



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:00 PM UTC

PDB ID : 8WDU / pdb\_00008wdu  
EMDB ID : EMD-37465  
Title : Photosynthetic LH1-RC complex from the purple sulfur bacterium *Allochro-  
matium vinosum* purified by sucrose density  
Authors : Tani, K.; Kanno, R.; Harada, A.; Kobayashi, A.; Minamino, A.; Nakamura,  
N.; Ji, X.-C.; Purba, E.R.; Hall, M.; Yu, L.-J.; Madigan, M.T.; Mizoguchi, A.;  
Iwasaki, K.; Humbel, B.M.; Kimura, Y.; Wang-Otomo, Z.-Y.  
Deposited on : 2023-09-16  
Resolution : 2.24 Å(reported)  
Based on initial model : 7VRJ

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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
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)

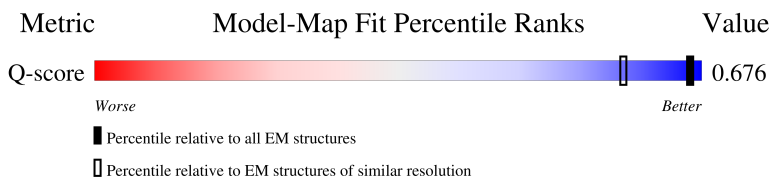
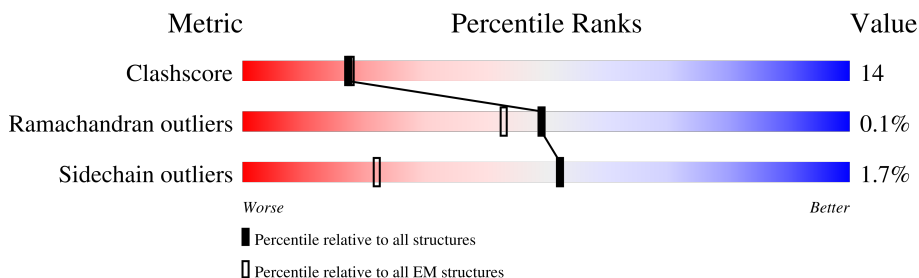
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.24 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                       | 3381 ( 1.75 - 2.74 )                                     |

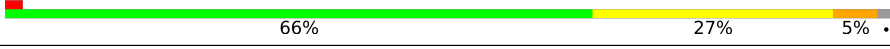
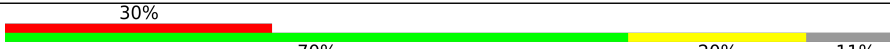
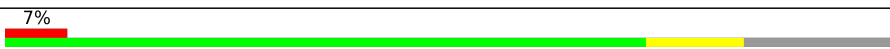
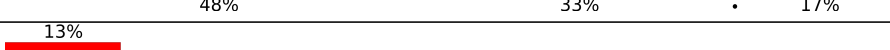
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey 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   | C     | 383    |                  |
| 2   | L     | 278    |                  |
| 3   | M     | 325    |                  |

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Validation Pipeline (wwPDB-VP) : 2.49

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | H     | 259    |    |
| 5   | 1     | 44     |    |
| 5   | 5     | 44     |    |
| 5   | 7     | 44     |    |
| 5   | 9     | 44     |    |
| 5   | A     | 44     |    |
| 5   | I     | 44     |    |
| 5   | K     | 44     |    |
| 5   | O     | 44     |    |
| 5   | Q     | 44     |    |
| 6   | 0     | 46     |    |
| 6   | 2     | 46     |   |
| 6   | 4     | 46     |  |
| 6   | 6     | 46     |  |
| 6   | 8     | 46     |  |
| 6   | B     | 46     |  |
| 6   | J     | 46     |  |
| 6   | N     | 46     |  |
| 6   | P     | 46     |  |
| 6   | R     | 46     |  |
| 7   | D     | 64     |  |
| 7   | F     | 64     |  |
| 7   | S     | 64     |  |
| 7   | U     | 64     |  |
| 7   | W     | 64     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 7   | Y     | 64     |                  |
| 8   | E     | 47     |                  |
| 8   | G     | 47     |                  |
| 8   | T     | 47     |                  |
| 8   | V     | 47     |                  |
| 8   | X     | 47     |                  |
| 8   | Z     | 47     |                  |
| 9   | 3     | 66     |                  |

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 26274 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 Photosynthetic reaction center cytochrome c subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | C     | 311      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2429  | 1535 | 418 | 460 | 16 |         |       |

- Molecule 2 is a protein called Reaction center protein L chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | L     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2210  | 1489 | 354 | 357 | 10 |         |       |

- Molecule 3 is a protein called Reaction center protein M chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | M     | 318      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2533  | 1702 | 405 | 414 | 12 |         |       |

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | H     | 259      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1993  | 1281 | 339 | 366 | 7 |         |       |

- Molecule 5 is a protein called Antenna complex alpha/beta subunit.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | A     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 359   | 248 | 58 | 52 | 1 |         |       |
| 5   | I     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 359   | 248 | 58 | 52 | 1 |         |       |
| 5   | K     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 366   | 251 | 59 | 55 | 1 |         |       |
| 5   | O     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 366   | 251 | 59 | 55 | 1 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | Q     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 359   | 248 | 58 | 52 | 1 |         |       |
| 5   | 1     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 359   | 248 | 58 | 52 | 1 |         |       |
| 5   | 5     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 355   | 245 | 57 | 52 | 1 |         |       |
| 5   | 7     | 42       | Total | C   | N  | O  | S | 1       | 0     |
|     |       |          | 359   | 251 | 56 | 51 | 1 |         |       |
| 5   | 9     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 359   | 248 | 58 | 52 | 1 |         |       |

- Molecule 6 is a protein called Antenna complex alpha/beta subunit.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | B     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 359   | 238 | 58 | 61 | 2 |         |       |
| 6   | J     | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 324   | 219 | 52 | 52 | 1 |         |       |
| 6   | N     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 320   | 217 | 51 | 51 | 1 |         |       |
| 6   | P     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 345   | 231 | 55 | 57 | 2 |         |       |
| 6   | R     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 331   | 223 | 53 | 54 | 1 |         |       |
| 6   | 2     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 339   | 228 | 54 | 55 | 2 |         |       |
| 6   | 4     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 345   | 231 | 55 | 57 | 2 |         |       |
| 6   | 6     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 320   | 217 | 51 | 51 | 1 |         |       |
| 6   | 8     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 339   | 228 | 54 | 55 | 2 |         |       |
| 6   | 0     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 351   | 234 | 56 | 59 | 2 |         |       |

- Molecule 7 is a protein called Antenna complex alpha/beta subunit.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | D     | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 397   | 270 | 62 | 64 | 1 |         |       |
| 7   | F     | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 397   | 270 | 62 | 64 | 1 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | S     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 402   | 273 | 63 | 65 | 1 |         |       |
| 7   | U     | 50       | Total | C   | N  | O  | S | 1       | 0     |
|     |       |          | 407   | 277 | 63 | 65 | 2 |         |       |
| 7   | W     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 402   | 273 | 63 | 65 | 1 |         |       |
| 7   | Y     | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 470   | 317 | 76 | 76 | 1 |         |       |

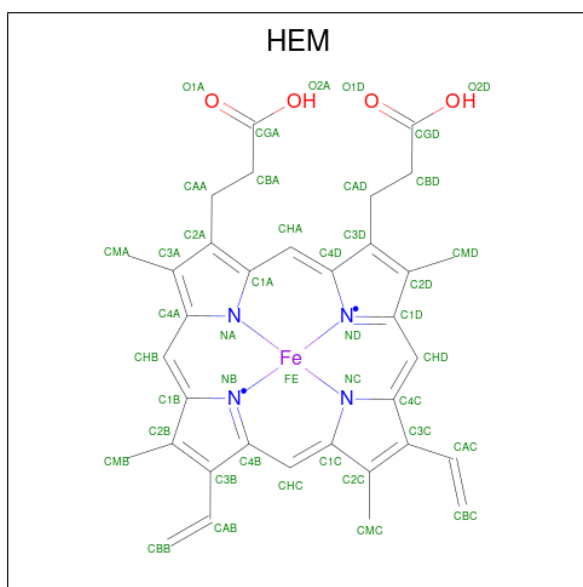
- Molecule 8 is a protein called Antenna complex alpha/beta subunit.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | E     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 343   | 231 | 53 | 56 | 3 |         |       |
| 8   | G     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 335   | 226 | 52 | 55 | 2 |         |       |
| 8   | T     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 343   | 231 | 53 | 56 | 3 |         |       |
| 8   | V     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 335   | 226 | 52 | 55 | 2 |         |       |
| 8   | X     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 343   | 231 | 53 | 56 | 3 |         |       |
| 8   | Z     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 343   | 231 | 53 | 56 | 3 |         |       |

- Molecule 9 is a protein called Antenna complex alpha/beta subunit.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | 3     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 498   | 337 | 78 | 80 | 3 |         |       |

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

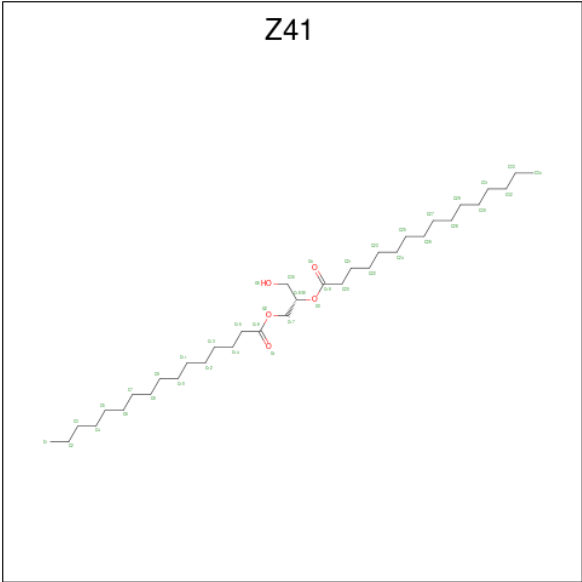


| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 10  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 10  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 10  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 10  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

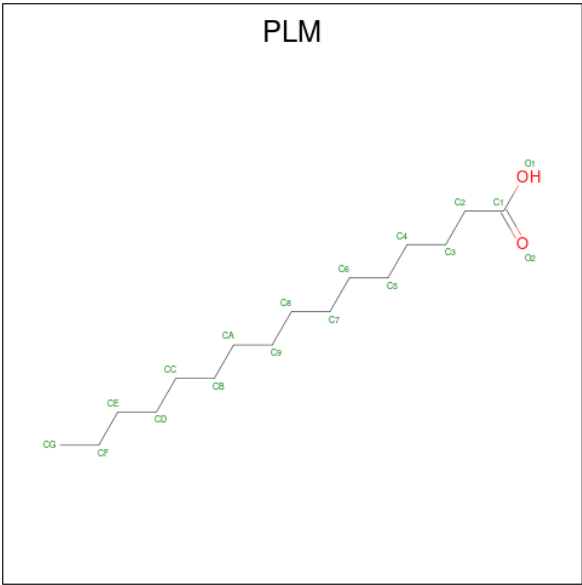
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 11  | C     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 12 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (CCD ID: Z41) (formula:  $C_{35}H_{68}O_5$ ).



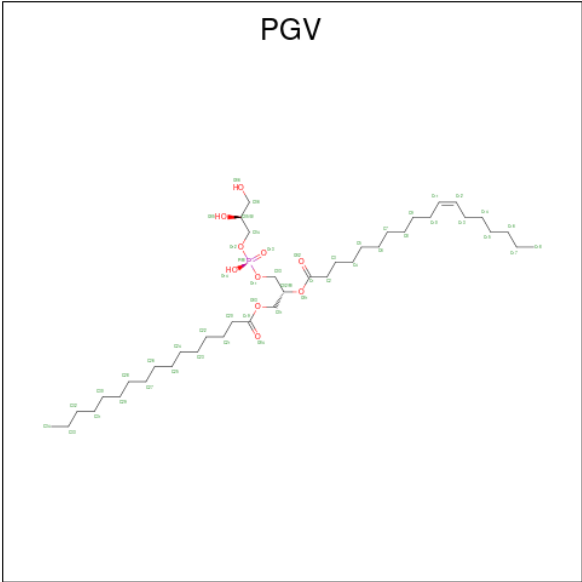
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 12  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |

- Molecule 13 is PALMITIC ACID (CCD ID: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



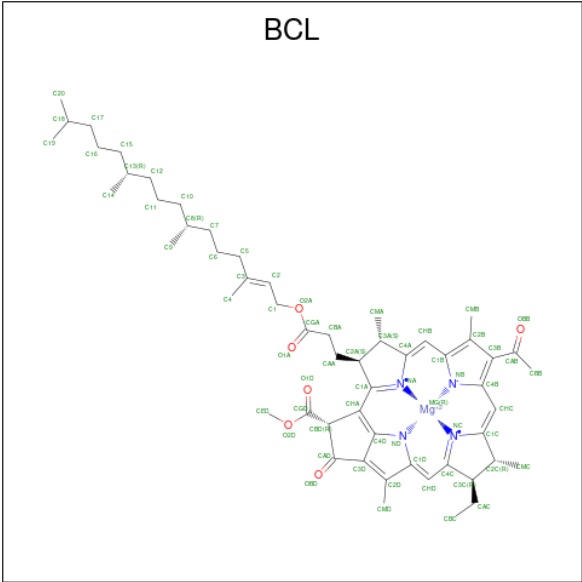
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 13  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 12    | 11 | 1 |         |

- Molecule 14 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 14  | C     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 31    | 20 | 10 | 1 |         |
| 14  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 29    | 18 | 10 | 1 |         |
| 14  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 35    | 24 | 10 | 1 |         |
| 14  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 14  | M     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 27    | 18 | 8  | 1 |         |
| 14  | H     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 36    | 25 | 10 | 1 |         |
| 14  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |
| 14  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 33    | 22 | 10 | 1 |         |
| 14  | F     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 31    | 22 | 8  | 1 |         |
| 14  | Q     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 24    | 15 | 8  | 1 |         |
| 14  | 1     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 27    | 18 | 8  | 1 |         |

- Molecule 15 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 15  | L     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | L     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | A     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | B     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | D     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | E     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | F     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | I     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | J     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | K     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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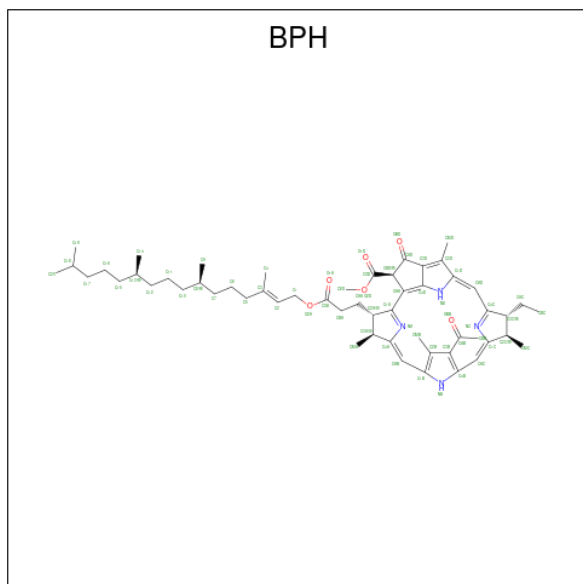
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 15  | O     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | P     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | Q     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | R     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | S     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | T     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | U     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | V     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | W     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | X     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | Y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | Z     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | 1     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | 2     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | 3     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | 4     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | 5     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | 6     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | 7     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | 8     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 15  | 9     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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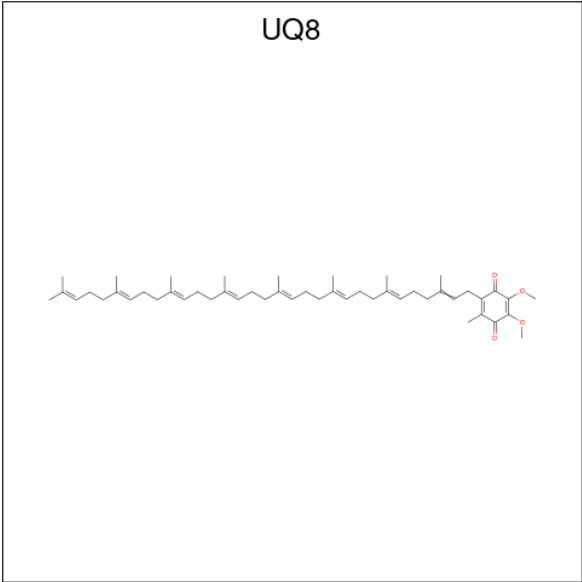
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
|     |       |          | Total | C  | Mg | N | O |         |
| 15  | 0     | 1        | 66    | 55 | 1  | 4 | 6 | 0       |

- Molecule 16 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



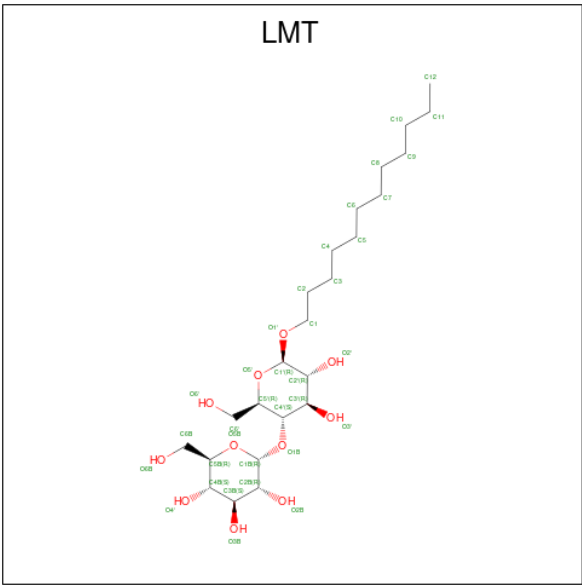
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
|     |       |          | Total | C  | N | O |         |
| 16  | L     | 1        | 65    | 55 | 4 | 6 | 0       |
| 16  | M     | 1        | 65    | 55 | 4 | 6 | 0       |

- Molecule 17 is Ubiquinone-8 (CCD ID: UQ8) (formula:  $C_{49}H_{74}O_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 17  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 29 | 4 |         |
| 17  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 53    | 49 | 4 |         |
| 17  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 53    | 49 | 4 |         |

- Molecule 18 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



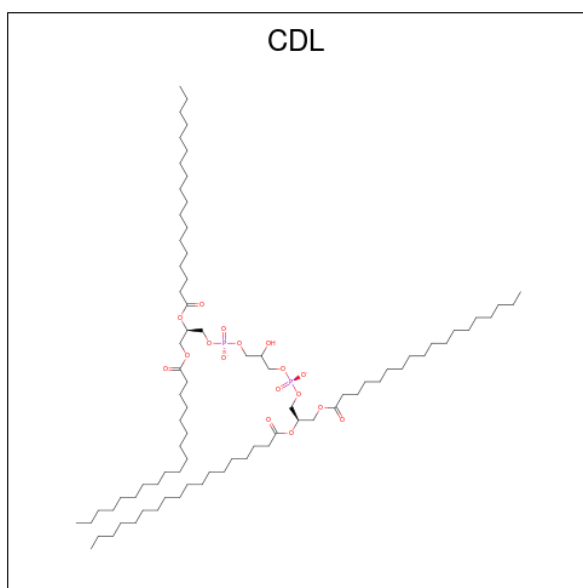
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 18  | L     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 18  | M     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | M     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 13 | 11 |         |
| 18  | H     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | E     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | P     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | P     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | R     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | S     | 1        | Total | C  | O  | 0       |
|     |       |          | 26    | 15 | 11 |         |
| 18  | T     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | X     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | Z     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | 2     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | 5     | 1        | Total | C  | O  | 0       |
|     |       |          | 31    | 20 | 11 |         |
| 18  | 8     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 18  | 8     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 19 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).

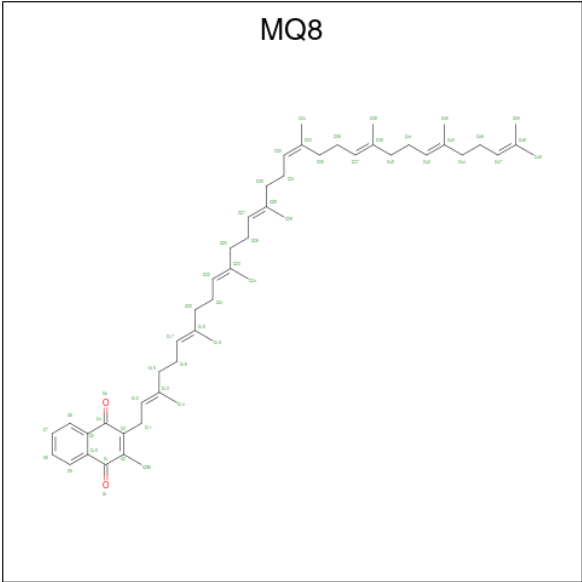


| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 19  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 80    | 61 | 17 | 2 |         |
| 19  | M     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 39    | 21 | 16 | 2 |         |
| 19  | M     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 95    | 76 | 17 | 2 |         |
| 19  | H     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 79    | 60 | 17 | 2 |         |
| 19  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 58    | 39 | 17 | 2 |         |

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

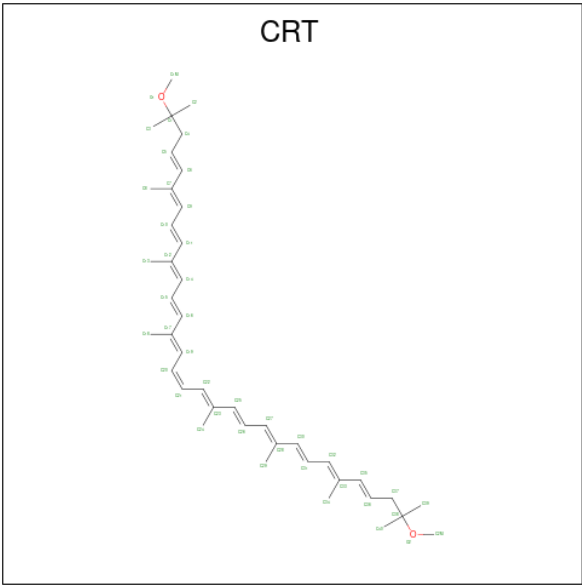
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 20  | M     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 21 is MENAQUINONE 8 (CCD ID: MQ8) (formula:  $C_{51}H_{72}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 21  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 53    | 51 | 2 |         |

- Molecule 22 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C<sub>42</sub>H<sub>60</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 22  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 22  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 22  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |

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| Mol | Chain | Residues | Atoms       |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
| 22  | G     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | J     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | N     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | P     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | R     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | T     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | V     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | Y     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | Z     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | 2     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | 4     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | 6     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | 9     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |
| 22  | 0     | 1        | Total<br>44 | C<br>42 | O<br>2 | 0       |

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca).

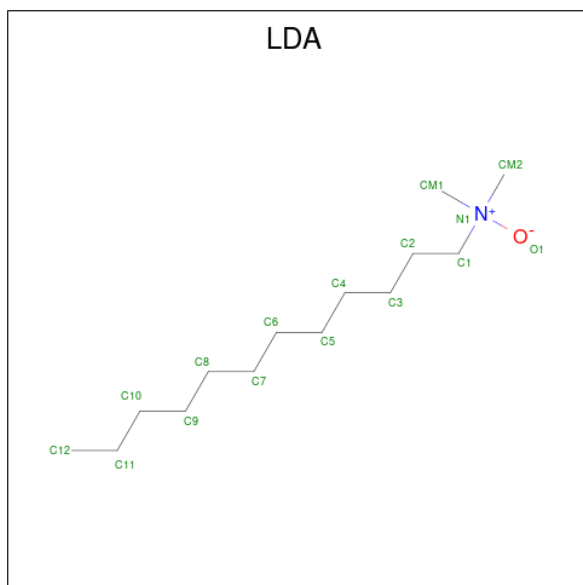
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 23  | D     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 23  | F     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 23  | S     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 23  | U     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 23  | W     | 1        | Total<br>1 | Ca<br>1 | 0       |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 23  | Y     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 24 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula:  $C_{14}H_{31}NO$ ).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 24  | K     | 1        | Total | C  | N | O | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |
| 24  | O     | 1        | Total | C  | N | O | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |

- Molecule 25 is water.

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 25  | C     | 119      | Total | O   | 0       |
|     |       |          | 119   | 119 |         |
| 25  | L     | 50       | Total | O   | 0       |
|     |       |          | 50    | 50  |         |
| 25  | M     | 77       | Total | O   | 0       |
|     |       |          | 77    | 77  |         |
| 25  | H     | 19       | Total | O   | 0       |
|     |       |          | 19    | 19  |         |
| 25  | A     | 2        | Total | O   | 0       |
|     |       |          | 2     | 2   |         |
| 25  | B     | 1        | Total | O   | 0       |
|     |       |          | 1     | 1   |         |

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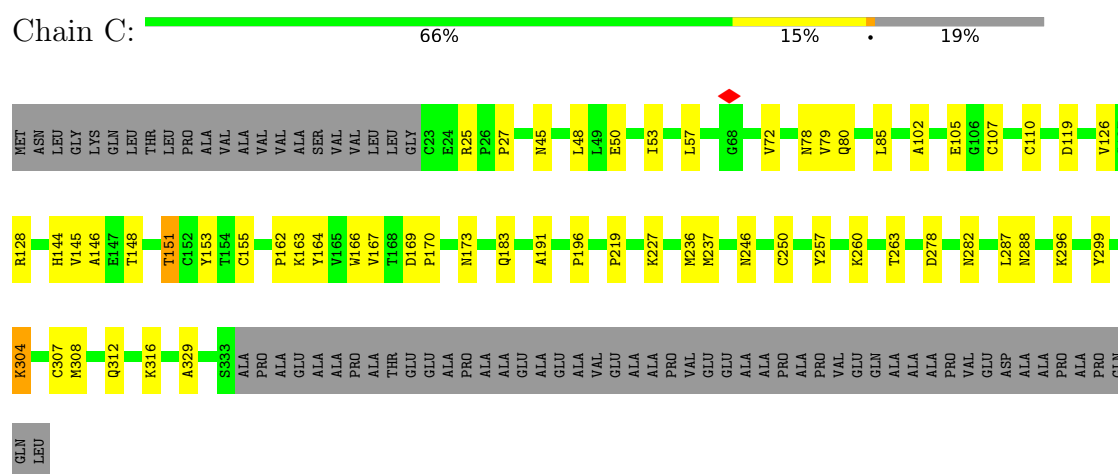
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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 25  | D     | 4        | Total<br>4  | O<br>4  | 0       |
| 25  | E     | 2        | Total<br>2  | O<br>2  | 0       |
| 25  | F     | 2        | Total<br>2  | O<br>2  | 0       |
| 25  | I     | 2        | Total<br>2  | O<br>2  | 0       |
| 25  | K     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | O     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | P     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | Q     | 2        | Total<br>2  | O<br>2  | 0       |
| 25  | R     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | S     | 5        | Total<br>5  | O<br>5  | 0       |
| 25  | T     | 3        | Total<br>3  | O<br>3  | 0       |
| 25  | U     | 10       | Total<br>10 | O<br>10 | 0       |
| 25  | V     | 3        | Total<br>3  | O<br>3  | 0       |
| 25  | W     | 7        | Total<br>7  | O<br>7  | 0       |
| 25  | X     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | Y     | 5        | Total<br>5  | O<br>5  | 0       |
| 25  | 1     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | 3     | 10       | Total<br>10 | O<br>10 | 0       |
| 25  | 7     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | 9     | 4        | Total<br>4  | O<br>4  | 0       |

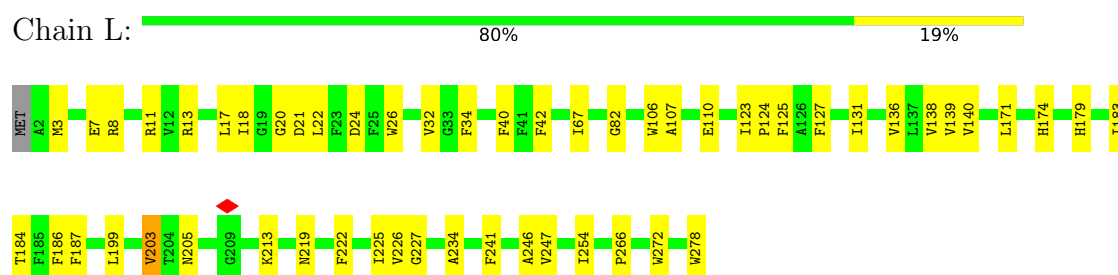
### 3 Residue-property plots

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.

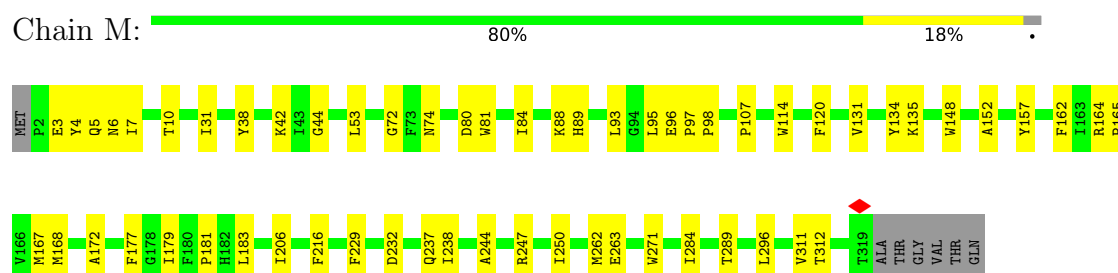
#### • Molecule 1: Photosynthetic reaction center cytochrome c subunit



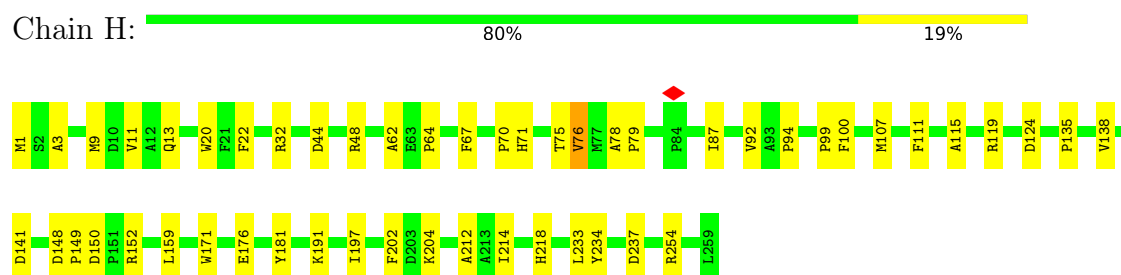
#### • Molecule 2: Reaction center protein L chain



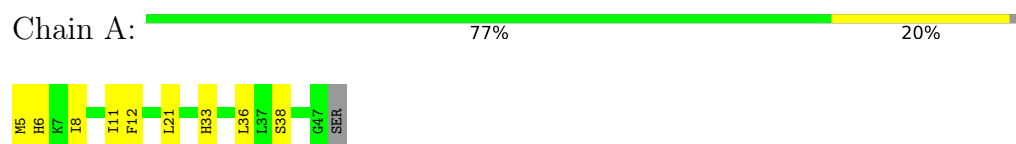
#### • Molecule 3: Reaction center protein M chain



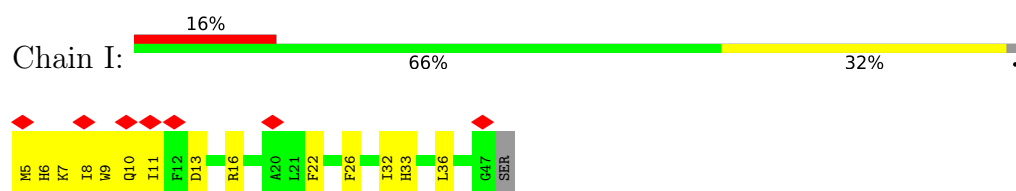
- Molecule 4: Photosynthetic reaction center H subunit



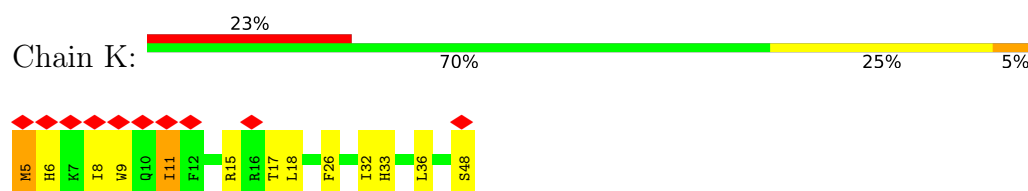
- Molecule 5: Antenna complex alpha/beta subunit



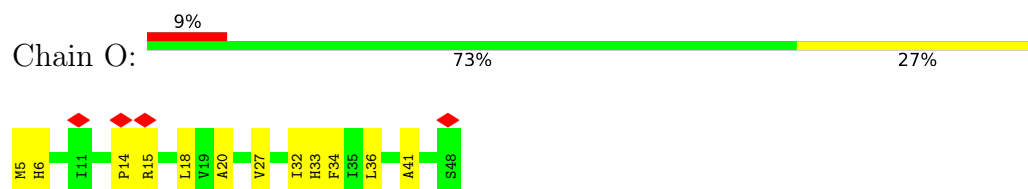
- Molecule 5: Antenna complex alpha/beta subunit



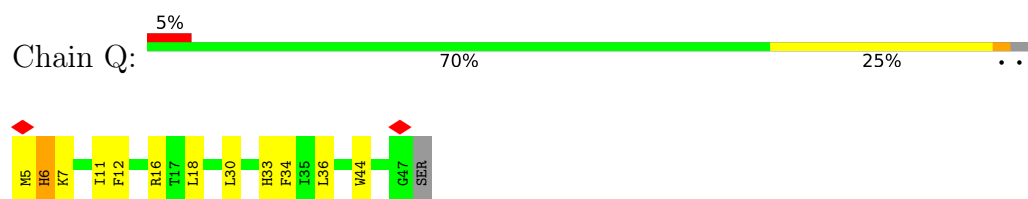
- Molecule 5: Antenna complex alpha/beta subunit



- Molecule 5: Antenna complex alpha/beta subunit



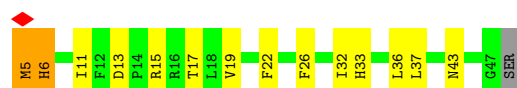
- Molecule 5: Antenna complex alpha/beta subunit



- Molecule 5: Antenna complex alpha/beta subunit



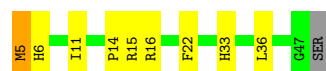
- Molecule 5: Antenna complex alpha/beta subunit



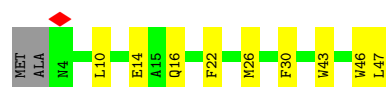
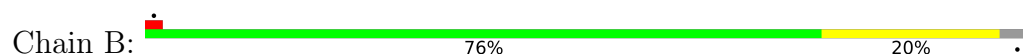
- Molecule 5: Antenna complex alpha/beta subunit



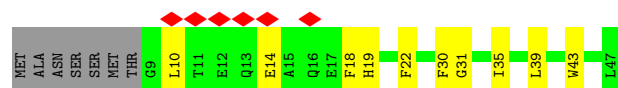
- Molecule 5: Antenna complex alpha/beta subunit



- Molecule 6: Antenna complex alpha/beta subunit



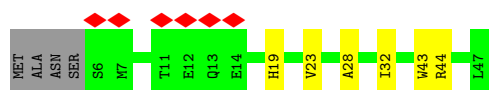
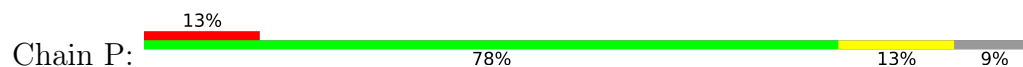
- Molecule 6: Antenna complex alpha/beta subunit



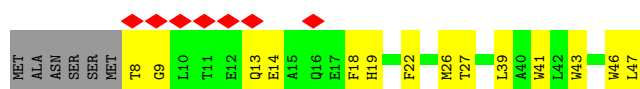
- Molecule 6: Antenna complex alpha/beta subunit



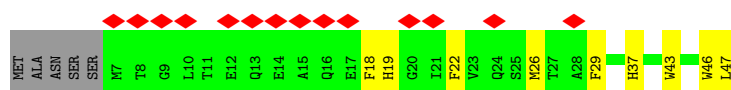
- Molecule 6: Antenna complex alpha/beta subunit



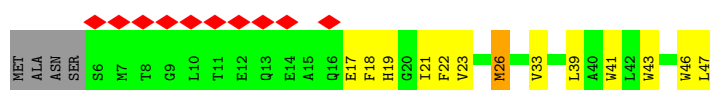
- Molecule 6: Antenna complex alpha/beta subunit



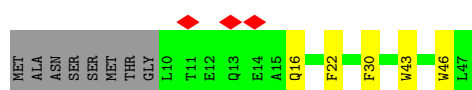
- Molecule 6: Antenna complex alpha/beta subunit



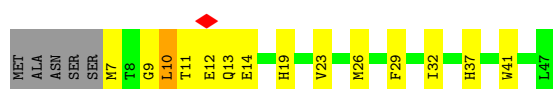
- Molecule 6: Antenna complex alpha/beta subunit



- Molecule 6: Antenna complex alpha/beta subunit



- Molecule 6: Antenna complex alpha/beta subunit

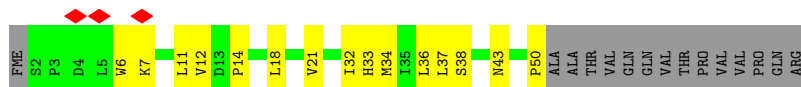


- Molecule 6: Antenna complex alpha/beta subunit





- Molecule 7: Antenna complex alpha/beta subunit



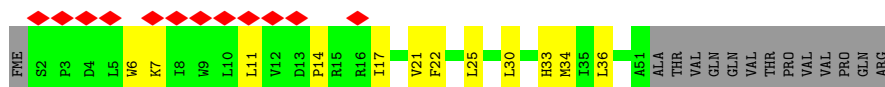
- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



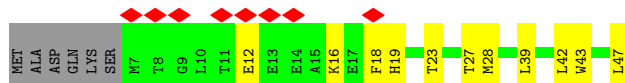
- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 8: Antenna complex alpha/beta subunit



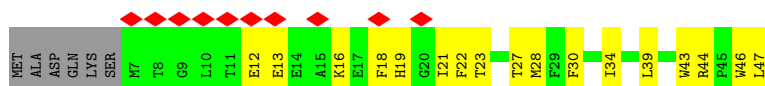
- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 8: Antenna complex alpha/beta subunit

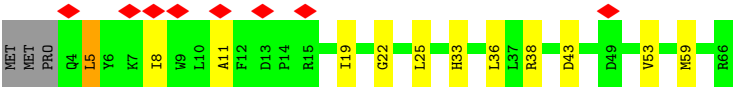


- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 9: Antenna complex alpha/beta subunit





## 4 Experimental information

| Property                             | Value                  | Source    |
|--------------------------------------|------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE        | Depositor |
| Imposed symmetry                     | POINT, Not provided    |           |
| Number of particles used             | 252230                 | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF      | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY    | Depositor |
| Microscope                           | JEOL CRYO ARM 300      | Depositor |
| Voltage (kV)                         | 300                    | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                     | Depositor |
| Minimum defocus (nm)                 | 700                    | Depositor |
| Maximum defocus (nm)                 | 3200                   | Depositor |
| Magnification                        | Not provided           |           |
| Image detector                       | GATAN K3 (6k x 4k)     | Depositor |
| Maximum map value                    | 0.143                  | Depositor |
| Minimum map value                    | -0.057                 | Depositor |
| Average map value                    | 0.000                  | Depositor |
| Map value standard deviation         | 0.004                  | Depositor |
| Recommended contour level            | 0.013                  | Depositor |
| Map size ( $\text{\AA}$ )            | 290.88, 290.88, 290.88 | wwPDB     |
| Map dimensions                       | 480, 480, 480          | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0       | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.606, 0.606, 0.606    | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CRT, FE, CA, BPH, UQ8, MQ8, BCL, PGV, PLM, Z41, LDA, CDL, FME, HEM, MG, LMT

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   | C     | 0.17         | 0/2502       | 0.34        | 0/3426       |
| 2   | L     | 0.18         | 0/2295       | 0.33        | 0/3135       |
| 3   | M     | 0.17         | 0/2632       | 0.30        | 0/3601       |
| 4   | H     | 0.15         | 0/2039       | 0.29        | 0/2776       |
| 5   | 1     | 0.13         | 0/362        | 0.26        | 0/492        |
| 5   | 5     | 0.12         | 0/358        | 0.24        | 0/488        |
| 5   | 7     | 0.15         | 0/366        | 0.28        | 0/499        |
| 5   | 9     | 0.15         | 0/362        | 0.33        | 0/492        |
| 5   | A     | 0.16         | 0/362        | 0.28        | 0/492        |
| 5   | I     | 0.15         | 0/362        | 0.32        | 0/492        |
| 5   | K     | 0.12         | 0/369        | 0.25        | 0/500        |
| 5   | O     | 0.15         | 0/369        | 0.26        | 0/500        |
| 5   | Q     | 0.15         | 0/362        | 0.26        | 0/492        |
| 6   | 0     | 0.12         | 0/363        | 0.20        | 0/493        |
| 6   | 2     | 0.14         | 0/351        | 0.34        | 0/477        |
| 6   | 4     | 0.11         | 0/357        | 0.22        | 0/485        |
| 6   | 6     | 0.10         | 0/332        | 0.19        | 0/452        |
| 6   | 8     | 0.13         | 0/351        | 0.26        | 0/477        |
| 6   | B     | 0.11         | 0/371        | 0.20        | 0/504        |
| 6   | J     | 0.13         | 0/336        | 0.24        | 0/457        |
| 6   | N     | 0.13         | 0/332        | 0.25        | 0/452        |
| 6   | P     | 0.11         | 0/357        | 0.18        | 0/485        |
| 6   | R     | 0.13         | 0/343        | 0.26        | 0/467        |
| 7   | D     | 0.13         | 0/409        | 0.30        | 0/561        |
| 7   | F     | 0.15         | 0/409        | 0.31        | 0/561        |
| 7   | S     | 0.13         | 0/414        | 0.29        | 0/568        |
| 7   | U     | 0.12         | 0/422        | 0.27        | 0/578        |
| 7   | W     | 0.13         | 0/414        | 0.28        | 0/568        |
| 7   | Y     | 0.44         | 1/483 (0.2%) | 0.82        | 3/663 (0.5%) |
| 8   | E     | 0.14         | 0/355        | 0.25        | 0/480        |
| 8   | G     | 0.12         | 0/347        | 0.25        | 0/470        |
| 8   | T     | 0.13         | 0/355        | 0.23        | 0/480        |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 8   | V     | 0.13         | 0/347          | 0.23        | 0/470          |
| 8   | X     | 0.13         | 0/355          | 0.24        | 0/480          |
| 8   | Z     | 0.14         | 0/355          | 0.33        | 0/480          |
| 9   | 3     | 0.17         | 0/515          | 0.42        | 0/700          |
| All | All   | 0.16         | 1/21413 (0.0%) | 0.32        | 3/29193 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | Y     | 59  | PRO  | CG-CD | -7.87 | 1.24        | 1.50     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 7   | Y     | 59  | PRO  | N-CD-CG  | -12.55 | 84.37       | 103.20   |
| 7   | Y     | 59  | PRO  | CA-CB-CG | -9.29  | 86.85       | 104.50   |
| 7   | Y     | 14  | PRO  | CA-N-CD  | -5.55  | 104.23      | 112.00   |

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   | C     | 2429  | 0        | 2327     | 57      | 0            |
| 2   | L     | 2210  | 0        | 2166     | 47      | 0            |
| 3   | M     | 2533  | 0        | 2490     | 53      | 0            |
| 4   | H     | 1993  | 0        | 1994     | 37      | 0            |
| 5   | 1     | 359   | 0        | 371      | 10      | 0            |
| 5   | 5     | 355   | 0        | 360      | 15      | 0            |
| 5   | 7     | 359   | 0        | 366      | 19      | 0            |
| 5   | 9     | 359   | 0        | 371      | 9       | 0            |
| 5   | A     | 359   | 0        | 371      | 8       | 0            |
| 5   | I     | 359   | 0        | 371      | 14      | 0            |
| 5   | K     | 366   | 0        | 376      | 13      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | O     | 366   | 0        | 376      | 14      | 0            |
| 5   | Q     | 359   | 0        | 371      | 16      | 0            |
| 6   | 0     | 351   | 0        | 339      | 10      | 0            |
| 6   | 2     | 339   | 0        | 329      | 14      | 0            |
| 6   | 4     | 345   | 0        | 334      | 14      | 0            |
| 6   | 6     | 320   | 0        | 310      | 5       | 0            |
| 6   | 8     | 339   | 0        | 329      | 13      | 0            |
| 6   | B     | 359   | 0        | 345      | 10      | 0            |
| 6   | J     | 324   | 0        | 313      | 10      | 0            |
| 6   | N     | 320   | 0        | 310      | 17      | 0            |
| 6   | P     | 345   | 0        | 334      | 4       | 0            |
| 6   | R     | 331   | 0        | 320      | 15      | 0            |
| 7   | D     | 397   | 0        | 413      | 15      | 0            |
| 7   | F     | 397   | 0        | 413      | 17      | 0            |
| 7   | S     | 402   | 0        | 418      | 13      | 0            |
| 7   | U     | 407   | 0        | 427      | 13      | 0            |
| 7   | W     | 402   | 0        | 418      | 14      | 0            |
| 7   | Y     | 470   | 0        | 494      | 27      | 0            |
| 8   | E     | 343   | 0        | 336      | 16      | 0            |
| 8   | G     | 335   | 0        | 327      | 10      | 0            |
| 8   | T     | 343   | 0        | 336      | 11      | 0            |
| 8   | V     | 335   | 0        | 327      | 13      | 0            |
| 8   | X     | 343   | 0        | 336      | 17      | 0            |
| 8   | Z     | 343   | 0        | 336      | 13      | 0            |
| 9   | 3     | 498   | 0        | 505      | 17      | 0            |
| 10  | C     | 172   | 0        | 120      | 19      | 0            |
| 11  | C     | 1     | 0        | 0        | 0       | 0            |
| 12  | C     | 35    | 0        | 0        | 0       | 0            |
| 13  | C     | 12    | 0        | 18       | 2       | 0            |
| 14  | 1     | 27    | 0        | 25       | 5       | 0            |
| 14  | A     | 72    | 0        | 87       | 7       | 0            |
| 14  | C     | 31    | 0        | 32       | 2       | 0            |
| 14  | F     | 31    | 0        | 35       | 0       | 0            |
| 14  | H     | 36    | 0        | 42       | 3       | 0            |
| 14  | L     | 101   | 0        | 115      | 13      | 0            |
| 14  | M     | 27    | 0        | 27       | 3       | 0            |
| 14  | Q     | 24    | 0        | 21       | 2       | 0            |
| 15  | 0     | 66    | 0        | 74       | 8       | 0            |
| 15  | 1     | 66    | 0        | 74       | 10      | 0            |
| 15  | 2     | 66    | 0        | 74       | 9       | 0            |
| 15  | 3     | 66    | 0        | 74       | 8       | 0            |
| 15  | 4     | 66    | 0        | 74       | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15  | 5     | 66    | 0        | 74       | 6       | 0            |
| 15  | 6     | 66    | 0        | 74       | 6       | 0            |
| 15  | 7     | 61    | 0        | 61       | 6       | 0            |
| 15  | 8     | 66    | 0        | 74       | 9       | 0            |
| 15  | 9     | 66    | 0        | 74       | 5       | 0            |
| 15  | A     | 66    | 0        | 74       | 3       | 0            |
| 15  | B     | 66    | 0        | 74       | 9       | 0            |
| 15  | D     | 66    | 0        | 74       | 4       | 0            |
| 15  | E     | 66    | 0        | 74       | 10      | 0            |
| 15  | F     | 66    | 0        | 74       | 0       | 0            |
| 15  | G     | 66    | 0        | 74       | 9       | 0            |
| 15  | I     | 66    | 0        | 74       | 5       | 0            |
| 15  | J     | 66    | 0        | 74       | 6       | 0            |
| 15  | K     | 66    | 0        | 74       | 6       | 0            |
| 15  | L     | 132   | 0        | 148      | 5       | 0            |
| 15  | M     | 132   | 0        | 148      | 5       | 0            |
| 15  | N     | 66    | 0        | 74       | 9       | 0            |
| 15  | O     | 66    | 0        | 74       | 3       | 0            |
| 15  | P     | 66    | 0        | 74       | 4       | 0            |
| 15  | Q     | 66    | 0        | 74       | 3       | 0            |
| 15  | R     | 66    | 0        | 74       | 6       | 0            |
| 15  | S     | 66    | 0        | 74       | 4       | 0            |
| 15  | T     | 66    | 0        | 74       | 4       | 0            |
| 15  | U     | 66    | 0        | 74       | 5       | 0            |
| 15  | V     | 66    | 0        | 74       | 6       | 0            |
| 15  | W     | 66    | 0        | 74       | 4       | 0            |
| 15  | X     | 66    | 0        | 74       | 5       | 0            |
| 15  | Y     | 66    | 0        | 74       | 3       | 0            |
| 15  | Z     | 66    | 0        | 74       | 6       | 0            |
| 16  | L     | 65    | 0        | 76       | 6       | 0            |
| 16  | M     | 65    | 0        | 76       | 6       | 0            |
| 17  | L     | 139   | 0        | 187      | 24      | 0            |
| 18  | 2     | 35    | 0        | 46       | 4       | 0            |
| 18  | 4     | 70    | 0        | 92       | 8       | 0            |
| 18  | 5     | 31    | 0        | 35       | 1       | 0            |
| 18  | 8     | 70    | 0        | 92       | 2       | 0            |
| 18  | B     | 35    | 0        | 46       | 3       | 0            |
| 18  | E     | 35    | 0        | 46       | 2       | 0            |
| 18  | G     | 35    | 0        | 46       | 1       | 0            |
| 18  | H     | 35    | 0        | 46       | 3       | 0            |
| 18  | J     | 70    | 0        | 92       | 4       | 0            |
| 18  | L     | 35    | 0        | 46       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18  | M     | 59    | 0        | 67       | 2       | 0            |
| 18  | P     | 70    | 0        | 92       | 4       | 0            |
| 18  | R     | 35    | 0        | 46       | 4       | 0            |
| 18  | S     | 26    | 0        | 25       | 4       | 0            |
| 18  | T     | 35    | 0        | 46       | 3       | 0            |
| 18  | X     | 35    | 0        | 46       | 3       | 0            |
| 18  | Z     | 35    | 0        | 46       | 2       | 0            |
| 19  | D     | 58    | 0        | 60       | 1       | 0            |
| 19  | H     | 79    | 0        | 105      | 3       | 0            |
| 19  | L     | 80    | 0        | 110      | 7       | 0            |
| 19  | M     | 134   | 0        | 168      | 9       | 0            |
| 20  | M     | 1     | 0        | 0        | 0       | 0            |
| 21  | M     | 53    | 0        | 72       | 9       | 0            |
| 22  | 0     | 44    | 0        | 60       | 7       | 0            |
| 22  | 2     | 44    | 0        | 60       | 12      | 0            |
| 22  | 4     | 44    | 0        | 60       | 10      | 0            |
| 22  | 6     | 44    | 0        | 60       | 5       | 0            |
| 22  | 9     | 44    | 0        | 60       | 5       | 0            |
| 22  | B     | 44    | 0        | 60       | 7       | 0            |
| 22  | E     | 44    | 0        | 60       | 6       | 0            |
| 22  | G     | 44    | 0        | 60       | 4       | 0            |
| 22  | J     | 44    | 0        | 60       | 8       | 0            |
| 22  | M     | 44    | 0        | 60       | 5       | 0            |
| 22  | N     | 44    | 0        | 60       | 9       | 0            |
| 22  | P     | 44    | 0        | 60       | 2       | 0            |
| 22  | R     | 44    | 0        | 60       | 4       | 0            |
| 22  | T     | 44    | 0        | 60       | 7       | 0            |
| 22  | V     | 44    | 0        | 60       | 10      | 0            |
| 22  | Y     | 44    | 0        | 60       | 6       | 0            |
| 22  | Z     | 44    | 0        | 60       | 7       | 0            |
| 23  | D     | 1     | 0        | 0        | 0       | 0            |
| 23  | F     | 1     | 0        | 0        | 0       | 0            |
| 23  | S     | 1     | 0        | 0        | 0       | 0            |
| 23  | U     | 1     | 0        | 0        | 0       | 0            |
| 23  | W     | 1     | 0        | 0        | 0       | 0            |
| 23  | Y     | 1     | 0        | 0        | 0       | 0            |
| 24  | K     | 16    | 0        | 31       | 0       | 0            |
| 24  | O     | 16    | 0        | 31       | 1       | 0            |
| 25  | 1     | 1     | 0        | 0        | 0       | 0            |
| 25  | 3     | 10    | 0        | 0        | 0       | 0            |
| 25  | 7     | 1     | 0        | 0        | 0       | 0            |
| 25  | 9     | 4     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25  | A     | 2     | 0        | 0        | 0       | 0            |
| 25  | B     | 1     | 0        | 0        | 0       | 0            |
| 25  | C     | 119   | 0        | 0        | 1       | 0            |
| 25  | D     | 4     | 0        | 0        | 0       | 0            |
| 25  | E     | 2     | 0        | 0        | 0       | 0            |
| 25  | F     | 2     | 0        | 0        | 0       | 0            |
| 25  | H     | 19    | 0        | 0        | 0       | 0            |
| 25  | I     | 2     | 0        | 0        | 0       | 0            |
| 25  | K     | 1     | 0        | 0        | 0       | 0            |
| 25  | L     | 50    | 0        | 0        | 0       | 0            |
| 25  | M     | 77    | 0        | 0        | 4       | 0            |
| 25  | O     | 1     | 0        | 0        | 0       | 0            |
| 25  | P     | 1     | 0        | 0        | 0       | 0            |
| 25  | Q     | 2     | 0        | 0        | 0       | 0            |
| 25  | R     | 1     | 0        | 0        | 0       | 0            |
| 25  | S     | 5     | 0        | 0        | 0       | 0            |
| 25  | T     | 3     | 0        | 0        | 0       | 0            |
| 25  | U     | 10    | 0        | 0        | 0       | 0            |
| 25  | V     | 3     | 0        | 0        | 0       | 0            |
| 25  | W     | 7     | 0        | 0        | 0       | 0            |
| 25  | X     | 1     | 0        | 0        | 0       | 0            |
| 25  | Y     | 5     | 0        | 0        | 0       | 0            |
| All | All   | 26274 | 0        | 26723    | 714     | 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 14.

