



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:00 PM UTC

PDB ID : 8WDV / pdb\_00008wdv  
EMDB ID : EMD-37466  
Title : Photosynthetic LH1-RC complex from the purple sulfur bacterium *Allochro-  
matium vinosum* purified by Ca<sup>2+</sup>-DEAE  
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:

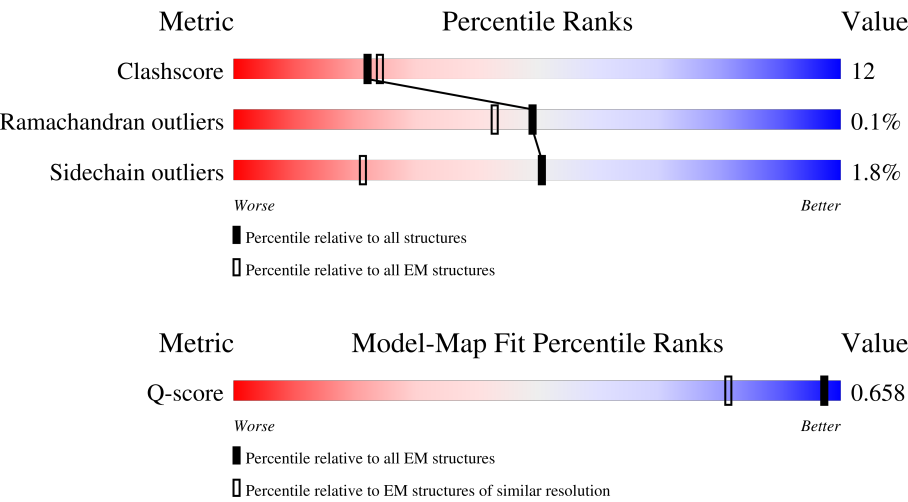
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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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| 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 26261 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     | 41       | Total | C   | N  | O  |   | 0       | 0     |
|     |       |          | 341   | 237 | 55 | 49 |   |         |       |
| 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     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 331   | 223 | 53 | 54 | 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     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 339   | 228 | 54 | 55 | 2 |         |       |
| 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     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 287   | 197 | 46 | 43 | 1 |         |       |
| 6   | 0     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 345   | 231 | 55 | 57 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | D     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 407   | 276 | 63 | 66 | 2 |         |       |
| 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     | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 412   | 279 | 64 | 67 | 2 |         |       |
| 7   | U     | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 412   | 279 | 64 | 67 | 2 |         |       |
| 7   | W     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 431   | 291 | 67 | 71 | 2 |         |       |
| 7   | Y     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 511   | 341 | 83 | 85 | 2 |         |       |

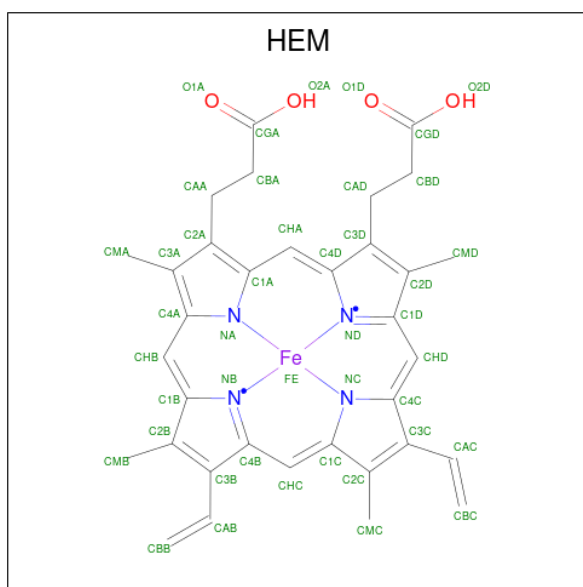
- Molecule 8 is a protein called Antenna complex alpha/beta subunit.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | E     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 343   | 231 | 53 | 56 | 3 |         |       |
| 8   | G     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 349   | 234 | 54 | 58 | 3 |         |       |
| 8   | T     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 349   | 234 | 54 | 58 | 3 |         |       |
| 8   | V     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 349   | 234 | 54 | 58 | 3 |         |       |
| 8   | X     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 349   | 234 | 54 | 58 | 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     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 489   | 332 | 76 | 78 | 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<br>1 | Mg<br>1 | 0       |

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

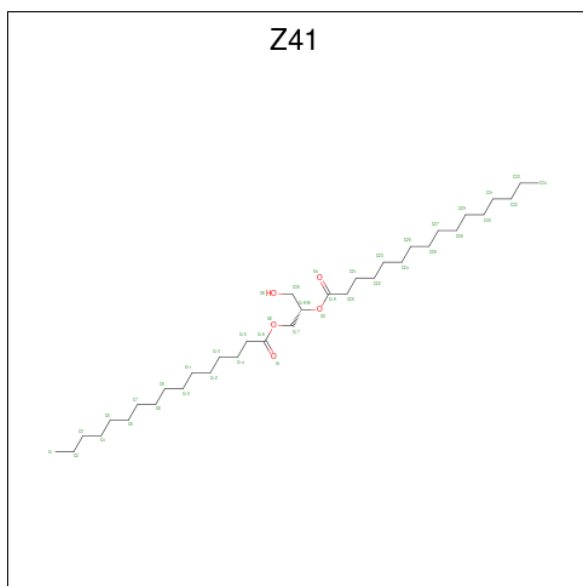
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 12  | C     | 1        | Total Ca<br>1 1 | 0       |
| 12  | M     | 1        | Total Ca<br>1 1 | 0       |
| 12  | D     | 1        | Total Ca<br>1 1 | 0       |
| 12  | F     | 1        | Total Ca<br>1 1 | 0       |

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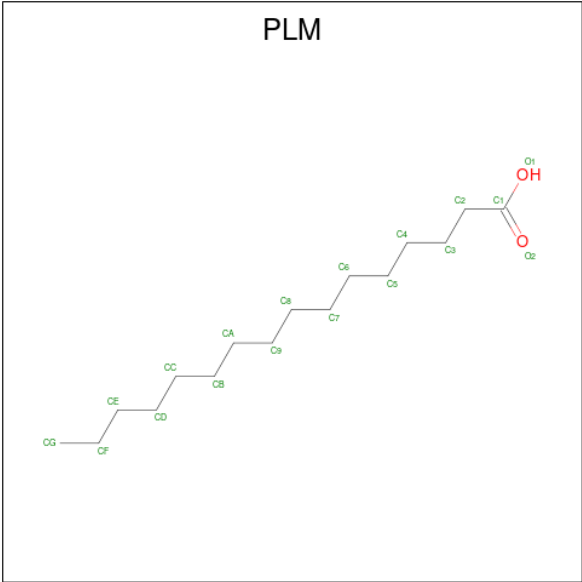
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 12  | S     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 12  | U     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 12  | W     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 12  | Y     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 13 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (CCD ID: Z41) (formula:  $C_{35}H_{68}O_5$ ).



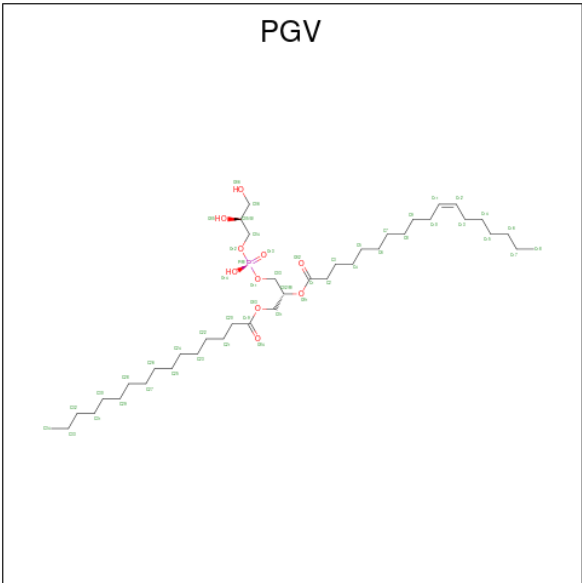
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 13  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |

- Molecule 14 is PALMITIC ACID (CCD ID: PLM) (formula:  $C_{16}H_{32}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 14  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 12    | 11 | 1 |         |

- Molecule 15 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).



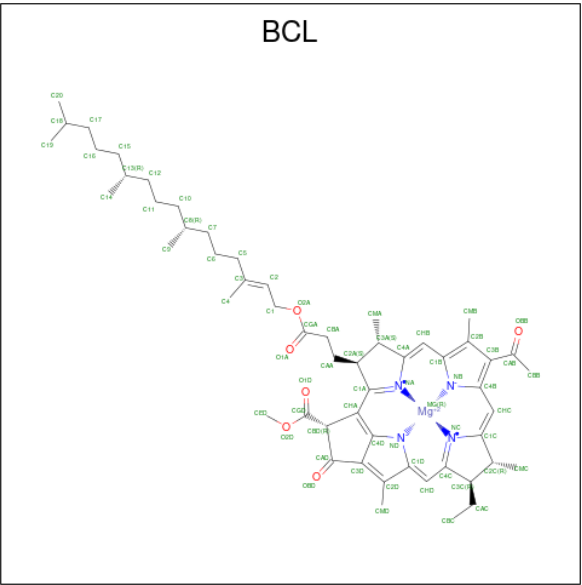
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 15  | C     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 31    | 20 | 10 | 1 |         |
| 15  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 29    | 18 | 10 | 1 |         |

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

- Molecule 16 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 16  | L     | 1        | Total | C  | Mg | N | O       |
|     |       |          | 66    | 55 | 1  | 4 | 6       |
| 16  | L     | 1        | Total | C  | Mg | N | O       |
|     |       |          | 66    | 55 | 1  | 4 | 6       |
| 16  | M     | 1        | Total | C  | Mg | N | O       |
|     |       |          | 66    | 55 | 1  | 4 | 6       |

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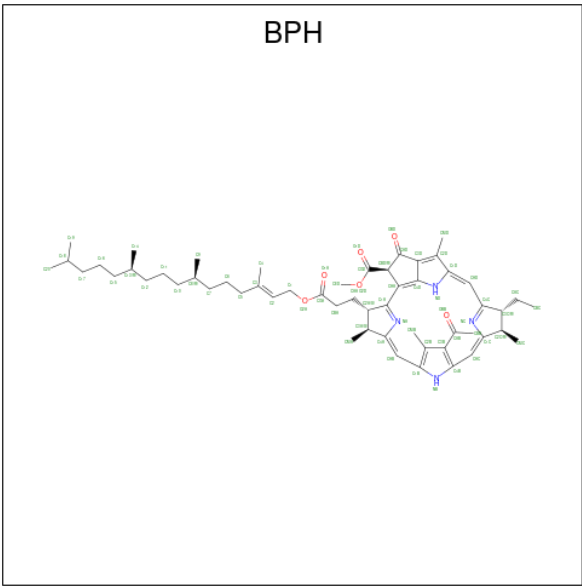
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 16  | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | A     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | B     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | D     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | E     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | F     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | I     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | J     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | K     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | O     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | P     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | Q     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | R     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | S     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | T     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | U     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | V     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | W     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 16  | X     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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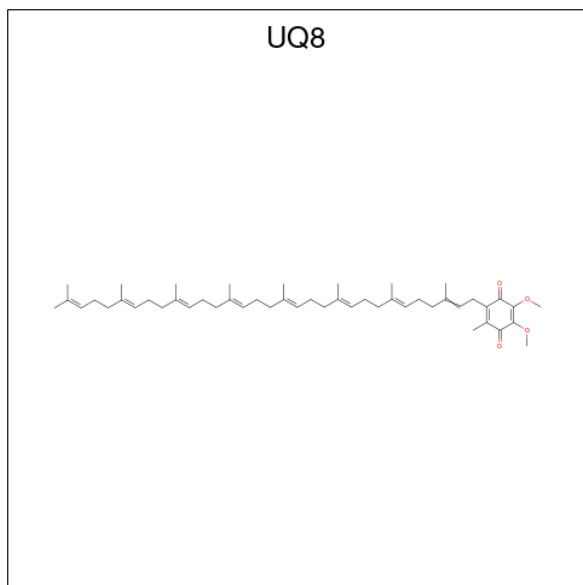
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 16  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 16  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 16  | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

- Molecule 17 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 17  | L     | 1        | Total | C  | N | O | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |
| 17  | M     | 1        | Total | C  | N | O | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |

- Molecule 18 is Ubiquinone-8 (CCD ID: UQ8) (formula:  $C_{49}H_{74}O_4$ ).

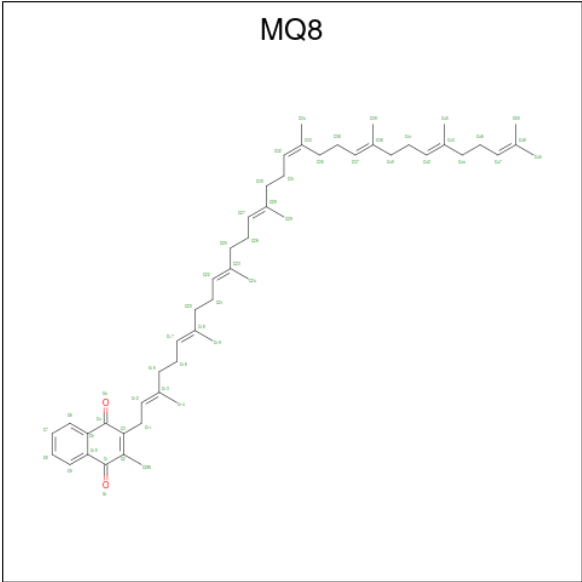


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 18  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 29 | 4 |         |
| 18  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 53    | 49 | 4 |         |
| 18  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 53    | 49 | 4 |         |

- Molecule 19 is FE (III) ION (CCD ID: FE) (formula: Fe).

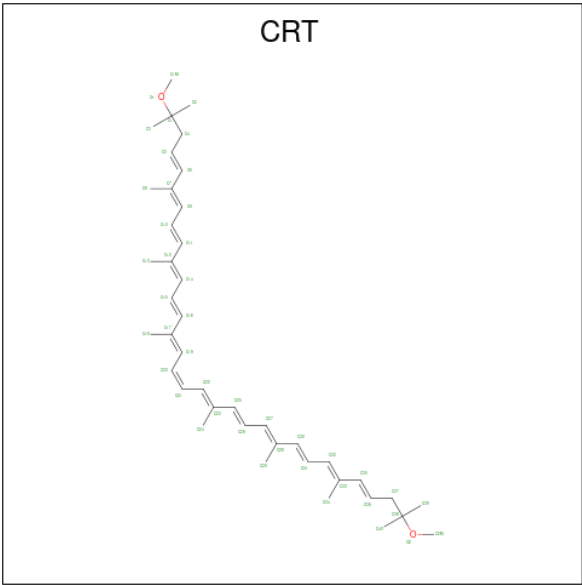
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 19  | M     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 20 is MENAQUINONE 8 (CCD ID: MQ8) (formula:  $C_{51}H_{72}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 20  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 53    | 51 | 2 |         |

- Molecule 21 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C<sub>42</sub>H<sub>60</sub>O<sub>2</sub>).



