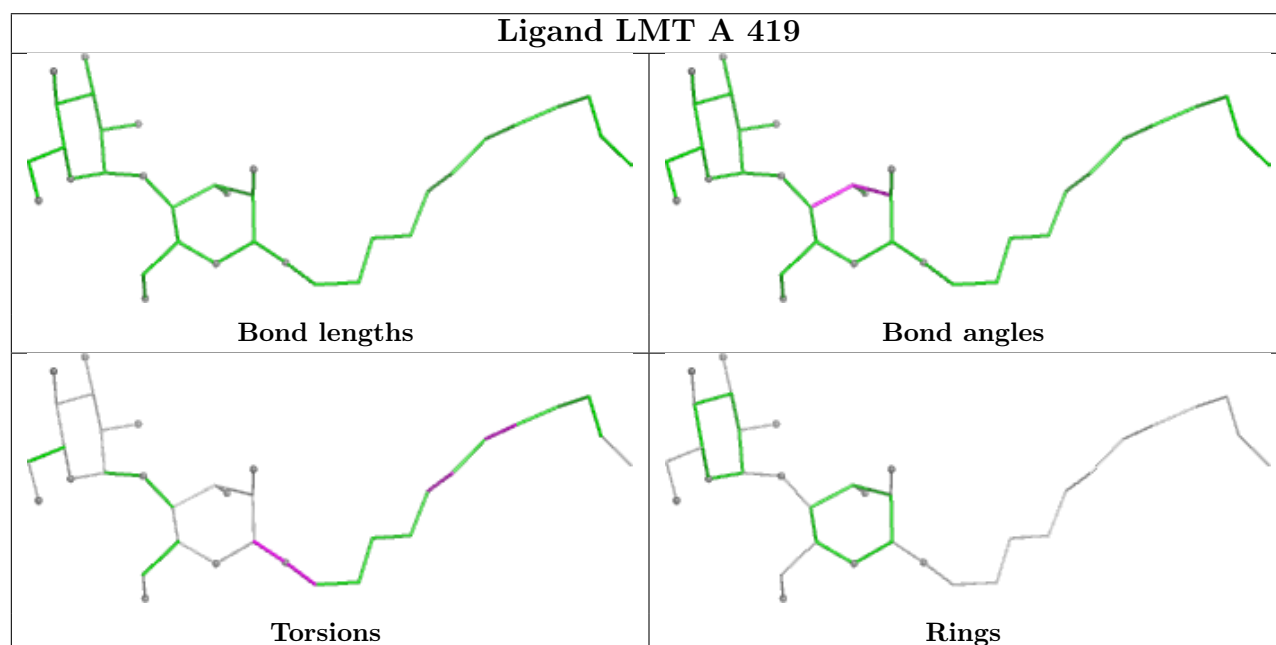
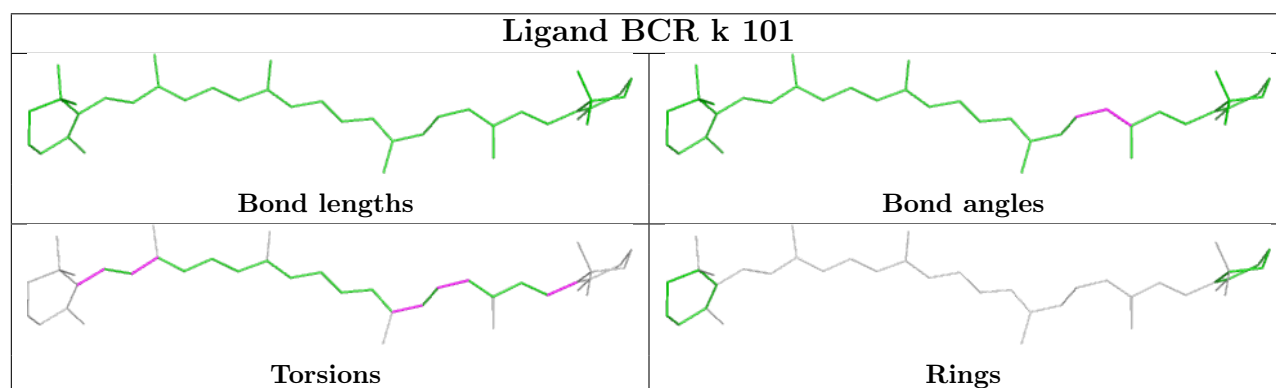
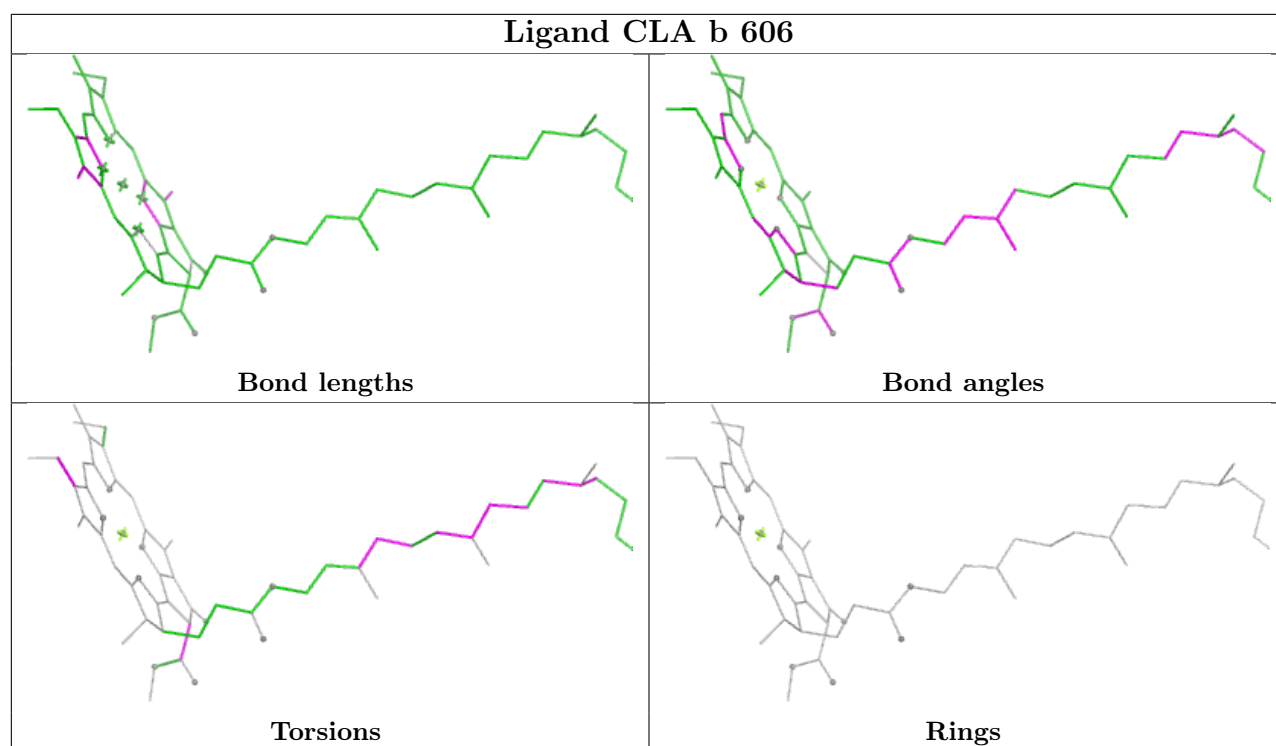