All (714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:C:155:CYS:SG | 10:C:402:HEM:HAC | 1.60                     | 1.42              |
| 1:C:155:CYS:SG | 10:C:402:HEM:CAC | 2.09                     | 1.41              |
| 1:C:250:CYS:SG | 10:C:403:HEM:HAC | 1.62                     | 1.39              |
| 1:C:110:CYS:SG | 10:C:401:HEM:HAC | 1.71                     | 1.30              |
| 1:C:250:CYS:SG | 10:C:403:HEM:CAC | 2.19                     | 1.29              |
| 1:C:110:CYS:SG | 10:C:401:HEM:CAC | 2.23                     | 1.27              |
| 3:M:96:GLU:OE1 | 25:M:501:HOH:O   | 1.77                     | 1.02              |
| 3:M:96:GLU:OE2 | 25:M:502:HOH:O   | 1.81                     | 0.97              |
| 1:C:250:CYS:HG | 10:C:403:HEM:HAC | 1.31                     | 0.96              |
| 3:M:72:GLY:HA3 | 22:M:406:CRT:H6  | 1.51                     | 0.92              |
| 1:C:155:CYS:SG | 10:C:402:HEM:C3C | 2.73                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:W:7:LYS:HG2     | 22:Z:103:CRT:H41  | 1.66                     | 0.77              |
| 7:S:7:LYS:HB3     | 22:V:102:CRT:H23  | 1.67                     | 0.77              |
| 18:R:103:LMT:H52  | 8:T:39:LEU:HB3    | 1.68                     | 0.75              |
| 2:L:219:ASN:HD21  | 4:H:176:GLU:HG2   | 1.51                     | 0.75              |
| 1:C:151:THR:HG22  | 1:C:153:TYR:H     | 1.54                     | 0.72              |
| 8:X:43:TRP:HB2    | 18:X:101:LMT:H22  | 1.72                     | 0.71              |
| 5:5:36:LEU:HD11   | 15:6:101:BCL:HHD  | 1.72                     | 0.70              |
| 15:0:101:BCL:H43  | 15:0:101:BCL:H3A  | 1.73                     | 0.70              |
| 7:Y:7:LYS:HD3     | 22:2:103:CRT:H32A | 1.74                     | 0.70              |
| 8:Z:21:ILE:HA     | 8:Z:24:GLN:HG2    | 1.74                     | 0.70              |
| 9:3:11:ALA:HB1    | 5:5:15:ARG:HG3    | 1.74                     | 0.70              |
| 1:C:307:CYS:O     | 25:C:501:HOH:O    | 2.09                     | 0.69              |
| 18:4:104:LMT:H22  | 6:6:43:TRP:HB2    | 1.73                     | 0.69              |
| 1:C:110:CYS:CB    | 10:C:401:HEM:HAC  | 2.23                     | 0.69              |
| 8:Z:18:PHE:HB2    | 22:Z:103:CRT:H23  | 1.76                     | 0.67              |
| 5:5:22:PHE:HB3    | 15:5:102:BCL:H51  | 1.75                     | 0.67              |
| 15:1:402:BCL:H92  | 6:2:29:PHE:HB2    | 1.75                     | 0.67              |
| 5:1:36:LEU:HD11   | 15:2:102:BCL:HHD  | 1.77                     | 0.66              |
| 9:3:22:GLY:HA3    | 15:3:101:BCL:H151 | 1.77                     | 0.66              |
| 3:M:5:GLN:HB2     | 19:M:407:CDL:HA32 | 1.77                     | 0.66              |
| 5:Q:6:HIS:HA      | 6:R:19:HIS:CD2    | 2.31                     | 0.66              |
| 5:I:10:GLN:NE2    | 6:J:10:LEU:O      | 2.29                     | 0.66              |
| 5:K:6:HIS:HA      | 6:N:19:HIS:ND1    | 2.10                     | 0.66              |
| 2:L:174:HIS:HB3   | 3:M:183:LEU:HD13  | 1.78                     | 0.66              |
| 18:P:104:LMT:H42  | 6:R:39:LEU:HB3    | 1.78                     | 0.65              |
| 15:U:101:BCL:H102 | 8:V:29:PHE:HB2    | 1.78                     | 0.65              |
| 3:M:98:PRO:HB3    | 3:M:107:PRO:HG3   | 1.78                     | 0.65              |
| 8:V:30:PHE:CE2    | 15:V:101:BCL:H11  | 2.31                     | 0.65              |
| 5:7:11:ILE:HD11   | 22:0:102:CRT:H23  | 1.79                     | 0.65              |
| 6:8:26:MET:HE1    | 15:9:102:BCL:H193 | 1.78                     | 0.65              |
| 21:M:405:MQ8:H491 | 14:A:503:PGV:H221 | 1.79                     | 0.65              |
| 7:D:11:LEU:HD11   | 22:G:103:CRT:H23  | 1.78                     | 0.65              |
| 8:G:21:ILE:O      | 8:G:25:SER:OG     | 2.14                     | 0.65              |
| 5:I:13:ASP:HB3    | 5:I:16:ARG:HD3    | 1.79                     | 0.65              |
| 2:L:7:GLU:HG3     | 3:M:250:ILE:HG12  | 1.80                     | 0.64              |
| 17:L:304:UQ8:H4M  | 5:7:21:LEU:HB2    | 1.80                     | 0.64              |
| 1:C:110:CYS:SG    | 10:C:401:HEM:CBC  | 2.84                     | 0.64              |
| 8:X:23:THR:O      | 8:X:27:THR:OG1    | 2.16                     | 0.64              |
| 5:I:36:LEU:HD11   | 15:J:102:BCL:HHD  | 1.80                     | 0.64              |
| 5:I:7:LYS:HG3     | 22:N:102:CRT:H41  | 1.80                     | 0.63              |
| 3:M:167:MET:HE3   | 3:M:289:THR:HG21  | 1.81                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:F:36:LEU:HD11   | 15:G:102:BCL:HHD  | 1.80                     | 0.63              |
| 6:J:43:TRP:HB2    | 18:J:101:LMT:H12  | 1.79                     | 0.63              |
| 5:Q:11:ILE:HD11   | 22:T:102:CRT:H82  | 1.79                     | 0.63              |
| 9:3:36:LEU:HD11   | 15:4:102:BCL:HHD  | 1.79                     | 0.63              |
| 4:H:64:PRO:HA     | 4:H:79:PRO:HD2    | 1.80                     | 0.63              |
| 6:8:19:HIS:O      | 6:8:23:VAL:HG23   | 1.99                     | 0.63              |
| 18:T:103:LMT:H31  | 8:V:43:TRP:HB2    | 1.80                     | 0.62              |
| 13:C:407:PLM:H61  | 14:L:305:PGV:H42  | 1.80                     | 0.62              |
| 2:L:8:ARG:HG2     | 4:H:87:ILE:HG21   | 1.80                     | 0.62              |
| 16:L:302:BPH:HHC  | 16:L:302:BPH:HBB3 | 1.82                     | 0.62              |
| 22:N:102:CRT:H393 | 5:O:33:HIS:HB3    | 1.82                     | 0.62              |
| 14:L:310:PGV:O13  | 18:S:101:LMT:O3'  | 2.16                     | 0.61              |
| 6:R:13:GLN:HE21   | 6:R:14:GLU:HG3    | 1.66                     | 0.61              |
| 9:3:8:ILE:H       | 9:3:8:ILE:HD12    | 1.66                     | 0.61              |
| 6:0:20:GLY:O      | 6:0:24:GLN:HG3    | 2.00                     | 0.61              |
| 1:C:236:MET:HB3   | 10:C:403:HEM:C4B  | 2.36                     | 0.60              |
| 1:C:191:ALA:HB3   | 1:C:237:MET:HE3   | 1.84                     | 0.60              |
| 14:L:305:PGV:H32  | 14:1:401:PGV:H51  | 1.84                     | 0.60              |
| 8:T:47:LEU:HD12   | 15:T:101:BCL:H172 | 1.83                     | 0.60              |
| 15:M:402:BCL:H61  | 21:M:405:MQ8:H243 | 1.83                     | 0.60              |
| 16:M:404:BPH:HHC  | 16:M:404:BPH:HBB3 | 1.83                     | 0.60              |
| 5:1:6:HIS:H       | 5:1:6:HIS:CD2     | 2.20                     | 0.60              |
| 2:L:107:ALA:HB1   | 19:L:311:CDL:H782 | 1.85                     | 0.59              |
| 1:C:27:PRO:HD3    | 9:3:38:ARG:HG3    | 1.84                     | 0.59              |
| 4:H:78:ALA:HB3    | 4:H:79:PRO:HD3    | 1.83                     | 0.59              |
| 6:R:13:GLN:NE2    | 6:R:14:GLU:HG3    | 2.17                     | 0.59              |
| 5:A:38:SER:O      | 14:A:501:PGV:O06  | 2.21                     | 0.59              |
| 22:Z:103:CRT:H372 | 5:1:33:HIS:CG     | 2.37                     | 0.58              |
| 6:8:10:LEU:HD13   | 6:8:14:GLU:HB2    | 1.85                     | 0.58              |
| 22:N:102:CRT:H35  | 15:O:502:BCL:HMB1 | 1.86                     | 0.58              |
| 18:L:307:LMT:H1'  | 5:7:43:ASN:HD21   | 1.67                     | 0.58              |
| 3:M:157:TYR:CZ    | 22:M:406:CRT:H293 | 2.37                     | 0.58              |
| 2:L:21:ASP:O      | 5:9:15:ARG:NH1    | 2.22                     | 0.58              |
| 1:C:288:ASN:O     | 1:C:296:LYS:NZ    | 2.35                     | 0.58              |
| 2:L:13:ARG:HD3    | 4:H:92:VAL:HG11   | 1.86                     | 0.58              |
| 15:N:101:BCL:H91  | 15:N:101:BCL:H143 | 1.86                     | 0.58              |
| 8:Z:43:TRP:HB2    | 18:Z:101:LMT:H12  | 1.86                     | 0.58              |
| 4:H:67:PHE:HB2    | 4:H:76:VAL:HG22   | 1.84                     | 0.57              |
| 8:E:18:PHE:HB2    | 22:E:103:CRT:H21A | 1.85                     | 0.57              |
| 5:O:36:LEU:HD11   | 15:P:102:BCL:HHD  | 1.86                     | 0.57              |
| 16:L:302:BPH:H171 | 14:A:501:PGV:H332 | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Y:36:LEU:HD11   | 15:Z:102:BCL:HHD  | 1.85                     | 0.57              |
| 8:T:19:HIS:O      | 8:T:23:THR:HG23   | 2.04                     | 0.57              |
| 22:M:406:CRT:H393 | 5:O:34:PHE:HD2    | 1.69                     | 0.57              |
| 15:4:102:BCL:HMA2 | 22:4:103:CRT:H30  | 1.85                     | 0.57              |
| 22:4:103:CRT:H32  | 22:4:103:CRT:H291 | 1.86                     | 0.57              |
| 7:Y:35:ILE:HD13   | 22:Z:103:CRT:H2M3 | 1.86                     | 0.57              |
| 6:2:43:TRP:HB2    | 18:2:101:LMT:H22  | 1.85                     | 0.57              |
| 8:G:10:LEU:HG     | 8:G:14:GLU:HG3    | 1.87                     | 0.57              |
| 8:V:22:PHE:CD2    | 22:V:102:CRT:H14  | 2.40                     | 0.57              |
| 1:C:45:ASN:HB3    | 1:C:48:LEU:HB2    | 1.87                     | 0.57              |
| 16:M:404:BPH:H192 | 18:S:101:LMT:H12  | 1.85                     | 0.57              |
| 15:2:102:BCL:HBB1 | 18:4:101:LMT:H62  | 1.86                     | 0.56              |
| 5:Q:36:LEU:HD11   | 15:R:101:BCL:HHD  | 1.86                     | 0.56              |
| 4:H:100:PHE:HB2   | 4:H:111:PHE:CZ    | 2.41                     | 0.56              |
| 3:M:95:LEU:HB3    | 3:M:177:PHE:HB2   | 1.88                     | 0.56              |
| 16:M:404:BPH:HBC3 | 16:M:404:BPH:HHD  | 1.88                     | 0.56              |
| 7:W:8:ILE:HA      | 22:Z:103:CRT:H83  | 1.88                     | 0.56              |
| 7:W:36:LEU:HD11   | 15:X:102:BCL:HHD  | 1.87                     | 0.56              |
| 5:5:43:ASN:HD21   | 18:5:101:LMT:H6E  | 1.70                     | 0.55              |
| 6:J:18:PHE:HB2    | 22:J:103:CRT:H32A | 1.88                     | 0.55              |
| 7:Y:9:TRP:HZ3     | 8:Z:19:HIS:CD2    | 2.24                     | 0.55              |
| 5:7:25:LEU:HB3    | 15:7:101:BCL:H12  | 1.88                     | 0.55              |
| 15:L:301:BCL:H202 | 21:M:405:MQ8:H292 | 1.87                     | 0.55              |
| 4:H:11:VAL:HG21   | 18:H:303:LMT:H31  | 1.87                     | 0.55              |
| 6:B:43:TRP:HB2    | 18:B:101:LMT:H12  | 1.87                     | 0.55              |
| 6:0:33:VAL:HG11   | 15:0:101:BCL:HBA2 | 1.87                     | 0.55              |
| 8:Z:30:PHE:O      | 8:Z:34:ILE:HD12   | 2.06                     | 0.55              |
| 17:L:304:UQ8:H1MA | 5:9:22:PHE:HB2    | 1.88                     | 0.55              |
| 8:E:18:PHE:HA     | 22:E:103:CRT:H6   | 1.88                     | 0.55              |
| 6:R:18:PHE:HA     | 22:R:102:CRT:H6   | 1.88                     | 0.55              |
| 1:C:246:ASN:HA    | 2:L:171:LEU:HD21  | 1.89                     | 0.55              |
| 9:3:33:HIS:CE1    | 15:4:102:BCL:HMD3 | 2.43                     | 0.55              |
| 2:L:26:TRP:HZ3    | 4:H:99:PRO:HB3    | 1.73                     | 0.54              |
| 3:M:3:GLU:O       | 3:M:5:GLN:NE2     | 2.39                     | 0.54              |
| 15:U:101:BCL:H161 | 8:V:32:ILE:HD11   | 1.88                     | 0.54              |
| 5:I:9:TRP:HE1     | 6:J:19:HIS:HB2    | 1.72                     | 0.54              |
| 22:T:102:CRT:H372 | 7:U:33:HIS:CG     | 2.42                     | 0.54              |
| 7:U:11:LEU:HD21   | 22:Y:101:CRT:H1M1 | 1.88                     | 0.54              |
| 7:D:12:VAL:HG12   | 7:F:15:ARG:HG2    | 1.90                     | 0.54              |
| 7:Y:30:LEU:O      | 7:Y:34:MET:HG2    | 2.08                     | 0.54              |
| 1:C:110:CYS:CB    | 10:C:401:HEM:CAC  | 2.84                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:W:41:GLU:O      | 8:X:44:ARG:NH1    | 2.40                     | 0.54              |
| 1:C:167:VAL:HG22  | 7:Y:62:PRO:HD2    | 1.89                     | 0.54              |
| 2:L:32:VAL:HG13   | 21:M:405:MQ8:H453 | 1.89                     | 0.54              |
| 3:M:148:TRP:HE1   | 19:M:409:CDL:H332 | 1.73                     | 0.54              |
| 3:M:271:TRP:CH2   | 19:M:409:CDL:H541 | 2.43                     | 0.54              |
| 5:K:6:HIS:HB3     | 6:N:16:GLN:HE22   | 1.72                     | 0.54              |
| 8:V:18:PHE:HD1    | 22:V:102:CRT:H6   | 1.73                     | 0.54              |
| 7:Y:5:LEU:HD13    | 15:1:402:BCL:H171 | 1.89                     | 0.54              |
| 4:H:70:PRO:HB2    | 4:H:71:HIS:CD2    | 2.43                     | 0.54              |
| 22:V:102:CRT:H35  | 15:W:101:BCL:HBB  | 1.89                     | 0.54              |
| 15:7:101:BCL:H141 | 6:8:32:ILE:HG21   | 1.89                     | 0.53              |
| 22:B:103:CRT:H23  | 5:9:11:ILE:HD11   | 1.90                     | 0.53              |
| 5:Q:11:ILE:O      | 7:S:15:ARG:NE     | 2.42                     | 0.53              |
| 22:2:103:CRT:H35  | 15:3:101:BCL:HMB1 | 1.91                     | 0.53              |
| 4:H:44:ASP:OD1    | 14:A:503:PGV:O05  | 2.15                     | 0.53              |
| 6:2:37:HIS:CG     | 15:2:102:BCL:H8   | 2.44                     | 0.53              |
| 2:L:227:GLY:HA3   | 14:L:310:PGV:H221 | 1.90                     | 0.53              |
| 6:J:10:LEU:HG     | 6:J:14:GLU:HG3    | 1.90                     | 0.53              |
| 7:Y:37:LEU:O      | 7:Y:43:ASN:ND2    | 2.38                     | 0.53              |
| 3:M:10:THR:HG21   | 4:H:202:PHE:HB2   | 1.91                     | 0.53              |
| 1:C:57:LEU:HD23   | 9:3:59:MET:HE1    | 1.89                     | 0.53              |
| 18:R:103:LMT:H2'  | 8:T:43:TRP:HD1    | 1.74                     | 0.53              |
| 7:S:11:LEU:HD21   | 7:U:14:PRO:HB2    | 1.90                     | 0.53              |
| 15:1:402:BCL:H122 | 15:1:402:BCL:H192 | 1.89                     | 0.53              |
| 5:7:36:LEU:HD11   | 15:8:102:BCL:HHD  | 1.91                     | 0.53              |
| 17:L:304:UQ8:H40B | 17:L:304:UQ8:H16A | 1.90                     | 0.53              |
| 7:D:33:HIS:CE1    | 15:E:102:BCL:HMD3 | 2.43                     | 0.53              |
| 2:L:187:PHE:HB3   | 16:M:404:BPH:HBB2 | 1.90                     | 0.52              |
| 7:S:33:HIS:CE1    | 15:T:101:BCL:HMD3 | 2.44                     | 0.52              |
| 6:J:22:PHE:CD2    | 22:J:103:CRT:H14  | 2.44                     | 0.52              |
| 5:K:11:ILE:HB     | 5:O:15:ARG:HH21   | 1.73                     | 0.52              |
| 4:H:13:GLN:NE2    | 14:H:301:PGV:O13  | 2.41                     | 0.52              |
| 7:U:22:PHE:HA     | 15:U:101:BCL:H41  | 1.91                     | 0.52              |
| 6:4:43:TRP:HA     | 18:4:101:LMT:H6D  | 1.92                     | 0.52              |
| 1:C:278:ASP:OD1   | 1:C:282:ASN:ND2   | 2.40                     | 0.52              |
| 8:X:13:GLU:HA     | 8:X:16:LYS:NZ     | 2.24                     | 0.52              |
| 6:6:30:PHE:CE2    | 15:6:101:BCL:H11  | 2.45                     | 0.52              |
| 5:A:33:HIS:CE1    | 15:B:102:BCL:HMD3 | 2.45                     | 0.52              |
| 8:E:20:GLY:O      | 8:E:24:GLN:HG3    | 2.10                     | 0.52              |
| 1:C:250:CYS:SG    | 10:C:403:HEM:C3C  | 2.99                     | 0.52              |
| 7:Y:9:TRP:CD1     | 7:Y:14:PRO:HB3    | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:53:LEU:O      | 5:Q:16:ARG:NH1    | 2.42                     | 0.52              |
| 6:N:11:THR:OG1    | 6:N:12:GLU:N      | 2.43                     | 0.52              |
| 4:H:67:PHE:HE2    | 4:H:78:ALA:HB2    | 1.76                     | 0.51              |
| 15:B:102:BCL:H43  | 15:B:102:BCL:H3A  | 1.93                     | 0.51              |
| 6:R:46:TRP:CD1    | 6:R:47:LEU:HG     | 2.45                     | 0.51              |
| 15:L:308:BCL:H171 | 3:M:179:ILE:HD11  | 1.91                     | 0.51              |
| 5:K:36:LEU:HD11   | 15:N:101:BCL:HHD  | 1.92                     | 0.51              |
| 15:2:102:BCL:H162 | 18:4:101:LMT:H21  | 1.93                     | 0.51              |
| 5:5:5:FME:HCN     | 22:9:101:CRT:H21A | 1.93                     | 0.51              |
| 3:M:31:ILE:HB     | 18:S:101:LMT:H3B  | 1.92                     | 0.51              |
| 4:H:94:PRO:HB2    | 6:0:9:GLY:HA3     | 1.92                     | 0.51              |
| 5:5:11:ILE:HG23   | 5:7:15:ARG:HE     | 1.76                     | 0.51              |
| 15:W:101:BCL:H172 | 8:X:28:MET:HE3    | 1.91                     | 0.51              |
| 6:4:22:PHE:HA     | 22:4:103:CRT:H14  | 1.93                     | 0.51              |
| 5:A:36:LEU:HD11   | 15:B:102:BCL:HHD  | 1.93                     | 0.51              |
| 2:L:138:VAL:HG23  | 2:L:139:VAL:HG23  | 1.92                     | 0.51              |
| 6:N:22:PHE:CD2    | 22:N:102:CRT:H14  | 2.46                     | 0.51              |
| 7:U:25:LEU:HB2    | 15:U:101:BCL:H43  | 1.93                     | 0.51              |
| 22:V:102:CRT:H372 | 7:W:33:HIS:CG     | 2.46                     | 0.51              |
| 6:2:43:TRP:HD1    | 18:2:101:LMT:H2'  | 1.75                     | 0.51              |
| 2:L:40:PHE:HB2    | 21:M:405:MQ8:H392 | 1.93                     | 0.51              |
| 5:K:11:ILE:HB     | 5:O:15:ARG:HE     | 1.76                     | 0.51              |
| 8:Z:46:TRP:CD2    | 15:Z:102:BCL:H2C  | 2.45                     | 0.51              |
| 1:C:110:CYS:HB2   | 10:C:401:HEM:C3C  | 2.46                     | 0.50              |
| 16:L:302:BPH:HHC  | 16:L:302:BPH:CBB  | 2.40                     | 0.50              |
| 4:H:70:PRO:HB2    | 4:H:71:HIS:HD2    | 1.76                     | 0.50              |
| 8:E:33:VAL:HG11   | 15:E:102:BCL:HAA1 | 1.92                     | 0.50              |
| 8:E:46:TRP:HZ2    | 15:E:102:BCL:H121 | 1.76                     | 0.50              |
| 7:D:18:LEU:HA     | 7:D:21:VAL:HG12   | 1.94                     | 0.50              |
| 6:N:46:TRP:CE2    | 15:N:101:BCL:H2C  | 2.47                     | 0.50              |
| 2:L:179:HIS:CE1   | 2:L:183:ILE:HD11  | 2.46                     | 0.50              |
| 15:4:102:BCL:O1A  | 22:4:103:CRT:H25  | 2.10                     | 0.50              |
| 5:O:41:ALA:O      | 6:P:44:ARG:NH1    | 2.36                     | 0.50              |
| 5:1:33:HIS:CE1    | 15:2:102:BCL:HMD1 | 2.46                     | 0.50              |
| 5:7:13:ASP:OD2    | 5:7:15:ARG:HG2    | 2.10                     | 0.50              |
| 14:M:408:PGV:H202 | 5:O:20:ALA:HA     | 1.93                     | 0.50              |
| 4:H:171:TRP:HB2   | 4:H:181:TYR:HB2   | 1.93                     | 0.50              |
| 7:S:6:TRP:CD1     | 8:T:16:LYS:HZ2    | 2.29                     | 0.50              |
| 7:U:33:HIS:CE1    | 15:V:101:BCL:HMD3 | 2.47                     | 0.50              |
| 7:S:2:SER:HB3     | 7:S:5:LEU:HG      | 1.94                     | 0.50              |
| 7:U:6:TRP:HH2     | 8:V:12:GLU:HG3    | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:L:136:VAL:HA    | 2:L:140:VAL:HB    | 1.93                     | 0.50              |
| 2:L:18:ILE:HD11   | 19:L:311:CDL:H672 | 1.94                     | 0.50              |
| 7:W:11:LEU:HB3    | 7:Y:15:ARG:HB2    | 1.94                     | 0.50              |
| 8:X:19:HIS:O      | 8:X:23:THR:OG1    | 2.21                     | 0.50              |
| 3:M:271:TRP:HH2   | 19:M:409:CDL:H541 | 1.77                     | 0.49              |
| 5:Q:33:HIS:CE1    | 15:R:101:BCL:HMD3 | 2.47                     | 0.49              |
| 6:R:22:PHE:CD2    | 22:R:102:CRT:H14  | 2.47                     | 0.49              |
| 8:X:21:ILE:H      | 8:X:21:ILE:HD12   | 1.76                     | 0.49              |
| 22:9:101:CRT:H82  | 22:9:101:CRT:H42  | 1.94                     | 0.49              |
| 5:1:15:ARG:HH11   | 5:1:15:ARG:HG2    | 1.77                     | 0.49              |
| 22:6:102:CRT:H372 | 5:7:33:HIS:CD2    | 2.48                     | 0.49              |
| 6:0:18:PHE:HB2    | 22:0:102:CRT:H21A | 1.94                     | 0.49              |
| 7:Y:10:LEU:HB2    | 22:2:103:CRT:H1M1 | 1.95                     | 0.49              |
| 8:G:37:HIS:CG     | 15:G:102:BCL:H8   | 2.47                     | 0.49              |
| 7:Y:5:LEU:HD22    | 15:1:402:BCL:H193 | 1.95                     | 0.49              |
| 6:8:11:THR:C      | 6:8:13:GLN:H      | 2.19                     | 0.49              |
| 2:L:225:ILE:HG22  | 2:L:226:VAL:HG13  | 1.94                     | 0.49              |
| 6:B:26:MET:HG3    | 22:B:103:CRT:C19  | 2.43                     | 0.49              |
| 7:F:12:VAL:HG22   | 7:F:17:ILE:HD11   | 1.95                     | 0.49              |
| 22:J:103:CRT:H342 | 15:K:102:BCL:HBA2 | 1.94                     | 0.49              |
| 8:X:39:LEU:HB3    | 18:X:101:LMT:H62  | 1.93                     | 0.49              |
| 6:2:46:TRP:CD2    | 15:2:102:BCL:H2C  | 2.48                     | 0.49              |
| 5:7:22[B]:PHE:CD1 | 15:7:101:BCL:H41  | 2.48                     | 0.49              |
| 14:L:305:PGV:H211 | 14:1:401:PGV:H42  | 1.95                     | 0.49              |
| 8:E:42:LEU:O      | 18:E:101:LMT:O3'  | 2.30                     | 0.49              |
| 7:U:17:ILE:O      | 7:U:21:VAL:HG12   | 2.12                     | 0.49              |
| 5:9:33:HIS:CE1    | 15:0:101:BCL:HMD3 | 2.48                     | 0.49              |
| 1:C:173:ASN:O     | 3:M:80:ASP:HB2    | 2.13                     | 0.49              |
| 15:M:403:BCL:HAA2 | 15:M:403:BCL:HBD  | 1.95                     | 0.49              |
| 6:4:39:LEU:HB3    | 18:4:101:LMT:H22  | 1.95                     | 0.49              |
| 1:C:85:LEU:HD11   | 1:C:329:ALA:HB2   | 1.95                     | 0.49              |
| 3:M:74:ASN:HD21   | 3:M:114:TRP:CD1   | 2.29                     | 0.49              |
| 8:X:43:TRP:O      | 18:X:101:LMT:O3'  | 2.28                     | 0.49              |
| 3:M:164:ARG:HD2   | 3:M:284:ILE:HG23  | 1.95                     | 0.49              |
| 5:O:33:HIS:CE1    | 15:P:102:BCL:HMD3 | 2.47                     | 0.49              |
| 7:U:36:LEU:HD11   | 15:V:101:BCL:HHD  | 1.95                     | 0.49              |
| 1:C:169:ASP:OD2   | 7:Y:64:ARG:NE     | 2.40                     | 0.48              |
| 17:L:304:UQ8:H4MB | 15:9:102:BCL:H112 | 1.95                     | 0.48              |
| 5:9:36:LEU:HD11   | 15:0:101:BCL:HHD  | 1.93                     | 0.48              |
| 1:C:308:MET:HA    | 1:C:312:GLN:H     | 1.78                     | 0.48              |
| 18:L:307:LMT:H122 | 18:L:307:LMT:H62  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:S:43:ASN:CG     | 7:S:46:GLU:HG2    | 2.38                     | 0.48              |
| 9:3:19:ILE:HA     | 15:3:101:BCL:H152 | 1.95                     | 0.48              |
| 8:G:37:HIS:CD2    | 15:G:102:BCL:H8   | 2.47                     | 0.48              |
| 15:1:402:BCL:H61  | 15:1:402:BCL:H101 | 1.55                     | 0.48              |
| 2:L:3:MET:HG2     | 2:L:11:ARG:CZ     | 2.43                     | 0.48              |
| 15:K:102:BCL:H193 | 6:N:25:SER:HA     | 1.94                     | 0.48              |
| 18:T:103:LMT:O3'  | 18:T:103:LMT:O2B  | 2.26                     | 0.48              |
| 16:M:404:BPH:H142 | 16:M:404:BPH:H8   | 1.94                     | 0.48              |
| 6:J:39:LEU:HB3    | 18:J:101:LMT:H42  | 1.95                     | 0.48              |
| 8:V:18:PHE:CD1    | 22:V:102:CRT:H6   | 2.48                     | 0.48              |
| 1:C:53:ILE:HG22   | 9:3:53:VAL:HG21   | 1.96                     | 0.48              |
| 15:G:102:BCL:H141 | 15:G:102:BCL:H161 | 1.67                     | 0.48              |
| 4:H:9:MET:HA      | 4:H:13:GLN:OE1    | 2.13                     | 0.48              |
| 5:A:6:HIS:CD2     | 6:B:16:GLN:HG2    | 2.48                     | 0.48              |
| 8:G:46:TRP:CE2    | 15:G:102:BCL:H2C  | 2.49                     | 0.48              |
| 15:R:101:BCL:H91  | 15:R:101:BCL:H111 | 1.71                     | 0.48              |
| 5:5:32:ILE:HD12   | 15:6:101:BCL:O1D  | 2.14                     | 0.48              |
| 18:8:103:LMT:H91  | 6:0:36:ALA:HB1    | 1.95                     | 0.48              |
| 14:A:503:PGV:H202 | 5:9:16:ARG:CZ     | 2.44                     | 0.48              |
| 5:I:33:HIS:CE1    | 15:J:102:BCL:HMD1 | 2.48                     | 0.48              |
| 18:T:103:LMT:H2'  | 8:V:43:TRP:HD1    | 1.79                     | 0.48              |
| 2:L:199:LEU:HD22  | 2:L:222:PHE:CE2   | 2.49                     | 0.48              |
| 4:H:149:PRO:HG3   | 4:H:204:LYS:HG2   | 1.95                     | 0.48              |
| 8:G:28:MET:O      | 8:G:32:ILE:HG13   | 2.14                     | 0.48              |
| 15:Y:102:BCL:H112 | 15:Y:102:BCL:H72  | 1.53                     | 0.48              |
| 16:L:302:BPH:HED1 | 21:M:405:MQ8:H211 | 1.96                     | 0.48              |
| 15:M:403:BCL:H141 | 16:M:404:BPH:H4C2 | 1.96                     | 0.48              |
| 6:R:46:TRP:CE2    | 15:R:101:BCL:H2C  | 2.49                     | 0.48              |
| 7:W:33:HIS:CE1    | 15:X:102:BCL:HMD3 | 2.49                     | 0.48              |
| 2:L:205:ASN:HB3   | 19:M:409:CDL:HB21 | 1.96                     | 0.47              |
| 6:P:43:TRP:HB2    | 18:P:101:LMT:H12  | 1.95                     | 0.47              |
| 18:P:104:LMT:H31  | 6:R:43:TRP:HB2    | 1.95                     | 0.47              |
| 6:4:19:HIS:O      | 6:4:23:VAL:HG23   | 2.13                     | 0.47              |
| 7:S:6:TRP:CD2     | 8:T:16:LYS:HG2    | 2.48                     | 0.47              |
| 9:3:8:ILE:HD12    | 9:3:8:ILE:N       | 2.29                     | 0.47              |
| 9:3:25:LEU:HB3    | 15:3:101:BCL:H12  | 1.96                     | 0.47              |
| 17:L:303:UQ8:H16  | 17:L:303:UQ8:H12  | 1.59                     | 0.47              |
| 4:H:20:TRP:NE1    | 14:H:301:PGV:H211 | 2.29                     | 0.47              |
| 5:I:16:ARG:HH22   | 5:K:15:ARG:CZ     | 2.27                     | 0.47              |
| 6:4:41:TRP:HH2    | 6:4:47:LEU:HB2    | 1.79                     | 0.47              |
| 17:L:304:UQ8:H12  | 17:L:304:UQ8:H16  | 1.68                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:197:ILE:HD11  | 4:H:202:PHE:HE2   | 1.79                     | 0.47              |
| 22:G:103:CRT:H371 | 15:I:101:BCL:C2B  | 2.45                     | 0.47              |
| 1:C:260:LYS:HE3   | 1:C:260:LYS:HB3   | 1.68                     | 0.47              |
| 4:H:135:PRO:HG3   | 4:H:171:TRP:CE2   | 2.49                     | 0.47              |
| 4:H:141:ASP:OD1   | 4:H:141:ASP:N     | 2.37                     | 0.47              |
| 5:A:21:LEU:HD11   | 22:B:103:CRT:H243 | 1.96                     | 0.47              |
| 6:N:46:TRP:CD2    | 15:N:101:BCL:H2C  | 2.50                     | 0.47              |
| 5:O:32:ILE:HD12   | 15:P:102:BCL:O1D  | 2.13                     | 0.47              |
| 8:T:12:GLU:O      | 8:T:16:LYS:HG3    | 2.14                     | 0.47              |
| 2:L:247:VAL:HG21  | 16:L:302:BPH:HBC3 | 1.96                     | 0.47              |
| 7:D:6:TRP:CH2     | 7:D:7:LYS:HD3     | 2.50                     | 0.47              |
| 22:4:103:CRT:H371 | 15:5:102:BCL:HMB2 | 1.96                     | 0.47              |
| 6:O:5:SER:OG      | 6:O:6:SER:N       | 2.45                     | 0.47              |
| 14:C:408:PGV:H211 | 5:1:31:LEU:HD22   | 1.97                     | 0.47              |
| 2:L:82:GLY:HA2    | 18:L:307:LMT:H21  | 1.97                     | 0.47              |
| 7:D:36:LEU:HD11   | 15:E:102:BCL:HHD  | 1.97                     | 0.47              |
| 7:F:9:TRP:HZ3     | 7:F:17:ILE:HG13   | 1.80                     | 0.47              |
| 6:J:30:PHE:CE1    | 15:J:102:BCL:H11  | 2.49                     | 0.47              |
| 15:Y:102:BCL:H101 | 15:Y:102:BCL:H13  | 1.55                     | 0.47              |
| 3:M:84:ILE:HG23   | 7:W:34:MET:HE3    | 1.97                     | 0.47              |
| 6:N:46:TRP:CZ3    | 15:N:101:BCL:HAC2 | 2.50                     | 0.47              |
| 8:T:28:MET:HA     | 8:T:28:MET:HE2    | 1.97                     | 0.47              |
| 5:7:6:HIS:NE2     | 6:8:12:GLU:OE2    | 2.37                     | 0.47              |
| 5:I:6:HIS:HA      | 6:J:19:HIS:CG     | 2.49                     | 0.47              |
| 6:N:43:TRP:CE2    | 6:N:44:ARG:HG3    | 2.50                     | 0.47              |
| 5:I:26:PHE:HA     | 15:I:101:BCL:H11  | 1.96                     | 0.47              |
| 7:Y:9:TRP:CZ3     | 8:Z:19:HIS:CD2    | 3.02                     | 0.47              |
| 6:2:47:LEU:HD13   | 18:4:101:LMT:H32  | 1.97                     | 0.47              |
| 2:L:241:PHE:HB2   | 19:L:311:CDL:H412 | 1.97                     | 0.46              |
| 3:M:247:ARG:NH2   | 4:H:115:ALA:O     | 2.47                     | 0.46              |
| 7:D:37:LEU:O      | 7:D:43:ASN:ND2    | 2.47                     | 0.46              |
| 8:E:17:GLU:HG2    | 22:E:103:CRT:H41  | 1.97                     | 0.46              |
| 15:N:101:BCL:H141 | 15:N:101:BCL:H162 | 1.70                     | 0.46              |
| 18:P:104:LMT:H5B  | 18:P:104:LMT:H6E  | 1.97                     | 0.46              |
| 5:Q:11:ILE:HG13   | 5:Q:12:PHE:CD1    | 2.51                     | 0.46              |
| 1:C:308:MET:O     | 1:C:308:MET:HG3   | 2.14                     | 0.46              |
| 17:L:303:UQ8:H22  | 17:L:303:UQ8:H25  | 1.66                     | 0.46              |
| 6:B:10:LEU:HD23   | 6:B:14:GLU:HB3    | 1.96                     | 0.46              |
| 7:Y:15:ARG:O      | 7:Y:19:ILE:HG12   | 2.15                     | 0.46              |
| 2:L:34:PHE:CZ     | 17:L:304:UQ8:H42A | 2.50                     | 0.46              |
| 5:5:33:HIS:CE1    | 15:6:101:BCL:HMD3 | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:S:41:GLU:OE2    | 7:S:41:GLU:N      | 2.48                     | 0.46              |
| 15:2:102:BCL:H62  | 15:2:102:BCL:H41  | 1.69                     | 0.46              |
| 6:4:17:GLU:O      | 6:4:21:ILE:HG13   | 2.16                     | 0.46              |
| 6:2:19:HIS:O      | 6:2:19:HIS:ND1    | 2.44                     | 0.46              |
| 1:C:78:ASN:HD21   | 1:C:80:GLN:HE21   | 1.63                     | 0.46              |
| 22:B:103:CRT:H371 | 15:D:102:BCL:HMB2 | 1.98                     | 0.46              |
| 6:N:19:HIS:HD2    | 6:N:19:HIS:O      | 1.97                     | 0.46              |
| 5:Q:16:ARG:HE     | 14:Q:101:PGV:H02  | 1.80                     | 0.46              |
| 15:Q:102:BCL:H61  | 15:Q:102:BCL:H41  | 1.59                     | 0.46              |
| 15:S:102:BCL:H93  | 15:S:102:BCL:H61  | 1.73                     | 0.46              |
| 8:Z:31:GLY:O      | 8:Z:35:ILE:HG13   | 2.16                     | 0.46              |
| 6:8:7:MET:HG3     | 6:8:9:GLY:H       | 1.80                     | 0.46              |
| 5:K:9:TRP:HZ3     | 5:K:17:THR:HG21   | 1.80                     | 0.46              |
| 15:G:102:BCL:H61  | 15:G:102:BCL:H2   | 1.61                     | 0.46              |
| 5:O:6:HIS:HA      | 6:P:19:HIS:ND1    | 2.31                     | 0.46              |
| 8:V:46:TRP:CD1    | 8:V:47:LEU:HG     | 2.51                     | 0.46              |
| 7:F:13:ASP:OD2    | 7:F:15:ARG:N      | 2.47                     | 0.46              |
| 22:J:103:CRT:H343 | 5:K:26:PHE:CE1    | 2.51                     | 0.46              |
| 3:M:4:TYR:CZ      | 3:M:6:ASN:HA      | 2.50                     | 0.46              |
| 15:D:102:BCL:H203 | 8:E:32:ILE:HD12   | 1.98                     | 0.46              |
| 15:I:101:BCL:H62  | 15:I:101:BCL:H41  | 1.63                     | 0.46              |
| 7:W:14:PRO:HB3    | 8:X:18:PHE:CZ     | 2.51                     | 0.46              |
| 7:Y:12:VAL:HB     | 7:Y:17:ILE:HD11   | 1.98                     | 0.46              |
| 6:2:18:PHE:HD2    | 22:2:103:CRT:C6   | 2.29                     | 0.46              |
| 5:5:13:ASP:O      | 5:5:17:THR:OG1    | 2.26                     | 0.46              |
| 5:5:37:LEU:O      | 5:5:43:ASN:ND2    | 2.48                     | 0.46              |
| 2:L:184:THR:HG22  | 17:L:303:UQ8:H25A | 1.97                     | 0.45              |
| 19:H:302:CDL:OA6  | 14:A:503:PGV:H21  | 2.16                     | 0.45              |
| 8:G:47:LEU:HD13   | 18:J:101:LMT:H32  | 1.97                     | 0.45              |
| 5:K:5:FME:O       | 5:K:8:ILE:HG12    | 2.16                     | 0.45              |
| 6:P:28:ALA:O      | 6:P:32:ILE:HD12   | 2.16                     | 0.45              |
| 7:S:12:VAL:HB     | 7:S:17:ILE:HD13   | 1.98                     | 0.45              |
| 6:8:37:HIS:CG     | 15:8:102:BCL:H91  | 2.51                     | 0.45              |
| 5:Q:7:LYS:HB2     | 5:Q:7:LYS:HE2     | 1.77                     | 0.45              |
| 7:Y:14:PRO:O      | 7:Y:18:LEU:HD12   | 2.16                     | 0.45              |
| 22:2:103:CRT:H372 | 9:3:33:HIS:CD2    | 2.51                     | 0.45              |
| 8:E:11:THR:OG1    | 8:E:13:GLU:HG3    | 2.16                     | 0.45              |
| 7:F:12:VAL:CG2    | 7:F:17:ILE:HD11   | 2.46                     | 0.45              |
| 21:M:405:MQ8:H2M3 | 21:M:405:MQ8:H121 | 1.98                     | 0.45              |
| 4:H:124:ASP:HB2   | 4:H:233:LEU:HD21  | 1.98                     | 0.45              |
| 18:2:101:LMT:H5B  | 18:2:101:LMT:H6E  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:32:ARG:HG2    | 4:H:62:ALA:HB2    | 1.99                     | 0.45              |
| 4:H:214:ILE:HB    | 4:H:218:HIS:HB2   | 1.98                     | 0.45              |
| 8:E:23:THR:O      | 8:E:27:THR:HG23   | 2.16                     | 0.45              |
| 15:E:102:BCL:H161 | 15:E:102:BCL:H141 | 1.67                     | 0.45              |
| 7:Y:14:PRO:HG2    | 22:Z:103:CRT:H1M1 | 1.98                     | 0.45              |
| 8:Z:46:TRP:CE2    | 15:Z:102:BCL:H2C  | 2.52                     | 0.45              |
| 1:C:227:LYS:NZ    | 3:M:97:PRO:O      | 2.48                     | 0.45              |
| 1:C:316:LYS:HG2   | 10:C:404:HEM:HAD2 | 1.98                     | 0.45              |
| 15:A:502:BCL:HAC2 | 15:A:502:BCL:HHD  | 1.73                     | 0.45              |
| 8:T:18:PHE:HB2    | 22:T:102:CRT:H1M2 | 1.98                     | 0.45              |
| 6:O:22:PHE:CD2    | 22:O:102:CRT:H14  | 2.52                     | 0.45              |
| 3:M:237:GLN:HB2   | 3:M:262:MET:HG2   | 1.99                     | 0.45              |
| 18:B:101:LMT:H62  | 18:B:101:LMT:H91  | 1.78                     | 0.45              |
| 7:W:14:PRO:HB3    | 8:X:18:PHE:CE1    | 2.52                     | 0.45              |
| 5:I:32:ILE:HD12   | 15:J:102:BCL:O1D  | 2.16                     | 0.45              |
| 15:O:502:BCL:H91  | 15:O:502:BCL:H112 | 1.67                     | 0.45              |
| 3:M:42:LYS:HE2    | 3:M:42:LYS:HB2    | 1.77                     | 0.45              |
| 15:D:102:BCL:HBC2 | 8:E:43:TRP:CZ3    | 2.51                     | 0.45              |
| 15:I:101:BCL:H143 | 15:I:101:BCL:H111 | 1.78                     | 0.45              |
| 22:P:103:CRT:H372 | 5:Q:33:HIS:CD2    | 2.52                     | 0.45              |
| 6:R:8:THR:OG1     | 6:R:9:GLY:N       | 2.49                     | 0.45              |
| 7:S:14:PRO:HB3    | 8:T:18:PHE:CZ     | 2.51                     | 0.45              |
| 2:L:272:TRP:CE2   | 17:L:309:UQ8:H4MA | 2.52                     | 0.44              |
| 7:Y:9:TRP:CE2     | 8:Z:18:PHE:HE1    | 2.35                     | 0.44              |
| 3:M:284:ILE:HD13  | 3:M:284:ILE:HA    | 1.81                     | 0.44              |
| 6:R:41:TRP:CZ2    | 15:R:101:BCL:H202 | 2.52                     | 0.44              |
| 5:5:11:ILE:HG23   | 5:7:15:ARG:NE     | 2.31                     | 0.44              |
| 15:5:102:BCL:H62  | 15:5:102:BCL:H93  | 1.72                     | 0.44              |
| 5:7:35:ILE:HD13   | 22:9:101:CRT:H391 | 1.98                     | 0.44              |
| 15:B:102:BCL:CHB  | 15:B:102:BCL:H71  | 2.48                     | 0.44              |
| 15:B:102:BCL:HBA2 | 15:B:102:BCL:HED3 | 1.98                     | 0.44              |
| 5:K:33:HIS:CE1    | 15:N:101:BCL:HMD1 | 2.52                     | 0.44              |
| 15:O:101:BCL:H3A  | 15:O:101:BCL:HBA1 | 1.63                     | 0.44              |
| 15:O:101:BCL:H62  | 15:O:101:BCL:H41  | 1.73                     | 0.44              |
| 2:L:234:ALA:HB2   | 3:M:44:GLY:HA2    | 1.99                     | 0.44              |
| 3:M:74:ASN:ND2    | 25:M:510:HOH:O    | 2.50                     | 0.44              |
| 5:I:22:PHE:HE1    | 22:J:103:CRT:H182 | 1.82                     | 0.44              |
| 1:C:163:LYS:HE3   | 1:C:163:LYS:HB2   | 1.73                     | 0.44              |
| 2:L:127:PHE:CE2   | 2:L:131:ILE:HD11  | 2.51                     | 0.44              |
| 17:L:304:UQ8:H7   | 17:L:304:UQ8:H1M  | 1.75                     | 0.44              |
| 3:M:229:PHE:HB2   | 3:M:244:ALA:HB2   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:M:409:CDL:H202 | 19:M:409:CDL:H171 | 1.89                     | 0.44              |
| 7:F:6:TRP:CD2     | 8:G:16:LYS:HD2    | 2.53                     | 0.44              |
| 7:F:33:HIS:CE1    | 15:G:102:BCL:HMD3 | 2.53                     | 0.44              |
| 7:F:37:LEU:O      | 7:F:43:ASN:ND2    | 2.43                     | 0.44              |
| 8:G:41:TRP:CE2    | 15:G:102:BCL:H192 | 2.52                     | 0.44              |
| 6:2:46:TRP:CD1    | 6:2:47:LEU:HG     | 2.53                     | 0.44              |
| 15:2:102:BCL:H91  | 15:2:102:BCL:H111 | 1.78                     | 0.44              |
| 15:3:101:BCL:HHD  | 15:3:101:BCL:HAC2 | 1.75                     | 0.44              |
| 2:L:17:LEU:C      | 2:L:18:ILE:HD12   | 2.42                     | 0.44              |
| 2:L:40:PHE:HD1    | 21:M:405:MQ8:H362 | 1.82                     | 0.44              |
| 2:L:110:GLU:HB3   | 2:L:124:PRO:HG3   | 1.99                     | 0.44              |
| 2:L:241:PHE:HB2   | 19:L:311:CDL:H382 | 1.99                     | 0.44              |
| 19:H:302:CDL:H821 | 19:H:302:CDL:H852 | 1.73                     | 0.44              |
| 15:1:402:BCL:H62  | 15:1:402:BCL:H41  | 1.79                     | 0.44              |
| 15:5:102:BCL:H192 | 15:5:102:BCL:H161 | 1.79                     | 0.44              |
| 3:M:38:TYR:OH     | 4:H:148:ASP:OD1   | 2.25                     | 0.44              |
| 3:M:206:ILE:HD13  | 15:M:402:BCL:HMD2 | 2.00                     | 0.44              |
| 5:A:12:PHE:HZ     | 7:D:18:LEU:HB2    | 1.82                     | 0.44              |
| 7:F:7:LYS:HB3     | 22:J:103:CRT:H41  | 1.99                     | 0.44              |
| 6:N:19:HIS:HD2    | 6:N:23:VAL:HG23   | 1.82                     | 0.44              |
| 6:R:47:LEU:HD13   | 18:R:103:LMT:H41  | 2.00                     | 0.44              |
| 7:Y:32:ILE:HD12   | 15:Z:102:BCL:O1D  | 2.17                     | 0.44              |
| 14:C:408:PGV:H52  | 22:2:103:CRT:H401 | 1.99                     | 0.44              |
| 15:D:102:BCL:H192 | 15:D:102:BCL:H162 | 1.83                     | 0.44              |
| 5:K:6:HIS:HB3     | 6:N:16:GLN:NE2    | 2.32                     | 0.44              |
| 6:N:19:HIS:CD2    | 6:N:23:VAL:HG23   | 2.53                     | 0.44              |
| 22:T:102:CRT:H15  | 22:T:102:CRT:H131 | 1.87                     | 0.44              |
| 15:V:101:BCL:H93  | 15:V:101:BCL:H62  | 1.75                     | 0.44              |
| 1:C:102:ALA:HB1   | 1:C:105:GLU:HB2   | 1.99                     | 0.43              |
| 2:L:42:PHE:CE1    | 17:L:304:UQ8:H18  | 2.53                     | 0.43              |
| 14:L:306:PGV:H22  | 7:D:34:MET:HB3    | 1.99                     | 0.43              |
| 22:Y:101:CRT:H291 | 15:Y:102:BCL:H11  | 2.00                     | 0.43              |
| 5:1:9:TRP:HZ3     | 5:1:17:THR:HG21   | 1.82                     | 0.43              |
| 6:2:22:PHE:CD2    | 22:2:103:CRT:H11  | 2.52                     | 0.43              |
| 15:6:101:BCL:H61  | 15:6:101:BCL:H93  | 1.65                     | 0.43              |
| 5:7:32:ILE:HG12   | 22:9:101:CRT:H403 | 2.00                     | 0.43              |
| 15:0:101:BCL:H61  | 15:0:101:BCL:H101 | 1.89                     | 0.43              |
| 2:L:203:VAL:HG13  | 2:L:213:LYS:HB2   | 1.99                     | 0.43              |
| 5:K:32:ILE:HD12   | 15:N:101:BCL:O1D  | 2.18                     | 0.43              |
| 8:V:31:GLY:O      | 8:V:35:ILE:HD12   | 2.19                     | 0.43              |
| 6:2:18:PHE:O      | 6:2:22:PHE:HB2    | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:5:102:BCL:HAC2 | 15:5:102:BCL:HHD  | 1.80                     | 0.43              |
| 1:C:162:PRO:HD2   | 10:C:402:HEM:HBD2 | 2.00                     | 0.43              |
| 19:L:311:CDL:H611 | 19:L:311:CDL:H582 | 1.79                     | 0.43              |
| 22:B:103:CRT:H20  | 22:B:103:CRT:H181 | 1.90                     | 0.43              |
| 7:Y:33:HIS:CE1    | 15:Z:102:BCL:HMD3 | 2.54                     | 0.43              |
| 22:4:103:CRT:H343 | 5:5:26:PHE:CD1    | 2.54                     | 0.43              |
| 5:7:33:HIS:CE1    | 15:8:102:BCL:HMD3 | 2.54                     | 0.43              |
| 1:C:50:GLU:OE1    | 9:3:53:VAL:HG12   | 2.18                     | 0.43              |
| 17:L:304:UQ8:H7   | 17:L:304:UQ8:H10  | 1.68                     | 0.43              |
| 19:M:409:CDL:H522 | 19:M:409:CDL:H552 | 1.63                     | 0.43              |
| 15:2:102:BCL:H93  | 15:2:102:BCL:H61  | 1.70                     | 0.43              |
| 5:9:5:FME:O       | 6:0:19:HIS:NE2    | 2.52                     | 0.43              |
| 1:C:144:HIS:HE1   | 10:C:404:HEM:C1C  | 2.37                     | 0.43              |
| 14:L:305:PGV:H41  | 14:1:401:PGV:H72  | 2.00                     | 0.43              |
| 14:L:310:PGV:H272 | 14:L:310:PGV:H242 | 1.68                     | 0.43              |
| 15:A:502:BCL:HBC3 | 15:A:502:BCL:H2C  | 1.86                     | 0.43              |
| 15:P:102:BCL:H93  | 15:P:102:BCL:H111 | 1.72                     | 0.43              |
| 15:Q:102:BCL:HBC2 | 6:R:43:TRP:CZ3    | 2.53                     | 0.43              |
| 5:7:37:LEU:O      | 5:7:43:ASN:ND2    | 2.47                     | 0.43              |
| 1:C:25:ARG:NH2    | 9:3:43:ASP:OD2    | 2.52                     | 0.43              |
| 1:C:145:VAL:O     | 10:C:404:HEM:HBD2 | 2.19                     | 0.43              |
| 1:C:126:VAL:HG13  | 1:C:287:LEU:HD13  | 2.00                     | 0.43              |
| 2:L:186:PHE:CD2   | 2:L:246:ALA:HB1   | 2.54                     | 0.43              |
| 22:E:103:CRT:H26  | 22:E:103:CRT:H241 | 1.89                     | 0.43              |
| 15:G:102:BCL:H93  | 15:G:102:BCL:H62  | 1.71                     | 0.43              |
| 6:J:31:GLY:O      | 6:J:35:ILE:HG13   | 2.18                     | 0.43              |
| 6:N:21:ILE:HA     | 6:N:24:GLN:OE1    | 2.19                     | 0.43              |
| 8:Z:12:GLU:O      | 8:Z:16:LYS:HG2    | 2.19                     | 0.43              |
| 6:4:33:VAL:HG11   | 15:4:102:BCL:HAA1 | 2.01                     | 0.43              |
| 1:C:151:THR:HG22  | 1:C:153:TYR:N     | 2.26                     | 0.43              |
| 3:M:134:TYR:CZ    | 14:M:408:PGV:H21  | 2.53                     | 0.43              |
| 3:M:232:ASP:OD1   | 3:M:232:ASP:N     | 2.51                     | 0.43              |
| 8:E:28:MET:O      | 8:E:32:ILE:HG13   | 2.18                     | 0.43              |
| 22:R:102:CRT:H20  | 22:R:102:CRT:H181 | 1.88                     | 0.43              |
| 18:R:103:LMT:H6E  | 8:T:42:LEU:O      | 2.19                     | 0.43              |
| 22:T:102:CRT:H20  | 22:T:102:CRT:H181 | 1.85                     | 0.43              |
| 15:X:102:BCL:H61  | 15:X:102:BCL:H2   | 1.63                     | 0.43              |
| 7:Y:30:LEU:HD23   | 22:Y:101:CRT:H36  | 2.01                     | 0.43              |
| 15:1:402:BCL:H122 | 15:1:402:BCL:H161 | 1.82                     | 0.43              |
| 22:2:103:CRT:H35  | 15:3:101:BCL:CMB  | 2.49                     | 0.43              |
| 6:4:22:PHE:CE1    | 6:4:26:MET:HE2    | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:4:23:VAL:HA     | 6:4:26:MET:HB2    | 1.99                     | 0.43              |
| 5:9:33:HIS:CD2    | 22:9:101:CRT:H372 | 2.53                     | 0.43              |
| 17:L:304:UQ8:H40  | 17:L:304:UQ8:H37  | 1.57                     | 0.43              |
| 14:A:501:PGV:H031 | 7:D:37:LEU:HB3    | 2.00                     | 0.43              |
| 15:S:102:BCL:H193 | 15:S:102:BCL:H161 | 1.88                     | 0.43              |
| 7:Y:35:ILE:HG12   | 14:1:401:PGV:H22  | 2.01                     | 0.43              |
| 6:2:26:MET:HG3    | 22:2:103:CRT:C19  | 2.48                     | 0.43              |
| 3:M:168:MET:HE3   | 3:M:168:MET:HB3   | 1.93                     | 0.43              |
| 7:D:32:ILE:HD12   | 15:E:102:BCL:O1D  | 2.19                     | 0.43              |
| 5:Q:6:HIS:HA      | 6:R:19:HIS:HD2    | 1.83                     | 0.43              |
| 6:6:22:PHE:CD1    | 22:6:102:CRT:H14  | 2.54                     | 0.43              |
| 6:8:41:TRP:CZ2    | 15:8:102:BCL:H202 | 2.54                     | 0.43              |
| 1:C:170:PRO:HB3   | 1:C:299:TYR:HE1   | 1.83                     | 0.42              |
| 6:B:46:TRP:CE2    | 15:B:102:BCL:H2C  | 2.54                     | 0.42              |
| 5:Q:18:LEU:HD23   | 5:Q:18:LEU:HA     | 1.85                     | 0.42              |
| 14:L:310:PGV:H291 | 14:L:310:PGV:H322 | 1.83                     | 0.42              |
| 8:E:7:MET:HE3     | 8:E:9:GLY:H       | 1.84                     | 0.42              |
| 7:F:13:ASP:O      | 7:F:17:ILE:HG12   | 2.18                     | 0.42              |
| 22:G:103:CRT:H372 | 5:I:33:HIS:CD2    | 2.54                     | 0.42              |
| 5:I:11:ILE:HG12   | 22:N:102:CRT:H1M1 | 2.00                     | 0.42              |
| 15:J:102:BCL:H91  | 15:J:102:BCL:H111 | 1.73                     | 0.42              |
| 22:Y:101:CRT:H10  | 22:Y:101:CRT:H81  | 1.78                     | 0.42              |
| 1:C:263:THR:HA    | 3:M:311:VAL:HG22  | 2.01                     | 0.42              |
| 19:L:311:CDL:H362 | 3:M:7:ILE:HD12    | 2.00                     | 0.42              |
| 3:M:238:ILE:HG12  | 3:M:263:GLU:HB2   | 2.00                     | 0.42              |
| 4:H:150:ASP:OD2   | 4:H:152:ARG:NH2   | 2.49                     | 0.42              |
| 6:B:46:TRP:CD2    | 15:B:102:BCL:H2C  | 2.53                     | 0.42              |
| 5:5:19:VAL:HA     | 15:5:102:BCL:H151 | 2.01                     | 0.42              |
| 22:6:102:CRT:H371 | 15:7:101:BCL:HMB2 | 2.00                     | 0.42              |
| 15:8:102:BCL:HBB2 | 18:8:103:LMT:H81  | 2.00                     | 0.42              |
| 13:C:407:PLM:H21  | 14:L:305:PGV:H031 | 2.01                     | 0.42              |
| 17:L:304:UQ8:H7A  | 15:9:102:BCL:H72  | 2.02                     | 0.42              |
| 7:F:13:ASP:OD2    | 7:F:13:ASP:C      | 2.63                     | 0.42              |
| 22:G:103:CRT:H20  | 22:G:103:CRT:H181 | 1.91                     | 0.42              |
| 5:Q:7:LYS:HB3     | 22:T:102:CRT:H41  | 2.02                     | 0.42              |
| 15:S:102:BCL:H143 | 15:S:102:BCL:H111 | 1.91                     | 0.42              |
| 22:T:102:CRT:H393 | 7:U:30:LEU:HD23   | 2.02                     | 0.42              |
| 15:V:101:BCL:O1A  | 22:V:102:CRT:H25  | 2.19                     | 0.42              |
| 5:7:24:PHE:O      | 5:7:27:VAL:HG12   | 2.19                     | 0.42              |
| 6:0:22:PHE:HA     | 22:0:102:CRT:H11  | 2.01                     | 0.42              |
| 1:C:250:CYS:SG    | 10:C:403:HEM:CBC  | 2.98                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:L:278:TRP:CG    | 3:M:88:LYS:HB2    | 2.54                     | 0.42              |
| 15:L:301:BCL:H2   | 16:L:302:BPH:HBB3 | 2.02                     | 0.42              |
| 17:L:304:UQ8:H3MB | 15:9:102:BCL:H142 | 2.00                     | 0.42              |
| 3:M:131:VAL:HG12  | 3:M:135:LYS:HD2   | 2.02                     | 0.42              |
| 22:M:406:CRT:H2M3 | 5:Q:34:PHE:CE1    | 2.54                     | 0.42              |
| 6:B:22:PHE:CD2    | 22:B:103:CRT:H14  | 2.55                     | 0.42              |
| 5:Q:44:TRP:CD2    | 15:Q:102:BCL:H2C  | 2.54                     | 0.42              |
| 6:4:18:PHE:HB2    | 22:4:103:CRT:H21A | 2.02                     | 0.42              |
| 17:L:309:UQ8:H22  | 17:L:309:UQ8:H25  | 1.79                     | 0.42              |
| 15:B:102:BCL:H93  | 15:B:102:BCL:H61  | 1.81                     | 0.42              |
| 15:K:102:BCL:H143 | 15:K:102:BCL:H111 | 1.80                     | 0.42              |
| 15:N:101:BCL:H91  | 15:N:101:BCL:H111 | 1.65                     | 0.42              |
| 7:S:15:ARG:HE     | 7:S:15:ARG:HB2    | 1.75                     | 0.42              |
| 8:X:47:LEU:HD13   | 18:Z:101:LMT:H32  | 2.00                     | 0.42              |
| 9:3:8:ILE:H       | 9:3:8:ILE:CD1     | 2.31                     | 0.42              |
| 5:5:11:ILE:O      | 5:7:15:ARG:NH2    | 2.53                     | 0.42              |
| 2:L:20:GLY:O      | 2:L:24:ASP:HB2    | 2.20                     | 0.42              |
| 4:H:107:MET:HE3   | 4:H:107:MET:HB3   | 1.77                     | 0.42              |
| 4:H:135:PRO:HG3   | 4:H:171:TRP:CZ2   | 2.54                     | 0.42              |
| 15:J:102:BCL:H93  | 15:J:102:BCL:H61  | 1.67                     | 0.42              |
| 22:N:102:CRT:H20  | 22:N:102:CRT:H181 | 1.79                     | 0.42              |
| 5:O:14:PRO:O      | 5:O:18:LEU:HB2    | 2.20                     | 0.42              |
| 15:R:101:BCL:H141 | 15:R:101:BCL:H161 | 1.80                     | 0.42              |
| 7:W:41:GLU:OE2    | 7:Y:52:ALA:HA     | 2.19                     | 0.42              |
| 22:4:103:CRT:H36  | 22:4:103:CRT:H341 | 1.82                     | 0.42              |
| 5:9:14:PRO:HB3    | 6:0:18:PHE:CZ     | 2.55                     | 0.42              |
| 2:L:125:PHE:HA    | 19:L:311:CDL:H752 | 2.02                     | 0.42              |
| 4:H:212:ALA:O     | 4:H:254:ARG:NH2   | 2.47                     | 0.42              |
| 22:J:103:CRT:H10  | 22:J:103:CRT:H81  | 1.86                     | 0.42              |
| 15:T:101:BCL:H102 | 15:T:101:BCL:C1B  | 2.49                     | 0.42              |
| 15:W:101:BCL:H143 | 15:W:101:BCL:H111 | 1.88                     | 0.42              |
| 8:Z:47:LEU:HD23   | 8:Z:47:LEU:HA     | 1.90                     | 0.42              |
| 22:4:103:CRT:H10  | 22:4:103:CRT:H81  | 1.87                     | 0.42              |
| 15:8:102:BCL:H111 | 15:8:102:BCL:H142 | 1.83                     | 0.42              |
| 15:T:101:BCL:H192 | 15:T:101:BCL:H162 | 1.79                     | 0.42              |
| 8:V:11:THR:OG1    | 8:V:13:GLU:HG3    | 2.20                     | 0.42              |
| 5:1:24:PHE:CD2    | 5:1:25:LEU:HD23   | 2.55                     | 0.42              |
| 6:4:46:TRP:CD2    | 15:4:102:BCL:H2C  | 2.55                     | 0.42              |
| 1:C:166:TRP:CZ2   | 1:C:304:LYS:HD2   | 2.55                     | 0.42              |
| 1:C:307:CYS:O     | 1:C:308:MET:HB3   | 2.20                     | 0.42              |
| 2:L:254:ILE:HD12  | 2:L:254:ILE:HA    | 1.90                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:152:ALA:HA    | 19:M:409:CDL:H191 | 2.02                     | 0.42              |
| 6:B:30:PHE:CE1    | 15:B:102:BCL:H11  | 2.55                     | 0.42              |
| 6:B:43:TRP:HB2    | 18:B:101:LMT:H31  | 2.02                     | 0.42              |
| 22:Z:103:CRT:H35  | 15:1:402:BCL:CHB  | 2.49                     | 0.42              |
| 15:4:102:BCL:H92  | 15:4:102:BCL:H61  | 1.81                     | 0.42              |
| 5:7:25:LEU:HB2    | 15:7:101:BCL:H43  | 2.00                     | 0.42              |
| 1:C:119:ASP:CG    | 1:C:128:ARG:HH12  | 2.28                     | 0.41              |
| 1:C:146:ALA:C     | 1:C:148:THR:H     | 2.27                     | 0.41              |
| 1:C:227:LYS:HG3   | 3:M:172:ALA:HB1   | 2.01                     | 0.41              |
| 17:L:309:UQ8:H42  | 17:L:309:UQ8:H46  | 1.75                     | 0.41              |
| 4:H:159:LEU:HD23  | 4:H:214:ILE:C     | 2.45                     | 0.41              |
| 6:N:46:TRP:CD1    | 6:N:47:LEU:HG     | 2.55                     | 0.41              |
| 8:X:12:GLU:H      | 8:X:12:GLU:HG2    | 1.66                     | 0.41              |
| 15:3:101:BCL:HBC3 | 15:3:101:BCL:H2C  | 1.89                     | 0.41              |
| 2:L:3:MET:HB3     | 2:L:7:GLU:HB3     | 2.02                     | 0.41              |
| 3:M:81:TRP:O      | 7:U:34[A]:MET:HB3 | 2.21                     | 0.41              |
| 5:A:8:ILE:HD13    | 22:E:103:CRT:H10  | 2.02                     | 0.41              |
| 6:B:47:LEU:O      | 7:D:50:PRO:HD3    | 2.20                     | 0.41              |
| 7:S:18:LEU:HD23   | 7:S:18:LEU:HA     | 1.91                     | 0.41              |
| 18:4:104:LMT:H1B  | 18:4:104:LMT:H3'  | 1.71                     | 0.41              |
| 6:6:46:TRP:CE2    | 15:6:101:BCL:H2C  | 2.55                     | 0.41              |
| 15:9:102:BCL:HAC2 | 15:9:102:BCL:HHD  | 1.81                     | 0.41              |
| 22:0:102:CRT:H20  | 22:0:102:CRT:H181 | 1.92                     | 0.41              |
| 14:M:408:PGV:H241 | 5:O:27:VAL:HG21   | 2.02                     | 0.41              |
| 8:E:41:TRP:CZ2    | 15:E:102:BCL:H18  | 2.54                     | 0.41              |
| 7:W:32:ILE:HD12   | 15:X:102:BCL:O1D  | 2.19                     | 0.41              |
| 5:1:9:TRP:CD1     | 6:2:18:PHE:HD1    | 2.38                     | 0.41              |
| 5:1:30:LEU:HD12   | 5:1:34:PHE:CE2    | 2.55                     | 0.41              |
| 6:8:37:HIS:CD2    | 15:8:102:BCL:H91  | 2.54                     | 0.41              |
| 15:0:101:BCL:H192 | 15:0:101:BCL:H161 | 1.69                     | 0.41              |
| 1:C:163:LYS:HG2   | 1:C:164:TYR:CE2   | 2.55                     | 0.41              |
| 18:J:104:LMT:H62  | 15:K:102:BCL:H3C  | 2.03                     | 0.41              |
| 15:K:102:BCL:H61  | 15:K:102:BCL:H102 | 1.49                     | 0.41              |
| 22:N:102:CRT:H10  | 22:N:102:CRT:H81  | 1.82                     | 0.41              |
| 22:P:103:CRT:H20  | 22:P:103:CRT:H181 | 1.82                     | 0.41              |
| 15:U:101:BCL:HBC3 | 15:U:101:BCL:HHD  | 2.01                     | 0.41              |
| 22:V:102:CRT:H26  | 22:V:102:CRT:H241 | 1.92                     | 0.41              |
| 8:X:22:PHE:HA     | 22:Y:101:CRT:H14  | 2.02                     | 0.41              |
| 6:4:41:TRP:CH2    | 6:4:47:LEU:HB2    | 2.54                     | 0.41              |
| 3:M:89:HIS:O      | 3:M:93:LEU:HG     | 2.20                     | 0.41              |
| 3:M:162:PHE:C     | 3:M:165:PRO:HD2   | 2.45                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:M:409:CDL:H822 | 4:H:22:PHE:HB2    | 2.01                     | 0.41              |
| 22:B:103:CRT:H10  | 22:B:103:CRT:H81  | 1.92                     | 0.41              |
| 22:V:102:CRT:H35  | 15:W:101:BCL:HMB1 | 2.02                     | 0.41              |
| 8:X:30:PHE:O      | 8:X:34:ILE:HD12   | 2.21                     | 0.41              |
| 8:X:46:TRP:CE2    | 15:X:102:BCL:H2C  | 2.56                     | 0.41              |
| 22:6:102:CRT:H20  | 22:6:102:CRT:H181 | 1.84                     | 0.41              |
| 6:8:41:TRP:CZ3    | 15:8:102:BCL:H172 | 2.56                     | 0.41              |
| 22:0:102:CRT:H15  | 22:0:102:CRT:H131 | 1.95                     | 0.41              |
| 17:L:304:UQ8:H46  | 17:L:304:UQ8:H42  | 1.78                     | 0.41              |
| 15:L:308:BCL:HED1 | 3:M:179:ILE:HG23  | 2.03                     | 0.41              |
| 22:M:406:CRT:H393 | 5:O:34:PHE:CD2    | 2.53                     | 0.41              |
| 19:H:302:CDL:OA3  | 19:D:101:CDL:O1   | 2.30                     | 0.41              |
| 7:F:5:LEU:HD13    | 15:I:101:BCL:H193 | 2.03                     | 0.41              |
| 7:W:18:LEU:HD23   | 7:W:18:LEU:HA     | 1.84                     | 0.41              |
| 22:2:103:CRT:H181 | 22:2:103:CRT:H20  | 1.80                     | 0.41              |
| 9:3:5:LEU:HB3     | 6:4:19:HIS:CE1    | 2.56                     | 0.41              |
| 6:4:43:TRP:HB2    | 18:4:101:LMT:H12  | 2.02                     | 0.41              |
| 1:C:257:TYR:OH    | 3:M:296:LEU:HD21  | 2.20                     | 0.41              |
| 18:M:410:LMT:H71  | 18:M:410:LMT:H101 | 1.84                     | 0.41              |
| 4:H:3:ALA:HB2     | 18:H:303:LMT:H6E  | 2.02                     | 0.41              |
| 4:H:64:PRO:HA     | 4:H:79:PRO:CD     | 2.50                     | 0.41              |
| 14:Q:101:PGV:O04  | 18:S:101:LMT:O2B  | 2.37                     | 0.41              |
| 8:V:46:TRP:CE2    | 15:V:101:BCL:H2C  | 2.55                     | 0.41              |
| 9:3:5:LEU:HD13    | 9:3:8:ILE:HD13    | 2.03                     | 0.41              |
| 2:L:272:TRP:CD1   | 17:L:309:UQ8:H4MA | 2.56                     | 0.41              |
| 17:L:303:UQ8:H21A | 17:L:303:UQ8:H17  | 1.71                     | 0.41              |
| 15:E:102:BCL:HBB2 | 18:G:101:LMT:H111 | 2.02                     | 0.41              |
| 22:V:102:CRT:H20  | 22:V:102:CRT:H181 | 1.85                     | 0.41              |
| 8:Z:47:LEU:HD13   | 18:2:101:LMT:H41  | 2.03                     | 0.41              |
| 5:7:32:ILE:HD12   | 15:8:102:BCL:O1D  | 2.21                     | 0.41              |
| 6:8:11:THR:O      | 6:8:13:GLN:N      | 2.52                     | 0.41              |
| 1:C:219:PRO:HG2   | 18:H:303:LMT:H6D  | 2.02                     | 0.41              |
| 15:A:502:BCL:H151 | 15:A:502:BCL:H18  | 1.89                     | 0.41              |
| 18:E:101:LMT:H1B  | 18:E:101:LMT:H3'  | 1.84                     | 0.41              |
| 15:E:102:BCL:H92  | 15:E:102:BCL:H62  | 1.87                     | 0.41              |
| 7:F:37:LEU:HG     | 7:F:44:TRP:CH2    | 2.56                     | 0.41              |
| 22:J:103:CRT:H20  | 22:J:103:CRT:H181 | 1.86                     | 0.41              |
| 6:N:26:MET:HG3    | 22:N:102:CRT:C19  | 2.51                     | 0.41              |
| 7:Y:9:TRP:HD1     | 7:Y:14:PRO:HB3    | 1.85                     | 0.41              |
| 7:Y:35:ILE:O      | 7:Y:39:THR:HG23   | 2.20                     | 0.41              |
| 15:1:402:BCL:HAC2 | 15:1:402:BCL:HHD  | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:2:103:CRT:H10  | 22:2:103:CRT:H81  | 1.94                     | 0.41              |
| 2:L:106:TRP:HH2   | 21:M:405:MQ8:H301 | 1.85                     | 0.41              |
| 17:L:309:UQ8:H35A | 17:L:309:UQ8:H37  | 1.71                     | 0.41              |
| 7:D:6:TRP:CZ2     | 7:D:7:LYS:HD3     | 2.56                     | 0.41              |
| 7:D:14:PRO:HB3    | 8:E:18:PHE:CZ     | 2.56                     | 0.41              |
| 7:F:14:PRO:HG2    | 8:G:10:LEU:HD22   | 2.03                     | 0.41              |
| 7:Y:35:ILE:HG13   | 14:1:401:PGV:H52  | 2.03                     | 0.41              |
| 15:Z:102:BCL:H162 | 15:Z:102:BCL:H192 | 1.81                     | 0.41              |
| 1:C:183:GLN:HB3   | 1:C:196:PRO:HA    | 2.03                     | 0.40              |
| 14:L:306:PGV:H042 | 7:D:38:SER:HB3    | 2.03                     | 0.40              |
| 14:L:306:PGV:H202 | 14:H:301:PGV:H062 | 2.02                     | 0.40              |
| 6:N:39:LEU:HD23   | 6:N:42:LEU:HD12   | 2.03                     | 0.40              |
| 15:S:102:BCL:HAC2 | 15:S:102:BCL:HHD  | 1.85                     | 0.40              |
| 2:L:67:ILE:HG12   | 14:L:306:PGV:H201 | 2.03                     | 0.40              |
| 5:A:33:HIS:CG     | 22:0:102:CRT:H372 | 2.56                     | 0.40              |
| 8:E:46:TRP:CE2    | 15:E:102:BCL:H2C  | 2.56                     | 0.40              |
| 5:I:7:LYS:CG      | 22:N:102:CRT:H41  | 2.49                     | 0.40              |
| 3:M:296:LEU:HD23  | 3:M:296:LEU:HA    | 1.92                     | 0.40              |
| 7:F:17:ILE:HG12   | 7:F:17:ILE:H      | 1.62                     | 0.40              |
| 15:K:102:BCL:HBA1 | 15:K:102:BCL:H3A  | 1.81                     | 0.40              |
| 6:R:26:MET:HG3    | 22:R:102:CRT:C19  | 2.51                     | 0.40              |
| 22:4:103:CRT:H31  | 22:4:103:CRT:H35  | 1.66                     | 0.40              |
| 15:L:301:BCL:H162 | 15:L:301:BCL:H141 | 1.85                     | 0.40              |
| 17:L:304:UQ8:H27A | 17:L:304:UQ8:H30  | 1.58                     | 0.40              |
| 3:M:181:PRO:HB3   | 25:M:502:HOH:O    | 2.22                     | 0.40              |
| 15:M:402:BCL:H162 | 15:M:402:BCL:H192 | 1.86                     | 0.40              |
| 22:E:103:CRT:H36  | 7:F:30:LEU:HD23   | 2.03                     | 0.40              |
| 5:O:34:PHE:HD1    | 24:O:501:LDA:H111 | 1.87                     | 0.40              |
| 8:X:12:GLU:O      | 8:X:16:LYS:HG3    | 2.22                     | 0.40              |
| 15:1:402:BCL:H93  | 15:1:402:BCL:H111 | 1.81                     | 0.40              |
| 6:2:22:PHE:CD2    | 22:2:103:CRT:H14  | 2.57                     | 0.40              |
| 5:5:6:HIS:CE1     | 6:6:16:GLN:HA     | 2.56                     | 0.40              |
| 15:7:101:BCL:H93  | 6:8:29:PHE:HB2    | 2.03                     | 0.40              |
| 1:C:72:VAL:HG11   | 1:C:79:VAL:HG11   | 2.03                     | 0.40              |
| 1:C:191:ALA:O     | 2:L:266:PRO:HB2   | 2.21                     | 0.40              |
| 2:L:42:PHE:HE2    | 17:L:304:UQ8:H37  | 1.85                     | 0.40              |
| 2:L:123:ILE:HB    | 2:L:124:PRO:HD3   | 2.03                     | 0.40              |
| 3:M:81:TRP:O      | 7:U:34[B]:MET:HB3 | 2.21                     | 0.40              |
| 3:M:120:PHE:HE2   | 5:Q:30:LEU:HD13   | 1.86                     | 0.40              |
| 3:M:167:MET:O     | 18:M:410:LMT:H3'  | 2.22                     | 0.40              |
| 4:H:119:ARG:O     | 4:H:234:TYR:HB2   | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:K:5:FME:HE2     | 15:O:502:BCL:H172 | 2.03                     | 0.40              |
| 7:U:7:LYS:HE2     | 7:U:7:LYS:HB3     | 1.87                     | 0.40              |
| 7:W:5:LEU:HD12    | 7:W:5:LEU:HA      | 1.92                     | 0.40              |
| 22:Y:101:CRT:H181 | 22:Y:101:CRT:H20  | 1.84                     | 0.40              |
| 15:3:101:BCL:H62  | 15:3:101:BCL:H41  | 1.54                     | 0.40              |
| 22:6:102:CRT:H5   | 22:6:102:CRT:H23  | 1.82                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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   | C     | 309/383 (81%)  | 297 (96%) | 12 (4%) | 0        | 100         | 100 |
| 2   | L     | 275/278 (99%)  | 268 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 3   | M     | 316/325 (97%)  | 311 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 4   | H     | 258/259 (100%) | 254 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 5   | 1     | 41/44 (93%)    | 41 (100%) | 0       | 0        | 100         | 100 |
| 5   | 5     | 41/44 (93%)    | 40 (98%)  | 0       | 1 (2%)   | 4           | 1   |
| 5   | 7     | 41/44 (93%)    | 41 (100%) | 0       | 0        | 100         | 100 |
| 5   | 9     | 41/44 (93%)    | 40 (98%)  | 0       | 1 (2%)   | 4           | 1   |
| 5   | A     | 41/44 (93%)    | 41 (100%) | 0       | 0        | 100         | 100 |
| 5   | I     | 41/44 (93%)    | 39 (95%)  | 2 (5%)  | 0        | 100         | 100 |
| 5   | K     | 42/44 (96%)    | 42 (100%) | 0       | 0        | 100         | 100 |
| 5   | O     | 42/44 (96%)    | 42 (100%) | 0       | 0        | 100         | 100 |
| 5   | Q     | 41/44 (93%)    | 39 (95%)  | 1 (2%)  | 1 (2%)   | 4           | 1   |
| 6   | 0     | 41/46 (89%)    | 41 (100%) | 0       | 0        | 100         | 100 |
| 6   | 2     | 39/46 (85%)    | 38 (97%)  | 1 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 6   | 4     | 40/46 (87%)     | 39 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 6   | 6     | 36/46 (78%)     | 36 (100%)  | 0       | 0        | 100         | 100 |
| 6   | 8     | 39/46 (85%)     | 37 (95%)   | 2 (5%)  | 0        | 100         | 100 |
| 6   | B     | 42/46 (91%)     | 41 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 6   | J     | 37/46 (80%)     | 37 (100%)  | 0       | 0        | 100         | 100 |
| 6   | N     | 36/46 (78%)     | 36 (100%)  | 0       | 0        | 100         | 100 |
| 6   | P     | 40/46 (87%)     | 40 (100%)  | 0       | 0        | 100         | 100 |
| 6   | R     | 38/46 (83%)     | 37 (97%)   | 1 (3%)  | 0        | 100         | 100 |
| 7   | D     | 47/64 (73%)     | 47 (100%)  | 0       | 0        | 100         | 100 |
| 7   | F     | 47/64 (73%)     | 47 (100%)  | 0       | 0        | 100         | 100 |
| 7   | S     | 48/64 (75%)     | 47 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 7   | U     | 49/64 (77%)     | 49 (100%)  | 0       | 0        | 100         | 100 |
| 7   | W     | 48/64 (75%)     | 48 (100%)  | 0       | 0        | 100         | 100 |
| 7   | Y     | 55/64 (86%)     | 52 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 8   | E     | 39/47 (83%)     | 39 (100%)  | 0       | 0        | 100         | 100 |
| 8   | G     | 38/47 (81%)     | 37 (97%)   | 1 (3%)  | 0        | 100         | 100 |
| 8   | T     | 39/47 (83%)     | 39 (100%)  | 0       | 0        | 100         | 100 |
| 8   | V     | 38/47 (81%)     | 38 (100%)  | 0       | 0        | 100         | 100 |
| 8   | X     | 39/47 (83%)     | 39 (100%)  | 0       | 0        | 100         | 100 |
| 8   | Z     | 39/47 (83%)     | 39 (100%)  | 0       | 0        | 100         | 100 |
| 9   | 3     | 61/66 (92%)     | 60 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| All | All   | 2504/2833 (88%) | 2458 (98%) | 43 (2%) | 3 (0%)   | 49          | 54  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | Q     | 6   | HIS  |
| 5   | 9     | 6   | HIS  |
| 5   | 5     | 6   | HIS  |

### 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   | C     | 265/311 (85%)  | 262 (99%) | 3 (1%)   | 65          | 74  |
| 2   | L     | 223/224 (100%) | 221 (99%) | 2 (1%)   | 70          | 78  |
| 3   | M     | 252/257 (98%)  | 250 (99%) | 2 (1%)   | 73          | 80  |
| 4   | H     | 206/206 (100%) | 200 (97%) | 6 (3%)   | 37          | 44  |
| 5   | 1     | 37/38 (97%)    | 36 (97%)  | 1 (3%)   | 39          | 47  |
| 5   | 5     | 36/38 (95%)    | 36 (100%) | 0        | 100         | 100 |
| 5   | 7     | 37/38 (97%)    | 37 (100%) | 0        | 100         | 100 |
| 5   | 9     | 37/38 (97%)    | 37 (100%) | 0        | 100         | 100 |
| 5   | A     | 37/38 (97%)    | 36 (97%)  | 1 (3%)   | 39          | 47  |
| 5   | I     | 37/38 (97%)    | 36 (97%)  | 1 (3%)   | 39          | 47  |
| 5   | K     | 38/38 (100%)   | 35 (92%)  | 3 (8%)   | 11          | 8   |
| 5   | O     | 38/38 (100%)   | 38 (100%) | 0        | 100         | 100 |
| 5   | Q     | 37/38 (97%)    | 37 (100%) | 0        | 100         | 100 |
| 6   | 0     | 36/38 (95%)    | 35 (97%)  | 1 (3%)   | 38          | 45  |
| 6   | 2     | 34/38 (90%)    | 34 (100%) | 0        | 100         | 100 |
| 6   | 4     | 35/38 (92%)    | 34 (97%)  | 1 (3%)   | 37          | 44  |
| 6   | 6     | 32/38 (84%)    | 32 (100%) | 0        | 100         | 100 |
| 6   | 8     | 34/38 (90%)    | 33 (97%)  | 1 (3%)   | 37          | 44  |
| 6   | B     | 37/38 (97%)    | 37 (100%) | 0        | 100         | 100 |
| 6   | J     | 32/38 (84%)    | 32 (100%) | 0        | 100         | 100 |
| 6   | N     | 32/38 (84%)    | 31 (97%)  | 1 (3%)   | 35          | 41  |
| 6   | P     | 35/38 (92%)    | 34 (97%)  | 1 (3%)   | 37          | 44  |
| 6   | R     | 33/38 (87%)    | 32 (97%)  | 1 (3%)   | 36          | 43  |
| 7   | D     | 43/55 (78%)    | 43 (100%) | 0        | 100         | 100 |
| 7   | F     | 43/55 (78%)    | 42 (98%)  | 1 (2%)   | 44          | 53  |
| 7   | S     | 43/55 (78%)    | 42 (98%)  | 1 (2%)   | 44          | 53  |
| 7   | U     | 44/55 (80%)    | 44 (100%) | 0        | 100         | 100 |
| 7   | W     | 43/55 (78%)    | 41 (95%)  | 2 (5%)   | 23          | 24  |
| 7   | Y     | 51/55 (93%)    | 50 (98%)  | 1 (2%)   | 48          | 58  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 8   | E     | 35/40 (88%)     | 34 (97%)   | 1 (3%)   | 37          | 44  |
| 8   | G     | 34/40 (85%)     | 34 (100%)  | 0        | 100         | 100 |
| 8   | T     | 35/40 (88%)     | 34 (97%)   | 1 (3%)   | 37          | 44  |
| 8   | V     | 34/40 (85%)     | 33 (97%)   | 1 (3%)   | 37          | 44  |
| 8   | X     | 35/40 (88%)     | 35 (100%)  | 0        | 100         | 100 |
| 8   | Z     | 35/40 (88%)     | 32 (91%)   | 3 (9%)   | 10          | 6   |
| 9   | 3     | 49/52 (94%)     | 48 (98%)   | 1 (2%)   | 48          | 58  |
| All | All   | 2144/2342 (92%) | 2107 (98%) | 37 (2%)  | 52          | 63  |

All (37) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 107 | CYS  |
| 1   | C     | 151 | THR  |
| 1   | C     | 304 | LYS  |
| 2   | L     | 22  | LEU  |
| 2   | L     | 203 | VAL  |
| 3   | M     | 216 | PHE  |
| 3   | M     | 312 | THR  |
| 4   | H     | 48  | ARG  |
| 4   | H     | 75  | THR  |
| 4   | H     | 76  | VAL  |
| 4   | H     | 138 | VAL  |
| 4   | H     | 191 | LYS  |
| 4   | H     | 237 | ASP  |
| 5   | A     | 11  | ILE  |
| 8   | E     | 11  | THR  |
| 7   | F     | 46  | GLU  |
| 5   | I     | 8   | ILE  |
| 5   | K     | 11  | ILE  |
| 5   | K     | 18  | LEU  |
| 5   | K     | 48  | SER  |
| 6   | N     | 24  | GLN  |
| 6   | P     | 23  | VAL  |
| 6   | R     | 27  | THR  |
| 7   | S     | 17  | ILE  |
| 8   | T     | 27  | THR  |
| 8   | V     | 23  | THR  |
| 7   | W     | 4   | ASP  |
| 7   | W     | 49  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | Y     | 58  | THR  |
| 8   | Z     | 11  | THR  |
| 8   | Z     | 28  | MET  |
| 8   | Z     | 33  | VAL  |
| 5   | 1     | 8   | ILE  |
| 9   | 3     | 5   | LEU  |
| 6   | 4     | 26  | MET  |
| 6   | 8     | 10  | LEU  |
| 6   | 0     | 10  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 78  | ASN  |
| 1   | C     | 184 | ASN  |
| 1   | C     | 206 | GLN  |
| 2   | L     | 207 | GLN  |
| 2   | L     | 219 | ASN  |
| 3   | M     | 74  | ASN  |
| 4   | H     | 71  | HIS  |
| 4   | H     | 178 | GLN  |
| 4   | H     | 192 | ASN  |
| 5   | A     | 6   | HIS  |
| 6   | B     | 4   | ASN  |
| 6   | B     | 13  | GLN  |
| 5   | I     | 10  | GLN  |
| 6   | J     | 24  | GLN  |
| 5   | K     | 6   | HIS  |
| 6   | N     | 19  | HIS  |
| 6   | P     | 24  | GLN  |
| 5   | Q     | 10  | GLN  |
| 6   | R     | 13  | GLN  |
| 6   | R     | 19  | HIS  |
| 6   | R     | 24  | GLN  |
| 5   | 1     | 6   | HIS  |
| 6   | 2     | 16  | GLN  |
| 6   | 8     | 16  | GLN  |
| 6   | 0     | 24  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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$ |
| 5   | FME  | 9     | 5   | 5    | 8,9,10       | 0.53 | 0           | 8,9,11      | 0.96 | 1 (12%)     |
| 5   | FME  | I     | 5   | 5    | 8,9,10       | 0.53 | 0           | 8,9,11      | 1.05 | 1 (12%)     |
| 4   | FME  | H     | 1   | 4    | 8,9,10       | 0.53 | 0           | 8,9,11      | 1.00 | 1 (12%)     |
| 5   | FME  | O     | 5   | 5    | 8,9,10       | 0.55 | 0           | 8,9,11      | 0.97 | 1 (12%)     |
| 5   | FME  | A     | 5   | 5    | 8,9,10       | 0.53 | 0           | 8,9,11      | 1.07 | 1 (12%)     |
| 5   | FME  | 1     | 5   | 5    | 8,9,10       | 0.56 | 0           | 8,9,11      | 0.79 | 1 (12%)     |
| 5   | FME  | 7     | 5   | 5    | 8,9,10       | 0.52 | 0           | 8,9,11      | 1.12 | 1 (12%)     |
| 5   | FME  | 5     | 5   | 5    | 8,9,10       | 0.56 | 0           | 8,9,11      | 0.91 | 1 (12%)     |
| 5   | FME  | Q     | 5   | 5    | 8,9,10       | 0.56 | 0           | 8,9,11      | 0.96 | 1 (12%)     |
| 5   | FME  | K     | 5   | 5    | 8,9,10       | 0.54 | 0           | 8,9,11      | 0.89 | 1 (12%)     |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 5   | FME  | 9     | 5   | 5    | -       | 0/7/9/11 | -     |
| 5   | FME  | I     | 5   | 5    | -       | 3/7/9/11 | -     |
| 4   | FME  | H     | 1   | 4    | -       | 0/7/9/11 | -     |
| 5   | FME  | O     | 5   | 5    | -       | 0/7/9/11 | -     |
| 5   | FME  | A     | 5   | 5    | -       | 0/7/9/11 | -     |
| 5   | FME  | 1     | 5   | 5    | -       | 2/7/9/11 | -     |
| 5   | FME  | 7     | 5   | 5    | -       | 1/7/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 5   | FME  | 5     | 5   | 5    | -       | 3/7/9/11 | -     |
| 5   | FME  | Q     | 5   | 5    | -       | 2/7/9/11 | -     |
| 5   | FME  | K     | 5   | 5    | -       | 3/7/9/11 | -     |

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | 7     | 5   | FME  | O-C-CA | -2.79 | 117.59      | 124.77   |
| 5   | I     | 5   | FME  | O-C-CA | -2.73 | 117.74      | 124.77   |
| 5   | A     | 5   | FME  | O-C-CA | -2.73 | 117.76      | 124.77   |
| 5   | 9     | 5   | FME  | O-C-CA | -2.55 | 118.22      | 124.77   |
| 5   | O     | 5   | FME  | O-C-CA | -2.53 | 118.27      | 124.77   |
| 5   | Q     | 5   | FME  | O-C-CA | -2.49 | 118.36      | 124.77   |
| 4   | H     | 1   | FME  | O-C-CA | -2.46 | 118.45      | 124.77   |
| 5   | K     | 5   | FME  | O-C-CA | -2.43 | 118.52      | 124.77   |
| 5   | 5     | 5   | FME  | O-C-CA | -2.38 | 118.65      | 124.77   |
| 5   | 1     | 5   | FME  | O-C-CA | -2.20 | 119.11      | 124.77   |

There are no chirality outliers.

All (14) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | I     | 5   | FME  | O-C-CA-CB   |
| 5   | K     | 5   | FME  | O1-CN-N-CA  |
| 5   | K     | 5   | FME  | CB-CA-N-CN  |
| 5   | Q     | 5   | FME  | O1-CN-N-CA  |
| 5   | Q     | 5   | FME  | CB-CA-N-CN  |
| 5   | 1     | 5   | FME  | O1-CN-N-CA  |
| 5   | 5     | 5   | FME  | O1-CN-N-CA  |
| 5   | 5     | 5   | FME  | N-CA-CB-CG  |
| 5   | 5     | 5   | FME  | C-CA-CB-CG  |
| 5   | I     | 5   | FME  | CA-CB-CG-SD |
| 5   | 7     | 5   | FME  | C-CA-CB-CG  |
| 5   | K     | 5   | FME  | N-CA-CB-CG  |
| 5   | 1     | 5   | FME  | N-CA-CB-CG  |
| 5   | I     | 5   | FME  | C-CA-CB-CG  |

There are no ring outliers.

3 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | 9     | 5   | FME  | 1       | 0            |
| 5   | 5     | 5   | FME  | 1       | 0            |
| 5   | K     | 5   | FME  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 8 are monoatomic - leaving 105 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 | $\# Z  > 2$ |
| 17  | UQ8  | L     | 303 | -    | 33,33,53     | 1.51 | 2 (6%)      | 42,43,67    | 1.68 | 10 (23%)    |
| 15  | BCL  | K     | 102 | -    | 69,74,74     | 1.78 | 18 (26%)    | 79,115,115  | 2.27 | 24 (30%)    |
| 15  | BCL  | 5     | 102 | -    | 69,74,74     | 1.78 | 17 (24%)    | 79,115,115  | 2.26 | 23 (29%)    |
| 18  | LMT  | G     | 101 | -    | 36,36,36     | 0.44 | 0           | 47,47,47    | 0.84 | 1 (2%)      |
| 19  | CDL  | M     | 409 | -    | 94,94,99     | 0.94 | 4 (4%)      | 100,106,111 | 1.10 | 8 (8%)      |
| 18  | LMT  | Z     | 101 | -    | 36,36,36     | 0.39 | 0           | 47,47,47    | 0.91 | 3 (6%)      |
| 22  | CRT  | 6     | 102 | -    | 43,43,43     | 0.62 | 0           | 48,54,54    | 2.04 | 15 (31%)    |
| 22  | CRT  | E     | 103 | -    | 43,43,43     | 0.60 | 0           | 48,54,54    | 2.25 | 17 (35%)    |
| 18  | LMT  | 2     | 101 | -    | 36,36,36     | 0.41 | 0           | 47,47,47    | 0.90 | 2 (4%)      |
| 14  | PGV  | L     | 305 | -    | 28,28,50     | 1.24 | 2 (7%)      | 31,34,56    | 1.33 | 4 (12%)     |
| 15  | BCL  | N     | 101 | -    | 69,74,74     | 1.76 | 16 (23%)    | 79,115,115  | 2.21 | 23 (29%)    |
| 22  | CRT  | Z     | 103 | -    | 43,43,43     | 0.65 | 0           | 48,54,54    | 1.96 | 12 (25%)    |
| 18  | LMT  | M     | 410 | -    | 36,36,36     | 0.41 | 0           | 47,47,47    | 0.80 | 1 (2%)      |
| 15  | BCL  | O     | 502 | -    | 69,74,74     | 1.77 | 17 (24%)    | 79,115,115  | 2.24 | 22 (27%)    |
| 18  | LMT  | P     | 104 | -    | 36,36,36     | 0.38 | 0           | 47,47,47    | 0.69 | 1 (2%)      |
| 17  | UQ8  | L     | 309 | -    | 53,53,53     | 1.27 | 2 (3%)      | 66,67,67    | 1.56 | 15 (22%)    |
| 15  | BCL  | U     | 101 | -    | 69,74,74     | 1.78 | 17 (24%)    | 79,115,115  | 2.29 | 21 (26%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 10  | HEM  | C     | 404 | 1    | 50,50,50     | 1.60 | 8 (16%)  | 67,82,82    | 1.58 | 11 (16%) |
| 19  | CDL  | H     | 302 | -    | 78,78,99     | 1.02 | 4 (5%)   | 84,90,111   | 1.08 | 5 (5%)   |
| 18  | LMT  | T     | 103 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.84 | 1 (2%)   |
| 19  | CDL  | M     | 407 | -    | 38,38,99     | 1.30 | 3 (7%)   | 43,49,111   | 1.21 | 5 (11%)  |
| 10  | HEM  | C     | 401 | 1    | 50,50,50     | 1.58 | 8 (16%)  | 67,82,82    | 1.65 | 13 (19%) |
| 15  | BCL  | 3     | 101 | -    | 69,74,74     | 1.77 | 18 (26%) | 79,115,115  | 2.25 | 23 (29%) |
| 12  | Z41  | C     | 406 | -    | 34,34,39     | 0.28 | 0        | 36,36,41    | 0.29 | 0        |
| 14  | PGV  | L     | 310 | -    | 36,36,50     | 1.07 | 2 (5%)   | 39,42,56    | 1.15 | 3 (7%)   |
| 18  | LMT  | 5     | 101 | -    | 32,32,36     | 0.41 | 0        | 43,43,47    | 1.31 | 5 (11%)  |
| 18  | LMT  | 8     | 103 | -    | 36,36,36     | 0.43 | 0        | 47,47,47    | 0.88 | 1 (2%)   |
| 18  | LMT  | L     | 307 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.80 | 1 (2%)   |
| 14  | PGV  | L     | 306 | -    | 34,34,50     | 1.09 | 2 (5%)   | 37,40,56    | 1.06 | 2 (5%)   |
| 18  | LMT  | S     | 101 | -    | 27,27,36     | 0.60 | 0        | 38,38,47    | 1.33 | 4 (10%)  |
| 15  | BCL  | 1     | 402 | -    | 69,74,74     | 1.79 | 17 (24%) | 79,115,115  | 2.22 | 23 (29%) |
| 22  | CRT  | N     | 102 | -    | 43,43,43     | 0.66 | 0        | 48,54,54    | 2.14 | 15 (31%) |
| 18  | LMT  | E     | 101 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.74 | 1 (2%)   |
| 18  | LMT  | 8     | 101 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.77 | 1 (2%)   |
| 22  | CRT  | R     | 102 | -    | 43,43,43     | 0.62 | 0        | 48,54,54    | 2.00 | 14 (29%) |
| 15  | BCL  | D     | 102 | -    | 69,74,74     | 1.77 | 17 (24%) | 79,115,115  | 2.22 | 24 (30%) |
| 15  | BCL  | L     | 301 | -    | 69,74,74     | 1.75 | 15 (21%) | 79,115,115  | 2.17 | 23 (29%) |
| 22  | CRT  | G     | 103 | -    | 43,43,43     | 0.69 | 0        | 48,54,54    | 1.86 | 12 (25%) |
| 18  | LMT  | 4     | 104 | -    | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.80 | 1 (2%)   |
| 19  | CDL  | L     | 311 | -    | 79,79,99     | 1.08 | 4 (5%)   | 85,91,111   | 1.13 | 6 (7%)   |
| 13  | PLM  | C     | 407 | 1    | 10,11,17     | 0.35 | 0        | 9,10,17     | 0.36 | 0        |
| 14  | PGV  | A     | 501 | -    | 38,38,50     | 1.02 | 2 (5%)   | 41,44,56    | 1.21 | 3 (7%)   |
| 15  | BCL  | Q     | 102 | -    | 69,74,74     | 1.76 | 17 (24%) | 79,115,115  | 2.27 | 22 (27%) |
| 18  | LMT  | M     | 411 | -    | 25,25,36     | 0.48 | 0        | 36,36,47    | 0.86 | 1 (2%)   |
| 15  | BCL  | 7     | 101 | -    | 64,69,74     | 1.83 | 17 (26%) | 73,109,115  | 2.29 | 23 (31%) |
| 22  | CRT  | 9     | 101 | -    | 43,43,43     | 0.65 | 0        | 48,54,54    | 1.99 | 16 (33%) |
| 18  | LMT  | P     | 101 | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.74 | 1 (2%)   |
| 15  | BCL  | M     | 402 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.19 | 24 (30%) |
| 15  | BCL  | Y     | 102 | -    | 69,74,74     | 1.77 | 18 (26%) | 79,115,115  | 2.27 | 22 (27%) |
| 24  | LDA  | K     | 101 | -    | 13,15,15     | 2.24 | 2 (15%)  | 14,17,17    | 0.52 | 0        |
| 18  | LMT  | J     | 104 | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.71 | 1 (2%)   |
| 21  | MQ8  | M     | 405 | -    | 54,54,54     | 1.36 | 2 (3%)   | 67,69,69    | 1.57 | 15 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | PGV  | H     | 301 | -    | 35,35,50     | 1.10 | 2 (5%)   | 38,41,56    | 1.41 | 4 (10%)  |
| 14  | PGV  | F     | 501 | -    | 30,30,50     | 1.23 | 2 (6%)   | 33,35,56    | 1.36 | 4 (12%)  |
| 15  | BCL  | M     | 403 | -    | 69,74,74     | 1.78 | 17 (24%) | 79,115,115  | 2.32 | 26 (32%) |
| 15  | BCL  | O     | 101 | -    | 69,74,74     | 1.75 | 15 (21%) | 79,115,115  | 2.16 | 22 (27%) |
| 15  | BCL  | Z     | 102 | -    | 69,74,74     | 1.77 | 16 (23%) | 79,115,115  | 2.21 | 21 (26%) |
| 15  | BCL  | B     | 102 | -    | 69,74,74     | 1.77 | 17 (24%) | 79,115,115  | 2.19 | 24 (30%) |
| 15  | BCL  | I     | 101 | -    | 69,74,74     | 1.80 | 17 (24%) | 79,115,115  | 2.26 | 22 (27%) |
| 18  | LMT  | 4     | 101 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.76 | 1 (2%)   |
| 22  | CRT  | O     | 102 | -    | 43,43,43     | 0.64 | 0        | 48,54,54    | 2.07 | 17 (35%) |
| 16  | BPH  | L     | 302 | -    | 59,70,70     | 0.82 | 3 (5%)   | 59,101,101  | 0.93 | 3 (5%)   |
| 15  | BCL  | 8     | 102 | -    | 69,74,74     | 1.75 | 15 (21%) | 79,115,115  | 2.16 | 24 (30%) |
| 18  | LMT  | B     | 101 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.76 | 1 (2%)   |
| 22  | CRT  | 4     | 103 | -    | 43,43,43     | 0.68 | 0        | 48,54,54    | 2.13 | 15 (31%) |
| 14  | PGV  | Q     | 101 | -    | 23,23,50     | 1.40 | 2 (8%)   | 26,28,56    | 1.30 | 3 (11%)  |
| 22  | CRT  | Y     | 101 | -    | 43,43,43     | 0.65 | 0        | 48,54,54    | 1.94 | 11 (22%) |
| 18  | LMT  | H     | 303 | -    | 36,36,36     | 0.43 | 0        | 47,47,47    | 0.80 | 2 (4%)   |
| 15  | BCL  | R     | 101 | -    | 69,74,74     | 1.77 | 17 (24%) | 79,115,115  | 2.10 | 23 (29%) |
| 15  | BCL  | X     | 102 | -    | 69,74,74     | 1.77 | 16 (23%) | 79,115,115  | 2.20 | 26 (32%) |
| 15  | BCL  | 2     | 102 | -    | 69,74,74     | 1.77 | 16 (23%) | 79,115,115  | 2.16 | 25 (31%) |
| 22  | CRT  | J     | 103 | -    | 43,43,43     | 0.67 | 0        | 48,54,54    | 2.18 | 15 (31%) |
| 10  | HEM  | C     | 402 | 1    | 50,50,50     | 1.59 | 8 (16%)  | 67,82,82    | 1.60 | 12 (17%) |
| 15  | BCL  | S     | 102 | -    | 69,74,74     | 1.77 | 16 (23%) | 79,115,115  | 2.24 | 22 (27%) |
| 15  | BCL  | T     | 101 | -    | 69,74,74     | 1.76 | 16 (23%) | 79,115,115  | 2.15 | 25 (31%) |
| 15  | BCL  | F     | 502 | -    | 69,74,74     | 1.78 | 17 (24%) | 79,115,115  | 2.24 | 22 (27%) |
| 17  | UQ8  | L     | 304 | -    | 53,53,53     | 1.24 | 2 (3%)   | 66,67,67    | 1.90 | 20 (30%) |
| 14  | PGV  | M     | 408 | -    | 26,26,50     | 1.29 | 2 (7%)   | 29,31,56    | 1.39 | 5 (17%)  |
| 15  | BCL  | 6     | 101 | -    | 69,74,74     | 1.76 | 17 (24%) | 79,115,115  | 2.22 | 22 (27%) |
| 15  | BCL  | G     | 102 | -    | 69,74,74     | 1.77 | 16 (23%) | 79,115,115  | 2.19 | 25 (31%) |
| 15  | BCL  | V     | 101 | -    | 69,74,74     | 1.76 | 16 (23%) | 79,115,115  | 2.20 | 23 (29%) |
| 15  | BCL  | J     | 102 | -    | 69,74,74     | 1.77 | 17 (24%) | 79,115,115  | 2.16 | 22 (27%) |
| 22  | CRT  | P     | 103 | -    | 43,43,43     | 0.68 | 0        | 48,54,54    | 2.16 | 14 (29%) |
| 16  | BPH  | M     | 404 | -    | 59,70,70     | 0.76 | 3 (5%)   | 59,101,101  | 0.90 | 3 (5%)   |
| 15  | BCL  | 4     | 102 | -    | 69,74,74     | 1.76 | 17 (24%) | 79,115,115  | 2.17 | 23 (29%) |
| 22  | CRT  | T     | 102 | -    | 43,43,43     | 0.61 | 0        | 48,54,54    | 2.01 | 15 (31%) |
| 15  | BCL  | P     | 102 | -    | 69,74,74     | 1.74 | 15 (21%) | 79,115,115  | 2.18 | 25 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | BCL  | L     | 308 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.16 | 23 (29%) |
| 14  | PGV  | C     | 408 | -    | 30,30,50     | 1.17 | 2 (6%)   | 33,36,56    | 1.11 | 4 (12%)  |
| 15  | BCL  | 9     | 102 | -    | 69,74,74     | 1.76 | 16 (23%) | 79,115,115  | 2.24 | 23 (29%) |
| 19  | CDL  | D     | 101 | -    | 57,57,99     | 1.12 | 4 (7%)   | 63,69,111   | 1.15 | 3 (4%)   |
| 18  | LMT  | R     | 103 | -    | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.72 | 1 (2%)   |
| 22  | CRT  | V     | 102 | -    | 43,43,43     | 0.65 | 0        | 48,54,54    | 2.26 | 19 (39%) |
| 22  | CRT  | 2     | 103 | -    | 43,43,43     | 0.72 | 0        | 48,54,54    | 2.09 | 10 (20%) |
| 10  | HEM  | C     | 403 | 1    | 50,50,50     | 1.61 | 9 (18%)  | 67,82,82    | 1.61 | 12 (17%) |
| 14  | PGV  | 1     | 401 | -    | 26,26,50     | 1.25 | 2 (7%)   | 29,31,56    | 1.25 | 4 (13%)  |
| 18  | LMT  | X     | 101 | -    | 36,36,36     | 0.45 | 0        | 47,47,47    | 0.85 | 1 (2%)   |
| 24  | LDA  | O     | 501 | -    | 13,15,15     | 2.25 | 2 (15%)  | 14,17,17    | 0.50 | 0        |
| 14  | PGV  | A     | 503 | -    | 32,32,50     | 1.14 | 2 (6%)   | 35,38,56    | 1.19 | 4 (11%)  |
| 15  | BCL  | A     | 502 | -    | 69,74,74     | 1.78 | 16 (23%) | 79,115,115  | 2.20 | 22 (27%) |
| 22  | CRT  | M     | 406 | -    | 43,43,43     | 0.60 | 0        | 48,54,54    | 2.21 | 14 (29%) |
| 22  | CRT  | B     | 103 | -    | 43,43,43     | 0.61 | 0        | 48,54,54    | 2.00 | 17 (35%) |
| 15  | BCL  | E     | 102 | -    | 69,74,74     | 1.77 | 16 (23%) | 79,115,115  | 2.19 | 23 (29%) |
| 15  | BCL  | W     | 101 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.24 | 23 (29%) |
| 18  | LMT  | J     | 101 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.72 | 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   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 17  | UQ8  | L     | 303 | -    | -       | 2/27/51/75     | 0/1/1/1 |
| 15  | BCL  | K     | 102 | -    | -       | 9/41/137/137   | -       |
| 15  | BCL  | 5     | 102 | -    | -       | 14/41/137/137  | -       |
| 18  | LMT  | G     | 101 | -    | -       | 5/21/61/61     | 0/2/2/2 |
| 19  | CDL  | M     | 409 | -    | -       | 30/105/105/110 | -       |
| 18  | LMT  | Z     | 101 | -    | -       | 4/21/61/61     | 0/2/2/2 |
| 22  | CRT  | 6     | 102 | -    | -       | 8/51/51/51     | -       |
| 22  | CRT  | E     | 103 | -    | -       | 7/51/51/51     | -       |
| 18  | LMT  | 2     | 101 | -    | -       | 4/21/61/61     | 0/2/2/2 |
| 14  | PGV  | L     | 305 | -    | -       | 11/33/33/55    | -       |
| 15  | BCL  | N     | 101 | -    | -       | 15/41/137/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 22  | CRT  | Z     | 103 | -    | -       | 14/51/51/51   | -       |
| 18  | LMT  | M     | 410 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 15  | BCL  | O     | 502 | -    | -       | 14/41/137/137 | -       |
| 18  | LMT  | P     | 104 | -    | -       | 1/21/61/61    | 0/2/2/2 |
| 17  | UQ8  | L     | 309 | -    | -       | 15/51/75/75   | 0/1/1/1 |
| 15  | BCL  | U     | 101 | -    | -       | 20/41/137/137 | -       |
| 10  | HEM  | C     | 404 | 1    | -       | 5/14/54/54    | -       |
| 19  | CDL  | H     | 302 | -    | -       | 23/89/89/110  | -       |
| 18  | LMT  | T     | 103 | -    | -       | 10/21/61/61   | 0/2/2/2 |
| 19  | CDL  | M     | 407 | -    | -       | 15/48/48/110  | -       |
| 10  | HEM  | C     | 401 | 1    | -       | 6/14/54/54    | -       |
| 15  | BCL  | 3     | 101 | -    | -       | 9/41/137/137  | -       |
| 12  | Z41  | C     | 406 | -    | -       | 6/35/35/41    | -       |
| 14  | PGV  | L     | 310 | -    | -       | 19/41/41/55   | -       |
| 18  | LMT  | 5     | 101 | -    | -       | 5/17/57/61    | 0/2/2/2 |
| 18  | LMT  | 8     | 103 | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 18  | LMT  | L     | 307 | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 14  | PGV  | L     | 306 | -    | -       | 8/39/39/55    | -       |
| 18  | LMT  | S     | 101 | -    | -       | 3/12/52/61    | 0/2/2/2 |
| 15  | BCL  | 1     | 402 | -    | -       | 9/41/137/137  | -       |
| 22  | CRT  | N     | 102 | -    | -       | 8/51/51/51    | -       |
| 18  | LMT  | E     | 101 | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 18  | LMT  | 8     | 101 | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 22  | CRT  | R     | 102 | -    | -       | 1/51/51/51    | -       |
| 15  | BCL  | D     | 102 | -    | -       | 13/41/137/137 | -       |
| 15  | BCL  | L     | 301 | -    | -       | 8/41/137/137  | -       |
| 22  | CRT  | G     | 103 | -    | -       | 9/51/51/51    | -       |
| 18  | LMT  | 4     | 104 | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 19  | CDL  | L     | 311 | -    | -       | 26/89/89/110  | -       |
| 13  | PLM  | C     | 407 | 1    | -       | 1/9/9/15      | -       |
| 14  | PGV  | A     | 501 | -    | -       | 12/43/43/55   | -       |
| 15  | BCL  | Q     | 102 | -    | -       | 17/41/137/137 | -       |
| 18  | LMT  | M     | 411 | -    | -       | 3/10/50/61    | 0/2/2/2 |
| 15  | BCL  | 7     | 101 | -    | -       | 11/35/131/137 | -       |
| 22  | CRT  | 9     | 101 | -    | -       | 3/51/51/51    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 18  | LMT  | P     | 101 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 15  | BCL  | M     | 402 | -    | -       | 5/41/137/137  | -       |
| 15  | BCL  | Y     | 102 | -    | -       | 14/41/137/137 | -       |
| 24  | LDA  | K     | 101 | -    | -       | 2/13/13/13    | -       |
| 18  | LMT  | J     | 104 | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 21  | MQ8  | M     | 405 | -    | -       | 4/47/67/67    | 0/2/2/2 |
| 14  | PGV  | H     | 301 | -    | -       | 12/40/40/55   | -       |
| 14  | PGV  | F     | 501 | -    | -       | 12/32/32/55   | -       |
| 15  | BCL  | M     | 403 | -    | -       | 5/41/137/137  | -       |
| 15  | BCL  | O     | 101 | -    | -       | 17/41/137/137 | -       |
| 15  | BCL  | Z     | 102 | -    | -       | 15/41/137/137 | -       |
| 15  | BCL  | B     | 102 | -    | -       | 11/41/137/137 | -       |
| 15  | BCL  | I     | 101 | -    | -       | 12/41/137/137 | -       |
| 18  | LMT  | 4     | 101 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 22  | CRT  | O     | 102 | -    | -       | 2/51/51/51    | -       |
| 16  | BPH  | L     | 302 | -    | -       | 5/37/105/105  | 0/5/6/6 |
| 15  | BCL  | 8     | 102 | -    | -       | 15/41/137/137 | -       |
| 18  | LMT  | B     | 101 | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 22  | CRT  | 4     | 103 | -    | -       | 5/51/51/51    | -       |
| 14  | PGV  | Q     | 101 | -    | -       | 9/25/25/55    | -       |
| 22  | CRT  | Y     | 101 | -    | -       | 2/51/51/51    | -       |
| 18  | LMT  | H     | 303 | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 15  | BCL  | R     | 101 | -    | -       | 13/41/137/137 | -       |
| 15  | BCL  | X     | 102 | -    | -       | 15/41/137/137 | -       |
| 15  | BCL  | 2     | 102 | -    | -       | 15/41/137/137 | -       |
| 22  | CRT  | J     | 103 | -    | -       | 10/51/51/51   | -       |
| 10  | HEM  | C     | 402 | 1    | -       | 7/14/54/54    | -       |
| 15  | BCL  | S     | 102 | -    | -       | 12/41/137/137 | -       |
| 15  | BCL  | T     | 101 | -    | -       | 15/41/137/137 | -       |
| 15  | BCL  | F     | 502 | -    | -       | 16/41/137/137 | -       |
| 17  | UQ8  | L     | 304 | -    | -       | 7/51/75/75    | 0/1/1/1 |
| 14  | PGV  | M     | 408 | -    | -       | 8/28/28/55    | -       |
| 15  | BCL  | 6     | 101 | -    | -       | 20/41/137/137 | -       |
| 15  | BCL  | G     | 102 | -    | -       | 17/41/137/137 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 15  | BCL  | V     | 101 | -    | -       | 18/41/137/137 | -       |
| 15  | BCL  | J     | 102 | -    | -       | 18/41/137/137 | -       |
| 22  | CRT  | P     | 103 | -    | -       | 7/51/51/51    | -       |
| 16  | BPH  | M     | 404 | -    | -       | 7/37/105/105  | 0/5/6/6 |
| 15  | BCL  | 4     | 102 | -    | -       | 15/41/137/137 | -       |
| 22  | CRT  | T     | 102 | -    | -       | 9/51/51/51    | -       |
| 15  | BCL  | P     | 102 | -    | -       | 15/41/137/137 | -       |
| 15  | BCL  | L     | 308 | -    | -       | 12/41/137/137 | -       |
| 14  | PGV  | C     | 408 | -    | -       | 8/35/35/55    | -       |
| 15  | BCL  | 9     | 102 | -    | -       | 11/41/137/137 | -       |
| 19  | CDL  | D     | 101 | -    | -       | 27/67/67/110  | -       |
| 18  | LMT  | R     | 103 | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 22  | CRT  | V     | 102 | -    | -       | 5/51/51/51    | -       |
| 22  | CRT  | 2     | 103 | -    | -       | 7/51/51/51    | -       |
| 10  | HEM  | C     | 403 | 1    | -       | 4/14/54/54    | -       |
| 14  | PGV  | 1     | 401 | -    | -       | 9/30/30/55    | -       |
| 18  | LMT  | X     | 101 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 24  | LDA  | O     | 501 | -    | -       | 2/13/13/13    | -       |
| 14  | PGV  | A     | 503 | -    | -       | 14/37/37/55   | -       |
| 15  | BCL  | A     | 502 | -    | -       | 12/41/137/137 | -       |
| 22  | CRT  | M     | 406 | -    | -       | 8/51/51/51    | -       |
| 22  | CRT  | B     | 103 | -    | -       | 4/51/51/51    | -       |
| 15  | BCL  | E     | 102 | -    | -       | 14/41/137/137 | -       |
| 15  | BCL  | W     | 101 | -    | -       | 14/41/137/137 | -       |
| 18  | LMT  | J     | 101 | -    | -       | 2/21/61/61    | 0/2/2/2 |