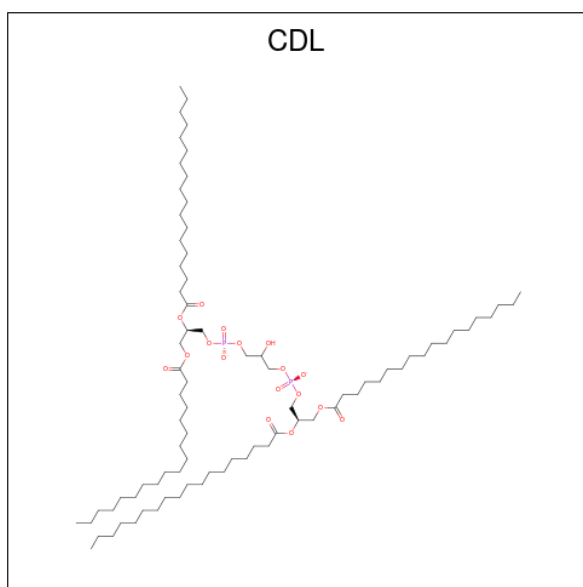
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 21  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |

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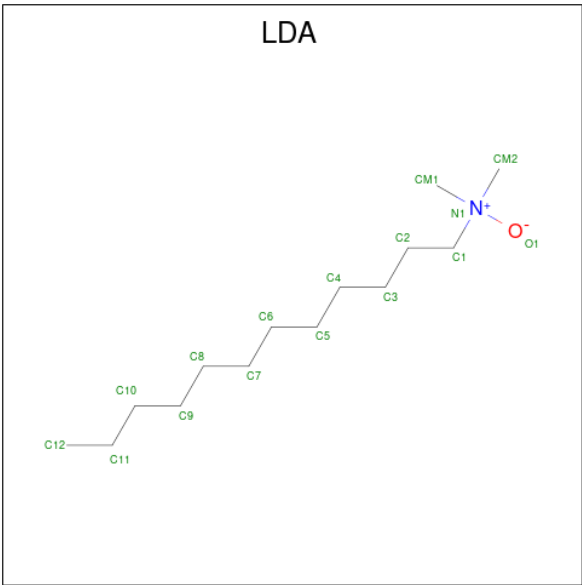
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 21  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | K     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | Q     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | T     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | V     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |
| 21  | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



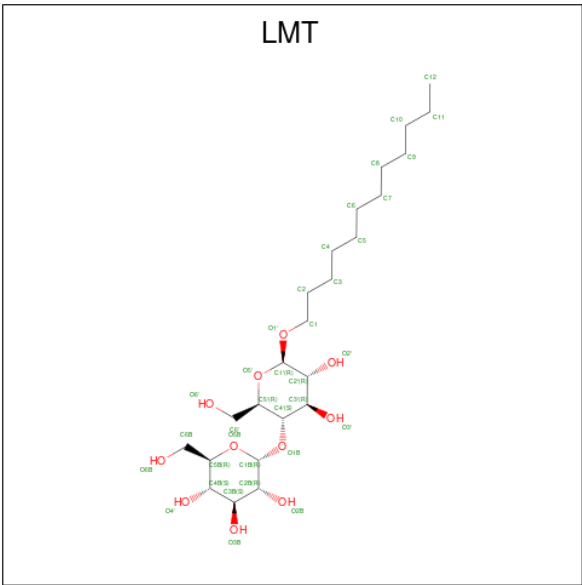
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
|     |       |          | Total | C  | O  | P |         |
| 22  | M     | 1        | 39    | 21 | 16 | 2 | 0       |
| 22  | M     | 1        | 95    | 76 | 17 | 2 | 0       |
| 22  | M     | 1        | 84    | 65 | 17 | 2 | 0       |
| 22  | H     | 1        | 79    | 60 | 17 | 2 | 0       |
| 22  | D     | 1        | 58    | 39 | 17 | 2 | 0       |

- Molecule 23 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula:  $C_{14}H_{31}NO$ ).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 23  | M     | 1        | Total | C  | N | O | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |
| 23  | O     | 1        | Total | C  | N | O | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |

- Molecule 24 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 |
|-----|-------|----------|-------|----|----|--|---------|
| 24  | M     | 1        | Total | C  | O  |  | 0       |
|     |       |          | 35    | 24 | 11 |  |         |
| 24  | H     | 1        | Total | C  | O  |  | 0       |
|     |       |          | 35    | 24 | 11 |  |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 24  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | E     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | P     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | P     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | R     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | V     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | X     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | Z     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | 2     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | 2     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | 5     | 1        | Total | C  | O  | 0       |
|     |       |          | 31    | 20 | 11 |         |
| 24  | 8     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 24  | 0     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 25 is water.

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 25  | C     | 134      | Total | O   | 0       |
|     |       |          | 134   | 134 |         |
| 25  | L     | 50       | Total | O   | 0       |
|     |       |          | 50    | 50  |         |

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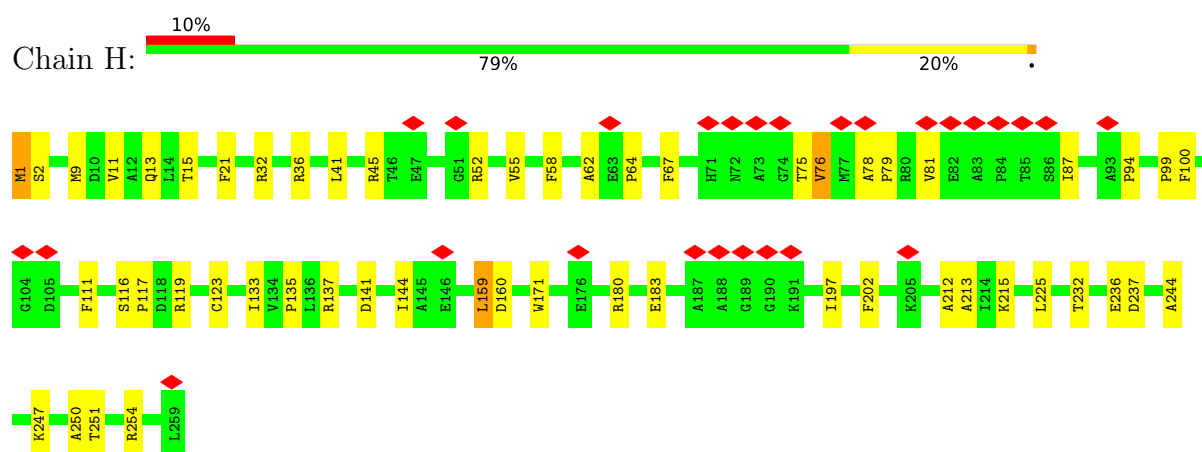
| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 25  | M     | 73       | Total<br>73 | O<br>73 | 0       |
| 25  | H     | 16       | Total<br>16 | O<br>16 | 0       |
| 25  | A     | 2        | Total<br>2  | O<br>2  | 0       |
| 25  | D     | 7        | Total<br>7  | O<br>7  | 0       |
| 25  | E     | 2        | Total<br>2  | O<br>2  | 0       |
| 25  | F     | 3        | Total<br>3  | O<br>3  | 0       |
| 25  | I     | 2        | Total<br>2  | O<br>2  | 0       |
| 25  | K     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | Q     | 3        | Total<br>3  | O<br>3  | 0       |
| 25  | R     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | S     | 6        | Total<br>6  | O<br>6  | 0       |
| 25  | T     | 4        | Total<br>4  | O<br>4  | 0       |
| 25  | U     | 12       | Total<br>12 | O<br>12 | 0       |
| 25  | V     | 3        | Total<br>3  | O<br>3  | 0       |
| 25  | W     | 6        | Total<br>6  | O<br>6  | 0       |
| 25  | X     | 2        | Total<br>2  | O<br>2  | 0       |
| 25  | Y     | 8        | Total<br>8  | O<br>8  | 0       |
| 25  | Z     | 2        | Total<br>2  | O<br>2  | 0       |
| 25  | 1     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | 2     | 1        | Total<br>1  | O<br>1  | 0       |
| 25  | 3     | 10       | Total<br>10 | O<br>10 | 0       |

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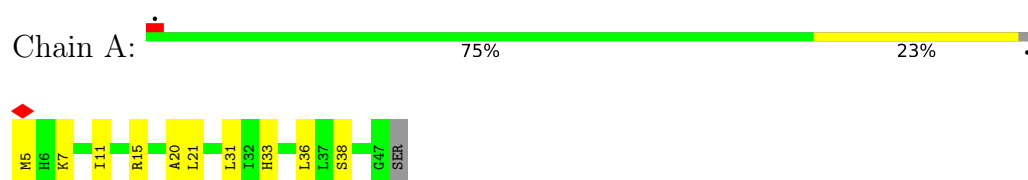
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| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 25  | 5     | 1        | Total<br>1 | O<br>1 | 0       |
| 25  | 7     | 1        | Total<br>1 | O<br>1 | 0       |
| 25  | 9     | 3        | Total<br>3 | O<br>3 | 0       |

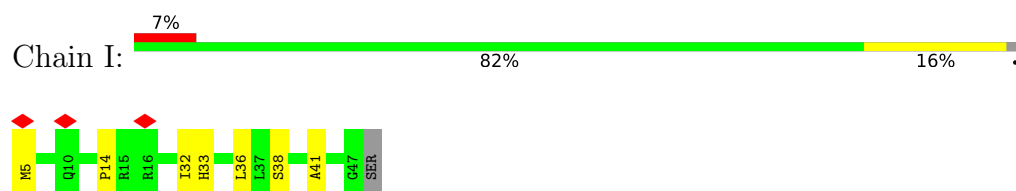




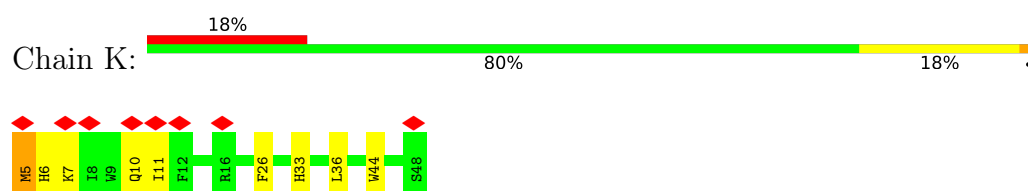
- Molecule 5: Antenna complex alpha/beta subunit



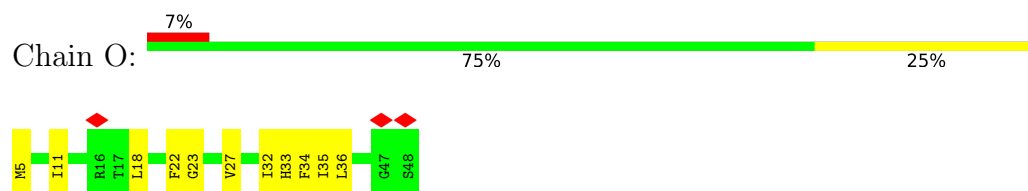
- Molecule 5: Antenna complex alpha/beta subunit



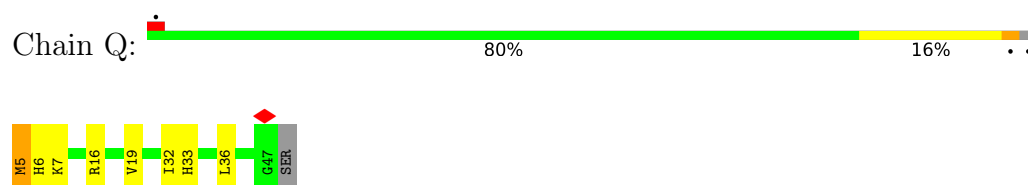
- Molecule 5: Antenna complex alpha/beta subunit



- Molecule 5: Antenna complex alpha/beta subunit



- Molecule 5: Antenna complex alpha/beta subunit



- Molecule 5: Antenna complex alpha/beta subunit

Chain 1:  70% 27% .



- Molecule 5: Antenna complex alpha/beta subunit

Chain 5:  11% 80% 16% ..



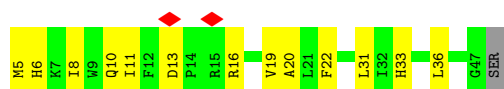
- Molecule 5: Antenna complex alpha/beta subunit

Chain 7:  11% 68% 23% . 7%



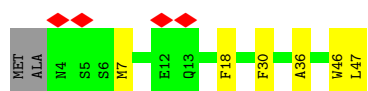
- Molecule 5: Antenna complex alpha/beta subunit

Chain 9:  5% 68% 30% .



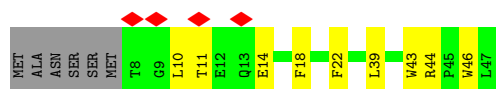
- Molecule 6: Antenna complex alpha/beta subunit

Chain B:  9% 83% 13% .