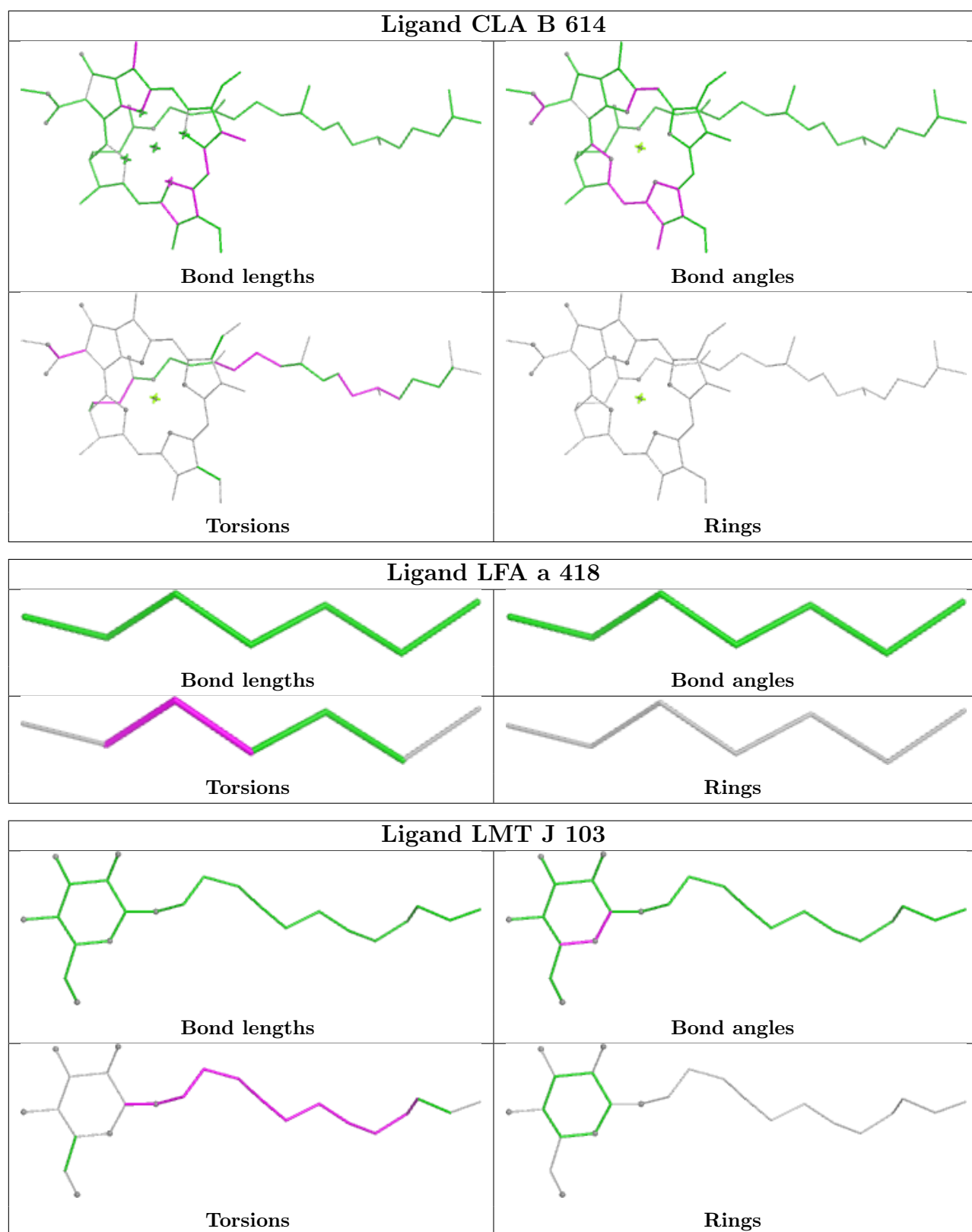


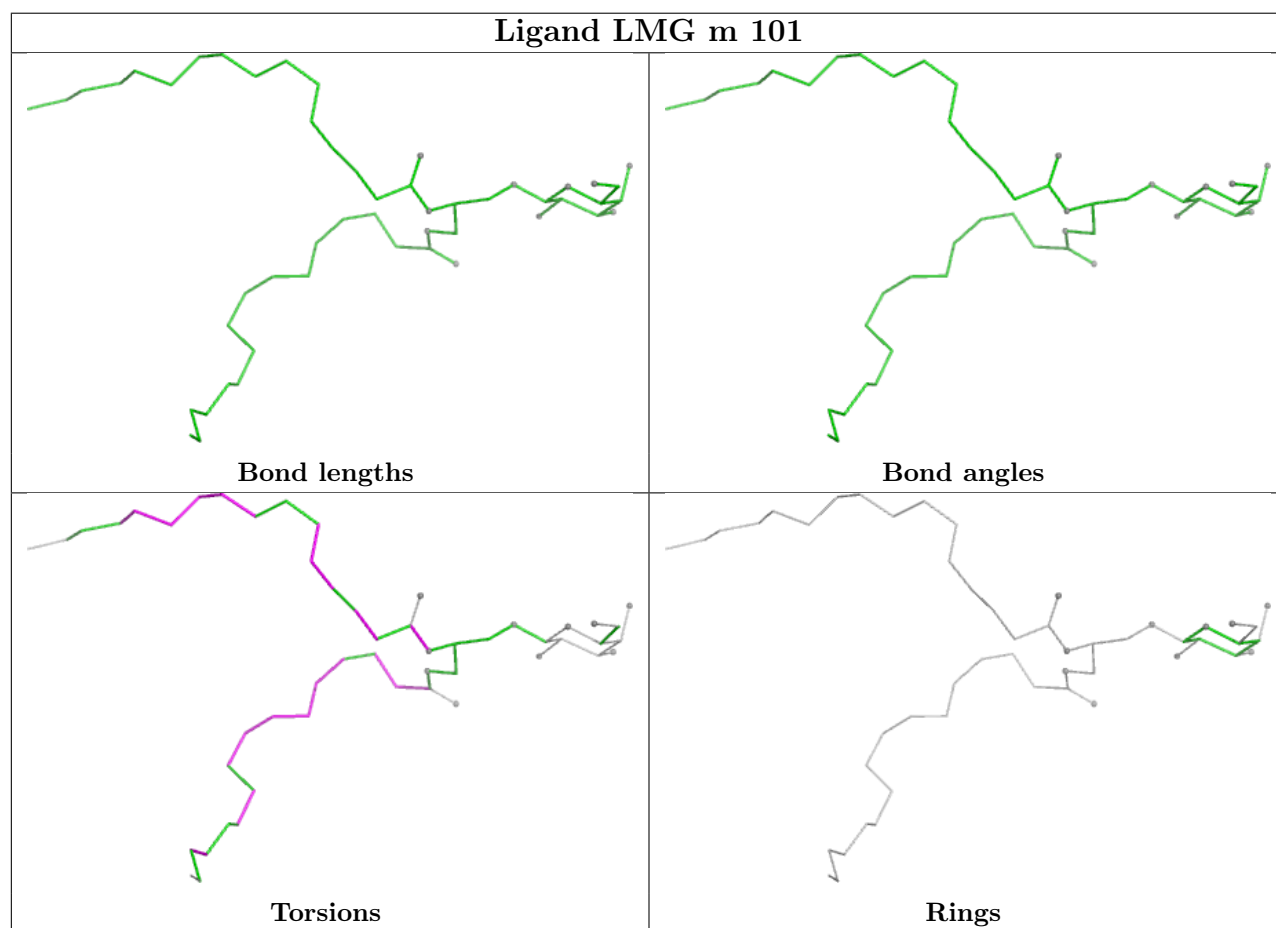
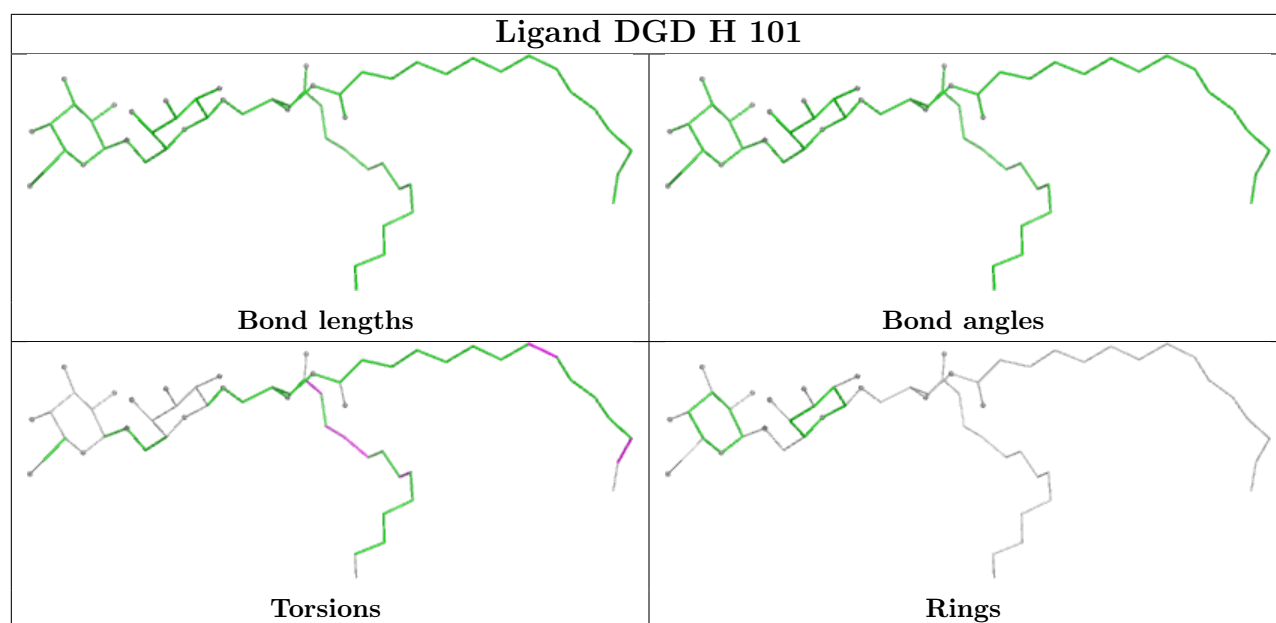