All (691) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 21  | M     | 405 | MQ8  | C3-C2 | 8.20  | 1.49        | 1.35     |
| 17  | L     | 309 | UQ8  | C6-C1 | 7.83  | 1.49        | 1.35     |
| 17  | L     | 304 | UQ8  | C6-C1 | 7.63  | 1.48        | 1.35     |
| 17  | L     | 303 | UQ8  | C6-C1 | 7.57  | 1.48        | 1.35     |
| 24  | O     | 501 | LDA  | O1-N1 | -6.98 | 1.25        | 1.42     |
| 24  | K     | 101 | LDA  | O1-N1 | -6.91 | 1.25        | 1.42     |
| 10  | C     | 404 | HEM  | FE-NB | 5.39  | 2.11        | 1.94     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | C     | 403 | HEM  | FE-NB   | 5.36  | 2.11        | 1.94     |
| 10  | C     | 402 | HEM  | FE-NB   | 5.33  | 2.11        | 1.94     |
| 10  | C     | 401 | HEM  | FE-NB   | 5.22  | 2.11        | 1.94     |
| 15  | L     | 301 | BCL  | O2D-CGD | 5.17  | 1.45        | 1.33     |
| 15  | T     | 101 | BCL  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 15  | 2     | 102 | BCL  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 19  | L     | 311 | CDL  | OA6-CA5 | 5.04  | 1.46        | 1.35     |
| 15  | 0     | 101 | BCL  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 15  | B     | 102 | BCL  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 15  | 3     | 101 | BCL  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 15  | 1     | 402 | BCL  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 15  | R     | 101 | BCL  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 15  | I     | 101 | BCL  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 15  | X     | 102 | BCL  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 15  | 6     | 101 | BCL  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 15  | W     | 101 | BCL  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 15  | J     | 102 | BCL  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 15  | O     | 502 | BCL  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 15  | V     | 101 | BCL  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 15  | 8     | 102 | BCL  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 15  | U     | 101 | BCL  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 15  | D     | 102 | BCL  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 15  | F     | 502 | BCL  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 15  | A     | 502 | BCL  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 15  | 7     | 101 | BCL  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 15  | 9     | 102 | BCL  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 15  | 4     | 102 | BCL  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 15  | 5     | 102 | BCL  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 15  | M     | 402 | BCL  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 15  | Q     | 102 | BCL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 15  | G     | 102 | BCL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 15  | S     | 102 | BCL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 15  | E     | 102 | BCL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 15  | Z     | 102 | BCL  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 15  | N     | 101 | BCL  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 21  | M     | 405 | MQ8  | C10-C5  | 4.90  | 1.48        | 1.40     |
| 15  | K     | 102 | BCL  | O2D-CGD | 4.88  | 1.45        | 1.33     |
| 15  | M     | 403 | BCL  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 15  | P     | 102 | BCL  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 15  | Y     | 102 | BCL  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 15  | L     | 308 | BCL  | C3D-C4D | -4.81 | 1.33        | 1.44     |
| 15  | M     | 403 | BCL  | C3D-C4D | -4.73 | 1.33        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | 9     | 102 | BCL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 15  | I     | 101 | BCL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 15  | U     | 101 | BCL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 15  | K     | 102 | BCL  | C3D-C4D | -4.69 | 1.33        | 1.44     |
| 15  | Y     | 102 | BCL  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 15  | M     | 402 | BCL  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 15  | S     | 102 | BCL  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 15  | 4     | 102 | BCL  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 15  | L     | 301 | BCL  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 15  | L     | 308 | BCL  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 15  | 3     | 101 | BCL  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 15  | B     | 102 | BCL  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 15  | 2     | 102 | BCL  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 15  | 1     | 402 | BCL  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 15  | 7     | 101 | BCL  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 15  | O     | 502 | BCL  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 15  | F     | 502 | BCL  | C3D-C4D | -4.59 | 1.33        | 1.44     |
| 15  | A     | 502 | BCL  | C3D-C4D | -4.58 | 1.33        | 1.44     |
| 15  | Q     | 102 | BCL  | C3D-C4D | -4.58 | 1.33        | 1.44     |
| 15  | 5     | 102 | BCL  | C3D-C4D | -4.58 | 1.33        | 1.44     |
| 15  | W     | 101 | BCL  | C3D-C4D | -4.56 | 1.33        | 1.44     |
| 15  | R     | 101 | BCL  | C3D-C4D | -4.56 | 1.33        | 1.44     |
| 15  | 6     | 101 | BCL  | C3D-C4D | -4.56 | 1.33        | 1.44     |
| 15  | E     | 102 | BCL  | C3D-C4D | -4.56 | 1.33        | 1.44     |
| 15  | D     | 102 | BCL  | C3D-C4D | -4.55 | 1.33        | 1.44     |
| 15  | T     | 101 | BCL  | C3D-C4D | -4.55 | 1.33        | 1.44     |
| 15  | Z     | 102 | BCL  | C3D-C4D | -4.55 | 1.33        | 1.44     |
| 15  | J     | 102 | BCL  | C3D-C4D | -4.54 | 1.34        | 1.44     |
| 15  | 8     | 102 | BCL  | C3D-C4D | -4.54 | 1.34        | 1.44     |
| 15  | G     | 102 | BCL  | C3D-C4D | -4.51 | 1.34        | 1.44     |
| 15  | V     | 101 | BCL  | C3D-C4D | -4.51 | 1.34        | 1.44     |
| 15  | P     | 102 | BCL  | C3D-C4D | -4.50 | 1.34        | 1.44     |
| 15  | X     | 102 | BCL  | C3D-C4D | -4.50 | 1.34        | 1.44     |
| 15  | 0     | 101 | BCL  | C3D-C4D | -4.50 | 1.34        | 1.44     |
| 15  | N     | 101 | BCL  | C3D-C4D | -4.50 | 1.34        | 1.44     |
| 15  | 4     | 102 | BCL  | O2A-CGA | 4.38  | 1.46        | 1.33     |
| 15  | M     | 402 | BCL  | O2A-CGA | 4.38  | 1.46        | 1.33     |
| 14  | L     | 305 | PGV  | O03-C19 | 4.37  | 1.46        | 1.33     |
| 15  | 9     | 102 | BCL  | O2A-CGA | 4.35  | 1.46        | 1.33     |
| 15  | W     | 101 | BCL  | O2A-CGA | 4.34  | 1.46        | 1.33     |
| 15  | O     | 502 | BCL  | O2A-CGA | 4.33  | 1.46        | 1.33     |
| 14  | M     | 408 | PGV  | O03-C19 | 4.31  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | Q     | 101 | PGV  | O03-C19 | 4.31 | 1.45        | 1.33     |
| 19  | D     | 101 | CDL  | OB8-CB7 | 4.31 | 1.45        | 1.33     |
| 10  | C     | 402 | HEM  | FE-NC   | 4.31 | 2.09        | 1.95     |
| 14  | F     | 501 | PGV  | O03-C19 | 4.30 | 1.45        | 1.33     |
| 19  | M     | 407 | CDL  | OA8-CA7 | 4.30 | 1.45        | 1.33     |
| 14  | Q     | 101 | PGV  | O01-C1  | 4.30 | 1.46        | 1.34     |
| 15  | I     | 402 | BCL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 10  | C     | 401 | HEM  | FE-NC   | 4.29 | 2.09        | 1.95     |
| 14  | H     | 301 | PGV  | O03-C19 | 4.28 | 1.45        | 1.33     |
| 15  | D     | 102 | BCL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 15  | K     | 102 | BCL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 15  | F     | 502 | BCL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 19  | M     | 407 | CDL  | OA6-CA5 | 4.26 | 1.46        | 1.34     |
| 15  | Z     | 102 | BCL  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 15  | S     | 102 | BCL  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 15  | N     | 101 | BCL  | O2A-CGA | 4.25 | 1.45        | 1.33     |
| 15  | E     | 102 | BCL  | O2A-CGA | 4.25 | 1.45        | 1.33     |
| 19  | M     | 409 | CDL  | OA8-CA7 | 4.25 | 1.45        | 1.33     |
| 14  | L     | 310 | PGV  | O03-C19 | 4.25 | 1.45        | 1.33     |
| 15  | 6     | 101 | BCL  | O2A-CGA | 4.25 | 1.45        | 1.33     |
| 19  | L     | 311 | CDL  | OB8-CB7 | 4.24 | 1.45        | 1.33     |
| 15  | T     | 101 | BCL  | O2A-CGA | 4.24 | 1.45        | 1.33     |
| 15  | I     | 101 | BCL  | C3B-C4B | 4.24 | 1.49        | 1.41     |
| 15  | X     | 102 | BCL  | O2A-CGA | 4.24 | 1.45        | 1.33     |
| 15  | G     | 102 | BCL  | O2A-CGA | 4.23 | 1.45        | 1.33     |
| 10  | C     | 404 | HEM  | FE-NC   | 4.23 | 2.09        | 1.95     |
| 14  | A     | 503 | PGV  | O03-C19 | 4.22 | 1.45        | 1.33     |
| 15  | A     | 502 | BCL  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 19  | M     | 409 | CDL  | OA6-CA5 | 4.22 | 1.46        | 1.34     |
| 15  | R     | 101 | BCL  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 14  | C     | 408 | PGV  | O03-C19 | 4.21 | 1.45        | 1.33     |
| 15  | L     | 308 | BCL  | O2A-CGA | 4.19 | 1.45        | 1.33     |
| 14  | L     | 306 | PGV  | O03-C19 | 4.19 | 1.45        | 1.33     |
| 15  | B     | 102 | BCL  | O2A-CGA | 4.19 | 1.45        | 1.33     |
| 15  | 3     | 101 | BCL  | O2A-CGA | 4.19 | 1.45        | 1.33     |
| 15  | V     | 101 | BCL  | O2A-CGA | 4.19 | 1.45        | 1.33     |
| 15  | 2     | 102 | BCL  | O2A-CGA | 4.18 | 1.45        | 1.33     |
| 19  | L     | 311 | CDL  | OA8-CA7 | 4.18 | 1.45        | 1.33     |
| 15  | L     | 301 | BCL  | O2A-CGA | 4.17 | 1.45        | 1.33     |
| 15  | J     | 102 | BCL  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 15  | U     | 101 | BCL  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 15  | Y     | 102 | BCL  | O2A-CGA | 4.15 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | D     | 101 | CDL  | OA6-CA5 | 4.15  | 1.46        | 1.34     |
| 14  | F     | 501 | PGV  | O01-C1  | 4.15  | 1.46        | 1.34     |
| 14  | 1     | 401 | PGV  | O03-C19 | 4.14  | 1.45        | 1.33     |
| 14  | A     | 501 | PGV  | O01-C1  | 4.14  | 1.46        | 1.34     |
| 15  | P     | 102 | BCL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 19  | H     | 302 | CDL  | OA6-CA5 | 4.14  | 1.46        | 1.34     |
| 24  | K     | 101 | LDA  | C1-N1   | -4.13 | 1.47        | 1.51     |
| 15  | M     | 403 | BCL  | O2A-CGA | 4.13  | 1.45        | 1.33     |
| 19  | M     | 407 | CDL  | OB6-CB5 | 4.13  | 1.45        | 1.34     |
| 19  | L     | 311 | CDL  | OB6-CB5 | 4.12  | 1.45        | 1.34     |
| 15  | 8     | 102 | BCL  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 19  | H     | 302 | CDL  | OA8-CA7 | 4.12  | 1.45        | 1.33     |
| 15  | Q     | 102 | BCL  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 15  | S     | 102 | BCL  | C3B-C4B | 4.10  | 1.49        | 1.41     |
| 15  | 0     | 101 | BCL  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 15  | 7     | 101 | BCL  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 24  | O     | 501 | LDA  | C1-N1   | -4.09 | 1.47        | 1.51     |
| 14  | L     | 305 | PGV  | O01-C1  | 4.08  | 1.45        | 1.34     |
| 10  | C     | 403 | HEM  | FE-NC   | 4.08  | 2.08        | 1.95     |
| 19  | M     | 409 | CDL  | OB8-CB7 | 4.08  | 1.45        | 1.33     |
| 14  | C     | 408 | PGV  | O01-C1  | 4.07  | 1.45        | 1.34     |
| 14  | 1     | 401 | PGV  | O01-C1  | 4.06  | 1.45        | 1.34     |
| 19  | H     | 302 | CDL  | OB8-CB7 | 4.06  | 1.45        | 1.33     |
| 15  | Z     | 102 | BCL  | C3B-C4B | 4.06  | 1.49        | 1.41     |
| 15  | I     | 101 | BCL  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 15  | U     | 101 | BCL  | C3B-C4B | 4.05  | 1.49        | 1.41     |
| 15  | X     | 102 | BCL  | C3B-C4B | 4.05  | 1.49        | 1.41     |
| 15  | 5     | 102 | BCL  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 14  | A     | 503 | PGV  | O01-C1  | 4.04  | 1.45        | 1.34     |
| 15  | L     | 301 | BCL  | C3B-C4B | 4.04  | 1.49        | 1.41     |
| 14  | L     | 306 | PGV  | O01-C1  | 4.04  | 1.45        | 1.34     |
| 14  | L     | 310 | PGV  | O01-C1  | 4.04  | 1.45        | 1.34     |
| 15  | 1     | 402 | BCL  | C3B-C4B | 4.02  | 1.49        | 1.41     |
| 19  | H     | 302 | CDL  | OB6-CB5 | 4.01  | 1.45        | 1.34     |
| 14  | H     | 301 | PGV  | O01-C1  | 4.01  | 1.45        | 1.34     |
| 15  | M     | 403 | BCL  | C3B-C4B | 4.01  | 1.49        | 1.41     |
| 15  | V     | 101 | BCL  | C3B-C4B | 4.01  | 1.49        | 1.41     |
| 15  | F     | 502 | BCL  | C3B-C4B | 4.00  | 1.49        | 1.41     |
| 19  | M     | 409 | CDL  | OB6-CB5 | 4.00  | 1.45        | 1.34     |
| 15  | 5     | 102 | BCL  | C3B-C4B | 3.99  | 1.49        | 1.41     |
| 19  | D     | 101 | CDL  | OB6-CB5 | 3.99  | 1.45        | 1.34     |
| 15  | E     | 102 | BCL  | C3B-C4B | 3.98  | 1.49        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | W     | 101 | BCL  | C3B-C4B | 3.98  | 1.49        | 1.41     |
| 15  | 9     | 102 | BCL  | C3B-C4B | 3.98  | 1.49        | 1.41     |
| 15  | A     | 502 | BCL  | C3B-C4B | 3.97  | 1.49        | 1.41     |
| 15  | 7     | 101 | BCL  | C3B-C4B | 3.96  | 1.48        | 1.41     |
| 15  | 0     | 101 | BCL  | C3B-C4B | 3.95  | 1.48        | 1.41     |
| 15  | Q     | 102 | BCL  | C3B-C4B | 3.94  | 1.48        | 1.41     |
| 14  | A     | 501 | PGV  | O03-C19 | 3.93  | 1.44        | 1.33     |
| 15  | B     | 102 | BCL  | C3B-C4B | 3.92  | 1.48        | 1.41     |
| 15  | K     | 102 | BCL  | C3B-C4B | 3.91  | 1.48        | 1.41     |
| 15  | T     | 101 | BCL  | C3B-C4B | 3.91  | 1.48        | 1.41     |
| 14  | M     | 408 | PGV  | O01-C1  | 3.90  | 1.45        | 1.34     |
| 15  | N     | 101 | BCL  | C3B-C4B | 3.90  | 1.48        | 1.41     |
| 15  | G     | 102 | BCL  | C3B-C4B | 3.89  | 1.48        | 1.41     |
| 15  | M     | 402 | BCL  | C3B-C4B | 3.89  | 1.48        | 1.41     |
| 15  | J     | 102 | BCL  | C3B-C4B | 3.89  | 1.48        | 1.41     |
| 15  | D     | 102 | BCL  | C3B-C4B | 3.88  | 1.48        | 1.41     |
| 15  | 6     | 101 | BCL  | C3B-C4B | 3.84  | 1.48        | 1.41     |
| 15  | P     | 102 | BCL  | C3B-C4B | 3.82  | 1.48        | 1.41     |
| 15  | R     | 101 | BCL  | C3B-C4B | 3.80  | 1.48        | 1.41     |
| 15  | O     | 502 | BCL  | C3B-C4B | 3.80  | 1.48        | 1.41     |
| 15  | 8     | 102 | BCL  | C3B-C4B | 3.79  | 1.48        | 1.41     |
| 15  | 3     | 101 | BCL  | C3B-C4B | 3.79  | 1.48        | 1.41     |
| 15  | 2     | 102 | BCL  | C3B-C4B | 3.77  | 1.48        | 1.41     |
| 15  | L     | 308 | BCL  | C3B-C4B | 3.76  | 1.48        | 1.41     |
| 15  | 4     | 102 | BCL  | C3B-C4B | 3.76  | 1.48        | 1.41     |
| 15  | Y     | 102 | BCL  | C3B-C4B | 3.70  | 1.48        | 1.41     |
| 17  | L     | 309 | UQ8  | C4-C3   | 3.67  | 1.49        | 1.36     |
| 15  | L     | 308 | BCL  | CHB-C1B | 3.66  | 1.47        | 1.39     |
| 15  | J     | 102 | BCL  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 15  | W     | 101 | BCL  | CHD-C1D | 3.62  | 1.45        | 1.38     |
| 10  | C     | 403 | HEM  | C1B-NB  | -3.61 | 1.34        | 1.40     |
| 15  | O     | 502 | BCL  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 15  | R     | 101 | BCL  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 15  | G     | 102 | BCL  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 15  | 2     | 102 | BCL  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 15  | X     | 102 | BCL  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 15  | 5     | 102 | BCL  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 15  | U     | 101 | BCL  | CHD-C1D | 3.57  | 1.45        | 1.38     |
| 15  | I     | 101 | BCL  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 15  | Z     | 102 | BCL  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 15  | 7     | 101 | BCL  | CHD-C1D | 3.56  | 1.45        | 1.38     |
| 15  | Q     | 102 | BCL  | OBD-CAD | 3.55  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | W     | 101 | BCL  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 15  | I     | 101 | BCL  | CHD-C1D | 3.55  | 1.45        | 1.38     |
| 15  | 1     | 402 | BCL  | CHD-C1D | 3.54  | 1.45        | 1.38     |
| 15  | 3     | 101 | BCL  | CHD-C1D | 3.54  | 1.45        | 1.38     |
| 15  | K     | 102 | BCL  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 15  | F     | 502 | BCL  | CHD-C1D | 3.53  | 1.45        | 1.38     |
| 15  | 3     | 101 | BCL  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 15  | 4     | 102 | BCL  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 10  | C     | 404 | HEM  | C1B-NB  | -3.52 | 1.34        | 1.40     |
| 15  | U     | 101 | BCL  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 15  | 0     | 101 | BCL  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 17  | L     | 304 | UQ8  | C4-C3   | 3.50  | 1.49        | 1.36     |
| 15  | F     | 502 | BCL  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 15  | M     | 403 | BCL  | CHD-C1D | 3.49  | 1.45        | 1.38     |
| 15  | Y     | 102 | BCL  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 15  | 8     | 102 | BCL  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 15  | S     | 102 | BCL  | CHD-C1D | 3.49  | 1.45        | 1.38     |
| 15  | E     | 102 | BCL  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 15  | V     | 101 | BCL  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 15  | A     | 502 | BCL  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 15  | D     | 102 | BCL  | CHD-C1D | 3.48  | 1.45        | 1.38     |
| 15  | 6     | 101 | BCL  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 15  | 1     | 402 | BCL  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 15  | N     | 101 | BCL  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 15  | A     | 502 | BCL  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 15  | M     | 402 | BCL  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 15  | K     | 102 | BCL  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 15  | 3     | 101 | BCL  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 15  | P     | 102 | BCL  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 15  | R     | 101 | BCL  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 15  | P     | 102 | BCL  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 15  | S     | 102 | BCL  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 15  | B     | 102 | BCL  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 15  | Q     | 102 | BCL  | CHD-C1D | 3.44  | 1.45        | 1.38     |
| 15  | 1     | 402 | BCL  | CHB-C1B | 3.44  | 1.47        | 1.39     |
| 15  | B     | 102 | BCL  | CHB-C1B | 3.44  | 1.47        | 1.39     |
| 15  | D     | 102 | BCL  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 15  | T     | 101 | BCL  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 15  | L     | 301 | BCL  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 15  | Y     | 102 | BCL  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 17  | L     | 303 | UQ8  | C4-C3   | 3.41  | 1.48        | 1.36     |
| 15  | 5     | 102 | BCL  | CHB-C1B | 3.41  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | M     | 402 | BCL  | CHD-C1D | 3.41  | 1.45        | 1.38     |
| 15  | 6     | 101 | BCL  | CHB-C1B | 3.40  | 1.47        | 1.39     |
| 15  | X     | 102 | BCL  | CHB-C1B | 3.40  | 1.47        | 1.39     |
| 15  | 9     | 102 | BCL  | CHD-C1D | 3.40  | 1.45        | 1.38     |
| 15  | G     | 102 | BCL  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 15  | L     | 308 | BCL  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 15  | T     | 101 | BCL  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 15  | 0     | 101 | BCL  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 15  | F     | 502 | BCL  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 15  | 9     | 102 | BCL  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 15  | A     | 502 | BCL  | CHD-C1D | 3.38  | 1.45        | 1.38     |
| 15  | K     | 102 | BCL  | CHD-C1D | 3.38  | 1.45        | 1.38     |
| 15  | V     | 101 | BCL  | CHB-C1B | 3.38  | 1.47        | 1.39     |
| 15  | O     | 502 | BCL  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 15  | Z     | 102 | BCL  | CHB-C1B | 3.38  | 1.47        | 1.39     |
| 15  | 5     | 102 | BCL  | CHD-C1D | 3.37  | 1.45        | 1.38     |
| 15  | 8     | 102 | BCL  | CHD-C1D | 3.37  | 1.45        | 1.38     |
| 15  | Y     | 102 | BCL  | CHD-C1D | 3.37  | 1.45        | 1.38     |
| 15  | L     | 308 | BCL  | C4B-NB  | -3.37 | 1.33        | 1.37     |
| 15  | E     | 102 | BCL  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 15  | 2     | 102 | BCL  | CHB-C1B | 3.36  | 1.47        | 1.39     |
| 15  | 9     | 102 | BCL  | CHB-C1B | 3.36  | 1.46        | 1.39     |
| 15  | M     | 403 | BCL  | CHC-C4B | 3.36  | 1.46        | 1.39     |
| 15  | 8     | 102 | BCL  | CHB-C1B | 3.36  | 1.46        | 1.39     |
| 15  | O     | 502 | BCL  | CHD-C1D | 3.35  | 1.44        | 1.38     |
| 15  | L     | 301 | BCL  | CHD-C1D | 3.35  | 1.44        | 1.38     |
| 15  | J     | 102 | BCL  | CHD-C1D | 3.35  | 1.44        | 1.38     |
| 15  | L     | 308 | BCL  | CHD-C1D | 3.34  | 1.44        | 1.38     |
| 15  | U     | 101 | BCL  | CHB-C1B | 3.34  | 1.46        | 1.39     |
| 15  | S     | 102 | BCL  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 15  | L     | 301 | BCL  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 10  | C     | 401 | HEM  | C1B-NB  | -3.32 | 1.34        | 1.40     |
| 15  | L     | 301 | BCL  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 15  | W     | 101 | BCL  | CHB-C1B | 3.31  | 1.46        | 1.39     |
| 15  | N     | 101 | BCL  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 15  | L     | 308 | BCL  | C1D-ND  | -3.30 | 1.33        | 1.37     |
| 10  | C     | 402 | HEM  | C1B-NB  | -3.29 | 1.34        | 1.40     |
| 15  | R     | 101 | BCL  | CHD-C1D | 3.29  | 1.44        | 1.38     |
| 15  | M     | 402 | BCL  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 15  | 7     | 101 | BCL  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 15  | G     | 102 | BCL  | CHD-C1D | 3.29  | 1.44        | 1.38     |
| 15  | 0     | 101 | BCL  | CHD-C1D | 3.28  | 1.44        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | T     | 101 | BCL  | CHD-C1D | 3.28  | 1.44        | 1.38     |
| 15  | B     | 102 | BCL  | CHD-C1D | 3.28  | 1.44        | 1.38     |
| 15  | M     | 403 | BCL  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 15  | I     | 101 | BCL  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 15  | V     | 101 | BCL  | CHC-C4B | 3.26  | 1.46        | 1.39     |
| 10  | C     | 403 | HEM  | C4D-ND  | -3.26 | 1.34        | 1.40     |
| 15  | 4     | 102 | BCL  | CHB-C1B | 3.26  | 1.46        | 1.39     |
| 15  | A     | 502 | BCL  | CHC-C4B | 3.26  | 1.46        | 1.39     |
| 15  | Z     | 102 | BCL  | CHD-C1D | 3.25  | 1.44        | 1.38     |
| 15  | I     | 101 | BCL  | CHC-C4B | 3.25  | 1.46        | 1.39     |
| 15  | D     | 102 | BCL  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 15  | 7     | 101 | BCL  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 15  | 6     | 101 | BCL  | CHD-C1D | 3.24  | 1.44        | 1.38     |
| 15  | 4     | 102 | BCL  | CHD-C1D | 3.23  | 1.44        | 1.38     |
| 15  | G     | 102 | BCL  | CHC-C4B | 3.22  | 1.46        | 1.39     |
| 15  | Z     | 102 | BCL  | CHC-C4B | 3.22  | 1.46        | 1.39     |
| 15  | Q     | 102 | BCL  | CHB-C1B | 3.21  | 1.46        | 1.39     |
| 15  | N     | 101 | BCL  | CHD-C1D | 3.20  | 1.44        | 1.38     |
| 15  | 2     | 102 | BCL  | CHD-C1D | 3.20  | 1.44        | 1.38     |
| 15  | S     | 102 | BCL  | CHC-C4B | 3.20  | 1.46        | 1.39     |
| 15  | 2     | 102 | BCL  | C1D-ND  | -3.20 | 1.33        | 1.37     |
| 10  | C     | 404 | HEM  | C4D-ND  | -3.20 | 1.34        | 1.40     |
| 15  | B     | 102 | BCL  | CHC-C4B | 3.20  | 1.46        | 1.39     |
| 15  | P     | 102 | BCL  | CHC-C4B | 3.20  | 1.46        | 1.39     |
| 15  | J     | 102 | BCL  | CHC-C4B | 3.20  | 1.46        | 1.39     |
| 15  | 1     | 402 | BCL  | CHC-C4B | 3.19  | 1.46        | 1.39     |
| 15  | E     | 102 | BCL  | CHD-C1D | 3.19  | 1.44        | 1.38     |
| 15  | X     | 102 | BCL  | CHC-C4B | 3.19  | 1.46        | 1.39     |
| 15  | F     | 502 | BCL  | CHC-C4B | 3.18  | 1.46        | 1.39     |
| 15  | J     | 102 | BCL  | CHB-C1B | 3.18  | 1.46        | 1.39     |
| 15  | N     | 101 | BCL  | CHC-C4B | 3.18  | 1.46        | 1.39     |
| 15  | M     | 402 | BCL  | CHC-C4B | 3.17  | 1.46        | 1.39     |
| 10  | C     | 401 | HEM  | C4D-ND  | -3.17 | 1.34        | 1.40     |
| 15  | 5     | 102 | BCL  | CHC-C4B | 3.17  | 1.46        | 1.39     |
| 15  | K     | 102 | BCL  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 15  | 3     | 101 | BCL  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 15  | P     | 102 | BCL  | CHD-C1D | 3.15  | 1.44        | 1.38     |
| 15  | X     | 102 | BCL  | CHD-C1D | 3.14  | 1.44        | 1.38     |
| 15  | M     | 402 | BCL  | C3D-C2D | 3.14  | 1.47        | 1.39     |
| 15  | 7     | 101 | BCL  | CHC-C4B | 3.14  | 1.46        | 1.39     |
| 15  | L     | 308 | BCL  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 15  | 6     | 101 | BCL  | CHC-C4B | 3.13  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | Q     | 102 | BCL  | CHC-C4B | 3.13  | 1.46        | 1.39     |
| 15  | 9     | 102 | BCL  | CHC-C4B | 3.13  | 1.46        | 1.39     |
| 15  | B     | 102 | BCL  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 15  | X     | 102 | BCL  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 15  | P     | 102 | BCL  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 15  | 4     | 102 | BCL  | CHC-C4B | 3.12  | 1.46        | 1.39     |
| 16  | L     | 302 | BPH  | C4D-CHA | 3.12  | 1.44        | 1.39     |
| 10  | C     | 402 | HEM  | C4D-ND  | -3.12 | 1.34        | 1.40     |
| 15  | D     | 102 | BCL  | C3D-C2D | 3.11  | 1.47        | 1.39     |
| 15  | 8     | 102 | BCL  | CHC-C4B | 3.11  | 1.46        | 1.39     |
| 15  | 0     | 101 | BCL  | CHC-C4B | 3.11  | 1.46        | 1.39     |
| 15  | M     | 402 | BCL  | C1D-ND  | -3.10 | 1.33        | 1.37     |
| 15  | T     | 101 | BCL  | C1D-ND  | -3.10 | 1.33        | 1.37     |
| 15  | Y     | 102 | BCL  | C4B-NB  | -3.10 | 1.33        | 1.37     |
| 15  | 2     | 102 | BCL  | CHC-C4B | 3.09  | 1.46        | 1.39     |
| 15  | U     | 101 | BCL  | CHC-C4B | 3.09  | 1.46        | 1.39     |
| 15  | L     | 308 | BCL  | CHC-C4B | 3.08  | 1.46        | 1.39     |
| 15  | M     | 403 | BCL  | OBD-CAD | 3.07  | 1.27        | 1.22     |
| 15  | G     | 102 | BCL  | C1D-ND  | -3.07 | 1.33        | 1.37     |
| 15  | J     | 102 | BCL  | C1D-ND  | -3.07 | 1.33        | 1.37     |
| 15  | E     | 102 | BCL  | CHC-C4B | 3.07  | 1.46        | 1.39     |
| 15  | V     | 101 | BCL  | C1D-ND  | -3.06 | 1.33        | 1.37     |
| 15  | 4     | 102 | BCL  | C4B-NB  | -3.06 | 1.33        | 1.37     |
| 15  | R     | 101 | BCL  | C1D-ND  | -3.05 | 1.33        | 1.37     |
| 15  | W     | 101 | BCL  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 15  | Y     | 102 | BCL  | CHC-C4B | 3.05  | 1.46        | 1.39     |
| 15  | G     | 102 | BCL  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 15  | O     | 502 | BCL  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 15  | V     | 101 | BCL  | CHD-C1D | 3.04  | 1.44        | 1.38     |
| 15  | 7     | 101 | BCL  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 15  | D     | 102 | BCL  | CHC-C4B | 3.03  | 1.46        | 1.39     |
| 15  | A     | 502 | BCL  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 16  | M     | 404 | BPH  | C4D-CHA | 3.03  | 1.44        | 1.39     |
| 15  | S     | 102 | BCL  | C3D-C2D | 3.03  | 1.47        | 1.39     |
| 15  | W     | 101 | BCL  | CHC-C4B | 3.03  | 1.46        | 1.39     |
| 15  | T     | 101 | BCL  | CHC-C4B | 3.03  | 1.46        | 1.39     |
| 15  | J     | 102 | BCL  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 15  | P     | 102 | BCL  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 15  | X     | 102 | BCL  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 15  | 4     | 102 | BCL  | C3D-C2D | 3.02  | 1.47        | 1.39     |
| 15  | M     | 402 | BCL  | C4B-NB  | -3.01 | 1.33        | 1.37     |
| 15  | E     | 102 | BCL  | C3D-C2D | 3.01  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | O     | 502 | BCL  | CHC-C4B | 3.01  | 1.46        | 1.39     |
| 15  | R     | 101 | BCL  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 15  | I     | 101 | BCL  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 15  | N     | 101 | BCL  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 15  | 8     | 102 | BCL  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 15  | 5     | 102 | BCL  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 15  | Q     | 102 | BCL  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 15  | K     | 102 | BCL  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 15  | 6     | 101 | BCL  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 15  | N     | 101 | BCL  | C1D-ND  | -2.97 | 1.34        | 1.37     |
| 15  | T     | 101 | BCL  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 15  | 1     | 402 | BCL  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 15  | V     | 101 | BCL  | C3D-C2D | 2.95  | 1.47        | 1.39     |
| 15  | 0     | 101 | BCL  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 15  | 4     | 102 | BCL  | C1D-ND  | -2.94 | 1.34        | 1.37     |
| 15  | E     | 102 | BCL  | C1D-ND  | -2.94 | 1.34        | 1.37     |
| 15  | U     | 101 | BCL  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 15  | 3     | 101 | BCL  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 15  | R     | 101 | BCL  | CHC-C4B | 2.94  | 1.46        | 1.39     |
| 15  | 2     | 102 | BCL  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 15  | Z     | 102 | BCL  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 15  | Y     | 102 | BCL  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 15  | 0     | 101 | BCL  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 15  | B     | 102 | BCL  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 15  | M     | 403 | BCL  | C3D-C2D | 2.92  | 1.47        | 1.39     |
| 15  | F     | 502 | BCL  | C3D-C2D | 2.92  | 1.46        | 1.39     |
| 15  | M     | 403 | BCL  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 15  | 8     | 102 | BCL  | C1D-ND  | -2.91 | 1.34        | 1.37     |
| 15  | 9     | 102 | BCL  | C3D-C2D | 2.91  | 1.46        | 1.39     |
| 15  | 6     | 101 | BCL  | C1D-ND  | -2.88 | 1.34        | 1.37     |
| 15  | 0     | 101 | BCL  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 15  | Q     | 102 | BCL  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 15  | F     | 502 | BCL  | CHD-C4C | 2.86  | 1.47        | 1.39     |
| 15  | 5     | 102 | BCL  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 15  | A     | 502 | BCL  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 15  | K     | 102 | BCL  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 15  | L     | 301 | BCL  | C3D-C2D | 2.83  | 1.46        | 1.39     |
| 15  | V     | 101 | BCL  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 15  | U     | 101 | BCL  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 15  | O     | 502 | BCL  | C1D-ND  | -2.82 | 1.34        | 1.37     |
| 15  | Z     | 102 | BCL  | C3D-C2D | 2.81  | 1.46        | 1.39     |
| 15  | B     | 102 | BCL  | C4B-NB  | -2.81 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | S     | 102 | BCL  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 15  | D     | 102 | BCL  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 15  | 3     | 101 | BCL  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 15  | I     | 101 | BCL  | CHD-C4C | 2.80  | 1.47        | 1.39     |
| 15  | W     | 101 | BCL  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 15  | U     | 101 | BCL  | CHD-C4C | 2.80  | 1.47        | 1.39     |
| 15  | F     | 502 | BCL  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 15  | 6     | 101 | BCL  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 15  | 7     | 101 | BCL  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 15  | R     | 101 | BCL  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 15  | 1     | 402 | BCL  | CHD-C4C | 2.78  | 1.47        | 1.39     |
| 15  | Z     | 102 | BCL  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 15  | G     | 102 | BCL  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 15  | Q     | 102 | BCL  | CHD-C4C | 2.76  | 1.47        | 1.39     |
| 15  | E     | 102 | BCL  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 15  | J     | 102 | BCL  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 15  | 8     | 102 | BCL  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 15  | F     | 502 | BCL  | C1D-C2D | 2.75  | 1.50        | 1.45     |
| 15  | M     | 403 | BCL  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 15  | N     | 101 | BCL  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 15  | 3     | 101 | BCL  | CHD-C4C | 2.73  | 1.46        | 1.39     |
| 15  | W     | 101 | BCL  | CHD-C4C | 2.73  | 1.46        | 1.39     |
| 15  | L     | 301 | BCL  | C1D-ND  | -2.73 | 1.34        | 1.37     |
| 15  | K     | 102 | BCL  | CHD-C4C | 2.72  | 1.46        | 1.39     |
| 15  | Y     | 102 | BCL  | CHD-C4C | 2.72  | 1.46        | 1.39     |
| 15  | 5     | 102 | BCL  | CHD-C4C | 2.72  | 1.46        | 1.39     |
| 15  | U     | 101 | BCL  | C1D-C2D | 2.71  | 1.50        | 1.45     |
| 15  | A     | 502 | BCL  | C1D-ND  | -2.71 | 1.34        | 1.37     |
| 15  | 1     | 402 | BCL  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 15  | I     | 101 | BCL  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 15  | O     | 502 | BCL  | CHD-C4C | 2.70  | 1.46        | 1.39     |
| 15  | D     | 102 | BCL  | C1D-ND  | -2.70 | 1.34        | 1.37     |
| 15  | 9     | 102 | BCL  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 15  | 9     | 102 | BCL  | CHD-C4C | 2.70  | 1.46        | 1.39     |
| 15  | I     | 101 | BCL  | C1D-ND  | -2.69 | 1.34        | 1.37     |
| 15  | I     | 101 | BCL  | C1D-C2D | 2.69  | 1.50        | 1.45     |
| 15  | 7     | 101 | BCL  | CHD-C4C | 2.69  | 1.46        | 1.39     |
| 15  | S     | 102 | BCL  | CHD-C4C | 2.69  | 1.46        | 1.39     |
| 15  | F     | 502 | BCL  | C1D-ND  | -2.69 | 1.34        | 1.37     |
| 15  | 1     | 402 | BCL  | C1D-ND  | -2.68 | 1.34        | 1.37     |
| 15  | L     | 308 | BCL  | MG-NA   | -2.67 | 1.99        | 2.06     |
| 15  | Q     | 102 | BCL  | C1D-C2D | 2.67  | 1.50        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | P     | 102 | BCL  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 15  | M     | 403 | BCL  | C1D-C2D | 2.66  | 1.50        | 1.45     |
| 15  | D     | 102 | BCL  | CHD-C4C | 2.66  | 1.46        | 1.39     |
| 15  | A     | 502 | BCL  | CHD-C4C | 2.65  | 1.46        | 1.39     |
| 15  | 2     | 102 | BCL  | C4B-NB  | -2.65 | 1.34        | 1.37     |
| 15  | T     | 101 | BCL  | C4B-NB  | -2.65 | 1.34        | 1.37     |
| 15  | W     | 101 | BCL  | C1D-ND  | -2.65 | 1.34        | 1.37     |
| 15  | 7     | 101 | BCL  | C1D-ND  | -2.64 | 1.34        | 1.37     |
| 15  | L     | 308 | BCL  | CHD-C4C | 2.64  | 1.46        | 1.39     |
| 15  | O     | 502 | BCL  | C1D-C2D | 2.64  | 1.50        | 1.45     |
| 15  | 5     | 102 | BCL  | C1D-ND  | -2.64 | 1.34        | 1.37     |
| 15  | S     | 102 | BCL  | C1D-ND  | -2.63 | 1.34        | 1.37     |
| 15  | 1     | 402 | BCL  | C1D-C2D | 2.63  | 1.50        | 1.45     |
| 15  | O     | 502 | BCL  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 15  | 2     | 102 | BCL  | C1B-NB  | -2.63 | 1.34        | 1.37     |
| 15  | K     | 102 | BCL  | C1D-ND  | -2.62 | 1.34        | 1.37     |
| 10  | C     | 404 | HEM  | C1C-C2C | -2.61 | 1.40        | 1.45     |
| 15  | X     | 102 | BCL  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 15  | Y     | 102 | BCL  | C1D-ND  | -2.61 | 1.34        | 1.37     |
| 15  | Q     | 102 | BCL  | C1D-ND  | -2.61 | 1.34        | 1.37     |
| 15  | M     | 403 | BCL  | CHD-C4C | 2.61  | 1.46        | 1.39     |
| 15  | W     | 101 | BCL  | C1D-C2D | 2.61  | 1.50        | 1.45     |
| 15  | D     | 102 | BCL  | C1D-C2D | 2.60  | 1.50        | 1.45     |
| 15  | M     | 403 | BCL  | C1B-NB  | -2.59 | 1.34        | 1.37     |
| 15  | K     | 102 | BCL  | C1D-C2D | 2.59  | 1.50        | 1.45     |
| 15  | U     | 101 | BCL  | C1D-ND  | -2.58 | 1.34        | 1.37     |
| 15  | 3     | 101 | BCL  | C1D-C2D | 2.57  | 1.50        | 1.45     |
| 10  | C     | 403 | HEM  | C1C-C2C | -2.57 | 1.40        | 1.45     |
| 15  | 5     | 102 | BCL  | C1D-C2D | 2.56  | 1.50        | 1.45     |
| 15  | L     | 301 | BCL  | C4B-NB  | -2.56 | 1.34        | 1.37     |
| 15  | Y     | 102 | BCL  | C1D-C2D | 2.56  | 1.50        | 1.45     |
| 15  | Q     | 102 | BCL  | C1B-NB  | -2.55 | 1.34        | 1.37     |
| 15  | M     | 402 | BCL  | CHD-C4C | 2.55  | 1.46        | 1.39     |
| 15  | R     | 101 | BCL  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 15  | T     | 101 | BCL  | C1B-NB  | -2.54 | 1.34        | 1.37     |
| 15  | E     | 102 | BCL  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 15  | S     | 102 | BCL  | C1D-C2D | 2.53  | 1.50        | 1.45     |
| 15  | Z     | 102 | BCL  | CHD-C4C | 2.53  | 1.46        | 1.39     |
| 15  | N     | 101 | BCL  | CHD-C4C | 2.53  | 1.46        | 1.39     |
| 15  | 5     | 102 | BCL  | MG-NA   | -2.53 | 2.00        | 2.06     |
| 15  | 9     | 102 | BCL  | C1B-NB  | -2.53 | 1.34        | 1.37     |
| 19  | D     | 101 | CDL  | OA8-CA7 | 2.52  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | G     | 102 | BCL  | CHD-C4C | 2.51  | 1.46        | 1.39     |
| 15  | 2     | 102 | BCL  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 15  | J     | 102 | BCL  | C1B-NB  | -2.51 | 1.34        | 1.37     |
| 15  | O     | 502 | BCL  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 10  | C     | 402 | HEM  | C1C-C2C | -2.51 | 1.40        | 1.45     |
| 15  | 9     | 102 | BCL  | C1D-ND  | -2.50 | 1.34        | 1.37     |
| 10  | C     | 401 | HEM  | C1C-C2C | -2.50 | 1.40        | 1.45     |
| 15  | 4     | 102 | BCL  | CHD-C4C | 2.49  | 1.46        | 1.39     |
| 15  | 0     | 101 | BCL  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 15  | K     | 102 | BCL  | MG-NA   | -2.48 | 2.00        | 2.06     |
| 15  | R     | 101 | BCL  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 15  | W     | 101 | BCL  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 15  | T     | 101 | BCL  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 15  | 9     | 102 | BCL  | C1D-C2D | 2.48  | 1.50        | 1.45     |
| 15  | A     | 502 | BCL  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 10  | C     | 401 | HEM  | FE-ND   | -2.48 | 1.87        | 1.94     |
| 15  | 6     | 101 | BCL  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 15  | U     | 101 | BCL  | C1B-NB  | -2.47 | 1.34        | 1.37     |
| 15  | 8     | 102 | BCL  | C1B-NB  | -2.47 | 1.34        | 1.37     |
| 15  | B     | 102 | BCL  | C1B-NB  | -2.47 | 1.34        | 1.37     |
| 15  | 8     | 102 | BCL  | CHD-C4C | 2.47  | 1.46        | 1.39     |
| 15  | L     | 301 | BCL  | CHD-C4C | 2.46  | 1.46        | 1.39     |
| 15  | 6     | 101 | BCL  | CHD-C4C | 2.46  | 1.46        | 1.39     |
| 15  | 2     | 102 | BCL  | CHD-C4C | 2.46  | 1.46        | 1.39     |
| 15  | R     | 101 | BCL  | CHD-C4C | 2.45  | 1.46        | 1.39     |
| 15  | A     | 502 | BCL  | C1D-C2D | 2.45  | 1.50        | 1.45     |
| 15  | P     | 102 | BCL  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 15  | I     | 101 | BCL  | C1B-NB  | -2.45 | 1.34        | 1.37     |
| 15  | G     | 102 | BCL  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 15  | Z     | 102 | BCL  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 15  | J     | 102 | BCL  | CHD-C4C | 2.45  | 1.46        | 1.39     |
| 15  | D     | 102 | BCL  | C1B-NB  | -2.45 | 1.34        | 1.37     |
| 15  | 7     | 101 | BCL  | C1D-C2D | 2.44  | 1.50        | 1.45     |
| 15  | 3     | 101 | BCL  | C1D-ND  | -2.43 | 1.34        | 1.37     |
| 15  | B     | 102 | BCL  | CHD-C4C | 2.43  | 1.46        | 1.39     |
| 15  | 3     | 101 | BCL  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 15  | 0     | 101 | BCL  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 15  | N     | 101 | BCL  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 15  | 7     | 101 | BCL  | C1B-NB  | -2.42 | 1.34        | 1.37     |
| 15  | Y     | 102 | BCL  | MG-NA   | -2.42 | 2.00        | 2.06     |
| 15  | 4     | 102 | BCL  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 15  | L     | 301 | BCL  | C1B-C2B | 2.42  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | E     | 102 | BCL  | CHD-C4C | 2.42  | 1.46        | 1.39     |
| 15  | Z     | 102 | BCL  | C1B-NB  | -2.42 | 1.34        | 1.37     |
| 15  | L     | 308 | BCL  | C1D-C2D | 2.41  | 1.50        | 1.45     |
| 15  | M     | 402 | BCL  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 15  | 3     | 101 | BCL  | MG-NA   | -2.41 | 2.00        | 2.06     |
| 15  | P     | 102 | BCL  | CHD-C4C | 2.40  | 1.45        | 1.39     |
| 15  | 0     | 101 | BCL  | CHD-C4C | 2.40  | 1.45        | 1.39     |
| 15  | V     | 101 | BCL  | C1B-NB  | -2.40 | 1.34        | 1.37     |
| 15  | W     | 101 | BCL  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 15  | X     | 102 | BCL  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 15  | B     | 102 | BCL  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 15  | X     | 102 | BCL  | CHD-C4C | 2.39  | 1.45        | 1.39     |
| 15  | Y     | 102 | BCL  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 15  | V     | 101 | BCL  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 15  | L     | 301 | BCL  | C1B-NB  | -2.38 | 1.34        | 1.37     |
| 15  | M     | 402 | BCL  | MG-NA   | -2.38 | 2.00        | 2.06     |
| 15  | E     | 102 | BCL  | C1B-NB  | -2.38 | 1.34        | 1.37     |
| 15  | 5     | 102 | BCL  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 15  | S     | 102 | BCL  | C1B-NB  | -2.38 | 1.34        | 1.37     |
| 15  | K     | 102 | BCL  | C1B-NB  | -2.38 | 1.34        | 1.37     |
| 15  | 1     | 402 | BCL  | C1B-NB  | -2.37 | 1.34        | 1.37     |
| 15  | 8     | 102 | BCL  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 15  | U     | 101 | BCL  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 15  | V     | 101 | BCL  | CHD-C4C | 2.36  | 1.45        | 1.39     |
| 15  | N     | 101 | BCL  | C1B-NB  | -2.36 | 1.34        | 1.37     |
| 15  | 1     | 402 | BCL  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 15  | X     | 102 | BCL  | C1B-NB  | -2.35 | 1.34        | 1.37     |
| 15  | J     | 102 | BCL  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 15  | F     | 502 | BCL  | C1B-NB  | -2.34 | 1.34        | 1.37     |
| 15  | D     | 102 | BCL  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 15  | 5     | 102 | BCL  | C1B-NB  | -2.34 | 1.34        | 1.37     |
| 15  | T     | 101 | BCL  | CHD-C4C | 2.34  | 1.45        | 1.39     |
| 15  | M     | 402 | BCL  | C1B-NB  | -2.33 | 1.34        | 1.37     |
| 15  | M     | 403 | BCL  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 15  | K     | 102 | BCL  | C1B-C2B | 2.32  | 1.48        | 1.43     |
| 15  | I     | 101 | BCL  | MG-NA   | -2.32 | 2.00        | 2.06     |
| 15  | I     | 101 | BCL  | MG-NC   | -2.32 | 2.00        | 2.06     |
| 15  | I     | 101 | BCL  | C1B-C2B | 2.31  | 1.48        | 1.43     |
| 15  | Y     | 102 | BCL  | C1B-NB  | -2.31 | 1.34        | 1.37     |
| 10  | C     | 403 | HEM  | FE-ND   | -2.30 | 1.87        | 1.94     |
| 15  | M     | 402 | BCL  | C1D-C2D | 2.30  | 1.49        | 1.45     |
| 15  | S     | 102 | BCL  | C1B-C2B | 2.29  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | L     | 302 | BPH  | C1B-C2B | 2.29  | 1.42        | 1.39     |
| 15  | O     | 502 | BCL  | C1B-NB  | -2.29 | 1.34        | 1.37     |
| 15  | X     | 102 | BCL  | MG-NA   | -2.29 | 2.00        | 2.06     |
| 15  | 4     | 102 | BCL  | C1B-NB  | -2.29 | 1.34        | 1.37     |
| 15  | 9     | 102 | BCL  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 15  | F     | 502 | BCL  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 15  | 2     | 102 | BCL  | MG-NA   | -2.28 | 2.00        | 2.06     |
| 15  | 1     | 402 | BCL  | MG-NA   | -2.28 | 2.00        | 2.06     |
| 10  | C     | 402 | HEM  | FE-ND   | -2.27 | 1.87        | 1.94     |
| 15  | F     | 502 | BCL  | MG-NA   | -2.26 | 2.00        | 2.06     |
| 15  | 7     | 101 | BCL  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 15  | P     | 102 | BCL  | C1B-NB  | -2.25 | 1.34        | 1.37     |
| 15  | G     | 102 | BCL  | C1B-NB  | -2.25 | 1.34        | 1.37     |
| 15  | O     | 502 | BCL  | MG-NA   | -2.24 | 2.00        | 2.06     |
| 15  | R     | 101 | BCL  | CHC-C1C | -2.24 | 1.32        | 1.37     |
| 15  | L     | 308 | BCL  | C1B-C2B | 2.23  | 1.48        | 1.43     |
| 15  | 6     | 101 | BCL  | C1B-NB  | -2.23 | 1.34        | 1.37     |
| 15  | S     | 102 | BCL  | MG-NA   | -2.23 | 2.01        | 2.06     |
| 15  | A     | 502 | BCL  | MG-NA   | -2.22 | 2.01        | 2.06     |
| 15  | L     | 301 | BCL  | C1D-C2D | 2.22  | 1.49        | 1.45     |
| 15  | Y     | 102 | BCL  | MG-NC   | -2.22 | 2.01        | 2.06     |
| 10  | C     | 402 | HEM  | C1D-ND  | -2.21 | 1.34        | 1.38     |
| 15  | 6     | 101 | BCL  | C1D-C2D | 2.21  | 1.49        | 1.45     |
| 15  | 7     | 101 | BCL  | MG-NA   | -2.21 | 2.01        | 2.06     |
| 10  | C     | 404 | HEM  | FE-ND   | -2.20 | 1.88        | 1.94     |
| 15  | W     | 101 | BCL  | MG-NA   | -2.20 | 2.01        | 2.06     |
| 15  | A     | 502 | BCL  | C1B-C2B | 2.20  | 1.48        | 1.43     |
| 15  | Z     | 102 | BCL  | C1D-C2D | 2.20  | 1.49        | 1.45     |
| 15  | N     | 101 | BCL  | C1D-C2D | 2.19  | 1.49        | 1.45     |
| 15  | M     | 403 | BCL  | MG-NA   | -2.18 | 2.01        | 2.06     |
| 15  | 6     | 101 | BCL  | MG-NA   | -2.18 | 2.01        | 2.06     |
| 15  | 7     | 101 | BCL  | MG-NC   | -2.18 | 2.01        | 2.06     |
| 15  | G     | 102 | BCL  | C1D-C2D | 2.18  | 1.49        | 1.45     |
| 15  | N     | 101 | BCL  | MG-NA   | -2.17 | 2.01        | 2.06     |
| 15  | 3     | 101 | BCL  | C1B-NB  | -2.17 | 1.35        | 1.37     |
| 15  | G     | 102 | BCL  | MG-NA   | -2.17 | 2.01        | 2.06     |
| 15  | J     | 102 | BCL  | MG-NA   | -2.17 | 2.01        | 2.06     |
| 15  | D     | 102 | BCL  | MG-NA   | -2.17 | 2.01        | 2.06     |
| 15  | 4     | 102 | BCL  | MG-NA   | -2.16 | 2.01        | 2.06     |
| 15  | V     | 101 | BCL  | MG-NA   | -2.16 | 2.01        | 2.06     |
| 16  | L     | 302 | BPH  | CBD-CGD | -2.16 | 1.49        | 1.52     |
| 10  | C     | 403 | HEM  | C1D-ND  | -2.15 | 1.34        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | 9     | 102 | BCL  | MG-NA   | -2.15 | 2.01        | 2.06     |
| 16  | M     | 404 | BPH  | C1B-C2B | 2.15  | 1.41        | 1.39     |
| 15  | P     | 102 | BCL  | MG-NA   | -2.14 | 2.01        | 2.06     |
| 15  | F     | 502 | BCL  | MG-NC   | -2.14 | 2.01        | 2.06     |
| 15  | 4     | 102 | BCL  | C1D-C2D | 2.13  | 1.49        | 1.45     |
| 10  | C     | 403 | HEM  | C3C-C4C | -2.13 | 1.42        | 1.46     |
| 10  | C     | 403 | HEM  | C4B-NB  | -2.13 | 1.34        | 1.38     |
| 15  | Q     | 102 | BCL  | MG-NA   | -2.13 | 2.01        | 2.06     |
| 15  | Z     | 102 | BCL  | MG-NA   | -2.13 | 2.01        | 2.06     |
| 15  | Q     | 102 | BCL  | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 15  | B     | 102 | BCL  | MG-NA   | -2.12 | 2.01        | 2.06     |
| 10  | C     | 401 | HEM  | C4B-NB  | -2.12 | 1.34        | 1.38     |
| 15  | E     | 102 | BCL  | MG-NA   | -2.12 | 2.01        | 2.06     |
| 15  | U     | 101 | BCL  | MG-NA   | -2.12 | 2.01        | 2.06     |
| 15  | 0     | 101 | BCL  | MG-NA   | -2.12 | 2.01        | 2.06     |
| 15  | 1     | 402 | BCL  | MG-NC   | -2.12 | 2.01        | 2.06     |
| 15  | R     | 101 | BCL  | C1D-C2D | 2.11  | 1.49        | 1.45     |
| 15  | J     | 102 | BCL  | C1D-C2D | 2.11  | 1.49        | 1.45     |
| 15  | W     | 101 | BCL  | MG-NC   | -2.10 | 2.01        | 2.06     |
| 15  | D     | 102 | BCL  | CHC-C1C | -2.10 | 1.32        | 1.37     |
| 15  | 2     | 102 | BCL  | CHC-C1C | -2.10 | 1.32        | 1.37     |
| 10  | C     | 402 | HEM  | C3C-C4C | -2.10 | 1.42        | 1.46     |
| 16  | M     | 404 | BPH  | C3A-C2A | -2.09 | 1.52        | 1.54     |
| 15  | R     | 101 | BCL  | MG-NA   | -2.08 | 2.01        | 2.06     |
| 15  | E     | 102 | BCL  | CHC-C1C | -2.08 | 1.32        | 1.37     |
| 15  | 5     | 102 | BCL  | MG-NC   | -2.07 | 2.01        | 2.06     |
| 15  | Y     | 102 | BCL  | CHC-C1C | -2.07 | 1.32        | 1.37     |
| 15  | M     | 403 | BCL  | MG-NC   | -2.06 | 2.01        | 2.06     |
| 15  | K     | 102 | BCL  | MG-NC   | -2.06 | 2.01        | 2.06     |
| 15  | B     | 102 | BCL  | CHC-C1C | -2.06 | 1.32        | 1.37     |
| 15  | J     | 102 | BCL  | MG-NC   | -2.06 | 2.01        | 2.06     |
| 15  | O     | 502 | BCL  | CHC-C1C | -2.06 | 1.32        | 1.37     |
| 15  | 8     | 102 | BCL  | MG-NA   | -2.05 | 2.01        | 2.06     |
| 15  | M     | 402 | BCL  | CHC-C1C | -2.05 | 1.32        | 1.37     |
| 15  | T     | 101 | BCL  | MG-NA   | -2.05 | 2.01        | 2.06     |
| 15  | T     | 101 | BCL  | CHC-C1C | -2.05 | 1.32        | 1.37     |
| 15  | W     | 101 | BCL  | CHC-C1C | -2.05 | 1.32        | 1.37     |
| 15  | L     | 308 | BCL  | C4D-CHA | 2.04  | 1.45        | 1.38     |
| 15  | B     | 102 | BCL  | MG-NC   | -2.04 | 2.01        | 2.06     |
| 10  | C     | 404 | HEM  | C3C-C4C | -2.03 | 1.42        | 1.46     |
| 15  | 3     | 101 | BCL  | C4D-CHA | 2.03  | 1.45        | 1.38     |
| 15  | 3     | 101 | BCL  | CHC-C1C | -2.03 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | L     | 308 | BCL  | C1B-NB  | -2.03 | 1.35        | 1.37     |
| 15  | 6     | 101 | BCL  | MG-NC   | -2.02 | 2.01        | 2.06     |
| 15  | M     | 402 | BCL  | MG-NC   | -2.02 | 2.01        | 2.06     |
| 10  | C     | 404 | HEM  | C4B-NB  | -2.02 | 1.34        | 1.38     |
| 15  | 4     | 102 | BCL  | CHC-C1C | -2.01 | 1.32        | 1.37     |
| 15  | K     | 102 | BCL  | CHC-C1C | -2.01 | 1.32        | 1.37     |
| 15  | V     | 101 | BCL  | C1D-C2D | 2.01  | 1.49        | 1.45     |
| 15  | L     | 308 | BCL  | CHC-C1C | -2.01 | 1.32        | 1.37     |
| 15  | U     | 101 | BCL  | MG-NC   | -2.00 | 2.01        | 2.06     |
| 15  | X     | 102 | BCL  | CHC-C1C | -2.00 | 1.32        | 1.37     |
| 10  | C     | 401 | HEM  | C1D-ND  | -2.00 | 1.34        | 1.38     |
| 15  | Q     | 102 | BCL  | CHB-C4A | -2.00 | 1.32        | 1.37     |