- Molecule 6: Antenna complex alpha/beta subunit

Chain J:  9% 67% 20% 13%

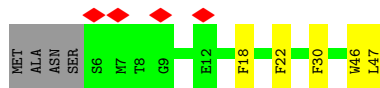
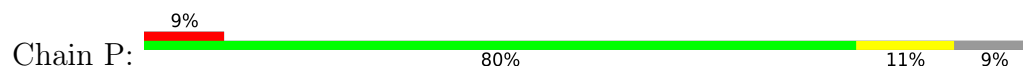


- Molecule 6: Antenna complex alpha/beta subunit

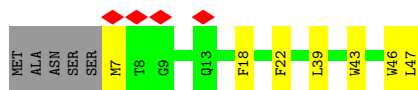
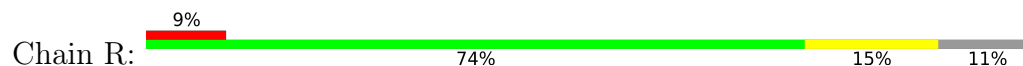
Chain N:  11% 67% 15% 17%



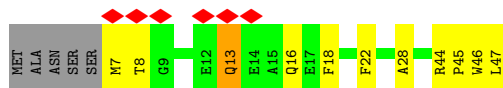
- Molecule 6: Antenna complex alpha/beta subunit



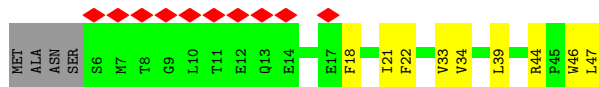
- Molecule 6: Antenna complex alpha/beta subunit



- Molecule 6: Antenna complex alpha/beta subunit



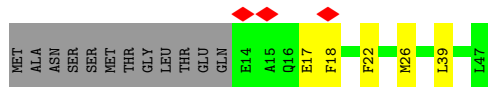
- Molecule 6: Antenna complex alpha/beta subunit



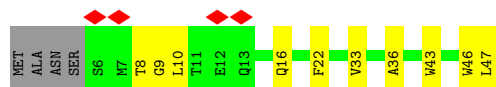
- Molecule 6: Antenna complex alpha/beta subunit



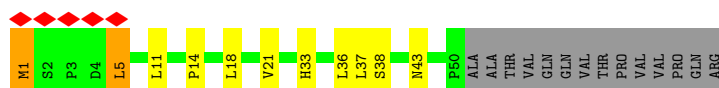
- Molecule 6: Antenna complex alpha/beta subunit



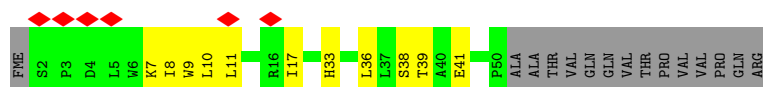
- Molecule 6: Antenna complex alpha/beta subunit



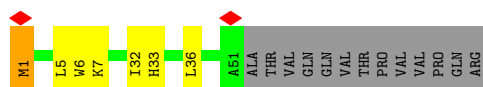
- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



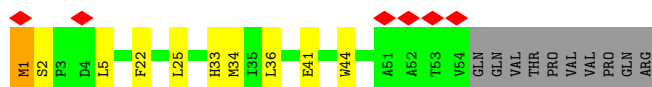
- Molecule 7: Antenna complex alpha/beta subunit



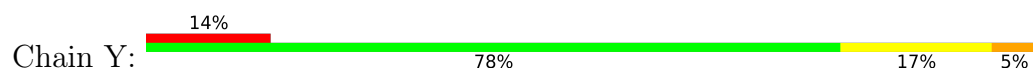
- Molecule 7: Antenna complex alpha/beta subunit

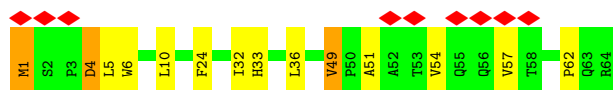


- Molecule 7: Antenna complex alpha/beta subunit

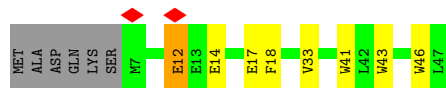


- Molecule 7: Antenna complex alpha/beta subunit

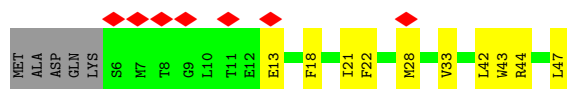




- Molecule 8: Antenna complex alpha/beta subunit



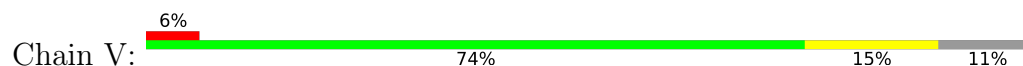
- Molecule 8: Antenna complex alpha/beta subunit



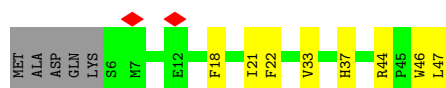
- Molecule 8: Antenna complex alpha/beta subunit



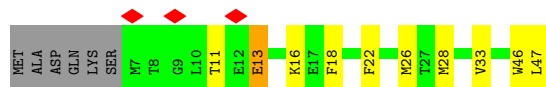
- Molecule 8: Antenna complex alpha/beta subunit



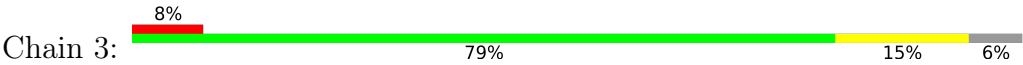
- Molecule 8: Antenna complex alpha/beta subunit



- 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             | 219233                             | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                  | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY                | Depositor |
| Microscope                           | FEI TITAN KRIOS                    | Depositor |
| Voltage (kV)                         | 300                                | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                 | Depositor |
| Minimum defocus (nm)                 | 500                                | Depositor |
| Maximum defocus (nm)                 | 2600                               | Depositor |
| Magnification                        | Not provided                       |           |
| Image detector                       | FEI FALCON III (4k x 4k)           | Depositor |
| Maximum map value                    | 0.244                              | Depositor |
| Minimum map value                    | -0.076                             | Depositor |
| Average map value                    | 0.000                              | Depositor |
| Map value standard deviation         | 0.006                              | Depositor |
| Recommended contour level            | 0.03                               | Depositor |
| Map size ( $\text{\AA}$ )            | 295.2, 295.2, 295.2                | wwPDB     |
| Map dimensions                       | 360, 360, 360                      | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                   | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.82000005, 0.82000005, 0.82000005 | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.19         | 0/2502  | 0.31        | 0/3426  |
| 2   | L     | 0.19         | 0/2295  | 0.29        | 0/3135  |
| 3   | M     | 0.20         | 0/2632  | 0.27        | 0/3601  |
| 4   | H     | 0.13         | 0/2039  | 0.24        | 0/2776  |
| 5   | 1     | 0.14         | 0/362   | 0.21        | 0/492   |
| 5   | 5     | 0.14         | 0/358   | 0.25        | 0/488   |
| 5   | 7     | 0.15         | 0/354   | 0.23        | 0/483   |
| 5   | 9     | 0.15         | 0/362   | 0.24        | 0/492   |
| 5   | A     | 0.16         | 0/362   | 0.23        | 0/492   |
| 5   | I     | 0.14         | 0/362   | 0.20        | 0/492   |
| 5   | K     | 0.13         | 0/369   | 0.20        | 0/500   |
| 5   | O     | 0.15         | 0/369   | 0.22        | 0/500   |
| 5   | Q     | 0.17         | 0/362   | 0.22        | 0/492   |
| 6   | 0     | 0.13         | 0/357   | 0.26        | 0/485   |
| 6   | 2     | 0.12         | 0/351   | 0.16        | 0/477   |
| 6   | 4     | 0.11         | 0/357   | 0.18        | 0/485   |
| 6   | 6     | 0.09         | 0/332   | 0.16        | 0/452   |
| 6   | 8     | 0.11         | 0/299   | 0.19        | 0/407   |
| 6   | B     | 0.12         | 0/371   | 0.17        | 0/504   |
| 6   | J     | 0.11         | 0/343   | 0.19        | 0/467   |
| 6   | N     | 0.11         | 0/332   | 0.16        | 0/452   |
| 6   | P     | 0.12         | 0/357   | 0.17        | 0/485   |
| 6   | R     | 0.13         | 0/351   | 0.15        | 0/477   |
| 7   | D     | 0.14         | 0/409   | 0.25        | 0/561   |
| 7   | F     | 0.13         | 0/409   | 0.23        | 0/561   |
| 7   | S     | 0.15         | 0/414   | 0.21        | 0/568   |
| 7   | U     | 0.15         | 0/414   | 0.21        | 0/568   |
| 7   | W     | 0.15         | 0/433   | 0.25        | 0/595   |
| 7   | Y     | 0.14         | 0/515   | 0.29        | 0/709   |
| 8   | E     | 0.12         | 0/355   | 0.17        | 0/480   |
| 8   | G     | 0.11         | 0/361   | 0.18        | 0/488   |
| 8   | T     | 0.14         | 0/361   | 0.18        | 0/488   |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 8   | V     | 0.13         | 0/361   | 0.17        | 0/488   |
| 8   | X     | 0.13         | 0/361   | 0.16        | 0/488   |
| 8   | Z     | 0.12         | 0/355   | 0.18        | 0/480   |
| 9   | 3     | 0.15         | 0/506   | 0.22        | 0/688   |
| All | All   | 0.16         | 0/21432 | 0.24        | 0/29222 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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        | 2328     | 55      | 0            |
| 2   | L     | 2210  | 0        | 2166     | 50      | 0            |
| 3   | M     | 2533  | 0        | 2490     | 51      | 0            |
| 4   | H     | 1993  | 0        | 1994     | 43      | 0            |
| 5   | 1     | 359   | 0        | 371      | 10      | 0            |
| 5   | 5     | 355   | 0        | 360      | 7       | 0            |
| 5   | 7     | 341   | 0        | 346      | 14      | 0            |
| 5   | 9     | 359   | 0        | 371      | 10      | 0            |
| 5   | A     | 359   | 0        | 371      | 8       | 0            |
| 5   | I     | 359   | 0        | 371      | 7       | 0            |
| 5   | K     | 366   | 0        | 376      | 12      | 0            |
| 5   | O     | 366   | 0        | 376      | 10      | 0            |
| 5   | Q     | 359   | 0        | 371      | 10      | 0            |
| 6   | 0     | 345   | 0        | 334      | 10      | 0            |
| 6   | 2     | 339   | 0        | 329      | 12      | 0            |
| 6   | 4     | 345   | 0        | 334      | 10      | 0            |
| 6   | 6     | 320   | 0        | 310      | 8       | 0            |
| 6   | 8     | 287   | 0        | 278      | 6       | 0            |
| 6   | B     | 359   | 0        | 345      | 7       | 0            |
| 6   | J     | 331   | 0        | 320      | 10      | 0            |
| 6   | N     | 320   | 0        | 310      | 8       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | P     | 345   | 0        | 334      | 5       | 0            |
| 6   | R     | 339   | 0        | 329      | 8       | 0            |
| 7   | D     | 407   | 0        | 424      | 10      | 0            |
| 7   | F     | 397   | 0        | 413      | 9       | 0            |
| 7   | S     | 412   | 0        | 429      | 7       | 0            |
| 7   | U     | 412   | 0        | 429      | 12      | 0            |
| 7   | W     | 431   | 0        | 450      | 12      | 0            |
| 7   | Y     | 511   | 0        | 535      | 11      | 0            |
| 8   | E     | 343   | 0        | 336      | 11      | 0            |
| 8   | G     | 349   | 0        | 341      | 10      | 0            |
| 8   | T     | 349   | 0        | 341      | 11      | 0            |
| 8   | V     | 349   | 0        | 341      | 10      | 0            |
| 8   | X     | 349   | 0        | 341      | 11      | 0            |
| 8   | Z     | 343   | 0        | 336      | 12      | 0            |
| 9   | 3     | 489   | 0        | 497      | 10      | 0            |
| 10  | C     | 172   | 0        | 120      | 22      | 0            |
| 11  | C     | 1     | 0        | 0        | 0       | 0            |
| 12  | C     | 1     | 0        | 0        | 0       | 0            |
| 12  | D     | 1     | 0        | 0        | 0       | 0            |
| 12  | F     | 1     | 0        | 0        | 0       | 0            |
| 12  | M     | 1     | 0        | 0        | 0       | 0            |
| 12  | S     | 1     | 0        | 0        | 0       | 0            |
| 12  | U     | 1     | 0        | 0        | 0       | 0            |
| 12  | W     | 1     | 0        | 0        | 0       | 0            |
| 12  | Y     | 1     | 0        | 0        | 0       | 0            |
| 13  | C     | 35    | 0        | 0        | 0       | 0            |
| 14  | C     | 12    | 0        | 18       | 3       | 0            |
| 15  | 1     | 27    | 0        | 25       | 3       | 0            |
| 15  | C     | 31    | 0        | 32       | 2       | 0            |
| 15  | D     | 39    | 0        | 51       | 4       | 0            |
| 15  | F     | 36    | 0        | 42       | 3       | 0            |
| 15  | H     | 36    | 0        | 42       | 3       | 0            |
| 15  | L     | 97    | 0        | 104      | 11      | 0            |
| 15  | M     | 64    | 0        | 74       | 3       | 0            |
| 16  | 0     | 66    | 0        | 74       | 8       | 0            |
| 16  | 1     | 66    | 0        | 74       | 3       | 0            |
| 16  | 2     | 66    | 0        | 74       | 10      | 0            |
| 16  | 3     | 66    | 0        | 74       | 6       | 0            |
| 16  | 4     | 66    | 0        | 74       | 6       | 0            |
| 16  | 5     | 66    | 0        | 74       | 6       | 0            |
| 16  | 6     | 66    | 0        | 74       | 6       | 0            |
| 16  | 7     | 61    | 0        | 61       | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | 8     | 66    | 0        | 74       | 4       | 0            |
| 16  | 9     | 66    | 0        | 74       | 4       | 0            |
| 16  | A     | 66    | 0        | 74       | 1       | 0            |
| 16  | B     | 66    | 0        | 74       | 8       | 0            |
| 16  | D     | 66    | 0        | 74       | 4       | 0            |
| 16  | E     | 66    | 0        | 74       | 7       | 0            |
| 16  | F     | 66    | 0        | 74       | 1       | 0            |
| 16  | G     | 66    | 0        | 74       | 5       | 0            |
| 16  | I     | 66    | 0        | 74       | 5       | 0            |
| 16  | J     | 66    | 0        | 74       | 5       | 0            |
| 16  | K     | 66    | 0        | 74       | 6       | 0            |
| 16  | L     | 132   | 0        | 148      | 8       | 0            |
| 16  | M     | 132   | 0        | 148      | 8       | 0            |
| 16  | N     | 66    | 0        | 74       | 7       | 0            |
| 16  | O     | 66    | 0        | 74       | 3       | 0            |
| 16  | P     | 66    | 0        | 74       | 8       | 0            |
| 16  | Q     | 66    | 0        | 74       | 4       | 0            |
| 16  | R     | 66    | 0        | 74       | 7       | 0            |
| 16  | S     | 66    | 0        | 74       | 6       | 0            |
| 16  | T     | 66    | 0        | 74       | 10      | 0            |
| 16  | U     | 66    | 0        | 74       | 5       | 0            |
| 16  | V     | 66    | 0        | 74       | 8       | 0            |
| 16  | W     | 66    | 0        | 74       | 2       | 0            |
| 16  | X     | 66    | 0        | 74       | 7       | 0            |
| 16  | Y     | 66    | 0        | 74       | 3       | 0            |
| 16  | Z     | 66    | 0        | 74       | 8       | 0            |
| 17  | L     | 65    | 0        | 76       | 5       | 0            |
| 17  | M     | 65    | 0        | 76       | 7       | 0            |
| 18  | L     | 139   | 0        | 187      | 25      | 0            |
| 19  | M     | 1     | 0        | 0        | 0       | 0            |
| 20  | M     | 53    | 0        | 72       | 4       | 0            |
| 21  | 0     | 44    | 0        | 60       | 4       | 0            |
| 21  | 2     | 44    | 0        | 60       | 7       | 0            |
| 21  | 4     | 44    | 0        | 60       | 11      | 0            |
| 21  | 7     | 44    | 0        | 60       | 10      | 0            |
| 21  | 8     | 44    | 0        | 60       | 7       | 0            |
| 21  | B     | 44    | 0        | 60       | 5       | 0            |
| 21  | E     | 44    | 0        | 60       | 4       | 0            |
| 21  | G     | 44    | 0        | 60       | 7       | 0            |
| 21  | K     | 44    | 0        | 60       | 9       | 0            |
| 21  | M     | 44    | 0        | 60       | 5       | 0            |
| 21  | N     | 44    | 0        | 60       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21  | Q     | 44    | 0        | 60       | 8       | 0            |
| 21  | R     | 44    | 0        | 60       | 5       | 0            |
| 21  | T     | 44    | 0        | 60       | 7       | 0            |
| 21  | V     | 44    | 0        | 60       | 3       | 0            |
| 21  | X     | 44    | 0        | 60       | 9       | 0            |
| 21  | Z     | 44    | 0        | 60       | 6       | 0            |
| 22  | D     | 58    | 0        | 60       | 3       | 0            |
| 22  | H     | 79    | 0        | 105      | 2       | 0            |
| 22  | M     | 218   | 0        | 289      | 13      | 0            |
| 23  | M     | 16    | 0        | 31       | 0       | 0            |
| 23  | O     | 16    | 0        | 31       | 1       | 0            |
| 24  | 0     | 35    | 0        | 46       | 3       | 0            |
| 24  | 2     | 70    | 0        | 92       | 4       | 0            |
| 24  | 4     | 35    | 0        | 46       | 2       | 0            |
| 24  | 5     | 31    | 0        | 35       | 1       | 0            |
| 24  | 8     | 35    | 0        | 46       | 4       | 0            |
| 24  | B     | 35    | 0        | 46       | 3       | 0            |
| 24  | E     | 35    | 0        | 46       | 2       | 0            |
| 24  | G     | 70    | 0        | 92       | 6       | 0            |
| 24  | H     | 35    | 0        | 46       | 3       | 0            |
| 24  | J     | 35    | 0        | 46       | 2       | 0            |
| 24  | M     | 35    | 0        | 46       | 2       | 0            |
| 24  | P     | 70    | 0        | 92       | 5       | 0            |
| 24  | R     | 35    | 0        | 46       | 2       | 0            |
| 24  | V     | 35    | 0        | 46       | 2       | 0            |
| 24  | X     | 35    | 0        | 46       | 0       | 0            |
| 24  | Z     | 35    | 0        | 46       | 2       | 0            |
| 25  | 1     | 1     | 0        | 0        | 0       | 0            |
| 25  | 2     | 1     | 0        | 0        | 0       | 0            |
| 25  | 3     | 10    | 0        | 0        | 0       | 0            |
| 25  | 5     | 1     | 0        | 0        | 0       | 0            |
| 25  | 7     | 1     | 0        | 0        | 0       | 0            |
| 25  | 9     | 3     | 0        | 0        | 0       | 0            |
| 25  | A     | 2     | 0        | 0        | 0       | 0            |
| 25  | C     | 134   | 0        | 0        | 1       | 0            |
| 25  | D     | 7     | 0        | 0        | 0       | 0            |
| 25  | E     | 2     | 0        | 0        | 0       | 0            |
| 25  | F     | 3     | 0        | 0        | 0       | 0            |
| 25  | H     | 16    | 0        | 0        | 0       | 0            |
| 25  | I     | 2     | 0        | 0        | 0       | 0            |
| 25  | K     | 1     | 0        | 0        | 0       | 0            |
| 25  | L     | 50    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25  | M     | 73    | 0        | 0        | 3       | 0            |
| 25  | Q     | 3     | 0        | 0        | 0       | 0            |
| 25  | R     | 1     | 0        | 0        | 0       | 0            |
| 25  | S     | 6     | 0        | 0        | 0       | 0            |
| 25  | T     | 4     | 0        | 0        | 0       | 0            |
| 25  | U     | 12    | 0        | 0        | 0       | 0            |
| 25  | V     | 3     | 0        | 0        | 0       | 0            |
| 25  | W     | 6     | 0        | 0        | 0       | 0            |
| 25  | X     | 2     | 0        | 0        | 0       | 0            |
| 25  | Y     | 8     | 0        | 0        | 0       | 0            |
| 25  | Z     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 26261 | 0        | 26696    | 606     | 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 12.