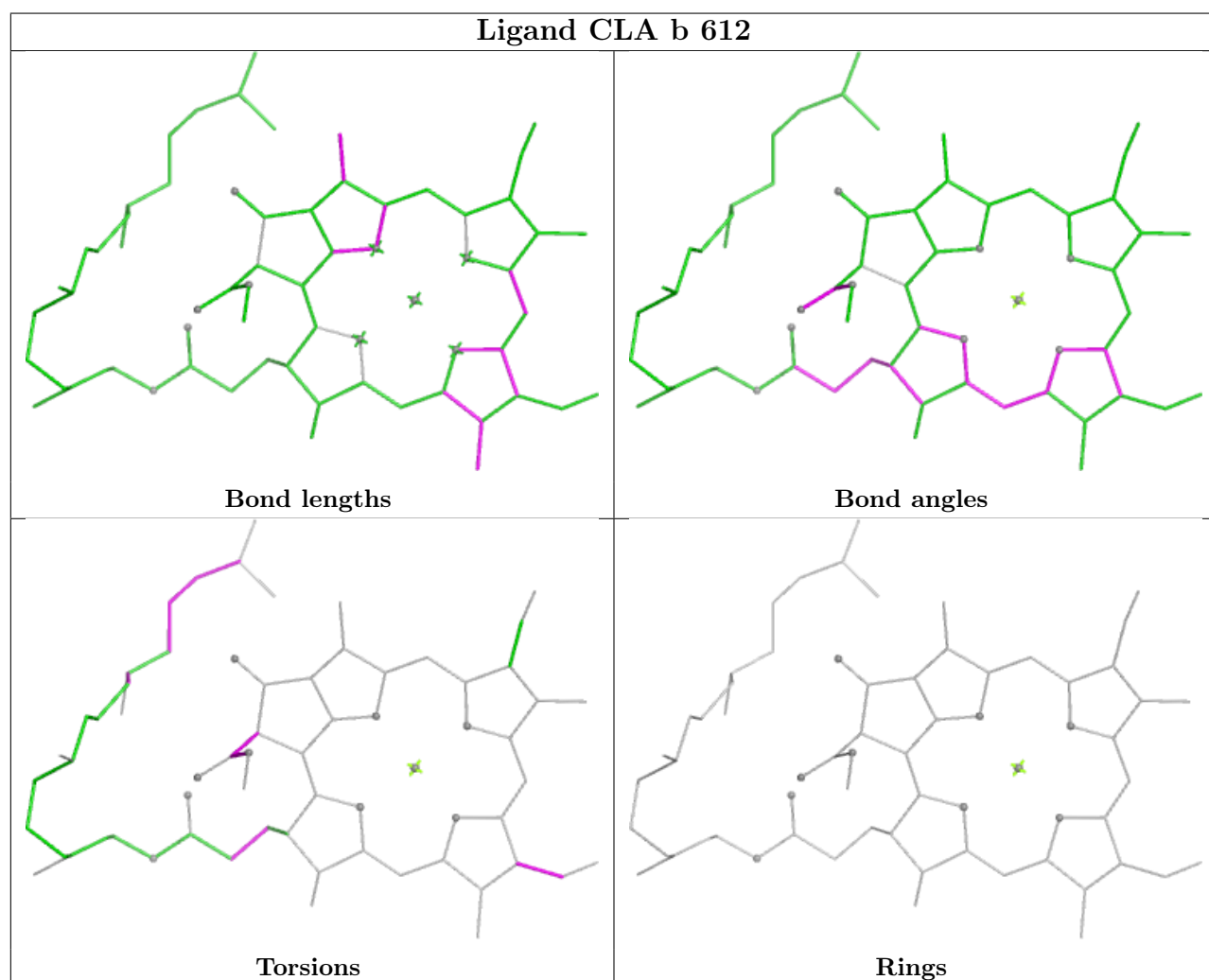
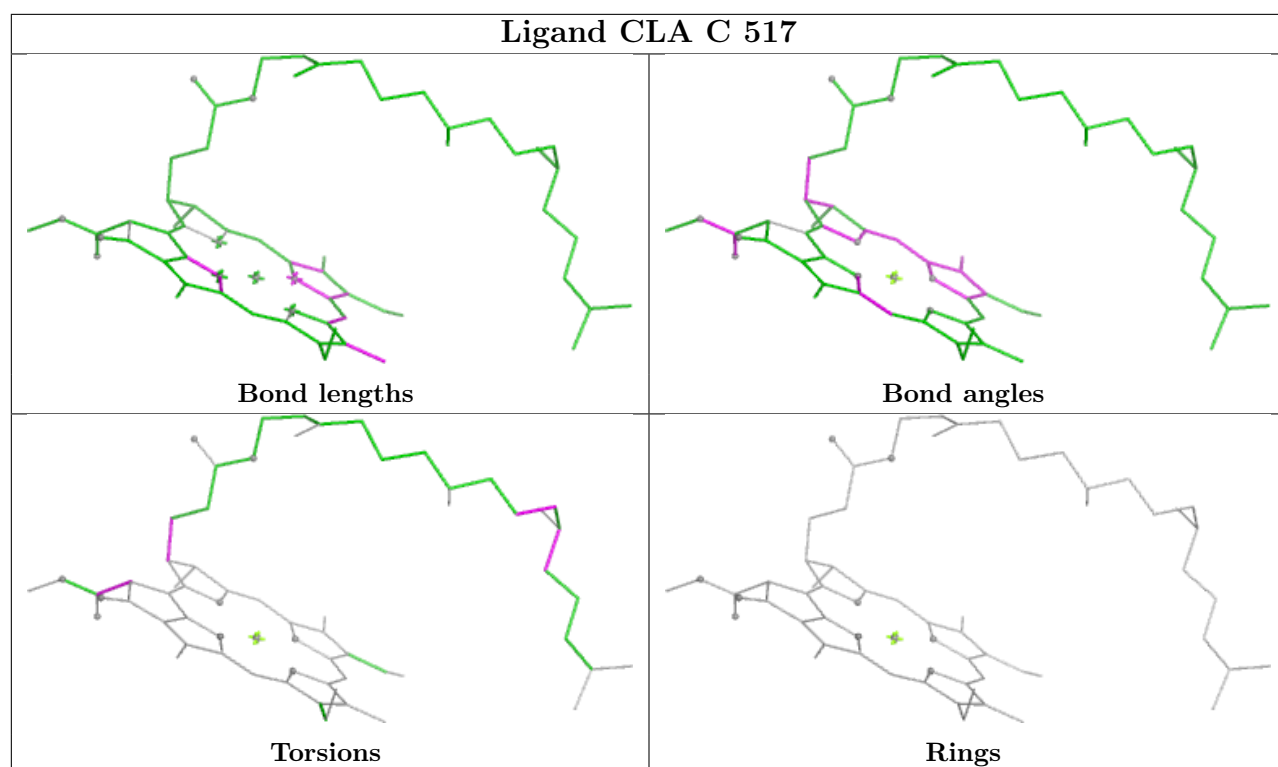