All (1294) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | U     | 101 | BCL  | CMD-C2D-C1D | 8.21  | 139.18      | 124.73   |
| 15  | M     | 403 | BCL  | CMD-C2D-C1D | 8.01  | 138.83      | 124.73   |
| 15  | K     | 102 | BCL  | CMD-C2D-C1D | 8.00  | 138.82      | 124.73   |
| 15  | 9     | 102 | BCL  | CMD-C2D-C1D | 7.99  | 138.80      | 124.73   |
| 15  | 3     | 101 | BCL  | CMD-C2D-C1D | 7.98  | 138.78      | 124.73   |
| 15  | F     | 502 | BCL  | CMD-C2D-C1D | 7.97  | 138.77      | 124.73   |
| 15  | Y     | 102 | BCL  | CMD-C2D-C1D | 7.95  | 138.73      | 124.73   |
| 15  | Q     | 102 | BCL  | CMD-C2D-C1D | 7.94  | 138.72      | 124.73   |
| 15  | 1     | 402 | BCL  | CMD-C2D-C1D | 7.82  | 138.49      | 124.73   |
| 15  | 5     | 102 | BCL  | CMD-C2D-C1D | 7.80  | 138.47      | 124.73   |
| 15  | D     | 102 | BCL  | CMD-C2D-C1D | 7.69  | 138.27      | 124.73   |
| 15  | W     | 101 | BCL  | CMD-C2D-C1D | 7.69  | 138.26      | 124.73   |
| 15  | I     | 101 | BCL  | CMD-C2D-C1D | 7.66  | 138.22      | 124.73   |
| 15  | O     | 502 | BCL  | CMD-C2D-C1D | 7.65  | 138.20      | 124.73   |
| 15  | S     | 102 | BCL  | CMD-C2D-C1D | 7.63  | 138.17      | 124.73   |
| 15  | L     | 301 | BCL  | CMD-C2D-C1D | 7.57  | 138.05      | 124.73   |
| 15  | 7     | 101 | BCL  | CMD-C2D-C1D | 7.44  | 137.84      | 124.73   |
| 15  | A     | 502 | BCL  | CMD-C2D-C1D | 7.37  | 137.70      | 124.73   |
| 15  | L     | 308 | BCL  | CMD-C2D-C1D | 7.33  | 137.63      | 124.73   |
| 22  | 4     | 103 | CRT  | C31-C32-C33 | -7.16 | 117.24      | 127.28   |
| 15  | 6     | 101 | BCL  | CMD-C2D-C1D | 7.03  | 137.10      | 124.73   |
| 15  | Z     | 102 | BCL  | CMD-C2D-C1D | 7.01  | 137.08      | 124.73   |
| 15  | 4     | 102 | BCL  | CMD-C2D-C1D | 6.93  | 136.93      | 124.73   |
| 15  | G     | 102 | BCL  | CMD-C2D-C1D | 6.92  | 136.92      | 124.73   |
| 15  | N     | 101 | BCL  | CMD-C2D-C1D | 6.89  | 136.87      | 124.73   |
| 15  | I     | 101 | BCL  | C2B-C1B-NB  | 6.81  | 117.39      | 110.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | N     | 102 | CRT  | C37-C36-C35 | -6.78 | 115.39      | 124.91   |
| 22  | 9     | 101 | CRT  | C37-C36-C35 | -6.72 | 115.48      | 124.91   |
| 15  | 7     | 101 | BCL  | C2B-C1B-NB  | 6.67  | 117.25      | 110.33   |
| 15  | F     | 502 | BCL  | C2B-C1B-NB  | 6.67  | 117.24      | 110.33   |
| 15  | Q     | 102 | BCL  | C2B-C1B-NB  | 6.66  | 117.23      | 110.33   |
| 15  | M     | 402 | BCL  | CMD-C2D-C1D | 6.64  | 136.43      | 124.73   |
| 15  | J     | 102 | BCL  | CMD-C2D-C1D | 6.64  | 136.43      | 124.73   |
| 15  | N     | 101 | BCL  | C2B-C1B-NB  | 6.64  | 117.21      | 110.33   |
| 15  | T     | 101 | BCL  | CMD-C2D-C1D | 6.63  | 136.41      | 124.73   |
| 15  | D     | 102 | BCL  | C2B-C1B-NB  | 6.62  | 117.19      | 110.33   |
| 15  | U     | 101 | BCL  | C2B-C1B-NB  | 6.59  | 117.16      | 110.33   |
| 15  | X     | 102 | BCL  | C2B-C1B-NB  | 6.59  | 117.16      | 110.33   |
| 15  | V     | 101 | BCL  | C2B-C1B-NB  | 6.57  | 117.14      | 110.33   |
| 15  | 0     | 101 | BCL  | CMD-C2D-C1D | 6.57  | 136.30      | 124.73   |
| 15  | 2     | 102 | BCL  | CMD-C2D-C1D | 6.56  | 136.28      | 124.73   |
| 22  | 6     | 102 | CRT  | C37-C36-C35 | -6.56 | 115.70      | 124.91   |
| 15  | V     | 101 | BCL  | CMD-C2D-C1D | 6.56  | 136.27      | 124.73   |
| 15  | 8     | 102 | BCL  | CMD-C2D-C1D | 6.55  | 136.26      | 124.73   |
| 15  | W     | 101 | BCL  | C2B-C1B-NB  | 6.54  | 117.11      | 110.33   |
| 15  | J     | 102 | BCL  | C2B-C1B-NB  | 6.52  | 117.09      | 110.33   |
| 15  | R     | 101 | BCL  | CMD-C2D-C1D | 6.52  | 136.22      | 124.73   |
| 15  | X     | 102 | BCL  | CMD-C2D-C1D | 6.52  | 136.22      | 124.73   |
| 22  | P     | 103 | CRT  | C37-C36-C35 | -6.52 | 115.75      | 124.91   |
| 15  | G     | 102 | BCL  | C2B-C1B-NB  | 6.52  | 117.09      | 110.33   |
| 15  | E     | 102 | BCL  | C2B-C1B-NB  | 6.50  | 117.06      | 110.33   |
| 15  | Z     | 102 | BCL  | C2B-C1B-NB  | 6.48  | 117.05      | 110.33   |
| 15  | S     | 102 | BCL  | C2B-C1B-NB  | 6.48  | 117.04      | 110.33   |
| 15  | 5     | 102 | BCL  | C2B-C1B-NB  | 6.48  | 117.04      | 110.33   |
| 15  | 4     | 102 | BCL  | C2B-C1B-NB  | 6.47  | 117.04      | 110.33   |
| 15  | P     | 102 | BCL  | CMD-C2D-C1D | 6.47  | 136.13      | 124.73   |
| 15  | B     | 102 | BCL  | C2B-C1B-NB  | 6.47  | 117.03      | 110.33   |
| 15  | 0     | 101 | BCL  | C2B-C1B-NB  | 6.46  | 117.02      | 110.33   |
| 15  | T     | 101 | BCL  | C2B-C1B-NB  | 6.43  | 116.99      | 110.33   |
| 15  | A     | 502 | BCL  | C2B-C1B-NB  | 6.42  | 116.99      | 110.33   |
| 15  | L     | 301 | BCL  | C2B-C1B-NB  | 6.42  | 116.98      | 110.33   |
| 15  | 9     | 102 | BCL  | C2B-C1B-NB  | 6.42  | 116.98      | 110.33   |
| 15  | E     | 102 | BCL  | CMD-C2D-C1D | 6.41  | 136.01      | 124.73   |
| 15  | M     | 403 | BCL  | C2B-C1B-NB  | 6.39  | 116.95      | 110.33   |
| 15  | 6     | 101 | BCL  | C2B-C1B-NB  | 6.39  | 116.95      | 110.33   |
| 15  | 8     | 102 | BCL  | C2B-C1B-NB  | 6.36  | 116.92      | 110.33   |
| 15  | B     | 102 | BCL  | CMD-C2D-C1D | 6.30  | 135.82      | 124.73   |
| 22  | Y     | 101 | CRT  | C37-C36-C35 | -6.28 | 116.09      | 124.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | 3     | 101 | BCL  | C2B-C1B-NB  | 6.26  | 116.82      | 110.33   |
| 15  | 2     | 102 | BCL  | C2B-C1B-NB  | 6.26  | 116.82      | 110.33   |
| 15  | Y     | 102 | BCL  | C2B-C1B-NB  | 6.24  | 116.79      | 110.33   |
| 15  | 1     | 402 | BCL  | C2B-C1B-NB  | 6.23  | 116.78      | 110.33   |
| 22  | G     | 103 | CRT  | C37-C36-C35 | -6.22 | 116.18      | 124.91   |
| 15  | P     | 102 | BCL  | C2B-C1B-NB  | 6.21  | 116.77      | 110.33   |
| 15  | M     | 402 | BCL  | C2B-C1B-NB  | 6.21  | 116.77      | 110.33   |
| 22  | J     | 103 | CRT  | C37-C36-C35 | -6.21 | 116.20      | 124.91   |
| 22  | E     | 103 | CRT  | C37-C36-C35 | -6.21 | 116.20      | 124.91   |
| 22  | R     | 102 | CRT  | C37-C36-C35 | -6.16 | 116.26      | 124.91   |
| 15  | K     | 102 | BCL  | C2B-C1B-NB  | 6.15  | 116.71      | 110.33   |
| 15  | R     | 101 | BCL  | C2B-C1B-NB  | 6.15  | 116.70      | 110.33   |
| 15  | L     | 308 | BCL  | C2B-C1B-NB  | 6.10  | 116.65      | 110.33   |
| 22  | 0     | 102 | CRT  | C37-C36-C35 | -6.05 | 116.42      | 124.91   |
| 15  | O     | 502 | BCL  | C2B-C1B-NB  | 6.00  | 116.55      | 110.33   |
| 15  | Q     | 102 | BCL  | CHD-C1D-ND  | -5.98 | 116.38      | 124.80   |
| 15  | F     | 502 | BCL  | CHD-C1D-ND  | -5.96 | 116.41      | 124.80   |
| 15  | 5     | 102 | BCL  | CHD-C1D-ND  | -5.94 | 116.44      | 124.80   |
| 15  | K     | 102 | BCL  | CHD-C1D-ND  | -5.92 | 116.47      | 124.80   |
| 15  | L     | 308 | BCL  | CHD-C1D-ND  | -5.92 | 116.48      | 124.80   |
| 22  | V     | 102 | CRT  | C37-C36-C35 | -5.89 | 116.64      | 124.91   |
| 15  | O     | 502 | BCL  | CHD-C1D-ND  | -5.89 | 116.51      | 124.80   |
| 22  | E     | 103 | CRT  | C4-C5-C6    | -5.86 | 116.68      | 124.91   |
| 15  | I     | 101 | BCL  | CHD-C1D-ND  | -5.86 | 116.56      | 124.80   |
| 15  | Y     | 102 | BCL  | CHD-C1D-ND  | -5.85 | 116.56      | 124.80   |
| 15  | U     | 101 | BCL  | CHD-C1D-ND  | -5.83 | 116.59      | 124.80   |
| 15  | 1     | 402 | BCL  | CHD-C1D-ND  | -5.82 | 116.61      | 124.80   |
| 22  | J     | 103 | CRT  | C3-C1-C2    | 5.80  | 121.03      | 110.43   |
| 15  | M     | 403 | BCL  | CHD-C1D-ND  | -5.78 | 116.67      | 124.80   |
| 15  | W     | 101 | BCL  | CHD-C1D-ND  | -5.77 | 116.68      | 124.80   |
| 22  | V     | 102 | CRT  | C40-C38-C39 | 5.77  | 120.97      | 110.43   |
| 15  | 3     | 101 | BCL  | CHD-C1D-ND  | -5.76 | 116.69      | 124.80   |
| 22  | 2     | 103 | CRT  | C37-C36-C35 | -5.76 | 116.83      | 124.91   |
| 22  | B     | 103 | CRT  | C37-C36-C35 | -5.75 | 116.83      | 124.91   |
| 15  | M     | 403 | BCL  | O2D-CGD-CBD | 5.74  | 121.27      | 111.23   |
| 15  | D     | 102 | BCL  | CHD-C1D-ND  | -5.74 | 116.73      | 124.80   |
| 15  | M     | 402 | BCL  | O2D-CGD-CBD | 5.72  | 121.23      | 111.23   |
| 15  | 9     | 102 | BCL  | CHD-C1D-ND  | -5.68 | 116.80      | 124.80   |
| 15  | S     | 102 | BCL  | CHD-C1D-ND  | -5.62 | 116.89      | 124.80   |
| 15  | M     | 402 | BCL  | CHD-C1D-ND  | -5.61 | 116.90      | 124.80   |
| 15  | 7     | 101 | BCL  | CHD-C1D-ND  | -5.57 | 116.96      | 124.80   |
| 22  | P     | 103 | CRT  | C3-C1-C2    | 5.57  | 120.61      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | M     | 406 | CRT  | C40-C38-C39 | 5.55  | 120.58      | 110.43   |
| 15  | A     | 502 | BCL  | CHD-C1D-ND  | -5.55 | 117.00      | 124.80   |
| 10  | C     | 401 | HEM  | CHC-C4B-NB  | 5.37  | 130.21      | 124.42   |
| 22  | 2     | 103 | CRT  | C40-C38-C39 | 5.36  | 120.22      | 110.43   |
| 15  | W     | 101 | BCL  | O2D-CGD-CBD | 5.35  | 120.59      | 111.23   |
| 15  | G     | 102 | BCL  | CHD-C1D-ND  | -5.28 | 117.37      | 124.80   |
| 15  | N     | 101 | BCL  | CHD-C1D-ND  | -5.27 | 117.38      | 124.80   |
| 14  | H     | 301 | PGV  | O01-C1-C2   | 5.27  | 122.89      | 111.48   |
| 15  | Z     | 102 | BCL  | CHD-C1D-ND  | -5.26 | 117.40      | 124.80   |
| 15  | 6     | 101 | BCL  | CHD-C1D-ND  | -5.23 | 117.44      | 124.80   |
| 15  | L     | 301 | BCL  | CHD-C1D-ND  | -5.19 | 117.50      | 124.80   |
| 22  | M     | 406 | CRT  | C36-C35-C33 | -5.18 | 118.06      | 125.89   |
| 15  | S     | 102 | BCL  | O2D-CGD-CBD | 5.14  | 120.22      | 111.23   |
| 22  | Z     | 103 | CRT  | C37-C36-C35 | -5.14 | 117.70      | 124.91   |
| 15  | 9     | 102 | BCL  | C3D-C2D-C1D | -5.11 | 98.86       | 105.83   |
| 15  | O     | 502 | BCL  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 15  | I     | 101 | BCL  | O2D-CGD-CBD | 5.09  | 120.14      | 111.23   |
| 15  | K     | 102 | BCL  | C3D-C2D-C1D | -5.09 | 98.88       | 105.83   |
| 15  | M     | 403 | BCL  | C3D-C2D-C1D | -5.08 | 98.90       | 105.83   |
| 15  | S     | 102 | BCL  | C3D-C2D-C1D | -5.08 | 98.90       | 105.83   |
| 15  | Y     | 102 | BCL  | C3D-C2D-C1D | -5.07 | 98.91       | 105.83   |
| 15  | U     | 101 | BCL  | C3D-C2D-C1D | -5.06 | 98.92       | 105.83   |
| 22  | T     | 102 | CRT  | C37-C36-C35 | -5.06 | 117.80      | 124.91   |
| 15  | X     | 102 | BCL  | CHD-C1D-ND  | -5.05 | 117.69      | 124.80   |
| 15  | K     | 102 | BCL  | O2D-CGD-CBD | 5.05  | 120.06      | 111.23   |
| 15  | 4     | 102 | BCL  | CHD-C1D-ND  | -5.05 | 117.69      | 124.80   |
| 15  | J     | 102 | BCL  | CHD-C1D-ND  | -5.04 | 117.71      | 124.80   |
| 22  | M     | 406 | CRT  | C21-C22-C23 | -5.04 | 120.21      | 127.28   |
| 15  | Q     | 102 | BCL  | O2D-CGD-CBD | 5.04  | 120.03      | 111.23   |
| 15  | F     | 502 | BCL  | C3D-C2D-C1D | -5.02 | 98.97       | 105.83   |
| 15  | 1     | 402 | BCL  | C3D-C2D-C1D | -5.02 | 98.97       | 105.83   |
| 22  | G     | 103 | CRT  | C4-C5-C6    | -5.02 | 117.86      | 124.91   |
| 15  | W     | 101 | BCL  | C3D-C2D-C1D | -5.02 | 98.98       | 105.83   |
| 15  | O     | 502 | BCL  | O2D-CGD-CBD | 5.02  | 120.01      | 111.23   |
| 15  | Q     | 102 | BCL  | C3D-C2D-C1D | -5.00 | 99.01       | 105.83   |
| 15  | V     | 101 | BCL  | CHD-C1D-ND  | -5.00 | 117.77      | 124.80   |
| 15  | A     | 502 | BCL  | C3D-C2D-C1D | -4.99 | 99.02       | 105.83   |
| 22  | 6     | 102 | CRT  | C5-C6-C7    | -4.99 | 118.36      | 125.89   |
| 15  | 8     | 102 | BCL  | CHD-C1D-ND  | -4.99 | 117.78      | 124.80   |
| 15  | U     | 101 | BCL  | O2D-CGD-CBD | 4.98  | 119.94      | 111.23   |
| 15  | 2     | 102 | BCL  | CHD-C1D-ND  | -4.96 | 117.82      | 124.80   |
| 15  | 3     | 101 | BCL  | C3D-C2D-C1D | -4.96 | 99.06       | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | P     | 102 | BCL  | CHD-C1D-ND  | -4.95 | 117.83      | 124.80   |
| 15  | L     | 301 | BCL  | C3D-C2D-C1D | -4.94 | 99.09       | 105.83   |
| 15  | N     | 101 | BCL  | C3D-C2D-C1D | -4.93 | 99.10       | 105.83   |
| 15  | E     | 102 | BCL  | CHD-C1D-ND  | -4.93 | 117.86      | 124.80   |
| 15  | V     | 101 | BCL  | C3C-C4C-CHD | -4.93 | 113.00      | 123.39   |
| 15  | 5     | 102 | BCL  | C3D-C2D-C1D | -4.93 | 99.11       | 105.83   |
| 15  | D     | 102 | BCL  | C3D-C2D-C1D | -4.92 | 99.11       | 105.83   |
| 15  | 5     | 102 | BCL  | O2D-CGD-CBD | 4.91  | 119.82      | 111.23   |
| 15  | 9     | 102 | BCL  | O2D-CGD-CBD | 4.91  | 119.81      | 111.23   |
| 15  | 0     | 101 | BCL  | CHD-C1D-ND  | -4.90 | 117.91      | 124.80   |
| 22  | 2     | 103 | CRT  | C4-C5-C6    | -4.90 | 118.04      | 124.91   |
| 15  | T     | 101 | BCL  | C3C-C4C-CHD | -4.89 | 113.07      | 123.39   |
| 10  | C     | 404 | HEM  | CHC-C4B-NB  | 4.89  | 129.68      | 124.42   |
| 15  | 7     | 101 | BCL  | C3D-C2D-C1D | -4.88 | 99.17       | 105.83   |
| 10  | C     | 403 | HEM  | CHC-C4B-NB  | 4.88  | 129.68      | 124.42   |
| 15  | P     | 102 | BCL  | C3C-C4C-CHD | -4.87 | 113.12      | 123.39   |
| 15  | I     | 101 | BCL  | C3D-C2D-C1D | -4.86 | 99.19       | 105.83   |
| 22  | E     | 103 | CRT  | C21-C22-C23 | -4.85 | 120.47      | 127.28   |
| 15  | X     | 102 | BCL  | C3C-C4C-CHD | -4.85 | 113.17      | 123.39   |
| 15  | R     | 101 | BCL  | CHD-C1D-ND  | -4.85 | 117.98      | 124.80   |
| 15  | A     | 502 | BCL  | O2D-CGD-CBD | 4.84  | 119.69      | 111.23   |
| 22  | 0     | 102 | CRT  | C21-C22-C23 | -4.84 | 120.50      | 127.28   |
| 15  | B     | 102 | BCL  | C3C-C4C-CHD | -4.83 | 113.21      | 123.39   |
| 15  | 6     | 101 | BCL  | C3D-C2D-C1D | -4.83 | 99.24       | 105.83   |
| 15  | T     | 101 | BCL  | CHD-C1D-ND  | -4.80 | 118.05      | 124.80   |
| 15  | E     | 102 | BCL  | C3C-C4C-CHD | -4.79 | 113.28      | 123.39   |
| 15  | B     | 102 | BCL  | CHD-C1D-ND  | -4.79 | 118.07      | 124.80   |
| 15  | P     | 102 | BCL  | C3D-C2D-C1D | -4.78 | 99.30       | 105.83   |
| 17  | L     | 304 | UQ8  | C7-C6-C5    | 4.78  | 124.07      | 118.52   |
| 15  | 8     | 102 | BCL  | C3D-C2D-C1D | -4.77 | 99.33       | 105.83   |
| 10  | C     | 402 | HEM  | CHC-C4B-NB  | 4.77  | 129.55      | 124.42   |
| 15  | L     | 308 | BCL  | C3D-C2D-C1D | -4.76 | 99.34       | 105.83   |
| 15  | 0     | 101 | BCL  | C3C-C4C-CHD | -4.75 | 113.37      | 123.39   |
| 15  | Y     | 102 | BCL  | O2D-CGD-CBD | 4.75  | 119.53      | 111.23   |
| 15  | F     | 502 | BCL  | O2D-CGD-CBD | 4.74  | 119.52      | 111.23   |
| 15  | Z     | 102 | BCL  | C3D-C2D-C1D | -4.74 | 99.36       | 105.83   |
| 15  | D     | 102 | BCL  | O2D-CGD-CBD | 4.74  | 119.52      | 111.23   |
| 22  | N     | 102 | CRT  | C21-C22-C23 | -4.74 | 120.63      | 127.28   |
| 15  | G     | 102 | BCL  | C3D-C2D-C1D | -4.74 | 99.37       | 105.83   |
| 17  | L     | 304 | UQ8  | C7-C6-C1    | -4.73 | 116.78      | 124.89   |
| 15  | M     | 402 | BCL  | C3D-C2D-C1D | -4.73 | 99.38       | 105.83   |
| 15  | 4     | 102 | BCL  | C3C-C4C-CHD | -4.72 | 113.44      | 123.39   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | 3     | 101 | BCL  | O2D-CGD-CBD | 4.72  | 119.48      | 111.23   |
| 22  | 4     | 103 | CRT  | C37-C36-C35 | -4.72 | 118.28      | 124.91   |
| 15  | V     | 101 | BCL  | C3D-C2D-C1D | -4.72 | 99.39       | 105.83   |
| 15  | E     | 102 | BCL  | C3D-C2D-C1D | -4.71 | 99.40       | 105.83   |
| 22  | N     | 102 | CRT  | C5-C6-C7    | -4.70 | 118.78      | 125.89   |
| 15  | N     | 101 | BCL  | C3C-C4C-CHD | -4.70 | 113.49      | 123.39   |
| 15  | G     | 102 | BCL  | C3C-C4C-CHD | -4.67 | 113.55      | 123.39   |
| 15  | 4     | 102 | BCL  | C3D-C2D-C1D | -4.65 | 99.48       | 105.83   |
| 15  | B     | 102 | BCL  | C3D-C2D-C1D | -4.65 | 99.48       | 105.83   |
| 22  | V     | 102 | CRT  | C21-C22-C23 | -4.64 | 120.77      | 127.28   |
| 22  | R     | 102 | CRT  | C4-C5-C6    | -4.64 | 118.40      | 124.91   |
| 15  | 0     | 101 | BCL  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 15  | T     | 101 | BCL  | C3D-C2D-C1D | -4.62 | 99.52       | 105.83   |
| 15  | Z     | 102 | BCL  | C3C-C4C-CHD | -4.62 | 113.66      | 123.39   |
| 15  | B     | 102 | BCL  | C1-C2-C3    | -4.62 | 118.64      | 126.20   |
| 15  | X     | 102 | BCL  | C3D-C2D-C1D | -4.61 | 99.53       | 105.83   |
| 15  | R     | 101 | BCL  | C3D-C2D-C1D | -4.58 | 99.58       | 105.83   |
| 15  | 6     | 101 | BCL  | C1D-ND-C4D  | -4.55 | 103.12      | 106.31   |
| 15  | 6     | 101 | BCL  | C3C-C4C-CHD | -4.55 | 113.80      | 123.39   |
| 15  | 2     | 102 | BCL  | C3C-C4C-CHD | -4.54 | 113.83      | 123.39   |
| 22  | B     | 103 | CRT  | C21-C22-C23 | -4.53 | 120.92      | 127.28   |
| 15  | J     | 102 | BCL  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 22  | E     | 103 | CRT  | C20-C19-C17 | -4.53 | 120.93      | 127.28   |
| 15  | L     | 301 | BCL  | C3C-C4C-CHD | -4.52 | 113.85      | 123.39   |
| 15  | J     | 102 | BCL  | C3C-C4C-CHD | -4.51 | 113.88      | 123.39   |
| 15  | Z     | 102 | BCL  | C1D-ND-C4D  | -4.50 | 103.16      | 106.31   |
| 10  | C     | 401 | HEM  | CHD-C1D-ND  | 4.48  | 129.25      | 124.42   |
| 15  | L     | 308 | BCL  | O2D-CGD-CBD | 4.48  | 119.06      | 111.23   |
| 15  | 7     | 101 | BCL  | O2D-CGD-CBD | 4.47  | 119.05      | 111.23   |
| 15  | 2     | 102 | BCL  | C3D-C2D-C1D | -4.46 | 99.74       | 105.83   |
| 15  | R     | 101 | BCL  | C3C-C4C-CHD | -4.46 | 113.99      | 123.39   |
| 15  | X     | 102 | BCL  | C1D-ND-C4D  | -4.44 | 103.20      | 106.31   |
| 15  | 8     | 102 | BCL  | C3C-C4C-CHD | -4.44 | 114.04      | 123.39   |
| 22  | Z     | 103 | CRT  | C5-C6-C7    | -4.44 | 119.19      | 125.89   |
| 19  | L     | 311 | CDL  | OA6-CA5-C11 | 4.43  | 118.99      | 111.09   |
| 22  | P     | 103 | CRT  | C21-C22-C23 | -4.43 | 121.07      | 127.28   |
| 22  | M     | 406 | CRT  | C4-C5-C6    | -4.42 | 118.70      | 124.91   |
| 22  | R     | 102 | CRT  | C21-C22-C23 | -4.42 | 121.08      | 127.28   |
| 22  | V     | 102 | CRT  | C4-C5-C6    | -4.41 | 118.71      | 124.91   |
| 19  | M     | 409 | CDL  | OA6-CA5-C11 | 4.40  | 121.00      | 111.48   |
| 15  | V     | 101 | BCL  | C1D-ND-C4D  | -4.39 | 103.23      | 106.31   |
| 15  | 1     | 402 | BCL  | O2D-CGD-CBD | 4.38  | 118.88      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | I     | 101 | BCL  | C1D-ND-C4D  | -4.38 | 103.24      | 106.31   |
| 22  | Y     | 101 | CRT  | C10-C9-C7   | -4.36 | 121.17      | 127.28   |
| 15  | J     | 102 | BCL  | O2D-CGD-CBD | 4.35  | 118.83      | 111.23   |
| 22  | T     | 102 | CRT  | C21-C22-C23 | -4.35 | 121.18      | 127.28   |
| 15  | P     | 102 | BCL  | C1D-ND-C4D  | -4.35 | 103.26      | 106.31   |
| 15  | M     | 403 | BCL  | C3C-C4C-CHD | -4.34 | 114.23      | 123.39   |
| 15  | E     | 102 | BCL  | O2D-CGD-CBD | 4.34  | 118.82      | 111.23   |
| 15  | N     | 101 | BCL  | C1D-ND-C4D  | -4.34 | 103.27      | 106.31   |
| 15  | L     | 308 | BCL  | C3C-C4C-CHD | -4.34 | 114.24      | 123.39   |
| 15  | Y     | 102 | BCL  | C1D-ND-C4D  | -4.34 | 103.27      | 106.31   |
| 15  | P     | 102 | BCL  | C2D-C1D-ND  | 4.32  | 114.40      | 110.13   |
| 15  | O     | 502 | BCL  | C3C-C4C-CHD | -4.31 | 114.30      | 123.39   |
| 19  | L     | 311 | CDL  | OB6-CB5-C51 | 4.31  | 120.81      | 111.48   |
| 22  | 2     | 103 | CRT  | C21-C22-C23 | -4.28 | 121.27      | 127.28   |
| 18  | S     | 101 | LMT  | C1B-O5B-C5B | 4.27  | 122.06      | 113.72   |
| 22  | J     | 103 | CRT  | C10-C9-C7   | -4.26 | 121.30      | 127.28   |
| 15  | N     | 101 | BCL  | C2D-C1D-ND  | 4.26  | 114.34      | 110.13   |
| 14  | L     | 305 | PGV  | O01-C1-C2   | 4.25  | 120.67      | 111.48   |
| 22  | J     | 103 | CRT  | C21-C22-C23 | -4.24 | 121.33      | 127.28   |
| 22  | 4     | 103 | CRT  | C4-C5-C6    | -4.24 | 118.97      | 124.91   |
| 15  | E     | 102 | BCL  | C1D-ND-C4D  | -4.23 | 103.34      | 106.31   |
| 22  | N     | 102 | CRT  | C10-C9-C7   | -4.23 | 121.34      | 127.28   |
| 15  | L     | 308 | BCL  | C1-C2-C3    | -4.23 | 119.26      | 126.20   |
| 15  | Q     | 102 | BCL  | C1D-ND-C4D  | -4.23 | 103.35      | 106.31   |
| 15  | O     | 502 | BCL  | C3B-C4B-NB  | 4.23  | 115.34      | 109.76   |
| 15  | M     | 403 | BCL  | O2D-CGD-O1D | -4.22 | 115.63      | 123.85   |
| 15  | G     | 102 | BCL  | C1D-ND-C4D  | -4.22 | 103.35      | 106.31   |
| 15  | F     | 502 | BCL  | C1D-ND-C4D  | -4.21 | 103.36      | 106.31   |
| 16  | L     | 302 | BPH  | C4D-CHA-CBD | -4.21 | 106.44      | 108.45   |
| 15  | U     | 101 | BCL  | C1D-ND-C4D  | -4.21 | 103.36      | 106.31   |
| 15  | 1     | 402 | BCL  | C1D-ND-C4D  | -4.19 | 103.37      | 106.31   |
| 15  | B     | 102 | BCL  | C1D-ND-C4D  | -4.18 | 103.38      | 106.31   |
| 15  | X     | 102 | BCL  | C2D-C1D-ND  | 4.17  | 114.26      | 110.13   |
| 15  | 6     | 101 | BCL  | C2D-C1D-ND  | 4.16  | 114.25      | 110.13   |
| 15  | W     | 101 | BCL  | C3B-C4B-NB  | 4.16  | 115.25      | 109.76   |
| 15  | 5     | 102 | BCL  | C1D-ND-C4D  | -4.16 | 103.39      | 106.31   |
| 22  | G     | 103 | CRT  | C21-C22-C23 | -4.16 | 121.44      | 127.28   |
| 10  | C     | 402 | HEM  | CHD-C1D-ND  | 4.16  | 128.90      | 124.42   |
| 15  | R     | 101 | BCL  | C3B-C4B-NB  | 4.16  | 115.25      | 109.76   |
| 15  | V     | 101 | BCL  | C2D-C1D-ND  | 4.15  | 114.24      | 110.13   |
| 15  | K     | 102 | BCL  | C1D-ND-C4D  | -4.15 | 103.40      | 106.31   |
| 19  | M     | 407 | CDL  | OB6-CB5-C51 | 4.14  | 120.44      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | T     | 101 | BCL  | C1D-ND-C4D  | -4.14 | 103.41      | 106.31   |
| 15  | D     | 102 | BCL  | C3B-C4B-NB  | 4.13  | 115.21      | 109.76   |
| 22  | M     | 406 | CRT  | C20-C19-C17 | -4.13 | 121.48      | 127.28   |
| 19  | M     | 409 | CDL  | OB6-CB5-C51 | 4.13  | 120.42      | 111.48   |
| 15  | O     | 502 | BCL  | C1D-ND-C4D  | -4.13 | 103.42      | 106.31   |
| 15  | 0     | 101 | BCL  | C1D-ND-C4D  | -4.12 | 103.42      | 106.31   |
| 19  | D     | 101 | CDL  | OA6-CA5-C11 | 4.12  | 120.39      | 111.48   |
| 22  | T     | 102 | CRT  | C5-C6-C7    | -4.12 | 119.67      | 125.89   |
| 15  | 6     | 101 | BCL  | O2D-CGD-CBD | 4.11  | 118.41      | 111.23   |
| 15  | Q     | 102 | BCL  | C3C-C4C-CHD | -4.10 | 114.74      | 123.39   |
| 15  | E     | 102 | BCL  | C2D-C1D-ND  | 4.10  | 114.19      | 110.13   |
| 15  | U     | 101 | BCL  | C3B-C4B-NB  | 4.10  | 115.16      | 109.76   |
| 15  | D     | 102 | BCL  | C3C-C4C-CHD | -4.09 | 114.76      | 123.39   |
| 15  | 2     | 102 | BCL  | C3B-C4B-NB  | 4.09  | 115.16      | 109.76   |
| 10  | C     | 404 | HEM  | CHD-C1D-ND  | 4.08  | 128.82      | 124.42   |
| 15  | G     | 102 | BCL  | C2D-C1D-ND  | 4.08  | 114.17      | 110.13   |
| 15  | W     | 101 | BCL  | C3C-C4C-CHD | -4.08 | 114.79      | 123.39   |
| 15  | 5     | 102 | BCL  | C1-C2-C3    | -4.07 | 119.53      | 126.20   |
| 22  | 9     | 101 | CRT  | C21-C22-C23 | -4.07 | 121.57      | 127.28   |
| 14  | 1     | 401 | PGV  | O01-C1-C2   | 4.07  | 120.28      | 111.48   |
| 22  | N     | 102 | CRT  | C20-C19-C17 | -4.06 | 121.58      | 127.28   |
| 15  | W     | 101 | BCL  | C1D-ND-C4D  | -4.06 | 103.47      | 106.31   |
| 15  | 7     | 101 | BCL  | C3B-C4B-NB  | 4.06  | 115.11      | 109.76   |
| 15  | Y     | 102 | BCL  | C3B-C4B-NB  | 4.05  | 115.11      | 109.76   |
| 15  | 8     | 102 | BCL  | C1D-ND-C4D  | -4.05 | 103.47      | 106.31   |
| 15  | M     | 402 | BCL  | C3C-C4C-CHD | -4.04 | 114.87      | 123.39   |
| 15  | Z     | 102 | BCL  | C2D-C1D-ND  | 4.04  | 114.12      | 110.13   |
| 15  | V     | 101 | BCL  | C1-C2-C3    | -4.04 | 119.58      | 126.20   |
| 15  | S     | 102 | BCL  | C3C-C4C-CHD | -4.04 | 114.88      | 123.39   |
| 15  | 4     | 102 | BCL  | C1D-ND-C4D  | -4.04 | 103.48      | 106.31   |
| 15  | B     | 102 | BCL  | C3B-C4B-NB  | 4.04  | 115.08      | 109.76   |
| 15  | E     | 102 | BCL  | C3B-C4B-NB  | 4.03  | 115.08      | 109.76   |
| 15  | T     | 101 | BCL  | C2D-C1D-ND  | 4.03  | 114.11      | 110.13   |
| 15  | T     | 101 | BCL  | C3B-C4B-NB  | 4.03  | 115.07      | 109.76   |
| 15  | 8     | 102 | BCL  | C2D-C1D-ND  | 4.03  | 114.11      | 110.13   |
| 22  | P     | 103 | CRT  | C5-C6-C7    | -4.02 | 119.82      | 125.89   |
| 14  | A     | 501 | PGV  | O01-C1-C2   | 4.02  | 120.17      | 111.48   |
| 14  | F     | 501 | PGV  | O01-C1-C2   | 4.01  | 120.16      | 111.48   |
| 15  | 4     | 102 | BCL  | O2D-CGD-CBD | 4.01  | 118.25      | 111.23   |
| 22  | 6     | 102 | CRT  | C10-C9-C7   | -4.01 | 121.65      | 127.28   |
| 15  | 7     | 101 | BCL  | C1D-ND-C4D  | -4.01 | 103.50      | 106.31   |
| 15  | O     | 502 | BCL  | C2D-C1D-ND  | 4.01  | 114.10      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | A     | 502 | BCL  | C1D-ND-C4D  | -4.01 | 103.50      | 106.31   |
| 10  | C     | 403 | HEM  | CHD-C1D-ND  | 4.00  | 128.73      | 124.42   |
| 15  | U     | 101 | BCL  | C3C-C4C-CHD | -3.99 | 114.97      | 123.39   |
| 18  | 5     | 101 | LMT  | C1-O1'-C1'  | -3.99 | 106.86      | 113.68   |
| 15  | B     | 102 | BCL  | C2D-C1D-ND  | 3.99  | 114.08      | 110.13   |
| 15  | S     | 102 | BCL  | C1D-ND-C4D  | -3.99 | 103.51      | 106.31   |
| 15  | 0     | 101 | BCL  | O2D-CGD-CBD | 3.99  | 118.20      | 111.23   |
| 15  | 0     | 101 | BCL  | C2D-C1D-ND  | 3.98  | 114.06      | 110.13   |
| 22  | Z     | 103 | CRT  | C10-C9-C7   | -3.98 | 121.70      | 127.28   |
| 22  | 0     | 102 | CRT  | C4-C5-C6    | -3.98 | 119.33      | 124.91   |
| 15  | 2     | 102 | BCL  | C1D-ND-C4D  | -3.98 | 103.52      | 106.31   |
| 22  | 4     | 103 | CRT  | C29-C28-C30 | 3.97  | 124.16      | 118.09   |
| 15  | 9     | 102 | BCL  | C1D-ND-C4D  | -3.97 | 103.53      | 106.31   |
| 15  | X     | 102 | BCL  | C3B-C4B-NB  | 3.96  | 114.98      | 109.76   |
| 15  | G     | 102 | BCL  | C3B-C4B-NB  | 3.95  | 114.98      | 109.76   |
| 19  | H     | 302 | CDL  | OB6-CB5-C51 | 3.95  | 120.03      | 111.48   |
| 15  | J     | 102 | BCL  | C1D-ND-C4D  | -3.95 | 103.54      | 106.31   |
| 15  | M     | 402 | BCL  | C1D-ND-C4D  | -3.94 | 103.55      | 106.31   |
| 15  | 9     | 102 | BCL  | C3C-C4C-CHD | -3.94 | 115.09      | 123.39   |
| 15  | Y     | 102 | BCL  | C2D-C1D-ND  | 3.94  | 114.02      | 110.13   |
| 14  | M     | 408 | PGV  | O01-C1-C2   | 3.93  | 119.98      | 111.48   |
| 15  | 0     | 101 | BCL  | C1-C2-C3    | -3.93 | 119.76      | 126.20   |
| 15  | Z     | 102 | BCL  | C3B-C4B-NB  | 3.92  | 114.94      | 109.76   |
| 15  | N     | 101 | BCL  | C3B-C4B-NB  | 3.92  | 114.93      | 109.76   |
| 15  | I     | 101 | BCL  | C3B-C4B-NB  | 3.92  | 114.93      | 109.76   |
| 22  | Z     | 103 | CRT  | C21-C22-C23 | -3.91 | 121.79      | 127.28   |
| 15  | S     | 102 | BCL  | C2D-C1D-ND  | 3.91  | 113.99      | 110.13   |
| 15  | 1     | 402 | BCL  | C3B-C4B-NB  | 3.91  | 114.92      | 109.76   |
| 15  | N     | 101 | BCL  | O2D-CGD-CBD | 3.91  | 118.06      | 111.23   |
| 15  | S     | 102 | BCL  | C3B-C4B-NB  | 3.91  | 114.91      | 109.76   |
| 15  | P     | 102 | BCL  | C1-C2-C3    | -3.90 | 119.80      | 126.20   |
| 22  | T     | 102 | CRT  | C10-C9-C7   | -3.90 | 121.81      | 127.28   |
| 15  | 8     | 102 | BCL  | C3B-C4B-NB  | 3.90  | 114.91      | 109.76   |
| 15  | 9     | 102 | BCL  | C3B-C4B-NB  | 3.89  | 114.90      | 109.76   |
| 15  | 1     | 402 | BCL  | C2D-C1D-ND  | 3.89  | 113.98      | 110.13   |
| 15  | 5     | 102 | BCL  | C3B-C4B-NB  | 3.89  | 114.89      | 109.76   |
| 15  | K     | 102 | BCL  | C2D-C1D-ND  | 3.89  | 113.97      | 110.13   |
| 15  | A     | 502 | BCL  | C2D-C1D-ND  | 3.89  | 113.97      | 110.13   |
| 15  | Y     | 102 | BCL  | C3C-C4C-CHD | -3.88 | 115.20      | 123.39   |
| 15  | W     | 101 | BCL  | C2D-C1D-ND  | 3.88  | 113.97      | 110.13   |
| 15  | Q     | 102 | BCL  | C3B-C4B-NB  | 3.88  | 114.88      | 109.76   |
| 15  | 6     | 101 | BCL  | C3B-C4B-NB  | 3.88  | 114.88      | 109.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | C     | 408 | PGV  | O01-C1-C2   | 3.87  | 119.86      | 111.48   |
| 22  | 6     | 102 | CRT  | C20-C19-C17 | -3.87 | 121.85      | 127.28   |
| 15  | Z     | 102 | BCL  | O2D-CGD-CBD | 3.87  | 117.99      | 111.23   |
| 15  | 0     | 101 | BCL  | C3B-C4B-NB  | 3.87  | 114.86      | 109.76   |
| 15  | J     | 102 | BCL  | C3B-C4B-NB  | 3.87  | 114.86      | 109.76   |
| 15  | Q     | 102 | BCL  | C2D-C1D-ND  | 3.86  | 113.95      | 110.13   |
| 15  | V     | 101 | BCL  | C3B-C4B-NB  | 3.86  | 114.85      | 109.76   |
| 15  | 5     | 102 | BCL  | C2D-C1D-ND  | 3.86  | 113.95      | 110.13   |
| 22  | 9     | 101 | CRT  | C8-C7-C6    | 3.86  | 123.98      | 118.09   |
| 15  | P     | 102 | BCL  | C3B-C4B-NB  | 3.85  | 114.84      | 109.76   |
| 15  | K     | 102 | BCL  | C3B-C4B-NB  | 3.85  | 114.83      | 109.76   |
| 15  | L     | 301 | BCL  | C1D-ND-C4D  | -3.84 | 103.62      | 106.31   |
| 15  | L     | 301 | BCL  | C2D-C1D-ND  | 3.84  | 113.92      | 110.13   |
| 15  | F     | 502 | BCL  | C2D-C1D-ND  | 3.84  | 113.92      | 110.13   |
| 21  | M     | 405 | MQ8  | C45-C43-C44 | 3.83  | 121.88      | 115.23   |
| 22  | 4     | 103 | CRT  | C21-C22-C23 | -3.83 | 121.90      | 127.28   |
| 15  | 9     | 102 | BCL  | C2D-C1D-ND  | 3.82  | 113.91      | 110.13   |
| 15  | 4     | 102 | BCL  | C2D-C1D-ND  | 3.82  | 113.91      | 110.13   |
| 15  | A     | 502 | BCL  | C3C-C4C-CHD | -3.82 | 115.34      | 123.39   |
| 15  | U     | 101 | BCL  | C2D-C1D-ND  | 3.82  | 113.90      | 110.13   |
| 15  | B     | 102 | BCL  | O2D-CGD-CBD | 3.82  | 117.90      | 111.23   |
| 14  | L     | 310 | PGV  | O01-C1-C2   | 3.81  | 119.73      | 111.48   |
| 15  | D     | 102 | BCL  | C1D-ND-C4D  | -3.81 | 103.64      | 106.31   |
| 15  | 3     | 101 | BCL  | C1D-ND-C4D  | -3.81 | 103.64      | 106.31   |
| 15  | K     | 102 | BCL  | C1-C2-C3    | -3.80 | 119.96      | 126.20   |
| 15  | R     | 101 | BCL  | C1D-ND-C4D  | -3.80 | 103.64      | 106.31   |
| 15  | A     | 502 | BCL  | C3B-C4B-NB  | 3.80  | 114.78      | 109.76   |
| 15  | 4     | 102 | BCL  | C3B-C4B-NB  | 3.80  | 114.78      | 109.76   |
| 15  | 3     | 101 | BCL  | C3B-C4B-NB  | 3.80  | 114.78      | 109.76   |
| 15  | 2     | 102 | BCL  | O2D-CGD-CBD | 3.80  | 117.87      | 111.23   |
| 15  | M     | 402 | BCL  | C2D-C1D-ND  | 3.80  | 113.88      | 110.13   |
| 15  | L     | 301 | BCL  | C3B-C4B-NB  | 3.80  | 114.77      | 109.76   |
| 15  | Y     | 102 | BCL  | C1-C2-C3    | -3.79 | 119.99      | 126.20   |
| 15  | F     | 502 | BCL  | C3B-C4B-NB  | 3.79  | 114.76      | 109.76   |
| 15  | J     | 102 | BCL  | C2D-C1D-ND  | 3.79  | 113.88      | 110.13   |
| 15  | 2     | 102 | BCL  | C2D-C1D-ND  | 3.79  | 113.88      | 110.13   |
| 14  | A     | 503 | PGV  | O01-C1-C2   | 3.79  | 119.67      | 111.48   |
| 15  | 7     | 101 | BCL  | C2D-C1D-ND  | 3.78  | 113.87      | 110.13   |
| 10  | C     | 401 | HEM  | CHA-C4D-ND  | 3.78  | 129.04      | 124.37   |
| 15  | M     | 402 | BCL  | C3B-C4B-NB  | 3.78  | 114.75      | 109.76   |
| 15  | I     | 101 | BCL  | C2D-C1D-ND  | 3.76  | 113.85      | 110.13   |
| 15  | D     | 102 | BCL  | C2D-C1D-ND  | 3.74  | 113.83      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | R     | 101 | BCL  | C2D-C1D-ND  | 3.74  | 113.83      | 110.13   |
| 15  | 7     | 101 | BCL  | C1-C2-C3    | -3.74 | 120.08      | 126.20   |
| 15  | 1     | 402 | BCL  | C3C-C4C-CHD | -3.73 | 115.53      | 123.39   |
| 22  | Y     | 101 | CRT  | C20-C19-C17 | -3.73 | 122.05      | 127.28   |
| 15  | G     | 102 | BCL  | O2D-CGD-CBD | 3.72  | 117.73      | 111.23   |
| 15  | K     | 102 | BCL  | C3C-C4C-CHD | -3.71 | 115.57      | 123.39   |
| 18  | 5     | 101 | LMT  | O1'-C1'-C2' | 3.70  | 113.90      | 108.27   |
| 15  | P     | 102 | BCL  | O2D-CGD-CBD | 3.70  | 117.70      | 111.23   |
| 15  | F     | 502 | BCL  | C3C-C4C-CHD | -3.70 | 115.59      | 123.39   |
| 15  | I     | 101 | BCL  | C3D-C4D-ND  | 3.69  | 115.99      | 109.99   |
| 15  | 8     | 102 | BCL  | O2D-CGD-CBD | 3.69  | 117.67      | 111.23   |
| 18  | G     | 101 | LMT  | C1B-O1B-C4' | -3.69 | 109.24      | 117.98   |
| 19  | D     | 101 | CDL  | OB6-CB5-C51 | 3.68  | 119.45      | 111.48   |
| 14  | Q     | 101 | PGV  | O01-C1-C2   | 3.68  | 119.44      | 111.48   |
| 15  | I     | 101 | BCL  | C1-C2-C3    | -3.65 | 120.22      | 126.20   |
| 22  | Z     | 103 | CRT  | C20-C19-C17 | -3.64 | 122.18      | 127.28   |
| 15  | M     | 402 | BCL  | C3D-C4D-ND  | 3.63  | 115.89      | 109.99   |
| 15  | 3     | 101 | BCL  | C2D-C1D-ND  | 3.63  | 113.72      | 110.13   |
| 17  | L     | 303 | UQ8  | C12-C13-C14 | -3.62 | 119.33      | 127.62   |
| 22  | 2     | 103 | CRT  | C20-C19-C17 | -3.62 | 122.20      | 127.28   |
| 16  | M     | 404 | BPH  | C4D-CHA-CBD | -3.61 | 106.72      | 108.45   |
| 15  | 6     | 101 | BCL  | C4-C3-C5    | 3.61  | 121.49      | 115.23   |
| 15  | T     | 101 | BCL  | O2D-CGD-CBD | 3.60  | 117.53      | 111.23   |
| 15  | X     | 102 | BCL  | C1-C2-C3    | -3.59 | 120.32      | 126.20   |
| 15  | X     | 102 | BCL  | O2D-CGD-CBD | 3.58  | 117.50      | 111.23   |
| 15  | 6     | 101 | BCL  | C3D-C4D-ND  | 3.56  | 115.77      | 109.99   |
| 15  | M     | 403 | BCL  | C1D-ND-C4D  | -3.56 | 103.82      | 106.31   |
| 14  | L     | 306 | PGV  | O01-C1-C2   | 3.56  | 119.17      | 111.48   |
| 22  | Y     | 101 | CRT  | C5-C6-C7    | -3.55 | 120.52      | 125.89   |
| 22  | G     | 103 | CRT  | C32-C31-C30 | -3.55 | 112.91      | 123.20   |
| 15  | Q     | 102 | BCL  | C3D-C4D-ND  | 3.55  | 115.76      | 109.99   |
| 15  | L     | 308 | BCL  | C2D-C1D-ND  | 3.55  | 113.64      | 110.13   |
| 10  | C     | 403 | HEM  | CHA-C4D-ND  | 3.55  | 128.76      | 124.37   |
| 15  | X     | 102 | BCL  | C3D-C4D-ND  | 3.54  | 115.75      | 109.99   |
| 15  | Y     | 102 | BCL  | C3D-C4D-ND  | 3.54  | 115.75      | 109.99   |
| 10  | C     | 402 | HEM  | CHB-C1B-NB  | 3.54  | 128.75      | 124.37   |
| 15  | I     | 101 | BCL  | C3C-C4C-CHD | -3.52 | 115.97      | 123.39   |
| 15  | Z     | 102 | BCL  | C3D-C4D-ND  | 3.52  | 115.71      | 109.99   |
| 15  | F     | 502 | BCL  | C3D-C4D-ND  | 3.52  | 115.70      | 109.99   |
| 15  | M     | 403 | BCL  | C2D-C1D-ND  | 3.52  | 113.61      | 110.13   |
| 15  | 7     | 101 | BCL  | C3C-C4C-CHD | -3.51 | 115.99      | 123.39   |
| 19  | H     | 302 | CDL  | OA6-CA5-C11 | 3.51  | 119.07      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | C     | 404 | HEM  | CHA-C4D-ND  | 3.50  | 128.70      | 124.37   |
| 15  | Q     | 102 | BCL  | C4-C3-C5    | 3.50  | 121.30      | 115.23   |
| 22  | P     | 103 | CRT  | C32-C31-C30 | -3.50 | 113.06      | 123.20   |
| 15  | 1     | 402 | BCL  | C3D-C4D-ND  | 3.50  | 115.67      | 109.99   |
| 22  | B     | 103 | CRT  | C4-C5-C6    | -3.49 | 120.01      | 124.91   |
| 15  | V     | 101 | BCL  | C3D-C4D-ND  | 3.49  | 115.66      | 109.99   |
| 15  | R     | 101 | BCL  | O2D-CGD-CBD | 3.48  | 117.32      | 111.23   |
| 15  | 5     | 102 | BCL  | C3C-C4C-CHD | -3.48 | 116.06      | 123.39   |
| 15  | U     | 101 | BCL  | C3D-C4D-ND  | 3.48  | 115.64      | 109.99   |
| 15  | Z     | 102 | BCL  | C1-C2-C3    | -3.47 | 120.51      | 126.20   |
| 15  | 7     | 101 | BCL  | C3D-C4D-ND  | 3.46  | 115.62      | 109.99   |
| 15  | W     | 101 | BCL  | C3D-C4D-ND  | 3.46  | 115.61      | 109.99   |
| 15  | K     | 102 | BCL  | C3D-C4D-ND  | 3.46  | 115.61      | 109.99   |
| 15  | 5     | 102 | BCL  | C3D-C4D-ND  | 3.45  | 115.59      | 109.99   |
| 15  | L     | 308 | BCL  | C3D-C4D-ND  | 3.44  | 115.59      | 109.99   |
| 15  | J     | 102 | BCL  | C3D-C4D-ND  | 3.44  | 115.58      | 109.99   |
| 15  | 4     | 102 | BCL  | C3D-C4D-ND  | 3.44  | 115.57      | 109.99   |
| 15  | G     | 102 | BCL  | C3D-C4D-ND  | 3.44  | 115.57      | 109.99   |
| 22  | E     | 103 | CRT  | C26-C27-C28 | -3.43 | 122.46      | 127.28   |
| 22  | P     | 103 | CRT  | C20-C19-C17 | -3.43 | 122.46      | 127.28   |
| 15  | 3     | 101 | BCL  | C3C-C4C-CHD | -3.43 | 116.15      | 123.39   |
| 15  | L     | 308 | BCL  | C1D-ND-C4D  | -3.43 | 103.91      | 106.31   |
| 17  | L     | 304 | UQ8  | C37-C38-C39 | -3.42 | 119.79      | 127.62   |
| 22  | J     | 103 | CRT  | C5-C6-C7    | -3.42 | 120.72      | 125.89   |
| 15  | N     | 101 | BCL  | C3D-C4D-ND  | 3.42  | 115.54      | 109.99   |
| 15  | D     | 102 | BCL  | C3D-C4D-ND  | 3.41  | 115.54      | 109.99   |
| 15  | O     | 502 | BCL  | C3D-C4D-ND  | 3.41  | 115.53      | 109.99   |
| 15  | B     | 102 | BCL  | C3D-C4D-ND  | 3.41  | 115.53      | 109.99   |
| 22  | T     | 102 | CRT  | C20-C19-C17 | -3.41 | 122.50      | 127.28   |
| 15  | A     | 502 | BCL  | C3D-C4D-ND  | 3.41  | 115.53      | 109.99   |
| 15  | M     | 403 | BCL  | C3B-C4B-NB  | 3.40  | 114.25      | 109.76   |
| 17  | L     | 303 | UQ8  | C7-C8-C9    | -3.40 | 120.97      | 126.83   |
| 15  | 2     | 102 | BCL  | C3D-C4D-ND  | 3.40  | 115.51      | 109.99   |
| 22  | Z     | 103 | CRT  | C15-C14-C12 | -3.39 | 122.52      | 127.28   |
| 15  | E     | 102 | BCL  | C3D-C4D-ND  | 3.39  | 115.49      | 109.99   |
| 10  | C     | 401 | HEM  | CHB-C1B-NB  | 3.39  | 128.56      | 124.37   |
| 15  | T     | 101 | BCL  | C3D-C4D-ND  | 3.38  | 115.48      | 109.99   |
| 22  | Y     | 101 | CRT  | C4-C5-C6    | -3.38 | 120.17      | 124.91   |
| 15  | P     | 102 | BCL  | C3D-C4D-ND  | 3.38  | 115.48      | 109.99   |
| 15  | 8     | 102 | BCL  | C1-C2-C3    | -3.37 | 120.67      | 126.20   |
| 14  | F     | 501 | PGV  | C02-O01-C1  | -3.37 | 109.73      | 117.80   |
| 10  | C     | 402 | HEM  | CHA-C4D-ND  | 3.37  | 128.53      | 124.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | P     | 103 | CRT  | C15-C14-C12 | -3.37 | 122.56      | 127.28   |
| 15  | V     | 101 | BCL  | O2D-CGD-CBD | 3.36  | 117.11      | 111.23   |
| 15  | R     | 101 | BCL  | C3D-C4D-ND  | 3.36  | 115.45      | 109.99   |
| 15  | M     | 403 | BCL  | C3D-C4D-ND  | 3.36  | 115.44      | 109.99   |
| 15  | L     | 308 | BCL  | C3B-C4B-NB  | 3.35  | 114.19      | 109.76   |
| 15  | 0     | 101 | BCL  | C3D-C4D-ND  | 3.35  | 115.43      | 109.99   |
| 22  | 9     | 101 | CRT  | C10-C9-C7   | -3.34 | 122.59      | 127.28   |
| 22  | M     | 406 | CRT  | C37-C36-C35 | -3.33 | 120.23      | 124.91   |
| 21  | M     | 405 | MQ8  | C41-C42-C43 | -3.33 | 120.00      | 127.62   |
| 15  | S     | 102 | BCL  | C3D-C4D-ND  | 3.33  | 115.40      | 109.99   |
| 15  | 8     | 102 | BCL  | C3D-C4D-ND  | 3.33  | 115.40      | 109.99   |
| 17  | L     | 304 | UQ8  | C27-C28-C29 | -3.33 | 120.00      | 127.62   |
| 17  | L     | 304 | UQ8  | C7-C8-C9    | -3.32 | 121.11      | 126.83   |
| 22  | B     | 103 | CRT  | C32-C31-C30 | -3.30 | 113.64      | 123.20   |
| 17  | L     | 304 | UQ8  | C17-C18-C19 | -3.29 | 120.09      | 127.62   |
| 15  | Q     | 102 | BCL  | C1-C2-C3    | -3.29 | 120.81      | 126.20   |
| 22  | 6     | 102 | CRT  | C32-C31-C30 | -3.29 | 113.68      | 123.20   |
| 15  | 3     | 101 | BCL  | C3D-C4D-ND  | 3.27  | 115.31      | 109.99   |
| 10  | C     | 401 | HEM  | C1B-NB-C4B  | 3.27  | 109.08      | 105.21   |
| 22  | M     | 406 | CRT  | C10-C9-C7   | -3.27 | 122.70      | 127.28   |
| 15  | T     | 101 | BCL  | C1C-NC-C4C  | -3.26 | 105.19      | 106.68   |
| 22  | 9     | 101 | CRT  | C20-C19-C17 | -3.25 | 122.71      | 127.28   |
| 10  | C     | 403 | HEM  | C1B-NB-C4B  | 3.25  | 109.06      | 105.21   |
| 15  | R     | 101 | BCL  | C1C-NC-C4C  | -3.25 | 105.19      | 106.68   |
| 15  | N     | 101 | BCL  | C4-C3-C5    | 3.25  | 120.87      | 115.23   |
| 22  | V     | 102 | CRT  | O2-C38-C39  | -3.25 | 86.65       | 108.97   |
| 15  | 8     | 102 | BCL  | O2A-CGA-CBA | 3.24  | 121.72      | 111.83   |
| 15  | 1     | 402 | BCL  | C4-C3-C5    | 3.24  | 120.85      | 115.23   |
| 15  | L     | 301 | BCL  | O2A-CGA-CBA | 3.24  | 121.71      | 111.83   |
| 17  | L     | 303 | UQ8  | C15-C14-C16 | 3.23  | 120.83      | 115.23   |
| 15  | L     | 301 | BCL  | O2D-CGD-CBD | 3.23  | 116.87      | 111.23   |
| 15  | M     | 402 | BCL  | C1-C2-C3    | -3.21 | 120.93      | 126.20   |
| 21  | M     | 405 | MQ8  | C36-C37-C38 | -3.21 | 120.28      | 127.62   |
| 15  | 9     | 102 | BCL  | C3D-C4D-ND  | 3.21  | 115.20      | 109.99   |
| 22  | M     | 406 | CRT  | O2-C38-C40  | -3.20 | 86.96       | 108.97   |
| 14  | A     | 503 | PGV  | C02-O01-C1  | -3.20 | 110.14      | 117.80   |
| 15  | L     | 301 | BCL  | C3D-C4D-ND  | 3.19  | 115.17      | 109.99   |
| 22  | 0     | 102 | CRT  | C32-C31-C30 | -3.17 | 114.01      | 123.20   |
| 10  | C     | 402 | HEM  | C1B-NB-C4B  | 3.17  | 108.96      | 105.21   |
| 21  | M     | 405 | MQ8  | C34-C33-C35 | 3.17  | 120.73      | 115.23   |
| 22  | 9     | 101 | CRT  | C32-C31-C30 | -3.17 | 114.02      | 123.20   |
| 22  | Y     | 101 | CRT  | C21-C22-C23 | -3.17 | 122.84      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | 2     | 102 | BCL  | C4-C3-C5    | 3.16  | 120.72      | 115.23   |
| 17  | L     | 309 | UQ8  | C7-C8-C9    | -3.16 | 121.39      | 126.83   |
| 22  | J     | 103 | CRT  | C20-C19-C17 | -3.16 | 122.85      | 127.28   |
| 22  | 6     | 102 | CRT  | C4-C5-C6    | -3.15 | 120.48      | 124.91   |
| 15  | M     | 403 | BCL  | CAA-C2A-C3A | -3.15 | 104.49      | 113.00   |
| 22  | T     | 102 | CRT  | C15-C14-C12 | -3.15 | 122.86      | 127.28   |
| 15  | 4     | 102 | BCL  | C1-C2-C3    | -3.15 | 121.04      | 126.20   |
| 15  | 3     | 101 | BCL  | C1C-NC-C4C  | -3.15 | 105.24      | 106.68   |
| 22  | E     | 103 | CRT  | C32-C31-C30 | -3.14 | 114.09      | 123.20   |
| 15  | 2     | 102 | BCL  | C1-C2-C3    | -3.14 | 121.05      | 126.20   |
| 15  | U     | 101 | BCL  | C1-C2-C3    | -3.14 | 121.05      | 126.20   |
| 15  | L     | 301 | BCL  | CED-O2D-CGD | 3.13  | 123.01      | 115.92   |
| 22  | V     | 102 | CRT  | C20-C19-C17 | -3.12 | 122.90      | 127.28   |
| 15  | 3     | 101 | BCL  | C4-C3-C5    | 3.12  | 120.64      | 115.23   |
| 10  | C     | 404 | HEM  | CHB-C1B-NB  | 3.12  | 128.22      | 124.37   |
| 15  | 2     | 102 | BCL  | O2A-CGA-CBA | 3.12  | 121.34      | 111.83   |
| 15  | J     | 102 | BCL  | C1-C2-C3    | -3.12 | 121.09      | 126.20   |
| 22  | B     | 103 | CRT  | C5-C6-C7    | -3.12 | 121.18      | 125.89   |
| 15  | X     | 102 | BCL  | O2A-CGA-CBA | 3.12  | 121.33      | 111.83   |
| 15  | L     | 301 | BCL  | C1-C2-C3    | -3.10 | 121.12      | 126.20   |
| 15  | G     | 102 | BCL  | O2A-CGA-CBA | 3.10  | 121.29      | 111.83   |
| 17  | L     | 304 | UQ8  | C12-C13-C14 | -3.10 | 120.53      | 127.62   |
| 15  | J     | 102 | BCL  | C4-C3-C5    | 3.10  | 120.60      | 115.23   |
| 22  | V     | 102 | CRT  | C9-C10-C11  | -3.09 | 114.26      | 123.20   |
| 17  | L     | 304 | UQ8  | C1M-C1-C6   | -3.08 | 119.38      | 124.45   |
| 15  | 6     | 101 | BCL  | O2A-CGA-CBA | 3.08  | 121.22      | 111.83   |
| 22  | 6     | 102 | CRT  | C21-C22-C23 | -3.07 | 122.97      | 127.28   |
| 22  | R     | 102 | CRT  | C32-C31-C30 | -3.06 | 114.33      | 123.20   |
| 22  | R     | 102 | CRT  | C9-C10-C11  | -3.05 | 114.36      | 123.20   |
| 18  | E     | 101 | LMT  | C1B-O1B-C4' | -3.05 | 110.75      | 117.98   |
| 22  | J     | 103 | CRT  | C32-C31-C30 | -3.04 | 114.38      | 123.20   |
| 22  | Z     | 103 | CRT  | C31-C32-C33 | -3.04 | 123.01      | 127.28   |
| 15  | M     | 402 | BCL  | C1C-NC-C4C  | -3.04 | 105.29      | 106.68   |
| 15  | O     | 502 | BCL  | CHC-C1C-NC  | 3.04  | 128.79      | 124.40   |
| 14  | L     | 305 | PGV  | C02-O01-C1  | -3.03 | 110.54      | 117.80   |
| 22  | M     | 406 | CRT  | C32-C31-C30 | -3.02 | 114.44      | 123.20   |
| 15  | D     | 102 | BCL  | CHC-C1C-NC  | 3.02  | 128.76      | 124.40   |
| 22  | R     | 102 | CRT  | C13-C12-C11 | 3.02  | 122.70      | 118.09   |
| 14  | L     | 310 | PGV  | O03-C19-C20 | 3.02  | 121.04      | 111.83   |
| 22  | E     | 103 | CRT  | C9-C10-C11  | -3.02 | 114.46      | 123.20   |
| 21  | M     | 405 | MQ8  | C29-C28-C30 | 3.02  | 120.46      | 115.23   |
| 22  | V     | 102 | CRT  | C14-C15-C16 | -3.01 | 114.47      | 123.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 2     | 103 | CRT  | O2-C38-C40  | -3.00 | 88.31       | 108.97   |
| 14  | H     | 301 | PGV  | O03-C19-C20 | 3.00  | 120.99      | 111.83   |
| 15  | 4     | 102 | BCL  | CHB-C4A-NA  | 3.00  | 128.73      | 124.40   |
| 22  | E     | 103 | CRT  | C14-C15-C16 | -3.00 | 114.51      | 123.20   |
| 15  | 1     | 402 | BCL  | C1-C2-C3    | -2.99 | 121.29      | 126.20   |
| 15  | U     | 101 | BCL  | C4-C3-C5    | 2.99  | 120.42      | 115.23   |
| 15  | E     | 102 | BCL  | O2A-CGA-CBA | 2.99  | 120.94      | 111.83   |
| 22  | V     | 102 | CRT  | O2-C38-C40  | -2.99 | 88.43       | 108.97   |
| 14  | H     | 301 | PGV  | C02-O01-C1  | -2.99 | 110.65      | 117.80   |
| 14  | M     | 408 | PGV  | C02-O01-C1  | -2.98 | 110.65      | 117.80   |
| 22  | 2     | 103 | CRT  | O2-C38-C39  | -2.98 | 88.45       | 108.97   |
| 14  | A     | 501 | PGV  | C02-O01-C1  | -2.98 | 110.66      | 117.80   |
| 22  | 4     | 103 | CRT  | C36-C35-C33 | -2.98 | 121.39      | 125.89   |
| 22  | P     | 103 | CRT  | C10-C9-C7   | -2.98 | 123.10      | 127.28   |
| 15  | M     | 403 | BCL  | O2A-CGA-CBA | 2.98  | 120.92      | 111.83   |
| 19  | L     | 311 | CDL  | CB4-OB6-CB5 | -2.98 | 110.67      | 117.80   |
| 19  | M     | 409 | CDL  | OB8-CB7-C71 | 2.97  | 120.90      | 111.83   |
| 17  | L     | 309 | UQ8  | C12-C13-C14 | -2.97 | 120.82      | 127.62   |
| 15  | X     | 102 | BCL  | CHB-C4A-NA  | 2.97  | 128.69      | 124.40   |
| 15  | E     | 102 | BCL  | C1C-NC-C4C  | -2.97 | 105.32      | 106.68   |
| 15  | Y     | 102 | BCL  | CHC-C1C-NC  | 2.97  | 128.68      | 124.40   |
| 17  | L     | 304 | UQ8  | C32-C33-C34 | -2.96 | 120.84      | 127.62   |
| 15  | 0     | 101 | BCL  | CHB-C4A-NA  | 2.96  | 128.68      | 124.40   |
| 14  | Q     | 101 | PGV  | O03-C19-C20 | 2.96  | 120.87      | 111.83   |
| 22  | R     | 102 | CRT  | C20-C19-C17 | -2.96 | 123.13      | 127.28   |
| 15  | A     | 502 | BCL  | C4-C3-C5    | 2.96  | 120.36      | 115.23   |
| 22  | T     | 102 | CRT  | C32-C31-C30 | -2.95 | 114.65      | 123.20   |
| 17  | L     | 303 | UQ8  | C10-C9-C11  | 2.95  | 120.34      | 115.23   |
| 21  | M     | 405 | MQ8  | C16-C17-C18 | -2.95 | 120.88      | 127.62   |
| 10  | C     | 404 | HEM  | C1B-NB-C4B  | 2.95  | 108.70      | 105.21   |
| 15  | 3     | 101 | BCL  | C1-C2-C3    | -2.95 | 121.37      | 126.20   |
| 15  | T     | 101 | BCL  | C1-C2-C3    | -2.95 | 121.37      | 126.20   |
| 15  | S     | 102 | BCL  | C4-C3-C5    | 2.94  | 120.34      | 115.23   |
| 15  | M     | 403 | BCL  | C1-C2-C3    | -2.94 | 121.38      | 126.20   |
| 15  | N     | 101 | BCL  | O2A-CGA-CBA | 2.94  | 120.80      | 111.83   |
| 15  | K     | 102 | BCL  | C4-C3-C5    | 2.94  | 120.33      | 115.23   |
| 15  | R     | 101 | BCL  | C1-C2-C3    | -2.94 | 121.38      | 126.20   |
| 14  | H     | 301 | PGV  | O01-C1-O02  | -2.94 | 116.84      | 123.70   |
| 15  | Y     | 102 | BCL  | O2A-CGA-CBA | 2.93  | 120.78      | 111.83   |
| 17  | L     | 304 | UQ8  | C15-C14-C16 | 2.93  | 120.32      | 115.23   |
| 15  | R     | 101 | BCL  | C4-C3-C5    | 2.93  | 120.31      | 115.23   |
| 18  | 4     | 104 | LMT  | C1B-O1B-C4' | -2.92 | 111.05      | 117.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | M     | 406 | CRT  | C14-C15-C16 | -2.92 | 114.73      | 123.20   |
| 19  | H     | 302 | CDL  | OB8-CB7-C71 | 2.92  | 120.75      | 111.83   |
| 15  | B     | 102 | BCL  | C4-C3-C5    | 2.92  | 120.30      | 115.23   |
| 14  | L     | 306 | PGV  | O03-C19-C20 | 2.92  | 120.74      | 111.83   |
| 15  | V     | 101 | BCL  | O2A-CGA-CBA | 2.92  | 120.73      | 111.83   |
| 17  | L     | 309 | UQ8  | C25-C24-C26 | 2.91  | 120.28      | 115.23   |
| 15  | A     | 502 | BCL  | C1-C2-C3    | -2.91 | 121.43      | 126.20   |
| 15  | B     | 102 | BCL  | C1C-NC-C4C  | -2.91 | 105.35      | 106.68   |
| 15  | N     | 101 | BCL  | C1C-NC-C4C  | -2.91 | 105.35      | 106.68   |
| 15  | I     | 101 | BCL  | CHC-C4B-NB  | -2.90 | 119.69      | 124.05   |
| 15  | L     | 301 | BCL  | C4-C3-C5    | 2.90  | 120.27      | 115.23   |
| 22  | N     | 102 | CRT  | C4-C5-C6    | -2.90 | 120.84      | 124.91   |
| 15  | E     | 102 | BCL  | C1-C2-C3    | -2.90 | 121.45      | 126.20   |
| 15  | T     | 101 | BCL  | CHB-C4A-NA  | 2.89  | 128.58      | 124.40   |
| 15  | V     | 101 | BCL  | CHB-C4A-NA  | 2.89  | 128.58      | 124.40   |
| 17  | L     | 304 | UQ8  | C10-C9-C11  | 2.89  | 120.25      | 115.23   |
| 15  | Z     | 102 | BCL  | O2A-CGA-CBA | 2.89  | 120.65      | 111.83   |
| 15  | V     | 101 | BCL  | C4-C3-C5    | 2.89  | 120.25      | 115.23   |
| 15  | L     | 308 | BCL  | C1C-NC-C4C  | -2.89 | 105.36      | 106.68   |
| 19  | D     | 101 | CDL  | OB8-CB7-C71 | 2.89  | 120.63      | 111.83   |
| 15  | G     | 102 | BCL  | C1-C2-C3    | -2.88 | 121.47      | 126.20   |
| 22  | Y     | 101 | CRT  | C32-C31-C30 | -2.88 | 114.85      | 123.20   |
| 15  | 9     | 102 | BCL  | C1-C2-C3    | -2.87 | 121.49      | 126.20   |
| 15  | A     | 502 | BCL  | C1C-NC-C4C  | -2.87 | 105.37      | 106.68   |
| 15  | Q     | 102 | BCL  | CHC-C1C-NC  | 2.87  | 128.54      | 124.40   |
| 22  | 0     | 102 | CRT  | C13-C12-C11 | 2.87  | 122.47      | 118.09   |
| 22  | 2     | 103 | CRT  | C32-C31-C30 | -2.87 | 114.89      | 123.20   |
| 17  | L     | 304 | UQ8  | C6-C1-C2    | 2.86  | 121.43      | 119.17   |
| 22  | T     | 102 | CRT  | C4-C5-C6    | -2.86 | 120.89      | 124.91   |
| 22  | 4     | 103 | CRT  | C10-C9-C7   | -2.86 | 123.27      | 127.28   |
| 19  | M     | 407 | CDL  | OA8-CA7-C31 | 2.85  | 119.81      | 111.15   |
| 10  | C     | 403 | HEM  | CHB-C1B-NB  | 2.85  | 127.90      | 124.37   |
| 17  | L     | 303 | UQ8  | C1M-C1-C6   | -2.85 | 119.77      | 124.45   |
| 22  | J     | 103 | CRT  | C14-C15-C16 | -2.85 | 114.95      | 123.20   |
| 15  | I     | 101 | BCL  | C4-C3-C5    | 2.85  | 120.17      | 115.23   |
| 15  | Y     | 102 | BCL  | C4-C3-C5    | 2.84  | 120.16      | 115.23   |
| 15  | M     | 403 | BCL  | C4A-NA-C1A  | 2.84  | 107.97      | 106.68   |
| 14  | L     | 305 | PGV  | O03-C19-C20 | 2.84  | 120.49      | 111.83   |
| 16  | M     | 404 | BPH  | C2B-C1B-NB  | -2.83 | 107.38      | 109.43   |
| 18  | 8     | 101 | LMT  | C1B-O1B-C4' | -2.83 | 111.27      | 117.98   |
| 15  | P     | 102 | BCL  | C1C-NC-C4C  | -2.83 | 105.39      | 106.68   |
| 22  | 0     | 102 | CRT  | C10-C9-C7   | -2.82 | 123.32      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 0     | 102 | CRT  | C14-C15-C16 | -2.82 | 115.02      | 123.20   |
| 15  | O     | 502 | BCL  | C1C-NC-C4C  | -2.82 | 105.39      | 106.68   |
| 22  | V     | 102 | CRT  | C32-C31-C30 | -2.82 | 115.04      | 123.20   |
| 15  | W     | 101 | BCL  | CHC-C1C-NC  | 2.82  | 128.46      | 124.40   |
| 17  | L     | 304 | UQ8  | C35-C34-C36 | 2.81  | 120.11      | 115.23   |
| 15  | N     | 101 | BCL  | CHC-C1C-NC  | 2.81  | 128.46      | 124.40   |
| 22  | Y     | 101 | CRT  | C14-C15-C16 | -2.81 | 115.06      | 123.20   |
| 17  | L     | 309 | UQ8  | C17-C18-C19 | -2.81 | 121.20      | 127.62   |
| 15  | 3     | 101 | BCL  | C4A-NA-C1A  | 2.81  | 107.96      | 106.68   |
| 15  | 4     | 102 | BCL  | O2A-CGA-CBA | 2.80  | 120.37      | 111.83   |
| 15  | F     | 502 | BCL  | C4-C3-C5    | 2.80  | 120.08      | 115.23   |
| 18  | 4     | 101 | LMT  | C1B-O1B-C4' | -2.79 | 111.35      | 117.98   |
| 15  | 0     | 101 | BCL  | C4-C3-C5    | 2.79  | 120.07      | 115.23   |
| 15  | W     | 101 | BCL  | O2A-CGA-CBA | 2.79  | 120.33      | 111.83   |
| 18  | S     | 101 | LMT  | O1B-C1B-C2B | 2.78  | 114.93      | 108.09   |
| 15  | 8     | 102 | BCL  | C4-C3-C5    | 2.78  | 120.06      | 115.23   |
| 17  | L     | 309 | UQ8  | C20-C19-C21 | 2.78  | 120.06      | 115.23   |
| 17  | L     | 309 | UQ8  | C7-C6-C1    | -2.78 | 120.12      | 124.89   |
| 21  | M     | 405 | MQ8  | C31-C32-C33 | -2.78 | 121.26      | 127.62   |
| 15  | 7     | 101 | BCL  | CHC-C1C-NC  | 2.78  | 128.41      | 124.40   |
| 22  | E     | 103 | CRT  | C34-C33-C35 | 2.78  | 122.33      | 118.09   |
| 22  | M     | 406 | CRT  | O2-C38-C39  | -2.78 | 89.87       | 108.97   |
| 14  | M     | 408 | PGV  | O03-C19-C20 | 2.78  | 120.30      | 111.83   |
| 15  | J     | 102 | BCL  | O2A-CGA-CBA | 2.77  | 120.29      | 111.83   |
| 15  | G     | 102 | BCL  | CHB-C4A-NA  | 2.77  | 128.40      | 124.40   |
| 15  | W     | 101 | BCL  | C4-C3-C5    | 2.77  | 120.03      | 115.23   |
| 15  | O     | 502 | BCL  | O2A-CGA-CBA | 2.77  | 120.27      | 111.83   |
| 22  | 0     | 102 | CRT  | C18-C17-C16 | 2.77  | 122.31      | 118.09   |
| 15  | N     | 101 | BCL  | C1-C2-C3    | -2.76 | 121.67      | 126.20   |
| 15  | U     | 101 | BCL  | CHC-C1C-NC  | 2.76  | 128.39      | 124.40   |
| 15  | 8     | 102 | BCL  | CHB-C4A-NA  | 2.76  | 128.38      | 124.40   |
| 15  | S     | 102 | BCL  | C1-C2-C3    | -2.76 | 121.68      | 126.20   |
| 15  | 1     | 402 | BCL  | CHC-C1C-NC  | 2.76  | 128.38      | 124.40   |
| 19  | M     | 407 | CDL  | CB4-OB6-CB5 | -2.76 | 111.20      | 117.80   |
| 15  | K     | 102 | BCL  | O2D-CGD-O1D | -2.75 | 118.49      | 123.85   |
| 15  | 2     | 102 | BCL  | CHB-C4A-NA  | 2.75  | 128.37      | 124.40   |
| 15  | 6     | 101 | BCL  | C2A-C1A-CHA | -2.75 | 119.09      | 123.87   |
| 15  | 6     | 101 | BCL  | C1-C2-C3    | -2.75 | 121.69      | 126.20   |
| 15  | 5     | 102 | BCL  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 22  | V     | 102 | CRT  | C13-C12-C11 | 2.75  | 122.29      | 118.09   |
| 15  | G     | 102 | BCL  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 15  | V     | 101 | BCL  | C1-O2A-CGA  | 2.75  | 123.30      | 116.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 103 | CRT  | C14-C15-C16 | -2.75 | 115.24      | 123.20   |
| 22  | N     | 102 | CRT  | C32-C31-C30 | -2.74 | 115.25      | 123.20   |
| 18  | S     | 101 | LMT  | C3'-C4'-C5' | -2.74 | 104.85      | 110.93   |
| 16  | L     | 302 | BPH  | C2B-C1B-NB  | -2.74 | 107.45      | 109.43   |
| 15  | S     | 102 | BCL  | CHC-C1C-NC  | 2.74  | 128.35      | 124.40   |
| 15  | 9     | 102 | BCL  | C1C-NC-C4C  | -2.74 | 105.43      | 106.68   |
| 22  | Z     | 103 | CRT  | C4-C5-C6    | -2.73 | 121.08      | 124.91   |
| 15  | L     | 308 | BCL  | CHC-C4B-NB  | -2.73 | 119.95      | 124.05   |
| 15  | K     | 102 | BCL  | CHC-C1C-NC  | 2.73  | 128.34      | 124.40   |
| 15  | 7     | 101 | BCL  | O2A-CGA-CBA | 2.73  | 120.16      | 111.83   |
| 15  | Z     | 102 | BCL  | C4-C3-C5    | 2.73  | 119.97      | 115.23   |
| 15  | E     | 102 | BCL  | CHB-C4A-NA  | 2.73  | 128.34      | 124.40   |
| 14  | A     | 503 | PGV  | O03-C19-C20 | 2.73  | 120.16      | 111.83   |
| 22  | B     | 103 | CRT  | C20-C19-C17 | -2.73 | 123.45      | 127.28   |
| 17  | L     | 304 | UQ8  | C20-C19-C21 | 2.73  | 119.96      | 115.23   |
| 15  | 0     | 101 | BCL  | C2A-C1A-CHA | -2.72 | 119.15      | 123.87   |
| 15  | P     | 102 | BCL  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 17  | L     | 304 | UQ8  | C30-C29-C31 | 2.71  | 119.94      | 115.23   |
| 17  | L     | 309 | UQ8  | C10-C9-C11  | 2.71  | 119.94      | 115.23   |
| 17  | L     | 303 | UQ8  | C7-C6-C1    | -2.71 | 120.24      | 124.89   |
| 15  | Q     | 102 | BCL  | O2D-CGD-O1D | -2.71 | 118.58      | 123.85   |
| 21  | M     | 405 | MQ8  | C19-C18-C20 | 2.71  | 119.93      | 115.23   |
| 15  | B     | 102 | BCL  | CHB-C4A-NA  | 2.71  | 128.30      | 124.40   |
| 15  | E     | 102 | BCL  | CHC-C1C-NC  | 2.71  | 128.30      | 124.40   |
| 17  | L     | 309 | UQ8  | C22-C23-C24 | -2.71 | 121.43      | 127.62   |
| 15  | 1     | 402 | BCL  | O2A-CGA-CBA | 2.70  | 120.07      | 111.83   |
| 15  | I     | 101 | BCL  | O2D-CGD-O1D | -2.70 | 118.60      | 123.85   |
| 15  | F     | 502 | BCL  | CHC-C1C-NC  | 2.69  | 128.29      | 124.40   |
| 15  | 6     | 101 | BCL  | CHB-C4A-NA  | 2.69  | 128.29      | 124.40   |
| 15  | 5     | 102 | BCL  | CHC-C1C-NC  | 2.69  | 128.28      | 124.40   |
| 15  | 0     | 101 | BCL  | C1C-NC-C4C  | -2.69 | 105.45      | 106.68   |
| 15  | V     | 101 | BCL  | C2A-C1A-CHA | -2.69 | 119.20      | 123.87   |
| 15  | B     | 102 | BCL  | C2A-C1A-CHA | -2.69 | 119.20      | 123.87   |
| 15  | F     | 502 | BCL  | O2D-CGD-O1D | -2.69 | 118.61      | 123.85   |
| 15  | V     | 101 | BCL  | C1C-NC-C4C  | -2.69 | 105.45      | 106.68   |
| 15  | K     | 102 | BCL  | O2A-CGA-CBA | 2.69  | 120.02      | 111.83   |
| 15  | D     | 102 | BCL  | C1-C2-C3    | -2.68 | 121.80      | 126.20   |
| 14  | A     | 501 | PGV  | O03-C19-C20 | 2.68  | 120.01      | 111.83   |
| 22  | 0     | 102 | CRT  | C27-C26-C25 | -2.68 | 115.43      | 123.20   |
| 15  | U     | 101 | BCL  | O2A-CGA-CBA | 2.68  | 120.01      | 111.83   |
| 15  | 2     | 102 | BCL  | C1C-NC-C4C  | -2.67 | 105.46      | 106.68   |
| 15  | 7     | 101 | BCL  | CHB-C4A-NA  | 2.67  | 128.26      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | 9     | 102 | BCL  | CHC-C1C-NC  | 2.67  | 128.26      | 124.40   |
| 15  | O     | 502 | BCL  | O2D-CGD-O1D | -2.67 | 118.65      | 123.85   |
| 21  | M     | 405 | MQ8  | C26-C27-C28 | -2.67 | 121.51      | 127.62   |
| 15  | 7     | 101 | BCL  | C4-C3-C5    | 2.67  | 119.86      | 115.23   |
| 15  | E     | 102 | BCL  | C4-C3-C5    | 2.67  | 119.86      | 115.23   |
| 15  | W     | 101 | BCL  | CHC-C4B-NB  | -2.67 | 120.05      | 124.05   |
| 15  | L     | 308 | BCL  | O2A-CGA-CBA | 2.67  | 119.97      | 111.83   |
| 22  | 9     | 101 | CRT  | C34-C33-C35 | 2.67  | 122.16      | 118.09   |
| 21  | M     | 405 | MQ8  | C21-C22-C23 | -2.66 | 121.52      | 127.62   |
| 15  | X     | 102 | BCL  | CHC-C1C-NC  | 2.66  | 128.24      | 124.40   |
| 10  | C     | 403 | HEM  | CHD-C4C-NC  | 2.66  | 127.35      | 124.45   |
| 18  | 5     | 101 | LMT  | O1B-C4'-C3' | 2.66  | 114.00      | 107.23   |
| 15  | M     | 403 | BCL  | C4-C3-C5    | 2.66  | 119.84      | 115.23   |
| 15  | I     | 101 | BCL  | CHC-C1C-NC  | 2.66  | 128.24      | 124.40   |
| 15  | J     | 102 | BCL  | O2D-CGD-O1D | -2.66 | 118.68      | 123.85   |
| 18  | T     | 103 | LMT  | C1B-O1B-C4' | -2.66 | 111.68      | 117.98   |
| 15  | P     | 102 | BCL  | C4-C3-C5    | 2.65  | 119.83      | 115.23   |
| 18  | P     | 104 | LMT  | C1B-O1B-C4' | -2.65 | 111.69      | 117.98   |
| 15  | M     | 402 | BCL  | CHC-C1C-NC  | 2.65  | 128.22      | 124.40   |
| 17  | L     | 309 | UQ8  | C37-C38-C39 | -2.65 | 121.56      | 127.62   |
| 22  | E     | 103 | CRT  | C21-C20-C19 | -2.65 | 118.10      | 123.52   |
| 22  | V     | 102 | CRT  | C26-C27-C28 | -2.65 | 123.56      | 127.28   |
| 15  | 5     | 102 | BCL  | C4A-NA-C1A  | 2.65  | 107.89      | 106.68   |
| 15  | O     | 502 | BCL  | C4-C3-C5    | 2.64  | 119.81      | 115.23   |
| 18  | B     | 101 | LMT  | C1B-O1B-C4' | -2.64 | 111.72      | 117.98   |
| 17  | L     | 303 | UQ8  | C25-C24-C26 | 2.63  | 120.65      | 114.59   |
| 15  | R     | 101 | BCL  | C2A-C1A-CHA | -2.63 | 119.30      | 123.87   |
| 15  | M     | 402 | BCL  | C1D-CHD-C4C | -2.63 | 120.27      | 126.62   |
| 15  | X     | 102 | BCL  | C1C-NC-C4C  | -2.63 | 105.48      | 106.68   |
| 15  | 9     | 102 | BCL  | CHC-C4B-NB  | -2.63 | 120.10      | 124.05   |
| 15  | O     | 502 | BCL  | C1-C2-C3    | -2.63 | 121.89      | 126.20   |
| 22  | B     | 103 | CRT  | C29-C28-C30 | 2.62  | 122.10      | 118.09   |
| 17  | L     | 304 | UQ8  | C42-C43-C44 | -2.62 | 118.90      | 127.64   |
| 15  | S     | 102 | BCL  | CHC-C4B-NB  | -2.62 | 120.12      | 124.05   |
| 15  | 9     | 102 | BCL  | O2A-CGA-CBA | 2.62  | 119.82      | 111.83   |
| 22  | 4     | 103 | CRT  | C31-C30-C28 | 2.62  | 133.54      | 126.36   |
| 15  | 3     | 101 | BCL  | O2A-CGA-CBA | 2.61  | 119.81      | 111.83   |
| 22  | B     | 103 | CRT  | C34-C33-C35 | 2.61  | 122.08      | 118.09   |
| 17  | L     | 304 | UQ8  | C40-C39-C41 | 2.61  | 119.77      | 115.23   |
| 19  | M     | 409 | CDL  | CA4-OA6-CA5 | -2.61 | 111.54      | 117.80   |
| 15  | 3     | 101 | BCL  | CHC-C1C-NC  | 2.61  | 128.16      | 124.40   |
| 15  | I     | 101 | BCL  | CHB-C4A-NA  | 2.60  | 128.16      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | R     | 101 | BCL  | CHB-C4A-NA  | 2.60  | 128.16      | 124.40   |
| 15  | 1     | 402 | BCL  | CHC-C4B-NB  | -2.60 | 120.14      | 124.05   |
| 15  | 7     | 101 | BCL  | CHC-C4B-NB  | -2.60 | 120.14      | 124.05   |
| 15  | G     | 102 | BCL  | CHC-C1C-NC  | 2.60  | 128.16      | 124.40   |
| 15  | B     | 102 | BCL  | CHC-C1C-NC  | 2.60  | 128.15      | 124.40   |
| 10  | C     | 402 | HEM  | CHD-C4C-NC  | 2.60  | 127.28      | 124.45   |
| 17  | L     | 309 | UQ8  | C30-C29-C28 | -2.60 | 116.96      | 123.63   |
| 14  | 1     | 401 | PGV  | O03-C19-C20 | 2.59  | 119.75      | 111.83   |
| 15  | P     | 102 | BCL  | C2A-C1A-CHA | -2.59 | 119.37      | 123.87   |
| 15  | 3     | 101 | BCL  | C1D-CHD-C4C | -2.59 | 120.37      | 126.62   |
| 22  | B     | 103 | CRT  | C9-C10-C11  | -2.59 | 115.69      | 123.20   |
| 15  | J     | 102 | BCL  | C2A-C1A-CHA | -2.59 | 119.37      | 123.87   |
| 15  | K     | 102 | BCL  | CHC-C4B-NB  | -2.59 | 120.17      | 124.05   |
| 15  | F     | 502 | BCL  | CHC-C4B-NB  | -2.59 | 120.17      | 124.05   |
| 15  | S     | 102 | BCL  | O2D-CGD-O1D | -2.59 | 118.81      | 123.85   |
| 15  | 6     | 101 | BCL  | O2D-CGD-O1D | -2.59 | 118.81      | 123.85   |
| 15  | G     | 102 | BCL  | C1C-NC-C4C  | -2.58 | 105.50      | 106.68   |
| 22  | 9     | 101 | CRT  | C27-C26-C25 | -2.58 | 115.72      | 123.20   |
| 22  | T     | 102 | CRT  | C27-C26-C25 | -2.58 | 115.73      | 123.20   |
| 22  | 9     | 101 | CRT  | C5-C6-C7    | 2.58  | 129.78      | 125.89   |
| 15  | J     | 102 | BCL  | CHB-C4A-NA  | 2.57  | 128.12      | 124.40   |
| 15  | F     | 502 | BCL  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |
| 22  | R     | 102 | CRT  | C14-C15-C16 | -2.57 | 115.75      | 123.20   |
| 15  | Q     | 102 | BCL  | CMB-C2B-C3B | 2.57  | 133.78      | 125.67   |
| 15  | D     | 102 | BCL  | CHC-C4B-NB  | -2.57 | 120.19      | 124.05   |
| 15  | X     | 102 | BCL  | C2A-C1A-CHA | -2.57 | 119.41      | 123.87   |
| 15  | K     | 102 | BCL  | C1C-NC-C4C  | -2.57 | 105.51      | 106.68   |
| 22  | 4     | 103 | CRT  | C21-C20-C19 | -2.56 | 118.27      | 123.52   |
| 15  | D     | 102 | BCL  | C1C-NC-C4C  | -2.56 | 105.51      | 106.68   |
| 15  | F     | 502 | BCL  | O2A-CGA-CBA | 2.56  | 119.64      | 111.83   |
| 17  | L     | 303 | UQ8  | C17-C18-C19 | -2.56 | 121.77      | 127.62   |
| 15  | N     | 101 | BCL  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 15  | X     | 102 | BCL  | CHC-C4B-NB  | -2.56 | 120.21      | 124.05   |
| 15  | 4     | 102 | BCL  | C2A-C1A-CHA | -2.56 | 119.43      | 123.87   |
| 22  | 0     | 102 | CRT  | C34-C33-C35 | 2.56  | 122.00      | 118.09   |
| 22  | Y     | 101 | CRT  | C26-C27-C28 | -2.56 | 123.69      | 127.28   |
| 22  | 0     | 102 | CRT  | C21-C20-C19 | -2.56 | 118.29      | 123.52   |
| 22  | 6     | 102 | CRT  | C34-C33-C35 | 2.55  | 121.99      | 118.09   |
| 22  | V     | 102 | CRT  | C5-C6-C7    | -2.55 | 122.03      | 125.89   |
| 15  | M     | 403 | BCL  | CHC-C4B-NB  | -2.55 | 120.22      | 124.05   |
| 15  | I     | 101 | BCL  | CMB-C2B-C3B | 2.55  | 133.71      | 125.67   |
| 15  | T     | 101 | BCL  | CHC-C1C-NC  | 2.55  | 128.08      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 103 | CRT  | C18-C17-C16 | 2.55  | 121.98      | 118.09   |
| 15  | W     | 101 | BCL  | C1-C2-C3    | -2.55 | 122.02      | 126.20   |
| 15  | Z     | 102 | BCL  | CHB-C4A-NA  | 2.55  | 128.07      | 124.40   |
| 15  | J     | 102 | BCL  | CHC-C1C-NC  | 2.55  | 128.07      | 124.40   |
| 15  | D     | 102 | BCL  | O2D-CGD-O1D | -2.54 | 118.90      | 123.85   |
| 15  | G     | 102 | BCL  | C2A-C1A-CHA | -2.54 | 119.46      | 123.87   |
| 15  | R     | 101 | BCL  | CHC-C1C-NC  | 2.54  | 128.06      | 124.40   |
| 15  | 8     | 102 | BCL  | CHC-C1C-NC  | 2.54  | 128.06      | 124.40   |
| 15  | F     | 502 | BCL  | C1-C2-C3    | -2.54 | 122.04      | 126.20   |
| 15  | U     | 101 | BCL  | CHC-C4B-NB  | -2.54 | 120.25      | 124.05   |
| 18  | 5     | 101 | LMT  | O1B-C4'-C5' | -2.53 | 102.84      | 109.48   |
| 15  | 0     | 101 | BCL  | CHC-C1C-NC  | 2.53  | 128.05      | 124.40   |
| 15  | U     | 101 | BCL  | CMD-C2D-C3D | -2.52 | 121.90      | 127.69   |
| 22  | P     | 103 | CRT  | C34-C33-C35 | 2.52  | 121.94      | 118.09   |
| 15  | 2     | 102 | BCL  | CHC-C1C-NC  | 2.52  | 128.04      | 124.40   |
| 15  | 6     | 101 | BCL  | CHC-C1C-NC  | 2.52  | 128.04      | 124.40   |
| 18  | L     | 307 | LMT  | C1B-O1B-C4' | -2.52 | 112.00      | 117.98   |
| 15  | 5     | 102 | BCL  | CHC-C4B-NB  | -2.52 | 120.27      | 124.05   |
| 15  | 4     | 102 | BCL  | C1C-NC-C4C  | -2.52 | 105.53      | 106.68   |
| 19  | L     | 311 | CDL  | OB8-CB7-C71 | 2.52  | 119.51      | 111.83   |
| 15  | 5     | 102 | BCL  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |
| 22  | 4     | 103 | CRT  | C32-C31-C30 | 2.52  | 130.49      | 123.20   |
| 15  | Q     | 102 | BCL  | CHC-C4B-NB  | -2.51 | 120.28      | 124.05   |
| 15  | Z     | 102 | BCL  | CHC-C1C-NC  | 2.51  | 128.03      | 124.40   |
| 15  | U     | 101 | BCL  | O2D-CGD-O1D | -2.51 | 118.95      | 123.85   |
| 15  | M     | 402 | BCL  | C4-C3-C5    | 2.51  | 119.59      | 115.23   |
| 15  | X     | 102 | BCL  | C4-C3-C5    | 2.51  | 119.58      | 115.23   |
| 15  | P     | 102 | BCL  | O2A-CGA-CBA | 2.51  | 119.48      | 111.83   |
| 15  | I     | 101 | BCL  | C2A-C1A-CHA | -2.50 | 119.53      | 123.87   |
| 15  | 2     | 102 | BCL  | C4A-NA-C1A  | 2.50  | 107.82      | 106.68   |
| 15  | Z     | 102 | BCL  | C2A-C1A-CHA | -2.50 | 119.53      | 123.87   |
| 15  | P     | 102 | BCL  | C1-O2A-CGA  | 2.50  | 122.70      | 116.65   |
| 15  | 9     | 102 | BCL  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |
| 15  | 9     | 102 | BCL  | CMB-C2B-C3B | 2.50  | 133.54      | 125.67   |
| 15  | S     | 102 | BCL  | C1C-NC-C4C  | -2.50 | 105.54      | 106.68   |
| 15  | P     | 102 | BCL  | CHC-C1C-NC  | 2.50  | 128.00      | 124.40   |
| 15  | Z     | 102 | BCL  | CHC-C4B-NB  | -2.50 | 120.31      | 124.05   |
| 22  | B     | 103 | CRT  | C13-C12-C11 | 2.49  | 121.90      | 118.09   |
| 18  | J     | 104 | LMT  | C1B-O1B-C4' | -2.49 | 112.07      | 117.98   |
| 15  | 8     | 102 | BCL  | C1C-NC-C4C  | -2.49 | 105.54      | 106.68   |
| 15  | 2     | 102 | BCL  | C2A-C1A-CHA | -2.49 | 119.55      | 123.87   |
| 22  | 9     | 101 | CRT  | C8-C7-C9    | -2.49 | 118.79      | 122.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | E     | 102 | BCL  | C2A-C1A-CHA | -2.49 | 119.55      | 123.87   |
| 15  | Y     | 102 | BCL  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 15  | M     | 403 | BCL  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 15  | 9     | 102 | BCL  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 18  | P     | 101 | LMT  | C1B-O1B-C4' | -2.48 | 112.10      | 117.98   |
| 19  | M     | 409 | CDL  | OA8-CA7-C31 | 2.48  | 119.39      | 111.83   |
| 15  | 1     | 402 | BCL  | CMB-C2B-C3B | 2.48  | 133.48      | 125.67   |
| 15  | L     | 301 | BCL  | O2A-CGA-O1A | -2.48 | 117.43      | 123.63   |
| 10  | C     | 402 | HEM  | C3B-C4B-NB  | -2.47 | 107.69      | 109.47   |
| 15  | 3     | 101 | BCL  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 22  | 0     | 102 | CRT  | C20-C19-C17 | -2.47 | 123.81      | 127.28   |
| 18  | 2     | 101 | LMT  | C1-O1'-C1'  | -2.47 | 109.46      | 113.68   |
| 22  | 0     | 102 | CRT  | C29-C28-C30 | 2.47  | 121.86      | 118.09   |
| 17  | L     | 303 | UQ8  | C20-C19-C21 | 2.47  | 119.51      | 115.23   |
| 22  | R     | 102 | CRT  | C21-C20-C19 | -2.46 | 118.48      | 123.52   |
| 15  | W     | 101 | BCL  | O2D-CGD-O1D | -2.46 | 119.05      | 123.85   |
| 15  | X     | 102 | BCL  | C4A-NA-C1A  | 2.46  | 107.80      | 106.68   |
| 21  | M     | 405 | MQ8  | C50-C48-C49 | 2.46  | 120.25      | 114.59   |
| 15  | S     | 102 | BCL  | CMB-C2B-C3B | 2.46  | 133.42      | 125.67   |
| 22  | 0     | 102 | CRT  | C5-C6-C7    | -2.46 | 122.18      | 125.89   |
| 15  | M     | 402 | BCL  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 18  | M     | 411 | LMT  | C1B-O1B-C4' | -2.45 | 112.17      | 117.98   |
| 22  | V     | 102 | CRT  | C34-C33-C35 | 2.45  | 121.83      | 118.09   |
| 17  | L     | 309 | UQ8  | C1M-C1-C6   | -2.45 | 120.42      | 124.45   |
| 15  | 9     | 102 | BCL  | C1D-CHD-C4C | -2.45 | 120.71      | 126.62   |
| 15  | A     | 502 | BCL  | CMB-C2B-C3B | 2.45  | 133.39      | 125.67   |
| 15  | M     | 402 | BCL  | O1D-CGD-CBD | -2.45 | 119.69      | 124.52   |
| 15  | V     | 101 | BCL  | CHC-C4B-NB  | -2.45 | 120.38      | 124.05   |
| 15  | J     | 102 | BCL  | C1C-NC-C4C  | -2.44 | 105.56      | 106.68   |
| 19  | H     | 302 | CDL  | OA8-CA7-C31 | 2.44  | 119.29      | 111.83   |
| 15  | M     | 403 | BCL  | CMB-C2B-C3B | 2.44  | 133.38      | 125.67   |
| 15  | M     | 403 | BCL  | C1D-CHD-C4C | -2.44 | 120.73      | 126.62   |
| 10  | C     | 401 | HEM  | CHD-C1D-C2D | -2.44 | 121.18      | 125.03   |
| 17  | L     | 304 | UQ8  | C22-C23-C24 | -2.44 | 122.05      | 127.62   |
| 14  | F     | 501 | PGV  | O03-C19-C20 | 2.43  | 119.26      | 111.83   |
| 15  | 7     | 101 | BCL  | C1C-NC-C4C  | -2.43 | 105.57      | 106.68   |
| 18  | 2     | 101 | LMT  | C1B-O1B-C4' | -2.43 | 112.22      | 117.98   |
| 21  | M     | 405 | MQ8  | C14-C13-C15 | 2.43  | 119.44      | 115.23   |
| 15  | 7     | 101 | BCL  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |
| 15  | T     | 101 | BCL  | C1-O2A-CGA  | 2.43  | 122.53      | 116.65   |
| 15  | D     | 102 | BCL  | CMB-C2B-C3B | 2.43  | 133.33      | 125.67   |
| 15  | 8     | 102 | BCL  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | N     | 101 | BCL  | CHC-C4B-NB  | -2.43 | 120.41      | 124.05   |
| 15  | E     | 102 | BCL  | CHC-C4B-NB  | -2.42 | 120.41      | 124.05   |
| 15  | T     | 101 | BCL  | C2A-C1A-CHA | -2.42 | 119.66      | 123.87   |
| 15  | Z     | 102 | BCL  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 15  | 8     | 102 | BCL  | C2A-C1A-CHA | -2.42 | 119.67      | 123.87   |
| 15  | U     | 101 | BCL  | CMB-C2B-C3B | 2.42  | 133.30      | 125.67   |
| 15  | Z     | 102 | BCL  | CMB-C2B-C3B | 2.42  | 133.29      | 125.67   |
| 15  | 7     | 101 | BCL  | CMB-C2B-C3B | 2.42  | 133.29      | 125.67   |
| 15  | R     | 101 | BCL  | C1-O2A-CGA  | 2.42  | 122.50      | 116.65   |
| 22  | Z     | 103 | CRT  | C32-C31-C30 | -2.42 | 116.20      | 123.20   |
| 15  | K     | 102 | BCL  | C4A-NA-C1A  | 2.42  | 107.78      | 106.68   |
| 15  | L     | 301 | BCL  | CHC-C1C-NC  | 2.41  | 127.88      | 124.40   |
| 15  | 3     | 101 | BCL  | CMD-C2D-C3D | -2.41 | 122.15      | 127.69   |
| 15  | 4     | 102 | BCL  | C4-C3-C5    | 2.41  | 119.42      | 115.23   |
| 15  | 5     | 102 | BCL  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 10  | C     | 401 | HEM  | C3B-C4B-NB  | -2.41 | 107.73      | 109.47   |
| 22  | 2     | 103 | CRT  | C26-C27-C28 | -2.41 | 123.90      | 127.28   |
| 15  | J     | 102 | BCL  | CMB-C2B-C3B | 2.41  | 133.27      | 125.67   |
| 15  | 5     | 102 | BCL  | C1D-CHD-C4C | -2.41 | 120.81      | 126.62   |
| 15  | N     | 101 | BCL  | CMB-C2B-C3B | 2.41  | 133.26      | 125.67   |
| 22  | R     | 102 | CRT  | C29-C28-C30 | 2.41  | 121.77      | 118.09   |
| 15  | A     | 502 | BCL  | CHC-C4B-NB  | -2.41 | 120.44      | 124.05   |
| 22  | R     | 102 | CRT  | C18-C17-C16 | 2.41  | 121.76      | 118.09   |
| 15  | V     | 101 | BCL  | CMB-C2B-C3B | 2.40  | 133.25      | 125.67   |
| 22  | 6     | 102 | CRT  | C9-C10-C11  | -2.40 | 116.23      | 123.20   |
| 15  | E     | 102 | BCL  | O2D-CGD-O1D | -2.40 | 119.17      | 123.85   |
| 22  | V     | 102 | CRT  | C27-C26-C25 | -2.40 | 116.24      | 123.20   |
| 15  | T     | 101 | BCL  | C4-C3-C5    | 2.40  | 119.40      | 115.23   |
| 18  | Z     | 101 | LMT  | C1-O1'-C1'  | -2.40 | 109.58      | 113.68   |
| 17  | L     | 309 | UQ8  | C40-C39-C41 | 2.40  | 119.40      | 115.23   |
| 15  | S     | 102 | BCL  | O2A-CGA-CBA | 2.40  | 119.16      | 111.83   |
| 22  | B     | 103 | CRT  | C10-C9-C7   | -2.40 | 123.91      | 127.28   |
| 15  | E     | 102 | BCL  | C1D-CHD-C4C | -2.40 | 120.83      | 126.62   |
| 15  | K     | 102 | BCL  | C1D-CHD-C4C | -2.40 | 120.84      | 126.62   |
| 14  | L     | 305 | PGV  | O01-C1-O02  | -2.40 | 118.10      | 123.70   |
| 15  | D     | 102 | BCL  | C4-C3-C5    | 2.40  | 119.39      | 115.23   |
| 15  | B     | 102 | BCL  | C1D-CHD-C4C | -2.40 | 120.84      | 126.62   |
| 17  | L     | 309 | UQ8  | C27-C26-C24 | -2.40 | 105.25      | 113.19   |
| 15  | A     | 502 | BCL  | O2D-CGD-O1D | -2.40 | 119.19      | 123.85   |
| 22  | V     | 102 | CRT  | C11-C12-C14 | -2.39 | 115.24      | 119.01   |
| 15  | 0     | 101 | BCL  | CMB-C2B-C3B | 2.39  | 133.22      | 125.67   |
| 17  | L     | 309 | UQ8  | C15-C14-C16 | 2.39  | 119.38      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | K     | 102 | BCL  | CMB-C2B-C3B | 2.39  | 133.20      | 125.67   |
| 15  | X     | 102 | BCL  | CMB-C2B-C3B | 2.39  | 133.20      | 125.67   |
| 15  | D     | 102 | BCL  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |
| 15  | A     | 502 | BCL  | CHC-C1C-NC  | 2.39  | 127.84      | 124.40   |
| 14  | C     | 408 | PGV  | O03-C19-C20 | 2.39  | 119.11      | 111.83   |
| 15  | K     | 102 | BCL  | C2A-C1A-CHA | -2.38 | 119.73      | 123.87   |
| 10  | C     | 402 | HEM  | CHD-C1D-C2D | -2.38 | 121.27      | 125.03   |
| 18  | M     | 410 | LMT  | C1B-O1B-C4' | -2.38 | 112.33      | 117.98   |
| 15  | T     | 101 | BCL  | C1D-CHD-C4C | -2.38 | 120.88      | 126.62   |
| 15  | A     | 502 | BCL  | O2A-CGA-CBA | 2.38  | 119.08      | 111.83   |
| 22  | E     | 103 | CRT  | C18-C17-C16 | 2.37  | 121.72      | 118.09   |
| 10  | C     | 402 | HEM  | CBA-CAA-C2A | -2.37 | 105.97      | 112.53   |
| 15  | N     | 101 | BCL  | C1D-CHD-C4C | -2.37 | 120.90      | 126.62   |
| 15  | M     | 402 | BCL  | O2A-CGA-CBA | 2.37  | 119.07      | 111.83   |
| 15  | L     | 301 | BCL  | C1C-NC-C4C  | -2.37 | 105.60      | 106.68   |
| 15  | F     | 502 | BCL  | CMD-C2D-C3D | -2.37 | 122.26      | 127.69   |
| 19  | M     | 409 | CDL  | CB4-OB6-CB5 | -2.37 | 112.13      | 117.80   |
| 22  | 2     | 103 | CRT  | C34-C33-C35 | 2.37  | 121.70      | 118.09   |
| 22  | N     | 102 | CRT  | C13-C12-C11 | 2.37  | 121.70      | 118.09   |
| 15  | M     | 403 | BCL  | CMD-C2D-C3D | -2.37 | 122.26      | 127.69   |
| 22  | T     | 102 | CRT  | C36-C35-C33 | -2.37 | 122.32      | 125.89   |
| 15  | M     | 402 | BCL  | CHC-C4B-NB  | -2.37 | 120.50      | 124.05   |
| 15  | B     | 102 | BCL  | CHC-C4B-NB  | -2.36 | 120.50      | 124.05   |
| 15  | B     | 102 | BCL  | CED-O2D-CGD | 2.36  | 121.28      | 115.92   |
| 22  | N     | 102 | CRT  | C21-C20-C19 | -2.36 | 118.69      | 123.52   |
| 15  | Q     | 102 | BCL  | CMD-C2D-C3D | -2.36 | 122.28      | 127.69   |
| 15  | 7     | 101 | BCL  | C1D-CHD-C4C | -2.36 | 120.93      | 126.62   |
| 15  | T     | 101 | BCL  | CHC-C4B-NB  | -2.36 | 120.51      | 124.05   |
| 15  | F     | 502 | BCL  | CMB-C2B-C3B | 2.36  | 133.11      | 125.67   |
| 15  | X     | 102 | BCL  | O2D-CGD-O1D | -2.36 | 119.26      | 123.85   |
| 15  | 4     | 102 | BCL  | O2D-CGD-O1D | -2.36 | 119.26      | 123.85   |
| 15  | A     | 502 | BCL  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 15  | 2     | 102 | BCL  | CHC-C4B-NB  | -2.36 | 120.51      | 124.05   |
| 15  | T     | 101 | BCL  | CED-O2D-CGD | 2.36  | 121.26      | 115.92   |
| 15  | I     | 101 | BCL  | O2A-CGA-CBA | 2.35  | 119.02      | 111.83   |
| 15  | K     | 102 | BCL  | CMD-C2D-C3D | -2.35 | 122.29      | 127.69   |
| 15  | M     | 402 | BCL  | CMB-C2B-C3B | 2.35  | 133.09      | 125.67   |
| 15  | B     | 102 | BCL  | CMB-C2B-C3B | 2.35  | 133.08      | 125.67   |
| 10  | C     | 403 | HEM  | CHD-C1D-C2D | -2.35 | 121.32      | 125.03   |
| 15  | D     | 102 | BCL  | O2A-CGA-CBA | 2.35  | 119.00      | 111.83   |
| 10  | C     | 404 | HEM  | CHD-C4C-NC  | 2.35  | 127.01      | 124.45   |
| 15  | 1     | 402 | BCL  | C1D-CHD-C4C | -2.35 | 120.96      | 126.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | 5     | 102 | BCL  | C1C-NC-C4C  | -2.35 | 105.61      | 106.68   |
| 15  | S     | 102 | BCL  | C1D-CHD-C4C | -2.35 | 120.96      | 126.62   |
| 15  | P     | 102 | BCL  | C1D-CHD-C4C | -2.34 | 120.97      | 126.62   |
| 15  | 4     | 102 | BCL  | C1D-CHD-C4C | -2.34 | 120.97      | 126.62   |
| 22  | T     | 102 | CRT  | C14-C15-C16 | -2.34 | 116.41      | 123.20   |
| 15  | V     | 101 | BCL  | CHC-C1C-NC  | 2.34  | 127.78      | 124.40   |
| 15  | J     | 102 | BCL  | CHC-C4B-NB  | -2.34 | 120.53      | 124.05   |
| 15  | 0     | 101 | BCL  | O2D-CGD-O1D | -2.34 | 119.29      | 123.85   |
| 15  | Z     | 102 | BCL  | C1D-CHD-C4C | -2.34 | 120.97      | 126.62   |
| 22  | 6     | 102 | CRT  | C21-C20-C19 | -2.34 | 118.73      | 123.52   |
| 10  | C     | 404 | HEM  | CHD-C1D-C2D | -2.34 | 121.34      | 125.03   |
| 10  | C     | 401 | HEM  | CHA-C4D-C3D | -2.34 | 120.92      | 125.23   |
| 15  | Q     | 102 | BCL  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 15  | Z     | 102 | BCL  | C1C-NC-C4C  | -2.34 | 105.61      | 106.68   |
| 15  | P     | 102 | BCL  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 22  | E     | 103 | CRT  | C13-C12-C11 | 2.34  | 121.66      | 118.09   |
| 15  | O     | 502 | BCL  | CHC-C4B-NB  | -2.33 | 120.55      | 124.05   |
| 15  | 9     | 102 | BCL  | CMD-C2D-C3D | -2.33 | 122.34      | 127.69   |
| 15  | G     | 102 | BCL  | CHC-C4B-NB  | -2.33 | 120.55      | 124.05   |
| 22  | Z     | 103 | CRT  | C36-C35-C33 | -2.33 | 122.37      | 125.89   |
| 10  | C     | 403 | HEM  | C1A-CHA-C4D | -2.33 | 120.77      | 126.25   |
| 22  | N     | 102 | CRT  | C14-C15-C16 | -2.33 | 116.46      | 123.20   |
| 22  | J     | 103 | CRT  | C18-C17-C16 | 2.33  | 121.64      | 118.09   |
| 15  | Y     | 102 | BCL  | CMD-C2D-C3D | -2.33 | 122.35      | 127.69   |
| 15  | 0     | 101 | BCL  | C1D-CHD-C4C | -2.33 | 121.01      | 126.62   |
| 15  | 3     | 101 | BCL  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 15  | 0     | 101 | BCL  | CHC-C4B-NB  | -2.32 | 120.57      | 124.05   |
| 22  | 4     | 103 | CRT  | C27-C26-C25 | -2.32 | 116.48      | 123.20   |
| 15  | Q     | 102 | BCL  | C2A-C1A-CHA | -2.32 | 119.84      | 123.87   |
| 15  | L     | 308 | BCL  | C4A-NA-C1A  | 2.32  | 107.74      | 106.68   |
| 18  | Z     | 101 | LMT  | O1'-C1'-C2' | 2.31  | 111.79      | 108.27   |
| 22  | G     | 103 | CRT  | C14-C15-C16 | -2.31 | 116.50      | 123.20   |
| 15  | U     | 101 | BCL  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 19  | L     | 311 | CDL  | OA8-CA7-C31 | 2.31  | 118.87      | 111.83   |
| 15  | A     | 502 | BCL  | C1D-CHD-C4C | -2.31 | 121.06      | 126.62   |
| 15  | T     | 101 | BCL  | C4A-NA-C1A  | 2.30  | 107.73      | 106.68   |
| 15  | R     | 101 | BCL  | CED-O2D-CGD | 2.30  | 121.14      | 115.92   |
| 15  | 5     | 102 | BCL  | CMB-C2B-C3B | 2.30  | 132.93      | 125.67   |
| 15  | L     | 308 | BCL  | CHC-C1C-NC  | 2.30  | 127.72      | 124.40   |
| 15  | 4     | 102 | BCL  | CMB-C2B-C3B | 2.30  | 132.93      | 125.67   |
| 22  | G     | 103 | CRT  | C34-C33-C35 | 2.30  | 121.60      | 118.09   |
| 15  | L     | 301 | BCL  | CMB-C2B-C3B | 2.30  | 132.92      | 125.67   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | W     | 101 | BCL  | CMB-C2B-C3B | 2.30  | 132.92      | 125.67   |
| 15  | B     | 102 | BCL  | O2D-CGD-O1D | -2.30 | 119.37      | 123.85   |
| 15  | 3     | 101 | BCL  | CHC-C4B-NB  | -2.30 | 120.60      | 124.05   |
| 15  | 2     | 102 | BCL  | CMB-C2B-C3B | 2.30  | 132.92      | 125.67   |
| 15  | 5     | 102 | BCL  | CMD-C2D-C3D | -2.30 | 122.42      | 127.69   |
| 15  | 4     | 102 | BCL  | CHC-C1C-NC  | 2.30  | 127.71      | 124.40   |
| 22  | 9     | 101 | CRT  | C35-C33-C32 | -2.30 | 115.40      | 119.01   |
| 15  | Q     | 102 | BCL  | O2A-CGA-CBA | 2.30  | 118.83      | 111.83   |
| 15  | L     | 308 | BCL  | O2D-CGD-O1D | -2.29 | 119.38      | 123.85   |
| 15  | L     | 308 | BCL  | CMB-C2B-C3B | 2.29  | 132.89      | 125.67   |
| 22  | Z     | 103 | CRT  | C26-C27-C28 | -2.29 | 124.07      | 127.28   |
| 22  | B     | 103 | CRT  | C27-C26-C25 | -2.29 | 116.57      | 123.20   |
| 15  | E     | 102 | BCL  | C4A-NA-C1A  | 2.29  | 107.72      | 106.68   |
| 14  | L     | 310 | PGV  | C02-O01-C1  | -2.29 | 112.32      | 117.80   |
| 16  | L     | 302 | BPH  | CMA-C3A-C4A | -2.28 | 109.69      | 114.61   |
| 22  | N     | 102 | CRT  | C34-C33-C35 | 2.28  | 121.57      | 118.09   |
| 15  | Y     | 102 | BCL  | CHC-C4B-NB  | -2.28 | 120.63      | 124.05   |
| 14  | F     | 501 | PGV  | O14-P-O13   | 2.28  | 119.71      | 110.83   |
| 22  | 6     | 102 | CRT  | C35-C33-C32 | -2.28 | 115.42      | 119.01   |
| 15  | T     | 101 | BCL  | O2D-CGD-O1D | -2.28 | 119.42      | 123.85   |
| 15  | 1     | 402 | BCL  | C1C-NC-C4C  | -2.27 | 105.64      | 106.68   |
| 15  | 6     | 101 | BCL  | C1C-NC-C4C  | -2.27 | 105.64      | 106.68   |
| 22  | 4     | 103 | CRT  | C30-C28-C27 | -2.27 | 115.44      | 119.01   |
| 19  | M     | 407 | CDL  | OB6-CB5-OB7 | -2.27 | 118.39      | 123.70   |
| 22  | Y     | 101 | CRT  | C34-C33-C35 | 2.27  | 121.56      | 118.09   |
| 19  | H     | 302 | CDL  | CB4-OB6-CB5 | -2.27 | 112.36      | 117.80   |
| 22  | J     | 103 | CRT  | C4-C5-C6    | -2.27 | 121.73      | 124.91   |
| 22  | E     | 103 | CRT  | C27-C26-C25 | -2.27 | 116.62      | 123.20   |
| 14  | M     | 408 | PGV  | O14-P-O13   | 2.27  | 119.68      | 110.83   |
| 15  | L     | 308 | BCL  | C1D-CHD-C4C | -2.27 | 121.15      | 126.62   |
| 15  | V     | 101 | BCL  | C1D-CHD-C4C | -2.27 | 121.15      | 126.62   |
| 15  | K     | 102 | BCL  | CHB-C4A-NA  | 2.27  | 127.67      | 124.40   |
| 22  | R     | 102 | CRT  | C11-C12-C14 | -2.27 | 115.45      | 119.01   |
| 15  | Y     | 102 | BCL  | C1C-NC-C4C  | -2.26 | 105.65      | 106.68   |
| 15  | 8     | 102 | BCL  | O2A-CGA-O1A | -2.26 | 117.97      | 123.63   |
| 22  | R     | 102 | CRT  | C27-C26-C25 | -2.26 | 116.65      | 123.20   |
| 22  | V     | 102 | CRT  | C29-C28-C30 | 2.26  | 121.54      | 118.09   |
| 15  | R     | 101 | BCL  | O2D-CGD-O1D | -2.26 | 119.45      | 123.85   |
| 15  | N     | 101 | BCL  | C4A-NA-C1A  | 2.26  | 107.71      | 106.68   |
| 22  | 6     | 102 | CRT  | C27-C26-C25 | -2.25 | 116.67      | 123.20   |
| 15  | T     | 101 | BCL  | CMB-C2B-C3B | 2.25  | 132.77      | 125.67   |
| 15  | 4     | 102 | BCL  | CHC-C4B-NB  | -2.25 | 120.67      | 124.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | Y     | 102 | BCL  | O2D-CGD-O1D | -2.25 | 119.47      | 123.85   |
| 15  | 1     | 402 | BCL  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 15  | 8     | 102 | BCL  | CMB-C2B-C3B | 2.25  | 132.76      | 125.67   |
| 15  | Y     | 102 | BCL  | C1D-CHD-C4C | -2.25 | 121.20      | 126.62   |
| 22  | P     | 103 | CRT  | C29-C28-C30 | 2.25  | 121.52      | 118.09   |
| 15  | 2     | 102 | BCL  | C1D-CHD-C4C | -2.25 | 121.20      | 126.62   |
| 15  | G     | 102 | BCL  | O2D-CGD-O1D | -2.25 | 119.48      | 123.85   |
| 15  | Q     | 102 | BCL  | CHB-C1B-C2B | -2.25 | 120.91      | 127.43   |
| 15  | G     | 102 | BCL  | CMB-C2B-C3B | 2.24  | 132.75      | 125.67   |
| 22  | B     | 103 | CRT  | C30-C28-C27 | -2.24 | 115.48      | 119.01   |
| 15  | L     | 301 | BCL  | CHC-C4B-NB  | -2.24 | 120.69      | 124.05   |
| 15  | R     | 101 | BCL  | C1D-CHD-C4C | -2.24 | 121.21      | 126.62   |
| 15  | B     | 102 | BCL  | O2A-CGA-CBA | 2.24  | 118.67      | 111.83   |
| 22  | G     | 103 | CRT  | C20-C19-C17 | -2.24 | 124.14      | 127.28   |
| 15  | 5     | 102 | BCL  | O2A-CGA-CBA | 2.24  | 118.66      | 111.83   |
| 15  | Y     | 102 | BCL  | C2A-C1A-CHA | -2.24 | 119.98      | 123.87   |
| 17  | L     | 304 | UQ8  | C42-C41-C39 | -2.24 | 105.77      | 113.19   |
| 15  | 6     | 101 | BCL  | CHC-C4B-NB  | -2.24 | 120.69      | 124.05   |
| 15  | 8     | 102 | BCL  | C1D-CHD-C4C | -2.24 | 121.22      | 126.62   |
| 22  | B     | 103 | CRT  | C21-C20-C19 | -2.24 | 118.94      | 123.52   |
| 15  | M     | 403 | BCL  | O2A-CGA-O1A | -2.23 | 118.05      | 123.63   |
| 21  | M     | 405 | MQ8  | C24-C23-C25 | 2.23  | 119.10      | 115.23   |
| 15  | F     | 502 | BCL  | C1D-CHD-C4C | -2.23 | 121.25      | 126.62   |
| 14  | 1     | 401 | PGV  | C02-O01-C1  | -2.23 | 112.47      | 117.80   |
| 15  | L     | 301 | BCL  | C1D-CHD-C4C | -2.23 | 121.25      | 126.62   |
| 15  | I     | 101 | BCL  | CMD-C2D-C3D | -2.23 | 122.58      | 127.69   |
| 22  | P     | 103 | CRT  | C27-C26-C25 | -2.22 | 116.75      | 123.20   |
| 15  | L     | 308 | BCL  | C4-C3-C5    | 2.22  | 119.09      | 115.23   |
| 22  | E     | 103 | CRT  | C20-C21-C22 | -2.22 | 118.97      | 123.52   |
| 22  | 4     | 103 | CRT  | C14-C15-C16 | -2.22 | 116.77      | 123.20   |
| 22  | E     | 103 | CRT  | C29-C28-C30 | 2.22  | 121.48      | 118.09   |
| 14  | Q     | 101 | PGV  | O14-P-O13   | 2.22  | 119.48      | 110.83   |
| 22  | T     | 102 | CRT  | C21-C20-C19 | -2.22 | 118.98      | 123.52   |
| 18  | S     | 101 | LMT  | O5B-C5B-C4B | 2.22  | 113.70      | 109.70   |
| 15  | J     | 102 | BCL  | C1D-CHD-C4C | -2.22 | 121.27      | 126.62   |
| 15  | U     | 101 | BCL  | C2A-C1A-CHA | -2.22 | 120.02      | 123.87   |
| 14  | 1     | 401 | PGV  | O01-C1-O02  | -2.21 | 118.54      | 123.70   |
| 15  | D     | 102 | BCL  | CMD-C2D-C3D | -2.21 | 122.62      | 127.69   |
| 15  | L     | 301 | BCL  | C2A-C1A-CHA | -2.21 | 120.03      | 123.87   |
| 22  | G     | 103 | CRT  | C29-C28-C30 | 2.21  | 121.46      | 118.09   |
| 22  | N     | 102 | CRT  | C15-C14-C12 | -2.20 | 124.19      | 127.28   |
| 22  | P     | 103 | CRT  | C35-C33-C32 | -2.20 | 115.54      | 119.01   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | N     | 102 | CRT  | C26-C27-C28 | -2.20 | 124.19      | 127.28   |
| 22  | 9     | 101 | CRT  | C15-C14-C12 | -2.20 | 124.19      | 127.28   |
| 15  | 2     | 102 | BCL  | O2D-CGD-O1D | -2.20 | 119.56      | 123.85   |
| 15  | M     | 403 | BCL  | CHB-C1B-NB  | -2.20 | 120.75      | 124.05   |
| 17  | L     | 309 | UQ8  | C46-C44-C45 | 2.20  | 119.65      | 114.59   |
| 15  | D     | 102 | BCL  | C1-O2A-CGA  | 2.20  | 121.98      | 116.65   |
| 16  | M     | 404 | BPH  | CMA-C3A-C4A | -2.20 | 109.88      | 114.61   |
| 15  | 6     | 101 | BCL  | C1D-CHD-C4C | -2.20 | 121.32      | 126.62   |
| 15  | P     | 102 | BCL  | CMB-C2B-C3B | 2.19  | 132.59      | 125.67   |
| 15  | N     | 101 | BCL  | O2D-CGD-O1D | -2.19 | 119.58      | 123.85   |
| 15  | 6     | 101 | BCL  | CMB-C2B-C3B | 2.19  | 132.59      | 125.67   |
| 15  | R     | 101 | BCL  | CMB-C2B-C3B | 2.19  | 132.59      | 125.67   |
| 10  | C     | 401 | HEM  | C1A-CHA-C4D | -2.19 | 121.09      | 126.25   |
| 10  | C     | 403 | HEM  | C3B-C4B-NB  | -2.19 | 107.89      | 109.47   |
| 22  | J     | 103 | CRT  | C21-C20-C19 | -2.19 | 119.04      | 123.52   |
| 14  | M     | 408 | PGV  | O01-C1-O02  | -2.19 | 118.58      | 123.70   |
| 15  | X     | 102 | BCL  | C1D-CHD-C4C | -2.19 | 121.34      | 126.62   |
| 22  | 0     | 102 | CRT  | C9-C10-C11  | -2.19 | 116.86      | 123.20   |
| 15  | P     | 102 | BCL  | CHC-C4B-NB  | -2.18 | 120.77      | 124.05   |
| 15  | R     | 101 | BCL  | CHC-C4B-NB  | -2.18 | 120.77      | 124.05   |
| 22  | V     | 102 | CRT  | C21-C20-C19 | -2.18 | 119.05      | 123.52   |
| 18  | R     | 103 | LMT  | C1B-O1B-C4' | -2.18 | 112.80      | 117.98   |
| 15  | N     | 101 | BCL  | C2A-C1A-CHA | -2.18 | 120.08      | 123.87   |
| 15  | O     | 502 | BCL  | CMB-C2B-C3B | 2.18  | 132.54      | 125.67   |
| 18  | 8     | 103 | LMT  | C3'-C4'-C5' | -2.18 | 106.11      | 110.93   |
| 22  | J     | 103 | CRT  | C8-C7-C9    | -2.18 | 119.29      | 122.82   |
| 15  | 8     | 102 | BCL  | CHC-C4B-NB  | -2.17 | 120.79      | 124.05   |
| 18  | H     | 303 | LMT  | O5'-C5'-C6' | 2.17  | 111.83      | 106.44   |
| 22  | 6     | 102 | CRT  | C15-C14-C12 | -2.17 | 124.23      | 127.28   |
| 21  | M     | 405 | MQ8  | C41-C40-C38 | -2.17 | 105.99      | 113.19   |
| 15  | 7     | 101 | BCL  | C4A-NA-C1A  | 2.17  | 107.67      | 106.68   |
| 15  | B     | 102 | BCL  | C1-O2A-CGA  | 2.17  | 121.91      | 116.65   |
| 22  | P     | 103 | CRT  | C4-C5-C6    | -2.17 | 121.87      | 124.91   |
| 15  | I     | 101 | BCL  | CHB-C1B-C2B | -2.17 | 121.13      | 127.43   |
| 15  | 2     | 102 | BCL  | CHB-C1B-NB  | -2.17 | 120.80      | 124.05   |
| 15  | L     | 308 | BCL  | CHB-C1B-C2B | -2.16 | 121.15      | 127.43   |
| 10  | C     | 404 | HEM  | CHA-C4D-C3D | -2.16 | 121.24      | 125.23   |
| 15  | M     | 403 | BCL  | CHC-C1C-NC  | 2.16  | 127.52      | 124.40   |
| 15  | 1     | 402 | BCL  | CED-O2D-CGD | 2.16  | 120.82      | 115.92   |
| 22  | 4     | 103 | CRT  | C5-C6-C7    | -2.16 | 122.62      | 125.89   |
| 10  | C     | 402 | HEM  | CHA-C4D-C3D | -2.16 | 121.25      | 125.23   |
| 15  | 2     | 102 | BCL  | C4D-CHA-C1A | -2.16 | 118.67      | 121.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | M     | 407 | CDL  | OA6-CA5-C11 | 2.16  | 118.85      | 110.93   |
| 15  | E     | 102 | BCL  | CMB-C2B-C3B | 2.16  | 132.47      | 125.67   |
| 22  | J     | 103 | CRT  | C29-C28-C30 | 2.15  | 121.38      | 118.09   |
| 15  | R     | 101 | BCL  | O2A-CGA-CBA | 2.15  | 118.40      | 111.83   |
| 10  | C     | 403 | HEM  | O2D-CGD-CBD | 2.15  | 120.80      | 114.00   |
| 15  | S     | 102 | BCL  | CHB-C4A-NA  | 2.15  | 127.50      | 124.40   |
| 15  | W     | 101 | BCL  | CMD-C2D-C3D | -2.15 | 122.76      | 127.69   |
| 15  | W     | 101 | BCL  | C1D-CHD-C4C | -2.15 | 121.44      | 126.62   |
| 15  | V     | 101 | BCL  | CED-O2D-CGD | 2.15  | 120.78      | 115.92   |
| 15  | 9     | 102 | BCL  | C4-C3-C5    | 2.15  | 118.95      | 115.23   |
| 18  | X     | 101 | LMT  | C1B-O1B-C4' | -2.15 | 112.89      | 117.98   |
| 22  | 6     | 102 | CRT  | C29-C28-C30 | 2.14  | 121.36      | 118.09   |
| 15  | 9     | 102 | BCL  | C4A-NA-C1A  | 2.14  | 107.66      | 106.68   |
| 10  | C     | 403 | HEM  | C4C-NC-C1C  | 2.14  | 109.31      | 105.82   |
| 15  | M     | 402 | BCL  | CHB-C4A-NA  | 2.14  | 127.49      | 124.40   |
| 22  | T     | 102 | CRT  | C34-C33-C35 | 2.14  | 121.36      | 118.09   |
| 15  | 2     | 102 | BCL  | O2A-CGA-O1A | -2.14 | 118.28      | 123.63   |
| 15  | O     | 502 | BCL  | CHB-C4A-NA  | 2.14  | 127.48      | 124.40   |
| 15  | M     | 402 | BCL  | C2A-C1A-CHA | -2.14 | 120.16      | 123.87   |
| 10  | C     | 403 | HEM  | CHA-C4D-C3D | -2.13 | 121.29      | 125.23   |
| 15  | G     | 102 | BCL  | C1D-CHD-C4C | -2.13 | 121.47      | 126.62   |
| 10  | C     | 404 | HEM  | C3B-C4B-NB  | -2.13 | 107.94      | 109.47   |
| 22  | G     | 103 | CRT  | C9-C10-C11  | -2.13 | 117.02      | 123.20   |
| 15  | G     | 102 | BCL  | CHB-C1B-NB  | -2.13 | 120.85      | 124.05   |
| 15  | F     | 502 | BCL  | C2A-C1A-CHA | -2.13 | 120.17      | 123.87   |
| 15  | 4     | 102 | BCL  | CED-O2D-CGD | 2.13  | 120.74      | 115.92   |
| 15  | 3     | 101 | BCL  | CMB-C2B-C3B | 2.13  | 132.38      | 125.67   |
| 15  | 0     | 101 | BCL  | CED-O2D-CGD | 2.13  | 120.74      | 115.92   |
| 22  | R     | 102 | CRT  | C34-C33-C35 | 2.12  | 121.33      | 118.09   |
| 15  | I     | 101 | BCL  | C1D-CHD-C4C | -2.12 | 121.50      | 126.62   |
| 15  | 8     | 102 | BCL  | CED-O2D-CGD | 2.12  | 120.73      | 115.92   |
| 15  | A     | 502 | BCL  | C2A-C1A-CHA | -2.12 | 120.19      | 123.87   |
| 22  | T     | 102 | CRT  | C29-C28-C30 | 2.12  | 121.33      | 118.09   |
| 15  | 3     | 101 | BCL  | CED-O2D-CGD | 2.12  | 120.71      | 115.92   |
| 15  | W     | 101 | BCL  | O1D-CGD-CBD | -2.11 | 120.35      | 124.52   |
| 17  | L     | 303 | UQ8  | C22-C23-C24 | -2.11 | 120.60      | 127.64   |
| 14  | A     | 503 | PGV  | O03-C19-O04 | -2.11 | 118.35      | 123.63   |
| 15  | L     | 308 | BCL  | CHD-C1D-C2D | 2.11  | 129.88      | 125.49   |
| 22  | Z     | 103 | CRT  | C27-C26-C25 | -2.11 | 117.08      | 123.20   |
| 15  | L     | 301 | BCL  | CHB-C4A-NA  | 2.11  | 127.44      | 124.40   |
| 15  | L     | 301 | BCL  | CMD-C2D-C3D | -2.11 | 122.86      | 127.69   |
| 22  | 4     | 103 | CRT  | C15-C14-C12 | -2.11 | 124.32      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 6     | 102 | CRT  | C26-C27-C28 | -2.11 | 124.33      | 127.28   |
| 22  | G     | 103 | CRT  | C21-C20-C19 | -2.11 | 119.21      | 123.52   |
| 22  | M     | 406 | CRT  | C27-C26-C25 | -2.10 | 117.11      | 123.20   |
| 21  | M     | 405 | MQ8  | C39-C38-C40 | 2.10  | 118.87      | 115.23   |
| 15  | F     | 502 | BCL  | CHB-C1B-C2B | -2.10 | 121.33      | 127.43   |
| 22  | N     | 102 | CRT  | C9-C10-C11  | -2.10 | 117.12      | 123.20   |
| 22  | 0     | 102 | CRT  | C24-C23-C25 | 2.10  | 121.29      | 118.09   |
| 10  | C     | 404 | HEM  | C1A-CHA-C4D | -2.10 | 121.32      | 126.25   |
| 18  | 5     | 101 | LMT  | O5'-C5'-C4' | 2.09  | 114.05      | 109.72   |
| 15  | Y     | 102 | BCL  | CMB-C2B-C3B | 2.09  | 132.27      | 125.67   |
| 22  | 9     | 101 | CRT  | C14-C15-C16 | -2.09 | 117.14      | 123.20   |
| 15  | D     | 102 | BCL  | CHB-C1B-C2B | -2.09 | 121.36      | 127.43   |
| 15  | E     | 102 | BCL  | CHB-C1B-NB  | -2.09 | 120.91      | 124.05   |
| 15  | G     | 102 | BCL  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 15  | P     | 102 | BCL  | C11-C12-C13 | -2.09 | 109.03      | 115.97   |
| 15  | 1     | 402 | BCL  | O2D-CGD-O1D | -2.09 | 119.79      | 123.85   |
| 10  | C     | 401 | HEM  | CBD-CAD-C3D | -2.08 | 106.77      | 112.53   |
| 15  | 6     | 101 | BCL  | CHB-C1B-NB  | -2.08 | 120.92      | 124.05   |
| 10  | C     | 401 | HEM  | CHD-C4C-NC  | 2.08  | 126.72      | 124.45   |
| 15  | O     | 502 | BCL  | CMD-C2D-C3D | -2.08 | 122.92      | 127.69   |
| 18  | H     | 303 | LMT  | O1B-C4'-C3' | 2.08  | 112.52      | 107.23   |
| 15  | V     | 101 | BCL  | O2D-CGD-O1D | -2.08 | 119.80      | 123.85   |
| 15  | S     | 102 | BCL  | CHB-C1B-C2B | -2.08 | 121.39      | 127.43   |
| 15  | 4     | 102 | BCL  | CHB-C1B-NB  | -2.08 | 120.93      | 124.05   |
| 22  | G     | 103 | CRT  | C35-C33-C32 | -2.08 | 115.74      | 119.01   |
| 15  | S     | 102 | BCL  | CMD-C2D-C3D | -2.07 | 122.93      | 127.69   |
| 22  | J     | 103 | CRT  | C27-C26-C25 | -2.07 | 117.19      | 123.20   |
| 22  | Y     | 101 | CRT  | C29-C28-C30 | 2.07  | 121.25      | 118.09   |
| 15  | A     | 502 | BCL  | CHB-C1B-C2B | -2.07 | 121.41      | 127.43   |
| 15  | W     | 101 | BCL  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 22  | V     | 102 | CRT  | C18-C17-C16 | 2.07  | 121.25      | 118.09   |
| 10  | C     | 401 | HEM  | CBA-CAA-C2A | -2.07 | 106.82      | 112.53   |
| 15  | 7     | 101 | BCL  | CHB-C1B-C2B | -2.07 | 121.43      | 127.43   |
| 17  | L     | 304 | UQ8  | C46-C44-C45 | 2.07  | 119.34      | 114.59   |
| 15  | 9     | 102 | BCL  | CHB-C1B-C2B | -2.07 | 121.43      | 127.43   |
| 10  | C     | 402 | HEM  | CHB-C1B-C2B | -2.06 | 121.08      | 126.95   |
| 22  | E     | 103 | CRT  | C11-C12-C14 | -2.06 | 115.77      | 119.01   |
| 19  | L     | 311 | CDL  | OB6-CB5-OB7 | -2.06 | 118.89      | 123.70   |
| 15  | J     | 102 | BCL  | C4D-CHA-C1A | -2.06 | 118.79      | 121.24   |
| 15  | 0     | 101 | BCL  | C4D-CHA-C1A | -2.06 | 118.79      | 121.24   |
| 10  | C     | 402 | HEM  | CHA-C1A-NA  | 2.05  | 127.58      | 123.86   |
| 22  | T     | 102 | CRT  | C31-C32-C33 | -2.05 | 124.40      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | M     | 409 | CDL  | OB8-CB7-OB9 | -2.05 | 118.49      | 123.63   |
| 22  | B     | 103 | CRT  | C20-C21-C22 | -2.05 | 119.32      | 123.52   |
| 15  | D     | 102 | BCL  | C1D-CHD-C4C | -2.05 | 121.68      | 126.62   |
| 22  | G     | 103 | CRT  | C13-C12-C11 | 2.05  | 121.22      | 118.09   |
| 22  | 9     | 101 | CRT  | C18-C17-C16 | 2.05  | 121.22      | 118.09   |
| 14  | C     | 408 | PGV  | C02-O01-C1  | -2.05 | 112.90      | 117.80   |
| 22  | 9     | 101 | CRT  | C21-C20-C19 | -2.05 | 119.33      | 123.52   |
| 15  | P     | 102 | BCL  | C4A-NA-C1A  | 2.05  | 107.61      | 106.68   |
| 15  | 7     | 101 | BCL  | CMD-C2D-C3D | -2.05 | 123.00      | 127.69   |
| 15  | 8     | 102 | BCL  | CHB-C1B-NB  | -2.05 | 120.98      | 124.05   |
| 15  | 1     | 402 | BCL  | CHB-C1B-C2B | -2.05 | 121.49      | 127.43   |
| 15  | P     | 102 | BCL  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 22  | N     | 102 | CRT  | C35-C33-C32 | -2.04 | 115.80      | 119.01   |
| 18  | Z     | 101 | LMT  | O5'-C1'-C2' | -2.04 | 106.18      | 110.37   |
| 15  | G     | 102 | BCL  | CED-O2D-CGD | 2.04  | 120.54      | 115.92   |
| 15  | W     | 101 | BCL  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 15  | X     | 102 | BCL  | C4D-CHA-C1A | -2.04 | 118.82      | 121.24   |
| 15  | O     | 502 | BCL  | O2A-CGA-O1A | -2.03 | 118.54      | 123.63   |
| 15  | L     | 308 | BCL  | CMD-C2D-C3D | -2.03 | 123.03      | 127.69   |
| 22  | M     | 406 | CRT  | C18-C17-C16 | 2.03  | 121.19      | 118.09   |
| 10  | C     | 404 | HEM  | O2A-CGA-CBA | 2.03  | 120.42      | 114.00   |
| 15  | W     | 101 | BCL  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 15  | X     | 102 | BCL  | CHB-C1B-NB  | -2.03 | 121.00      | 124.05   |
| 10  | C     | 401 | HEM  | O2A-CGA-CBA | 2.03  | 120.42      | 114.00   |
| 15  | U     | 101 | BCL  | CHB-C1B-C2B | -2.03 | 121.54      | 127.43   |
| 14  | C     | 408 | PGV  | O01-C1-O02  | -2.03 | 118.97      | 123.70   |
| 15  | M     | 403 | BCL  | CHD-C1D-C2D | 2.03  | 129.70      | 125.49   |
| 22  | 0     | 102 | CRT  | C16-C17-C19 | -2.03 | 115.82      | 119.01   |
| 15  | T     | 101 | BCL  | CHB-C1B-NB  | -2.03 | 121.01      | 124.05   |
| 15  | G     | 102 | BCL  | C4D-CHA-C1A | -2.02 | 118.83      | 121.24   |
| 22  | J     | 103 | CRT  | C26-C27-C28 | -2.02 | 124.44      | 127.28   |
| 22  | E     | 103 | CRT  | C8-C7-C6    | 2.02  | 121.18      | 118.09   |
| 15  | M     | 403 | BCL  | C1C-NC-C4C  | -2.02 | 105.76      | 106.68   |
| 15  | D     | 102 | BCL  | C2A-C1A-CHA | -2.02 | 120.36      | 123.87   |
| 15  | M     | 402 | BCL  | CHB-C1B-C2B | -2.02 | 121.56      | 127.43   |
| 19  | M     | 409 | CDL  | OB6-CB5-OB7 | -2.02 | 118.98      | 123.70   |
| 22  | 9     | 101 | CRT  | C9-C10-C11  | -2.02 | 117.35      | 123.20   |
| 15  | 1     | 402 | BCL  | C2A-C1A-CHA | -2.02 | 120.36      | 123.87   |
| 15  | X     | 102 | BCL  | CED-O2D-CGD | 2.02  | 120.49      | 115.92   |
| 22  | M     | 406 | CRT  | C5-C6-C7    | -2.02 | 122.84      | 125.89   |
| 15  | O     | 502 | BCL  | C1D-CHD-C4C | -2.01 | 121.76      | 126.62   |
| 15  | M     | 402 | BCL  | C1-O2A-CGA  | 2.01  | 121.53      | 116.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | 5     | 102 | BCL  | CHB-C1B-C2B | -2.01 | 121.58      | 127.43   |
| 15  | X     | 102 | BCL  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 15  | B     | 102 | BCL  | C4D-CHA-C1A | -2.01 | 118.85      | 121.24   |
| 15  | K     | 102 | BCL  | CHB-C1B-C2B | -2.01 | 121.60      | 127.43   |
| 22  | P     | 103 | CRT  | C30-C28-C27 | -2.00 | 115.86      | 119.01   |
| 15  | N     | 101 | BCL  | CHB-C1B-C2B | -2.00 | 121.61      | 127.43   |
| 15  | Q     | 102 | BCL  | CHD-C1D-C2D | 2.00  | 129.65      | 125.49   |
| 15  | T     | 101 | BCL  | O2A-CGA-CBA | 2.00  | 117.94      | 111.83   |

There are no chirality outliers.