All (606) 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  | 1.62                     | 1.39              |
| 1:C:250:CYS:SG   | 10:C:403:HEM:HAC  | 1.60                     | 1.39              |
| 1:C:310:CYS:SG   | 10:C:404:HEM:CAC  | 2.15                     | 1.34              |
| 1:C:155:CYS:SG   | 10:C:402:HEM:CAC  | 2.15                     | 1.33              |
| 1:C:250:CYS:SG   | 10:C:403:HEM:CAC  | 2.19                     | 1.30              |
| 1:C:110:CYS:SG   | 10:C:401:HEM:HAC  | 1.72                     | 1.28              |
| 1:C:310:CYS:SG   | 10:C:404:HEM:HAC  | 1.73                     | 1.25              |
| 1:C:110:CYS:SG   | 10:C:401:HEM:CAC  | 2.24                     | 1.24              |
| 1:C:155:CYS:HG   | 10:C:402:HEM:HAC  | 0.81                     | 0.93              |
| 1:C:155:CYS:HG   | 10:C:402:HEM:CAC  | 1.70                     | 0.87              |
| 6:O:8:THR:HG23   | 6:O:10:LEU:H      | 1.45                     | 0.81              |
| 1:C:151:THR:HG22 | 1:C:153:TYR:H     | 1.48                     | 0.77              |
| 14:C:408:PLM:H51 | 15:L:305:PGV:H42  | 1.66                     | 0.75              |
| 1:C:155:CYS:SG   | 10:C:402:HEM:C3C  | 2.80                     | 0.73              |
| 1:C:310:CYS:SG   | 10:C:404:HEM:C3C  | 2.82                     | 0.73              |
| 16:L:307:BCL:HHC | 16:M:404:BCL:H42  | 1.71                     | 0.72              |
| 8:V:43:TRP:HB2   | 24:V:101:LMT:H31  | 1.72                     | 0.72              |
| 4:H:45:ARG:NH1   | 6:B:7:MET:O       | 2.22                     | 0.72              |
| 2:L:203:VAL:HG13 | 2:L:213:LYS:HB2   | 1.73                     | 0.71              |
| 5:A:31:LEU:HD11  | 15:D:501:PGV:H201 | 1.73                     | 0.70              |
| 4:H:58:PHE:HB3   | 22:D:502:CDL:H141 | 1.72                     | 0.70              |
| 3:M:81:TRP:HB3   | 7:U:34:MET:HE3    | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:2:104:LMT:H42  | 6:4:39:LEU:HB3    | 1.75                     | 0.69              |
| 7:U:2:SER:H       | 7:U:5:LEU:HD23    | 1.56                     | 0.69              |
| 8:G:47:LEU:HD13   | 24:G:104:LMT:H32  | 1.76                     | 0.68              |
| 6:2:18:PHE:HA     | 21:2:103:CRT:H6   | 1.76                     | 0.68              |
| 7:F:39:THR:HG22   | 7:F:41:GLU:H      | 1.59                     | 0.67              |
| 4:H:133:ILE:HD12  | 4:H:180:ARG:HG3   | 1.76                     | 0.66              |
| 7:D:11:LEU:HD11   | 21:G:103:CRT:H23  | 1.77                     | 0.66              |
| 24:P:103:LMT:H42  | 6:R:39:LEU:HB3    | 1.77                     | 0.66              |
| 17:M:405:BPH:HBB3 | 17:M:405:BPH:HHC  | 1.76                     | 0.65              |
| 22:M:411:CDL:H141 | 22:M:411:CDL:H532 | 1.77                     | 0.65              |
| 4:H:137:ARG:NH2   | 4:H:183:GLU:OE1   | 2.30                     | 0.65              |
| 1:C:110:CYS:HG    | 10:C:401:HEM:CAC  | 2.08                     | 0.65              |
| 2:L:237:ARG:HH21  | 3:M:6:ASN:HD22    | 1.46                     | 0.64              |
| 8:G:42:LEU:O      | 24:G:101:LMT:O3'  | 2.14                     | 0.64              |
| 2:L:23:PHE:HE1    | 5:9:19:VAL:HG21   | 1.61                     | 0.64              |
| 15:L:306:PGV:H232 | 15:H:301:PGV:H201 | 1.78                     | 0.64              |
| 5:A:11:ILE:HD11   | 21:E:103:CRT:H23  | 1.79                     | 0.63              |
| 8:X:22:PHE:HA     | 21:X:103:CRT:H14  | 1.79                     | 0.63              |
| 15:1:401:PGV:H011 | 15:1:401:PGV:H32  | 1.80                     | 0.63              |
| 7:U:11:LEU:HD12   | 21:X:103:CRT:H82  | 1.81                     | 0.63              |
| 3:M:98:PRO:HB3    | 3:M:107:PRO:HG3   | 1.80                     | 0.63              |
| 5:1:13:ASP:HB3    | 5:1:16:ARG:HG2    | 1.80                     | 0.63              |
| 1:C:278:ASP:OD1   | 1:C:282:ASN:ND2   | 2.30                     | 0.62              |
| 6:N:47:LEU:HD13   | 24:P:101:LMT:H32  | 1.81                     | 0.62              |
| 8:T:33:VAL:HG11   | 16:T:101:BCL:HBA2 | 1.81                     | 0.62              |
| 9:3:36:LEU:HD11   | 16:4:101:BCL:HHD  | 1.80                     | 0.62              |
| 1:C:72:VAL:HG13   | 1:C:76:TYR:HD2    | 1.65                     | 0.62              |
| 15:M:410:PGV:H251 | 5:O:27:VAL:HG21   | 1.82                     | 0.61              |
| 8:G:43:TRP:HB2    | 24:G:101:LMT:H52  | 1.80                     | 0.61              |
| 15:L:309:PGV:O14  | 5:A:15:ARG:NH1    | 2.32                     | 0.61              |
| 21:G:103:CRT:H393 | 5:I:33:HIS:HB3    | 1.83                     | 0.61              |
| 2:L:97:ILE:HG21   | 18:L:304:UQ8:H22A | 1.83                     | 0.61              |
| 4:H:212:ALA:O     | 4:H:254:ARG:NH2   | 2.25                     | 0.61              |
| 5:Q:7:LYS:NZ      | 8:T:17:GLU:OE2    | 2.26                     | 0.61              |
| 5:K:7:LYS:HB3     | 21:Q:101:CRT:H41  | 1.81                     | 0.61              |
| 7:F:41:GLU:O      | 8:G:44:ARG:NH1    | 2.33                     | 0.61              |
| 24:G:104:LMT:H31  | 6:J:43:TRP:HB2    | 1.83                     | 0.61              |
| 5:I:36:LEU:HD11   | 16:J:101:BCL:HHD  | 1.83                     | 0.60              |
| 7:Y:1:FME:SD      | 7:Y:1:FME:N       | 2.74                     | 0.60              |
| 4:H:32:ARG:HG2    | 4:H:62:ALA:HB2    | 1.83                     | 0.60              |
| 17:M:405:BPH:HBC3 | 17:M:405:BPH:HHD  | 1.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:78:ALA:HB3    | 4:H:79:PRO:HD3    | 1.83                     | 0.60              |
| 24:4:103:LMT:H22  | 6:6:43:TRP:HB2    | 1.82                     | 0.60              |
| 2:L:174:HIS:HB3   | 3:M:183:LEU:HD13  | 1.84                     | 0.60              |
| 14:C:408:PLM:H32  | 15:L:305:PGV:H21  | 1.84                     | 0.59              |
| 3:M:28:LEU:HD12   | 3:M:54:GLY:HA2    | 1.82                     | 0.59              |
| 1:C:250:CYS:SG    | 10:C:403:HEM:C3C  | 2.94                     | 0.59              |
| 16:U:101:BCL:H152 | 8:V:28:MET:HB3    | 1.84                     | 0.59              |
| 7:Y:4:ASP:OD1     | 7:Y:4:ASP:N       | 2.35                     | 0.59              |
| 1:C:191:ALA:HB3   | 1:C:237:MET:HE3   | 1.83                     | 0.59              |
| 7:U:8:ILE:HA      | 21:X:103:CRT:H83  | 1.84                     | 0.59              |
| 8:V:7:MET:SD      | 8:V:7:MET:N       | 2.70                     | 0.59              |
| 7:F:38:SER:OG     | 15:F:501:PGV:O04  | 2.21                     | 0.59              |
| 4:H:67:PHE:HB2    | 4:H:76:VAL:HG13   | 1.84                     | 0.59              |
| 5:O:36:LEU:HD11   | 16:P:102:BCL:HHD  | 1.84                     | 0.59              |
| 24:R:103:LMT:H31  | 8:T:43:TRP:HB2    | 1.83                     | 0.59              |
| 3:M:229:PHE:HB2   | 3:M:244:ALA:HB2   | 1.84                     | 0.59              |
| 16:M:404:BCL:H12  | 17:M:405:BPH:HBB3 | 1.84                     | 0.58              |
| 6:R:7:MET:SD      | 6:R:7:MET:N       | 2.75                     | 0.58              |
| 22:H:302:CDL:OA3  | 22:D:502:CDL:O1   | 2.20                     | 0.58              |
| 5:O:11:ILE:HD11   | 21:R:102:CRT:H23  | 1.86                     | 0.58              |
| 5:Q:5:FME:O       | 5:Q:7:LYS:N       | 2.31                     | 0.58              |
| 5:5:22:PHE:HE1    | 21:7:101:CRT:H182 | 1.68                     | 0.58              |
| 5:A:7:LYS:NZ      | 8:E:17:GLU:OE2    | 2.26                     | 0.58              |
| 1:C:27:PRO:HD3    | 9:3:38:ARG:HG2    | 1.85                     | 0.58              |
| 17:L:302:BPH:HHC  | 17:L:302:BPH:HBB3 | 1.85                     | 0.58              |
| 21:N:102:CRT:H35  | 16:O:502:BCL:HMB1 | 1.86                     | 0.58              |
| 7:D:5:LEU:HD23    | 8:G:21:ILE:HD11   | 1.86                     | 0.58              |
| 2:L:8:ARG:HG2     | 4:H:87:ILE:HG21   | 1.85                     | 0.57              |
| 18:L:304:UQ8:H20A | 5:7:31:LEU:HA     | 1.86                     | 0.57              |
| 3:M:233:ARG:NH1   | 4:H:236:GLU:OE1   | 2.37                     | 0.57              |
| 21:Z:103:CRT:H36  | 5:1:30:LEU:HD23   | 1.86                     | 0.57              |
| 5:5:36:LEU:HD11   | 16:6:101:BCL:HHD  | 1.86                     | 0.57              |
| 21:B:103:CRT:H23  | 5:9:11:ILE:HD11   | 1.87                     | 0.57              |
| 4:H:13:GLN:NE2    | 15:H:301:PGV:O13  | 2.38                     | 0.57              |
| 2:L:13:ARG:HH11   | 2:L:13:ARG:HB2    | 1.70                     | 0.56              |
| 6:6:37:HIS:HB3    | 16:6:101:BCL:H92  | 1.86                     | 0.56              |
| 5:7:36:LEU:HD11   | 16:8:102:BCL:HHD  | 1.88                     | 0.56              |
| 1:C:129:ARG:NH1   | 1:C:132:GLU:OE1   | 2.38                     | 0.56              |
| 7:F:36:LEU:HD11   | 16:G:102:BCL:HHD  | 1.88                     | 0.56              |
| 24:P:101:LMT:H5B  | 24:P:101:LMT:H6E  | 1.87                     | 0.56              |
| 4:H:159:LEU:HD22  | 4:H:215:LYS:HG2   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Q:36:LEU:HD11   | 16:R:101:BCL:HHD  | 1.88                     | 0.56              |
| 15:M:410:PGV:H201 | 5:O:23:GLY:HA3    | 1.86                     | 0.56              |
| 24:G:104:LMT:H42  | 6:J:39:LEU:HB3    | 1.88                     | 0.55              |
| 5:1:11:ILE:HD11   | 21:4:102:CRT:H23  | 1.88                     | 0.55              |
| 15:L:305:PGV:H22  | 15:1:401:PGV:H202 | 1.87                     | 0.55              |
| 4:H:1:FME:HB2     | 24:H:303:LMT:H21  | 1.89                     | 0.55              |
| 1:C:25:ARG:NH2    | 9:3:43:ASP:OD2    | 2.40                     | 0.55              |
| 6:P:47:LEU:HD13   | 24:P:103:LMT:H32  | 1.88                     | 0.55              |
| 2:L:179:HIS:CE1   | 2:L:183:ILE:HD11  | 2.42                     | 0.55              |
| 24:P:103:LMT:H31  | 6:R:43:TRP:HB2    | 1.88                     | 0.55              |
| 6:B:18:PHE:HB2    | 21:B:103:CRT:H21A | 1.87                     | 0.55              |
| 1:C:246:ASN:HA    | 2:L:171:LEU:HD21  | 1.90                     | 0.54              |
| 22:M:412:CDL:H801 | 22:M:412:CDL:H561 | 1.89                     | 0.54              |
| 8:G:18:PHE:HA     | 21:G:103:CRT:H6   | 1.88                     | 0.54              |
| 7:S:33:HIS:CE1    | 16:T:101:BCL:HMD3 | 2.42                     | 0.54              |
| 24:R:103:LMT:H52  | 8:T:39:LEU:HB3    | 1.90                     | 0.54              |
| 5:1:36:LEU:HD11   | 16:2:102:BCL:HHD  | 1.90                     | 0.54              |
| 7:Y:10:LEU:HB2    | 21:2:103:CRT:H1M1 | 1.89                     | 0.54              |
| 8:E:18:PHE:HB2    | 21:E:103:CRT:H21A | 1.89                     | 0.54              |
| 3:M:61:ILE:HG23   | 17:M:405:BPH:H121 | 1.89                     | 0.54              |
| 5:K:5:FME:HE2     | 16:O:502:BCL:H18  | 1.90                     | 0.54              |
| 16:Y:101:BCL:H3C  | 24:Z:101:LMT:H62  | 1.90                     | 0.54              |