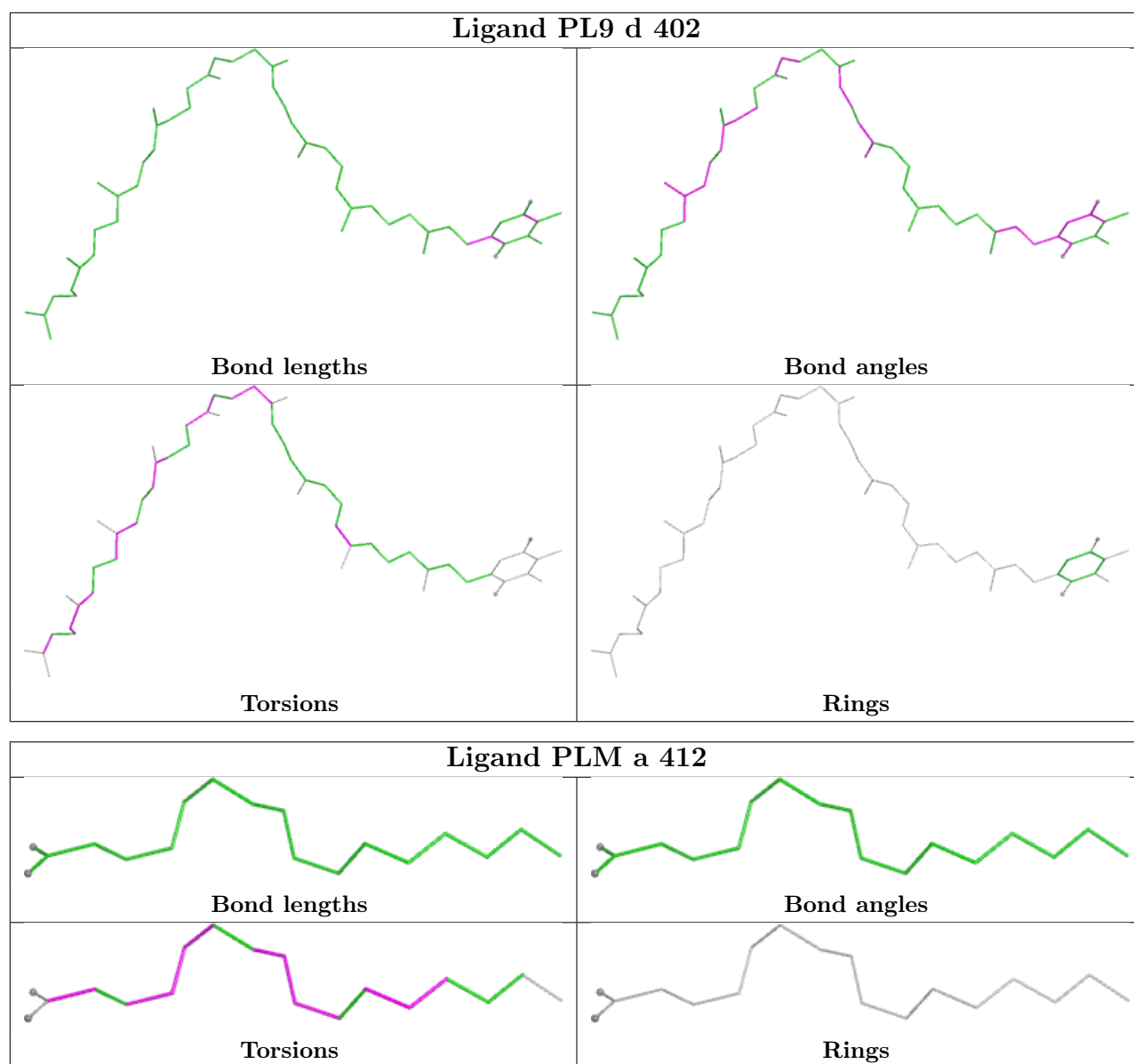


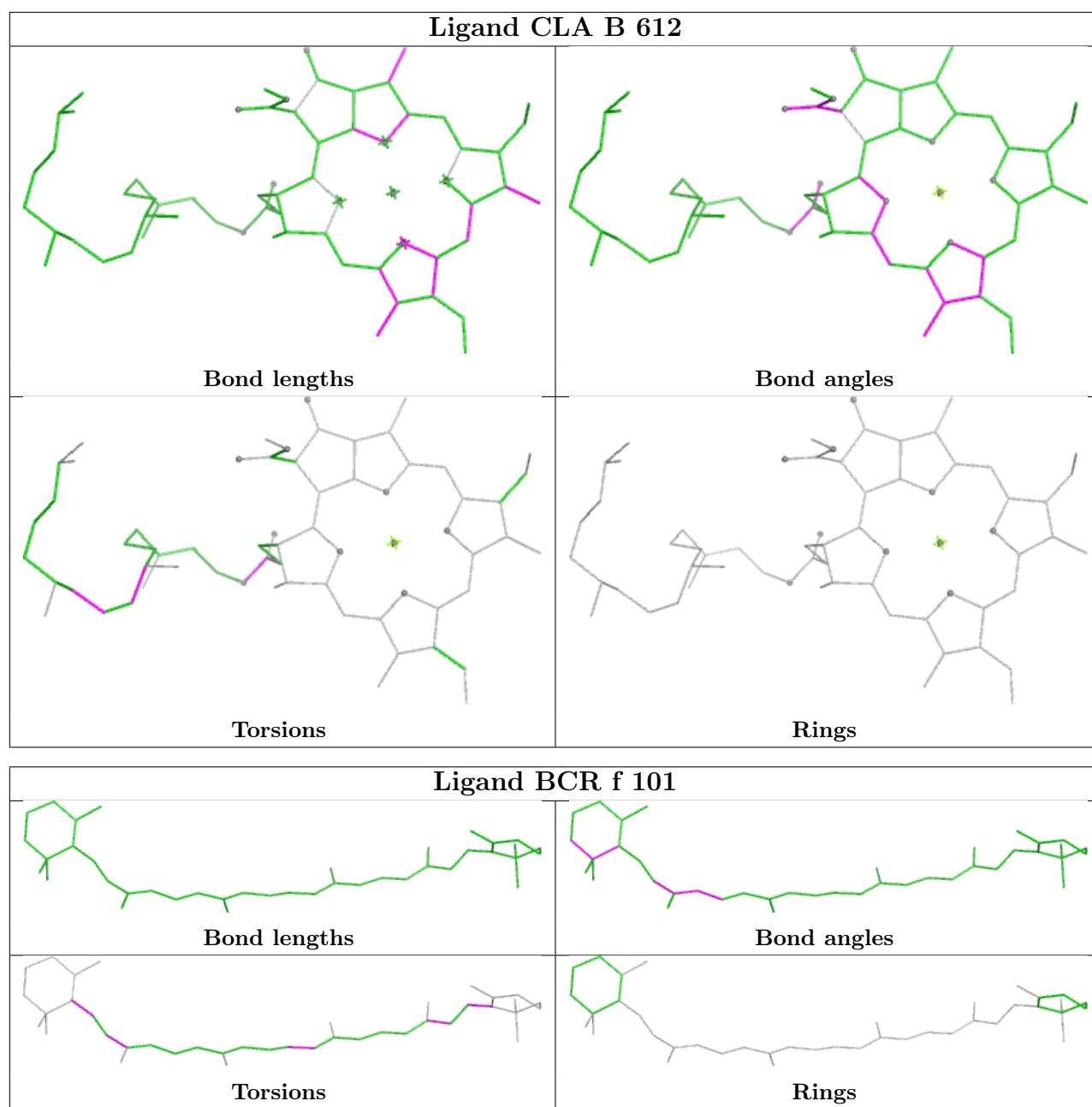












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

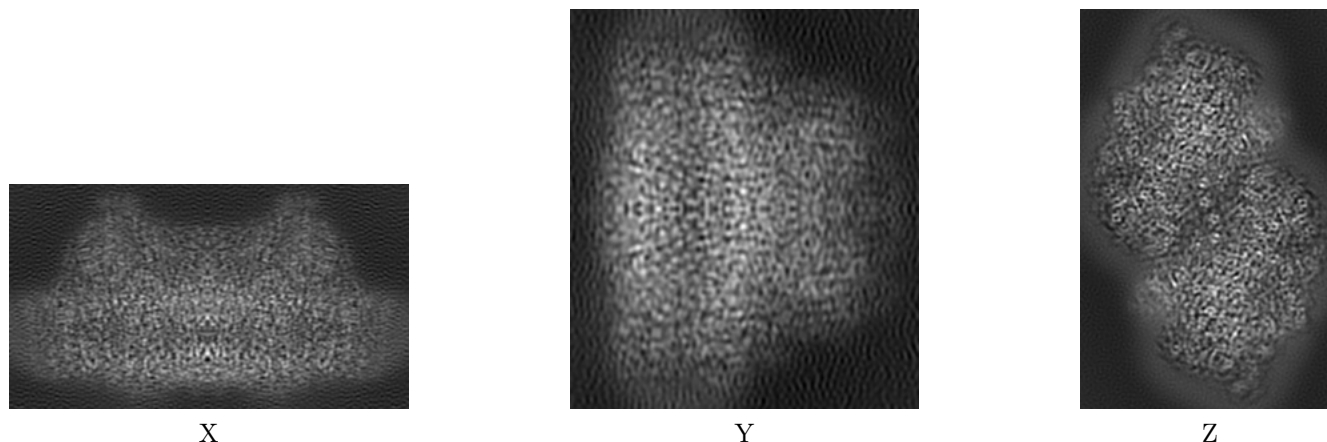
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51102. These allow visual inspection of the internal detail of the map and identification of artifacts.

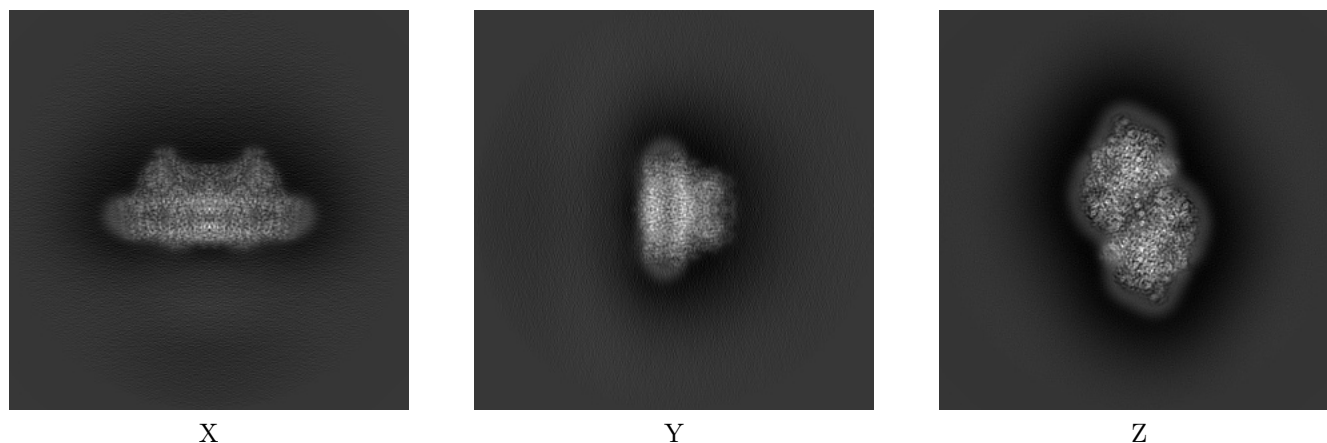
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