All (1013) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | C     | 401 | HEM  | C2B-C3B-CAB-CBB |
| 10  | C     | 402 | HEM  | C2B-C3B-CAB-CBB |
| 10  | C     | 403 | HEM  | C2B-C3B-CAB-CBB |
| 10  | C     | 403 | HEM  | C4B-C3B-CAB-CBB |
| 10  | C     | 404 | HEM  | C2B-C3B-CAB-CBB |
| 10  | C     | 404 | HEM  | C2C-C3C-CAC-CBC |
| 14  | L     | 305 | PGV  | C03-O11-P-O13   |
| 14  | L     | 305 | PGV  | C04-O12-P-O13   |
| 14  | L     | 305 | PGV  | O12-C04-C05-C06 |
| 14  | L     | 306 | PGV  | C04-O12-P-O14   |
| 14  | L     | 310 | PGV  | C03-O11-P-O12   |
| 14  | L     | 310 | PGV  | C03-O11-P-O14   |
| 14  | L     | 310 | PGV  | C04-O12-P-O14   |
| 14  | H     | 301 | PGV  | C04-O12-P-O11   |
| 14  | H     | 301 | PGV  | C04-C05-C06-O06 |
| 14  | A     | 501 | PGV  | C03-O11-P-O12   |
| 14  | A     | 501 | PGV  | C03-O11-P-O13   |
| 14  | A     | 501 | PGV  | C03-O11-P-O14   |
| 14  | A     | 501 | PGV  | C04-O12-P-O11   |
| 14  | A     | 501 | PGV  | C04-O12-P-O13   |
| 14  | A     | 501 | PGV  | O02-C1-O01-C02  |
| 14  | A     | 501 | PGV  | C2-C1-O01-C02   |
| 14  | A     | 503 | PGV  | C04-O12-P-O13   |
| 14  | Q     | 101 | PGV  | C03-O11-P-O12   |
| 14  | Q     | 101 | PGV  | C03-O11-P-O14   |
| 15  | M     | 403 | BCL  | CAD-CBD-CGD-O1D |
| 15  | M     | 403 | BCL  | CAD-CBD-CGD-O2D |
| 15  | A     | 502 | BCL  | C2C-C3C-CAC-CBC |
| 15  | D     | 102 | BCL  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | D     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 15  | E     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | G     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 15  | G     | 102 | BCL  | C11-C12-C13-C14 |
| 15  | J     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 15  | N     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 15  | N     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 15  | O     | 502 | BCL  | C1A-C2A-CAA-CBA |
| 15  | O     | 502 | BCL  | C3A-C2A-CAA-CBA |
| 15  | O     | 502 | BCL  | C4C-C3C-CAC-CBC |
| 15  | Q     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 15  | Q     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 15  | R     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 15  | R     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 15  | T     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 15  | T     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 15  | T     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 15  | T     | 101 | BCL  | C6-C7-C8-C9     |
| 15  | U     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 15  | U     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 15  | V     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 15  | W     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 15  | W     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 15  | W     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 15  | X     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 15  | Z     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 15  | Z     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 15  | Z     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | 2     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 15  | 2     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | 3     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 15  | 3     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 15  | 4     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | 6     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 15  | 6     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 15  | 8     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 15  | 0     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 17  | L     | 304 | UQ8  | C1-C6-C7-C8     |
| 17  | L     | 304 | UQ8  | C5-C6-C7-C8     |
| 18  | M     | 411 | LMT  | O5'-C1'-O1'-C1  |
| 18  | H     | 303 | LMT  | O5'-C1'-O1'-C1  |
| 18  | J     | 104 | LMT  | O5'-C1'-O1'-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | L     | 311 | CDL  | CA2-OA2-PA1-OA4 |
| 19  | L     | 311 | CDL  | CA2-OA2-PA1-OA5 |
| 19  | L     | 311 | CDL  | CA3-OA5-PA1-OA3 |
| 19  | L     | 311 | CDL  | C11-CA5-OA6-CA4 |
| 19  | L     | 311 | CDL  | CB3-OB5-PB2-OB2 |
| 19  | M     | 407 | CDL  | CA2-OA2-PA1-OA4 |
| 19  | M     | 407 | CDL  | CA2-OA2-PA1-OA5 |
| 19  | M     | 407 | CDL  | CB2-OB2-PB2-OB3 |
| 19  | M     | 407 | CDL  | CB2-OB2-PB2-OB4 |
| 19  | M     | 407 | CDL  | CB2-OB2-PB2-OB5 |
| 19  | M     | 407 | CDL  | CB3-OB5-PB2-OB2 |
| 19  | M     | 407 | CDL  | CB3-OB5-PB2-OB4 |
| 19  | M     | 409 | CDL  | CA2-OA2-PA1-OA4 |
| 19  | M     | 409 | CDL  | CA2-OA2-PA1-OA5 |
| 19  | M     | 409 | CDL  | CA3-OA5-PA1-OA2 |
| 19  | M     | 409 | CDL  | CB3-OB5-PB2-OB2 |
| 19  | M     | 409 | CDL  | CB3-OB5-PB2-OB3 |
| 19  | M     | 409 | CDL  | CB3-OB5-PB2-OB4 |
| 19  | M     | 409 | CDL  | OB5-CB3-CB4-OB6 |
| 19  | H     | 302 | CDL  | O1-C1-CB2-OB2   |
| 19  | H     | 302 | CDL  | CA3-OA5-PA1-OA2 |
| 19  | H     | 302 | CDL  | CA3-OA5-PA1-OA3 |
| 19  | H     | 302 | CDL  | CB3-OB5-PB2-OB2 |
| 19  | H     | 302 | CDL  | CB3-OB5-PB2-OB4 |
| 19  | D     | 101 | CDL  | O1-C1-CB2-OB2   |
| 19  | D     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 19  | D     | 101 | CDL  | CA2-OA2-PA1-OA4 |
| 19  | D     | 101 | CDL  | CA2-OA2-PA1-OA5 |
| 19  | D     | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 19  | D     | 101 | CDL  | CA3-OA5-PA1-OA4 |
| 19  | D     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 19  | D     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 19  | D     | 101 | CDL  | CB3-OB5-PB2-OB2 |
| 19  | D     | 101 | CDL  | CB3-OB5-PB2-OB3 |
| 22  | M     | 406 | CRT  | C32-C33-C35-C36 |
| 22  | M     | 406 | CRT  | C34-C33-C35-C36 |
| 22  | M     | 406 | CRT  | C36-C37-C38-C39 |
| 22  | M     | 406 | CRT  | C36-C37-C38-O2  |
| 22  | B     | 103 | CRT  | C5-C6-C7-C9     |
| 22  | E     | 103 | CRT  | C2-C1-O1-C1M    |
| 22  | E     | 103 | CRT  | C36-C37-C38-C39 |
| 22  | E     | 103 | CRT  | C36-C37-C38-C40 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | E     | 103 | CRT  | C36-C37-C38-O2  |
| 22  | G     | 103 | CRT  | C5-C6-C7-C9     |
| 22  | G     | 103 | CRT  | C40-C38-O2-C2M  |
| 22  | J     | 103 | CRT  | C2-C1-O1-C1M    |
| 22  | J     | 103 | CRT  | O1-C1-C4-C5     |
| 22  | J     | 103 | CRT  | C2-C1-C4-C5     |
| 22  | J     | 103 | CRT  | C3-C1-C4-C5     |
| 22  | J     | 103 | CRT  | C40-C38-O2-C2M  |
| 22  | N     | 102 | CRT  | O1-C1-C4-C5     |
| 22  | N     | 102 | CRT  | C2-C1-C4-C5     |
| 22  | N     | 102 | CRT  | C3-C1-C4-C5     |
| 22  | N     | 102 | CRT  | C36-C37-C38-C39 |
| 22  | N     | 102 | CRT  | C36-C37-C38-C40 |
| 22  | N     | 102 | CRT  | C36-C37-C38-O2  |
| 22  | P     | 103 | CRT  | C2-C1-O1-C1M    |
| 22  | P     | 103 | CRT  | C10-C11-C12-C13 |
| 22  | P     | 103 | CRT  | C10-C11-C12-C14 |
| 22  | P     | 103 | CRT  | C15-C16-C17-C19 |
| 22  | T     | 102 | CRT  | O1-C1-C4-C5     |
| 22  | T     | 102 | CRT  | C2-C1-C4-C5     |
| 22  | T     | 102 | CRT  | C3-C1-C4-C5     |
| 22  | T     | 102 | CRT  | C10-C11-C12-C13 |
| 22  | T     | 102 | CRT  | C10-C11-C12-C14 |
| 22  | T     | 102 | CRT  | C15-C16-C17-C19 |
| 22  | V     | 102 | CRT  | O1-C1-C4-C5     |
| 22  | V     | 102 | CRT  | C2-C1-C4-C5     |
| 22  | V     | 102 | CRT  | C3-C1-C4-C5     |
| 22  | V     | 102 | CRT  | C36-C37-C38-C39 |
| 22  | V     | 102 | CRT  | C36-C37-C38-C40 |
| 22  | Y     | 101 | CRT  | C10-C11-C12-C13 |
| 22  | Y     | 101 | CRT  | C10-C11-C12-C14 |
| 22  | Z     | 103 | CRT  | O1-C1-C4-C5     |
| 22  | Z     | 103 | CRT  | C2-C1-C4-C5     |
| 22  | Z     | 103 | CRT  | C3-C1-C4-C5     |
| 22  | Z     | 103 | CRT  | C10-C11-C12-C14 |
| 22  | Z     | 103 | CRT  | C32-C33-C35-C36 |
| 22  | Z     | 103 | CRT  | C36-C37-C38-C39 |
| 22  | Z     | 103 | CRT  | C36-C37-C38-O2  |
| 22  | 2     | 103 | CRT  | C5-C6-C7-C8     |
| 22  | 2     | 103 | CRT  | C5-C6-C7-C9     |
| 22  | 2     | 103 | CRT  | C36-C37-C38-C40 |
| 22  | 4     | 103 | CRT  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 4     | 103 | CRT  | C5-C6-C7-C9     |
| 22  | 6     | 102 | CRT  | O1-C1-C4-C5     |
| 22  | 6     | 102 | CRT  | C2-C1-C4-C5     |
| 22  | 6     | 102 | CRT  | C5-C6-C7-C9     |
| 22  | 9     | 101 | CRT  | C5-C6-C7-C8     |
| 22  | 9     | 101 | CRT  | C5-C6-C7-C9     |
| 18  | 5     | 101 | LMT  | C3'-C4'-O1B-C1B |
| 19  | L     | 311 | CDL  | OA7-CA5-OA6-CA4 |
| 18  | S     | 101 | LMT  | C2B-C1B-O1B-C4' |
| 15  | T     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 14  | L     | 310 | PGV  | O04-C19-O03-C01 |
| 19  | D     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 15  | A     | 502 | BCL  | C3-C5-C6-C7     |
| 15  | E     | 102 | BCL  | C3-C5-C6-C7     |
| 15  | U     | 101 | BCL  | C3-C5-C6-C7     |
| 14  | L     | 310 | PGV  | C20-C19-O03-C01 |
| 18  | E     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 15  | 4     | 102 | BCL  | CBD-CGD-O2D-CED |
| 15  | 7     | 101 | BCL  | CBD-CGD-O2D-CED |
| 15  | F     | 502 | BCL  | C4-C3-C5-C6     |
| 15  | I     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | N     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | R     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | S     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | 2     | 102 | BCL  | C4-C3-C5-C6     |
| 17  | L     | 309 | UQ8  | C40-C39-C41-C42 |
| 17  | L     | 309 | UQ8  | C35-C34-C36-C37 |
| 21  | M     | 405 | MQ8  | C45-C43-C44-C46 |
| 15  | I     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | N     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | R     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | 2     | 102 | BCL  | C2-C3-C5-C6     |
| 17  | L     | 309 | UQ8  | C38-C39-C41-C42 |
| 21  | M     | 405 | MQ8  | C42-C43-C44-C46 |
| 18  | L     | 307 | LMT  | O5B-C5B-C6B-O6B |
| 15  | D     | 102 | BCL  | C3-C5-C6-C7     |
| 14  | A     | 503 | PGV  | C20-C19-O03-C01 |
| 14  | A     | 503 | PGV  | O04-C19-O03-C01 |
| 15  | 0     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 19  | D     | 101 | CDL  | OA9-CA7-OA8-CA6 |
| 15  | Z     | 102 | BCL  | C3-C5-C6-C7     |
| 15  | B     | 102 | BCL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | S     | 102 | BCL  | CBD-CGD-O2D-CED |
| 14  | L     | 306 | PGV  | O12-C04-C05-O05 |
| 19  | L     | 311 | CDL  | O1-C1-CA2-OA2   |
| 15  | 0     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 18  | L     | 307 | LMT  | C4B-C5B-C6B-O6B |
| 18  | E     | 101 | LMT  | C4B-C5B-C6B-O6B |
| 19  | D     | 101 | CDL  | C31-CA7-OA8-CA6 |
| 18  | M     | 410 | LMT  | O5'-C5'-C6'-O6' |
| 15  | 1     | 402 | BCL  | C4-C3-C5-C6     |
| 15  | 3     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | 0     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | S     | 102 | BCL  | C2-C3-C5-C6     |
| 15  | 3     | 101 | BCL  | C2-C3-C5-C6     |
| 17  | L     | 309 | UQ8  | C33-C34-C36-C37 |
| 18  | P     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 17  | L     | 303 | UQ8  | C19-C21-C22-C23 |
| 17  | L     | 304 | UQ8  | C9-C11-C12-C13  |
| 17  | L     | 309 | UQ8  | C39-C41-C42-C43 |
| 17  | L     | 309 | UQ8  | C24-C26-C27-C28 |
| 17  | L     | 309 | UQ8  | C19-C21-C22-C23 |
| 18  | R     | 103 | LMT  | O5'-C1'-O1'-C1  |
| 15  | W     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 15  | L     | 308 | BCL  | CBD-CGD-O2D-CED |
| 15  | J     | 102 | BCL  | CBD-CGD-O2D-CED |
| 15  | I     | 101 | BCL  | CBD-CGD-O2D-CED |
| 15  | W     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 19  | D     | 101 | CDL  | CA2-C1-CB2-OB2  |
| 15  | K     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 15  | U     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 15  | 7     | 101 | BCL  | O1D-CGD-O2D-CED |
| 15  | Q     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | F     | 502 | BCL  | C2-C3-C5-C6     |
| 15  | Q     | 102 | BCL  | C2-C3-C5-C6     |
| 15  | 1     | 402 | BCL  | C2-C3-C5-C6     |
| 15  | 0     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | L     | 308 | BCL  | C11-C10-C8-C9   |
| 15  | B     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | G     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | G     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | I     | 101 | BCL  | C11-C10-C8-C9   |
| 15  | J     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | N     | 101 | BCL  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | P     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | R     | 101 | BCL  | C6-C7-C8-C9     |
| 15  | R     | 101 | BCL  | C11-C10-C8-C9   |
| 15  | V     | 101 | BCL  | C6-C7-C8-C9     |
| 15  | X     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | 6     | 101 | BCL  | C6-C7-C8-C9     |
| 15  | 6     | 101 | BCL  | C11-C10-C8-C9   |
| 15  | 8     | 102 | BCL  | C11-C12-C13-C14 |
| 15  | 9     | 102 | BCL  | C11-C10-C8-C9   |
| 14  | 1     | 401 | PGV  | C19-C20-C21-C22 |
| 19  | M     | 407 | CDL  | O1-C1-CB2-OB2   |
| 22  | B     | 103 | CRT  | C5-C6-C7-C8     |
| 22  | G     | 103 | CRT  | C5-C6-C7-C8     |
| 22  | P     | 103 | CRT  | C15-C16-C17-C18 |
| 22  | T     | 102 | CRT  | C15-C16-C17-C18 |
| 22  | Z     | 103 | CRT  | C10-C11-C12-C13 |
| 22  | Z     | 103 | CRT  | C34-C33-C35-C36 |
| 22  | 6     | 102 | CRT  | C5-C6-C7-C8     |
| 15  | 6     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 15  | K     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 15  | U     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 14  | M     | 408 | PGV  | O01-C02-C03-O11 |
| 15  | T     | 101 | BCL  | CBD-CGD-O2D-CED |
| 15  | 0     | 101 | BCL  | C10-C11-C12-C13 |
| 15  | J     | 102 | BCL  | C5-C6-C7-C8     |
| 15  | U     | 101 | BCL  | C10-C11-C12-C13 |
| 19  | D     | 101 | CDL  | CA5-C11-C12-C13 |
| 15  | P     | 102 | BCL  | C8-C10-C11-C12  |
| 15  | I     | 101 | BCL  | C6-C7-C8-C10    |
| 15  | N     | 101 | BCL  | C6-C7-C8-C10    |
| 15  | Y     | 102 | BCL  | C11-C10-C8-C7   |
| 15  | 4     | 102 | BCL  | C11-C10-C8-C7   |
| 15  | 0     | 101 | BCL  | C6-C7-C8-C10    |
| 17  | L     | 303 | UQ8  | C14-C16-C17-C18 |
| 17  | L     | 309 | UQ8  | C34-C36-C37-C38 |
| 17  | L     | 309 | UQ8  | C14-C16-C17-C18 |
| 15  | O     | 502 | BCL  | C5-C6-C7-C8     |
| 15  | O     | 502 | BCL  | C10-C11-C12-C13 |
| 15  | 4     | 102 | BCL  | O1D-CGD-O2D-CED |
| 15  | A     | 502 | BCL  | C10-C11-C12-C13 |
| 15  | O     | 502 | BCL  | C8-C10-C11-C12  |
| 15  | S     | 102 | BCL  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | 6     | 101 | BCL  | C15-C16-C17-C18 |
| 15  | 7     | 101 | BCL  | C5-C6-C7-C8     |
| 15  | E     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 15  | N     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 15  | Z     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 15  | B     | 102 | BCL  | C15-C16-C17-C18 |
| 15  | D     | 102 | BCL  | C10-C11-C12-C13 |
| 15  | F     | 502 | BCL  | C10-C11-C12-C13 |
| 15  | F     | 502 | BCL  | C15-C16-C17-C18 |
| 15  | G     | 102 | BCL  | C5-C6-C7-C8     |
| 15  | 5     | 102 | BCL  | C5-C6-C7-C8     |
| 15  | 6     | 101 | BCL  | C5-C6-C7-C8     |
| 14  | M     | 408 | PGV  | C19-C20-C21-C22 |
| 19  | M     | 409 | CDL  | CA5-C11-C12-C13 |
| 15  | P     | 102 | BCL  | C3-C5-C6-C7     |
| 15  | S     | 102 | BCL  | C3-C5-C6-C7     |
| 18  | T     | 103 | LMT  | O5'-C1'-O1'-C1  |
| 15  | B     | 102 | BCL  | C5-C6-C7-C8     |
| 15  | E     | 102 | BCL  | C13-C15-C16-C17 |
| 15  | W     | 101 | BCL  | C5-C6-C7-C8     |
| 15  | Z     | 102 | BCL  | C5-C6-C7-C8     |
| 15  | 3     | 101 | BCL  | C5-C6-C7-C8     |
| 15  | 5     | 102 | BCL  | C15-C16-C17-C18 |
| 14  | L     | 305 | PGV  | O12-C04-C05-O05 |
| 15  | A     | 502 | BCL  | C13-C15-C16-C17 |
| 15  | W     | 101 | BCL  | C10-C11-C12-C13 |
| 15  | X     | 102 | BCL  | C3-C5-C6-C7     |
| 15  | T     | 101 | BCL  | C5-C6-C7-C8     |
| 15  | S     | 102 | BCL  | O1D-CGD-O2D-CED |
| 14  | A     | 501 | PGV  | C20-C19-O03-C01 |
| 15  | B     | 102 | BCL  | O1D-CGD-O2D-CED |
| 15  | N     | 101 | BCL  | C3-C5-C6-C7     |
| 18  | 4     | 104 | LMT  | C5'-C4'-O1B-C1B |
| 19  | M     | 409 | CDL  | C52-C53-C54-C55 |
| 14  | L     | 306 | PGV  | O12-C04-C05-C06 |
| 15  | E     | 102 | BCL  | C5-C6-C7-C8     |
| 15  | E     | 102 | BCL  | C10-C11-C12-C13 |
| 15  | T     | 101 | BCL  | C10-C11-C12-C13 |
| 15  | Y     | 102 | BCL  | C5-C6-C7-C8     |
| 15  | 2     | 102 | BCL  | C15-C16-C17-C18 |
| 15  | 0     | 101 | BCL  | C15-C16-C17-C18 |
| 15  | P     | 102 | BCL  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | U     | 101 | BCL  | C5-C6-C7-C8     |
| 15  | 4     | 102 | BCL  | C15-C16-C17-C18 |
| 18  | S     | 101 | LMT  | O1'-C1-C2-C3    |
| 18  | S     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 18  | M     | 410 | LMT  | C4'-C5'-C6'-O6' |
| 15  | F     | 502 | BCL  | C13-C15-C16-C17 |
| 15  | N     | 101 | BCL  | C8-C10-C11-C12  |
| 15  | V     | 101 | BCL  | C10-C11-C12-C13 |
| 15  | 6     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | R     | 101 | BCL  | C13-C15-C16-C17 |
| 15  | 2     | 102 | BCL  | C13-C15-C16-C17 |
| 14  | Q     | 101 | PGV  | C2-C1-O01-C02   |
| 15  | Z     | 102 | BCL  | C11-C12-C13-C14 |
| 18  | 2     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 14  | Q     | 101 | PGV  | O02-C1-O01-C02  |
| 15  | V     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 18  | 4     | 104 | LMT  | C3'-C4'-O1B-C1B |
| 22  | M     | 406 | CRT  | C5-C6-C7-C8     |
| 22  | J     | 103 | CRT  | C5-C6-C7-C8     |
| 22  | M     | 406 | CRT  | C5-C6-C7-C9     |
| 22  | J     | 103 | CRT  | C5-C6-C7-C9     |
| 15  | G     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 15  | J     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 15  | V     | 101 | BCL  | C15-C16-C17-C18 |
| 18  | L     | 307 | LMT  | C4-C5-C6-C7     |
| 14  | A     | 503 | PGV  | C04-C05-C06-O06 |
| 15  | 5     | 102 | BCL  | CBD-CGD-O2D-CED |
| 19  | L     | 311 | CDL  | CA6-CA4-OA6-CA5 |
| 18  | P     | 101 | LMT  | C4-C5-C6-C7     |
| 18  | 2     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 14  | H     | 301 | PGV  | C2-C1-O01-C02   |
| 15  | U     | 101 | BCL  | C13-C15-C16-C17 |
| 15  | O     | 502 | BCL  | CBA-CGA-O2A-C1  |
| 14  | A     | 501 | PGV  | O04-C19-O03-C01 |
| 15  | J     | 102 | BCL  | O1D-CGD-O2D-CED |
| 18  | R     | 103 | LMT  | O5B-C5B-C6B-O6B |
| 18  | 2     | 101 | LMT  | O1'-C1-C2-C3    |
| 14  | C     | 408 | PGV  | C3-C4-C5-C6     |
| 14  | M     | 408 | PGV  | C21-C22-C23-C24 |
| 18  | T     | 103 | LMT  | C6-C7-C8-C9     |
| 18  | 5     | 101 | LMT  | C3-C4-C5-C6     |
| 19  | L     | 311 | CDL  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | L     | 311 | CDL  | C54-C55-C56-C57 |
| 19  | D     | 101 | CDL  | C54-C55-C56-C57 |
| 19  | L     | 311 | CDL  | C62-C63-C64-C65 |
| 14  | H     | 301 | PGV  | O05-C05-C06-O06 |
| 19  | H     | 302 | CDL  | C59-C60-C61-C62 |
| 18  | M     | 411 | LMT  | C2'-C1'-O1'-C1  |
| 12  | C     | 406 | Z41  | C25-C26-C27-C28 |
| 19  | M     | 407 | CDL  | C11-CA5-OA6-CA4 |
| 15  | K     | 102 | BCL  | C6-C7-C8-C10    |
| 15  | Q     | 102 | BCL  | C12-C13-C15-C16 |
| 15  | 9     | 102 | BCL  | C6-C7-C8-C10    |
| 19  | H     | 302 | CDL  | C16-C17-C18-C19 |
| 14  | L     | 310 | PGV  | O12-C04-C05-O05 |
| 14  | A     | 503 | PGV  | C19-C20-C21-C22 |
| 14  | 1     | 401 | PGV  | C1-C2-C3-C4     |
| 15  | L     | 301 | BCL  | C15-C16-C17-C18 |
| 18  | R     | 103 | LMT  | C2-C3-C4-C5     |
| 15  | 7     | 101 | BCL  | C3-C5-C6-C7     |
| 15  | J     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 15  | V     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 15  | W     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 15  | X     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 15  | Y     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 15  | 1     | 402 | BCL  | C3A-C2A-CAA-CBA |
| 15  | 2     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 15  | 3     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 15  | 8     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 15  | L     | 308 | BCL  | O1D-CGD-O2D-CED |
| 15  | 6     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | R     | 101 | BCL  | C8-C10-C11-C12  |
| 15  | Y     | 102 | BCL  | C8-C10-C11-C12  |
| 15  | 6     | 101 | BCL  | C8-C10-C11-C12  |
| 15  | 0     | 101 | BCL  | C13-C15-C16-C17 |
| 18  | 4     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 15  | V     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 14  | H     | 301 | PGV  | O02-C1-O01-C02  |
| 19  | H     | 302 | CDL  | CA2-C1-CB2-OB2  |
| 15  | 6     | 101 | BCL  | C3-C5-C6-C7     |
| 15  | O     | 502 | BCL  | O1A-CGA-O2A-C1  |
| 19  | L     | 311 | CDL  | C79-C80-C81-C82 |
| 14  | C     | 408 | PGV  | C1-C2-C3-C4     |
| 19  | L     | 311 | CDL  | CB5-C51-C52-C53 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | 8     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 15  | X     | 102 | BCL  | C15-C16-C17-C18 |
| 15  | Q     | 102 | BCL  | C3-C5-C6-C7     |
| 18  | L     | 307 | LMT  | C3-C4-C5-C6     |
| 19  | L     | 311 | CDL  | C63-C64-C65-C66 |
| 19  | M     | 409 | CDL  | C55-C56-C57-C58 |
| 18  | T     | 103 | LMT  | C5-C6-C7-C8     |
| 19  | M     | 407 | CDL  | OA7-CA5-OA6-CA4 |
| 15  | 8     | 102 | BCL  | C15-C16-C17-C18 |
| 18  | L     | 307 | LMT  | C2-C3-C4-C5     |
| 18  | H     | 303 | LMT  | C4-C5-C6-C7     |
| 18  | Z     | 101 | LMT  | C6-C7-C8-C9     |
| 15  | D     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | 5     | 102 | BCL  | C8-C10-C11-C12  |
| 19  | L     | 311 | CDL  | C80-C81-C82-C83 |
| 18  | 4     | 101 | LMT  | C5-C6-C7-C8     |
| 22  | Z     | 103 | CRT  | C11-C10-C9-C7   |
| 15  | N     | 101 | BCL  | C16-C17-C18-C19 |
| 15  | U     | 101 | BCL  | C16-C17-C18-C20 |
| 14  | L     | 305 | PGV  | C2-C1-O01-C02   |
| 14  | L     | 310 | PGV  | C2-C1-O01-C02   |
| 14  | A     | 503 | PGV  | C2-C1-O01-C02   |
| 14  | F     | 501 | PGV  | C2-C1-O01-C02   |
| 18  | G     | 101 | LMT  | C3'-C4'-O1B-C1B |
| 15  | F     | 502 | BCL  | CBD-CGD-O2D-CED |
| 22  | B     | 103 | CRT  | C15-C16-C17-C18 |
| 14  | L     | 310 | PGV  | C25-C26-C27-C28 |
| 19  | H     | 302 | CDL  | C17-C18-C19-C20 |
| 19  | H     | 302 | CDL  | CA7-C31-C32-C33 |
| 22  | M     | 406 | CRT  | C1-C4-C5-C6     |
| 22  | Z     | 103 | CRT  | C1-C4-C5-C6     |
| 15  | 5     | 102 | BCL  | C10-C11-C12-C13 |
| 15  | 2     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 10  | C     | 402 | HEM  | C2C-C3C-CAC-CBC |
| 19  | M     | 409 | CDL  | C36-C37-C38-C39 |
| 14  | L     | 310 | PGV  | O02-C1-O01-C02  |
| 18  | 8     | 103 | LMT  | O5B-C5B-C6B-O6B |
| 19  | M     | 409 | CDL  | C42-C43-C44-C45 |
| 10  | C     | 401 | HEM  | C4B-C3B-CAB-CBB |
| 10  | C     | 402 | HEM  | C4B-C3B-CAB-CBB |
| 10  | C     | 404 | HEM  | C4B-C3B-CAB-CBB |
| 10  | C     | 404 | HEM  | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | L     | 305 | PGV  | C2-C3-C4-C5     |
| 15  | 8     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 15  | I     | 101 | BCL  | O1D-CGD-O2D-CED |
| 14  | C     | 408 | PGV  | C2-C3-C4-C5     |
| 18  | M     | 411 | LMT  | O5'-C5'-C6'-O6' |
| 18  | R     | 103 | LMT  | O5'-C5'-C6'-O6' |
| 15  | 3     | 101 | BCL  | C3-C5-C6-C7     |
| 19  | D     | 101 | CDL  | OB6-CB4-CB6-OB8 |
| 19  | M     | 409 | CDL  | C16-C17-C18-C19 |
| 18  | E     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 18  | E     | 101 | LMT  | C3'-C4'-O1B-C1B |
| 19  | H     | 302 | CDL  | C54-C55-C56-C57 |
| 19  | H     | 302 | CDL  | C58-C59-C60-C61 |
| 18  | X     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 15  | V     | 101 | BCL  | C16-C17-C18-C20 |
| 18  | X     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 15  | V     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | 5     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | G     | 102 | BCL  | C2-C3-C5-C6     |
| 14  | F     | 501 | PGV  | O02-C1-O01-C02  |
| 14  | A     | 503 | PGV  | O12-C04-C05-C06 |
| 19  | L     | 311 | CDL  | CB2-C1-CA2-OA2  |
| 14  | 1     | 401 | PGV  | C2-C3-C4-C5     |
| 15  | T     | 101 | BCL  | O1D-CGD-O2D-CED |
| 15  | M     | 402 | BCL  | C10-C11-C12-C13 |
| 18  | T     | 103 | LMT  | O5B-C5B-C6B-O6B |
| 19  | L     | 311 | CDL  | C38-C39-C40-C41 |
| 15  | Y     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 15  | 1     | 402 | BCL  | C1A-C2A-CAA-CBA |
| 15  | 0     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 15  | J     | 102 | BCL  | C8-C10-C11-C12  |
| 19  | L     | 311 | CDL  | C71-C72-C73-C74 |
| 14  | L     | 310 | PGV  | C01-C02-C03-O11 |
| 14  | M     | 408 | PGV  | C01-C02-C03-O11 |
| 14  | L     | 305 | PGV  | O02-C1-O01-C02  |
| 15  | G     | 102 | BCL  | C3-C5-C6-C7     |
| 15  | B     | 102 | BCL  | C11-C10-C8-C7   |
| 15  | D     | 102 | BCL  | C11-C12-C13-C15 |
| 15  | G     | 102 | BCL  | C6-C7-C8-C10    |
| 15  | K     | 102 | BCL  | C11-C10-C8-C7   |
| 15  | Q     | 102 | BCL  | C11-C10-C8-C7   |
| 15  | Q     | 102 | BCL  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | S     | 102 | BCL  | C11-C10-C8-C7   |
| 15  | U     | 101 | BCL  | C6-C7-C8-C10    |
| 15  | W     | 101 | BCL  | C11-C10-C8-C7   |
| 15  | 2     | 102 | BCL  | C11-C10-C8-C7   |
| 15  | 5     | 102 | BCL  | C11-C10-C8-C7   |
| 18  | J     | 104 | LMT  | C4-C5-C6-C7     |
| 15  | B     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 15  | G     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 15  | J     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 15  | O     | 502 | BCL  | C2C-C3C-CAC-CBC |
| 15  | 7     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 15  | 8     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 22  | G     | 103 | CRT  | C36-C37-C38-C39 |
| 22  | Z     | 103 | CRT  | C36-C37-C38-C40 |
| 22  | 6     | 102 | CRT  | C3-C1-C4-C5     |
| 19  | M     | 409 | CDL  | C51-C52-C53-C54 |
| 18  | 5     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 15  | L     | 308 | BCL  | C8-C10-C11-C12  |
| 15  | Y     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | 7     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | 9     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | U     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | G     | 102 | BCL  | C13-C15-C16-C17 |
| 15  | X     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 15  | Q     | 102 | BCL  | C14-C13-C15-C16 |
| 15  | U     | 101 | BCL  | C6-C7-C8-C9     |
| 15  | 5     | 102 | BCL  | C11-C10-C8-C9   |
| 19  | M     | 409 | CDL  | C59-C60-C61-C62 |
| 19  | M     | 409 | CDL  | C31-CA7-OA8-CA6 |
| 15  | V     | 101 | BCL  | C5-C6-C7-C8     |
| 14  | F     | 501 | PGV  | O03-C01-C02-C03 |
| 19  | M     | 409 | CDL  | CB3-CB4-CB6-OB8 |
| 13  | C     | 407 | PLM  | C6-C7-C8-C9     |
| 15  | L     | 308 | BCL  | C5-C6-C7-C8     |
| 15  | 2     | 102 | BCL  | C5-C6-C7-C8     |
| 18  | T     | 103 | LMT  | O5'-C5'-C6'-O6' |
| 15  | N     | 101 | BCL  | C16-C17-C18-C20 |
| 15  | U     | 101 | BCL  | C16-C17-C18-C19 |
| 18  | G     | 101 | LMT  | C5'-C4'-O1B-C1B |
| 15  | N     | 101 | BCL  | C13-C15-C16-C17 |
| 18  | G     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 18  | 8     | 103 | LMT  | O5'-C5'-C6'-O6' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | G     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | V     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | Y     | 102 | BCL  | C2-C3-C5-C6     |
| 15  | 5     | 102 | BCL  | C2-C3-C5-C6     |
| 15  | 7     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | 9     | 102 | BCL  | C2-C3-C5-C6     |
| 15  | A     | 502 | BCL  | C16-C17-C18-C19 |
| 18  | L     | 307 | LMT  | C11-C10-C9-C8   |
| 19  | M     | 409 | CDL  | OA9-CA7-OA8-CA6 |
| 18  | E     | 101 | LMT  | C5'-C4'-O1B-C1B |
| 15  | O     | 502 | BCL  | C2A-CAA-CBA-CGA |
| 14  | F     | 501 | PGV  | O01-C02-C03-O11 |
| 19  | M     | 407 | CDL  | OB5-CB3-CB4-OB6 |
| 14  | M     | 408 | PGV  | C20-C19-O03-C01 |
| 15  | U     | 101 | BCL  | C4-C3-C5-C6     |
| 17  | L     | 304 | UQ8  | C38-C39-C41-C42 |
| 14  | L     | 310 | PGV  | O03-C01-C02-O01 |
| 14  | A     | 503 | PGV  | O12-C04-C05-O05 |
| 18  | 8     | 101 | LMT  | C3-C4-C5-C6     |
| 15  | V     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 18  | Z     | 101 | LMT  | C7-C8-C9-C10    |
| 22  | E     | 103 | CRT  | C3-C1-O1-C1M    |
| 22  | G     | 103 | CRT  | C39-C38-O2-C2M  |
| 22  | J     | 103 | CRT  | C3-C1-O1-C1M    |
| 22  | J     | 103 | CRT  | C39-C38-O2-C2M  |
| 22  | N     | 102 | CRT  | C39-C38-O2-C2M  |
| 22  | P     | 103 | CRT  | C3-C1-O1-C1M    |
| 22  | Z     | 103 | CRT  | C39-C38-O2-C2M  |
| 12  | C     | 406 | Z41  | C11-C10-C9-C8   |
| 15  | 2     | 102 | BCL  | C16-C17-C18-C19 |
| 15  | W     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | 8     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | 1     | 402 | BCL  | CBA-CGA-O2A-C1  |
| 18  | L     | 307 | LMT  | C7-C8-C9-C10    |
| 14  | A     | 503 | PGV  | O02-C1-O01-C02  |
| 18  | 8     | 101 | LMT  | C2-C1-O1'-C1'   |
| 15  | M     | 402 | BCL  | C11-C10-C8-C9   |
| 15  | D     | 102 | BCL  | C11-C12-C13-C14 |
| 15  | G     | 102 | BCL  | C14-C13-C15-C16 |
| 15  | K     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | O     | 502 | BCL  | C11-C10-C8-C9   |
| 15  | Q     | 102 | BCL  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | Q     | 102 | BCL  | C11-C12-C13-C14 |
| 15  | S     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | W     | 101 | BCL  | C11-C10-C8-C9   |
| 15  | Y     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | 4     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | 9     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | 0     | 101 | BCL  | C6-C7-C8-C9     |
| 18  | M     | 410 | LMT  | C2-C3-C4-C5     |
| 15  | K     | 102 | BCL  | C15-C16-C17-C18 |
| 15  | Q     | 102 | BCL  | C15-C16-C17-C18 |
| 15  | Y     | 102 | BCL  | C10-C11-C12-C13 |
| 18  | B     | 101 | LMT  | C4B-C5B-C6B-O6B |
| 14  | L     | 310 | PGV  | C21-C22-C23-C24 |
| 14  | L     | 305 | PGV  | C4-C5-C6-C7     |
| 14  | C     | 408 | PGV  | C01-C02-C03-O11 |
| 19  | M     | 409 | CDL  | OB5-CB3-CB4-CB6 |
| 14  | 1     | 401 | PGV  | C21-C22-C23-C24 |
| 15  | E     | 102 | BCL  | C6-C7-C8-C10    |
| 15  | F     | 502 | BCL  | C11-C10-C8-C7   |
| 15  | G     | 102 | BCL  | C11-C12-C13-C15 |
| 15  | T     | 101 | BCL  | C6-C7-C8-C10    |
| 15  | V     | 101 | BCL  | C6-C7-C8-C10    |
| 15  | Z     | 102 | BCL  | C6-C7-C8-C10    |
| 16  | M     | 404 | BPH  | C11-C12-C13-C15 |
| 15  | P     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 16  | M     | 404 | BPH  | C4-C3-C5-C6     |
| 17  | L     | 304 | UQ8  | C40-C39-C41-C42 |
| 15  | J     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 15  | A     | 502 | BCL  | C16-C17-C18-C20 |
| 22  | E     | 103 | CRT  | C34-C33-C35-C36 |
| 18  | B     | 101 | LMT  | C2-C3-C4-C5     |
| 18  | P     | 101 | LMT  | C4B-C5B-C6B-O6B |
| 18  | H     | 303 | LMT  | O1'-C1-C2-C3    |
| 14  | F     | 501 | PGV  | C20-C19-O03-C01 |
| 19  | H     | 302 | CDL  | C71-C72-C73-C74 |
| 15  | L     | 301 | BCL  | C16-C17-C18-C19 |
| 15  | X     | 102 | BCL  | C2-C3-C5-C6     |
| 14  | C     | 408 | PGV  | C21-C22-C23-C24 |
| 14  | A     | 501 | PGV  | C24-C25-C26-C27 |
| 14  | L     | 310 | PGV  | O01-C02-C03-O11 |
| 18  | P     | 101 | LMT  | O1'-C1-C2-C3    |
| 15  | 2     | 102 | BCL  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | 5     | 102 | BCL  | O1D-CGD-O2D-CED |
| 19  | L     | 311 | CDL  | C33-C34-C35-C36 |
| 19  | H     | 302 | CDL  | C78-C79-C80-C81 |
| 19  | M     | 409 | CDL  | OB6-CB4-CB6-OB8 |
| 15  | X     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | W     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | 2     | 102 | BCL  | C16-C17-C18-C20 |
| 19  | L     | 311 | CDL  | CB7-C71-C72-C73 |
| 15  | J     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | V     | 101 | BCL  | C11-C10-C8-C9   |
| 19  | L     | 311 | CDL  | C81-C82-C83-C84 |
| 15  | V     | 101 | BCL  | C16-C17-C18-C19 |
| 21  | M     | 405 | MQ8  | C28-C30-C31-C32 |
| 15  | M     | 402 | BCL  | C4C-C3C-CAC-CBC |
| 18  | X     | 101 | LMT  | C3'-C4'-O1B-C1B |
| 12  | C     | 406 | Z41  | C21-C22-C23-C24 |
| 15  | X     | 102 | BCL  | C8-C10-C11-C12  |
| 16  | M     | 404 | BPH  | C3-C5-C6-C7     |
| 16  | L     | 302 | BPH  | C4-C3-C5-C6     |
| 15  | 8     | 102 | BCL  | C2-C3-C5-C6     |
| 15  | W     | 101 | BCL  | C8-C10-C11-C12  |
| 15  | F     | 502 | BCL  | O1D-CGD-O2D-CED |
| 19  | M     | 409 | CDL  | C43-C44-C45-C46 |
| 15  | 7     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 14  | L     | 306 | PGV  | C01-C02-C03-O11 |
| 15  | V     | 101 | BCL  | C8-C10-C11-C12  |
| 15  | 4     | 102 | BCL  | C5-C6-C7-C8     |
| 15  | L     | 308 | BCL  | C6-C7-C8-C10    |
| 15  | L     | 308 | BCL  | C11-C10-C8-C7   |
| 15  | A     | 502 | BCL  | C11-C12-C13-C15 |
| 15  | F     | 502 | BCL  | C6-C7-C8-C10    |
| 15  | R     | 101 | BCL  | C6-C7-C8-C10    |
| 15  | Y     | 102 | BCL  | C6-C7-C8-C10    |
| 15  | 9     | 102 | BCL  | C12-C13-C15-C16 |
| 18  | Z     | 101 | LMT  | C1-C2-C3-C4     |
| 12  | C     | 406 | Z41  | C13-C14-C15-C16 |
| 22  | 6     | 102 | CRT  | C1-C4-C5-C6     |
| 22  | 9     | 101 | CRT  | C1-C4-C5-C6     |
| 22  | B     | 103 | CRT  | C15-C16-C17-C19 |
| 15  | I     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 15  | I     | 101 | BCL  | C8-C10-C11-C12  |
| 14  | M     | 408 | PGV  | O04-C19-O03-C01 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | P     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 10  | C     | 401 | HEM  | C2C-C3C-CAC-CBC |
| 10  | C     | 403 | HEM  | C2C-C3C-CAC-CBC |
| 15  | I     | 101 | BCL  | C3-C5-C6-C7     |
| 19  | M     | 407 | CDL  | CA6-CA4-OA6-CA5 |
| 15  | Z     | 102 | BCL  | CBD-CGD-O2D-CED |
| 14  | 1     | 401 | PGV  | C20-C21-C22-C23 |
| 15  | Y     | 102 | BCL  | C16-C17-C18-C19 |
| 15  | 0     | 101 | BCL  | C16-C17-C18-C19 |
| 18  | P     | 101 | LMT  | C9-C10-C11-C12  |
| 15  | 1     | 402 | BCL  | O1A-CGA-O2A-C1  |
| 18  | T     | 103 | LMT  | C4-C5-C6-C7     |
| 14  | L     | 306 | PGV  | O01-C02-C03-O11 |
| 14  | F     | 501 | PGV  | C20-C21-C22-C23 |
| 14  | H     | 301 | PGV  | C3-C4-C5-C6     |
| 10  | C     | 402 | HEM  | C4C-C3C-CAC-CBC |
| 15  | J     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 15  | O     | 502 | BCL  | C4-C3-C5-C6     |
| 15  | Z     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | 4     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | M     | 404 | BPH  | C2-C3-C5-C6     |
| 14  | A     | 503 | PGV  | C2-C3-C4-C5     |
| 14  | C     | 408 | PGV  | O03-C01-C02-O01 |
| 15  | F     | 502 | BCL  | C6-C7-C8-C9     |
| 15  | F     | 502 | BCL  | C11-C10-C8-C9   |
| 15  | 9     | 102 | BCL  | C14-C13-C15-C16 |
| 15  | 0     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | M     | 404 | BPH  | C11-C12-C13-C14 |
| 14  | L     | 305 | PGV  | C3-C4-C5-C6     |
| 14  | F     | 501 | PGV  | O04-C19-O03-C01 |
| 18  | H     | 303 | LMT  | C2'-C1'-O1'-C1  |
| 15  | R     | 101 | BCL  | C16-C17-C18-C19 |
| 15  | 4     | 102 | BCL  | C16-C17-C18-C19 |
| 10  | C     | 402 | HEM  | C3D-CAD-CBD-CGD |
| 18  | 4     | 101 | LMT  | C6-C7-C8-C9     |
| 15  | 8     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 15  | 7     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 15  | Q     | 102 | BCL  | CBD-CGD-O2D-CED |
| 15  | I     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 15  | L     | 301 | BCL  | C16-C17-C18-C20 |
| 18  | R     | 103 | LMT  | C5-C6-C7-C8     |
| 15  | Z     | 102 | BCL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 101 | LMT  | C6-C7-C8-C9     |
| 15  | 0     | 101 | BCL  | CBD-CGD-O2D-CED |
| 19  | H     | 302 | CDL  | C53-C54-C55-C56 |
| 14  | A     | 503 | PGV  | C01-C02-C03-O11 |
| 19  | M     | 407 | CDL  | OB5-CB3-CB4-CB6 |
| 19  | M     | 409 | CDL  | OA5-CA3-CA4-CA6 |
| 15  | F     | 502 | BCL  | C11-C12-C13-C15 |
| 15  | J     | 102 | BCL  | C12-C13-C15-C16 |
| 15  | N     | 101 | BCL  | C11-C10-C8-C7   |
| 15  | P     | 102 | BCL  | C11-C12-C13-C15 |
| 15  | R     | 101 | BCL  | C11-C10-C8-C7   |
| 15  | 3     | 101 | BCL  | C16-C17-C18-C19 |
| 15  | 4     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 15  | 5     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 22  | G     | 103 | CRT  | C36-C37-C38-C40 |
| 15  | 6     | 101 | BCL  | C13-C15-C16-C17 |
| 14  | F     | 501 | PGV  | C23-C24-C25-C26 |
| 18  | T     | 103 | LMT  | O1'-C1-C2-C3    |
| 15  | 4     | 102 | BCL  | C2-C3-C5-C6     |
| 14  | C     | 408 | PGV  | O01-C02-C03-O11 |
| 14  | A     | 503 | PGV  | O01-C02-C03-O11 |
| 19  | M     | 409 | CDL  | OA5-CA3-CA4-OA6 |
| 19  | D     | 101 | CDL  | OB5-CB3-CB4-OB6 |
| 15  | A     | 502 | BCL  | C11-C12-C13-C14 |
| 15  | J     | 102 | BCL  | C14-C13-C15-C16 |
| 15  | 0     | 101 | BCL  | C16-C17-C18-C20 |
| 18  | X     | 101 | LMT  | C5'-C4'-O1B-C1B |
| 15  | 9     | 102 | BCL  | C5-C6-C7-C8     |
| 15  | 0     | 101 | BCL  | O1D-CGD-O2D-CED |
| 14  | F     | 501 | PGV  | O03-C01-C02-O01 |
| 15  | D     | 102 | BCL  | C5-C6-C7-C8     |
| 14  | 1     | 401 | PGV  | C4-C5-C6-C7     |
| 15  | Q     | 102 | BCL  | O1D-CGD-O2D-CED |
| 14  | L     | 310 | PGV  | O03-C01-C02-C03 |
| 19  | D     | 101 | CDL  | CB3-CB4-CB6-OB8 |
| 18  | R     | 103 | LMT  | C3-C4-C5-C6     |
| 15  | J     | 102 | BCL  | C16-C17-C18-C19 |
| 17  | L     | 309 | UQ8  | C5-C4-O4-C4M    |
| 14  | H     | 301 | PGV  | C23-C24-C25-C26 |
| 15  | 6     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 14  | L     | 306 | PGV  | C04-O12-P-O11   |
| 14  | L     | 306 | PGV  | C04-O12-P-O13   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | L     | 310 | PGV  | C03-O11-P-O13   |
| 14  | L     | 310 | PGV  | C04-O12-P-O11   |
| 14  | L     | 310 | PGV  | C04-O12-P-O13   |
| 14  | H     | 301 | PGV  | C04-O12-P-O13   |
| 14  | A     | 503 | PGV  | C04-O12-P-O11   |
| 15  | L     | 308 | BCL  | CHA-CBD-CGD-O1D |
| 15  | L     | 308 | BCL  | CHA-CBD-CGD-O2D |
| 19  | L     | 311 | CDL  | CB3-OB5-PB2-OB3 |
| 19  | M     | 407 | CDL  | CA3-OA5-PA1-OA4 |
| 19  | M     | 409 | CDL  | CA3-OA5-PA1-OA3 |
| 19  | H     | 302 | CDL  | CB3-OB5-PB2-OB3 |
| 19  | D     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 19  | D     | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 24  | K     | 101 | LDA  | C4-C5-C6-C7     |
| 15  | O     | 502 | BCL  | C2-C3-C5-C6     |
| 15  | Z     | 102 | BCL  | C2-C3-C5-C6     |
| 19  | L     | 311 | CDL  | CA4-CA3-OA5-PA1 |
| 22  | 0     | 102 | CRT  | C15-C16-C17-C18 |
| 18  | B     | 101 | LMT  | C4-C5-C6-C7     |
| 18  | T     | 103 | LMT  | C2-C3-C4-C5     |
| 14  | 1     | 401 | PGV  | C04-O12-P-O13   |
| 14  | Q     | 101 | PGV  | C01-C02-O01-C1  |
| 19  | D     | 101 | CDL  | CA6-CA4-OA6-CA5 |
| 22  | 4     | 103 | CRT  | C28-C30-C31-C32 |
| 15  | P     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 17  | L     | 304 | UQ8  | C14-C16-C17-C18 |
| 18  | B     | 101 | LMT  | O1'-C1-C2-C3    |
| 14  | F     | 501 | PGV  | C01-C02-C03-O11 |
| 15  | L     | 308 | BCL  | C6-C7-C8-C9     |
| 15  | T     | 101 | BCL  | C11-C10-C8-C9   |
| 15  | U     | 101 | BCL  | C14-C13-C15-C16 |
| 15  | Y     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | E     | 102 | BCL  | O1D-CGD-O2D-CED |
| 15  | J     | 102 | BCL  | C6-C7-C8-C10    |
| 19  | M     | 407 | CDL  | CA2-C1-CB2-OB2  |
| 18  | E     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 18  | G     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 18  | 8     | 103 | LMT  | C6-C7-C8-C9     |
| 14  | M     | 408 | PGV  | C1-C2-C3-C4     |
| 19  | L     | 311 | CDL  | C73-C74-C75-C76 |
| 22  | J     | 103 | CRT  | C11-C10-C9-C7   |
| 15  | T     | 101 | BCL  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | Q     | 101 | PGV  | O03-C19-C20-C21 |
| 22  | N     | 102 | CRT  | C40-C38-O2-C2M  |
| 22  | Z     | 103 | CRT  | C40-C38-O2-C2M  |
| 22  | 2     | 103 | CRT  | C1-C4-C5-C6     |
| 14  | L     | 306 | PGV  | C6-C7-C8-C9     |
| 15  | F     | 502 | BCL  | C8-C10-C11-C12  |
| 15  | 2     | 102 | BCL  | O1D-CGD-O2D-CED |
| 22  | 6     | 102 | CRT  | C11-C10-C9-C7   |
| 15  | F     | 502 | BCL  | C16-C17-C18-C19 |
| 16  | L     | 302 | BPH  | C2-C3-C5-C6     |
| 15  | B     | 102 | BCL  | C13-C15-C16-C17 |
| 15  | 6     | 101 | BCL  | O1D-CGD-O2D-CED |
| 14  | Q     | 101 | PGV  | O01-C1-C2-C3    |
| 18  | J     | 101 | LMT  | C4-C5-C6-C7     |
| 15  | A     | 502 | BCL  | C6-C7-C8-C9     |
| 18  | J     | 104 | LMT  | O1'-C1-C2-C3    |
| 18  | Z     | 101 | LMT  | O1'-C1-C2-C3    |
| 15  | Y     | 102 | BCL  | C16-C17-C18-C20 |
| 18  | 4     | 104 | LMT  | C5-C6-C7-C8     |
| 15  | E     | 102 | BCL  | C4-C3-C5-C6     |
| 17  | L     | 309 | UQ8  | C30-C29-C31-C32 |
| 18  | 2     | 101 | LMT  | C2-C3-C4-C5     |
| 17  | L     | 309 | UQ8  | C29-C31-C32-C33 |
| 19  | M     | 409 | CDL  | C11-CA5-OA6-CA4 |
| 15  | X     | 102 | BCL  | C6-C7-C8-C10    |
| 15  | 8     | 102 | BCL  | C11-C12-C13-C15 |
| 19  | M     | 409 | CDL  | OA7-CA5-OA6-CA4 |
| 15  | E     | 102 | BCL  | C8-C10-C11-C12  |
| 15  | 6     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 19  | H     | 302 | CDL  | C60-C61-C62-C63 |
| 15  | U     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 15  | T     | 101 | BCL  | C2-C3-C5-C6     |
| 14  | L     | 310 | PGV  | C29-C30-C31-C32 |
| 18  | 4     | 101 | LMT  | C4-C5-C6-C7     |
| 22  | 4     | 103 | CRT  | C31-C32-C33-C34 |
| 18  | 5     | 101 | LMT  | C5'-C4'-O1B-C1B |
| 14  | Q     | 101 | PGV  | C19-C20-C21-C22 |
| 18  | 8     | 101 | LMT  | C3'-C4'-O1B-C1B |
| 15  | D     | 102 | BCL  | C2-C1-O2A-CGA   |
| 15  | S     | 102 | BCL  | C8-C10-C11-C12  |
| 14  | A     | 501 | PGV  | C05-C04-O12-P   |
| 15  | 8     | 102 | BCL  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | T     | 103 | LMT  | C2B-C1B-O1B-C4' |
| 16  | M     | 404 | BPH  | C5-C6-C7-C8     |
| 15  | A     | 502 | BCL  | C11-C10-C8-C9   |
| 15  | E     | 102 | BCL  | C14-C13-C15-C16 |
| 15  | F     | 502 | BCL  | C11-C12-C13-C14 |
| 15  | P     | 102 | BCL  | C11-C12-C13-C14 |
| 15  | Q     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | S     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | X     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | Z     | 102 | BCL  | C14-C13-C15-C16 |
| 15  | 4     | 102 | BCL  | C14-C13-C15-C16 |
| 15  | J     | 102 | BCL  | C16-C17-C18-C20 |
| 15  | 3     | 101 | BCL  | C15-C16-C17-C18 |
| 18  | M     | 410 | LMT  | O5B-C1B-O1B-C4' |
| 18  | 4     | 101 | LMT  | C7-C8-C9-C10    |
| 19  | M     | 409 | CDL  | CB5-C51-C52-C53 |
| 15  | 6     | 101 | BCL  | CBD-CGD-O2D-CED |
| 17  | L     | 309 | UQ8  | C28-C29-C31-C32 |
| 15  | B     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 15  | G     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 15  | U     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 15  | Z     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 22  | 4     | 103 | CRT  | C31-C32-C33-C35 |
| 15  | L     | 308 | BCL  | C16-C17-C18-C20 |
| 14  | F     | 501 | PGV  | C19-C20-C21-C22 |
| 19  | H     | 302 | CDL  | CA4-CA3-OA5-PA1 |
| 19  | D     | 101 | CDL  | OB5-CB3-CB4-CB6 |
| 15  | E     | 102 | BCL  | C2-C3-C5-C6     |
| 18  | B     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 15  | A     | 502 | BCL  | C6-C7-C8-C10    |
| 15  | D     | 102 | BCL  | C6-C7-C8-C10    |
| 15  | P     | 102 | BCL  | C11-C10-C8-C7   |
| 15  | U     | 101 | BCL  | C12-C13-C15-C16 |
| 15  | 6     | 101 | BCL  | C6-C7-C8-C10    |
| 15  | 6     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | L     | 302 | BPH  | C11-C12-C13-C15 |
| 15  | Y     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 10  | C     | 401 | HEM  | CAA-CBA-CGA-O2A |
| 15  | 0     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 10  | C     | 401 | HEM  | CAA-CBA-CGA-O1A |
| 15  | N     | 101 | BCL  | C10-C11-C12-C13 |
| 22  | M     | 406 | CRT  | C29-C28-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | G     | 103 | CRT  | C15-C16-C17-C18 |
| 22  | T     | 102 | CRT  | C5-C6-C7-C8     |
| 22  | 2     | 103 | CRT  | C15-C16-C17-C18 |
| 10  | C     | 402 | HEM  | CAD-CBD-CGD-O1D |
| 15  | D     | 102 | BCL  | C15-C16-C17-C18 |
| 15  | 1     | 402 | BCL  | C13-C15-C16-C17 |
| 15  | S     | 102 | BCL  | C2-C1-O2A-CGA   |
| 15  | P     | 102 | BCL  | C16-C17-C18-C19 |
| 15  | L     | 301 | BCL  | C3-C5-C6-C7     |
| 15  | L     | 301 | BCL  | C11-C10-C8-C9   |
| 15  | Q     | 102 | BCL  | C13-C15-C16-C17 |
| 15  | T     | 101 | BCL  | C13-C15-C16-C17 |
| 19  | H     | 302 | CDL  | C31-CA7-OA8-CA6 |
| 15  | K     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | U     | 101 | BCL  | C15-C16-C17-C18 |
| 14  | C     | 408 | PGV  | O03-C01-C02-C03 |
| 15  | B     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 15  | J     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 15  | 8     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 15  | P     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 14  | A     | 503 | PGV  | C22-C23-C24-C25 |
| 15  | D     | 102 | BCL  | C16-C17-C18-C19 |
| 10  | C     | 402 | HEM  | CAD-CBD-CGD-O2D |
| 15  | M     | 403 | BCL  | C5-C6-C7-C8     |
| 14  | L     | 305 | PGV  | O01-C02-C03-O11 |
| 15  | V     | 101 | BCL  | CAA-CBA-CGA-O1A |
| 24  | K     | 101 | LDA  | C2-C3-C4-C5     |
| 24  | O     | 501 | LDA  | C2-C3-C4-C5     |
| 19  | H     | 302 | CDL  | OA9-CA7-OA8-CA6 |
| 15  | L     | 308 | BCL  | C16-C17-C18-C19 |
| 16  | L     | 302 | BPH  | C16-C17-C18-C20 |
| 15  | K     | 102 | BCL  | C2-C3-C5-C6     |
| 14  | H     | 301 | PGV  | C02-C03-O11-P   |
| 18  | 8     | 103 | LMT  | C11-C10-C9-C8   |
| 15  | L     | 301 | BCL  | C11-C10-C8-C7   |
| 15  | X     | 102 | BCL  | C11-C10-C8-C7   |
| 15  | S     | 102 | BCL  | C10-C11-C12-C13 |
| 12  | C     | 406 | Z41  | C30-C31-C32-C33 |
| 22  | 0     | 102 | CRT  | C15-C16-C17-C19 |
| 15  | 5     | 102 | BCL  | C6-C7-C8-C9     |
| 15  | 5     | 102 | BCL  | C14-C13-C15-C16 |
| 19  | M     | 409 | CDL  | C58-C59-C60-C61 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | P     | 104 | LMT  | C2-C3-C4-C5     |
| 15  | U     | 101 | BCL  | C2-C1-O2A-CGA   |
| 15  | 5     | 102 | BCL  | C2-C1-O2A-CGA   |
| 15  | G     | 102 | BCL  | O1D-CGD-O2D-CED |
| 18  | J     | 101 | LMT  | C11-C10-C9-C8   |
| 15  | G     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 19  | L     | 311 | CDL  | C84-C85-C86-C87 |
| 18  | J     | 104 | LMT  | C4'-C5'-C6'-O6' |
| 15  | R     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 18  | 8     | 101 | LMT  | C5'-C4'-O1B-C1B |
| 15  | X     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 17  | L     | 304 | UQ8  | C19-C21-C22-C23 |
| 15  | E     | 102 | BCL  | CBD-CGD-O2D-CED |
| 10  | C     | 401 | HEM  | C4C-C3C-CAC-CBC |
| 10  | C     | 403 | HEM  | C4C-C3C-CAC-CBC |
| 18  | X     | 101 | LMT  | C7-C8-C9-C10    |
| 15  | 8     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 14  | Q     | 101 | PGV  | C01-C02-C03-O11 |
| 22  | G     | 103 | CRT  | C36-C37-C38-O2  |
| 15  | L     | 301 | BCL  | C2A-CAA-CBA-CGA |
| 15  | M     | 402 | BCL  | C6-C7-C8-C10    |
| 15  | M     | 403 | BCL  | C12-C13-C15-C16 |
| 15  | A     | 502 | BCL  | C11-C10-C8-C7   |
| 15  | 4     | 102 | BCL  | C6-C7-C8-C10    |
| 15  | 9     | 102 | BCL  | C11-C10-C8-C7   |
| 19  | M     | 409 | CDL  | C17-C18-C19-C20 |
| 15  | W     | 101 | BCL  | C2-C1-O2A-CGA   |
| 15  | 6     | 101 | BCL  | C2-C1-O2A-CGA   |
| 15  | 7     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 15  | F     | 502 | BCL  | C16-C17-C18-C20 |
| 15  | 2     | 102 | BCL  | CBD-CGD-O2D-CED |
| 14  | 1     | 401 | PGV  | O01-C1-C2-C3    |
| 15  | N     | 101 | BCL  | C15-C16-C17-C18 |
| 15  | 4     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 14  | L     | 310 | PGV  | C23-C24-C25-C26 |
| 19  | D     | 101 | CDL  | C52-C51-CB5-OB6 |
| 15  | M     | 402 | BCL  | C6-C7-C8-C9     |
| 15  | D     | 102 | BCL  | C6-C7-C8-C9     |
| 21  | M     | 405 | MQ8  | C43-C44-C46-C47 |
| 14  | A     | 501 | PGV  | C25-C26-C27-C28 |
| 15  | P     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 15  | 6     | 101 | BCL  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | L     | 309 | UQ8  | C20-C19-C21-C22 |
| 18  | 5     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 22  | E     | 103 | CRT  | C32-C33-C35-C36 |
| 22  | R     | 102 | CRT  | C22-C23-C25-C26 |
| 22  | 2     | 103 | CRT  | C15-C16-C17-C19 |
| 14  | H     | 301 | PGV  | C6-C7-C8-C9     |
| 19  | D     | 101 | CDL  | C72-C71-CB7-OB8 |
| 15  | I     | 101 | BCL  | C2-C1-O2A-CGA   |
| 15  | O     | 502 | BCL  | C2-C1-O2A-CGA   |
| 15  | 9     | 102 | BCL  | C2-C1-O2A-CGA   |
| 15  | I     | 101 | BCL  | C11-C10-C8-C7   |
| 15  | V     | 101 | BCL  | C11-C12-C13-C15 |
| 15  | 1     | 402 | BCL  | C6-C7-C8-C10    |
| 15  | P     | 102 | BCL  | C15-C16-C17-C18 |
| 15  | 4     | 102 | BCL  | C16-C17-C18-C20 |
| 15  | 9     | 102 | BCL  | C16-C17-C18-C19 |
| 16  | L     | 302 | BPH  | O2A-C1-C2-C3    |
| 15  | 1     | 402 | BCL  | C5-C6-C7-C8     |
| 22  | P     | 103 | CRT  | C36-C37-C38-C39 |
| 22  | 2     | 103 | CRT  | C36-C37-C38-C39 |
| 22  | 6     | 102 | CRT  | C36-C37-C38-C39 |
| 17  | L     | 309 | UQ8  | C9-C11-C12-C13  |
| 12  | C     | 406 | Z41  | C28-C29-C30-C31 |
| 15  | E     | 102 | BCL  | C15-C16-C17-C18 |
| 16  | M     | 404 | BPH  | C10-C11-C12-C13 |
| 15  | B     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 15  | Z     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 19  | H     | 302 | CDL  | C55-C56-C57-C58 |
| 19  | H     | 302 | CDL  | C72-C73-C74-C75 |
| 14  | 1     | 401 | PGV  | O02-C1-C2-C3    |
| 18  | M     | 410 | LMT  | C2B-C1B-O1B-C4' |
| 19  | M     | 409 | CDL  | C77-C78-C79-C80 |
| 15  | K     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 15  | M     | 403 | BCL  | C14-C13-C15-C16 |
| 15  | T     | 101 | BCL  | C14-C13-C15-C16 |
| 18  | 8     | 103 | LMT  | C5'-C4'-O1B-C1B |
| 19  | H     | 302 | CDL  | C82-C83-C84-C85 |
| 15  | P     | 102 | BCL  | C16-C17-C18-C20 |
| 24  | O     | 501 | LDA  | C4-C5-C6-C7     |
| 19  | L     | 311 | CDL  | C75-C76-C77-C78 |
| 22  | G     | 103 | CRT  | C15-C16-C17-C19 |
| 22  | T     | 102 | CRT  | C5-C6-C7-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | 7     | 101 | BCL  | CAA-CBA-CGA-O1A |
| 14  | H     | 301 | PGV  | O12-C04-C05-C06 |
| 19  | D     | 101 | CDL  | C72-C71-CB7-OB9 |
| 14  | M     | 408 | PGV  | O03-C19-C20-C21 |
| 15  | R     | 101 | BCL  | C16-C17-C18-C20 |
| 10  | C     | 404 | HEM  | CAA-CBA-CGA-O2A |
| 18  | T     | 103 | LMT  | O5B-C1B-O1B-C4' |
| 19  | D     | 101 | CDL  | C52-C51-CB5-OB7 |
| 15  | 8     | 102 | BCL  | C16-C17-C18-C19 |
| 15  | Q     | 102 | BCL  | C10-C11-C12-C13 |
| 14  | L     | 305 | PGV  | C01-C02-C03-O11 |
| 15  | L     | 301 | BCL  | C2-C1-O2A-CGA   |
| 14  | H     | 301 | PGV  | O03-C19-C20-C21 |
| 15  | X     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 15  | X     | 102 | BCL  | C10-C11-C12-C13 |
| 18  | 8     | 103 | LMT  | C4-C5-C6-C7     |
| 18  | G     | 101 | LMT  | C6-C7-C8-C9     |
| 14  | F     | 501 | PGV  | O03-C19-C20-C21 |

There are no ring outliers.

99 monomers are involved in 445 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | L     | 303 | UQ8  | 4       | 0            |
| 15  | K     | 102 | BCL  | 6       | 0            |
| 15  | 5     | 102 | BCL  | 6       | 0            |
| 18  | G     | 101 | LMT  | 1       | 0            |
| 19  | M     | 409 | CDL  | 8       | 0            |
| 18  | Z     | 101 | LMT  | 2       | 0            |
| 22  | 6     | 102 | CRT  | 5       | 0            |
| 22  | E     | 103 | CRT  | 6       | 0            |
| 18  | 2     | 101 | LMT  | 4       | 0            |
| 14  | L     | 305 | PGV  | 5       | 0            |
| 15  | N     | 101 | BCL  | 9       | 0            |
| 22  | Z     | 103 | CRT  | 7       | 0            |
| 18  | M     | 410 | LMT  | 2       | 0            |
| 15  | O     | 502 | BCL  | 3       | 0            |
| 18  | P     | 104 | LMT  | 3       | 0            |
| 17  | L     | 309 | UQ8  | 5       | 0            |
| 15  | U     | 101 | BCL  | 5       | 0            |
| 10  | C     | 404 | HEM  | 3       | 0            |
| 19  | H     | 302 | CDL  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | T     | 103 | LMT  | 3       | 0            |
| 19  | M     | 407 | CDL  | 1       | 0            |
| 10  | C     | 401 | HEM  | 6       | 0            |
| 15  | 3     | 101 | BCL  | 8       | 0            |
| 14  | L     | 310 | PGV  | 4       | 0            |
| 18  | 5     | 101 | LMT  | 1       | 0            |
| 18  | 8     | 103 | LMT  | 2       | 0            |
| 18  | L     | 307 | LMT  | 3       | 0            |
| 14  | L     | 306 | PGV  | 4       | 0            |
| 18  | S     | 101 | LMT  | 4       | 0            |
| 15  | 1     | 402 | BCL  | 10      | 0            |
| 22  | N     | 102 | CRT  | 9       | 0            |
| 18  | E     | 101 | LMT  | 2       | 0            |
| 22  | R     | 102 | CRT  | 4       | 0            |
| 15  | D     | 102 | BCL  | 4       | 0            |
| 15  | L     | 301 | BCL  | 3       | 0            |
| 22  | G     | 103 | CRT  | 4       | 0            |
| 18  | 4     | 104 | LMT  | 2       | 0            |
| 19  | L     | 311 | CDL  | 7       | 0            |
| 13  | C     | 407 | PLM  | 2       | 0            |
| 14  | A     | 501 | PGV  | 3       | 0            |
| 15  | Q     | 102 | BCL  | 3       | 0            |
| 15  | 7     | 101 | BCL  | 6       | 0            |
| 22  | 9     | 101 | CRT  | 5       | 0            |
| 18  | P     | 101 | LMT  | 1       | 0            |
| 15  | M     | 402 | BCL  | 3       | 0            |
| 15  | Y     | 102 | BCL  | 3       | 0            |
| 18  | J     | 104 | LMT  | 1       | 0            |
| 21  | M     | 405 | MQ8  | 9       | 0            |
| 14  | H     | 301 | PGV  | 3       | 0            |
| 15  | M     | 403 | BCL  | 2       | 0            |
| 15  | 0     | 101 | BCL  | 8       | 0            |
| 15  | Z     | 102 | BCL  | 6       | 0            |
| 15  | B     | 102 | BCL  | 9       | 0            |
| 15  | I     | 101 | BCL  | 5       | 0            |
| 18  | 4     | 101 | LMT  | 6       | 0            |
| 22  | 0     | 102 | CRT  | 7       | 0            |
| 16  | L     | 302 | BPH  | 6       | 0            |
| 15  | 8     | 102 | BCL  | 9       | 0            |
| 18  | B     | 101 | LMT  | 3       | 0            |
| 22  | 4     | 103 | CRT  | 10      | 0            |
| 14  | Q     | 101 | PGV  | 2       | 0            |

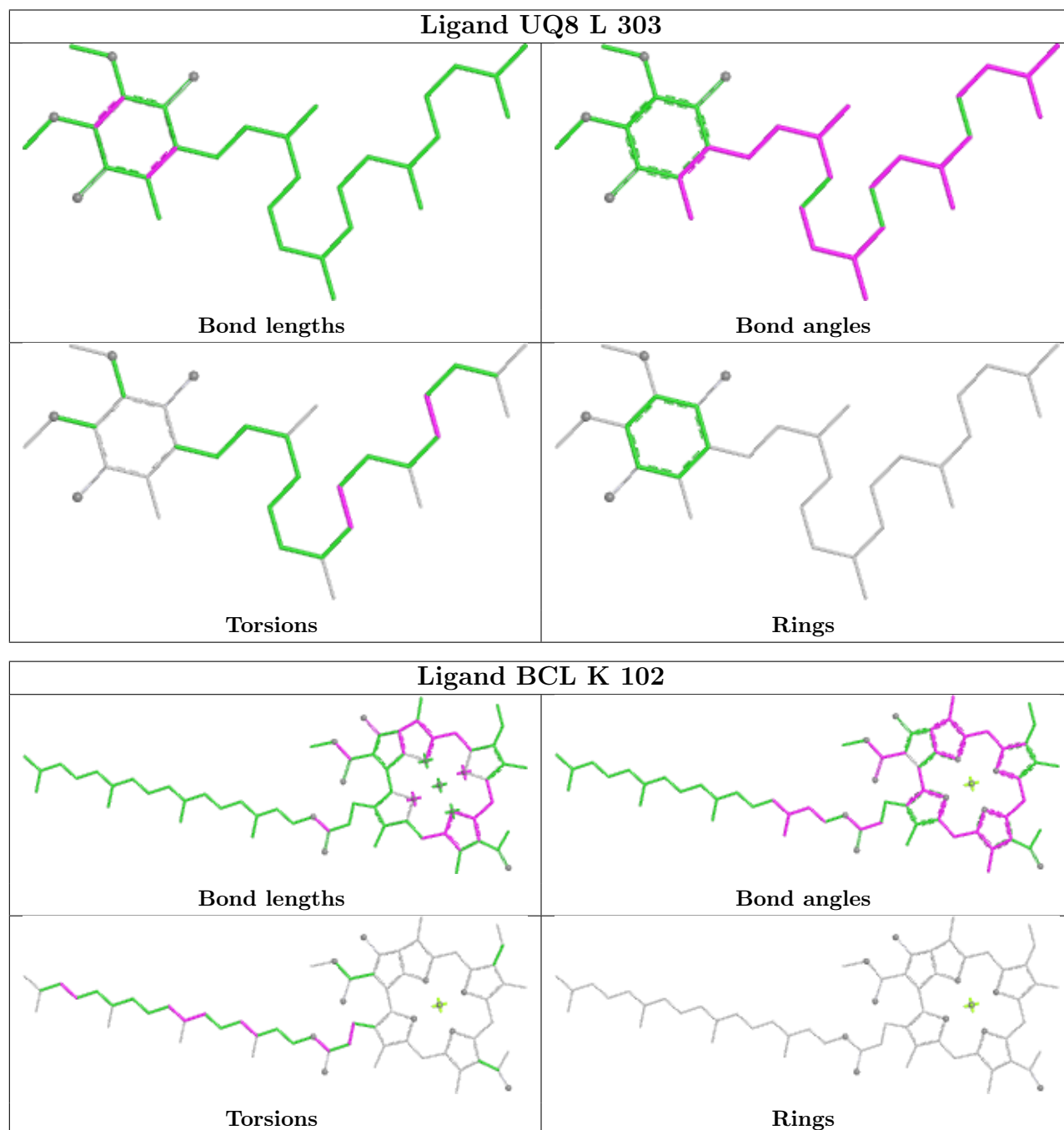
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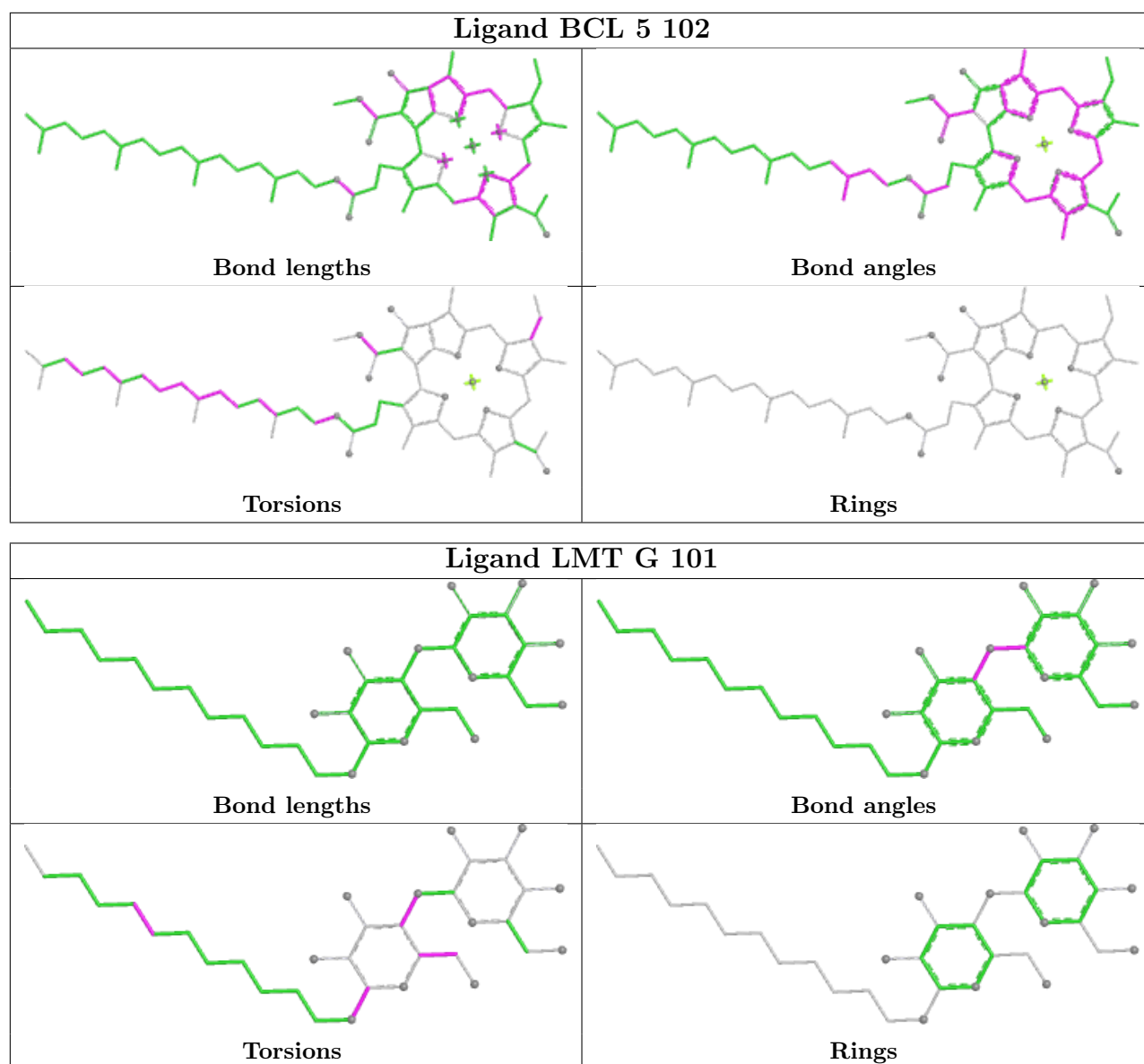
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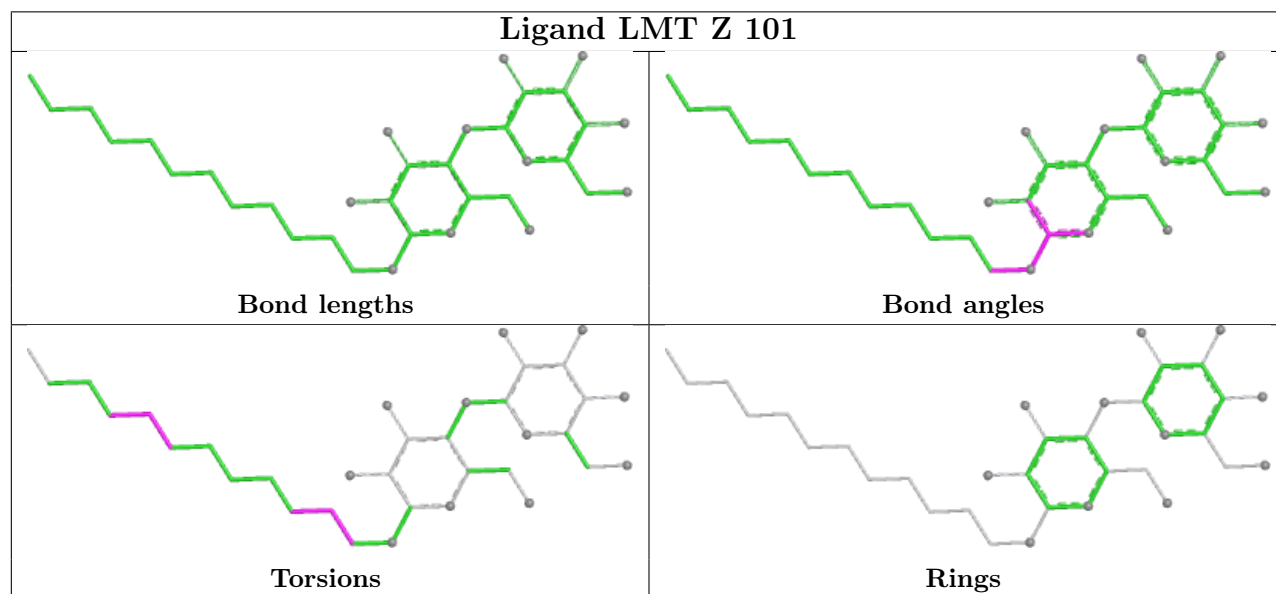
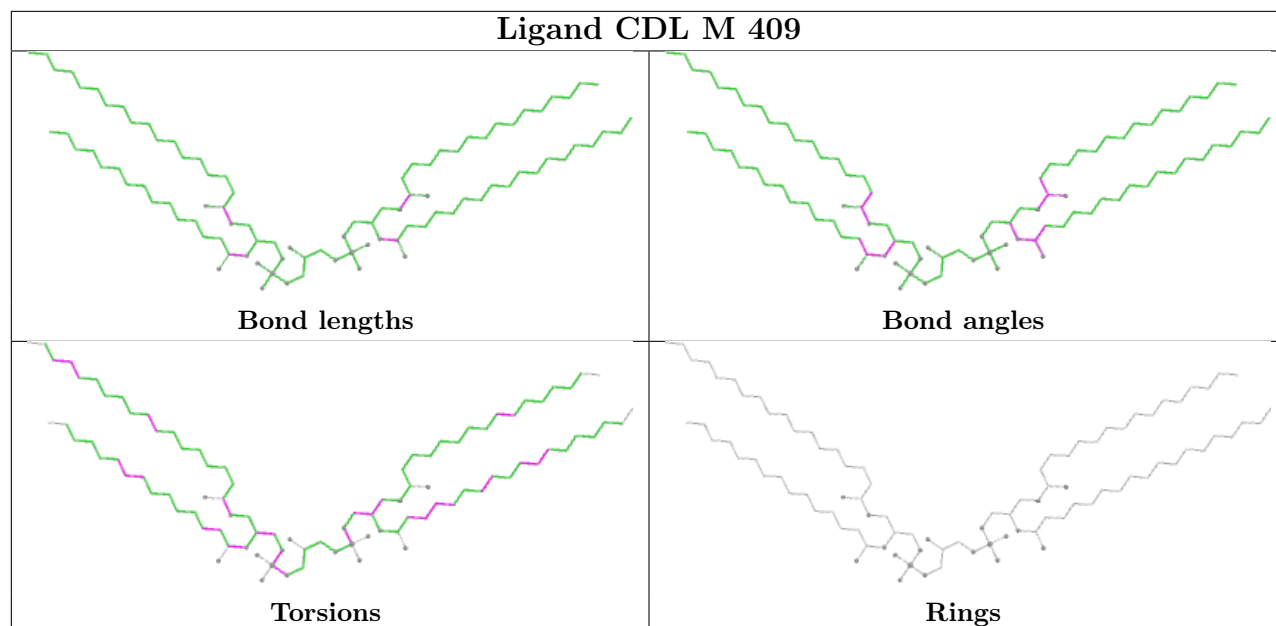
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | Y     | 101 | CRT  | 6       | 0            |
| 18  | H     | 303 | LMT  | 3       | 0            |
| 15  | R     | 101 | BCL  | 6       | 0            |
| 15  | X     | 102 | BCL  | 5       | 0            |
| 15  | 2     | 102 | BCL  | 9       | 0            |
| 22  | J     | 103 | CRT  | 8       | 0            |
| 10  | C     | 402 | HEM  | 4       | 0            |
| 15  | S     | 102 | BCL  | 4       | 0            |
| 15  | T     | 101 | BCL  | 4       | 0            |
| 17  | L     | 304 | UQ8  | 15      | 0            |
| 14  | M     | 408 | PGV  | 3       | 0            |
| 15  | 6     | 101 | BCL  | 6       | 0            |
| 15  | G     | 102 | BCL  | 9       | 0            |
| 15  | V     | 101 | BCL  | 6       | 0            |
| 15  | J     | 102 | BCL  | 6       | 0            |
| 22  | P     | 103 | CRT  | 2       | 0            |
| 16  | M     | 404 | BPH  | 6       | 0            |
| 15  | 4     | 102 | BCL  | 7       | 0            |
| 22  | T     | 102 | CRT  | 7       | 0            |
| 15  | P     | 102 | BCL  | 4       | 0            |
| 15  | L     | 308 | BCL  | 2       | 0            |
| 14  | C     | 408 | PGV  | 2       | 0            |
| 15  | 9     | 102 | BCL  | 5       | 0            |
| 19  | D     | 101 | CDL  | 1       | 0            |
| 18  | R     | 103 | LMT  | 4       | 0            |
| 22  | V     | 102 | CRT  | 10      | 0            |
| 22  | 2     | 103 | CRT  | 12      | 0            |
| 10  | C     | 403 | HEM  | 6       | 0            |
| 14  | 1     | 401 | PGV  | 5       | 0            |
| 18  | X     | 101 | LMT  | 3       | 0            |
| 24  | O     | 501 | LDA  | 1       | 0            |
| 14  | A     | 503 | PGV  | 4       | 0            |
| 15  | A     | 502 | BCL  | 3       | 0            |
| 22  | M     | 406 | CRT  | 5       | 0            |
| 22  | B     | 103 | CRT  | 7       | 0            |
| 15  | E     | 102 | BCL  | 10      | 0            |
| 15  | W     | 101 | BCL  | 4       | 0            |
| 18  | J     | 101 | LMT  | 3       | 0            |