| 5:A:38:SER:O      | 15:D:501:PGV:O06  | 2.25                     | 0.54              |
| 1:C:32:GLN:HB2    | 2:L:77:LEU:HD12   | 1.90                     | 0.53              |
| 8:G:18:PHE:HB2    | 21:G:103:CRT:H21A | 1.90                     | 0.53              |
| 24:2:101:LMT:H5B  | 24:2:101:LMT:H6E  | 1.90                     | 0.53              |
| 6:6:18:PHE:HB2    | 21:7:101:CRT:H21A | 1.89                     | 0.53              |
| 5:7:25:LEU:HB2    | 16:7:102:BCL:H43  | 1.90                     | 0.53              |
| 3:M:13:VAL:HG12   | 4:H:144:ILE:HD13  | 1.90                     | 0.53              |
| 7:F:7:LYS:HA      | 7:F:10:LEU:HD13   | 1.90                     | 0.53              |
| 7:W:41:GLU:O      | 8:X:44:ARG:NH1    | 2.40                     | 0.53              |
| 16:6:101:BCL:H172 | 24:8:101:LMT:H41  | 1.91                     | 0.53              |
| 1:C:205:ASP:OD1   | 1:C:281:GLN:NE2   | 2.42                     | 0.53              |
| 5:9:33:HIS:CE1    | 16:0:102:BCL:HMD3 | 2.44                     | 0.53              |
| 21:B:103:CRT:H35  | 16:D:503:BCL:HMB1 | 1.91                     | 0.53              |
| 7:Y:1:FME:HG2     | 6:2:28:ALA:HB2    | 1.91                     | 0.53              |
| 3:M:157:TYR:CZ    | 21:M:407:CRT:H293 | 2.43                     | 0.53              |
| 7:W:36:LEU:HD11   | 16:X:102:BCL:HHD  | 1.90                     | 0.53              |
| 7:W:2:SER:HB3     | 7:W:5:LEU:HG      | 1.91                     | 0.53              |
| 21:K:101:CRT:H342 | 16:K:102:BCL:HBA2 | 1.91                     | 0.53              |
| 21:Z:103:CRT:H372 | 5:1:33:HIS:CG     | 2.44                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:18:LEU:HD21   | 21:7:101:CRT:H132 | 1.90                     | 0.53              |
| 5:I:41:ALA:O      | 6:J:44:ARG:NH1    | 2.39                     | 0.52              |
| 3:M:10:THR:HG21   | 4:H:202:PHE:HB2   | 1.91                     | 0.52              |
| 8:Z:18:PHE:HA     | 21:Z:103:CRT:H6   | 1.92                     | 0.52              |
| 7:D:33:HIS:CE1    | 16:E:102:BCL:HMD3 | 2.44                     | 0.52              |
| 6:8:22:PHE:CD1    | 21:8:103:CRT:H14  | 2.45                     | 0.52              |
| 22:H:302:CDL:H862 | 22:H:302:CDL:H592 | 1.91                     | 0.52              |
| 5:7:10:GLN:HB2    | 21:0:103:CRT:H1M1 | 1.91                     | 0.52              |
| 1:C:167:VAL:HG22  | 7:Y:62:PRO:HD2    | 1.91                     | 0.52              |
| 2:L:32:VAL:HG23   | 2:L:33:GLY:H      | 1.75                     | 0.52              |
| 6:0:36:ALA:HB1    | 24:0:101:LMT:H101 | 1.92                     | 0.52              |
| 4:H:41:LEU:HD12   | 4:H:55:VAL:HG12   | 1.91                     | 0.52              |
| 7:W:22:PHE:HE1    | 21:X:103:CRT:H182 | 1.75                     | 0.52              |
| 1:C:236:MET:HB3   | 10:C:403:HEM:C4B  | 2.45                     | 0.52              |
| 1:C:25:ARG:HD3    | 15:C:409:PGV:H31  | 1.92                     | 0.51              |
| 24:2:104:LMT:H61  | 16:3:101:BCL:H3C  | 1.91                     | 0.51              |
| 21:4:102:CRT:H291 | 21:4:102:CRT:H32  | 1.93                     | 0.51              |
| 2:L:13:ARG:NH1    | 2:L:21:ASP:OD1    | 2.43                     | 0.51              |
| 15:L:309:PGV:H41  | 5:A:20:ALA:HB2    | 1.93                     | 0.51              |
| 8:Z:11:THR:OG1    | 8:Z:13:GLU:OE1    | 2.24                     | 0.51              |
| 4:H:141:ASP:OD1   | 4:H:141:ASP:N     | 2.38                     | 0.51              |
| 6:0:43:TRP:HB2    | 24:0:101:LMT:H22  | 1.92                     | 0.51              |
| 7:D:37:LEU:O      | 7:D:43:ASN:ND2    | 2.40                     | 0.51              |
| 7:S:1:FME:O       | 8:V:24:GLN:NE2    | 2.44                     | 0.51              |
| 1:C:110:CYS:HB2   | 10:C:401:HEM:C3C  | 2.45                     | 0.51              |
| 4:H:64:PRO:HA     | 4:H:79:PRO:HD2    | 1.92                     | 0.51              |
| 6:4:21:ILE:HD11   | 21:4:102:CRT:H6   | 1.93                     | 0.51              |
| 6:4:21:ILE:HG13   | 21:4:102:CRT:H9   | 1.92                     | 0.51              |
| 1:C:184:ASN:ND2   | 3:M:96:GLU:HG2    | 2.26                     | 0.50              |
| 1:C:119:ASP:OD1   | 1:C:124:LYS:NZ    | 2.41                     | 0.50              |
| 17:L:302:BPH:HHC  | 17:L:302:BPH:CBB  | 2.40                     | 0.50              |
| 5:Q:5:FME:C       | 5:Q:7:LYS:H       | 2.23                     | 0.50              |
| 8:X:21:ILE:HD12   | 21:X:103:CRT:H6   | 1.92                     | 0.50              |
| 2:L:83:MET:HB3    | 5:7:38:SER:HB3    | 1.93                     | 0.50              |
| 3:M:148:TRP:HE1   | 22:M:411:CDL:H361 | 1.76                     | 0.50              |
| 22:M:411:CDL:H801 | 4:H:21:PHE:HB3    | 1.94                     | 0.50              |
| 16:2:102:BCL:H203 | 16:2:102:BCL:H13  | 1.93                     | 0.50              |
| 5:O:22:PHE:HE1    | 21:Q:101:CRT:H182 | 1.77                     | 0.50              |
| 1:C:48:LEU:HD21   | 15:C:409:PGV:H05  | 1.94                     | 0.50              |
| 2:L:207:GLN:HB2   | 2:L:210:GLU:HG3   | 1.93                     | 0.50              |
| 21:R:102:CRT:H372 | 7:S:33:HIS:CG     | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:11:VAL:HG21   | 24:H:303:LMT:H32  | 1.94                     | 0.50              |
| 5:K:33:HIS:CE1    | 16:N:101:BCL:HMD1 | 2.47                     | 0.50              |
| 1:C:45:ASN:HB3    | 1:C:48:LEU:HB2    | 1.94                     | 0.50              |
| 5:A:33:HIS:CE1    | 16:B:102:BCL:HMD3 | 2.47                     | 0.50              |
| 3:M:65:PHE:HD1    | 17:M:405:BPH:H112 | 1.77                     | 0.49              |
| 5:I:33:HIS:CE1    | 16:J:101:BCL:HMD3 | 2.45                     | 0.49              |
| 5:K:36:LEU:HD11   | 16:N:101:BCL:HHD  | 1.94                     | 0.49              |
| 1:C:184:ASN:HD21  | 3:M:96:GLU:HG2    | 1.76                     | 0.49              |
| 3:M:131:VAL:HG21  | 15:M:410:PGV:H212 | 1.94                     | 0.49              |
| 22:M:411:CDL:H672 | 24:H:303:LMT:H123 | 1.94                     | 0.49              |
| 7:D:36:LEU:HD11   | 16:E:102:BCL:HHD  | 1.94                     | 0.49              |
| 4:H:215:LYS:NZ    | 4:H:250:ALA:O     | 2.45                     | 0.49              |
| 8:T:22:PHE:HA     | 21:T:102:CRT:H14  | 1.94                     | 0.49              |
| 3:M:65:PHE:CD1    | 17:M:405:BPH:H112 | 2.47                     | 0.49              |
| 7:W:33:HIS:CE1    | 16:X:102:BCL:HMD3 | 2.48                     | 0.49              |
| 1:C:151:THR:HG22  | 1:C:153:TYR:N     | 2.23                     | 0.49              |
| 18:L:304:UQ8:H23  | 5:7:27:VAL:HG13   | 1.94                     | 0.49              |
| 8:E:33:VAL:HG11   | 16:E:102:BCL:HAA1 | 1.95                     | 0.49              |
| 6:R:46:TRP:CD1    | 6:R:47:LEU:HG     | 2.46                     | 0.49              |
| 4:H:36:ARG:HG2    | 4:H:79:PRO:HG3    | 1.94                     | 0.49              |
| 7:S:7:LYS:HB3     | 21:V:103:CRT:H23  | 1.95                     | 0.49              |
| 2:L:108:LEU:HD11  | 22:M:412:CDL:H602 | 1.95                     | 0.49              |
| 3:M:74:ASN:HD21   | 3:M:114:TRP:CD1   | 2.30                     | 0.49              |
| 3:M:289:THR:HB    | 24:M:414:LMT:H11  | 1.95                     | 0.49              |
| 4:H:197:ILE:HD11  | 4:H:202:PHE:HE2   | 1.77                     | 0.49              |
| 6:2:22:PHE:HA     | 21:2:103:CRT:H11  | 1.93                     | 0.49              |
| 2:L:136:VAL:HA    | 2:L:140:VAL:HB    | 1.95                     | 0.49              |
| 2:L:187:PHE:HB3   | 17:M:405:BPH:HBB2 | 1.93                     | 0.49              |
| 5:K:10:GLN:HE21   | 6:N:12:GLU:HG2    | 1.78                     | 0.49              |
| 7:U:36:LEU:HD11   | 16:V:102:BCL:HHD  | 1.94                     | 0.49              |
| 2:L:104:VAL:HG22  | 22:M:412:CDL:H821 | 1.93                     | 0.49              |
| 6:B:46:TRP:CD1    | 6:B:47:LEU:HG     | 2.48                     | 0.49              |
| 5:O:33:HIS:CE1    | 16:P:102:BCL:HMD3 | 2.47                     | 0.49              |
| 1:C:292:PRO:HD2   | 1:C:295:ARG:HG2   | 1.95                     | 0.48              |
| 6:B:46:TRP:CE2    | 16:B:102:BCL:H2C  | 2.48                     | 0.48              |
| 6:P:30:PHE:CE1    | 16:P:102:BCL:H11  | 2.48                     | 0.48              |
| 9:3:31:PHE:HE2    | 21:4:102:CRT:H2M2 | 1.77                     | 0.48              |
| 1:C:162:PRO:HD2   | 10:C:402:HEM:HBD2 | 1.94                     | 0.48              |
| 3:M:52:TYR:O      | 3:M:132:ARG:NH1   | 2.41                     | 0.48              |
| 2:L:25:PHE:CE1    | 2:L:32:VAL:HG21   | 2.48                     | 0.48              |
| 22:M:411:CDL:H371 | 22:M:411:CDL:H121 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:102:BCL:H93  | 16:P:102:BCL:HMB2 | 1.95                     | 0.48              |
| 1:C:110:CYS:CB    | 10:C:401:HEM:HAC  | 2.40                     | 0.48              |
| 15:L:306:PGV:H202 | 15:H:301:PGV:H062 | 1.95                     | 0.48              |
| 7:F:9:TRP:HZ3     | 7:F:17:ILE:HG21   | 1.78                     | 0.48              |
| 6:2:18:PHE:HB2    | 21:2:103:CRT:H21A | 1.94                     | 0.48              |
| 16:L:301:BCL:H2   | 17:L:302:BPH:HBB3 | 1.96                     | 0.48              |
| 4:H:52:ARG:NH2    | 8:E:14:GLU:OE1    | 2.47                     | 0.48              |
| 6:J:11:THR:N      | 6:J:14:GLU:OE2    | 2.44                     | 0.48              |
| 8:T:33:VAL:HG11   | 16:T:101:BCL:CBA  | 2.44                     | 0.48              |
| 6:4:18:PHE:HB2    | 21:4:102:CRT:H21A | 1.95                     | 0.48              |
| 1:C:144:HIS:HE1   | 10:C:404:HEM:C1C  | 2.32                     | 0.48              |
| 16:L:307:BCL:CHC  | 16:M:404:BCL:H42  | 2.43                     | 0.48              |
| 3:M:202:HIS:CE1   | 3:M:206:ILE:HD11  | 2.49                     | 0.48              |
| 6:P:18:PHE:HB2    | 21:Q:101:CRT:H32A | 1.96                     | 0.48              |
| 8:G:22:PHE:CD2    | 21:G:103:CRT:H14  | 2.49                     | 0.48              |
| 16:R:101:BCL:H41  | 16:R:101:BCL:H61  | 1.54                     | 0.48              |
| 5:1:33:HIS:CE1    | 16:2:102:BCL:HMD3 | 2.49                     | 0.48              |
| 3:M:229:PHE:HE1   | 4:H:244:ALA:HB2   | 1.79                     | 0.47              |
| 18:L:303:UQ8:H22  | 18:L:303:UQ8:H25  | 1.62                     | 0.47              |
| 18:L:308:UQ8:H41A | 7:U:27:VAL:HG12   | 1.96                     | 0.47              |
| 8:E:43:TRP:O      | 24:E:101:LMT:O3'  | 2.31                     | 0.47              |
| 8:Z:26:MET:HE1    | 16:1:402:BCL:H162 | 1.97                     | 0.47              |
| 9:3:33:HIS:CE1    | 16:4:101:BCL:HMD3 | 2.49                     | 0.47              |
| 2:L:247:VAL:HG21  | 17:L:302:BPH:HBC3 | 1.96                     | 0.47              |