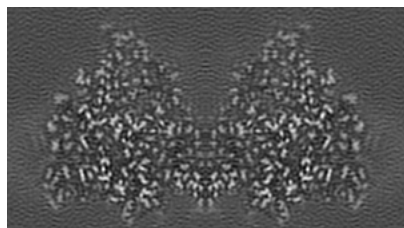
#### 6.1.2 Raw map



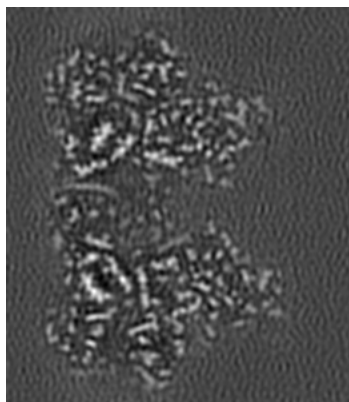
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

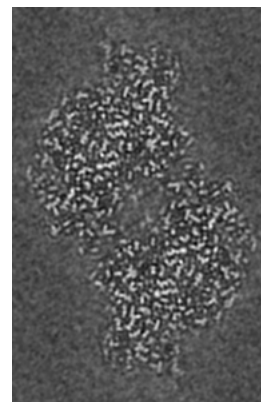
### 6.2.1 Primary map



X Index: 135

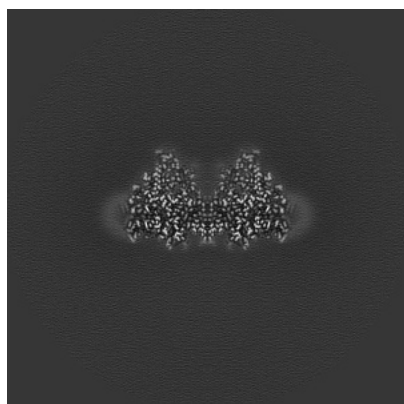


Y Index: 210

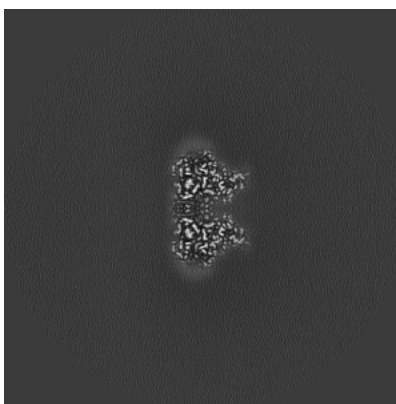


Z Index: 118

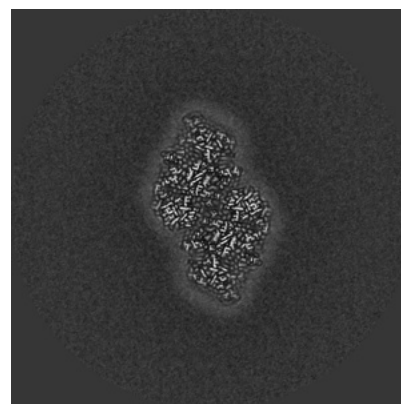
### 6.2.2 Raw map



X Index: 200



Y Index: 200

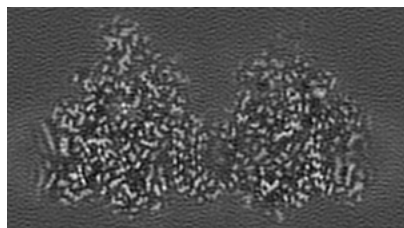


Z Index: 200

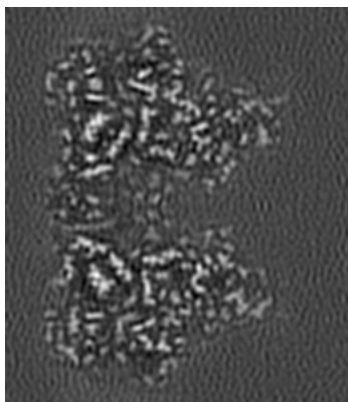
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

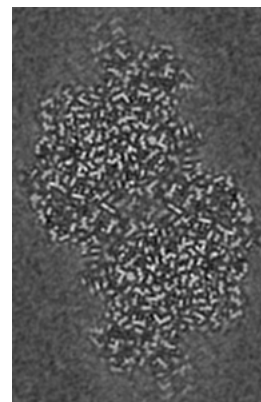
### 6.3.1 Primary map



X Index: 141

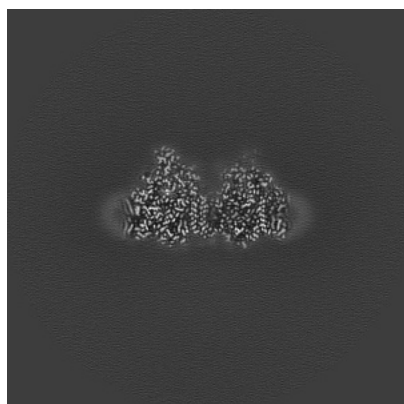


Y Index: 207

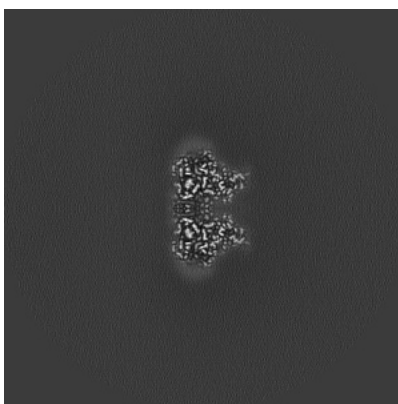


Z Index: 110

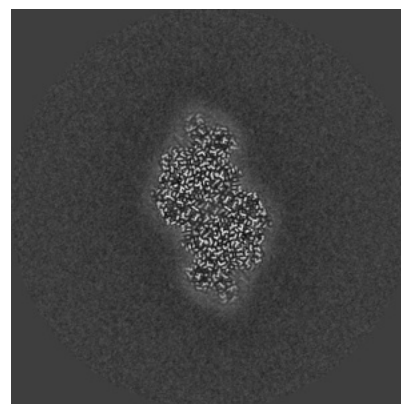
### 6.3.2 Raw map



X Index: 203



Y Index: 200



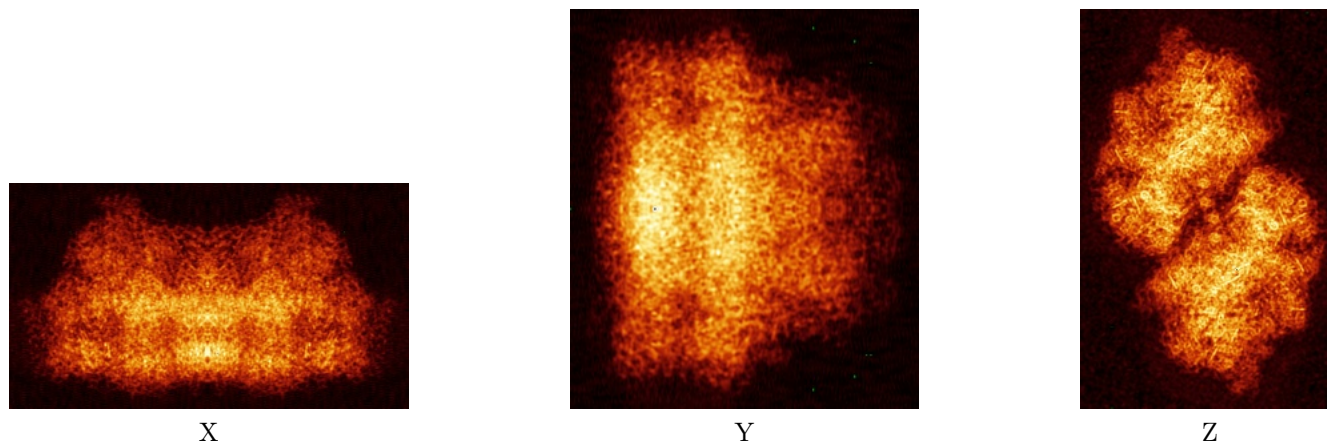
Z Index: 207

The images above show the largest variance slices of the map in three orthogonal directions.