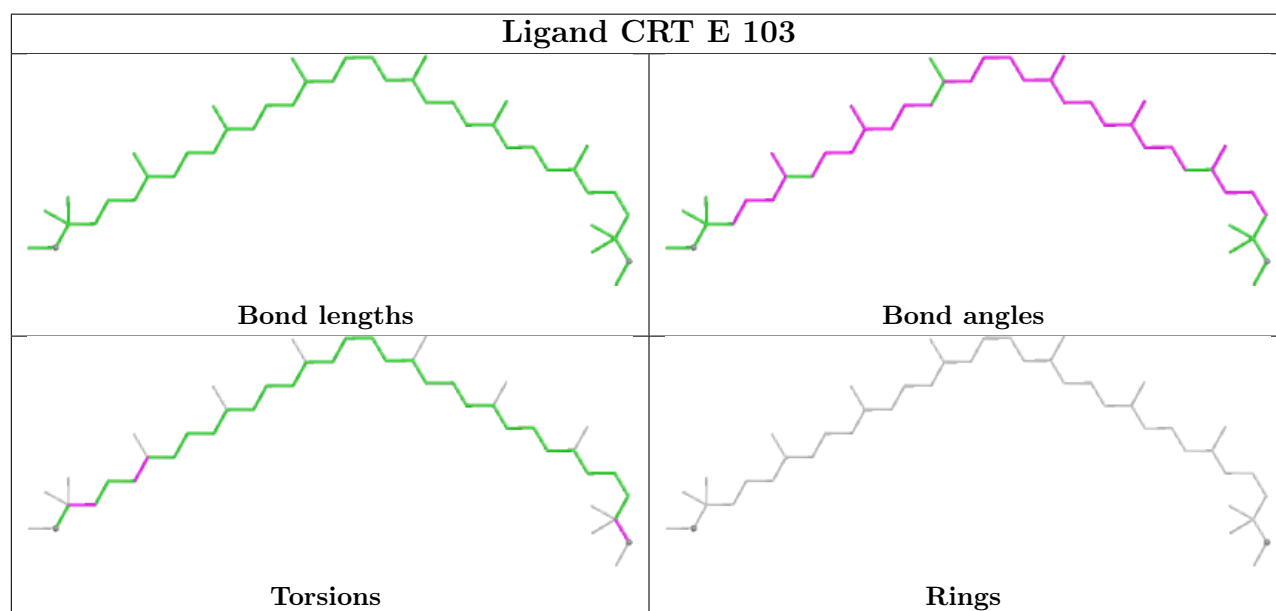
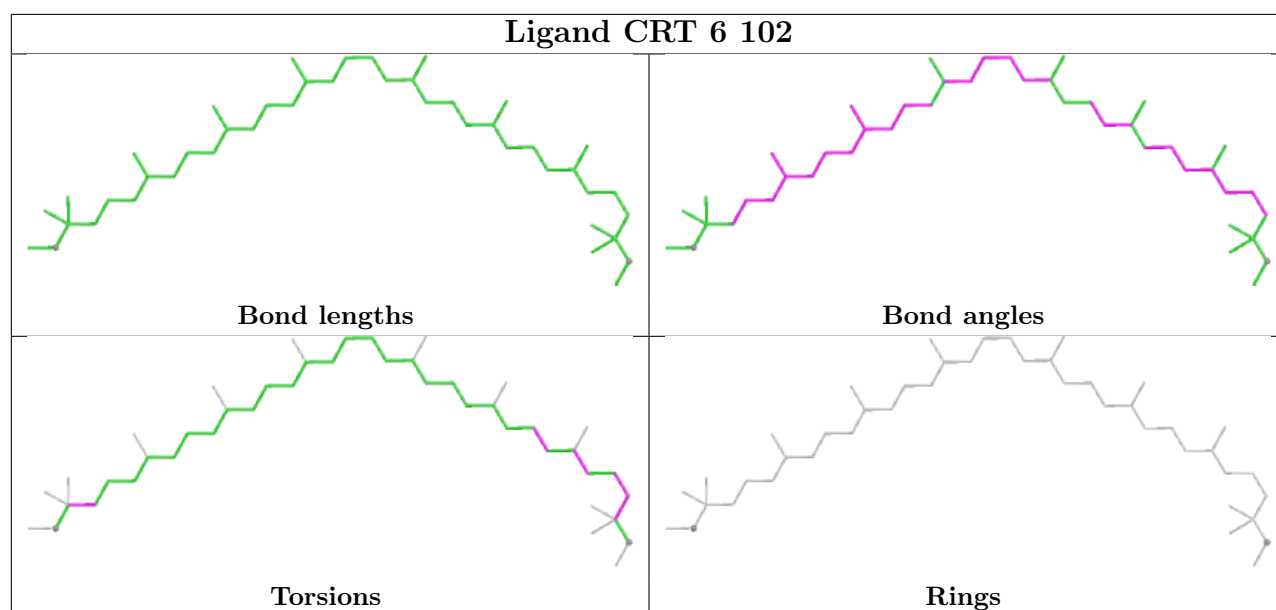
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

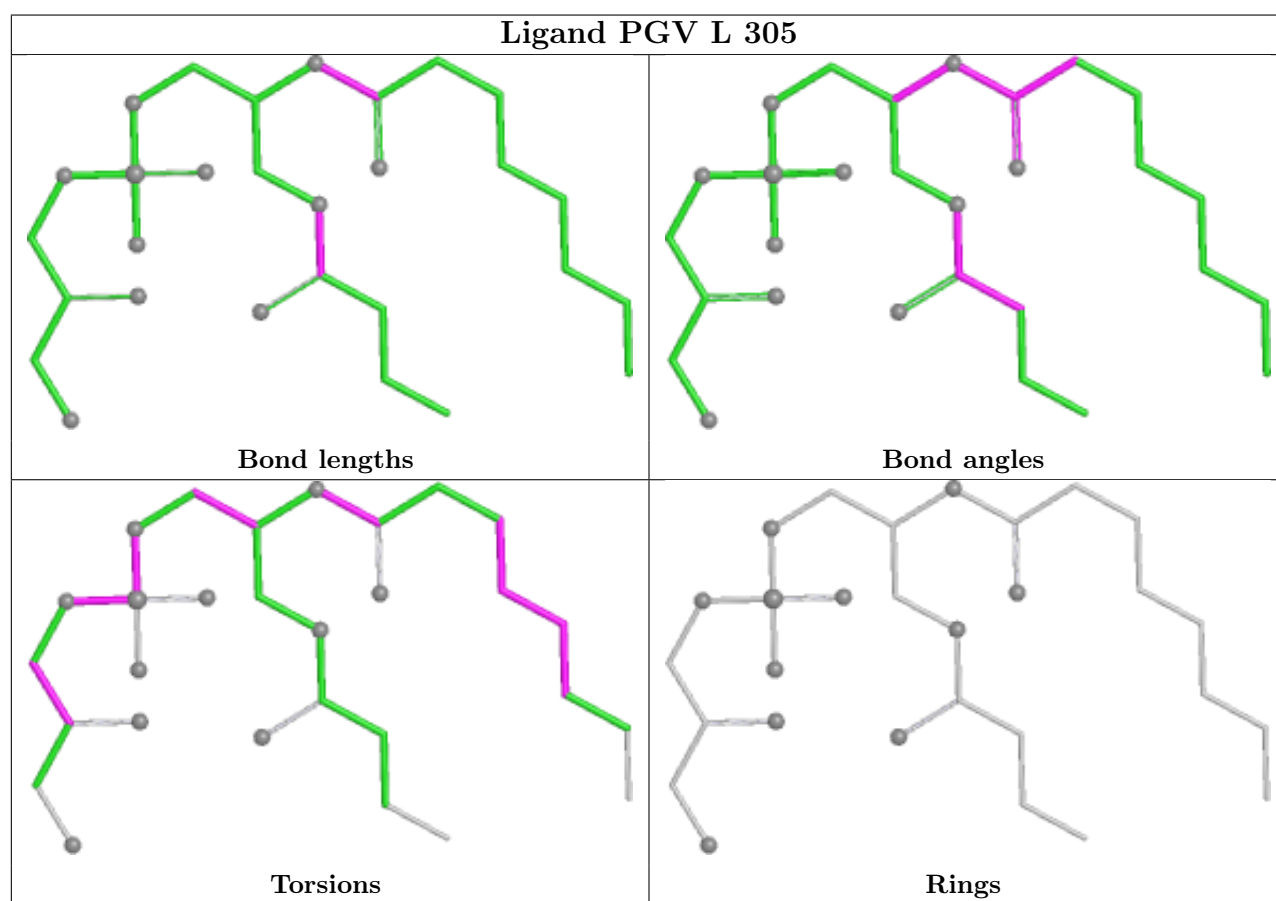
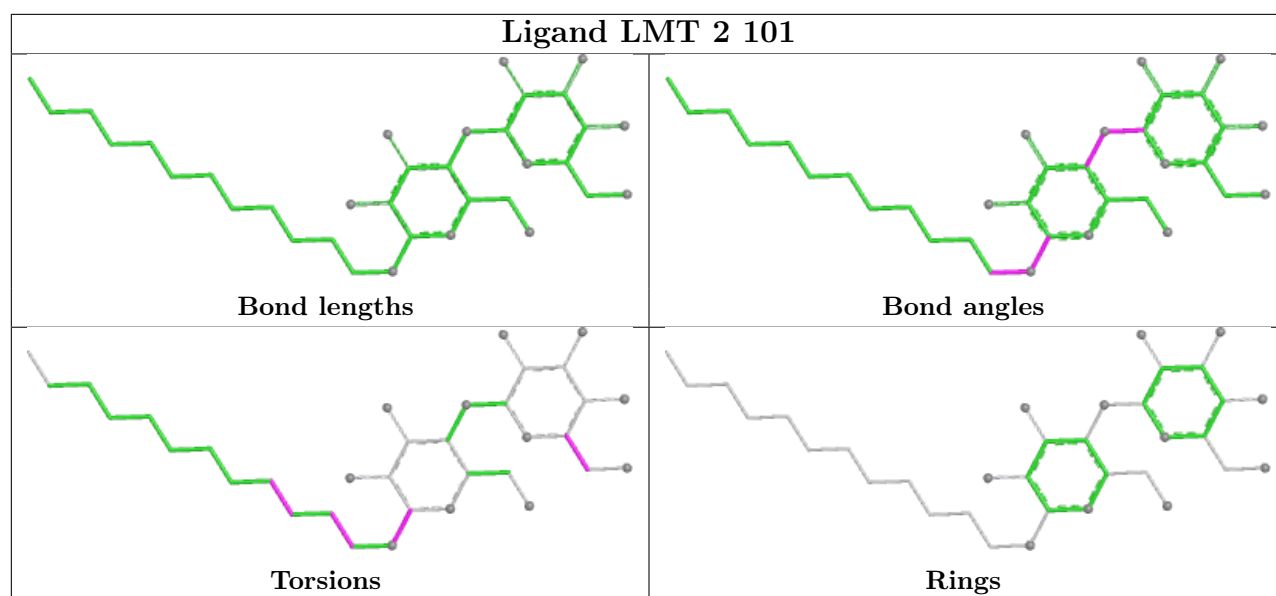
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

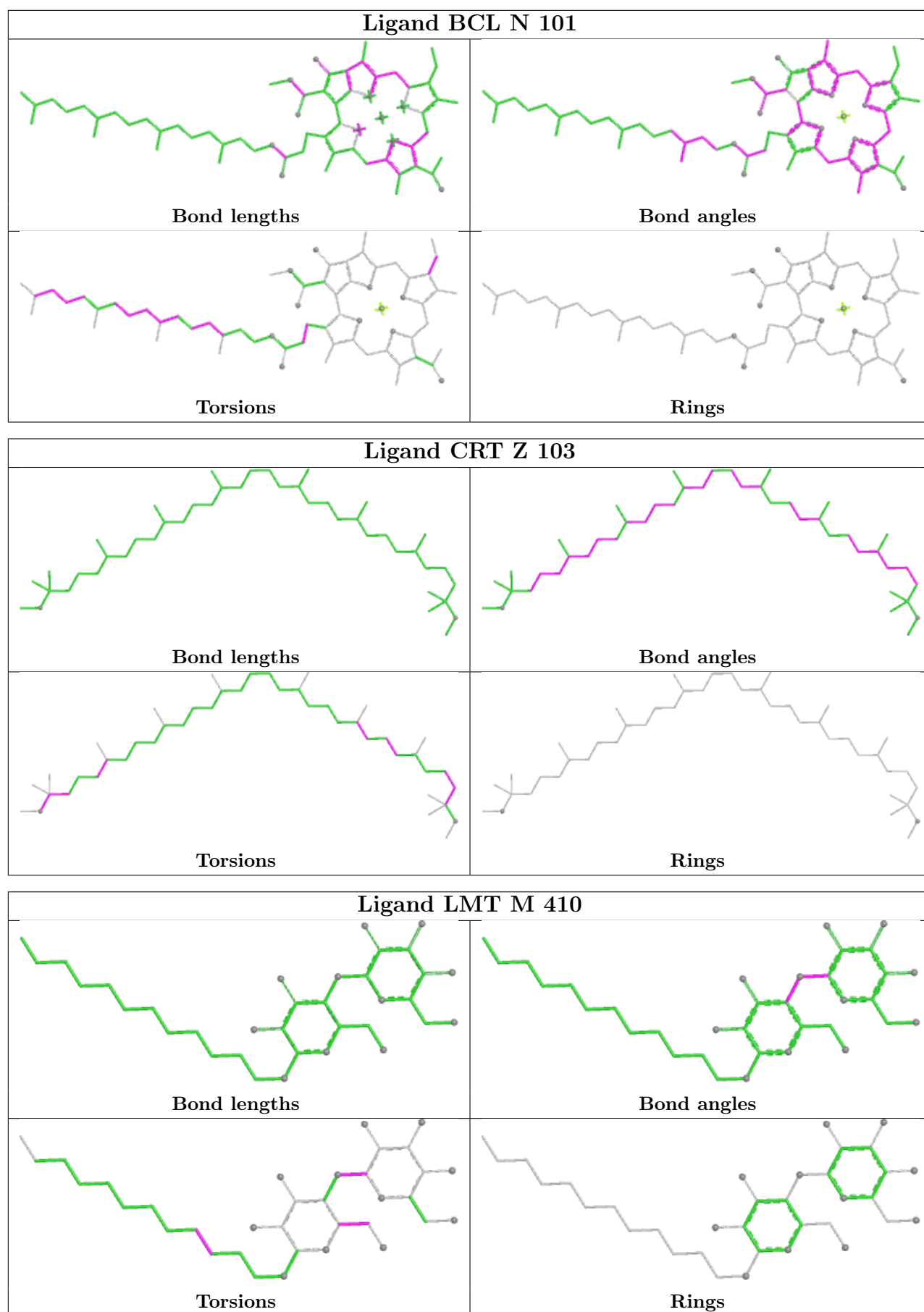


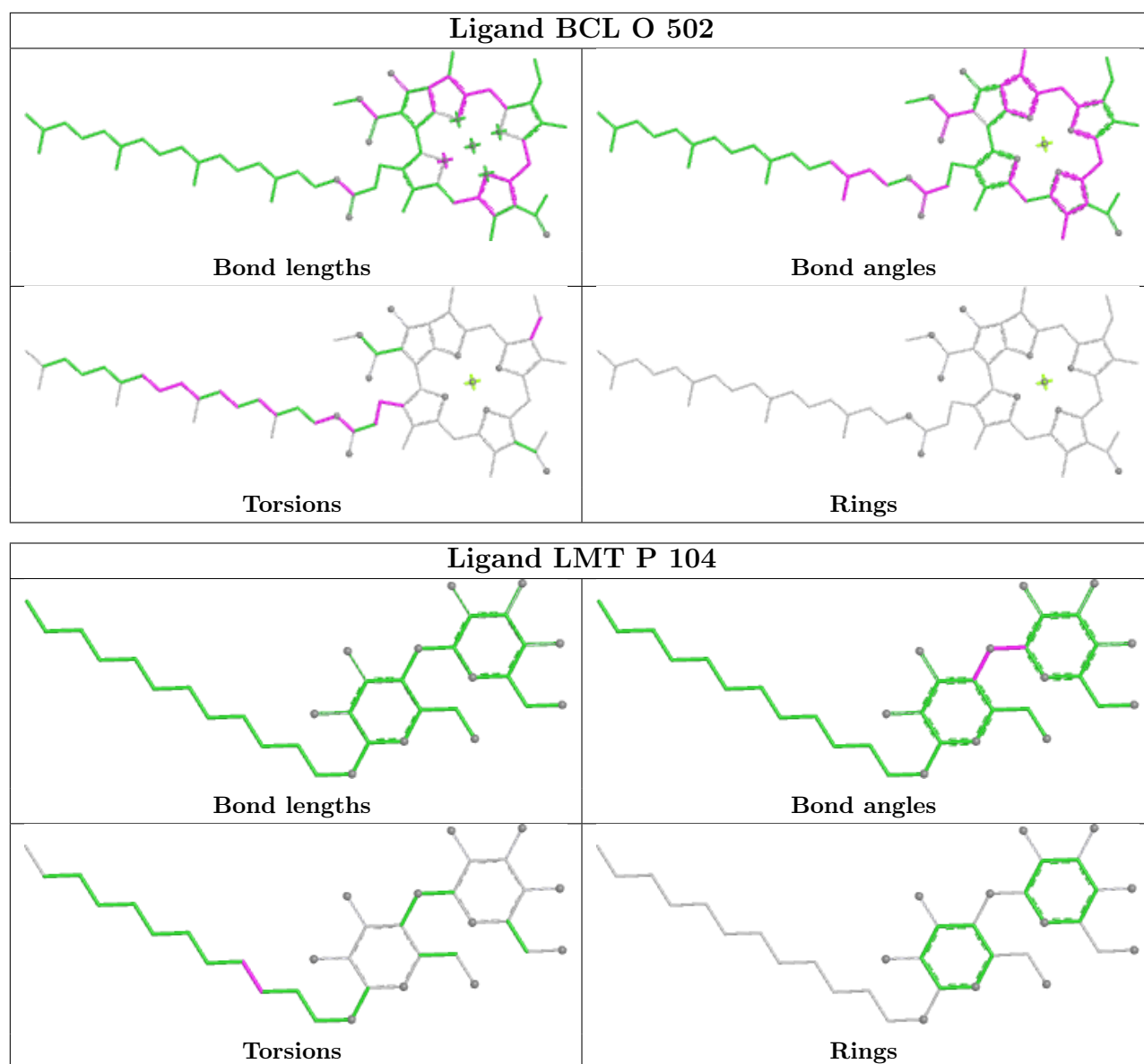


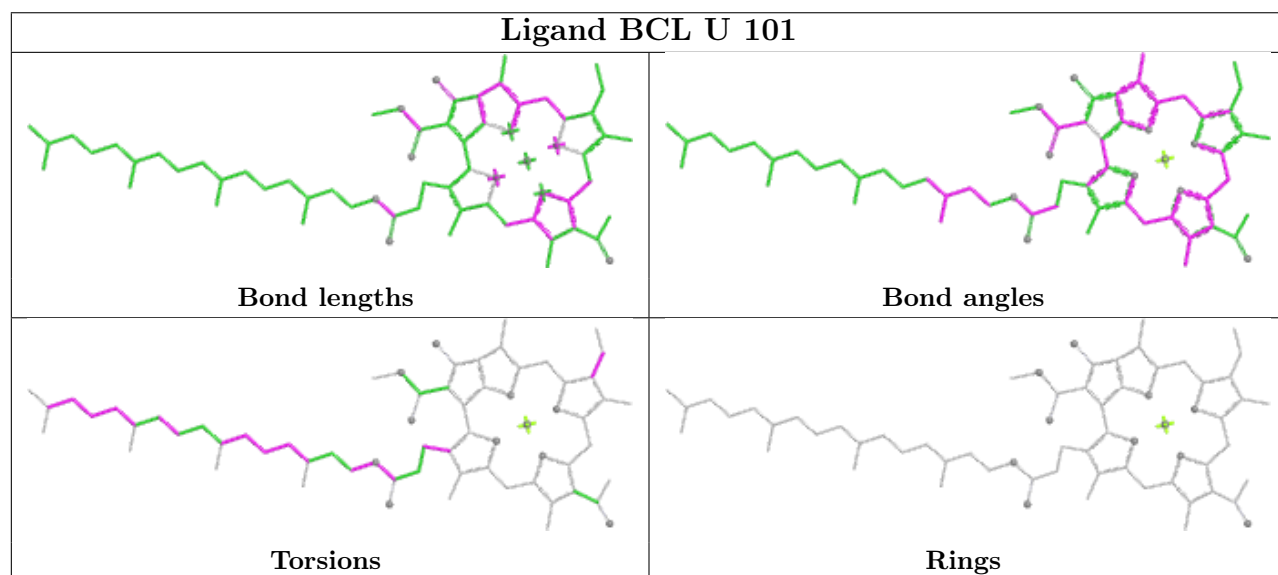
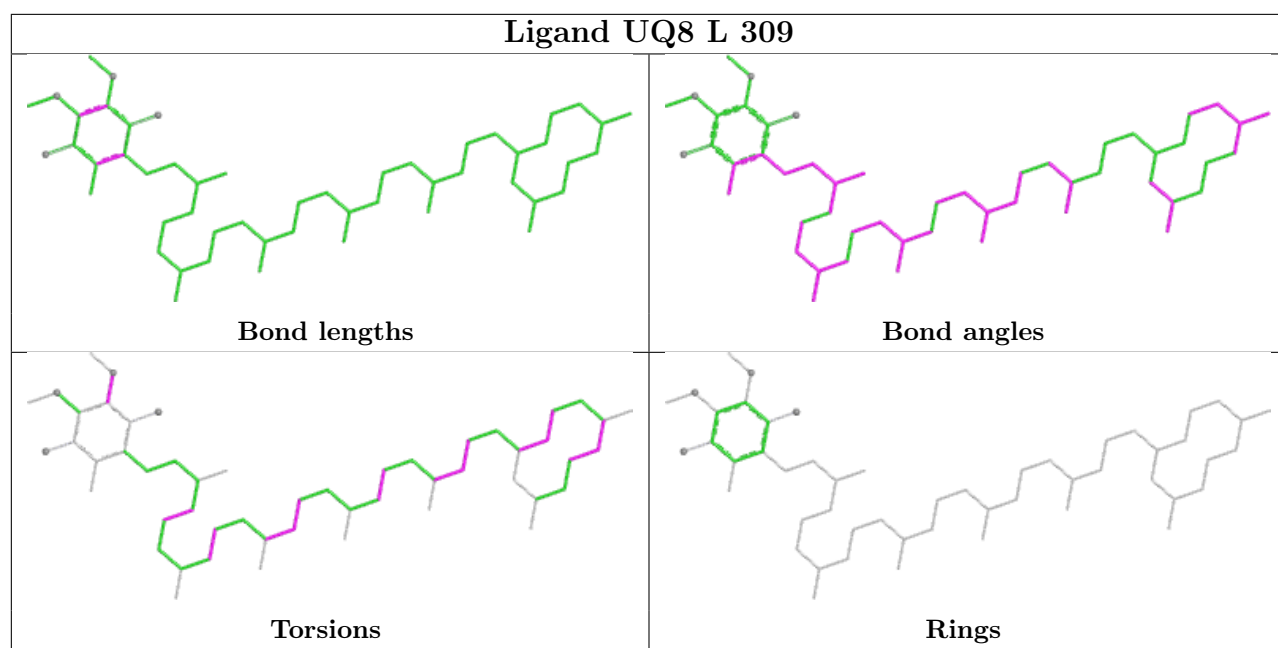


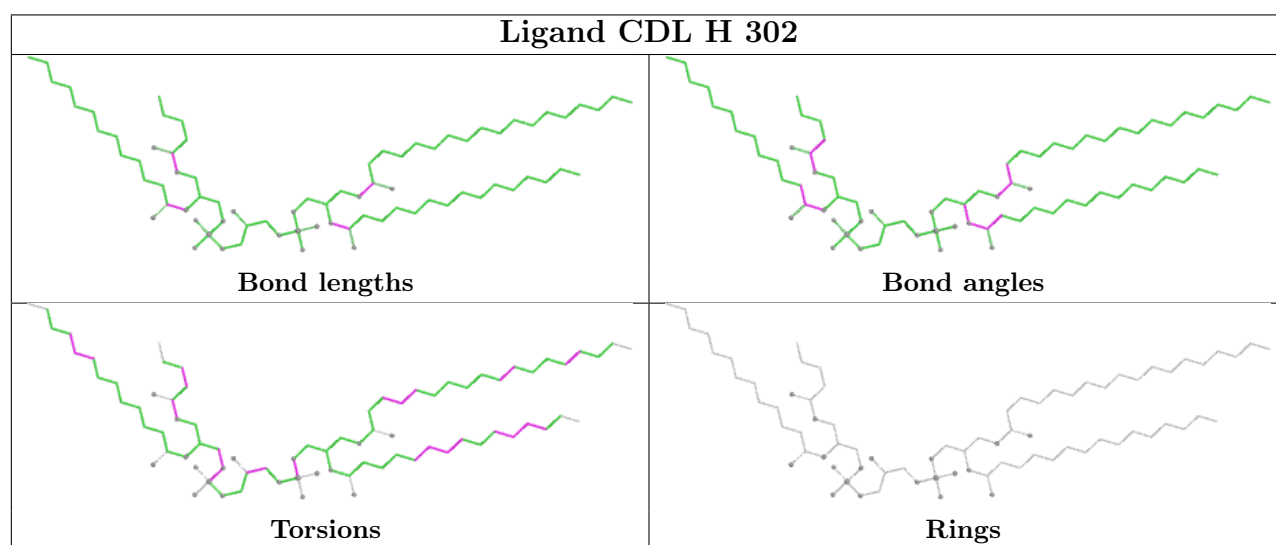
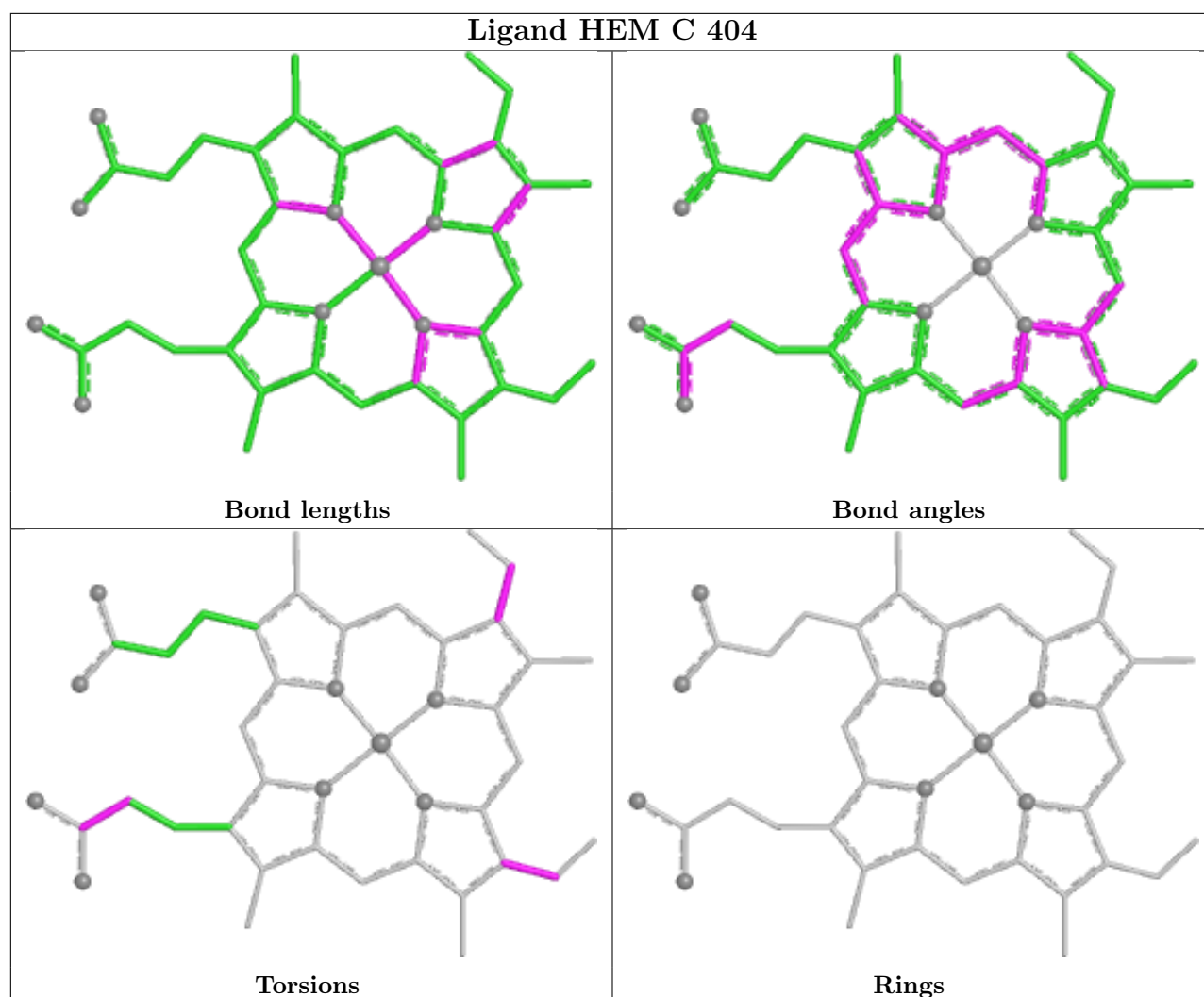


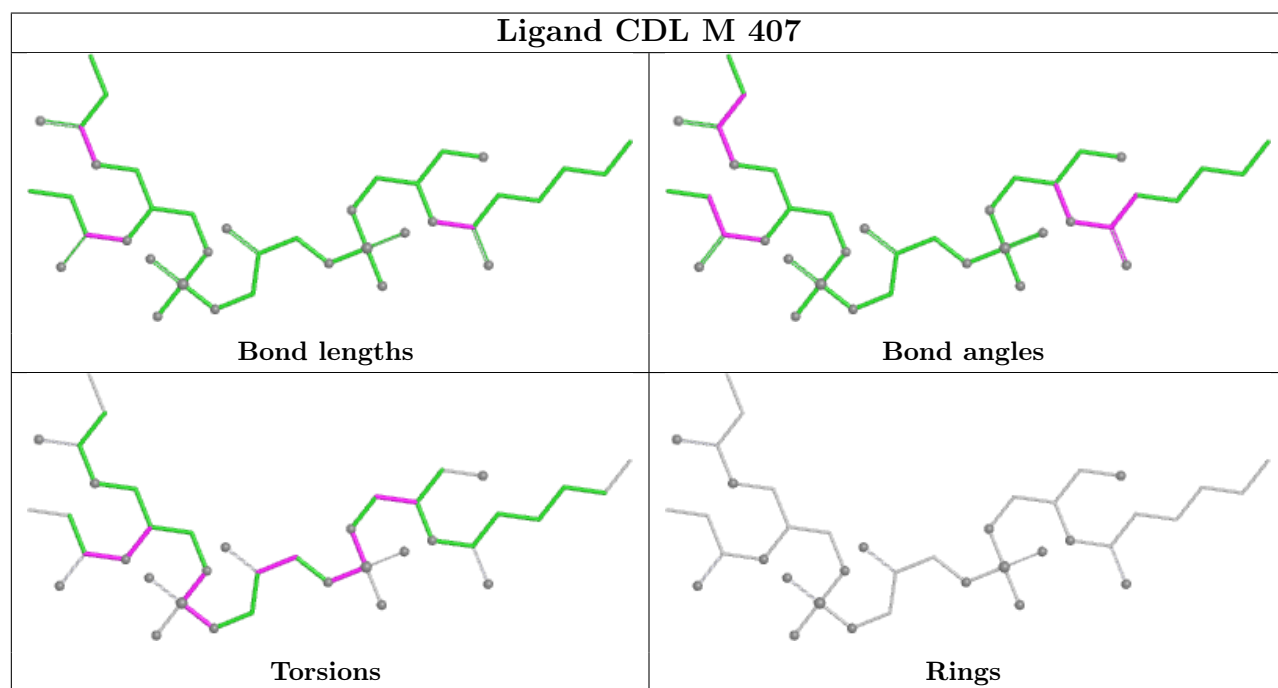
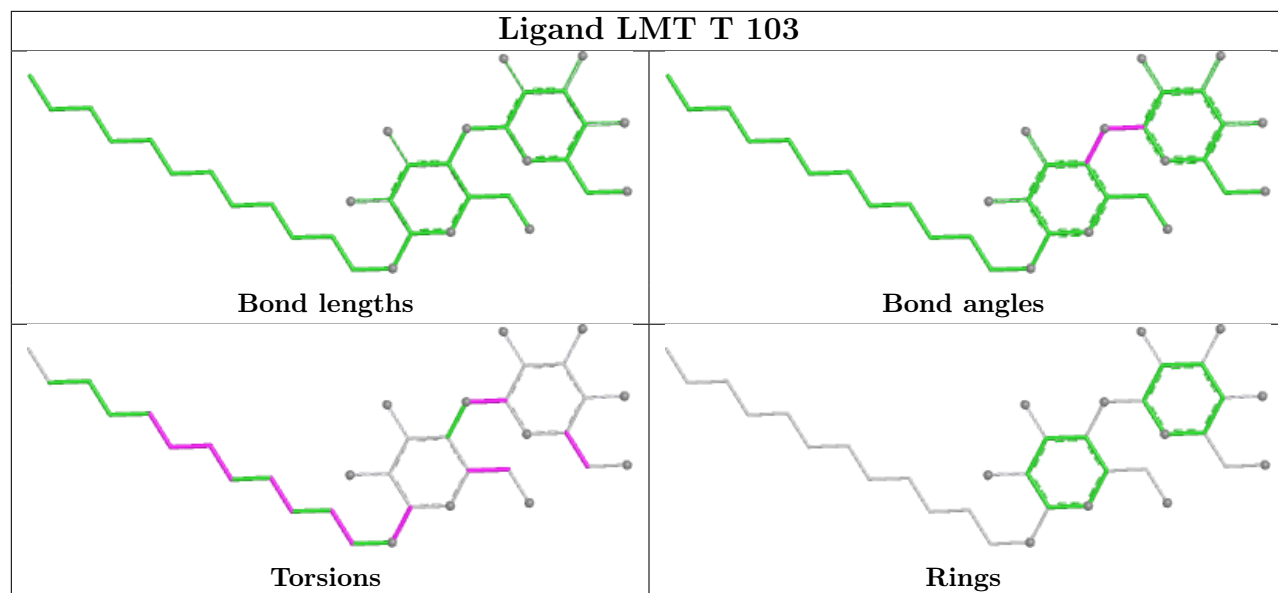


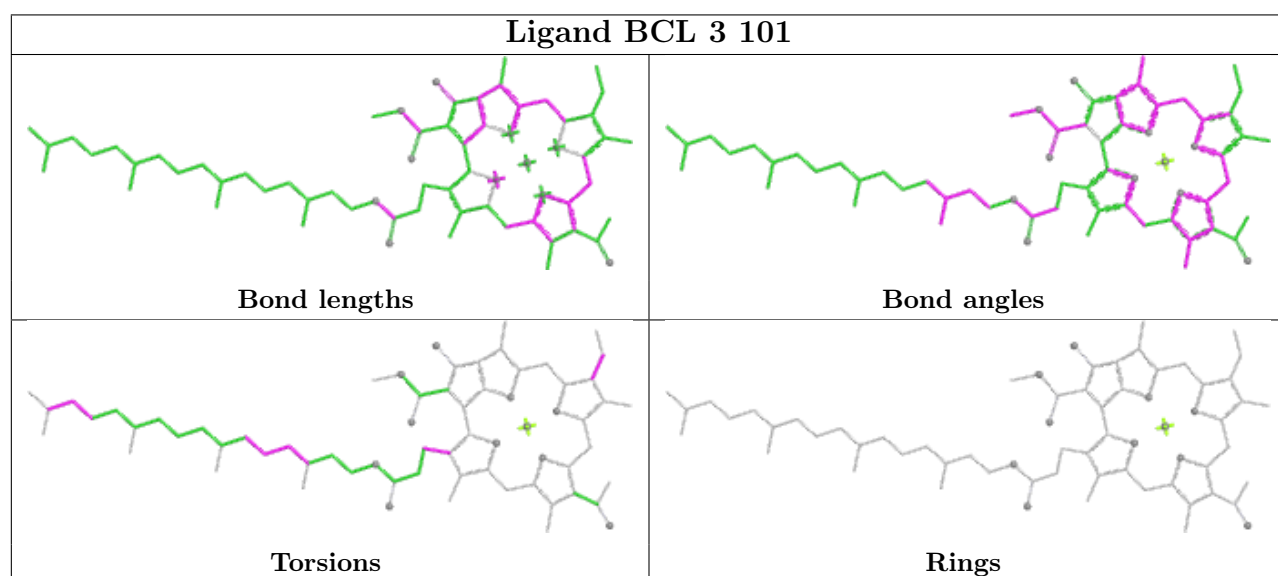
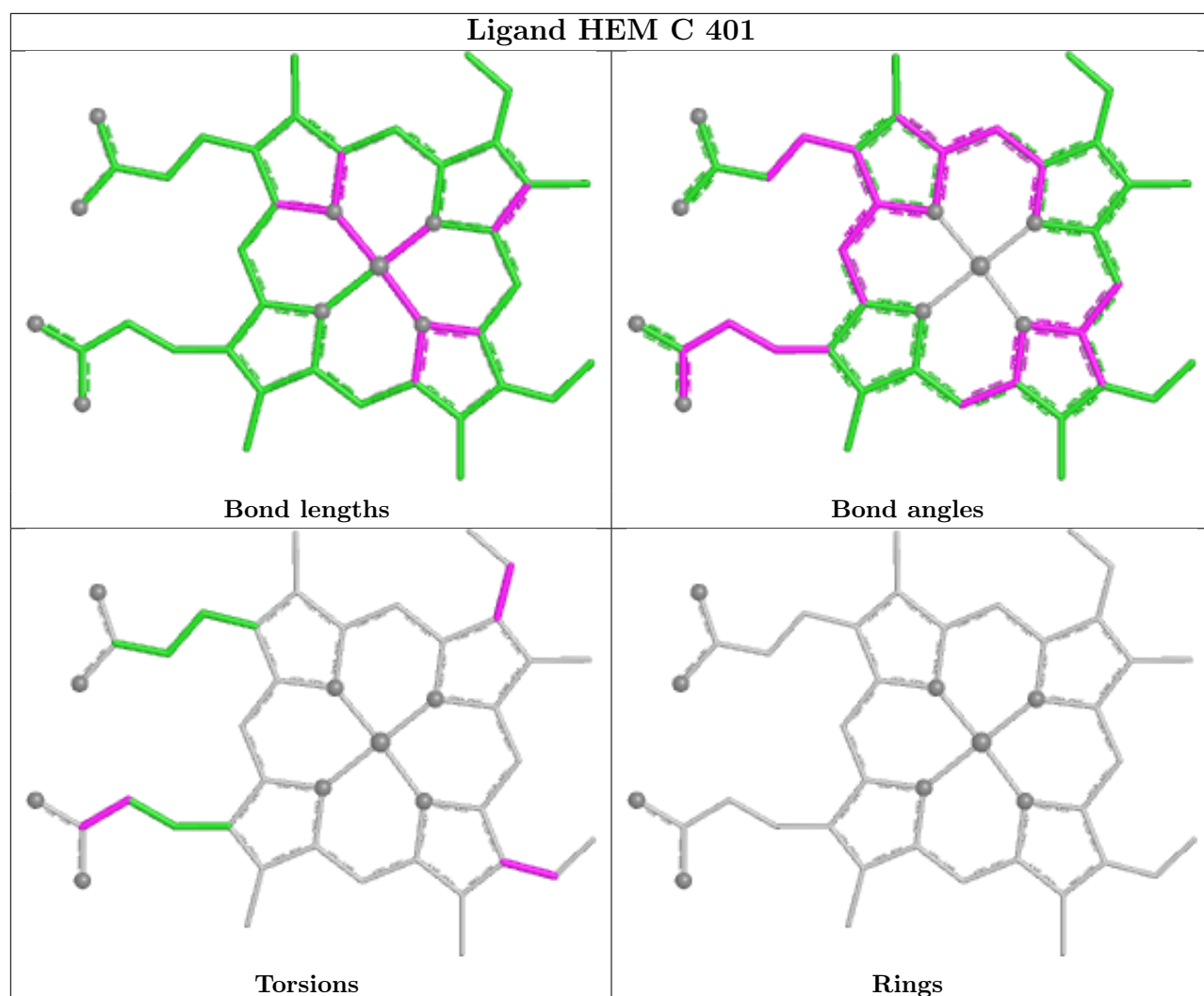


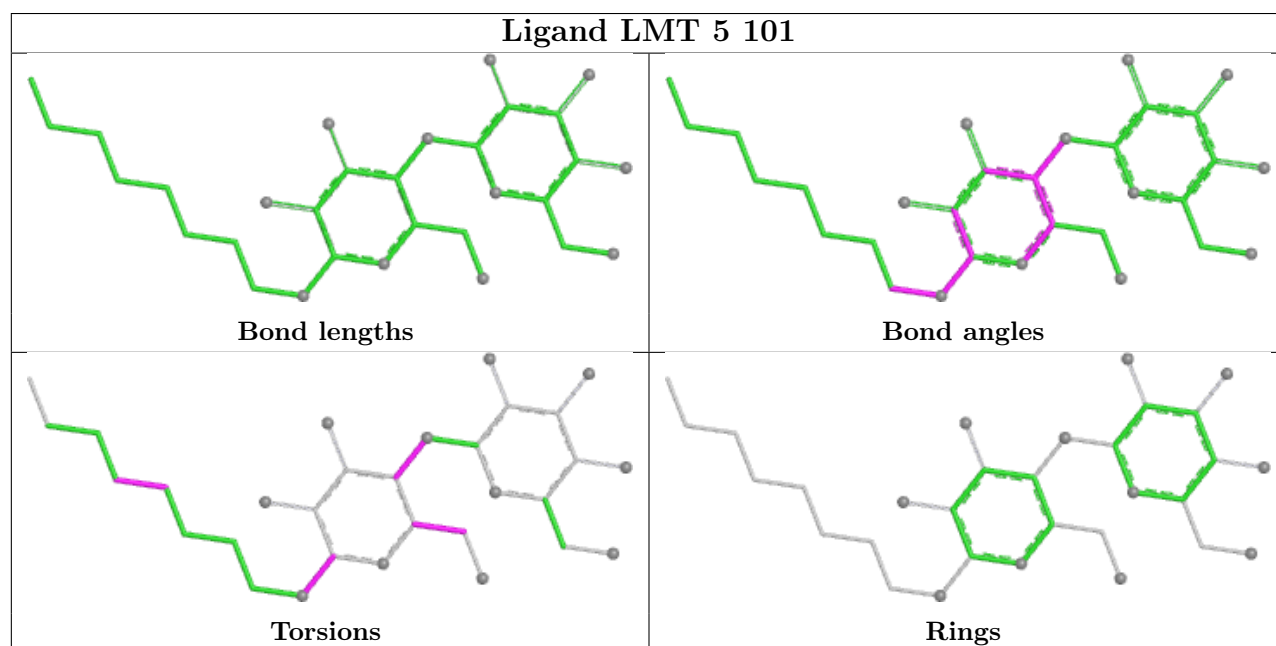
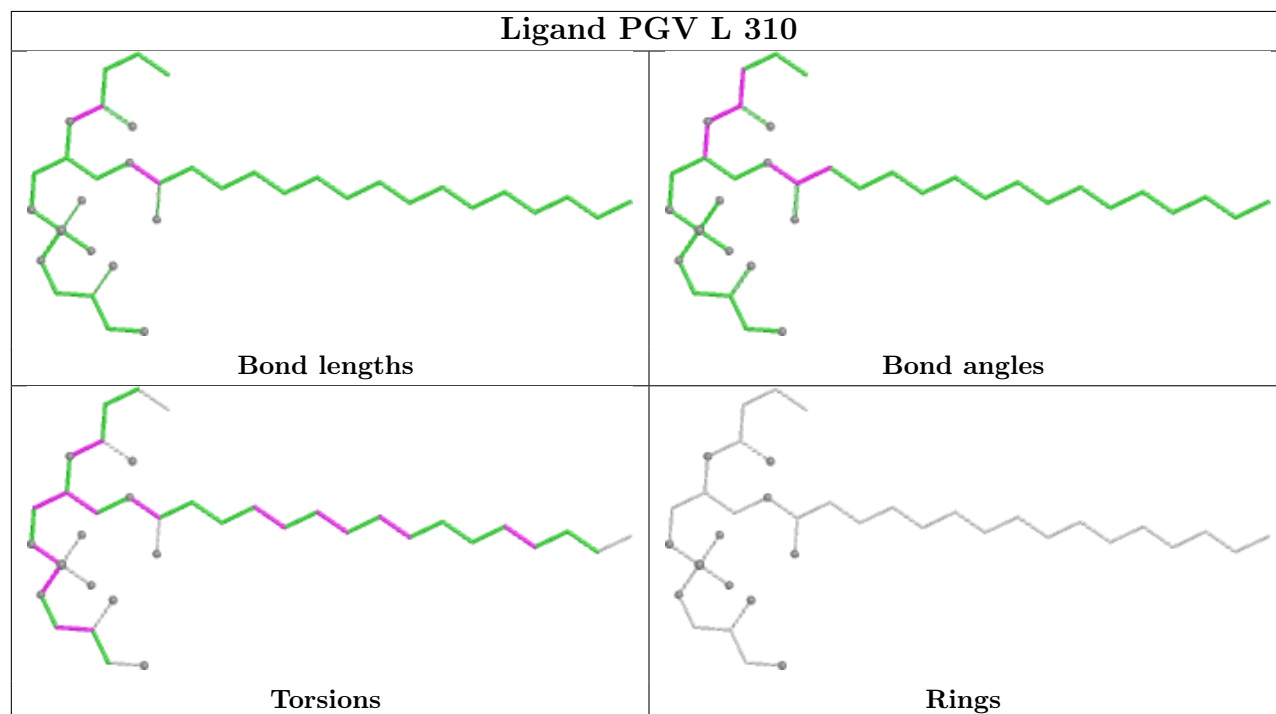
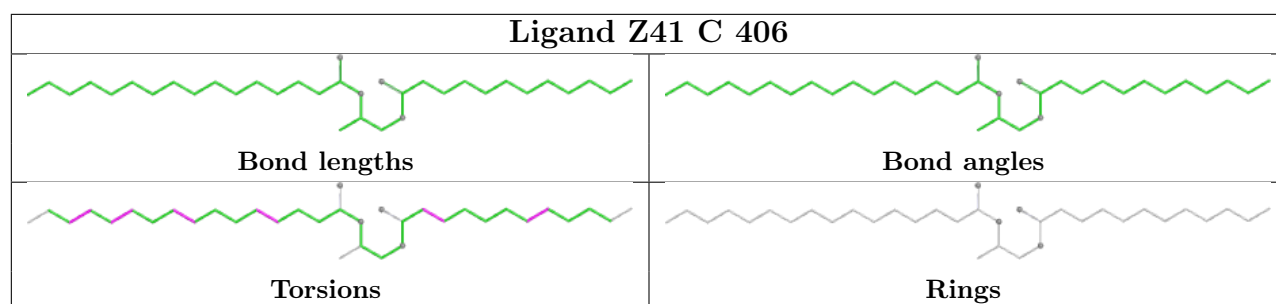


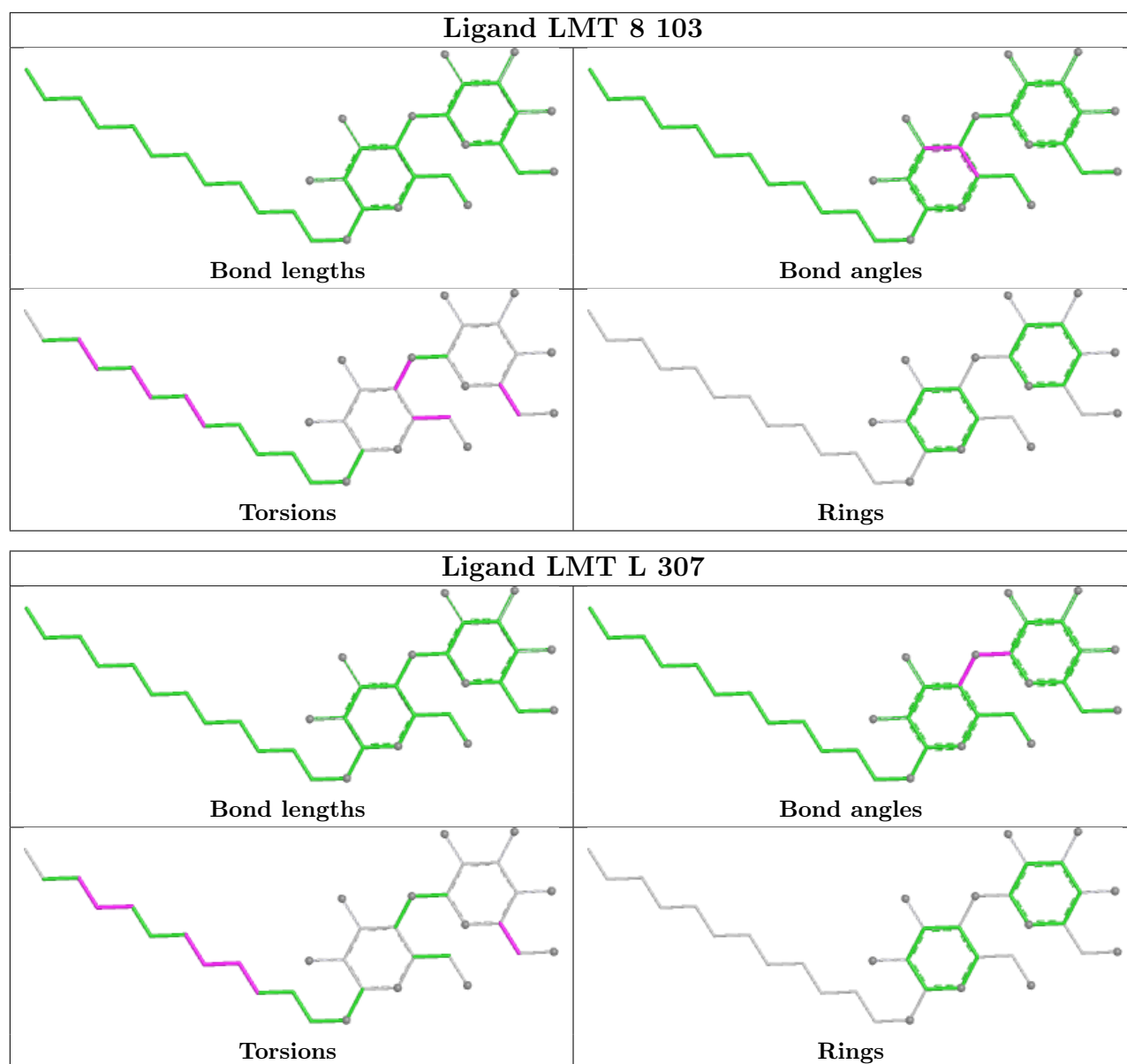


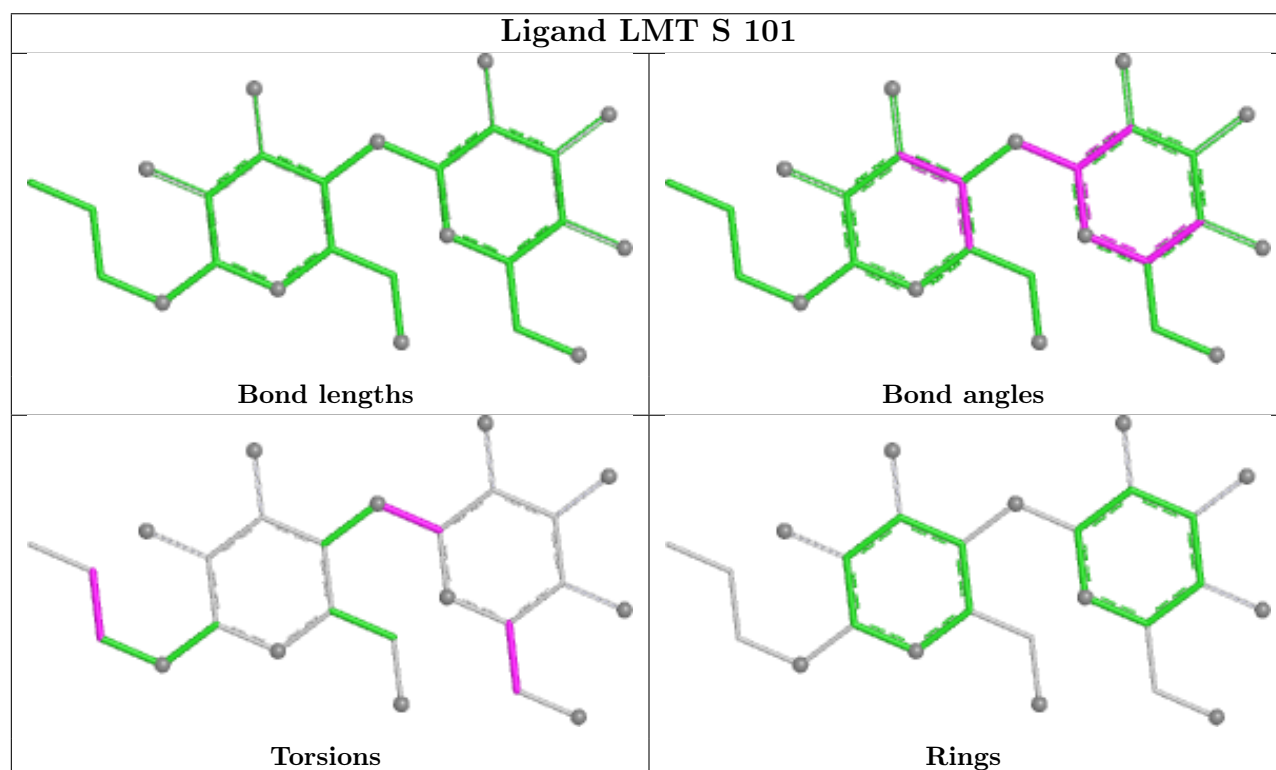
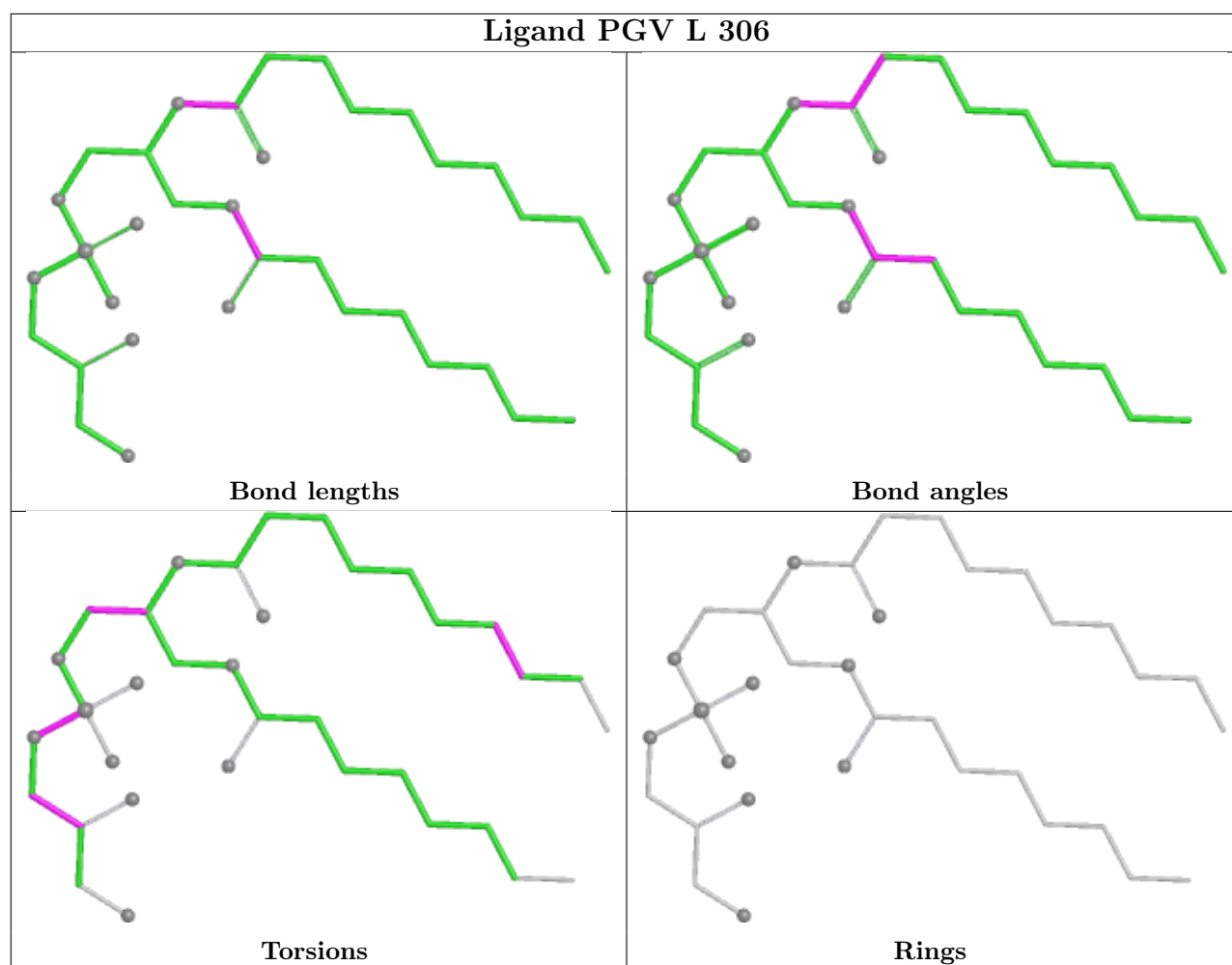


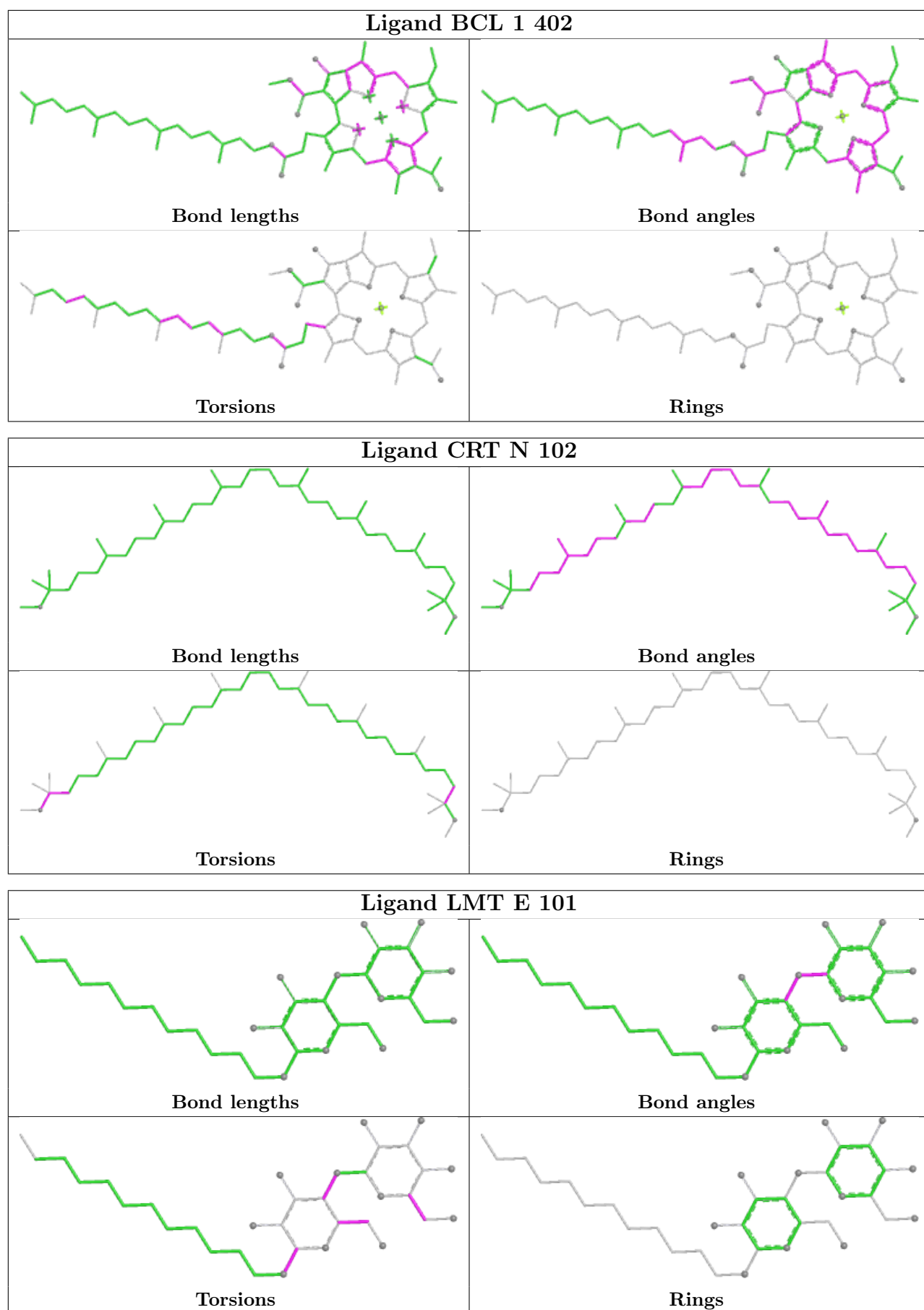


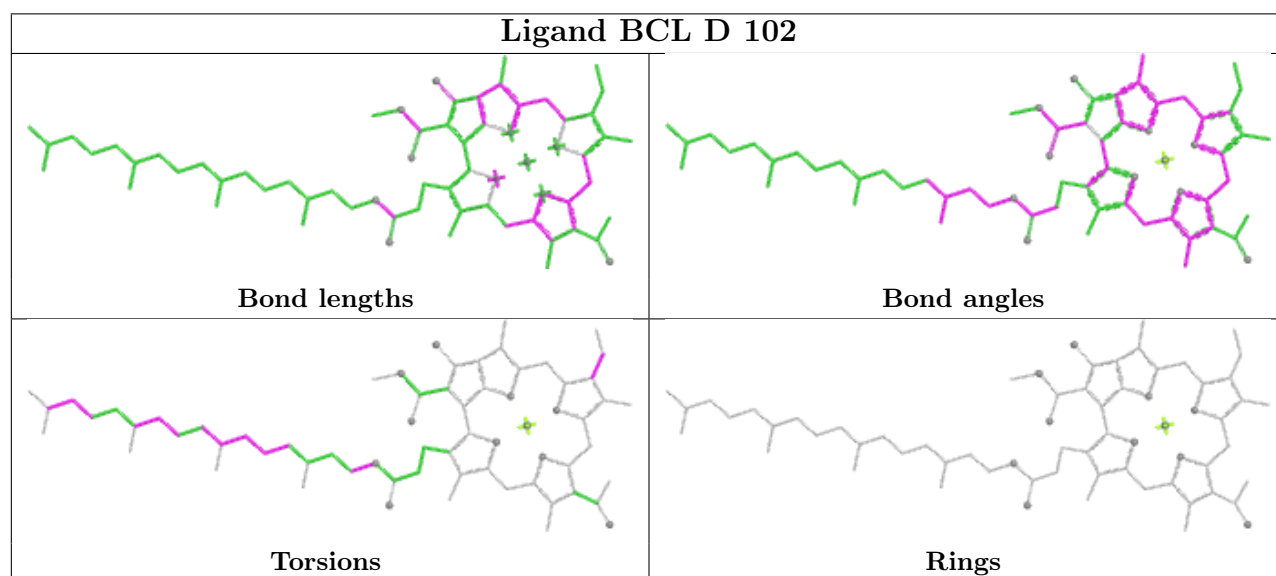
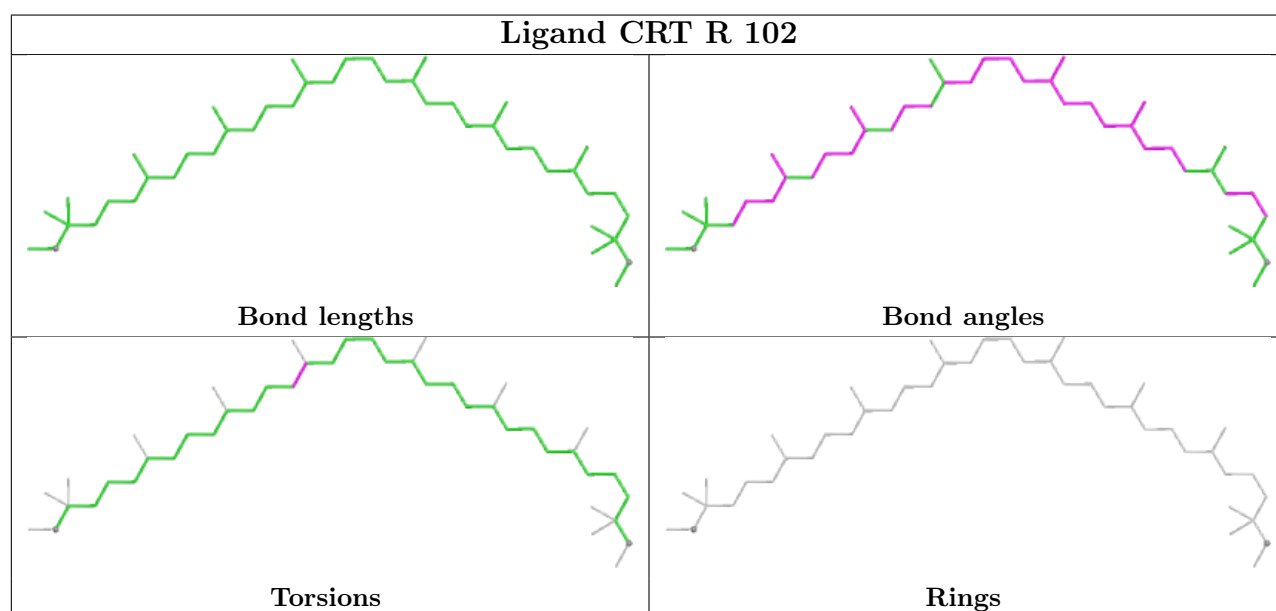
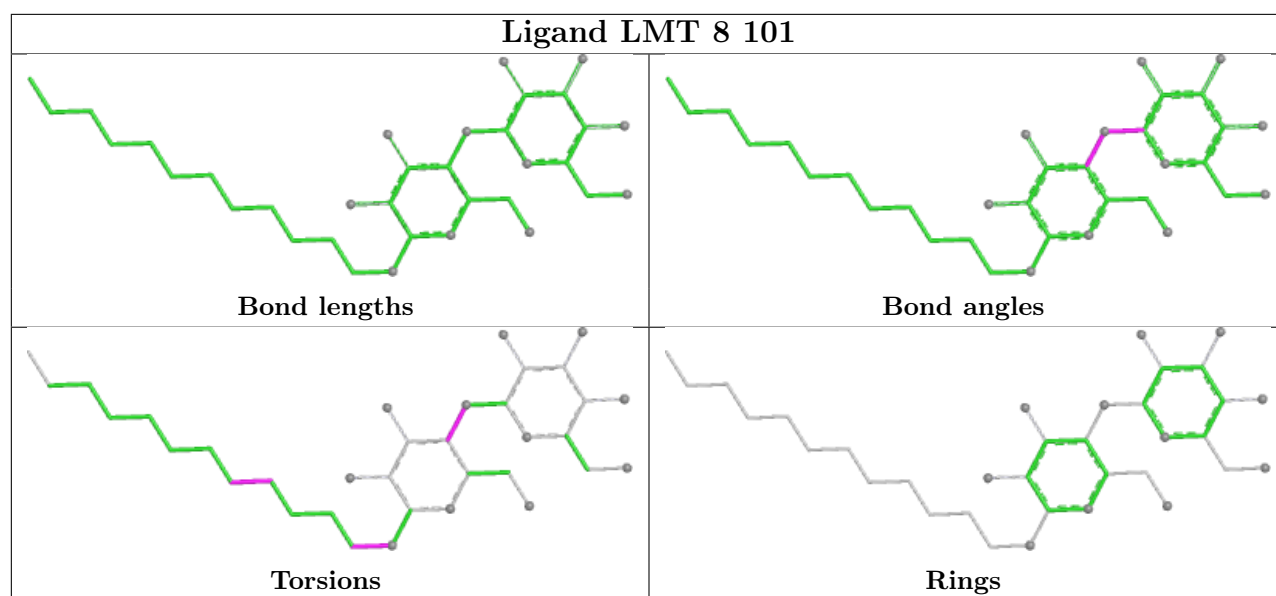


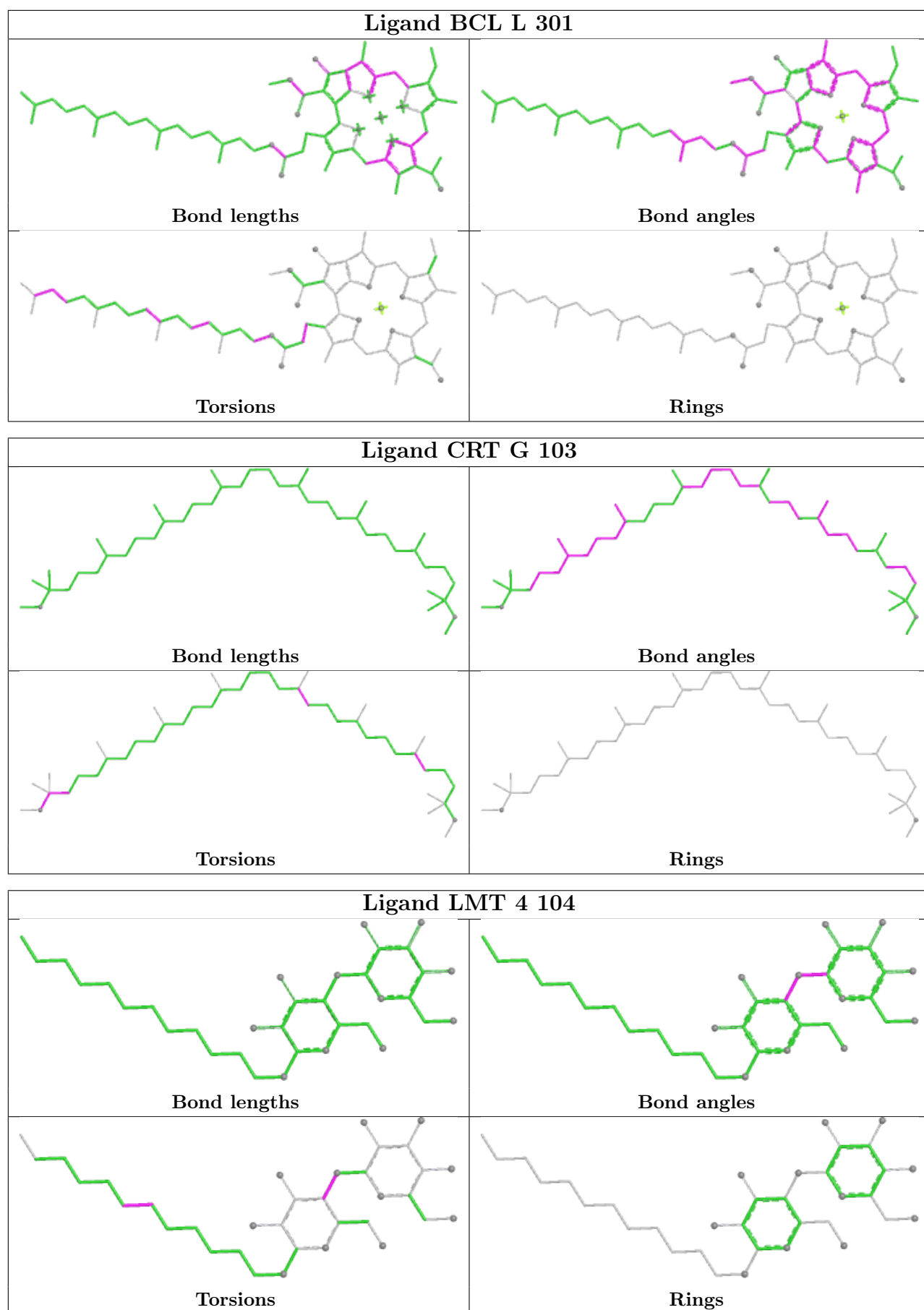


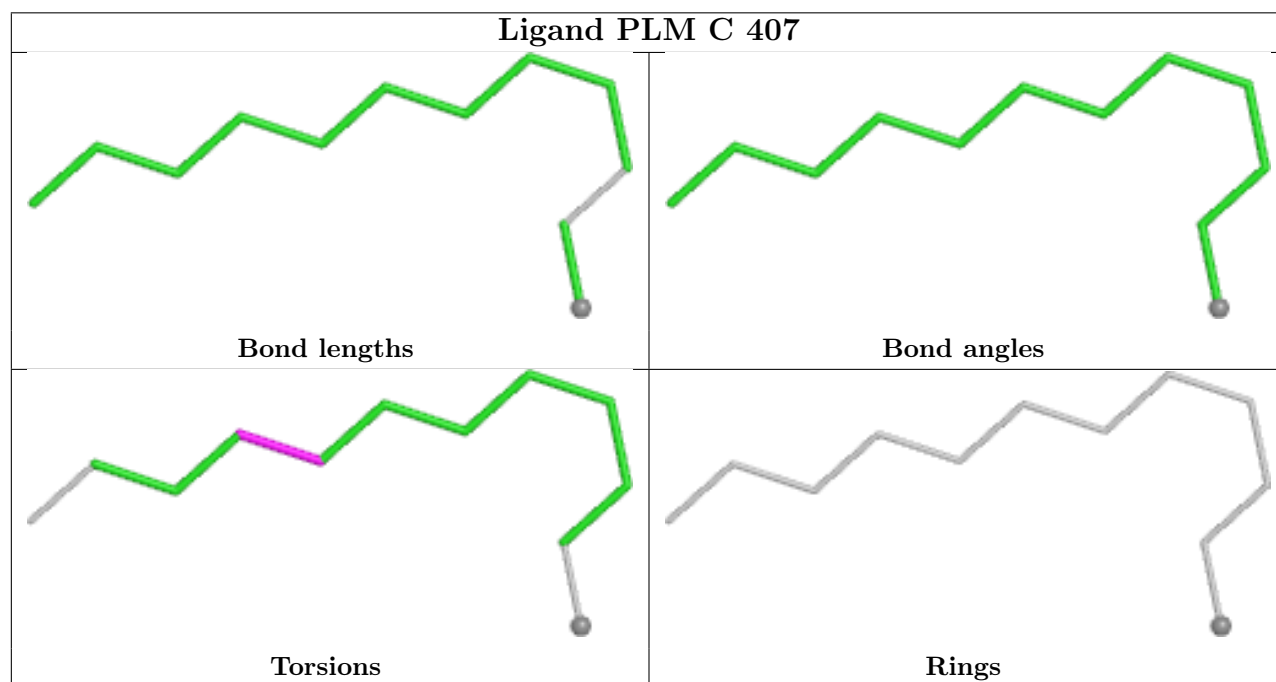
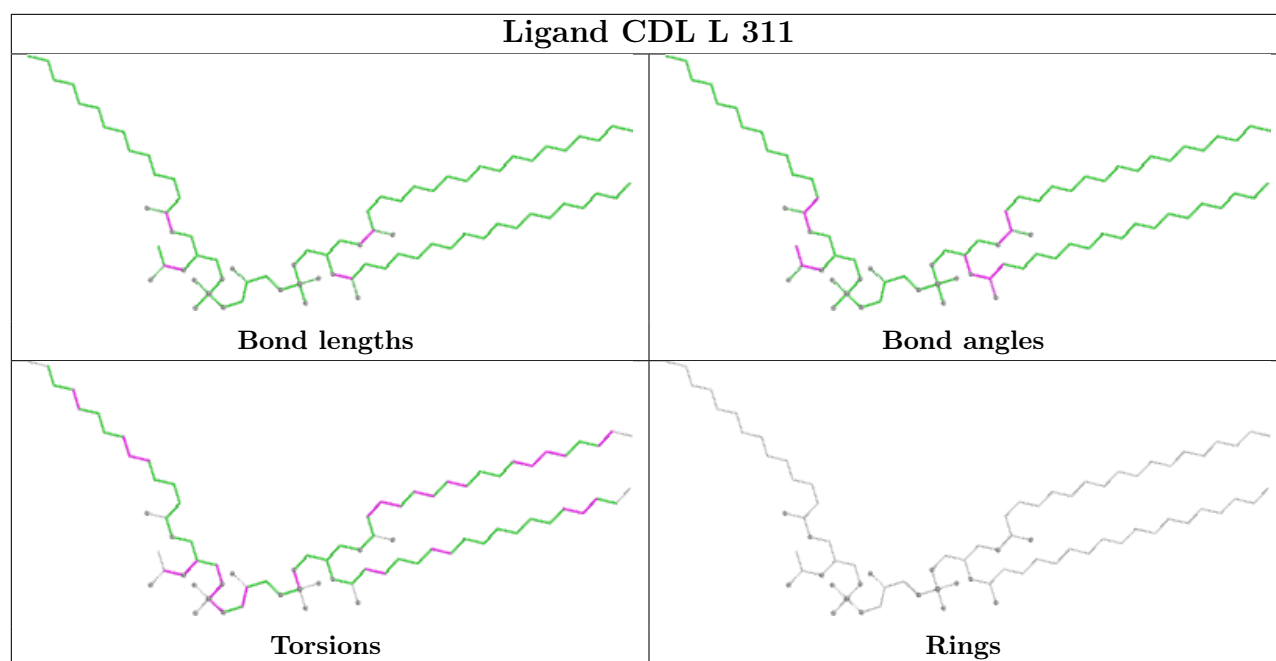


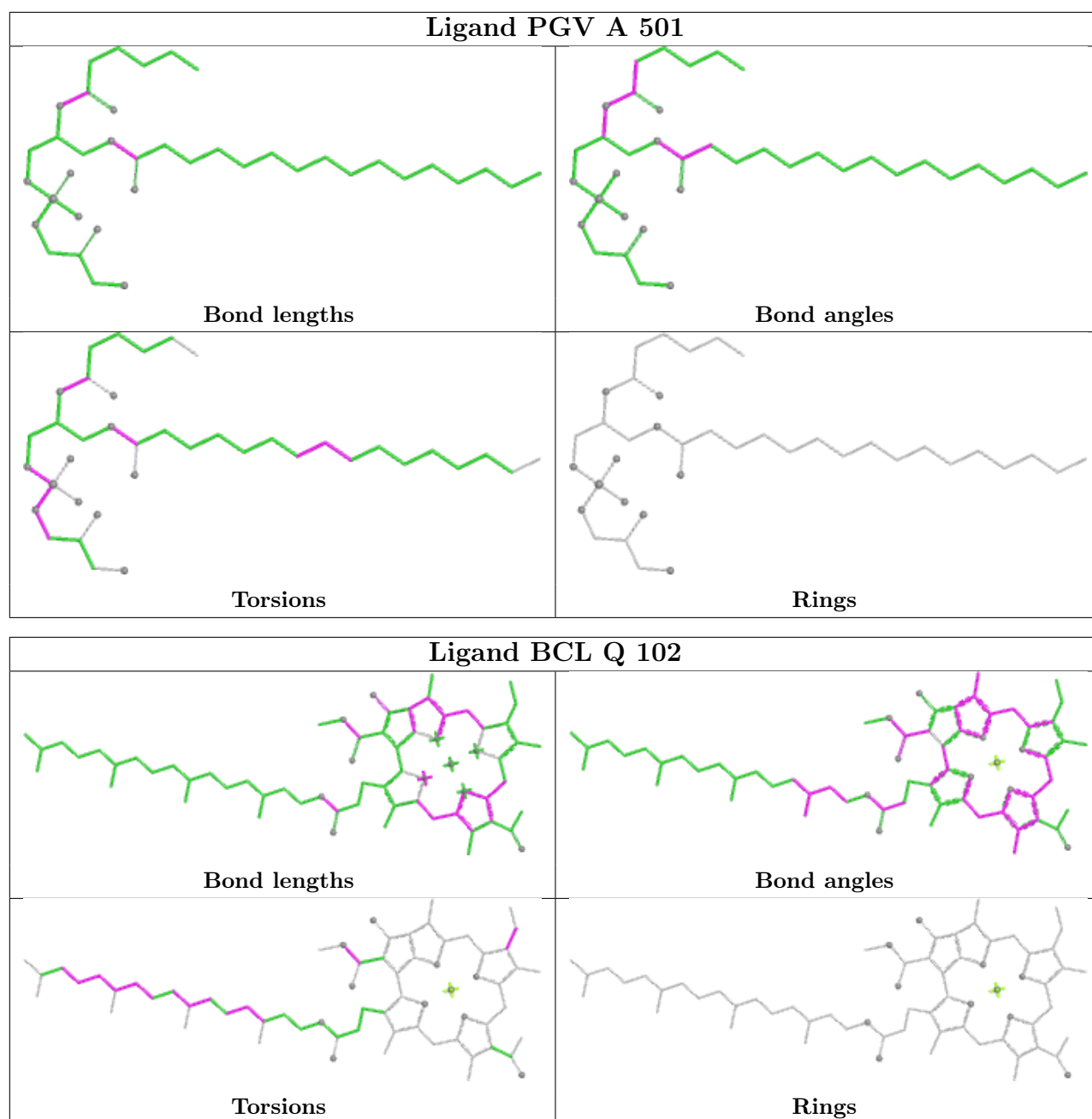


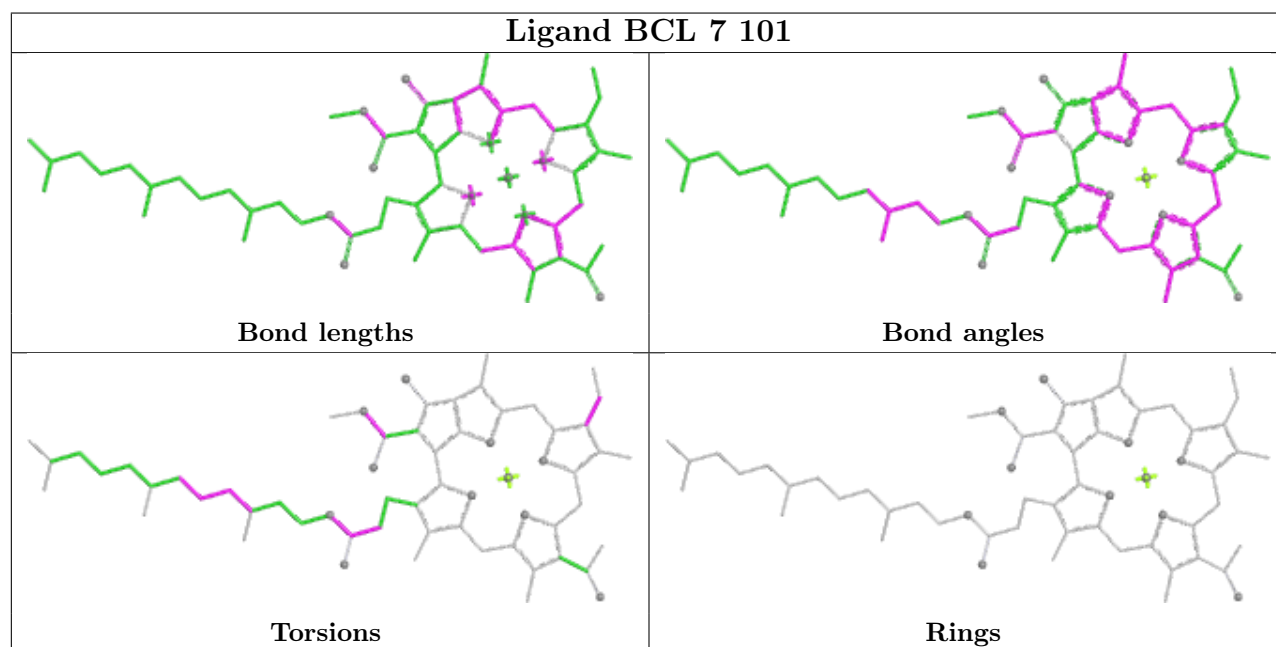
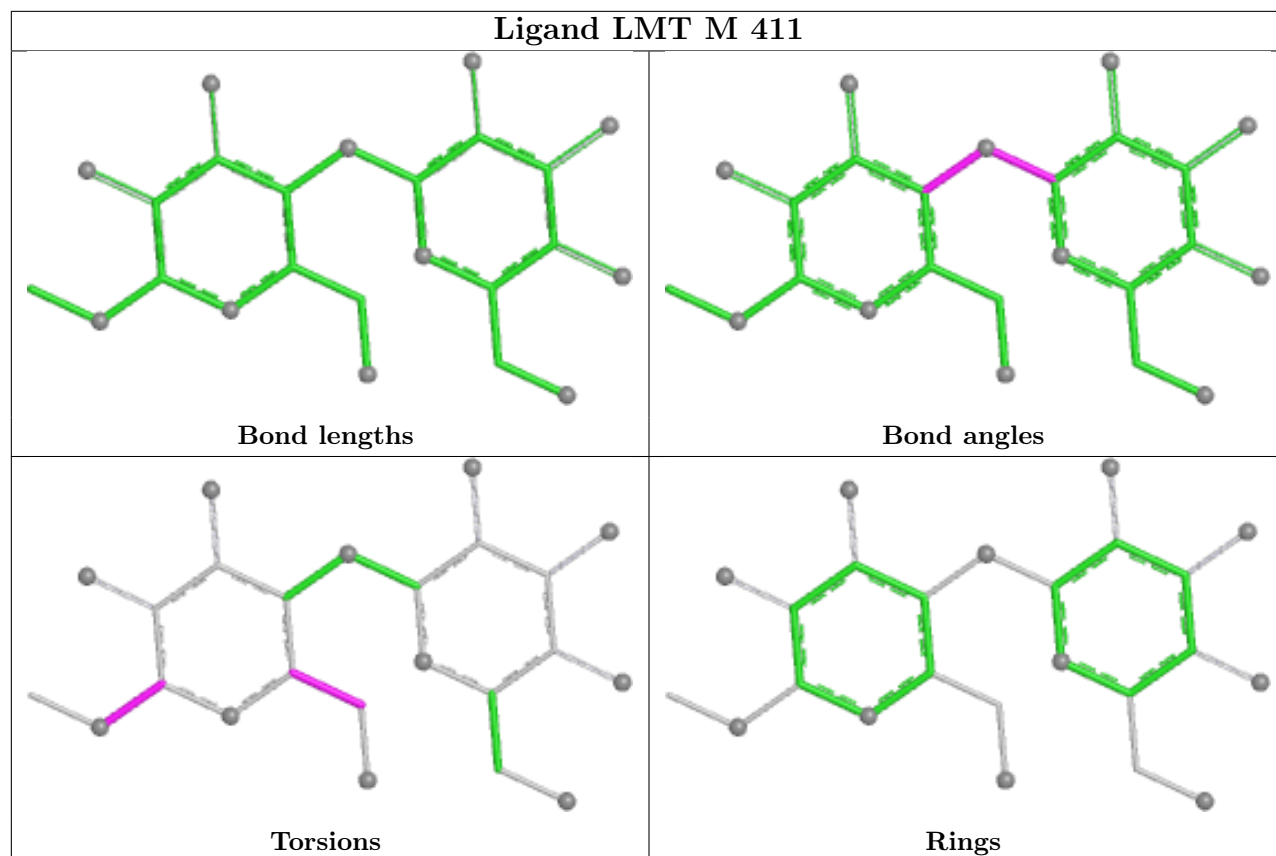