| 16:2:102:BCL:H162 | 24:2:104:LMT:H41  | 1.96                     | 0.47              |
| 5:9:13:ASP:OD2    | 5:9:16:ARG:HG3    | 2.15                     | 0.47              |
| 1:C:100:TRP:CD1   | 1:C:153:TYR:HB2   | 2.49                     | 0.47              |
| 8:T:46:TRP:CE2    | 16:T:101:BCL:H2C  | 2.50                     | 0.47              |
| 16:Y:101:BCL:H112 | 16:Y:101:BCL:H72  | 1.49                     | 0.47              |
| 6:8:22:PHE:CE1    | 21:8:103:CRT:H16  | 2.49                     | 0.47              |
| 16:8:102:BCL:HBB2 | 24:0:101:LMT:H111 | 1.95                     | 0.47              |
| 4:H:9:MET:HA      | 4:H:13:GLN:OE1    | 2.14                     | 0.47              |
| 21:T:102:CRT:H392 | 7:U:33:HIS:HB2    | 1.96                     | 0.47              |
| 7:U:33:HIS:CE1    | 16:V:102:BCL:HMD3 | 2.50                     | 0.47              |
| 8:X:18:PHE:HB2    | 21:X:103:CRT:H21A | 1.96                     | 0.47              |
| 4:H:2:SER:H       | 5:I:38:SER:HB2    | 1.80                     | 0.47              |
| 5:Q:33:HIS:CE1    | 16:R:101:BCL:HMD3 | 2.50                     | 0.47              |
| 7:W:25:LEU:HB2    | 16:W:101:BCL:H43  | 1.97                     | 0.47              |
| 6:6:46:TRP:HZ2    | 16:6:101:BCL:H91  | 1.78                     | 0.47              |
| 16:I:101:BCL:H141 | 16:I:101:BCL:H161 | 1.75                     | 0.47              |
| 16:T:101:BCL:HBA1 | 16:T:101:BCL:H3A  | 1.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:U:25:LEU:HB2    | 16:U:101:BCL:H43  | 1.96                     | 0.47              |
| 9:3:41:GLU:O      | 6:4:44:ARG:NH1    | 2.46                     | 0.47              |
| 3:M:243:THR:HB    | 4:H:117:PRO:HD2   | 1.96                     | 0.47              |
| 4:H:100:PHE:HB2   | 4:H:111:PHE:CZ    | 2.50                     | 0.47              |
| 21:Q:101:CRT:H371 | 16:Q:102:BCL:HMB2 | 1.97                     | 0.47              |
| 5:9:36:LEU:HD11   | 16:0:102:BCL:HHD  | 1.96                     | 0.47              |
| 1:C:115:ASN:ND2   | 1:C:118:SER:HB2   | 2.30                     | 0.46              |
| 2:L:119:ILE:HG22  | 3:M:229:PHE:HE2   | 1.80                     | 0.46              |
| 18:L:304:UQ8:H40A | 5:9:22:PHE:HB3    | 1.97                     | 0.46              |
| 21:M:407:CRT:H2M3 | 5:O:35:ILE:HG12   | 1.97                     | 0.46              |
| 21:G:103:CRT:H35  | 16:I:101:BCL:HMB2 | 1.96                     | 0.46              |
| 8:V:30:PHE:CE1    | 16:V:102:BCL:H11  | 2.51                     | 0.46              |
| 6:2:46:TRP:CD2    | 16:2:102:BCL:H2C  | 2.50                     | 0.46              |
| 6:4:34:VAL:HG22   | 16:4:101:BCL:H62  | 1.97                     | 0.46              |
| 6:6:47:LEU:HD13   | 24:8:101:LMT:H51  | 1.96                     | 0.46              |
| 2:L:12:VAL:O      | 2:L:116:LYS:NZ    | 2.40                     | 0.46              |
| 4:H:94:PRO:HB2    | 6:0:9:GLY:HA3     | 1.97                     | 0.46              |
| 5:I:32:ILE:HD12   | 16:J:101:BCL:O1D  | 2.15                     | 0.46              |
| 7:Y:36:LEU:HD11   | 16:Z:102:BCL:HHD  | 1.97                     | 0.46              |
| 6:4:21:ILE:HD11   | 21:4:102:CRT:C6   | 2.45                     | 0.46              |
| 6:4:46:TRP:CD1    | 6:4:47:LEU:HG     | 2.51                     | 0.46              |
| 5:9:10:GLN:HA     | 6:0:8:THR:HG21    | 1.97                     | 0.46              |
| 5:A:36:LEU:HD11   | 16:B:102:BCL:HHD  | 1.97                     | 0.46              |
| 7:Y:33:HIS:CE1    | 16:Z:102:BCL:HMD3 | 2.50                     | 0.46              |
| 7:Y:49:VAL:HA     | 7:Y:51:ALA:H      | 1.80                     | 0.46              |
| 16:0:102:BCL:H3A  | 16:0:102:BCL:H43  | 1.97                     | 0.46              |
| 1:C:110:CYS:SG    | 10:C:401:HEM:CBC  | 2.96                     | 0.46              |
| 18:L:308:UQ8:H33  | 7:W:34:MET:SD     | 2.55                     | 0.46              |
| 5:I:14:PRO:HB3    | 6:J:18:PHE:CZ     | 2.51                     | 0.46              |
| 8:V:46:TRP:CE2    | 16:V:102:BCL:H2C  | 2.51                     | 0.46              |
| 3:M:42:LYS:NZ     | 25:M:506:HOH:O    | 2.44                     | 0.46              |
| 5:K:11:ILE:HD13   | 21:Q:101:CRT:H1M1 | 1.96                     | 0.46              |
| 8:X:37:HIS:CG     | 16:X:102:BCL:H91  | 2.50                     | 0.46              |
| 16:4:101:BCL:H192 | 16:4:101:BCL:H161 | 1.74                     | 0.46              |
| 18:L:303:UQ8:H16  | 18:L:303:UQ8:H12  | 1.66                     | 0.46              |
| 15:L:309:PGV:H241 | 5:9:20:ALA:HB2    | 1.98                     | 0.46              |
| 3:M:89:HIS:O      | 3:M:93:LEU:HG     | 2.16                     | 0.46              |
| 6:6:22:PHE:HA     | 21:7:101:CRT:H14  | 1.98                     | 0.46              |
| 2:L:218:GLU:CD    | 3:M:235:ILE:HD11  | 2.40                     | 0.46              |
| 7:D:18:LEU:HA     | 7:D:21:VAL:HG12   | 1.98                     | 0.46              |
| 5:7:32:ILE:HD12   | 16:8:102:BCL:O1D  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:7:101:CRT:H392 | 16:7:102:BCL:HBB2 | 1.98                     | 0.46              |
| 6:8:18:PHE:CE1    | 21:8:103:CRT:H9   | 2.51                     | 0.46              |
| 18:L:304:UQ8:H17A | 5:7:30:LEU:HD13   | 1.98                     | 0.46              |
| 16:G:102:BCL:H192 | 16:G:102:BCL:H161 | 1.72                     | 0.46              |
| 6:N:33:VAL:HG11   | 16:N:101:BCL:HAA1 | 1.98                     | 0.46              |
| 5:O:34:PHE:HD1    | 23:O:501:LDA:H111 | 1.80                     | 0.46              |
| 8:T:46:TRP:CD2    | 16:T:101:BCL:H2C  | 2.51                     | 0.46              |
| 6:0:22:PHE:CD1    | 21:0:103:CRT:H14  | 2.51                     | 0.46              |
| 1:C:173:ASN:O     | 3:M:80:ASP:HB2    | 2.15                     | 0.45              |
| 4:H:55:VAL:HG13   | 22:D:502:CDL:HA21 | 1.98                     | 0.45              |
| 21:B:103:CRT:H372 | 7:D:33:HIS:CG     | 2.51                     | 0.45              |
| 16:D:503:BCL:HBC2 | 8:E:43:TRP:CZ3    | 2.51                     | 0.45              |
| 16:N:101:BCL:H91  | 16:N:101:BCL:H111 | 1.73                     | 0.45              |
| 8:Z:28:MET:HE3    | 8:Z:28:MET:HB2    | 1.85                     | 0.45              |
| 4:H:247:LYS:HE2   | 4:H:247:LYS:HA    | 1.97                     | 0.45              |
| 7:S:6:TRP:CD2     | 8:T:16:LYS:HG2    | 2.51                     | 0.45              |
| 16:3:101:BCL:H62  | 16:3:101:BCL:H41  | 1.50                     | 0.45              |
| 1:C:183:GLN:HB3   | 1:C:196:PRO:HA    | 1.98                     | 0.45              |
| 16:L:307:BCL:H201 | 18:L:308:UQ8:H13  | 1.98                     | 0.45              |
| 18:L:308:UQ8:H17  | 18:L:308:UQ8:H20  | 1.75                     | 0.45              |
| 16:A:101:BCL:H61  | 16:A:101:BCL:H102 | 1.40                     | 0.45              |
| 16:K:102:BCL:H102 | 16:K:102:BCL:H61  | 1.48                     | 0.45              |
| 16:Z:102:BCL:O2A  | 16:Z:102:BCL:H3A  | 2.15                     | 0.45              |
| 6:8:39:LEU:HB3    | 24:8:101:LMT:H42  | 1.98                     | 0.45              |
| 15:L:305:PGV:H211 | 15:1:401:PGV:H71  | 1.99                     | 0.45              |
| 16:G:102:BCL:H161 | 16:G:102:BCL:H143 | 1.74                     | 0.45              |
| 7:U:30:LEU:O      | 7:U:34:MET:HG2    | 2.17                     | 0.45              |
| 16:V:102:BCL:H93  | 16:V:102:BCL:H62  | 1.78                     | 0.45              |
| 21:2:103:CRT:H10  | 21:2:103:CRT:H81  | 1.85                     | 0.45              |
| 5:5:33:HIS:CE1    | 16:6:101:BCL:HMD3 | 2.51                     | 0.45              |
| 6:J:22:PHE:CD2    | 21:K:101:CRT:H14  | 2.52                     | 0.45              |
| 16:S:101:BCL:H8   | 16:S:101:BCL:H122 | 1.73                     | 0.45              |
| 8:V:46:TRP:CD1    | 8:V:47:LEU:HG     | 2.52                     | 0.45              |
| 21:Z:103:CRT:H20  | 21:Z:103:CRT:H181 | 1.86                     | 0.45              |
| 6:2:7:MET:SD      | 6:2:8:THR:N       | 2.90                     | 0.45              |
| 2:L:26:TRP:HZ3    | 4:H:99:PRO:HB3    | 1.81                     | 0.45              |
| 5:5:18:LEU:HD23   | 16:5:102:BCL:H203 | 1.99                     | 0.45              |
| 6:0:33:VAL:HG11   | 16:0:102:BCL:HBA2 | 1.98                     | 0.45              |
| 16:B:102:BCL:H141 | 16:B:102:BCL:H161 | 1.79                     | 0.45              |
| 6:R:47:LEU:HD12   | 16:R:101:BCL:H162 | 1.99                     | 0.45              |
| 21:T:102:CRT:H372 | 7:U:33:HIS:CG     | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:X:21:ILE:HB     | 21:X:103:CRT:H9   | 1.97                     | 0.45              |
| 2:L:202:SER:HA    | 3:M:143:SER:HB2   | 1.99                     | 0.45              |
| 16:L:307:BCL:H91  | 16:L:307:BCL:H111 | 1.83                     | 0.45              |
| 16:M:403:BCL:H61  | 20:M:406:MQ8:H243 | 1.99                     | 0.45              |
| 6:J:46:TRP:CD2    | 16:J:101:BCL:H2C  | 2.52                     | 0.45              |
| 21:Q:101:CRT:H10  | 21:Q:101:CRT:H81  | 1.82                     | 0.45              |
| 21:E:103:CRT:H35  | 16:F:502:BCL:HMB2 | 1.99                     | 0.45              |
| 16:L:307:BCL:H201 | 18:L:308:UQ8:H15  | 1.98                     | 0.45              |
| 3:M:284:ILE:HD13  | 3:M:284:ILE:HA    | 1.82                     | 0.45              |
| 7:F:8:ILE:HD12    | 7:F:11:LEU:HD11   | 2.00                     | 0.45              |
| 16:I:101:BCL:H62  | 16:I:101:BCL:H41  | 1.57                     | 0.45              |
| 16:S:101:BCL:H61  | 16:S:101:BCL:H41  | 1.54                     | 0.45              |
| 7:W:1:FME:HB3     | 8:Z:28:MET:HE1    | 1.97                     | 0.45              |
| 6:2:45:PRO:O      | 9:3:48:PRO:HG3    | 2.17                     | 0.45              |
| 2:L:106:TRP:HH2   | 20:M:406:MQ8:H301 | 1.82                     | 0.44              |
| 18:L:308:UQ8:H27  | 18:L:308:UQ8:H30  | 1.75                     | 0.44              |
| 21:B:103:CRT:H20  | 21:B:103:CRT:H181 | 1.88                     | 0.44              |
| 21:X:103:CRT:H20  | 21:X:103:CRT:H181 | 1.85                     | 0.44              |
| 9:3:32:ILE:HD12   | 16:4:101:BCL:O1D  | 2.17                     | 0.44              |
| 16:5:102:BCL:HBC3 | 16:5:102:BCL:H2C  | 1.81                     | 0.44              |
| 1:C:110:CYS:CB    | 10:C:401:HEM:CAC  | 2.95                     | 0.44              |
| 2:L:277:LEU:HB3   | 7:W:34:MET:HE2    | 1.99                     | 0.44              |
| 3:M:80:ASP:OD1    | 25:M:502:HOH:O    | 2.20                     | 0.44              |
| 3:M:197:TYR:OH    | 16:M:404:BCL:OBB  | 2.33                     | 0.44              |
| 7:D:14:PRO:HB3    | 8:E:18:PHE:CZ     | 2.53                     | 0.44              |
| 6:J:10:LEU:HG     | 6:J:14:GLU:HG2    | 1.98                     | 0.44              |
| 8:X:33:VAL:HG11   | 16:X:102:BCL:HAA1 | 1.99                     | 0.44              |