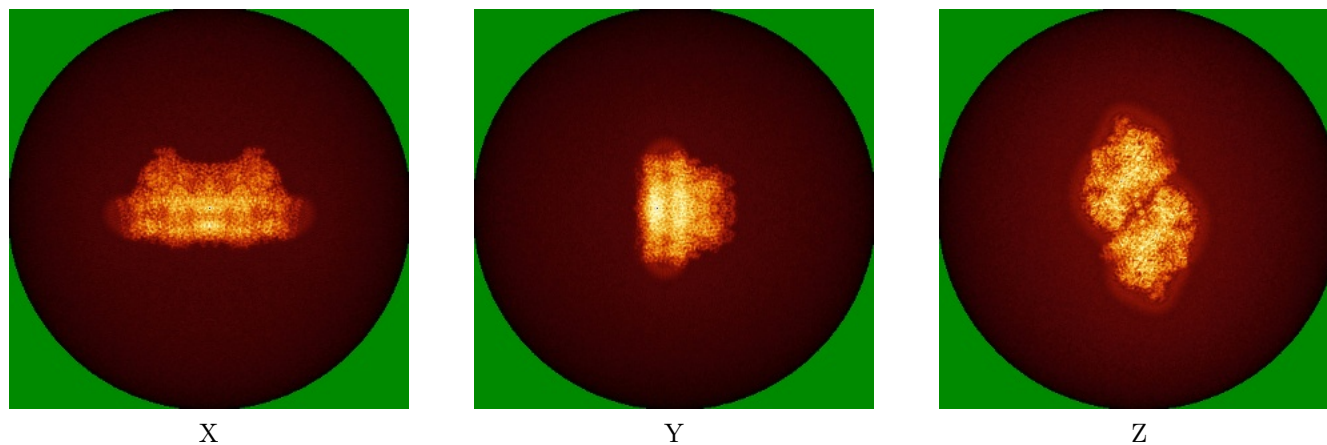


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



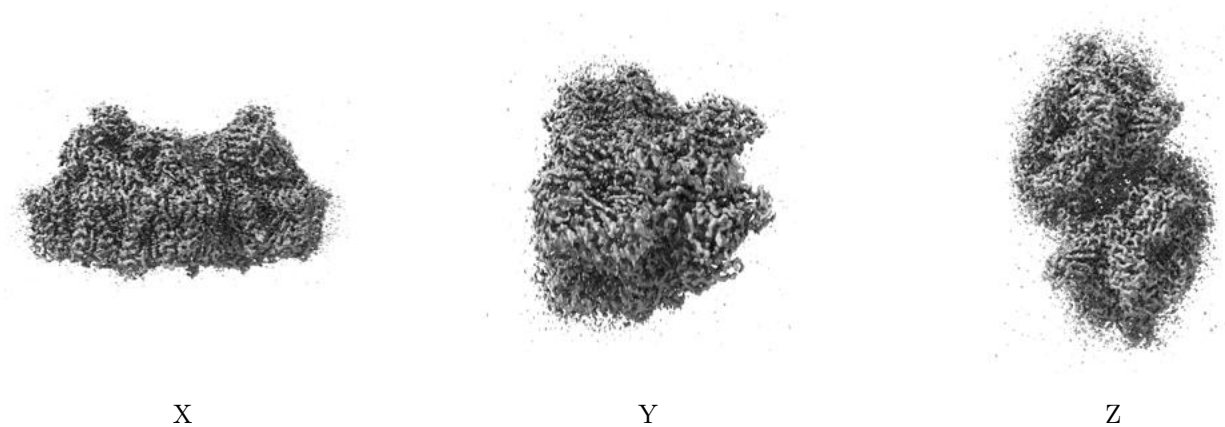
### 6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

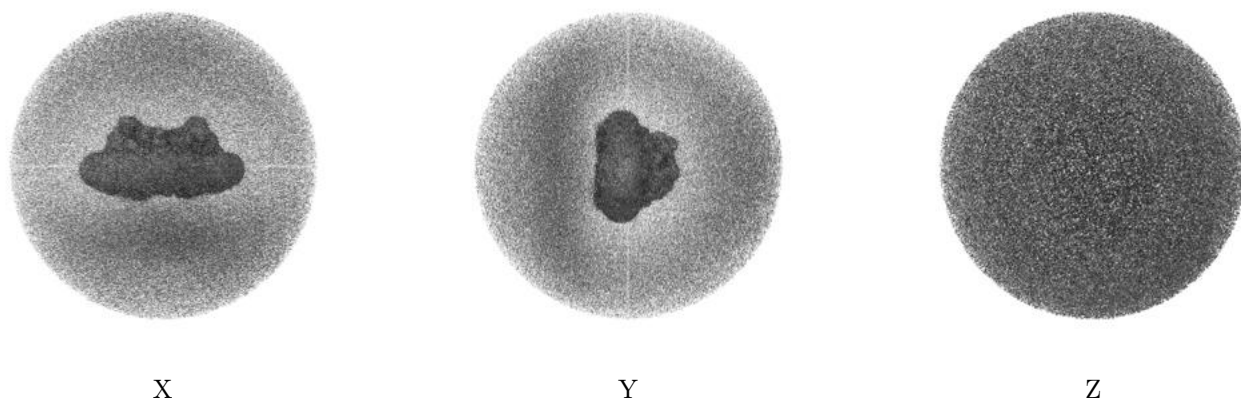
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.043. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

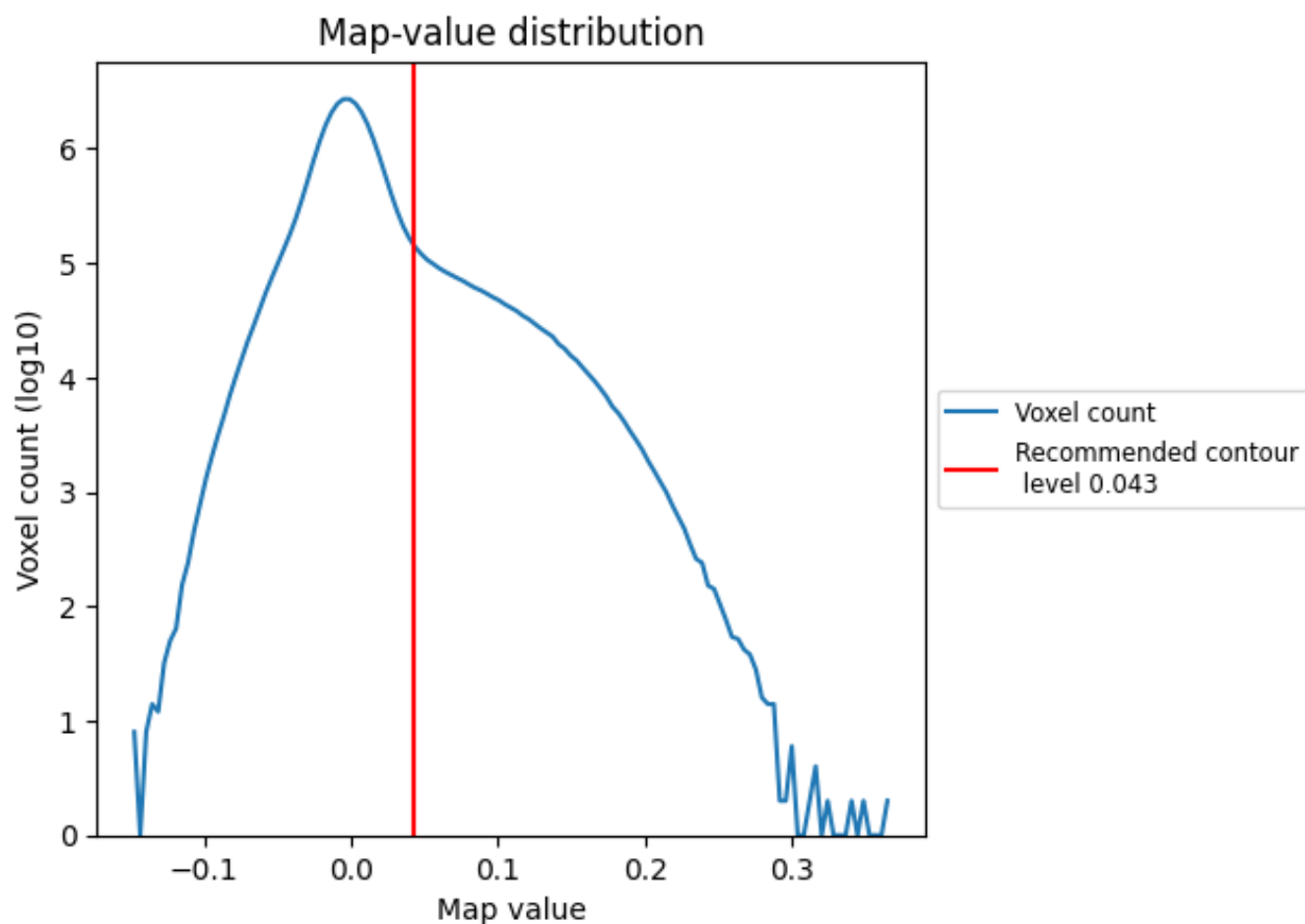
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