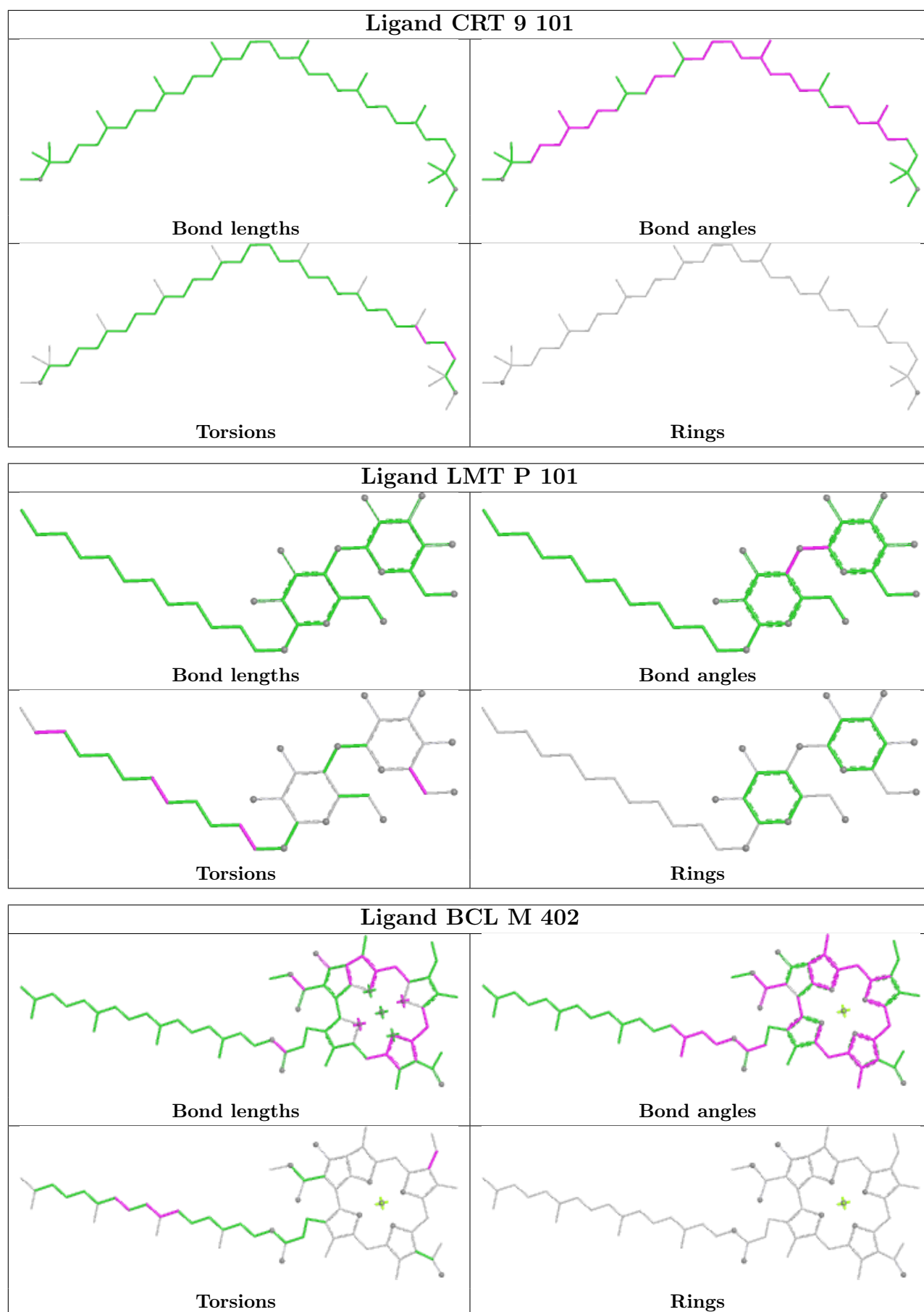


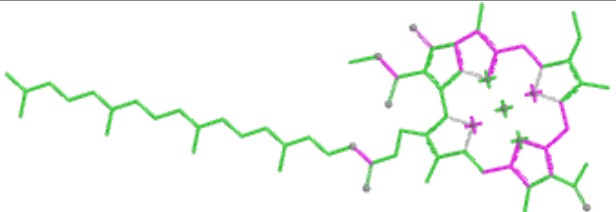
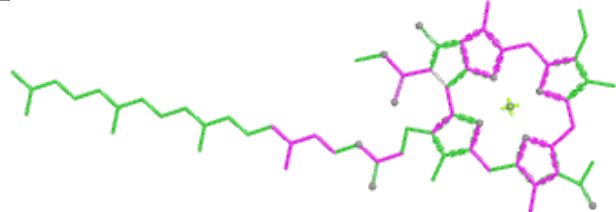
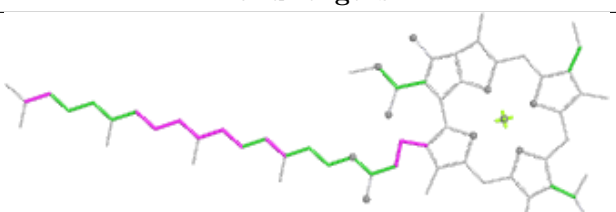
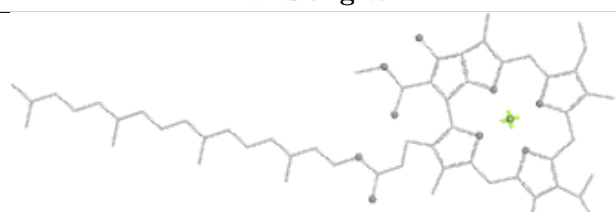


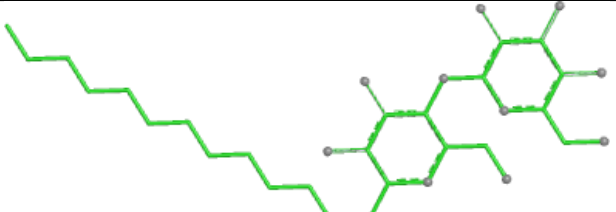
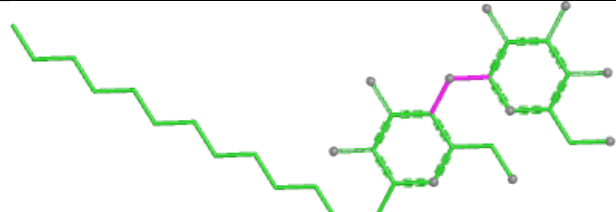
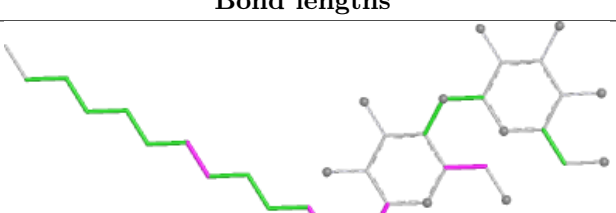
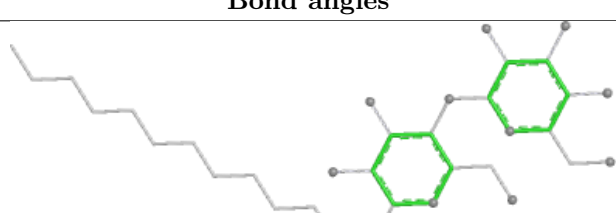


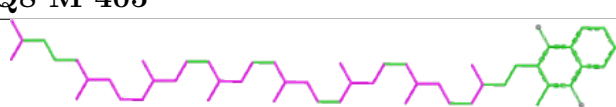
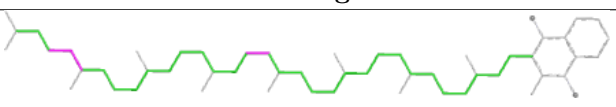
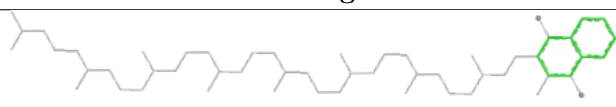


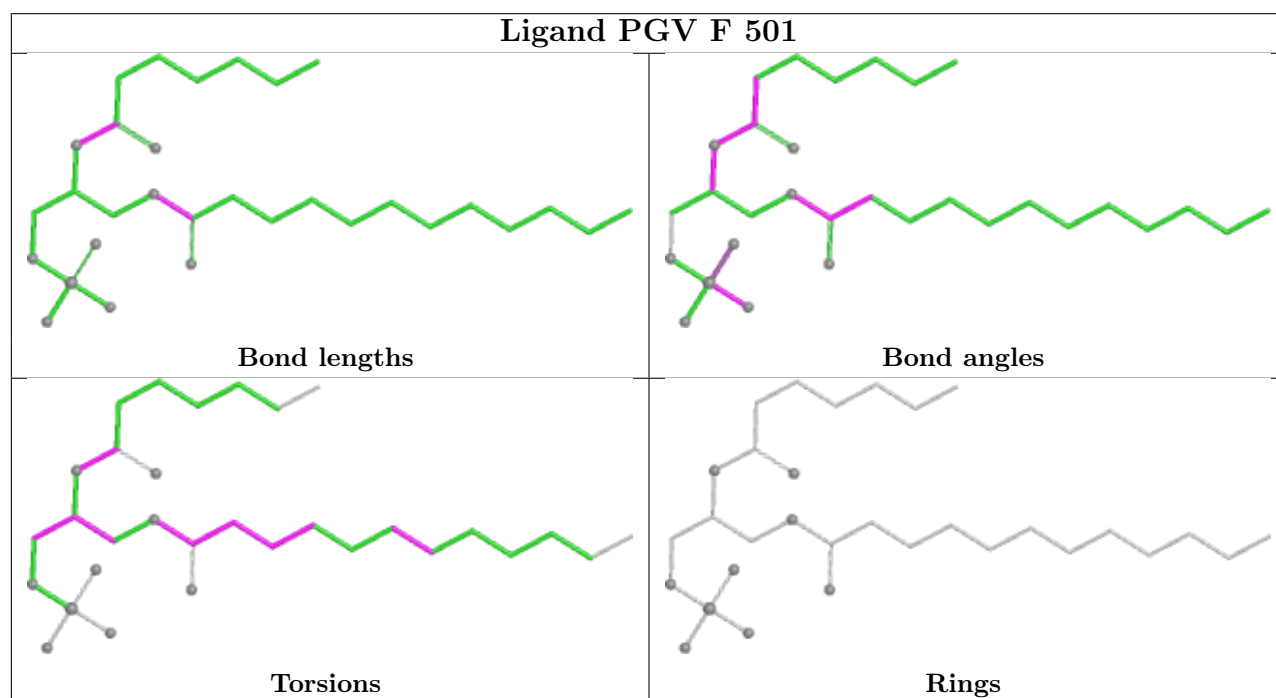
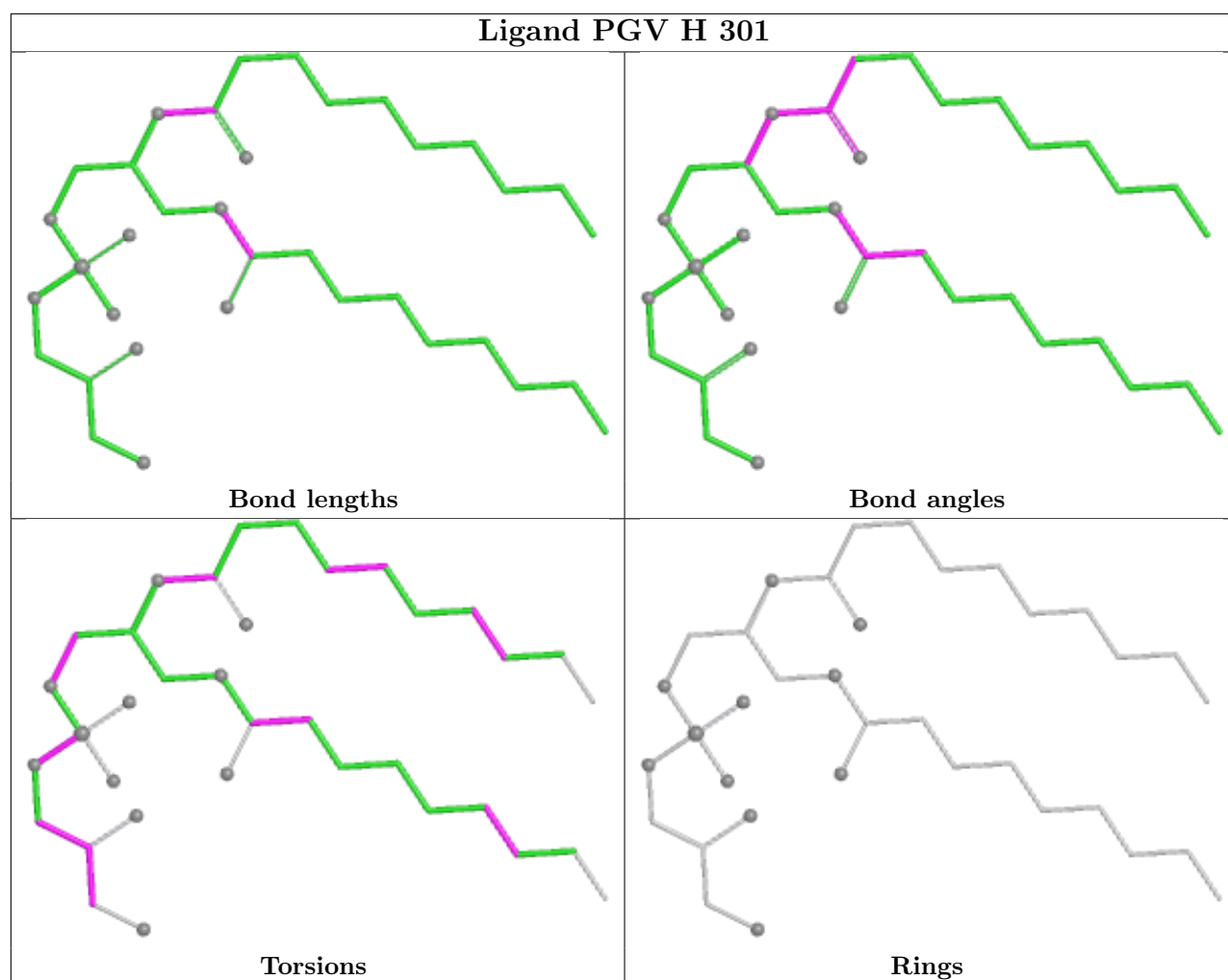


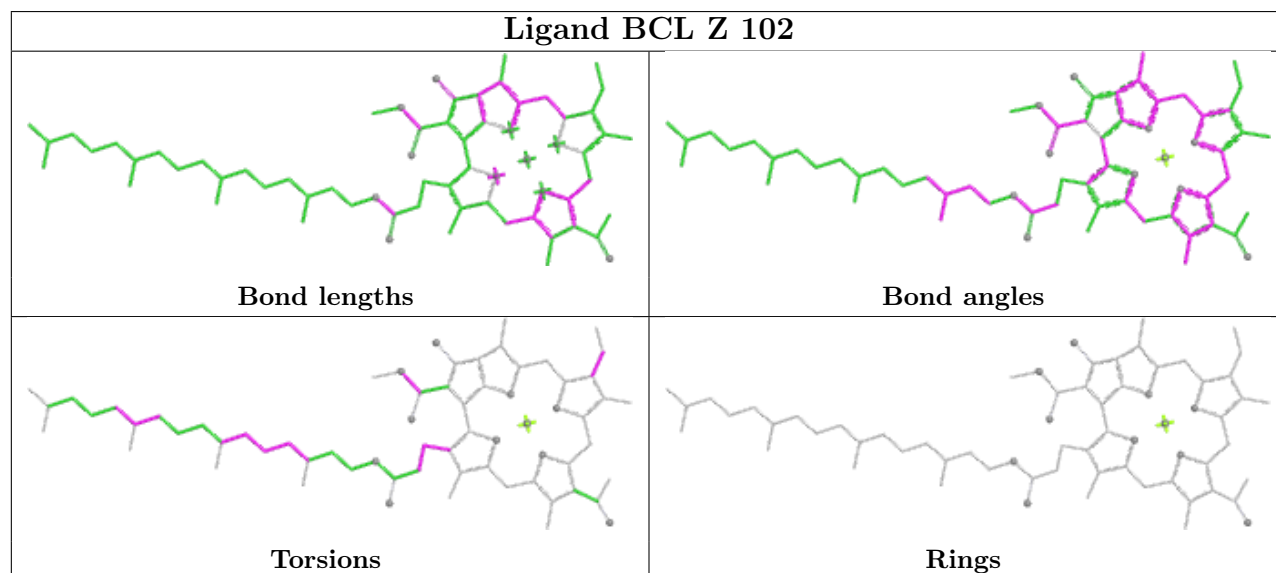
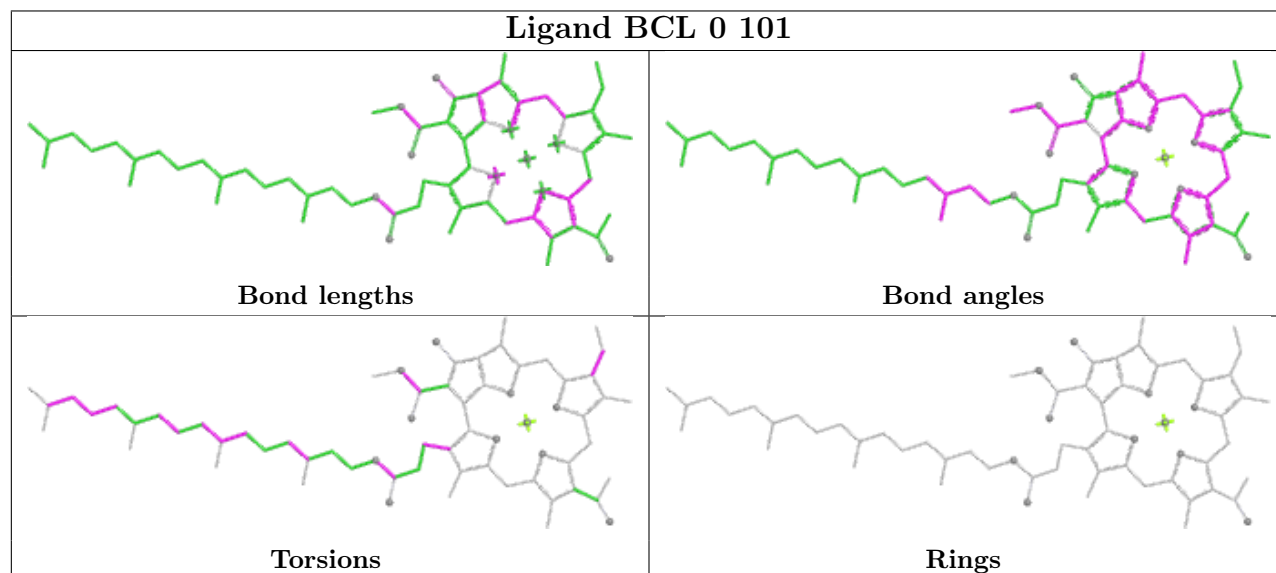
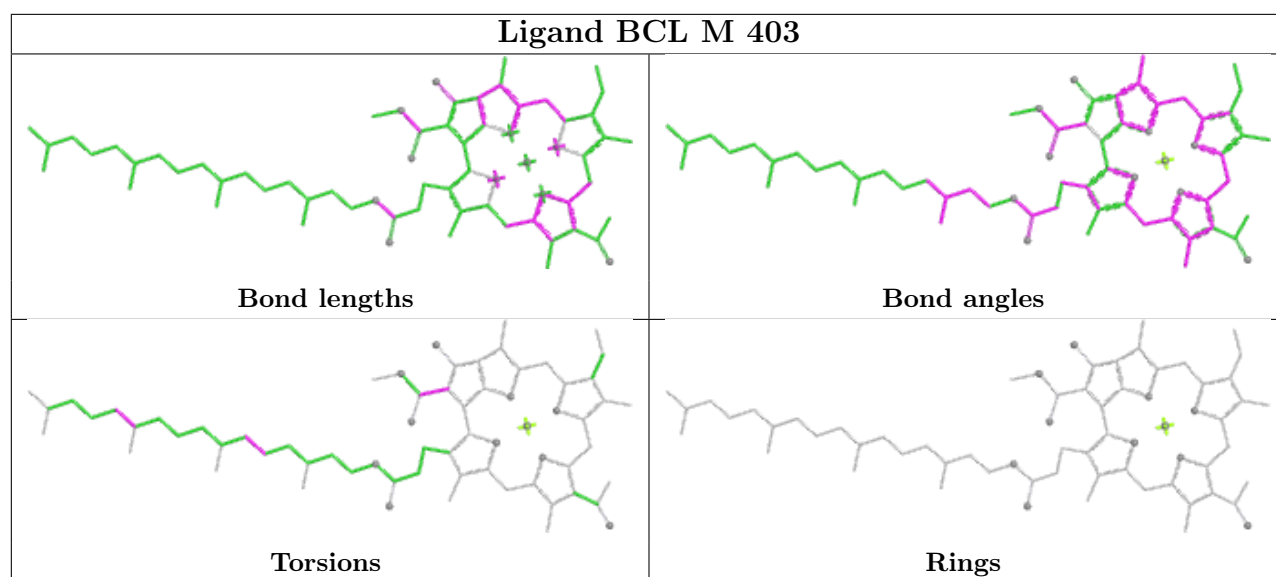


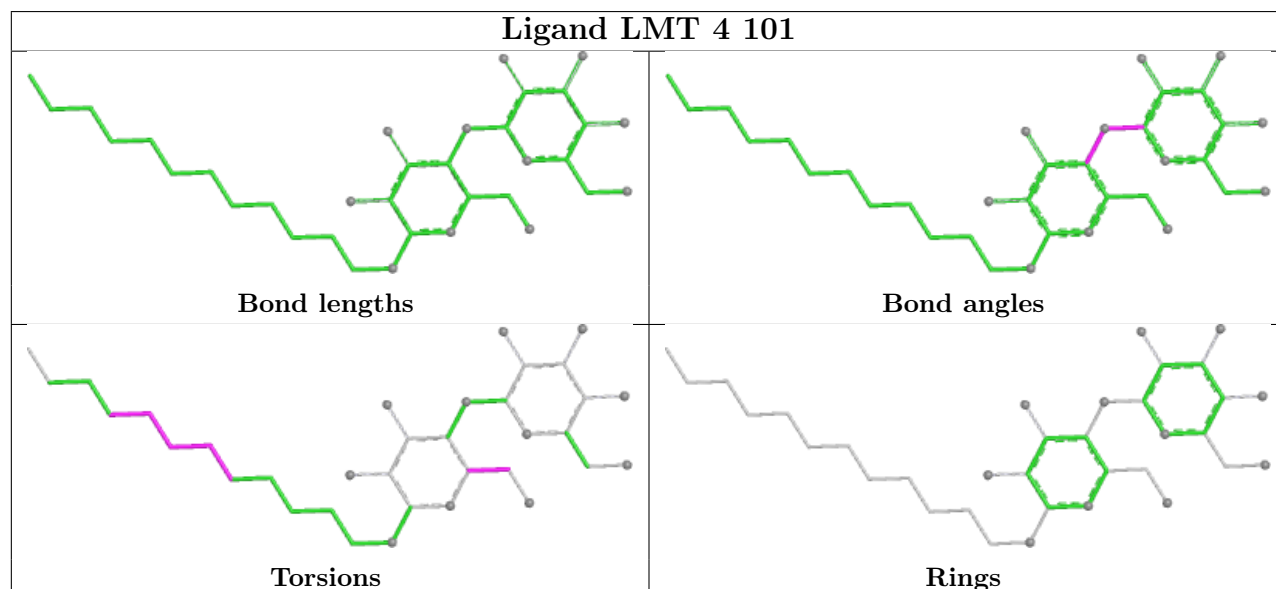
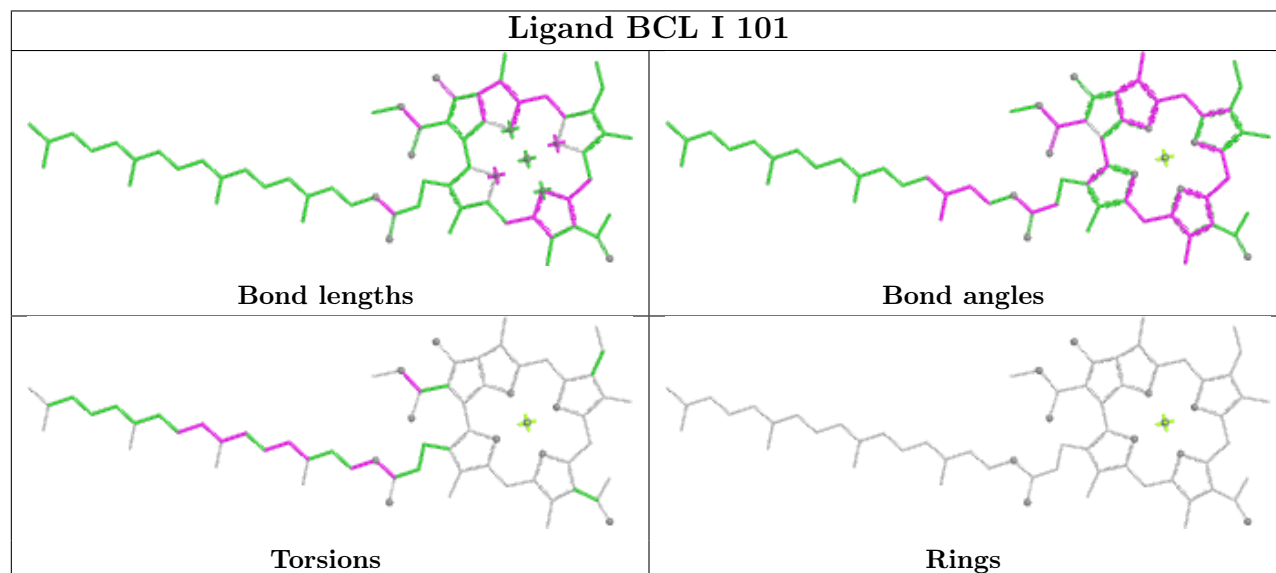
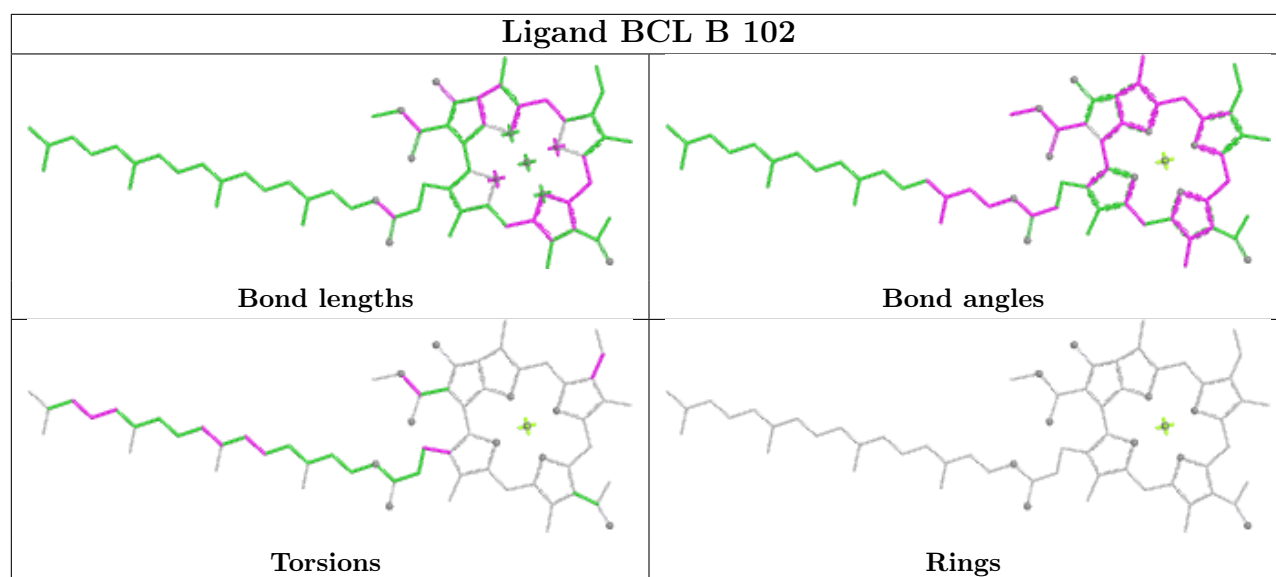
| Ligand BCL Y 102                                                                  |                                                                                    |
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|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

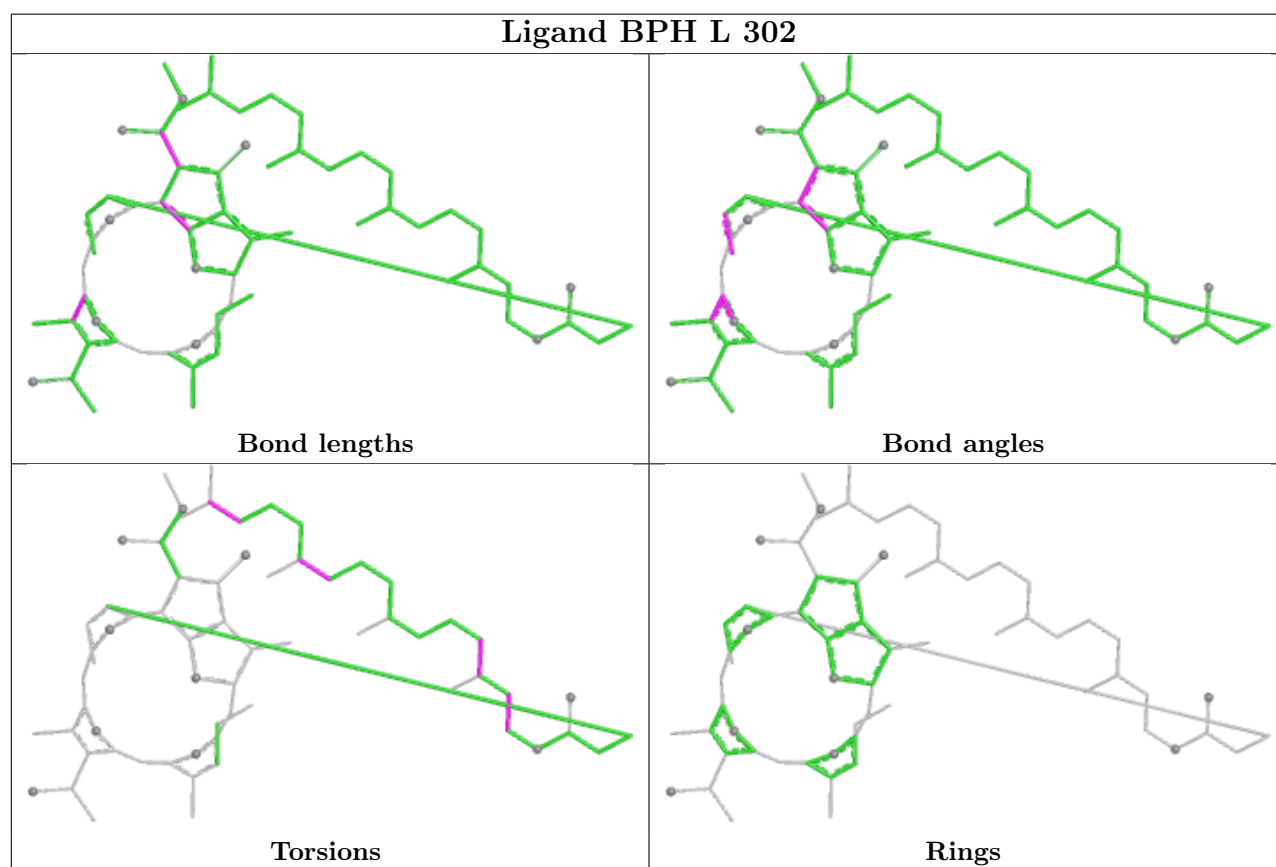
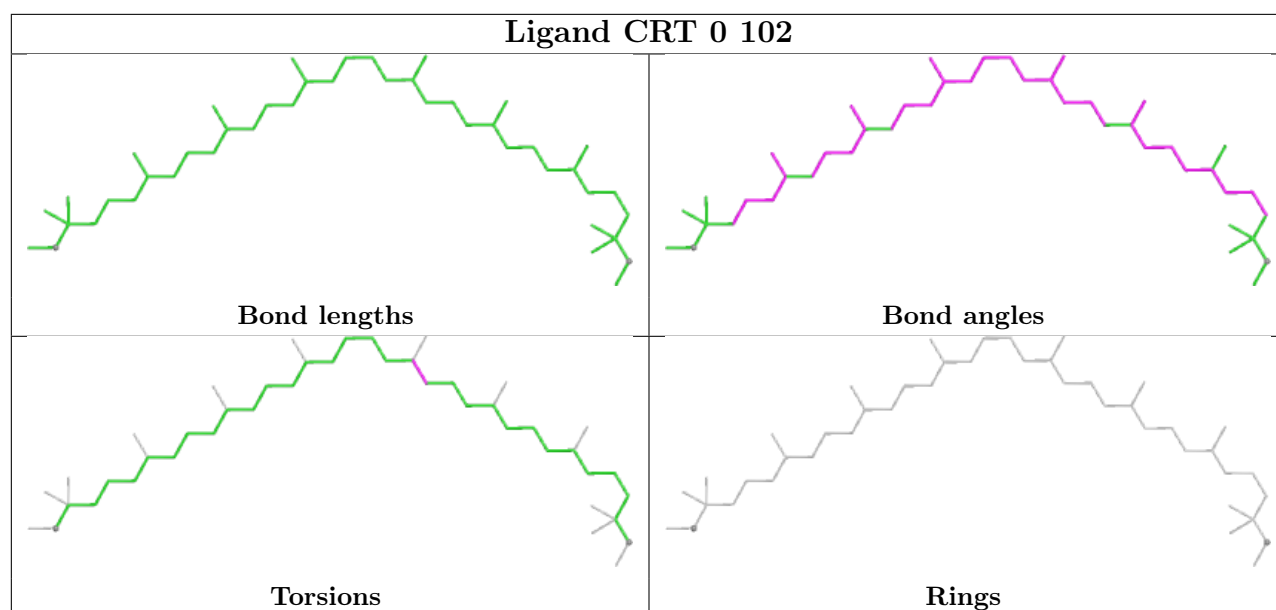
| Ligand LMT J 104                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

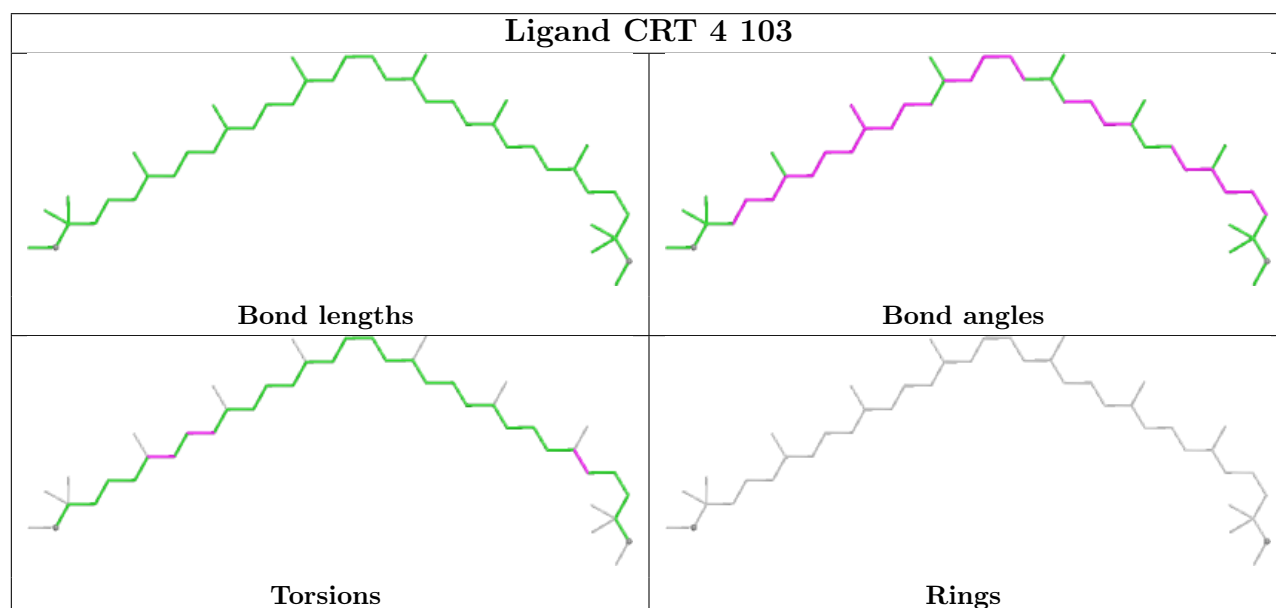
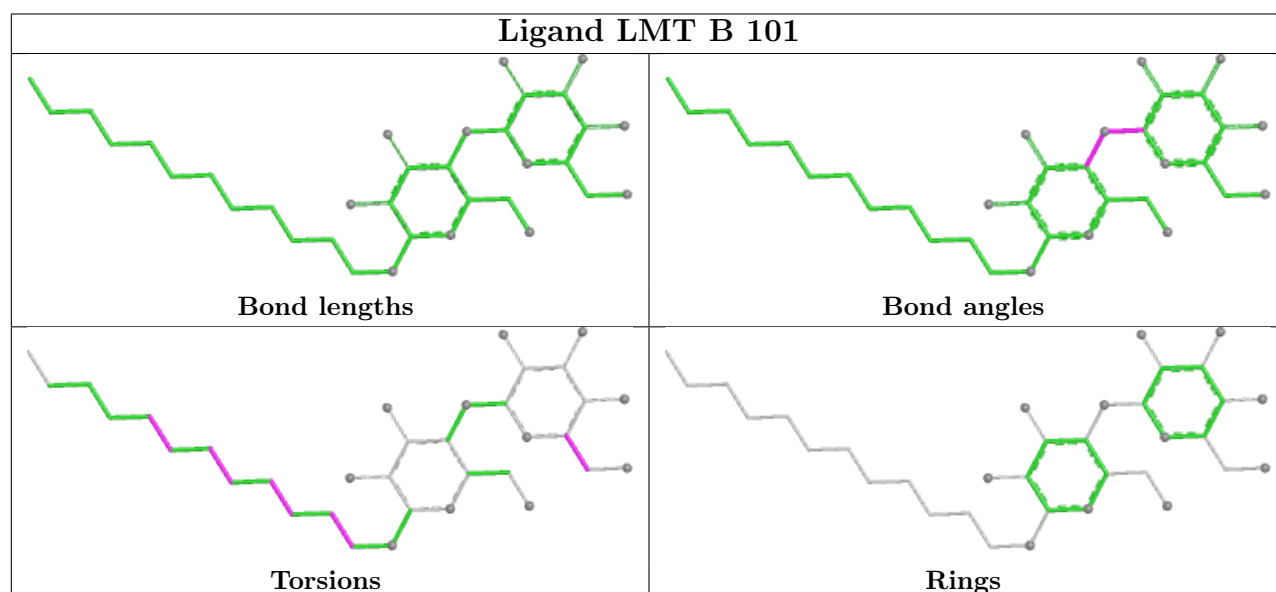
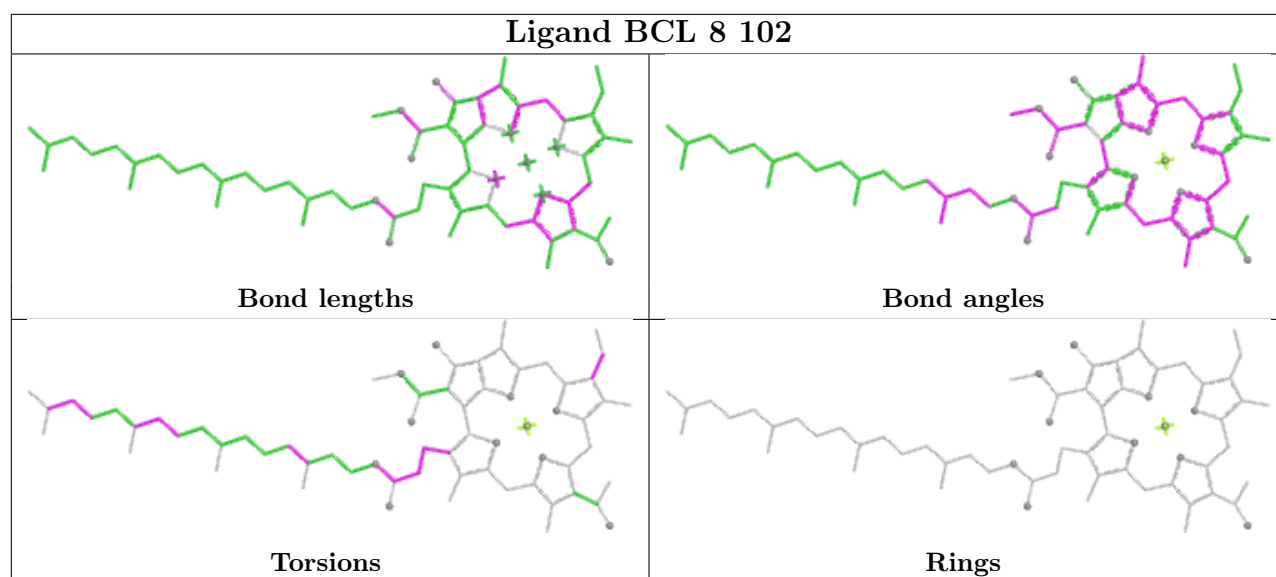
| Ligand MQ8 M 405                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

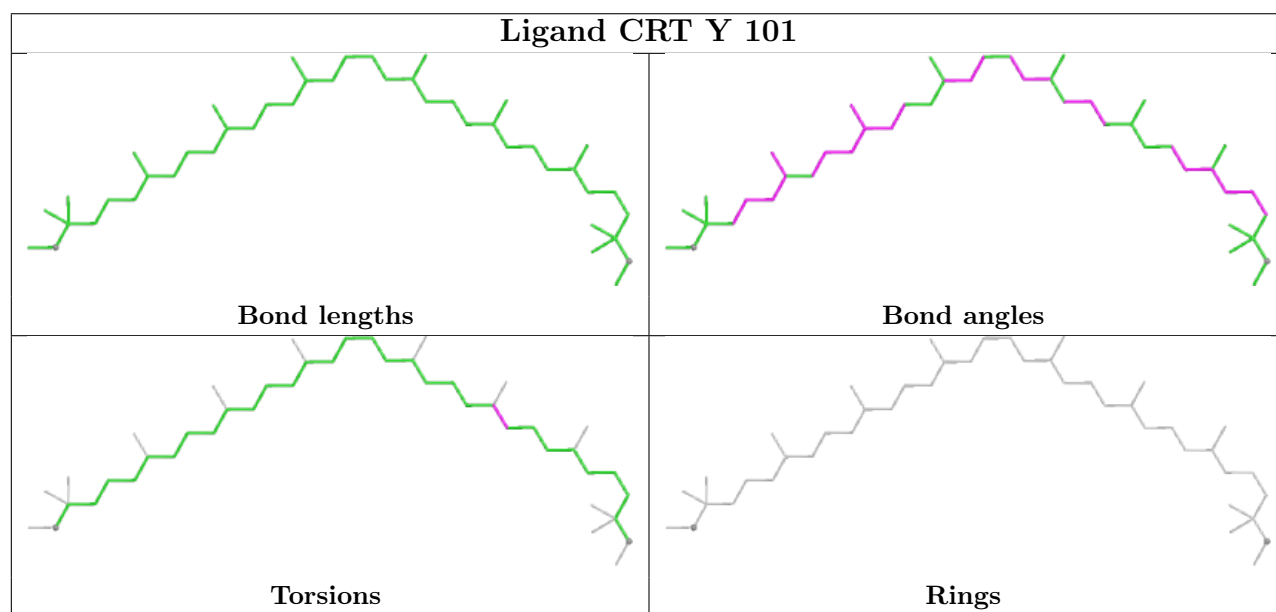
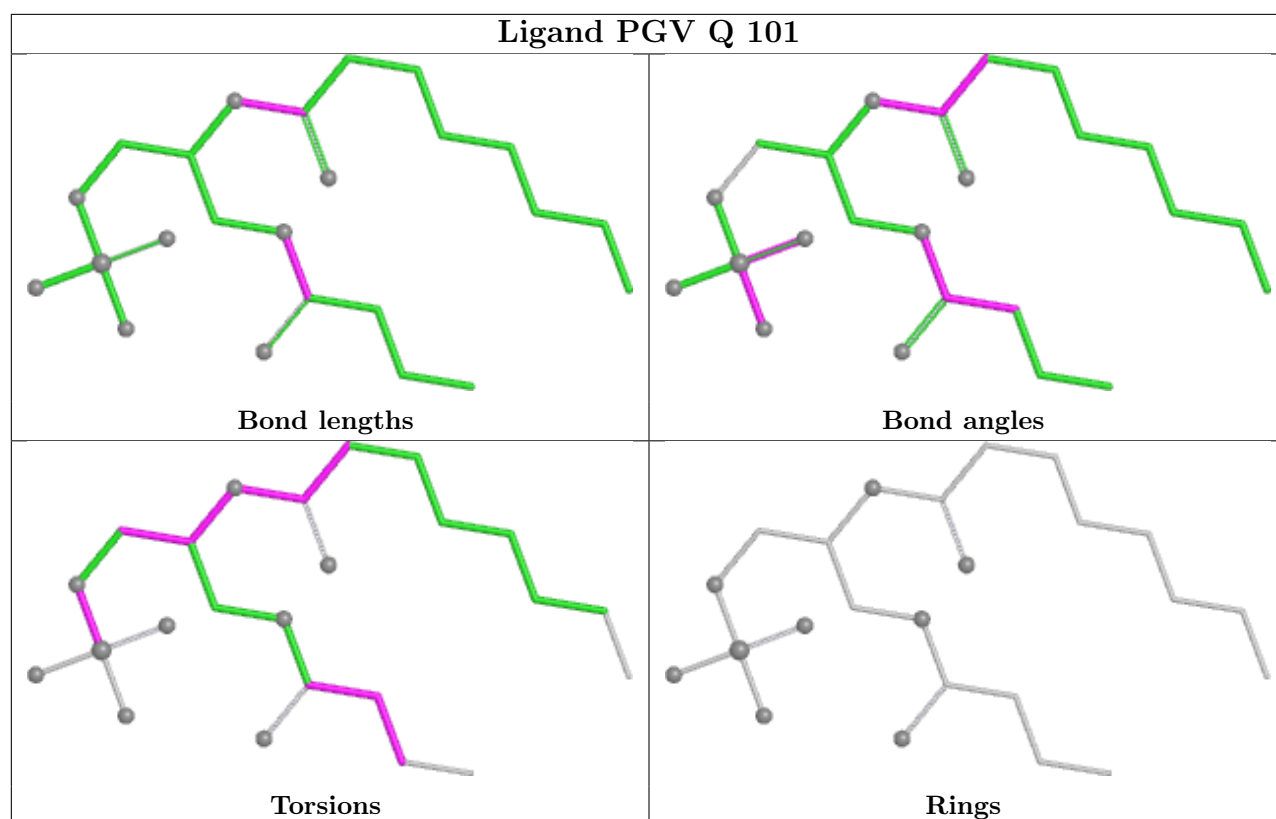


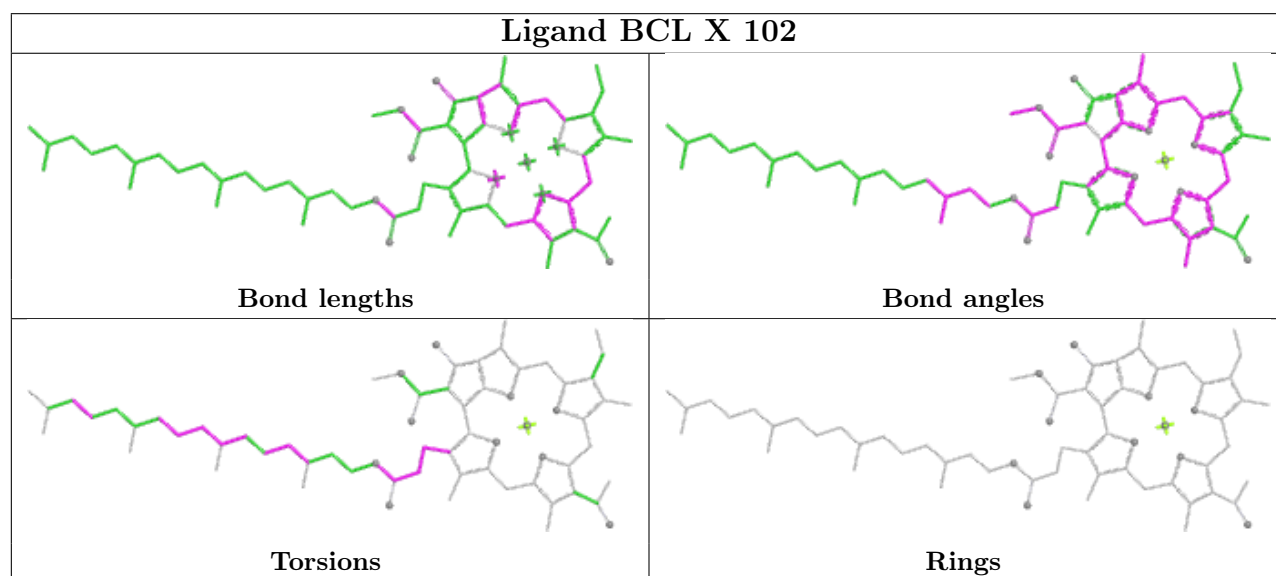
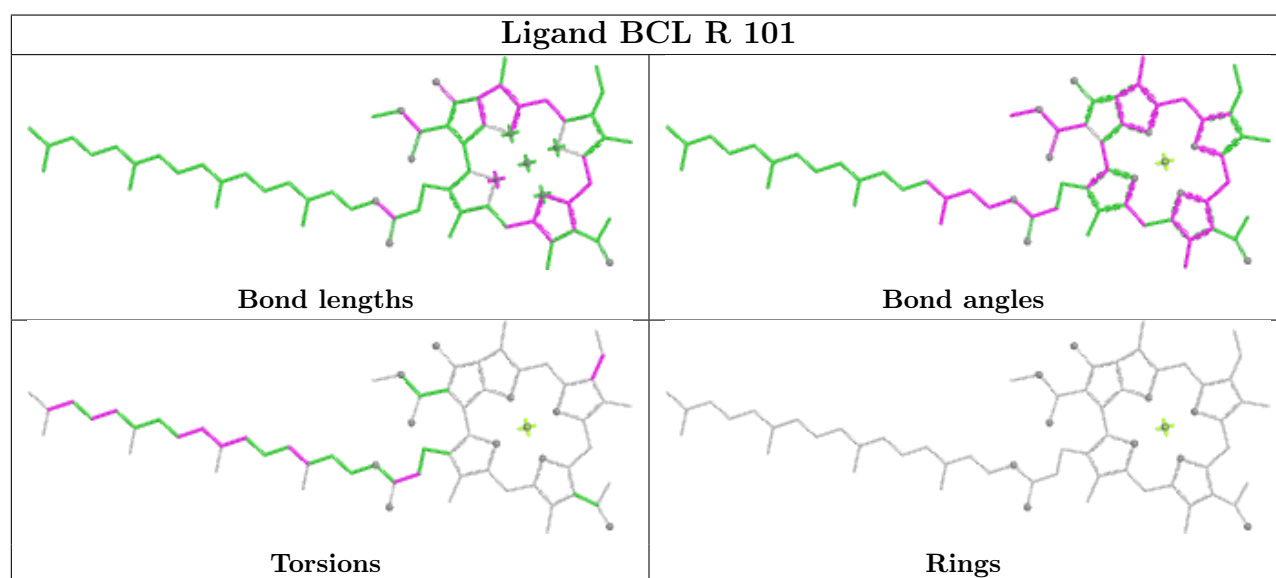
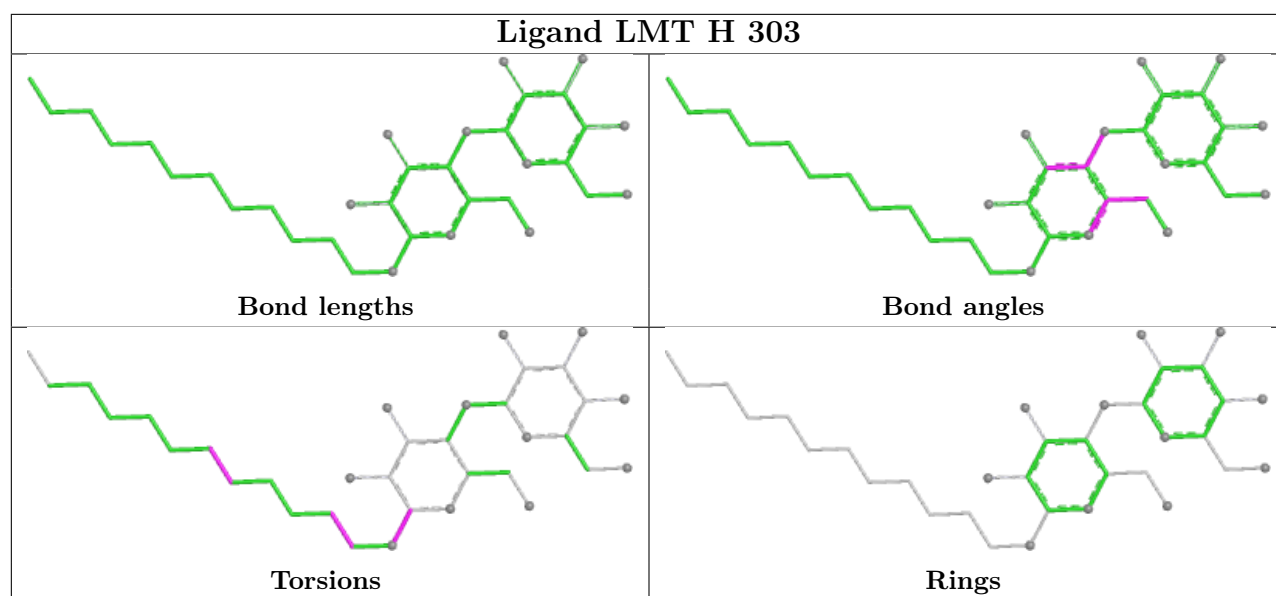


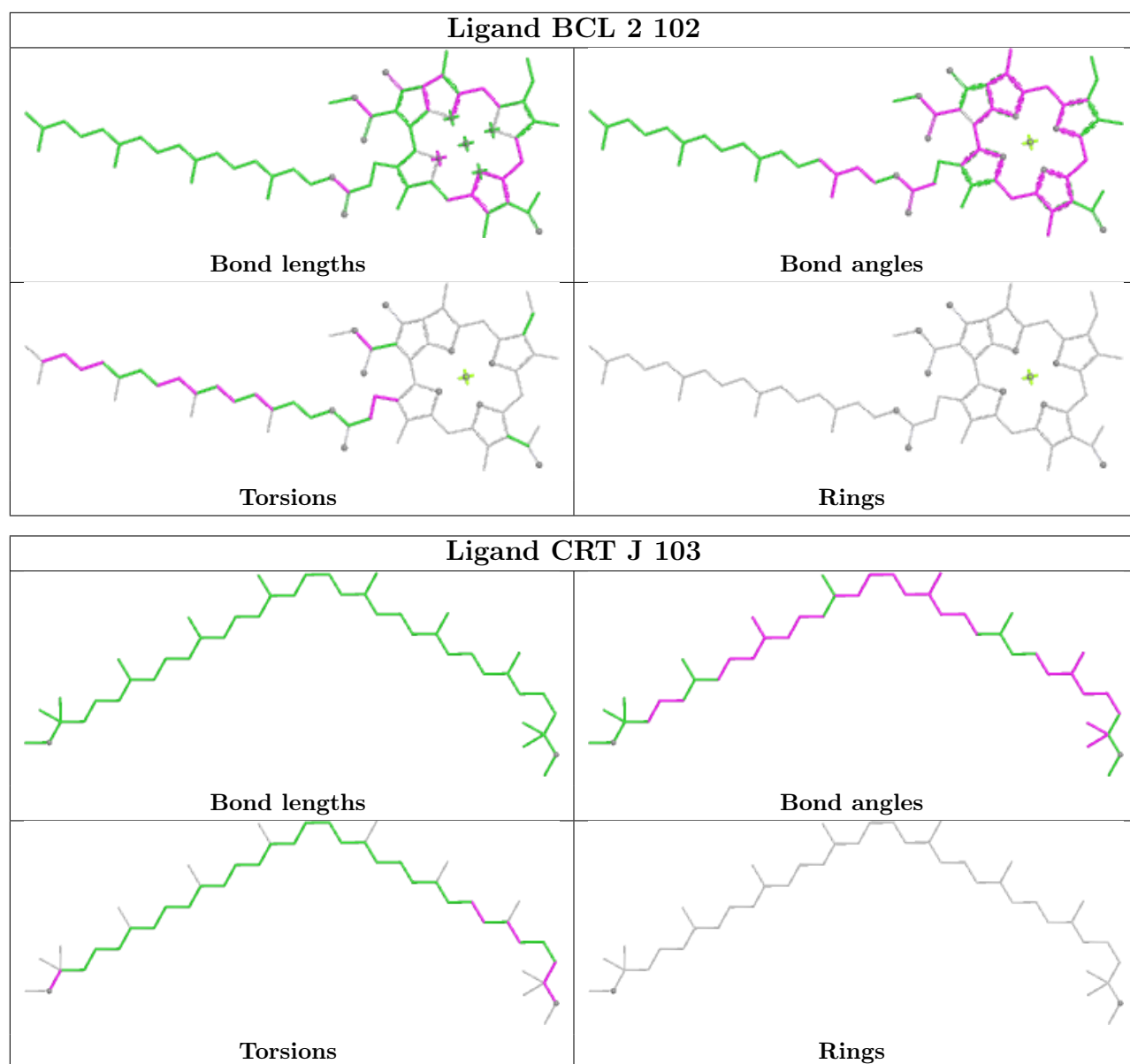


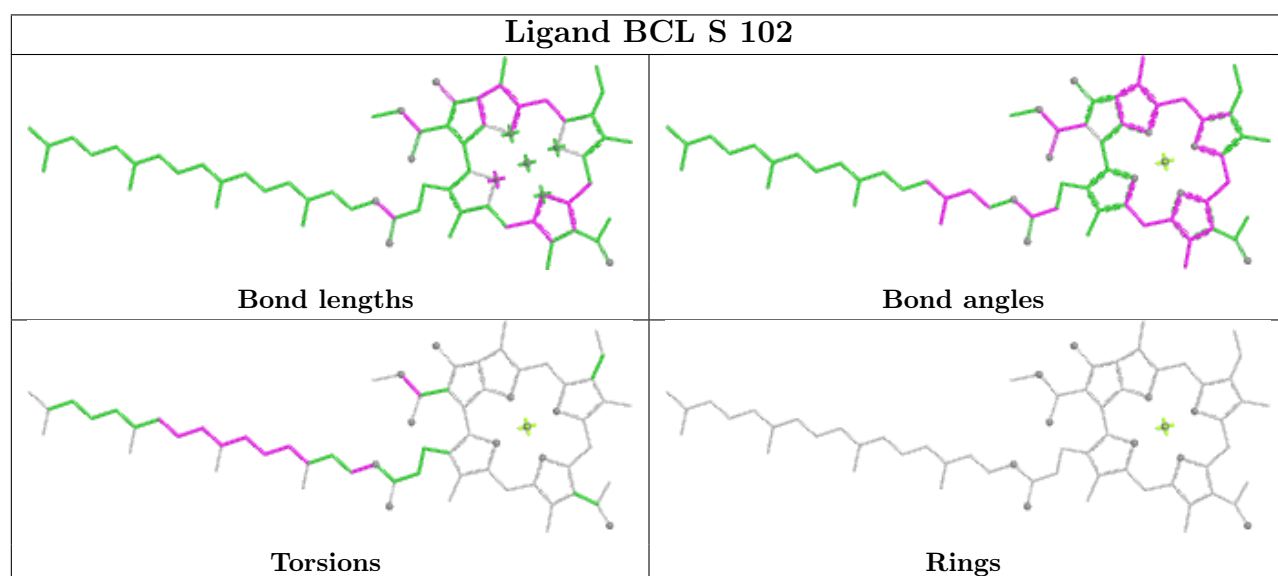
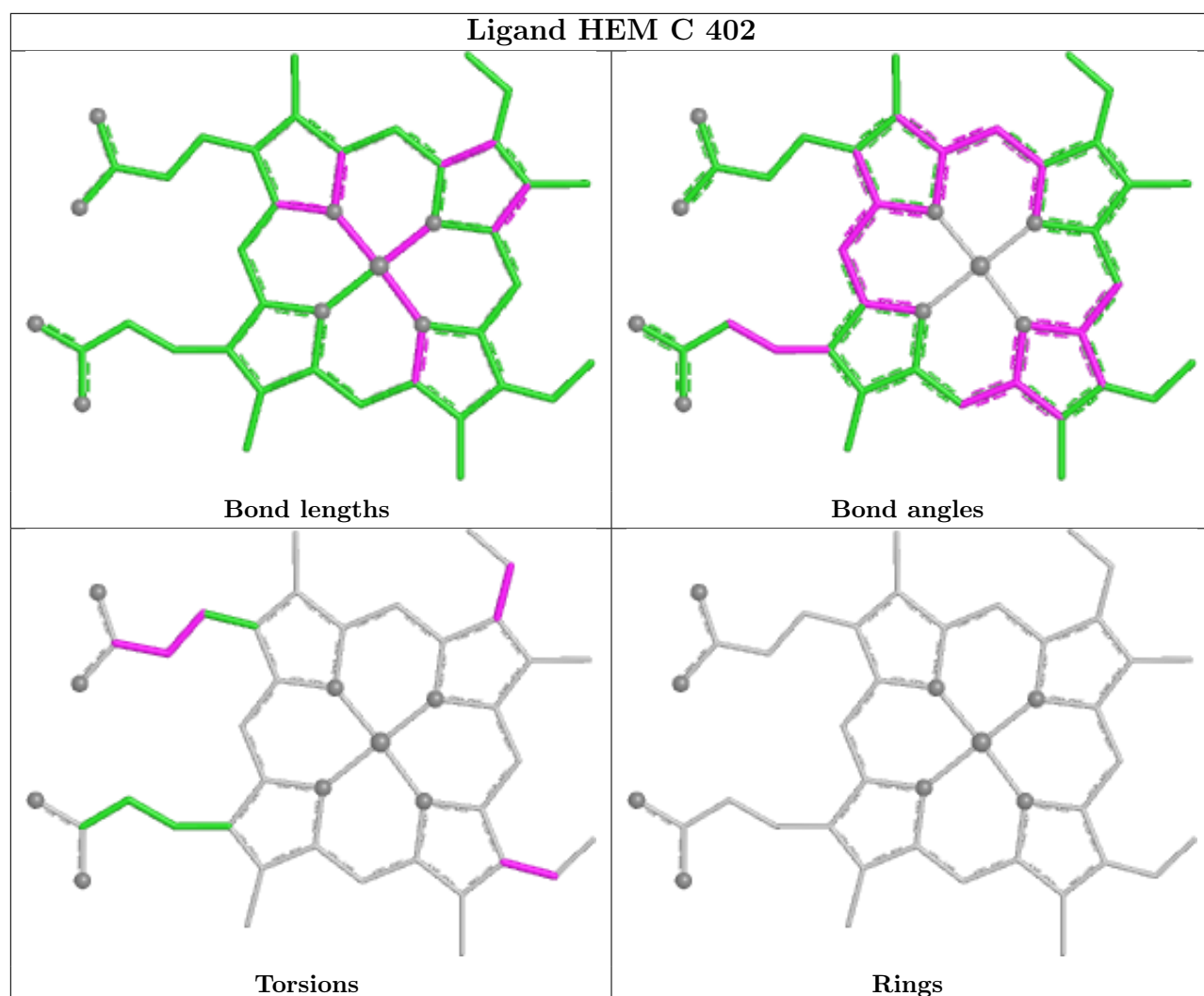


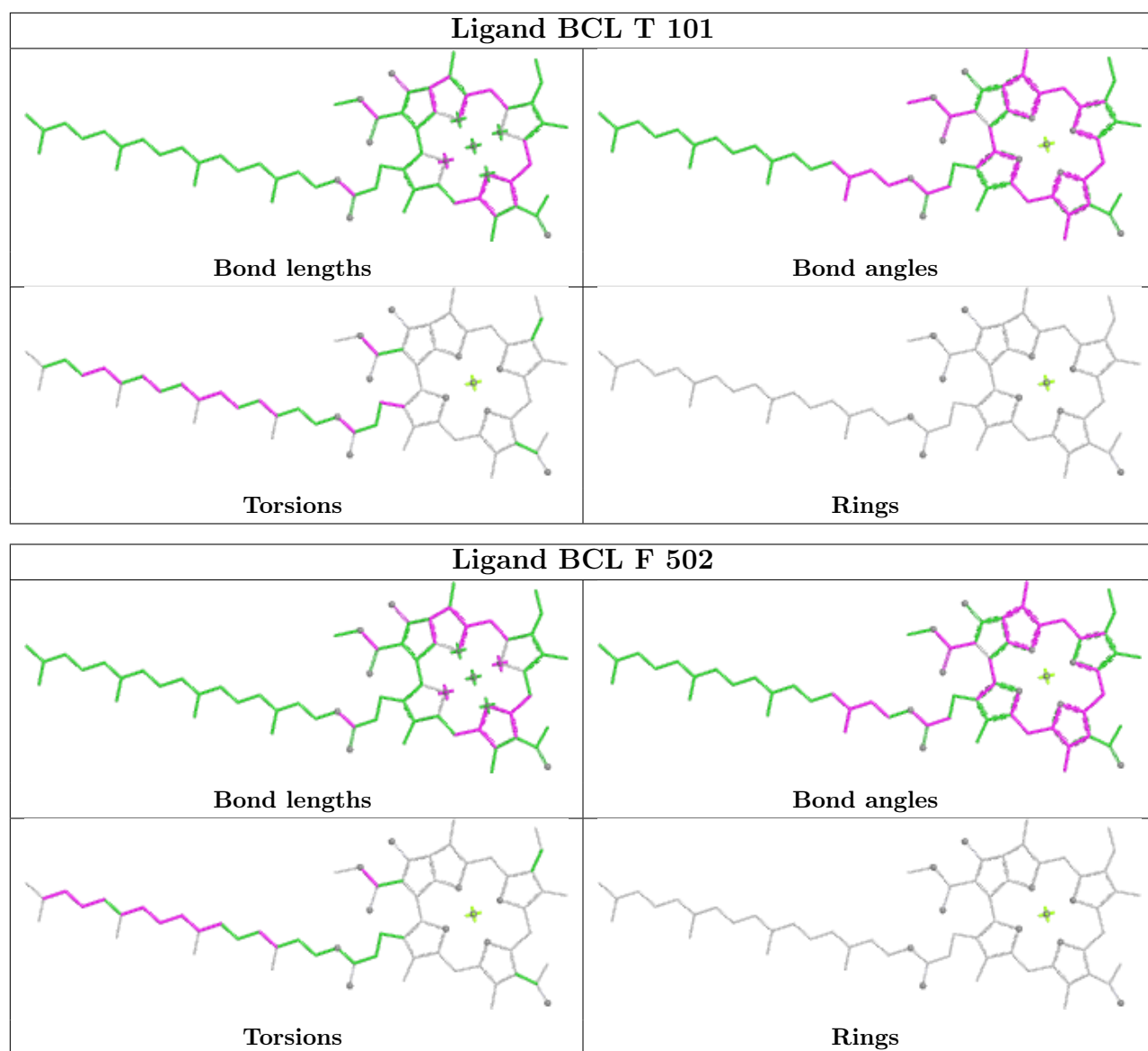


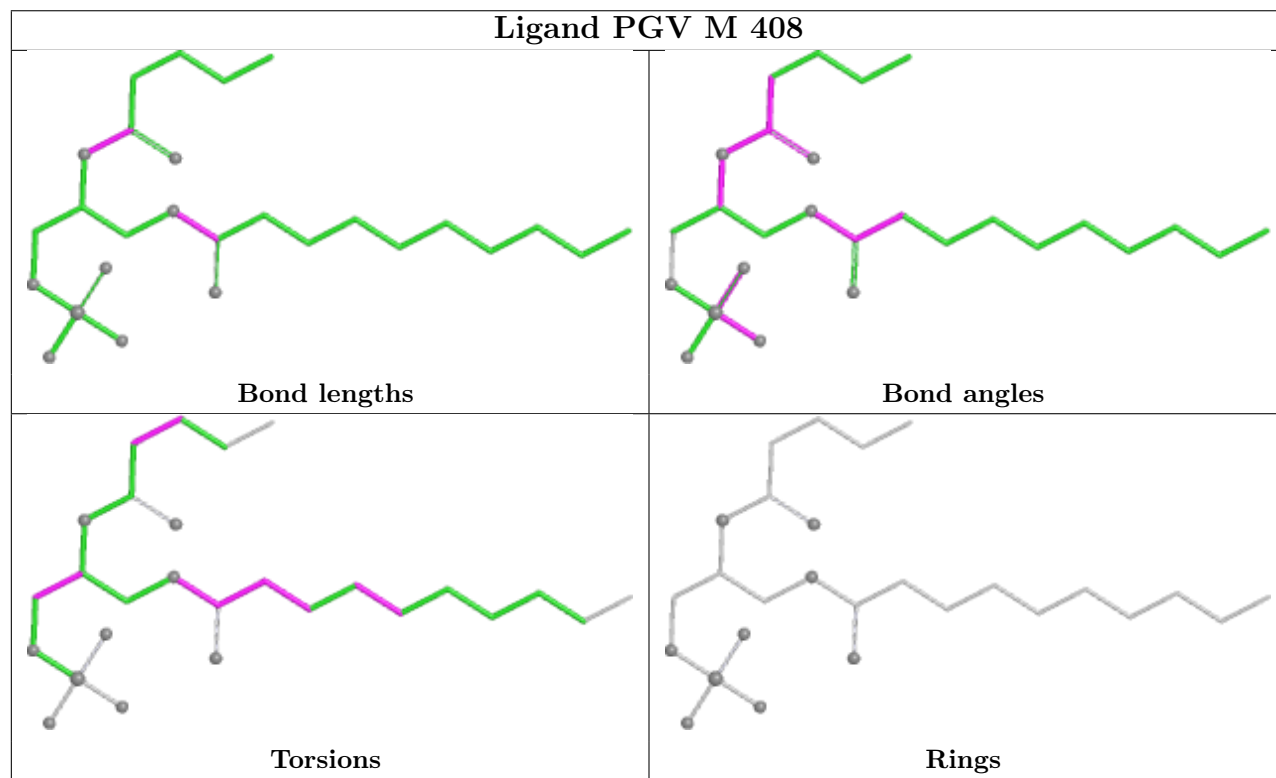
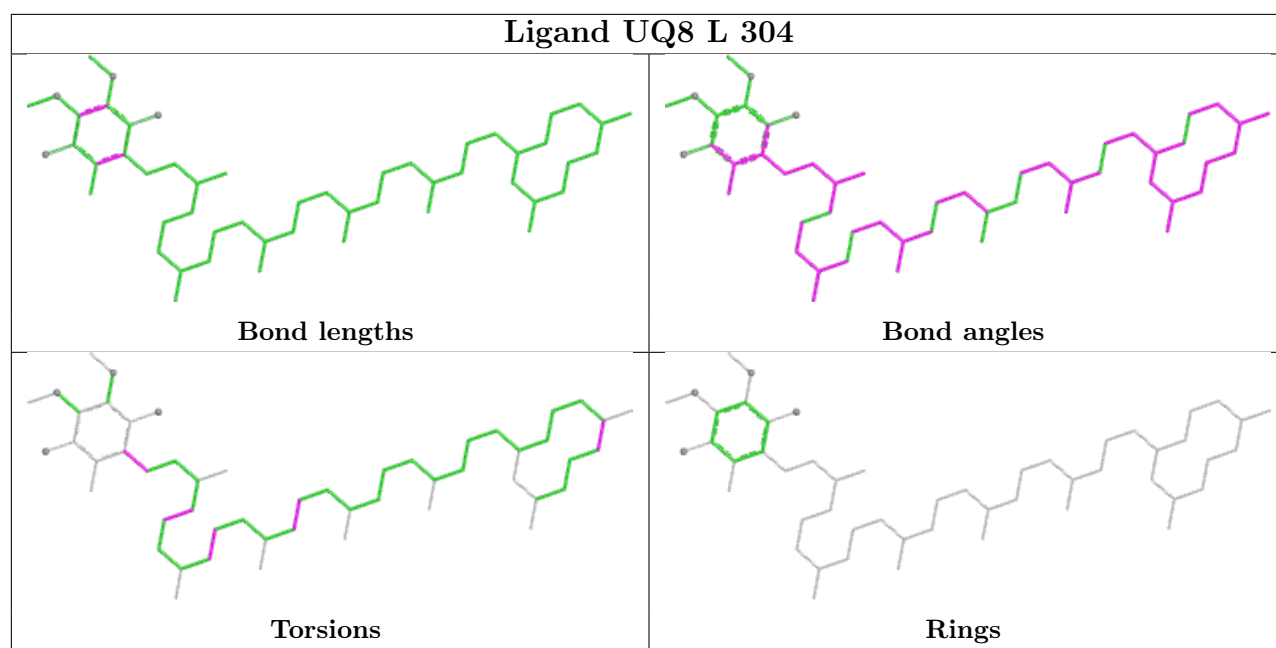


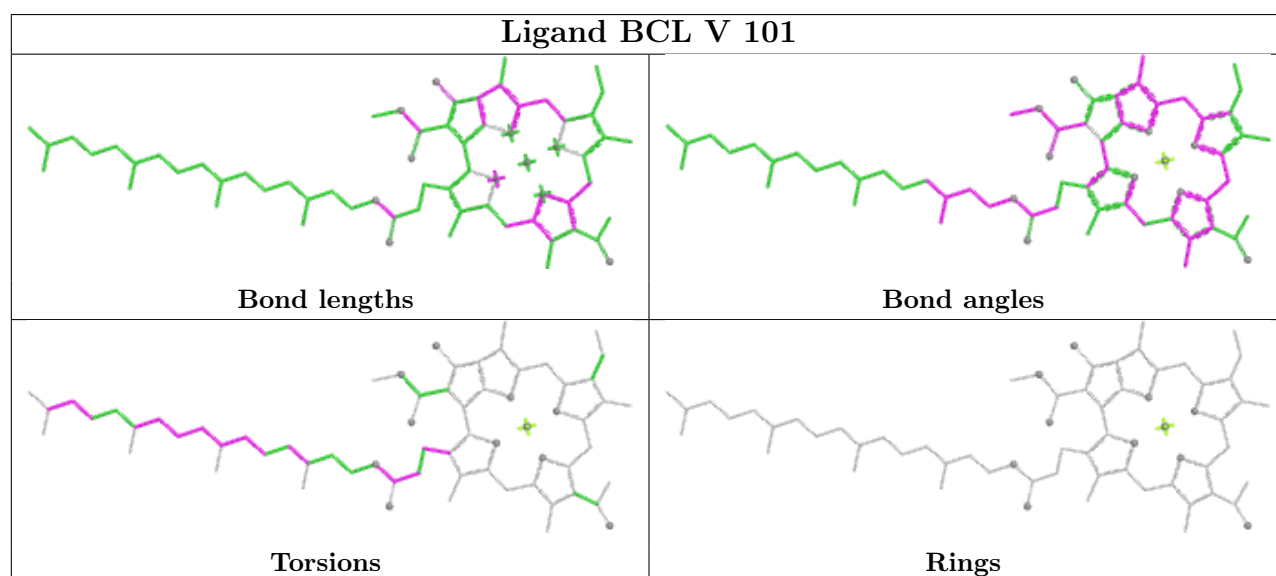
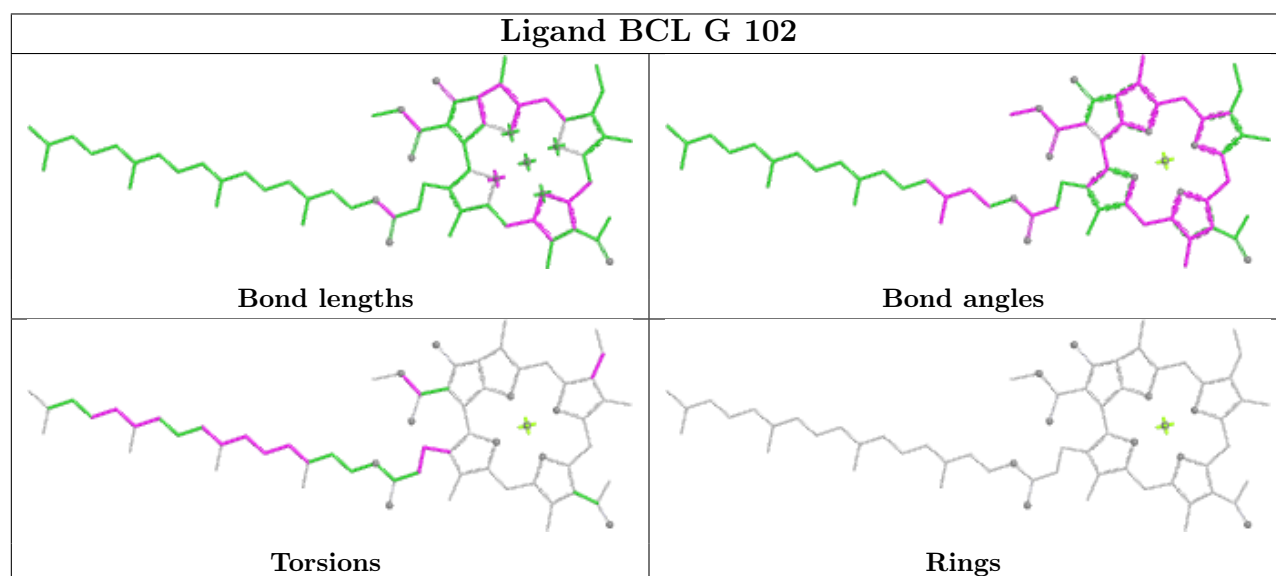
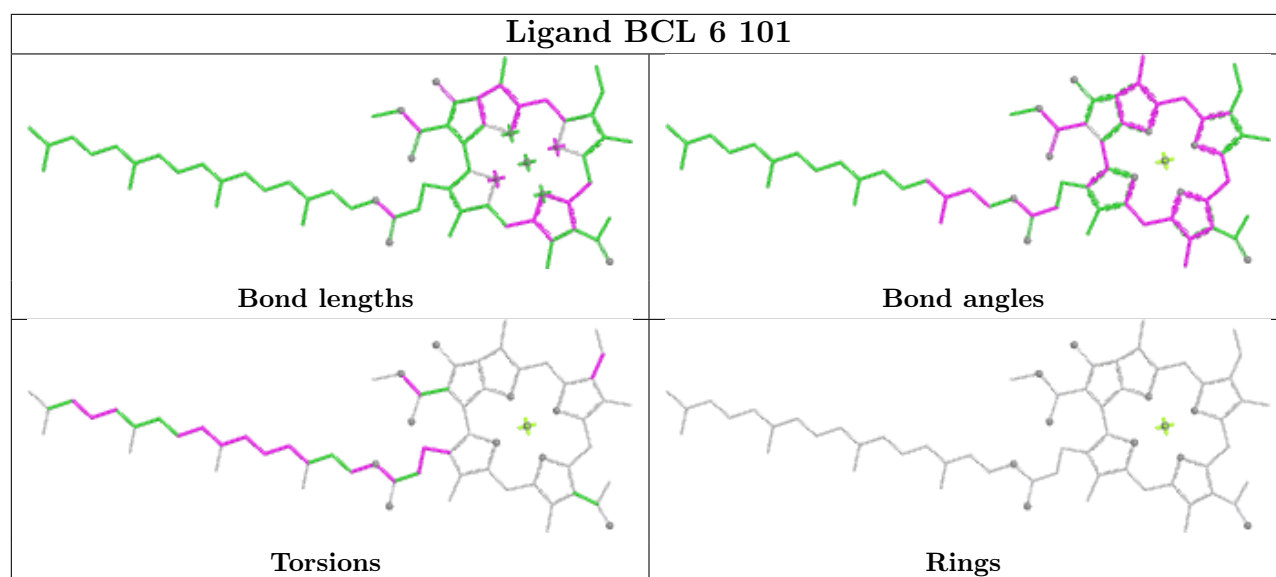


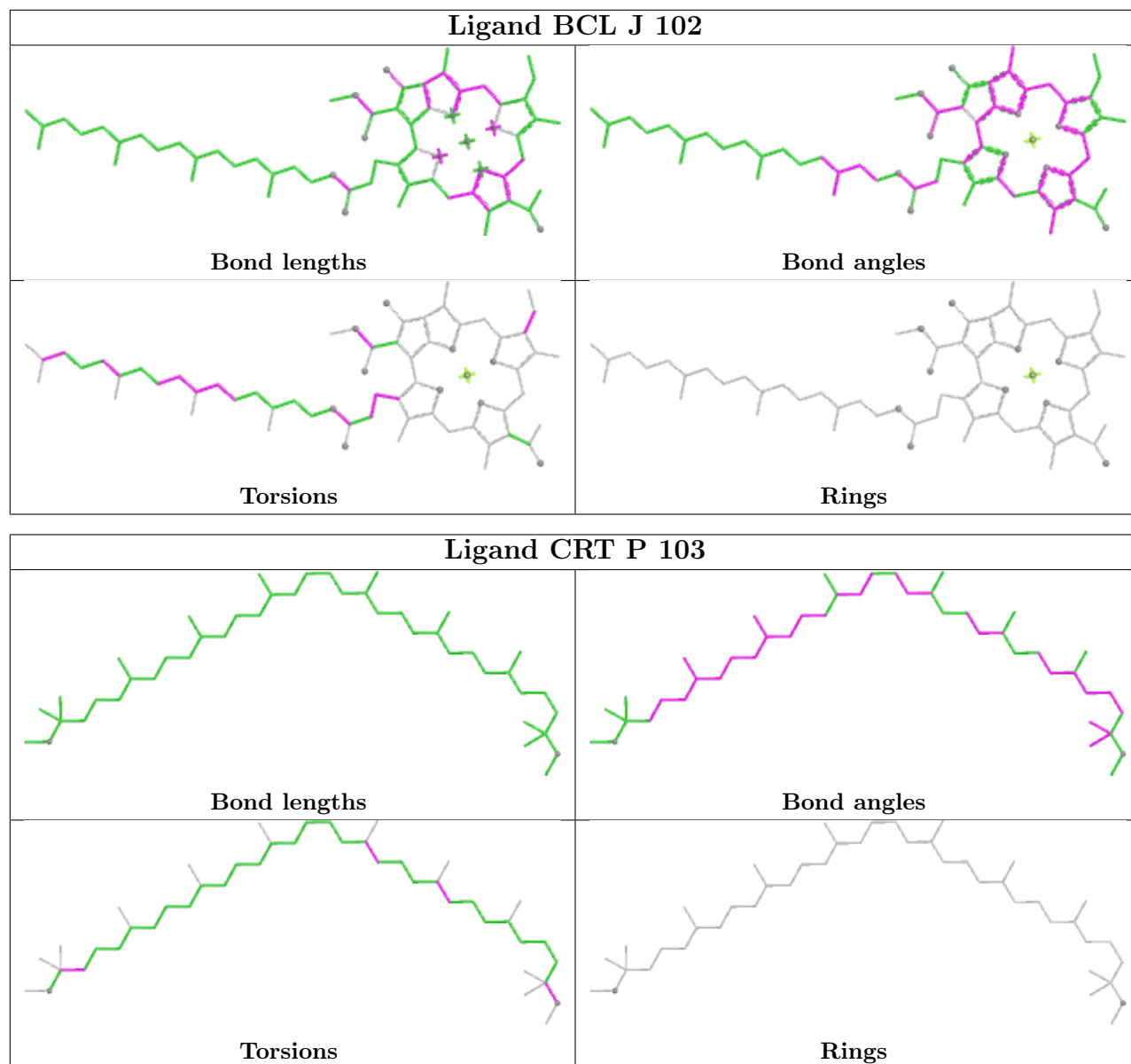


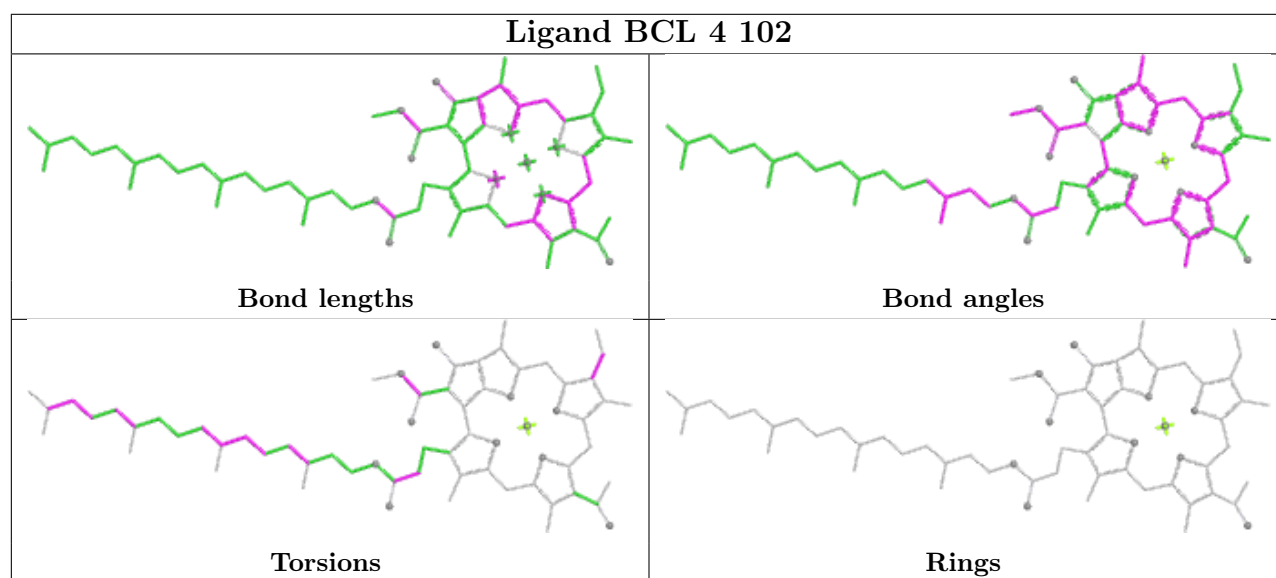
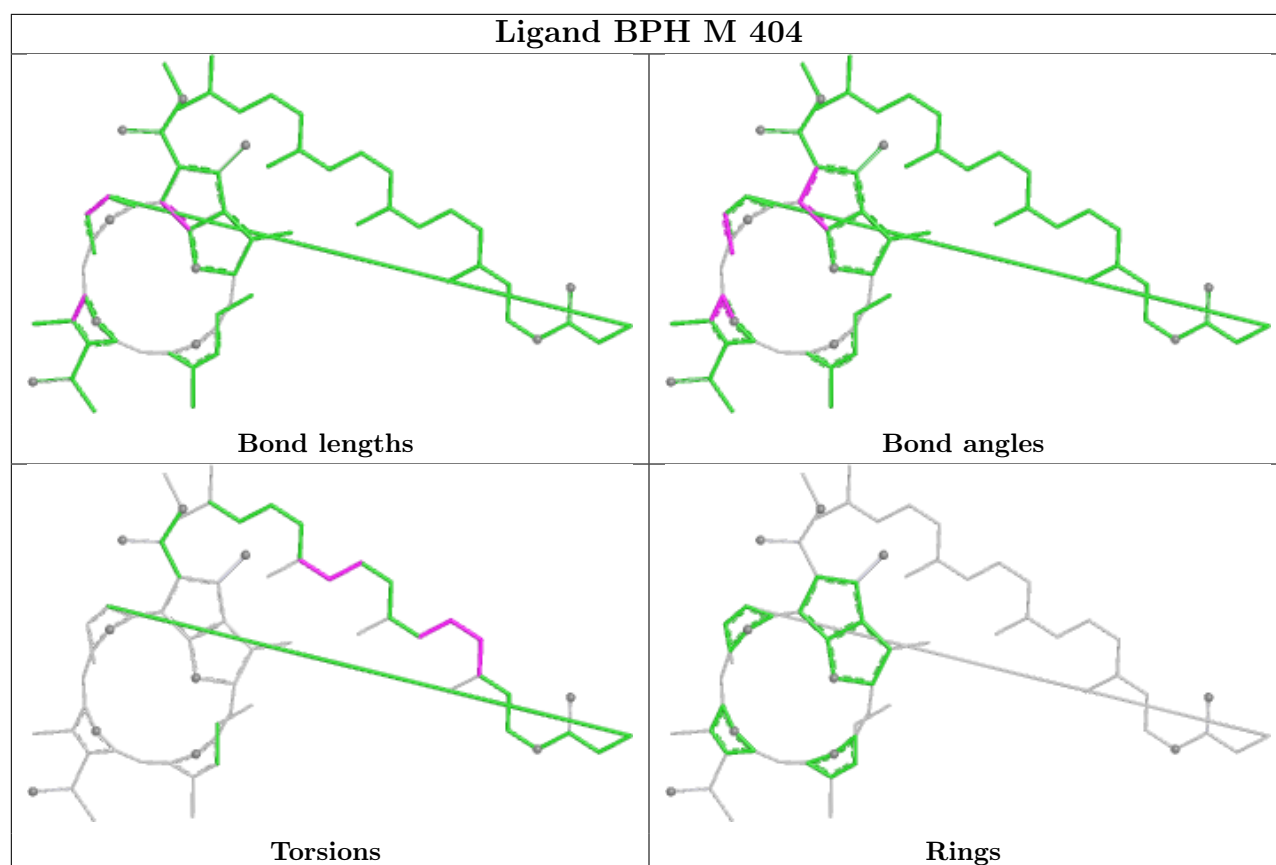