| 8:Z:22:PHE:HA     | 21:Z:103:CRT:H14  | 1.98                     | 0.44              |
| 8:X:46:TRP:CE2    | 16:X:102:BCL:H2C  | 2.52                     | 0.44              |
| 16:U:101:BCL:H2   | 16:U:101:BCL:H61  | 1.73                     | 0.44              |
| 8:Z:46:TRP:CD2    | 16:Z:102:BCL:H2C  | 2.51                     | 0.44              |
| 16:5:102:BCL:H93  | 16:5:102:BCL:H61  | 1.72                     | 0.44              |
| 16:Q:102:BCL:H172 | 16:Q:102:BCL:H111 | 1.98                     | 0.44              |
| 16:1:402:BCL:H152 | 16:1:402:BCL:H18  | 1.53                     | 0.44              |
| 16:2:102:BCL:H62  | 16:2:102:BCL:H41  | 1.72                     | 0.44              |
| 18:L:304:UQ8:H45B | 5:7:21:LEU:HD23   | 1.98                     | 0.44              |
| 16:B:102:BCL:H93  | 16:B:102:BCL:H61  | 1.69                     | 0.44              |
| 6:2:46:TRP:CE2    | 16:2:102:BCL:H2C  | 2.53                     | 0.44              |
| 21:2:103:CRT:H26  | 21:2:103:CRT:H241 | 1.86                     | 0.44              |
| 16:0:102:BCL:H93  | 16:0:102:BCL:H61  | 1.69                     | 0.44              |
| 2:L:186:PHE:CD2   | 2:L:246:ALA:HB1   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:206:ILE:HD13  | 16:M:403:BCL:HMD2 | 2.00                     | 0.44              |
| 7:Y:6:TRP:CD2     | 8:Z:16:LYS:HG2    | 2.53                     | 0.44              |
| 7:Y:32:ILE:HD12   | 16:Z:102:BCL:O1D  | 2.17                     | 0.44              |
| 8:Z:46:TRP:CE2    | 16:Z:102:BCL:H2C  | 2.53                     | 0.44              |
| 5:7:11:ILE:HG23   | 21:0:103:CRT:H1M2 | 2.00                     | 0.44              |
| 24:G:104:LMT:H122 | 16:I:101:BCL:HMA3 | 2.00                     | 0.44              |
| 16:S:101:BCL:HBC3 | 16:S:101:BCL:H2C  | 1.87                     | 0.44              |
| 21:T:102:CRT:H10  | 21:T:102:CRT:H81  | 1.75                     | 0.44              |
| 18:L:308:UQ8:H46  | 18:L:308:UQ8:H42  | 1.64                     | 0.44              |
| 7:F:33:HIS:CE1    | 16:G:102:BCL:HMD1 | 2.53                     | 0.44              |
| 5:K:33:HIS:CD2    | 21:K:101:CRT:H372 | 2.53                     | 0.44              |
| 6:6:21:ILE:HD12   | 21:7:101:CRT:H6   | 2.00                     | 0.44              |
| 5:7:33:HIS:CD2    | 21:7:101:CRT:H372 | 2.53                     | 0.44              |
| 2:L:193:LEU:HD13  | 3:M:216:PHE:CG    | 2.53                     | 0.43              |
| 2:L:199:LEU:HD22  | 2:L:222:PHE:CE2   | 2.53                     | 0.43              |
| 18:L:304:UQ8:H32  | 18:L:304:UQ8:H35  | 1.67                     | 0.43              |
| 16:3:101:BCL:H192 | 16:3:101:BCL:H161 | 1.82                     | 0.43              |
| 16:9:101:BCL:HBC3 | 16:9:101:BCL:H2C  | 1.82                     | 0.43              |
| 18:L:304:UQ8:H7A  | 18:L:304:UQ8:H10  | 1.52                     | 0.43              |
| 20:M:406:MQ8:H2M3 | 20:M:406:MQ8:H121 | 2.00                     | 0.43              |
| 8:Z:33:VAL:HG11   | 16:Z:102:BCL:HAA1 | 2.00                     | 0.43              |
| 16:0:102:BCL:H41  | 16:0:102:BCL:H62  | 1.84                     | 0.43              |
| 18:L:308:UQ8:H40  | 18:L:308:UQ8:H37  | 1.77                     | 0.43              |
| 6:2:22:PHE:CD2    | 21:2:103:CRT:H14  | 2.53                     | 0.43              |
| 3:M:4:TYR:HE1     | 22:M:409:CDL:HA22 | 1.82                     | 0.43              |
| 16:O:502:BCL:H192 | 16:O:502:BCL:H162 | 1.76                     | 0.43              |
| 16:Q:102:BCL:H41  | 16:Q:102:BCL:H61  | 1.54                     | 0.43              |
| 16:2:102:BCL:H91  | 16:2:102:BCL:H111 | 1.77                     | 0.43              |
| 1:C:191:ALA:O     | 2:L:266:PRO:HB2   | 2.18                     | 0.43              |
| 2:L:195:MET:HE3   | 2:L:222:PHE:CE1   | 2.54                     | 0.43              |
| 8:E:46:TRP:CD2    | 16:E:102:BCL:H2C  | 2.54                     | 0.43              |
| 21:K:101:CRT:H10  | 21:K:101:CRT:H81  | 1.88                     | 0.43              |
| 21:T:102:CRT:H20  | 21:T:102:CRT:H181 | 1.86                     | 0.43              |
| 16:V:102:BCL:HBA2 | 16:V:102:BCL:HED3 | 2.00                     | 0.43              |
| 5:1:9:TRP:HZ3     | 5:1:17:THR:HG21   | 1.83                     | 0.43              |
| 5:7:33:HIS:CE1    | 16:8:102:BCL:HMD3 | 2.54                     | 0.43              |
| 21:7:101:CRT:H371 | 16:7:102:BCL:C2B  | 2.48                     | 0.43              |
| 18:L:308:UQ8:H32  | 18:L:308:UQ8:H35  | 1.75                     | 0.43              |
| 3:M:201:PHE:CZ    | 4:H:15:THR:HG22   | 2.54                     | 0.43              |
| 5:K:26:PHE:CE1    | 21:K:101:CRT:H343 | 2.53                     | 0.43              |
| 2:L:42:PHE:HA     | 18:L:304:UQ8:H30B | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:L:48:LEU:HD13   | 5:9:31:LEU:HD22   | 2.00                     | 0.43              |
| 2:L:113:ILE:HG23  | 3:M:254:TRP:HE3   | 1.83                     | 0.43              |
| 8:T:47:LEU:HD12   | 16:T:101:BCL:H161 | 2.00                     | 0.43              |
| 5:Q:32:ILE:HD12   | 16:R:101:BCL:O1D  | 2.19                     | 0.43              |
| 6:R:18:PHE:HA     | 21:R:102:CRT:H6   | 2.01                     | 0.43              |
| 16:3:101:BCL:HHD  | 16:3:101:BCL:HAC2 | 1.80                     | 0.43              |
| 6:J:14:GLU:OE1    | 6:J:14:GLU:N      | 2.50                     | 0.43              |
| 6:P:22:PHE:HA     | 21:Q:101:CRT:H14  | 2.00                     | 0.43              |
| 16:S:101:BCL:HAC2 | 16:S:101:BCL:HHD  | 1.82                     | 0.43              |
| 7:W:41:GLU:HA     | 7:Y:54:VAL:HG11   | 2.01                     | 0.43              |
| 5:1:14:PRO:HA     | 5:1:17:THR:HG22   | 2.01                     | 0.43              |
| 5:1:41:ALA:O      | 6:2:44:ARG:NH1    | 2.52                     | 0.43              |
| 6:6:11:THR:HG22   | 6:6:12:GLU:H      | 1.83                     | 0.43              |
| 3:M:55:PHE:CD1    | 5:Q:19:VAL:HG21   | 2.55                     | 0.42              |
| 16:S:101:BCL:H202 | 16:S:101:BCL:H162 | 1.79                     | 0.42              |
| 8:X:46:TRP:CD1    | 8:X:47:LEU:HG     | 2.54                     | 0.42              |
| 3:M:240:ASP:OD2   | 4:H:119:ARG:HB3   | 2.19                     | 0.42              |
| 4:H:213:ALA:HA    | 4:H:247:LYS:HE3   | 2.00                     | 0.42              |
| 24:V:101:LMT:O3'  | 24:V:101:LMT:O2B  | 2.24                     | 0.42              |
| 8:X:47:LEU:HD13   | 24:Z:101:LMT:H32  | 2.00                     | 0.42              |
| 14:C:408:PLM:H62  | 2:L:268:TRP:CZ2   | 2.54                     | 0.42              |
| 3:M:53:LEU:O      | 5:Q:16:ARG:NH1    | 2.34                     | 0.42              |
| 4:H:123:CYS:HA    | 4:H:232:THR:HA    | 2.01                     | 0.42              |
| 7:W:44:TRP:CD2    | 16:W:101:BCL:H2C  | 2.55                     | 0.42              |
| 9:3:34:TYR:CE2    | 9:3:38:ARG:HD2    | 2.55                     | 0.42              |
| 21:4:102:CRT:H36  | 21:4:102:CRT:H341 | 1.85                     | 0.42              |
| 2:L:117:LEU:O     | 3:M:247:ARG:NH1   | 2.51                     | 0.42              |
| 4:H:67:PHE:HE2    | 4:H:78:ALA:HB2    | 1.84                     | 0.42              |
| 8:E:12:GLU:H      | 8:E:12:GLU:HG3    | 1.67                     | 0.42              |
| 16:I:101:BCL:H192 | 16:I:101:BCL:H162 | 1.76                     | 0.42              |
| 16:J:101:BCL:H111 | 16:J:101:BCL:H91  | 1.65                     | 0.42              |
| 5:Q:5:FME:C       | 5:Q:7:LYS:N       | 2.82                     | 0.42              |
| 16:7:102:BCL:HBC3 | 16:7:102:BCL:H2C  | 1.83                     | 0.42              |
| 6:0:46:TRP:CE2    | 16:0:102:BCL:H2C  | 2.55                     | 0.42              |
| 21:M:407:CRT:H10  | 21:M:407:CRT:H81  | 1.85                     | 0.42              |
| 8:X:46:TRP:HZ2    | 16:X:102:BCL:H13  | 1.84                     | 0.42              |
| 16:1:402:BCL:HAC2 | 16:1:402:BCL:HHD  | 1.85                     | 0.42              |
| 16:3:101:BCL:HBC3 | 16:3:101:BCL:H2C  | 1.79                     | 0.42              |
| 21:7:101:CRT:H20  | 21:7:101:CRT:H181 | 1.81                     | 0.42              |
| 16:9:101:BCL:H8   | 16:9:101:BCL:H52  | 1.75                     | 0.42              |
| 2:L:135:LEU:HD12  | 22:M:412:CDL:H861 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:72:GLY:HA3    | 21:M:407:CRT:C6   | 2.50                     | 0.42              |
| 4:H:21:PHE:HE2    | 15:F:501:PGV:H292 | 1.83                     | 0.42              |
| 6:J:22:PHE:CE2    | 21:K:101:CRT:H16  | 2.54                     | 0.42              |
| 16:L:307:BCL:H202 | 16:L:307:BCL:H162 | 1.76                     | 0.42              |
| 7:D:1:FME:HG3     | 8:G:28:MET:SD     | 2.59                     | 0.42              |
| 8:E:43:TRP:HB2    | 24:E:101:LMT:H22  | 2.01                     | 0.42              |
| 16:K:102:BCL:H202 | 16:K:102:BCL:H162 | 1.88                     | 0.42              |
| 21:R:102:CRT:H20  | 21:R:102:CRT:H181 | 1.89                     | 0.42              |
| 16:7:102:BCL:H71  | 16:7:102:BCL:H112 | 1.69                     | 0.42              |
| 6:8:18:PHE:HE1    | 21:8:103:CRT:H9   | 1.85                     | 0.42              |
| 21:8:103:CRT:H292 | 16:9:101:BCL:H61  | 2.02                     | 0.42              |
| 4:H:13:GLN:NE2    | 15:F:501:PGV:H211 | 2.35                     | 0.42              |
| 8:E:41:TRP:CZ2    | 16:E:102:BCL:H18  | 2.54                     | 0.42              |
| 1:C:39:ALA:O      | 2:L:169:GLN:NE2   | 2.45                     | 0.42              |
| 15:L:306:PGV:H061 | 7:D:38:SER:HA     | 2.02                     | 0.42              |
| 21:M:407:CRT:H20  | 21:M:407:CRT:H181 | 1.77                     | 0.42              |
| 24:J:102:LMT:H122 | 16:K:102:BCL:HMA3 | 2.02                     | 0.42              |
| 16:P:102:BCL:O2A  | 16:P:102:BCL:H3A  | 2.20                     | 0.42              |
| 6:R:46:TRP:CE2    | 16:R:101:BCL:H2C  | 2.55                     | 0.42              |
| 7:S:32:ILE:HD12   | 16:T:101:BCL:O1D  | 2.20                     | 0.42              |
| 16:X:102:BCL:H161 | 16:X:102:BCL:H192 | 1.82                     | 0.42              |
| 16:Y:101:BCL:H101 | 16:Y:101:BCL:H13  | 1.62                     | 0.42              |
| 8:Z:22:PHE:HA     | 21:Z:103:CRT:H11  | 2.02                     | 0.42              |
| 16:2:102:BCL:H93  | 16:2:102:BCL:H61  | 1.67                     | 0.42              |
| 2:L:63:GLN:OE1    | 15:D:501:PGV:H05  | 2.19                     | 0.42              |
| 3:M:34:PRO:HG3    | 3:M:50:PRO:HD3    | 2.02                     | 0.42              |
| 3:M:286:LEU:HD23  | 24:M:414:LMT:H52  | 2.01                     | 0.42              |
| 16:D:503:BCL:H162 | 16:D:503:BCL:H122 | 1.74                     | 0.42              |
| 7:F:7:LYS:HD3     | 21:K:101:CRT:H31A | 2.02                     | 0.42              |
| 5:K:33:HIS:CG     | 21:K:101:CRT:H372 | 2.55                     | 0.42              |