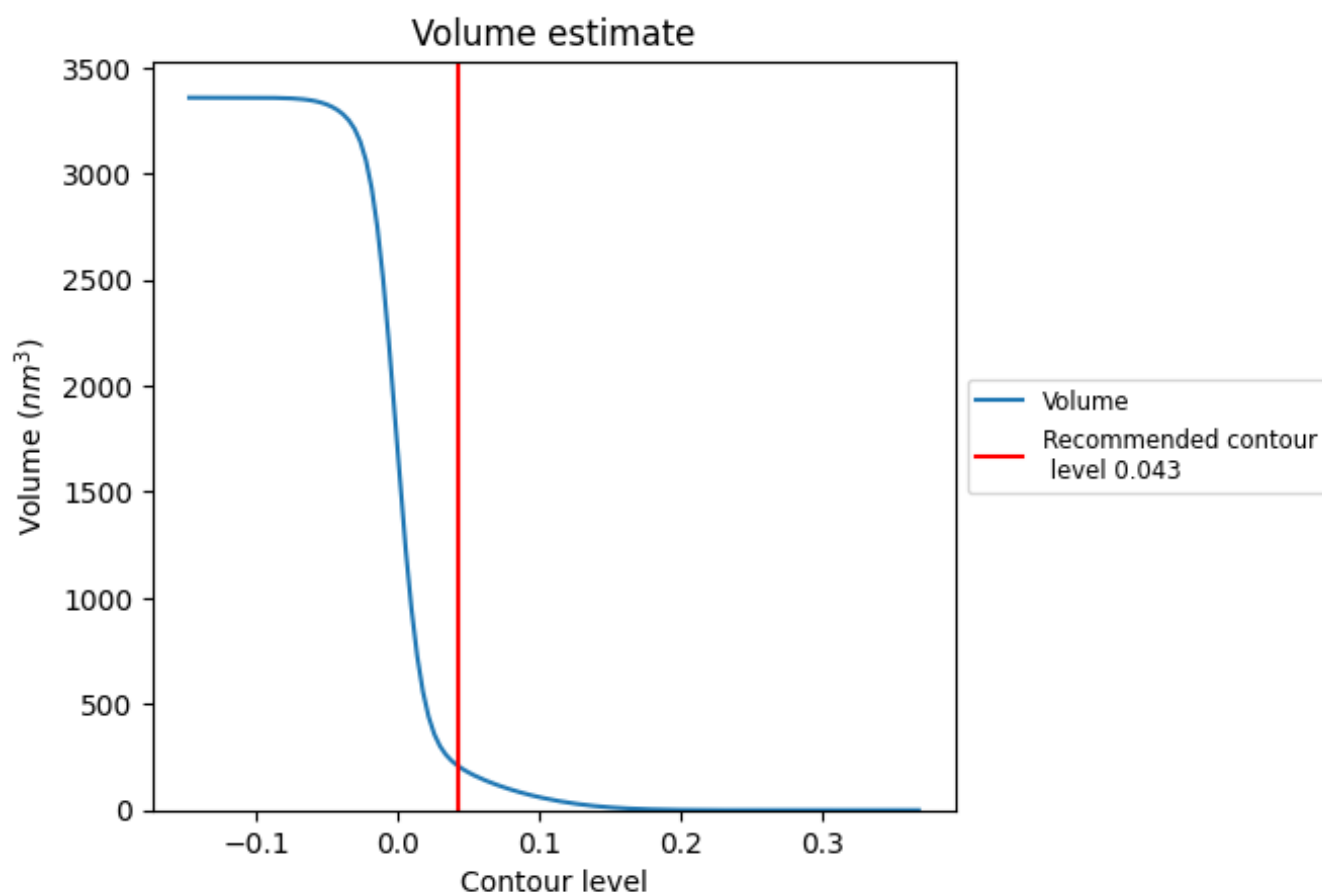
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm<sup>3</sup>; this corresponds to an approximate mass of 188 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

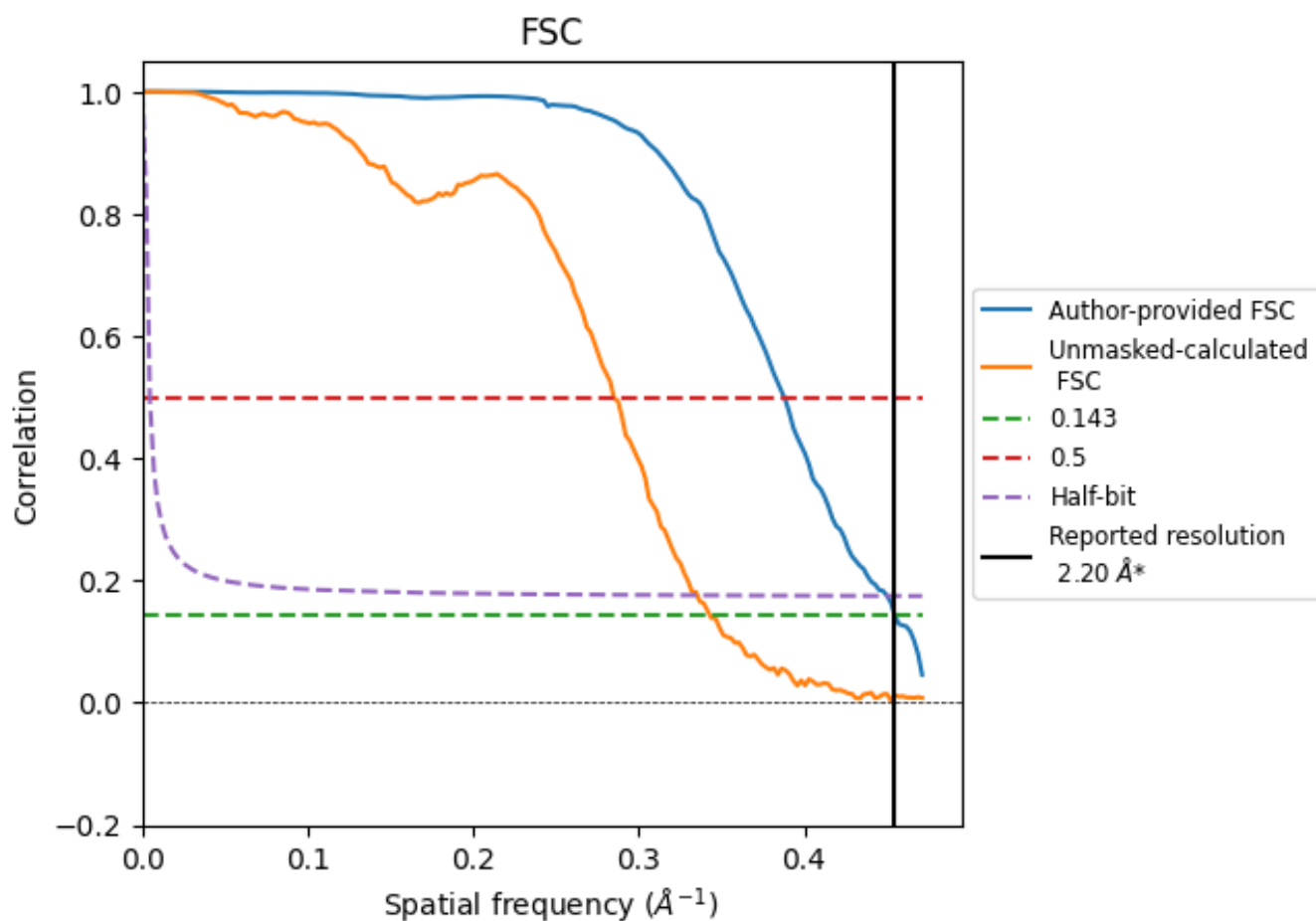
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

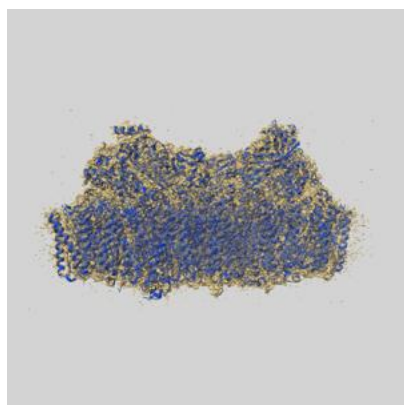
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.20                               | -    | -        |
| Author-provided FSC curve | 2.20                               | 2.58 | 2.22     |
| Unmasked-calculated*      | 2.91                               | 3.51 | 2.98     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.91 differs from the reported value 2.2 by more than 10 %

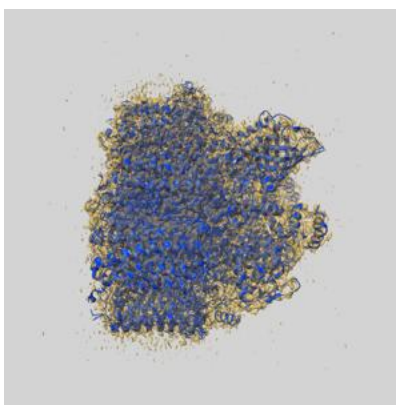
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51102 and PDB model 9G6H. Per-residue inclusion information can be found in section 3 on page 30.