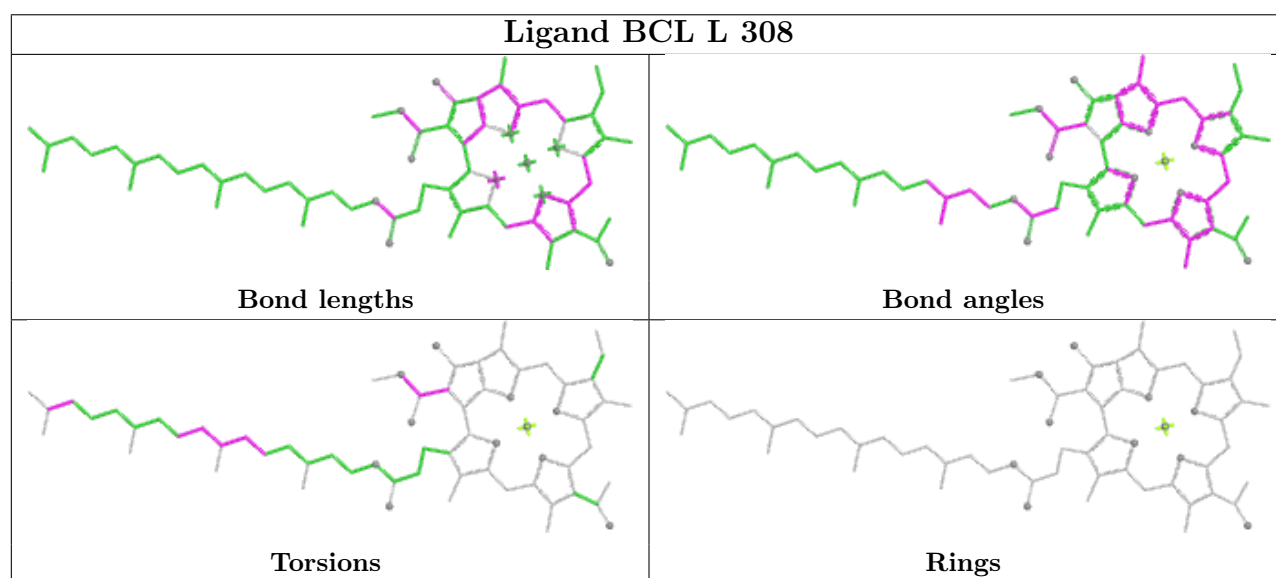
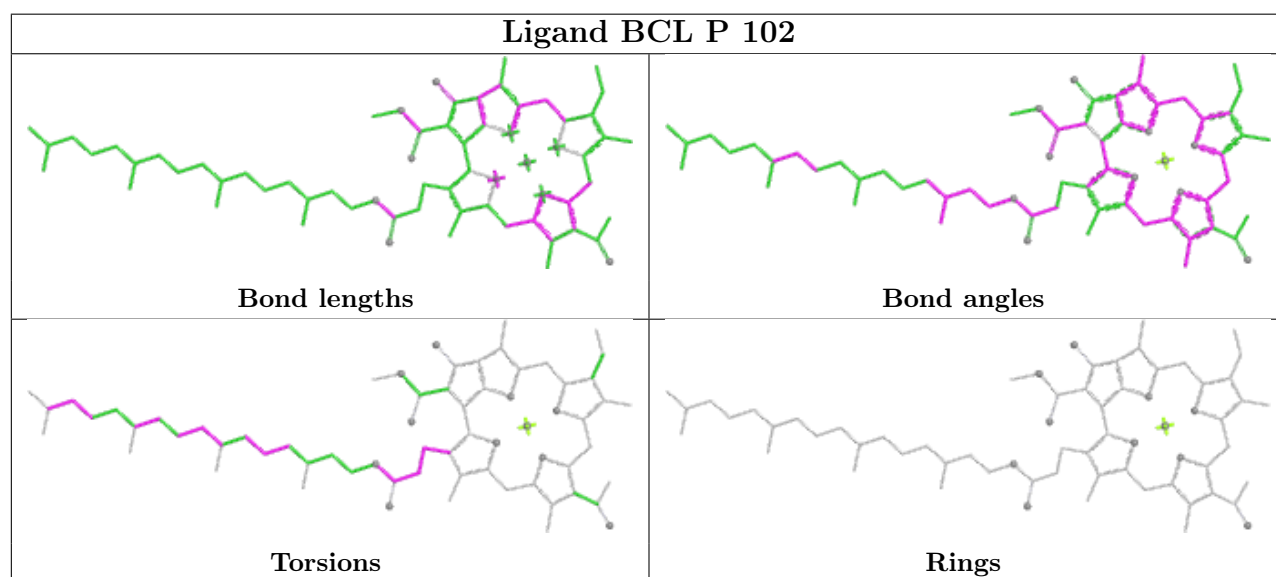
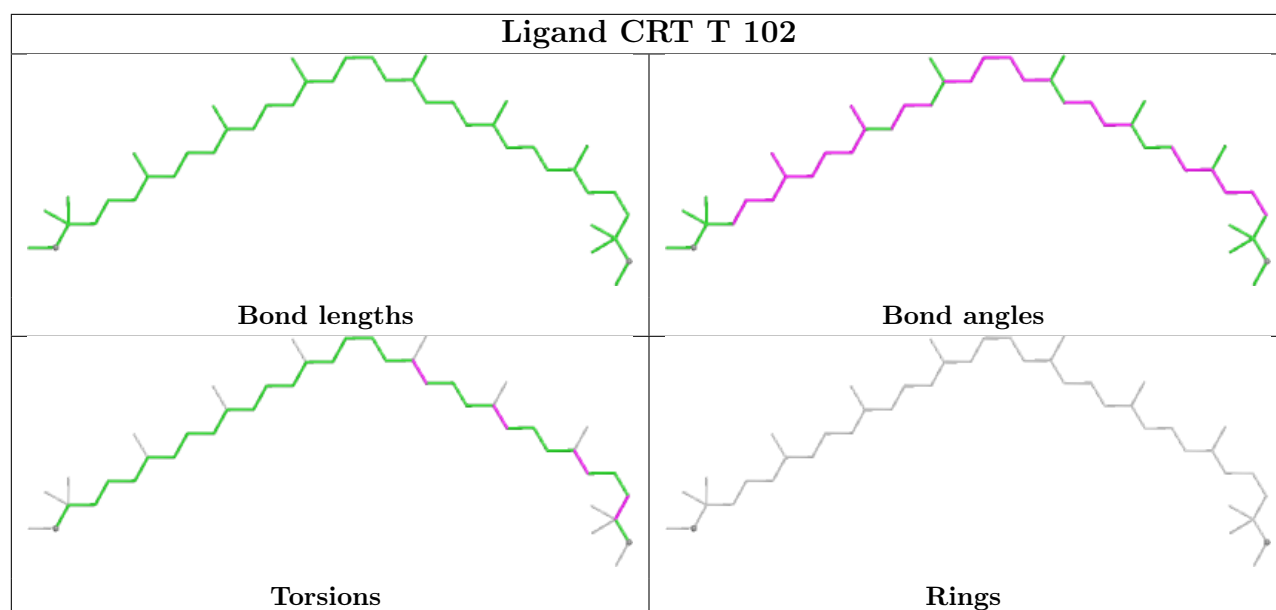


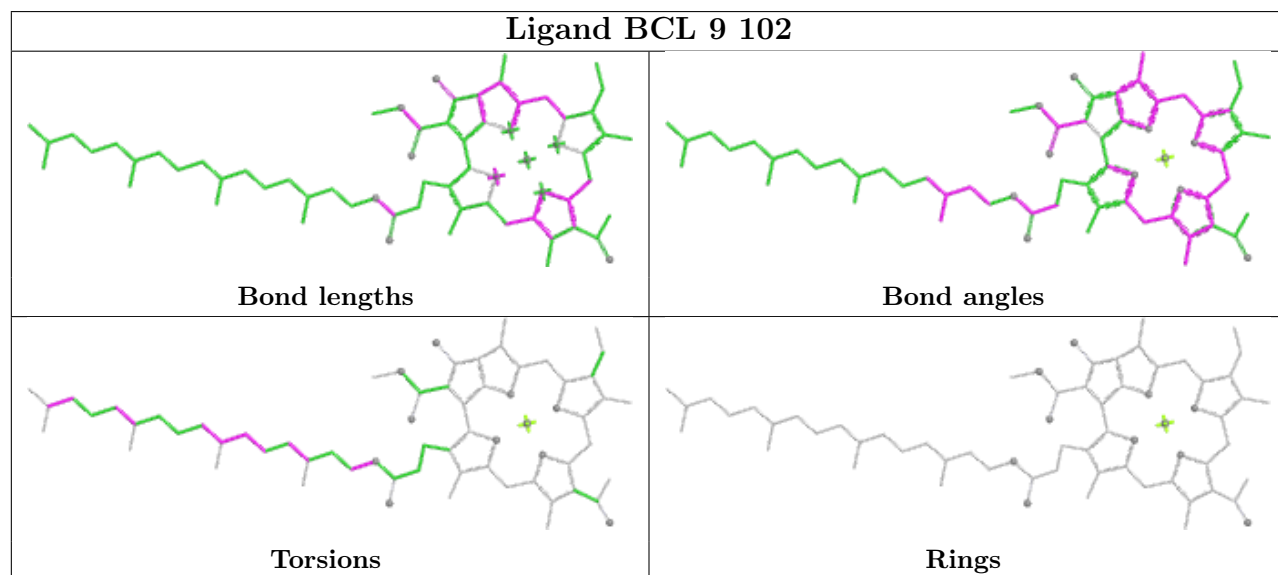
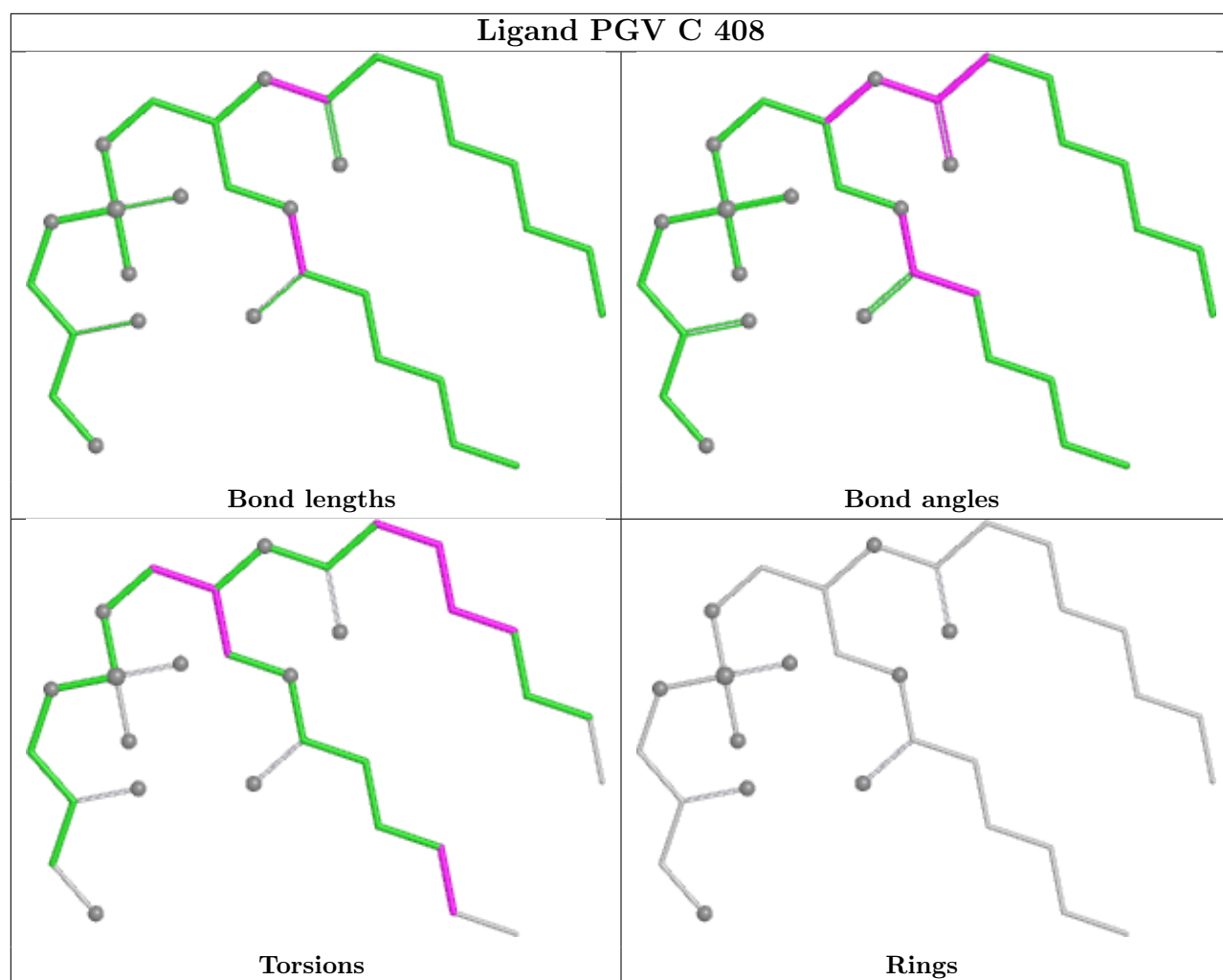


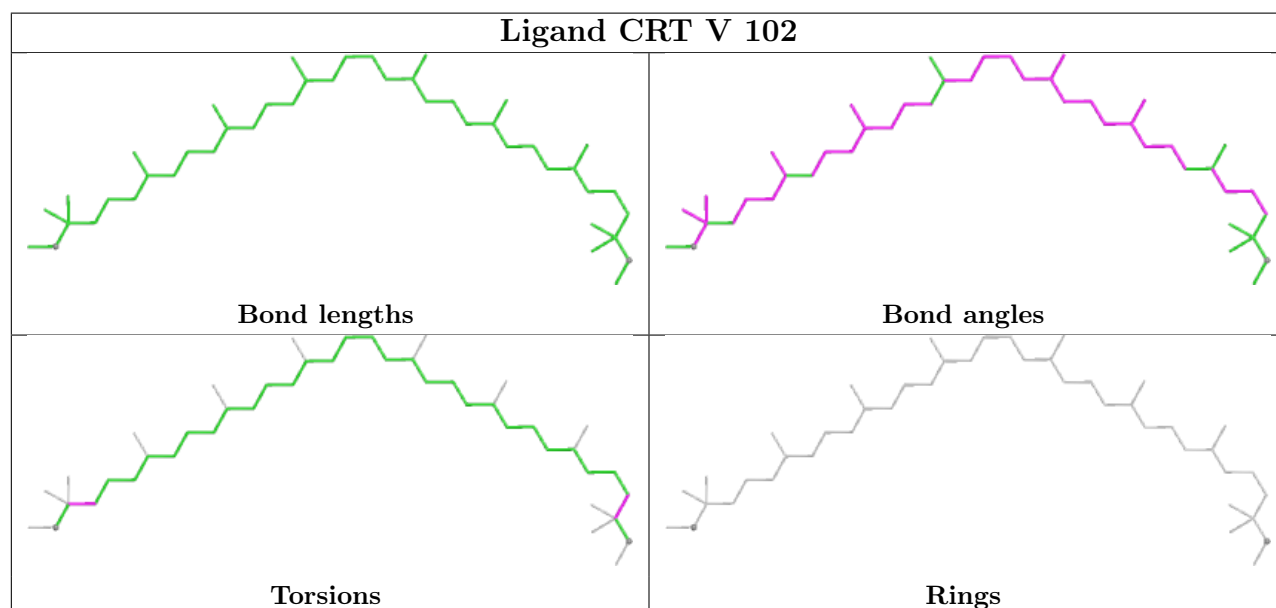
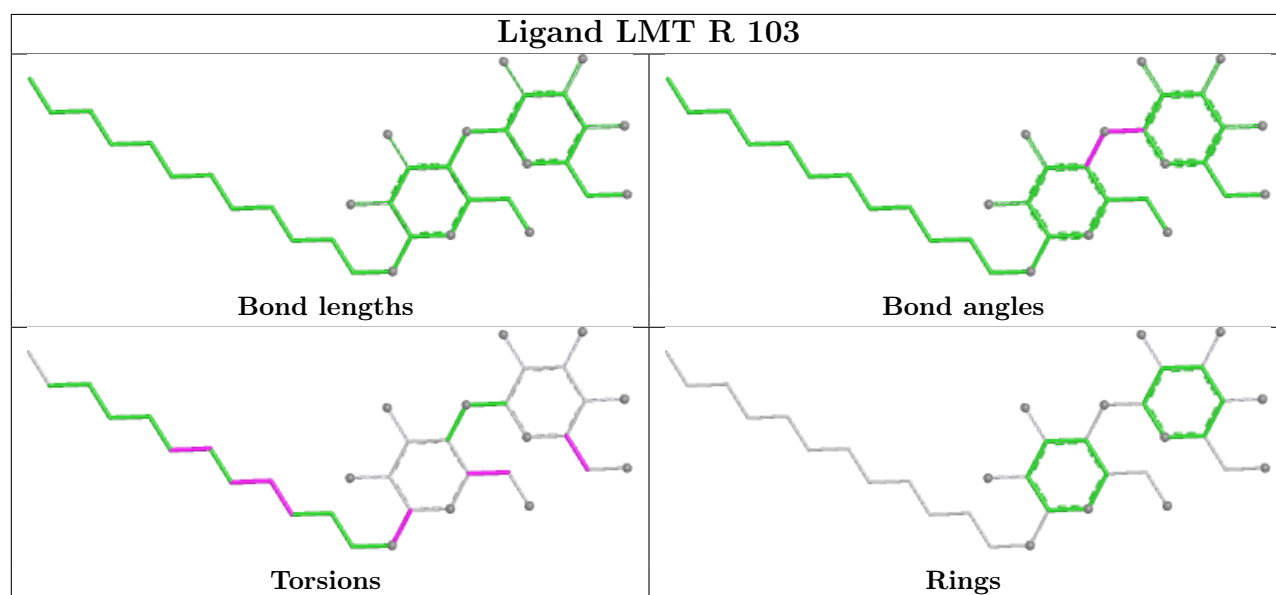
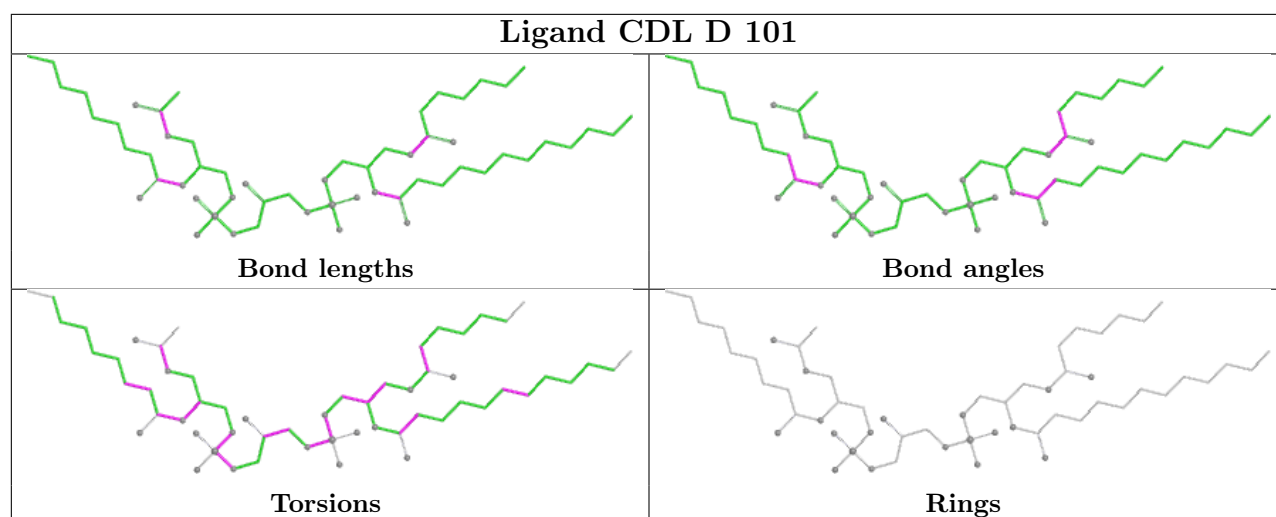


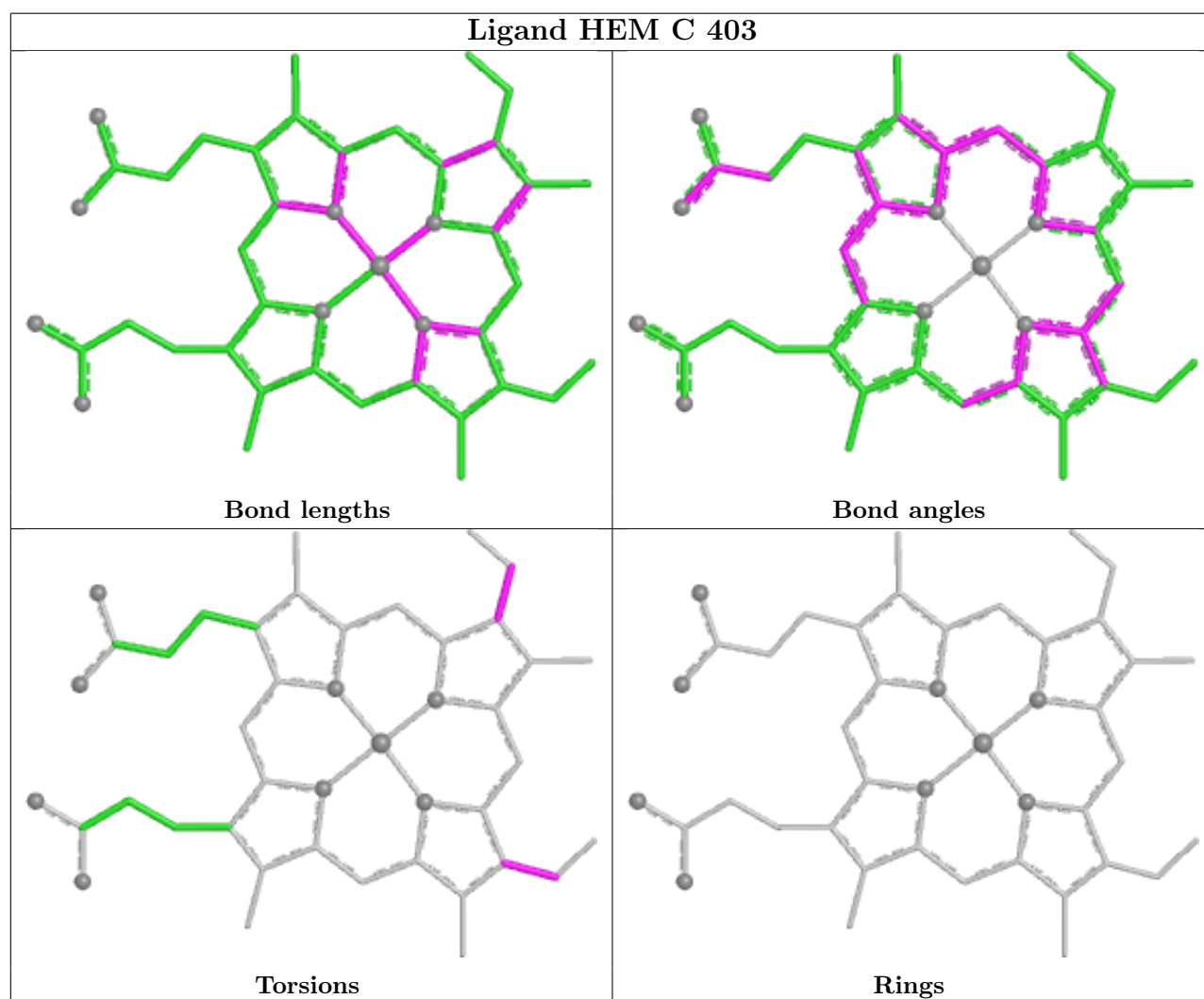
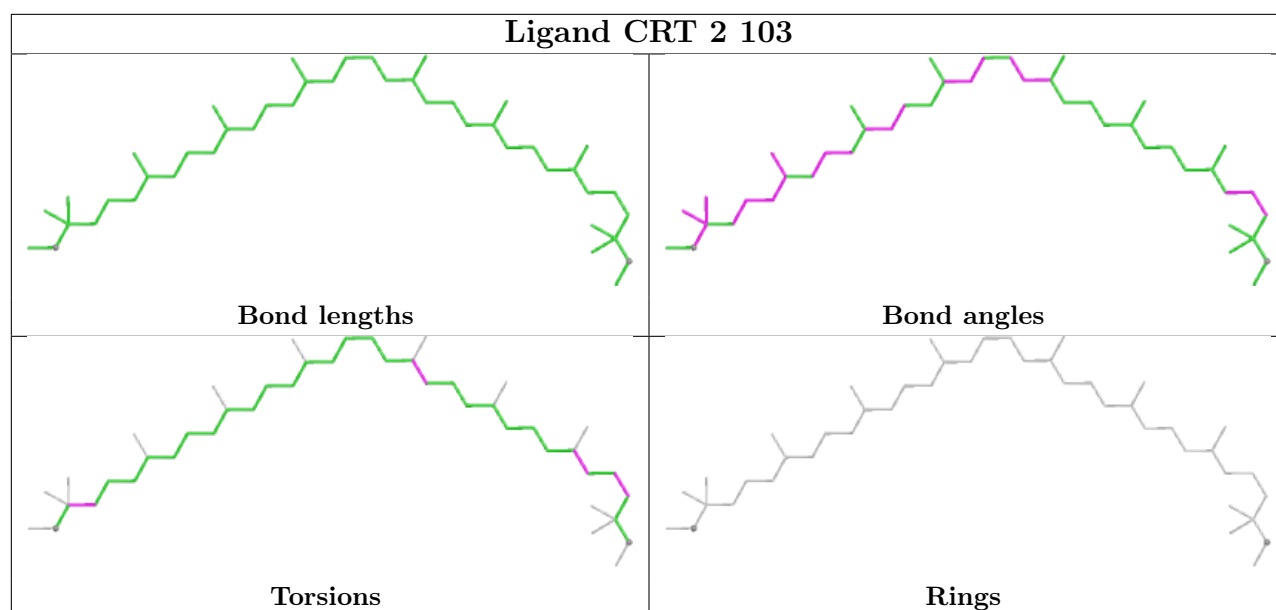


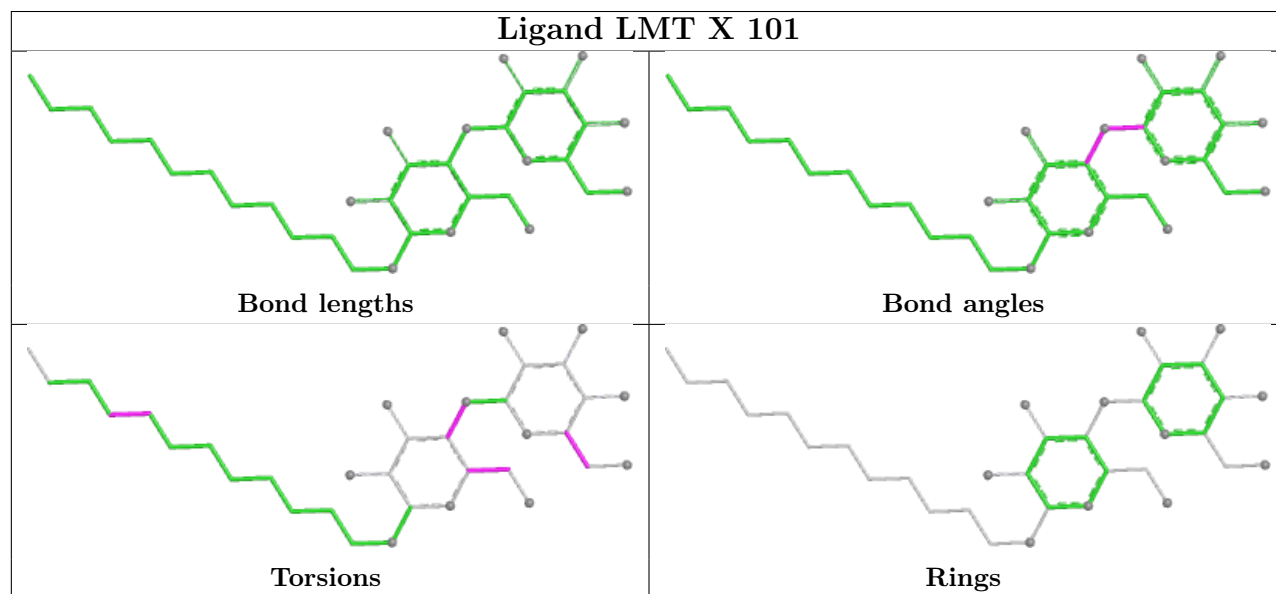
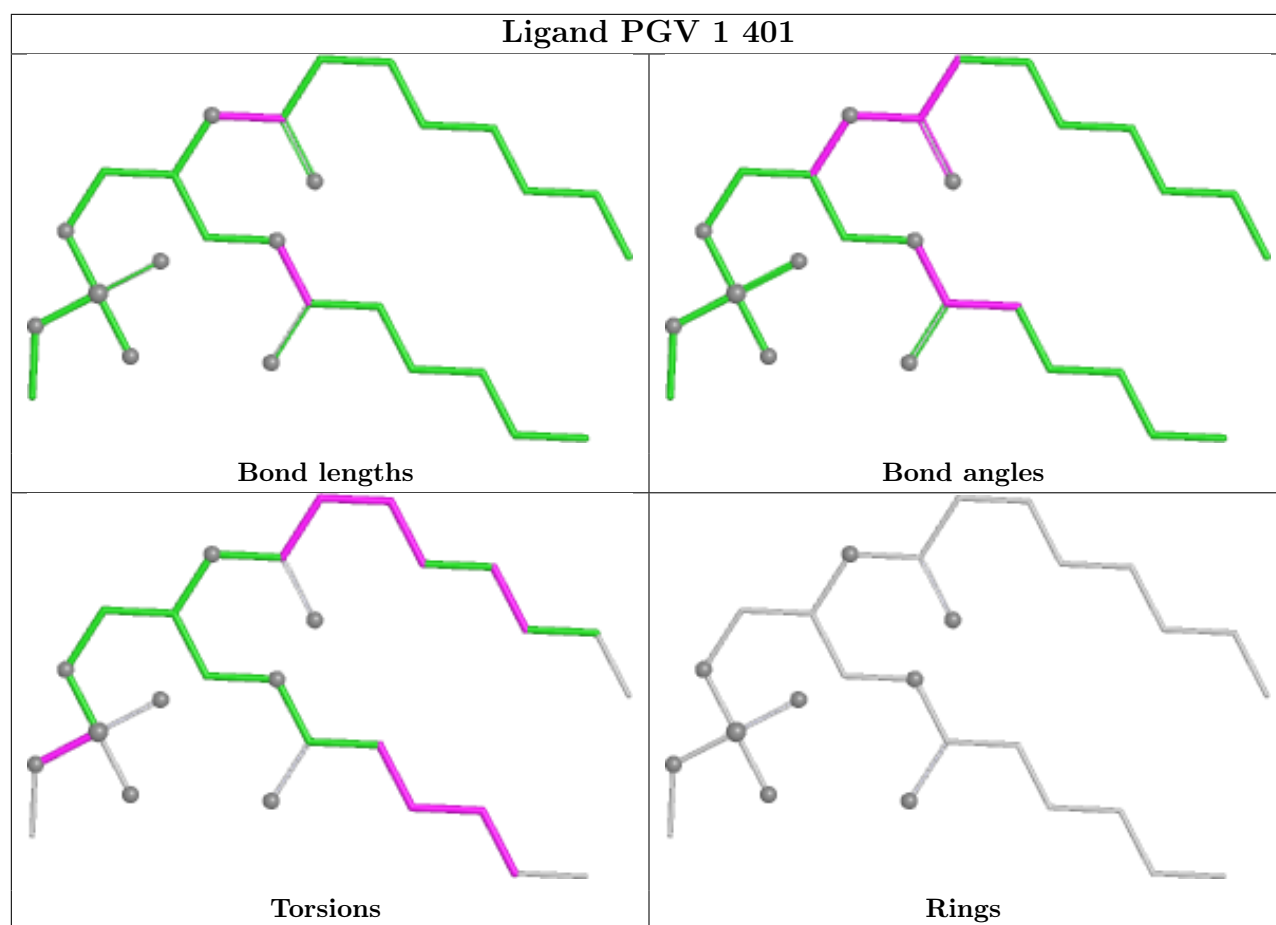


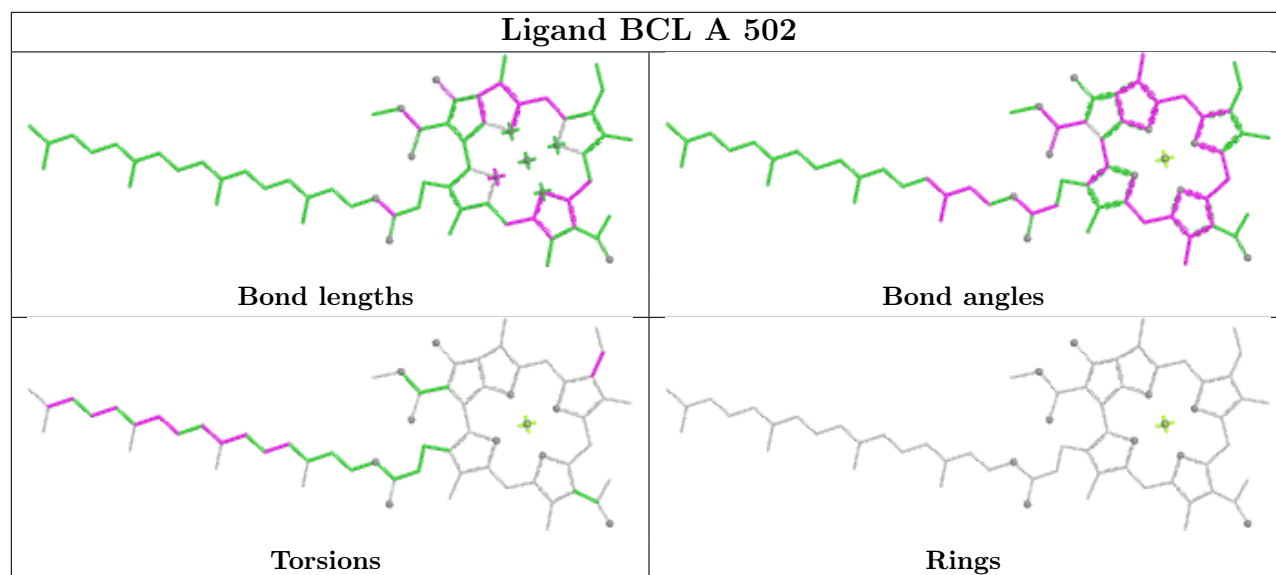
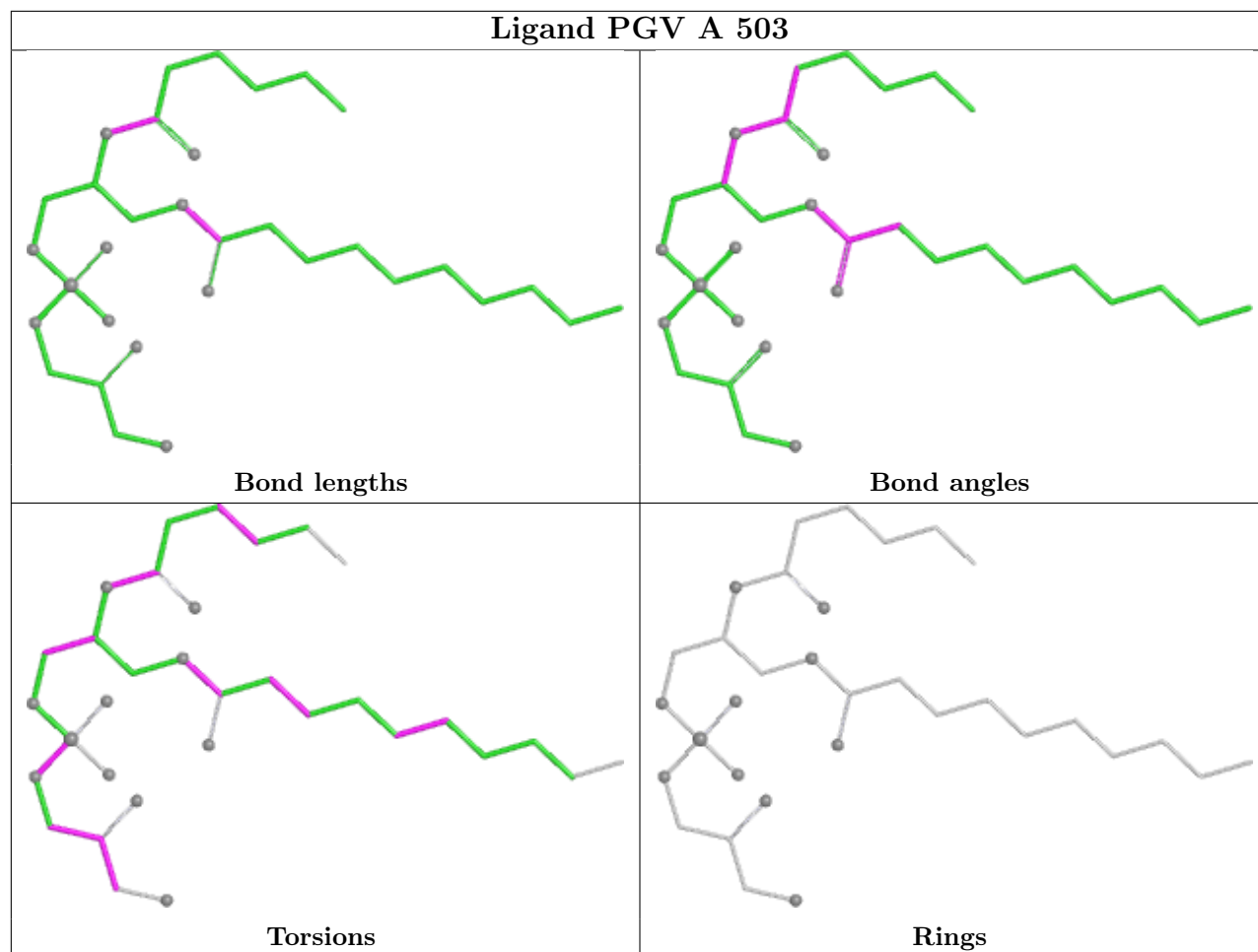


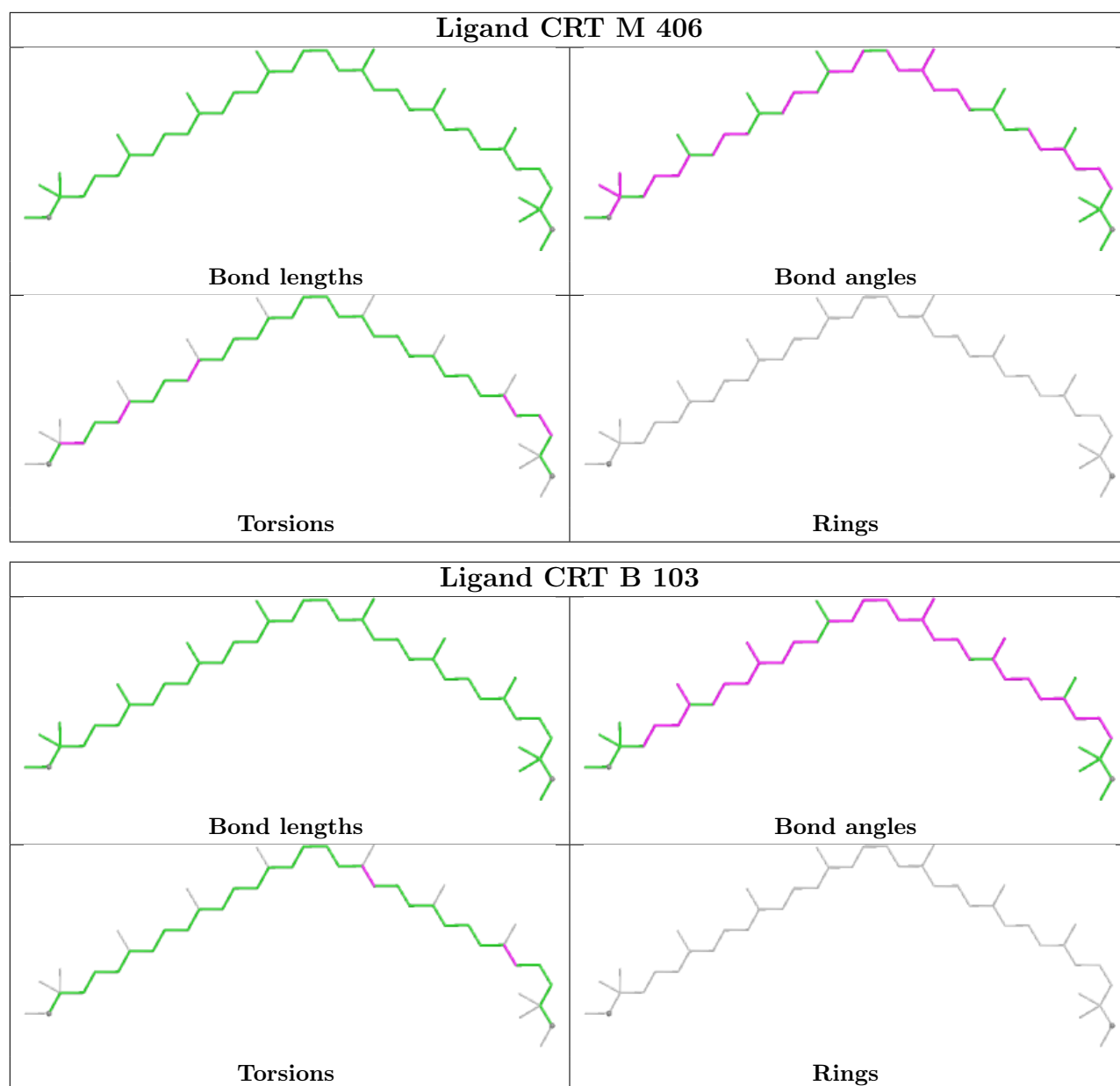


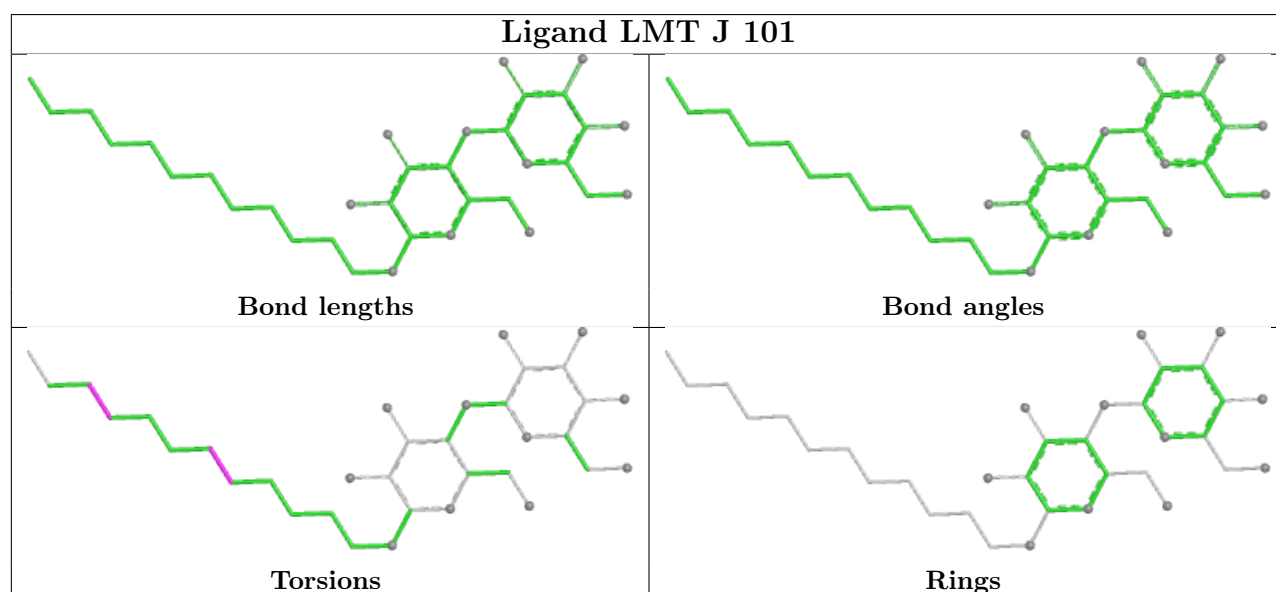
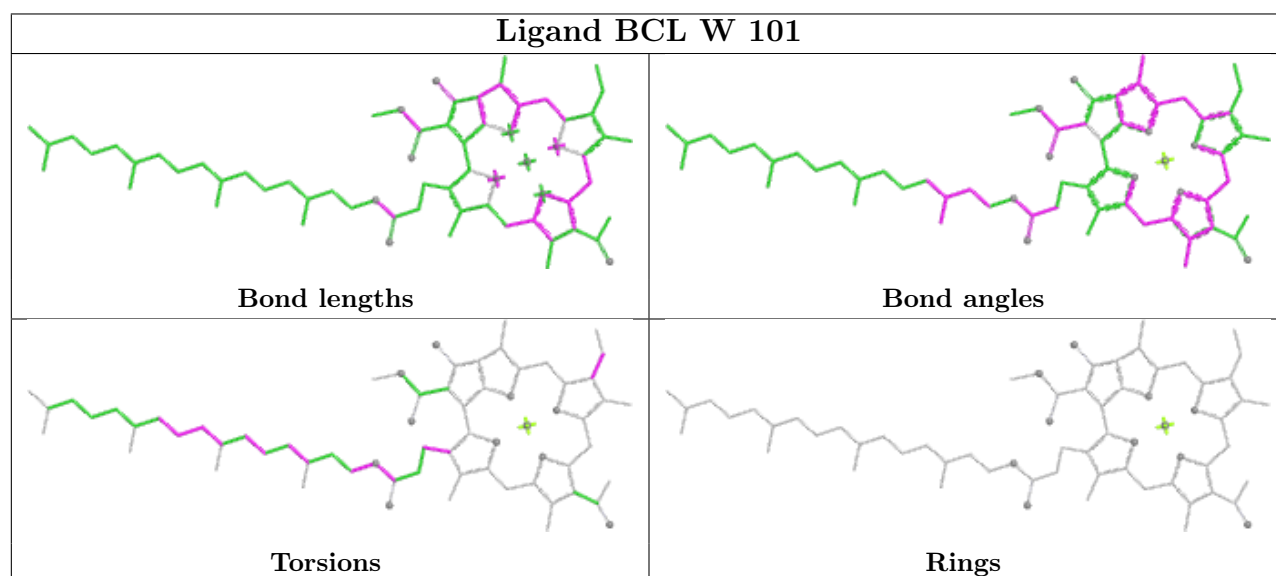
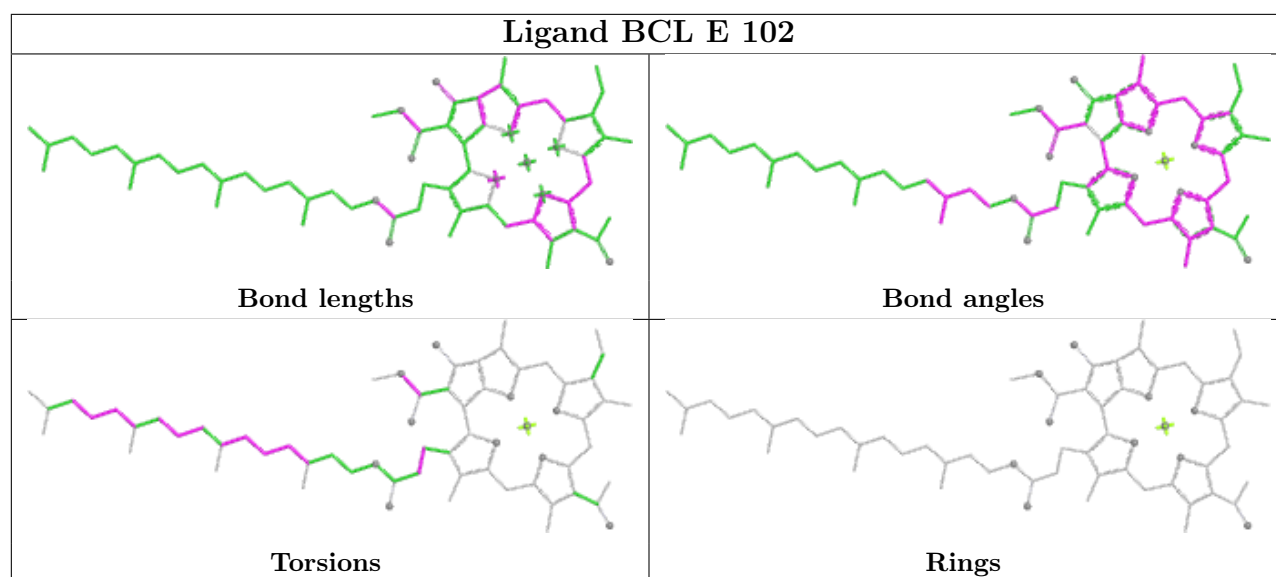












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

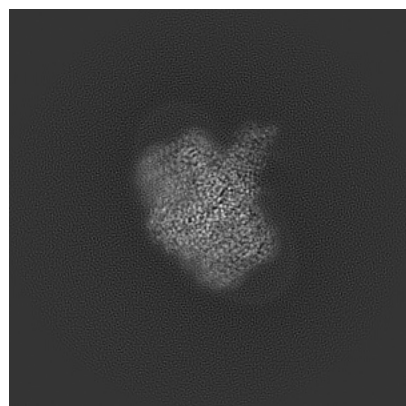
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37465. These allow visual inspection of the internal detail of the map and identification of artifacts.

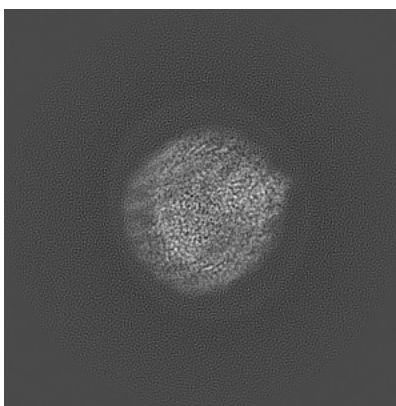
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

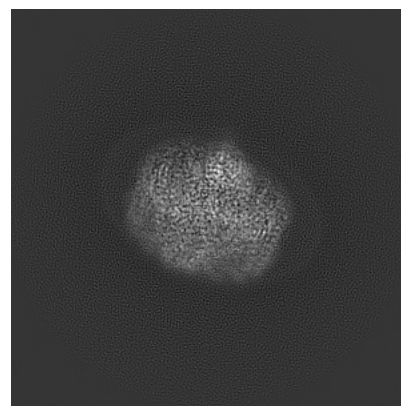
#### 6.1.1 Primary map



X

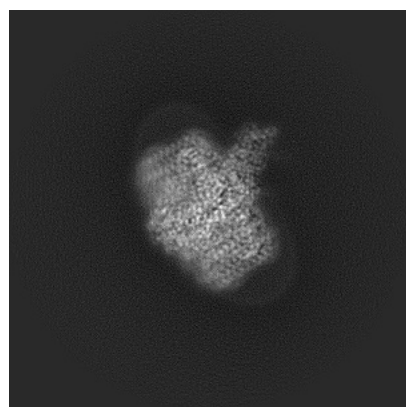


Y

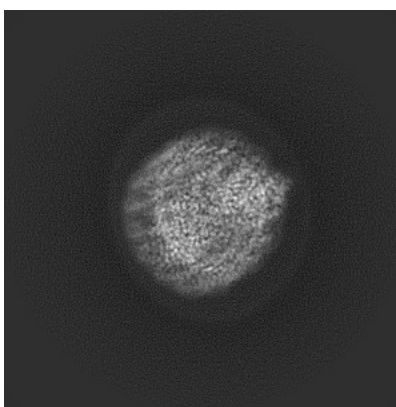


Z

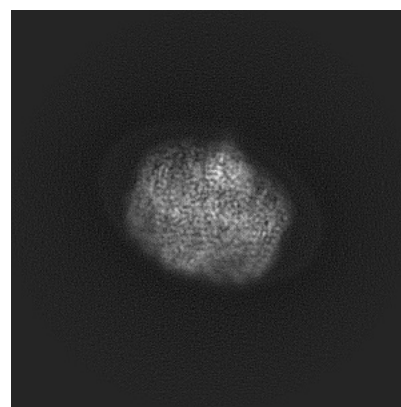
#### 6.1.2 Raw map



X



Y

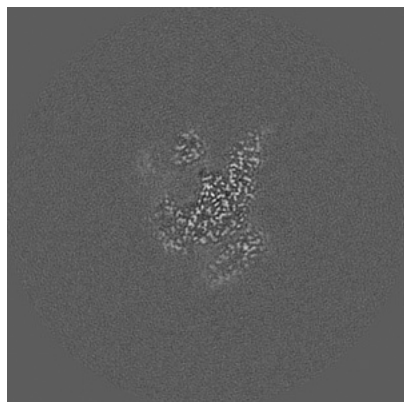


Z

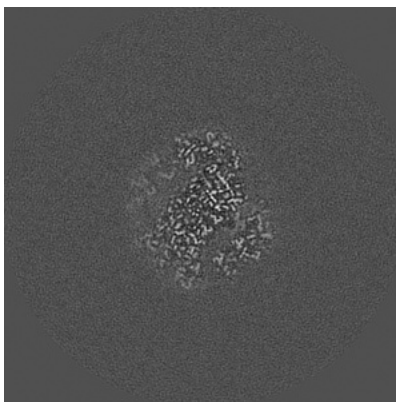
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

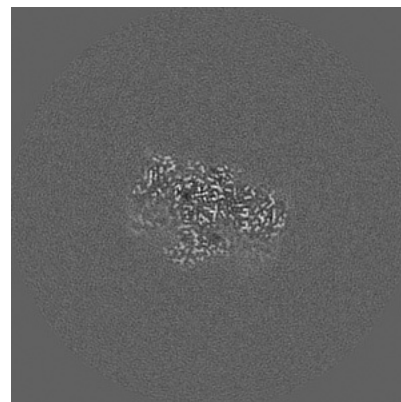
### 6.2.1 Primary map



X Index: 240

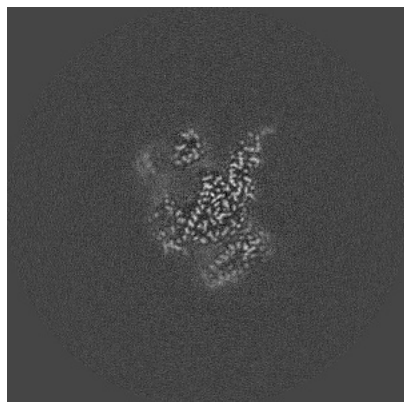


Y Index: 240

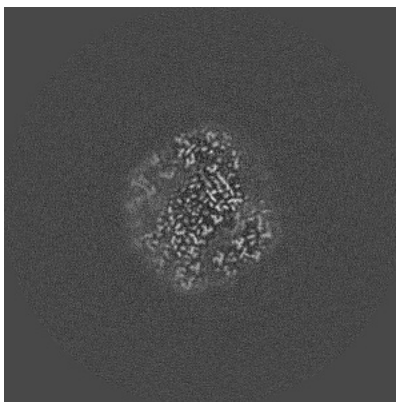


Z Index: 240

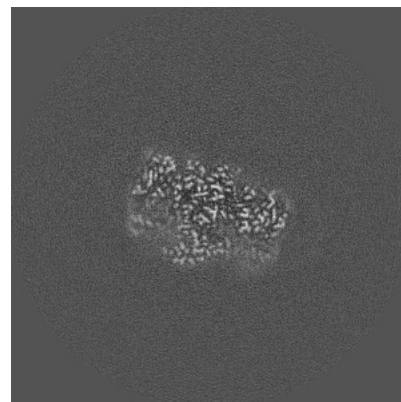
### 6.2.2 Raw map



X Index: 240



Y Index: 240

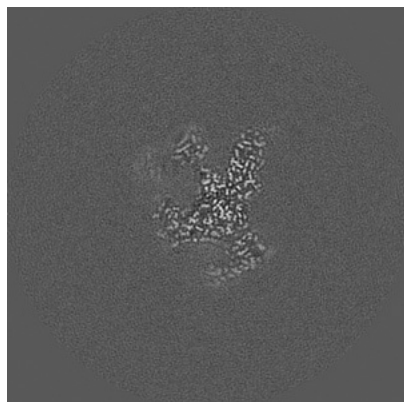


Z Index: 240

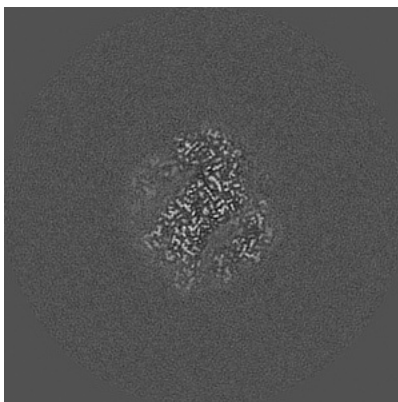
The images above show central slices of the map in three orthogonal directions.

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

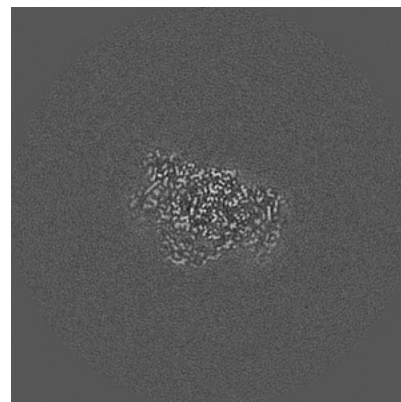
### 6.3.1 Primary map



X Index: 246

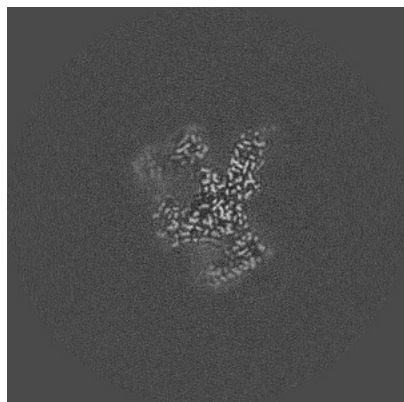


Y Index: 238

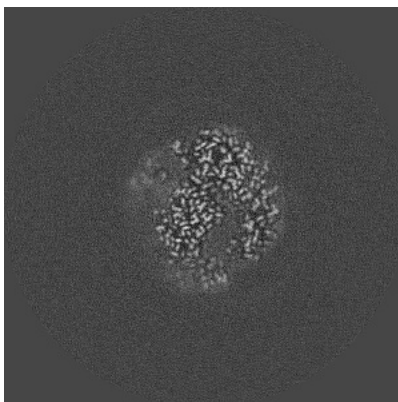


Z Index: 231

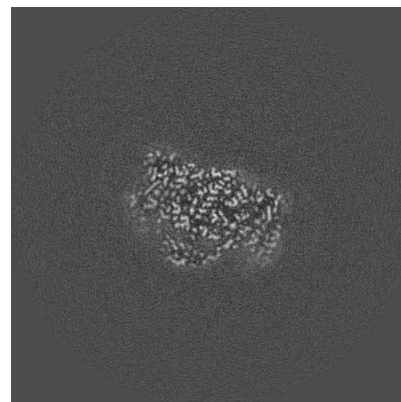
### 6.3.2 Raw map



X Index: 246



Y Index: 228

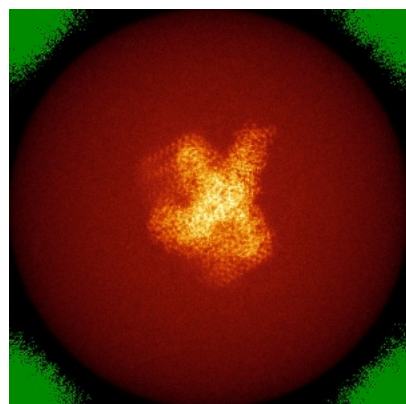


Z Index: 231

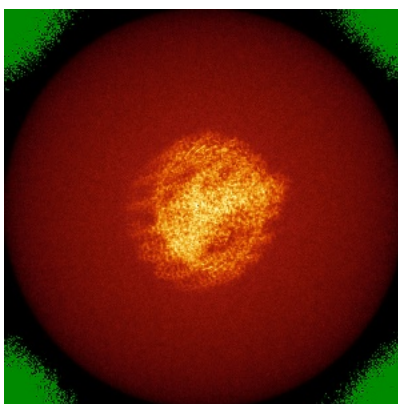
The images above show the largest variance slices of the map in three orthogonal directions.

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

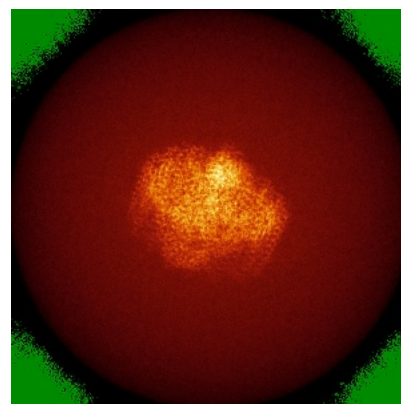
### 6.4.1 Primary map



X

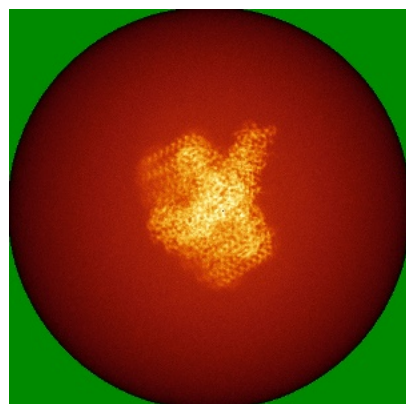


Y

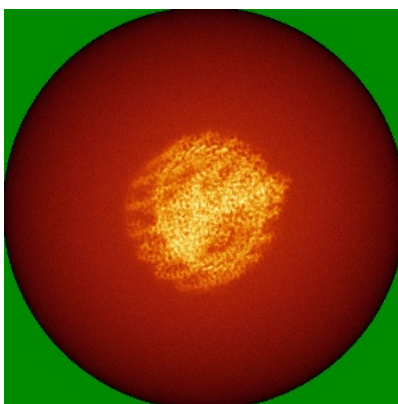


Z

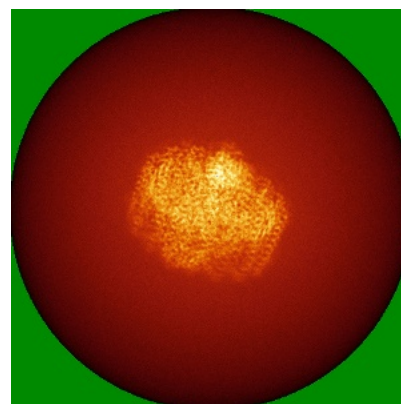
### 6.4.2 Raw map



X



Y

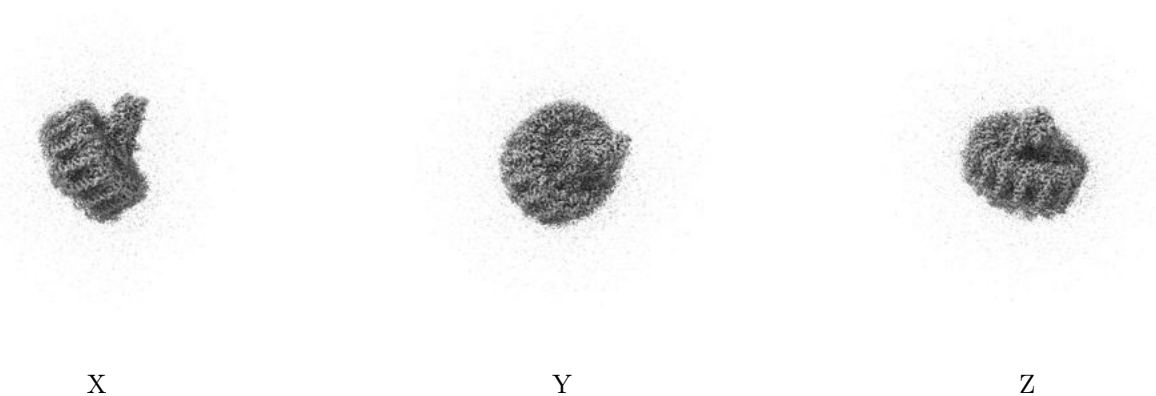


Z

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.

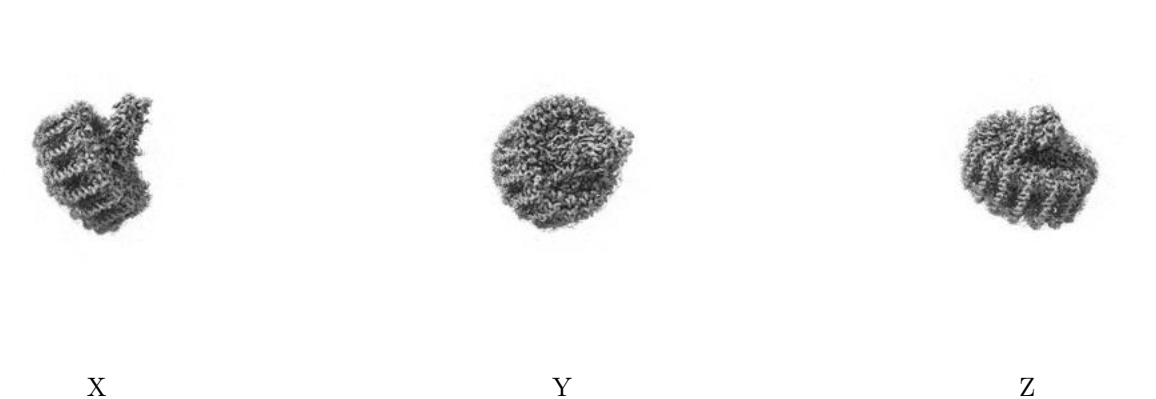
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

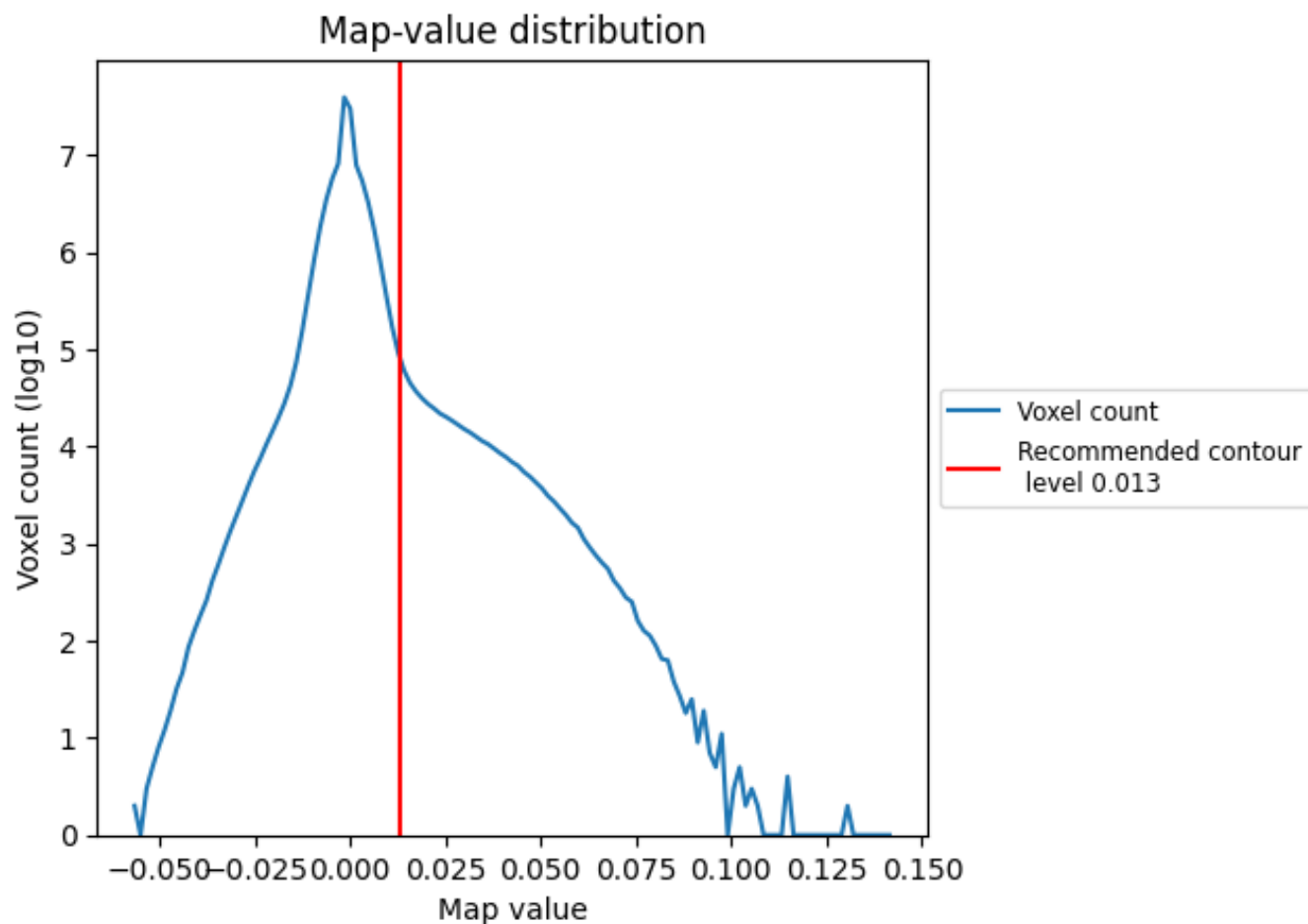
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

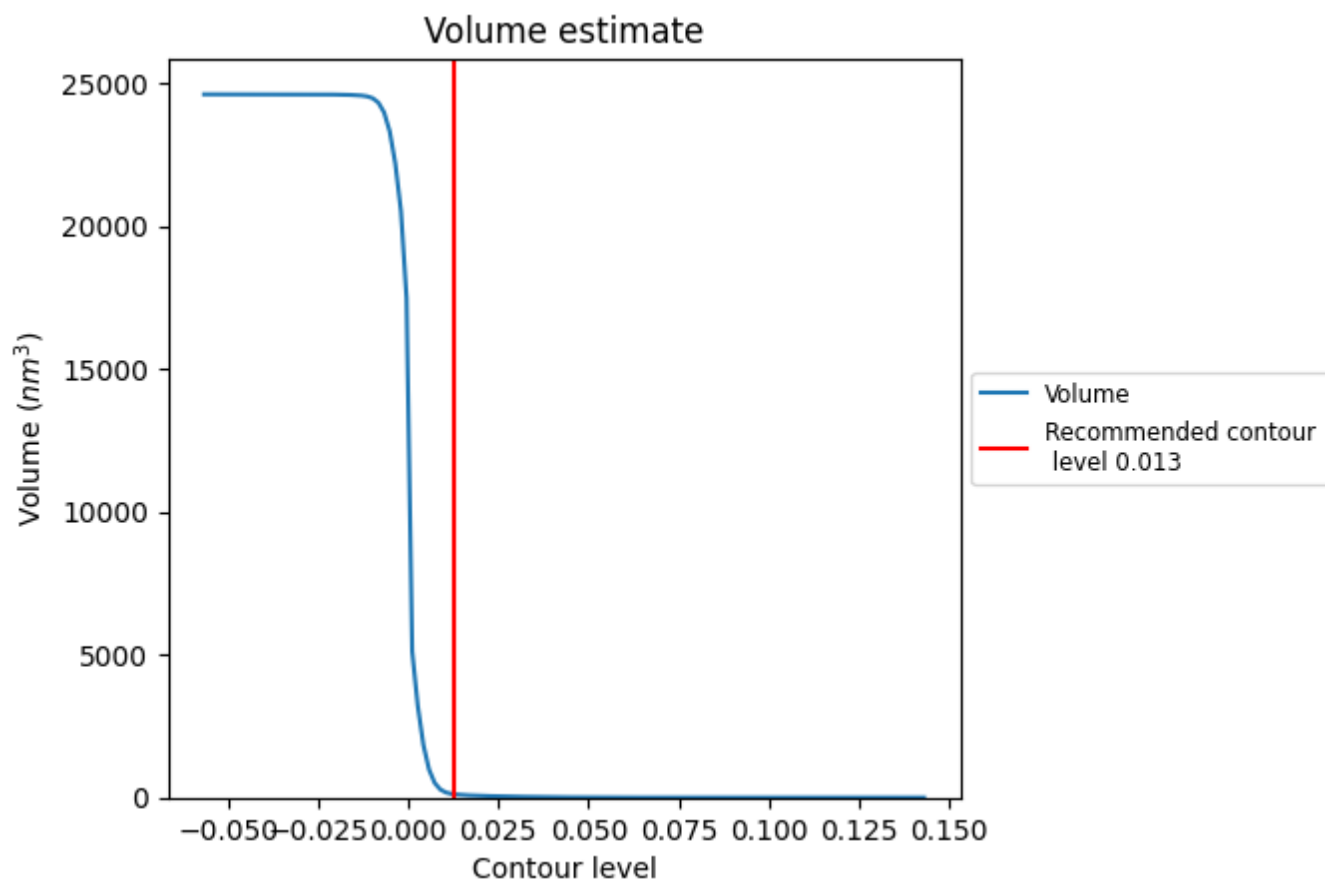
This section contains the results of statistical analysis of the map.

### 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.

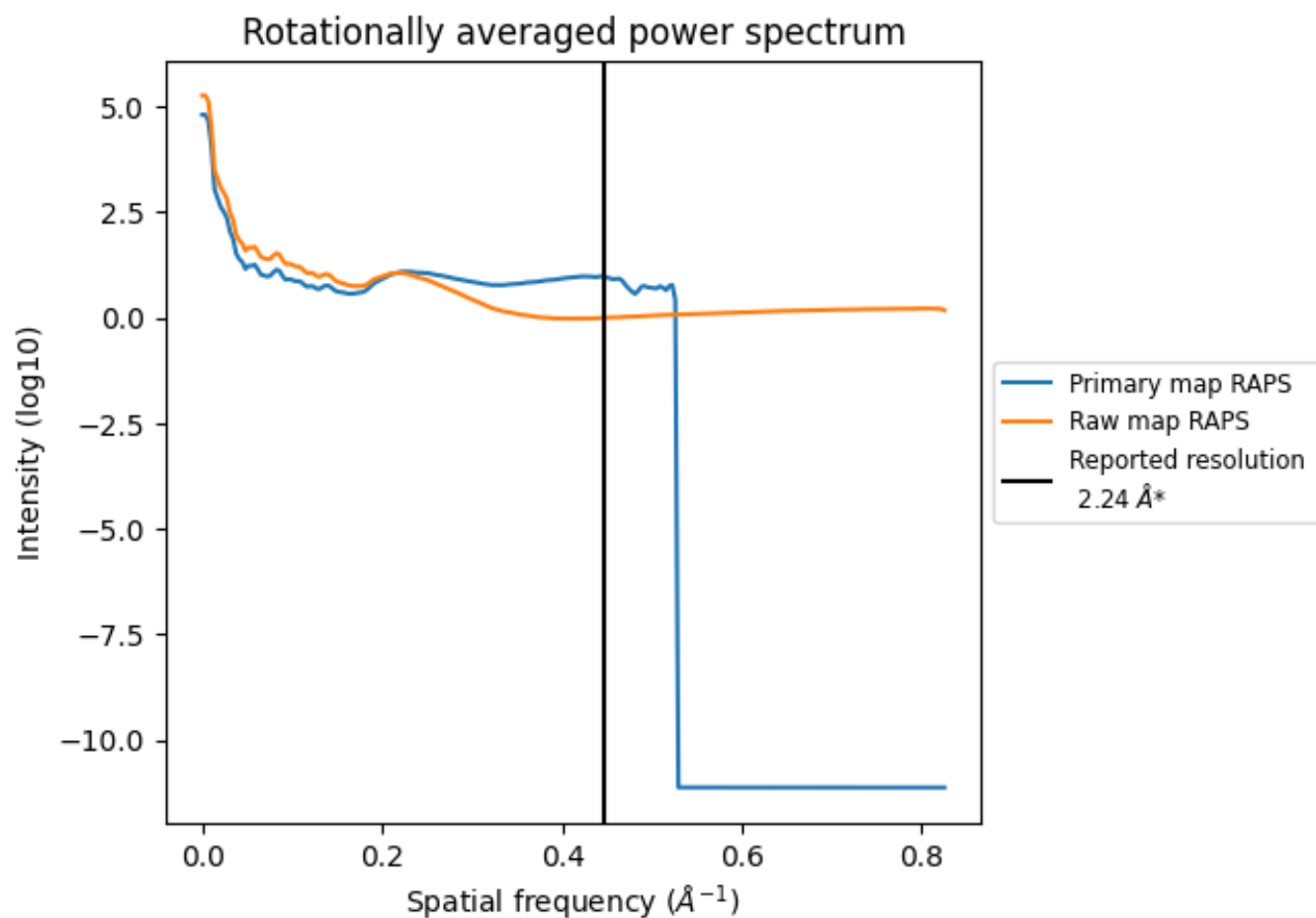
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115  $\text{nm}^3$ ; this corresponds to an approximate mass of 103 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 ⓘ

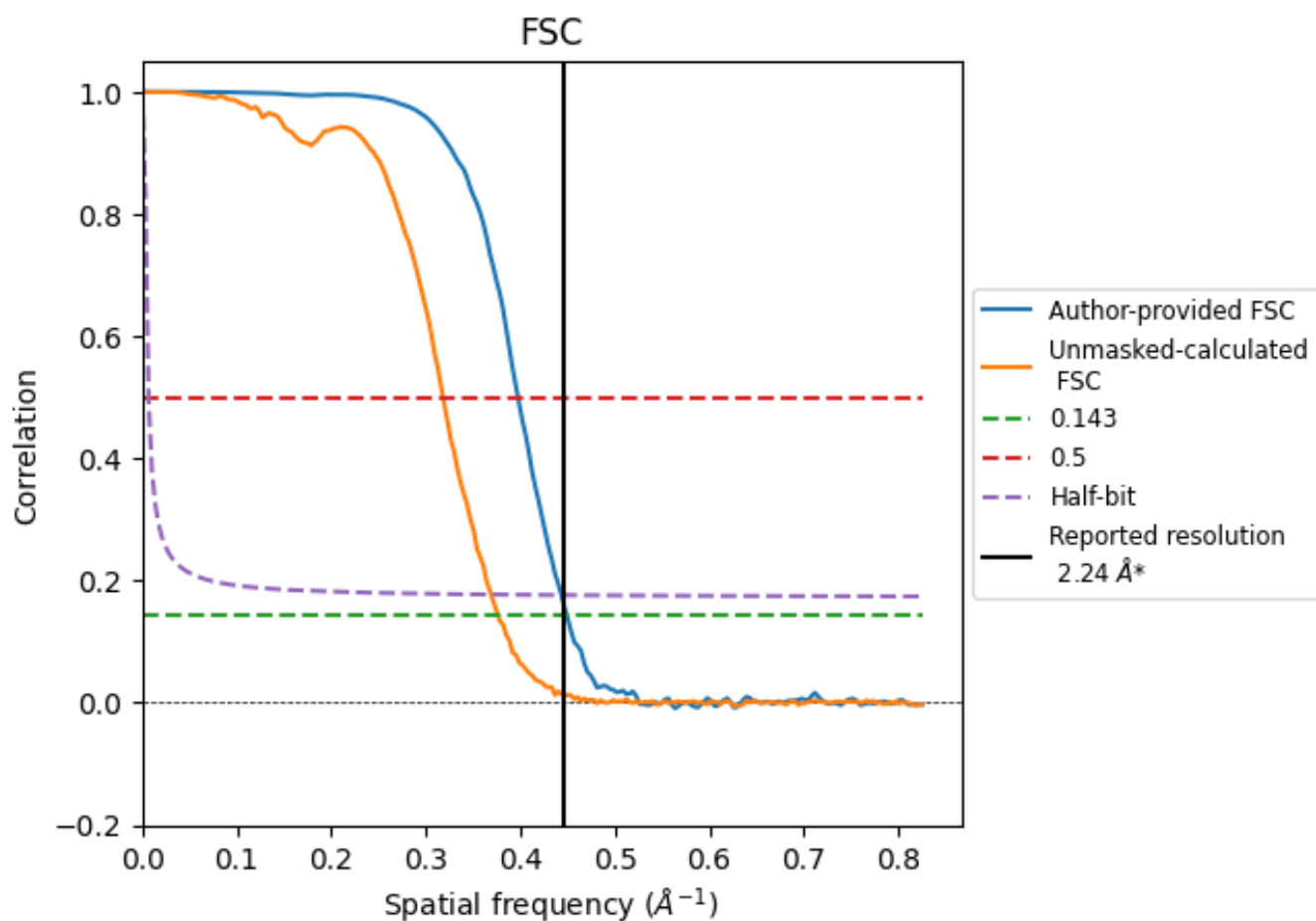


\*Reported resolution corresponds to spatial frequency of 0.446 Å<sup>-1</sup>

## 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  $0.446 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

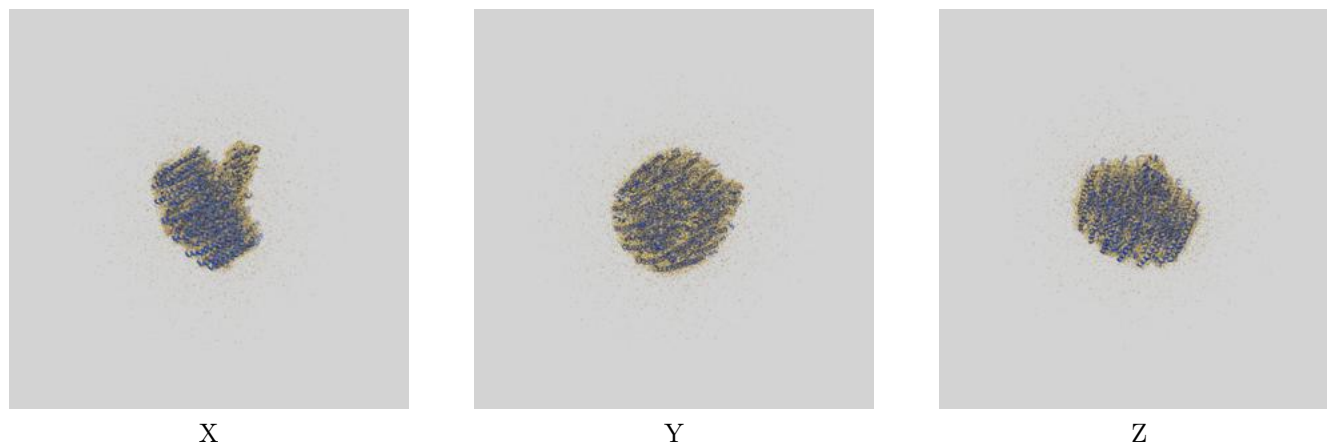
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.24                               | -    | -        |
| Author-provided FSC curve | 2.23                               | 2.52 | 2.25     |
| Unmasked-calculated*      | 2.66                               | 3.14 | 2.71     |

\*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 2.66 differs from the reported value 2.24 by more than 10 %

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

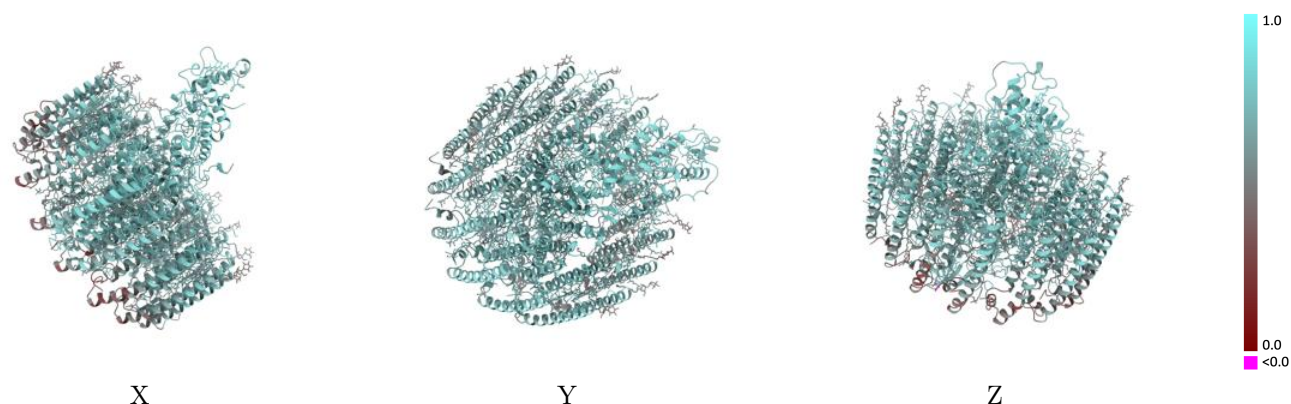
This section contains information regarding the fit between EMDB map EMD-37465 and PDB model 8WDU. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.013 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](#)

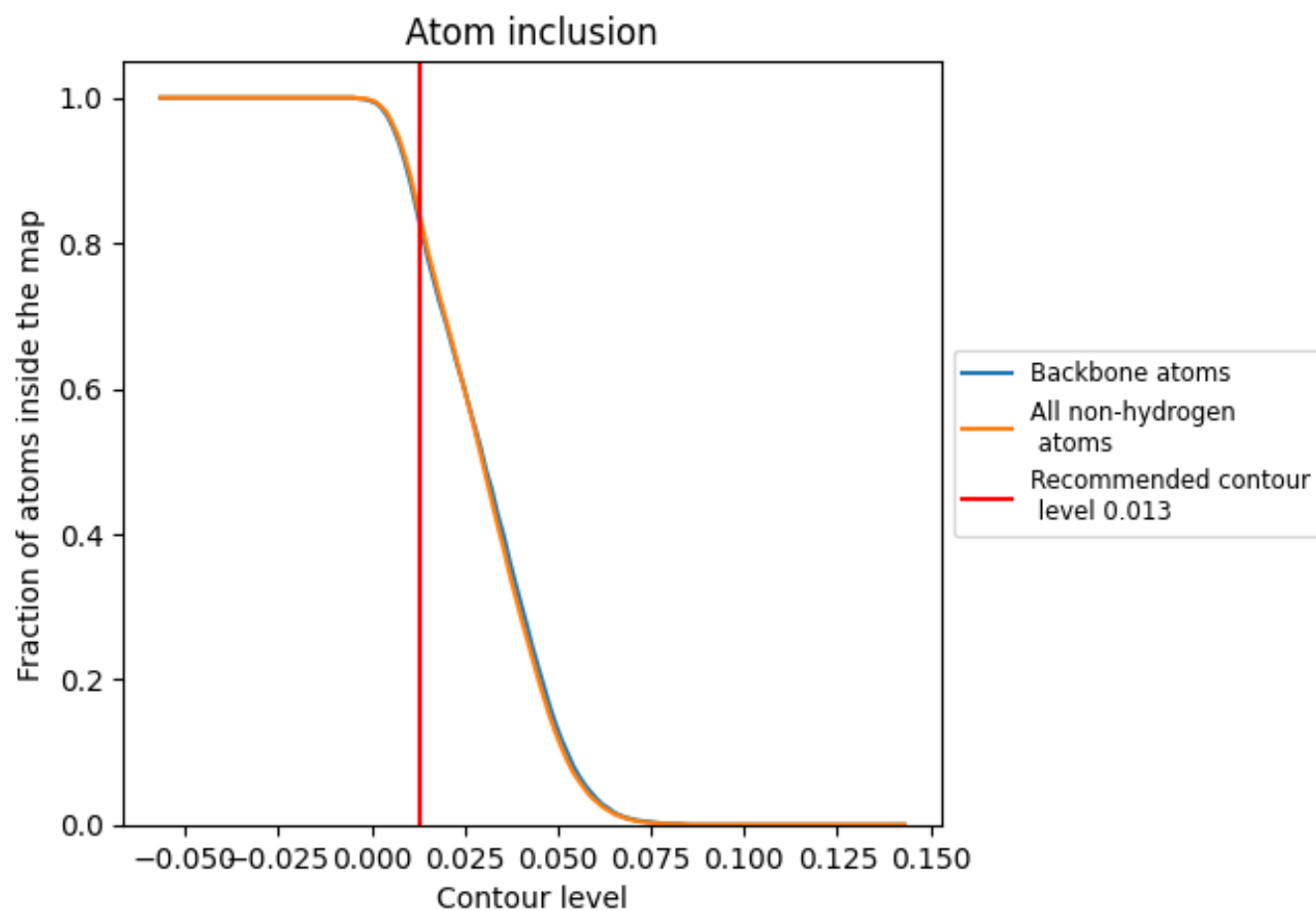


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.013) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8360   |  0.6760   |
| 0     |  0.9090   |  0.7090   |
| 1     |  0.7440   |  0.6370   |
| 2     |  0.5920   |  0.5390   |
| 3     |  0.7870   |  0.6490   |
| 4     |  0.6360   |  0.5700   |
| 5     |  0.8460   |  0.6710   |
| 6     |  0.8050   |  0.6540   |
| 7     |  0.9350   |  0.7170   |
| 8     |  0.8050   |  0.6450   |
| 9     |  0.9480   |  0.7270   |
| A     |  0.9240   |  0.7070   |
| B     |  0.8770   |  0.6870   |
| C     |  0.9620   |  0.7430   |
| D     |  0.8530  |  0.6830  |
| E     |  0.7970 |  0.6520 |
| F     |  0.7340 |  0.6280 |
| G     |  0.7390 |  0.6240 |
| H     |  0.9220 |  0.7140 |
| I     |  0.7470 |  0.6370 |
| J     |  0.6730 |  0.5870 |
| K     |  0.6900 |  0.5930 |
| L     |  0.9300 |  0.7400 |
| M     |  0.9460 |  0.7430 |
| N     |  0.6370 |  0.5700 |
| O     |  0.8080 |  0.6510 |
| P     |  0.7110 |  0.5980 |
| Q     |  0.8220 |  0.6620 |
| R     |  0.7710 |  0.6370 |
| S     |  0.7500 |  0.6510 |
| T     |  0.7120 |  0.6050 |
| U     |  0.7360 |  0.6320 |
| V     |  0.7320 |  0.6130 |
| W     |  0.7180 |  0.6230 |
| X     |  0.6760 |  0.5960 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Y     |  0.6850 |  0.5950 |
| Z     |  0.6680 |  0.5650 |