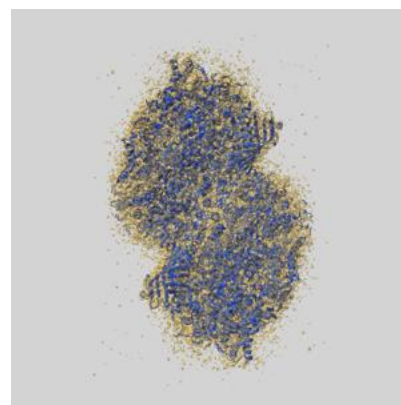
### 9.1 Map-model overlay [i](#)



X



Y

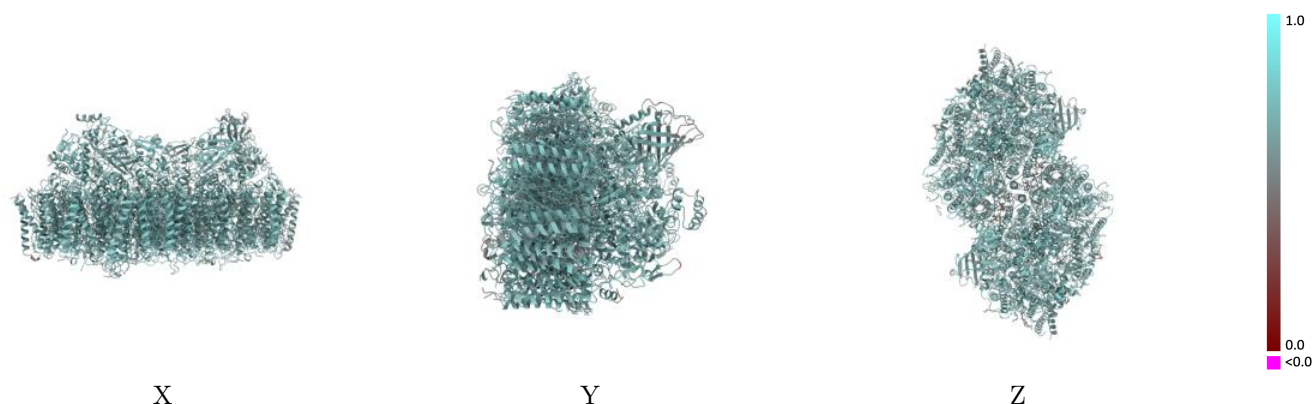


Z

The images above show the 3D surface view of the map at the recommended contour level 0.043 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

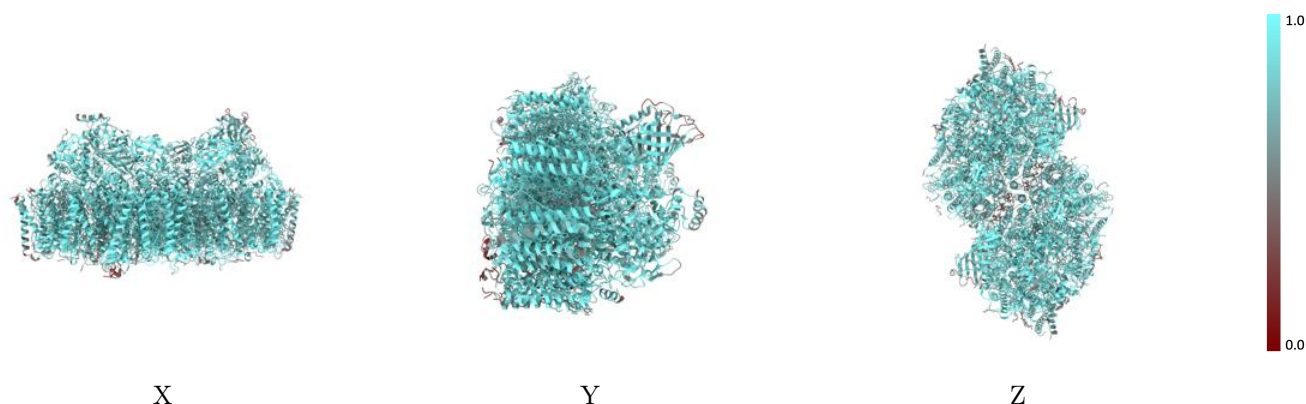


## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

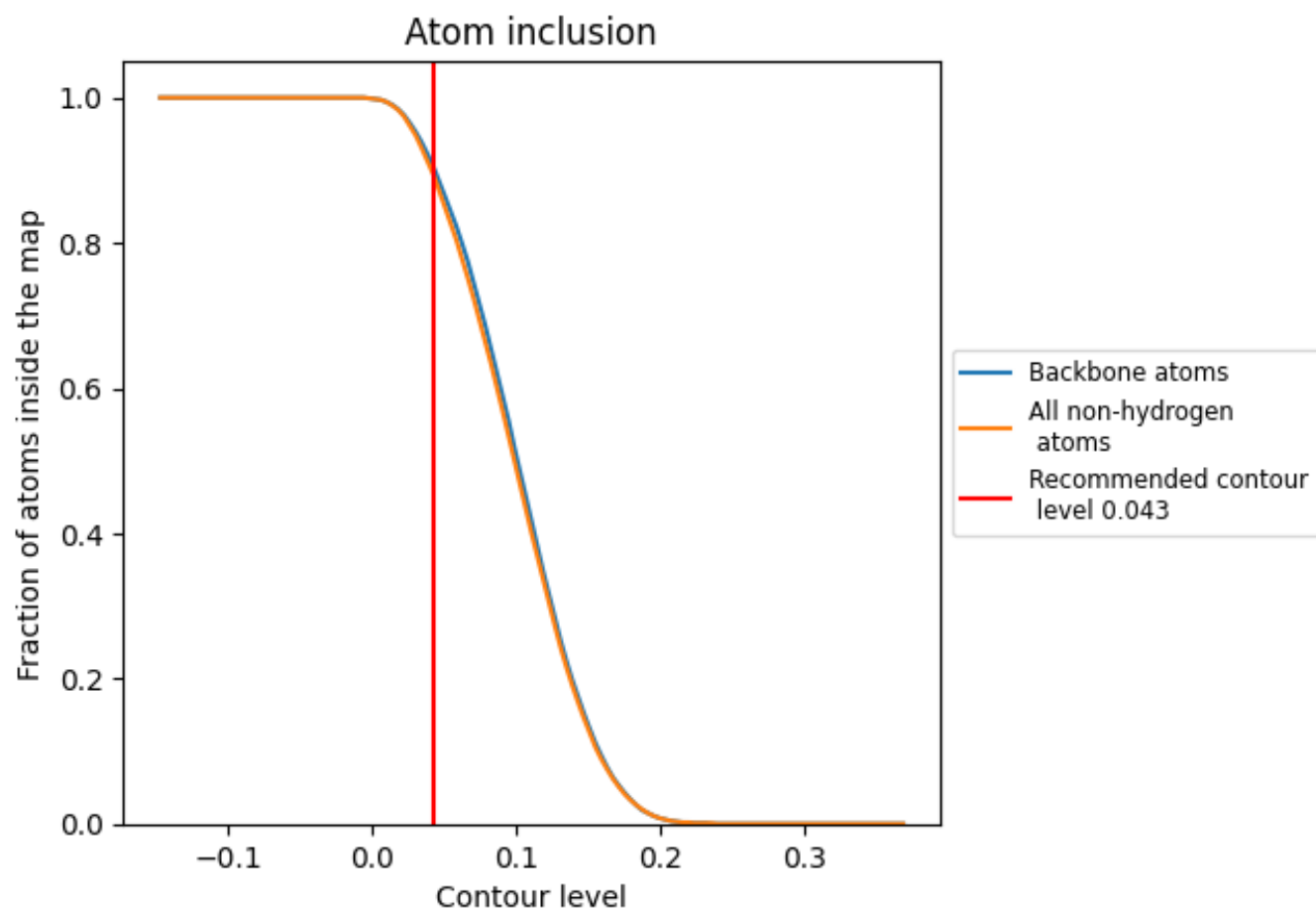
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.043).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.043) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8910   |  0.6750   |
| A     |  0.9290   |  0.6920   |
| B     |  0.9020   |  0.6840   |
| C     |  0.9120   |  0.6720   |
| D     |  0.9410   |  0.7010   |
| E     |  0.8180   |  0.6390   |
| F     |  0.8700   |  0.6710   |
| H     |  0.9370   |  0.6870   |
| I     |  0.8590   |  0.6510   |
| J     |  0.8580   |  0.6480   |
| K     |  0.9170   |  0.6600   |
| L     |  0.8850   |  0.6850   |
| M     |  0.8820   |  0.6790   |
| O     |  0.7840   |  0.6190   |
| T     |  0.8090  |  0.6570  |
| U     |  0.8060 |  0.6350 |
| V     |  0.8710 |  0.6520 |
| X     |  0.8060 |  0.6460 |
| Y     |  0.7430 |  0.6010 |
| Z     |  0.7220 |  0.6020 |
| a     |  0.9340 |  0.7020 |
| b     |  0.9100 |  0.6800 |
| c     |  0.9250 |  0.6900 |
| d     |  0.9370 |  0.6980 |
| e     |  0.8460 |  0.6510 |
| f     |  0.8490 |  0.6620 |
| h     |  0.9360 |  0.6790 |
| i     |  0.8280 |  0.6660 |
| j     |  0.8490 |  0.6640 |
| k     |  0.9080 |  0.6710 |
| l     |  0.8550 |  0.6720 |
| m     |  0.8730 |  0.6780 |
| o     |  0.7940 |  0.6320 |
| t     |  0.9100 |  0.6970 |
| u     |  0.8210 |  0.6440 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| v     |  0.8840 |  0.6620 |
| x     |  0.8110 |  0.6410 |
| y     |  0.7430 |  0.6080 |
| z     |  0.7650 |  0.6220 |