| 16:Z:102:BCL:H141 | 16:Z:102:BCL:H162 | 1.68                     | 0.42              |
| 21:4:102:CRT:H35  | 21:4:102:CRT:H31  | 1.67                     | 0.42              |
| 6:8:22:PHE:O      | 6:8:26:MET:HG3    | 2.20                     | 0.42              |
| 1:C:186:ALA:HB2   | 3:M:92:TRP:CD2    | 2.55                     | 0.41              |
| 20:M:406:MQ8:H241 | 20:M:406:MQ8:H261 | 1.80                     | 0.41              |
| 24:B:101:LMT:H62  | 24:B:101:LMT:H91  | 1.89                     | 0.41              |
| 16:E:102:BCL:H141 | 16:E:102:BCL:H161 | 1.79                     | 0.41              |
| 6:N:37:HIS:CG     | 16:N:101:BCL:H92  | 2.55                     | 0.41              |
| 6:N:46:TRP:CE2    | 16:N:101:BCL:H2C  | 2.55                     | 0.41              |
| 7:S:36:LEU:HD11   | 16:T:101:BCL:HHD  | 2.01                     | 0.41              |
| 21:T:102:CRT:H15  | 21:T:102:CRT:H131 | 1.97                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:4:22:PHE:HA     | 21:4:102:CRT:H14  | 2.01                     | 0.41              |
| 24:8:101:LMT:H81  | 24:8:101:LMT:H52  | 1.88                     | 0.41              |
| 1:C:137:THR:HG23  | 1:C:275:HIS:CE1   | 2.55                     | 0.41              |
| 18:L:304:UQ8:H42  | 18:L:304:UQ8:H46  | 1.72                     | 0.41              |
| 3:M:96:GLU:CD     | 25:M:503:HOH:O    | 2.63                     | 0.41              |
| 3:M:237:GLN:HB2   | 3:M:262:MET:HG2   | 2.02                     | 0.41              |
| 4:H:116:SER:OG    | 4:H:237:ASP:HB3   | 2.20                     | 0.41              |
| 4:H:160:ASP:OD1   | 4:H:160:ASP:N     | 2.44                     | 0.41              |
| 6:B:36:ALA:HB1    | 24:B:101:LMT:H111 | 2.02                     | 0.41              |
| 16:K:102:BCL:H193 | 6:N:25:SER:HA     | 2.01                     | 0.41              |
| 16:P:102:BCL:H162 | 16:P:102:BCL:H192 | 1.74                     | 0.41              |
| 24:4:103:LMT:H1B  | 24:4:103:LMT:H3'  | 1.73                     | 0.41              |
| 16:5:102:BCL:HAC2 | 16:5:102:BCL:HHD  | 1.84                     | 0.41              |
| 5:7:33:HIS:CG     | 21:7:101:CRT:H372 | 2.54                     | 0.41              |
| 21:0:103:CRT:H20  | 21:0:103:CRT:H181 | 1.92                     | 0.41              |
| 17:L:302:BPH:H6C1 | 17:L:302:BPH:H102 | 1.85                     | 0.41              |
| 18:L:303:UQ8:H15B | 18:L:303:UQ8:H17A | 1.95                     | 0.41              |
| 6:B:46:TRP:CD2    | 16:B:102:BCL:H2C  | 2.55                     | 0.41              |
| 5:O:18:LEU:HD12   | 5:O:18:LEU:HA     | 1.92                     | 0.41              |
| 5:O:32:ILE:HD12   | 16:P:102:BCL:O1D  | 2.20                     | 0.41              |
| 21:V:103:CRT:H372 | 7:W:33:HIS:CG     | 2.55                     | 0.41              |
| 21:X:103:CRT:H15  | 21:X:103:CRT:H131 | 1.93                     | 0.41              |
| 6:4:33:VAL:HG11   | 16:4:101:BCL:HAA1 | 2.03                     | 0.41              |
| 24:5:101:LMT:H3'  | 24:5:101:LMT:H1B  | 1.77                     | 0.41              |
| 16:9:101:BCL:H13  | 16:9:101:BCL:H102 | 1.72                     | 0.41              |
| 16:0:102:BCL:H3A  | 16:0:102:BCL:HBA1 | 1.63                     | 0.41              |
| 18:L:304:UQ8:H27  | 18:L:304:UQ8:H30  | 1.66                     | 0.41              |
| 3:M:164:ARG:HH12  | 3:M:173:GLU:HB3   | 1.85                     | 0.41              |
| 22:M:412:CDL:H802 | 22:M:412:CDL:H831 | 1.77                     | 0.41              |
| 8:G:33:VAL:HG11   | 16:G:102:BCL:HAA1 | 2.02                     | 0.41              |
| 16:R:101:BCL:H141 | 16:R:101:BCL:H161 | 1.79                     | 0.41              |
| 21:4:102:CRT:H15  | 21:4:102:CRT:H131 | 1.97                     | 0.41              |
| 2:L:108:LEU:HD21  | 22:M:412:CDL:H562 | 2.02                     | 0.41              |
| 2:L:244:LEU:HD12  | 22:M:412:CDL:H392 | 2.02                     | 0.41              |
| 5:K:33:HIS:HB3    | 21:K:101:CRT:H393 | 2.01                     | 0.41              |
| 5:Q:36:LEU:HD13   | 16:Q:102:BCL:HBC1 | 2.02                     | 0.41              |
| 16:S:101:BCL:H162 | 16:S:101:BCL:H141 | 1.85                     | 0.41              |
| 6:2:13:GLN:HE21   | 6:2:13:GLN:HB3    | 1.62                     | 0.41              |
| 5:9:6:HIS:HB2     | 6:0:16:GLN:HA     | 2.03                     | 0.41              |
| 1:C:288:ASN:O     | 1:C:296:LYS:NZ    | 2.41                     | 0.41              |
| 2:L:199:LEU:HD22  | 2:L:222:PHE:CD2   | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:T:101:BCL:H62  | 16:T:101:BCL:H92  | 1.82                     | 0.41              |
| 1:C:25:ARG:NH1    | 25:C:521:HOH:O    | 2.54                     | 0.41              |
| 16:M:404:BCL:H41  | 16:M:404:BCL:H62  | 1.64                     | 0.41              |
| 8:T:46:TRP:CD1    | 8:T:47:LEU:HG     | 2.56                     | 0.41              |
| 16:5:102:BCL:H192 | 16:5:102:BCL:H162 | 1.76                     | 0.41              |
| 6:P:46:TRP:CE2    | 16:P:102:BCL:H2C  | 2.55                     | 0.41              |
| 21:Q:101:CRT:H26  | 21:Q:101:CRT:H241 | 1.93                     | 0.41              |
| 6:2:46:TRP:CD1    | 6:2:47:LEU:HG     | 2.56                     | 0.41              |
| 5:7:32:ILE:HG12   | 21:8:103:CRT:H403 | 2.03                     | 0.41              |
| 1:C:195:LEU:HD12  | 1:C:237:MET:HG3   | 2.03                     | 0.41              |
| 2:L:7:GLU:OE2     | 3:M:254:TRP:NE1   | 2.36                     | 0.41              |
| 2:L:67:ILE:HG23   | 15:D:501:PGV:H41  | 2.03                     | 0.41              |
| 2:L:150:HIS:HE1   | 25:L:441:HOH:O    | 2.03                     | 0.41              |
| 18:L:304:UQ8:H37  | 18:L:304:UQ8:H40  | 1.57                     | 0.41              |
| 16:E:102:BCL:H142 | 16:E:102:BCL:H111 | 1.83                     | 0.41              |
| 24:J:102:LMT:H42  | 6:N:39:LEU:HB3    | 2.02                     | 0.41              |
| 5:K:6:HIS:CE1     | 5:K:7:LYS:HD3     | 2.56                     | 0.41              |
| 21:T:102:CRT:H393 | 7:U:30:LEU:HD23   | 2.02                     | 0.41              |
| 5:1:32:ILE:HD12   | 16:2:102:BCL:O1D  | 2.20                     | 0.41              |
| 16:7:102:BCL:H92  | 16:7:102:BCL:H61  | 1.88                     | 0.41              |
| 2:L:4:LEU:HB2     | 2:L:7:GLU:HB2     | 2.03                     | 0.41              |
| 21:G:103:CRT:H10  | 21:G:103:CRT:H81  | 1.90                     | 0.41              |
| 8:Z:46:TRP:CD1    | 8:Z:47:LEU:HG     | 2.56                     | 0.41              |
| 5:5:22:PHE:HB3    | 16:5:102:BCL:H71  | 2.03                     | 0.41              |
| 6:N:37:HIS:CD2    | 16:N:101:BCL:H92  | 2.56                     | 0.40              |
| 1:C:250:CYS:HB3   | 1:C:266:ARG:HB2   | 2.04                     | 0.40              |
| 2:L:254:ILE:HD12  | 2:L:254:ILE:HA    | 1.92                     | 0.40              |
| 16:L:307:BCL:H152 | 16:M:404:BCL:H193 | 2.03                     | 0.40              |
| 21:V:103:CRT:H20  | 21:V:103:CRT:H181 | 1.87                     | 0.40              |
| 1:C:82:LEU:HB3    | 1:C:85:LEU:HD12   | 2.03                     | 0.40              |
| 4:H:135:PRO:HA    | 4:H:171:TRP:HA    | 2.03                     | 0.40              |
| 21:E:103:CRT:H26  | 21:E:103:CRT:H241 | 1.91                     | 0.40              |
| 5:K:44:TRP:NE1    | 16:K:102:BCL:OBB  | 2.53                     | 0.40              |
| 15:L:309:PGV:H231 | 15:L:309:PGV:H202 | 1.88                     | 0.40              |
| 3:M:56:THR:HG21   | 3:M:131:VAL:HB    | 2.03                     | 0.40              |
| 16:D:503:BCL:H162 | 16:D:503:BCL:H192 | 1.69                     | 0.40              |
| 16:U:101:BCL:HBC2 | 8:V:43:TRP:CZ3    | 2.56                     | 0.40              |
| 8:V:46:TRP:CD2    | 16:V:102:BCL:H2C  | 2.56                     | 0.40              |
| 8:V:46:TRP:HZ2    | 16:V:102:BCL:H122 | 1.87                     | 0.40              |
| 9:3:22:GLY:HA3    | 16:3:101:BCL:H172 | 2.03                     | 0.40              |
| 5:5:32:ILE:HD12   | 16:6:101:BCL:O1D  | 2.20                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:8:103:CRT:H15  | 21:8:103:CRT:H131 | 1.91                     | 0.40              |
| 1:C:257:TYR:OH    | 3:M:296:LEU:HD21  | 2.21                     | 0.40              |
| 1:C:303:PHE:HB2   | 10:C:402:HEM:HBD1 | 2.04                     | 0.40              |
| 2:L:74:PRO:HG3    | 2:L:151:GLY:O     | 2.21                     | 0.40              |
| 2:L:196:HIS:ND1   | 18:L:303:UQ8:O2   | 2.38                     | 0.40              |
| 6:B:30:PHE:CE1    | 16:B:102:BCL:H11  | 2.57                     | 0.40              |
| 24:B:101:LMT:H41  | 6:O:47:LEU:HD13   | 2.03                     | 0.40              |
| 16:B:102:BCL:H91  | 16:B:102:BCL:H111 | 1.85                     | 0.40              |
| 6:R:22:PHE:HA     | 21:R:102:CRT:H14  | 2.03                     | 0.40              |
| 16:U:101:BCL:H112 | 16:U:101:BCL:H72  | 1.95                     | 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%)  | 301 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | L     | 275/278 (99%)  | 269 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 3   | M     | 316/325 (97%)  | 311 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 4   | H     | 258/259 (100%) | 249 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 5   | 1     | 41/44 (93%)    | 41 (100%) | 0       | 0        | 100         | 100 |
| 5   | 5     | 41/44 (93%)    | 38 (93%)  | 2 (5%)  | 1 (2%)   | 4           | 1   |
| 5   | 7     | 39/44 (89%)    | 39 (100%) | 0       | 0        | 100         | 100 |
| 5   | 9     | 41/44 (93%)    | 40 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 5   | A     | 41/44 (93%)    | 41 (100%) | 0       | 0        | 100         | 100 |
| 5   | I     | 41/44 (93%)    | 41 (100%) | 0       | 0        | 100         | 100 |
| 5   | K     | 42/44 (96%)    | 42 (100%) | 0       | 0        | 100         | 100 |
| 5   | O     | 42/44 (96%)    | 41 (98%)  | 1 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 5   | Q     | 41/44 (93%)     | 40 (98%)   | 0       | 1 (2%)   | 4           | 1   |
| 6   | 0     | 40/46 (87%)     | 38 (95%)   | 2 (5%)  | 0        | 100         | 100 |
| 6   | 2     | 39/46 (85%)     | 38 (97%)   | 1 (3%)  | 0        | 100         | 100 |
| 6   | 4     | 40/46 (87%)     | 40 (100%)  | 0       | 0        | 100         | 100 |
| 6   | 6     | 36/46 (78%)     | 36 (100%)  | 0       | 0        | 100         | 100 |
| 6   | 8     | 32/46 (70%)     | 32 (100%)  | 0       | 0        | 100         | 100 |
| 6   | B     | 42/46 (91%)     | 42 (100%)  | 0       | 0        | 100         | 100 |
| 6   | J     | 38/46 (83%)     | 38 (100%)  | 0       | 0        | 100         | 100 |
| 6   | N     | 36/46 (78%)     | 36 (100%)  | 0       | 0        | 100         | 100 |
| 6   | P     | 40/46 (87%)     | 39 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 6   | R     | 39/46 (85%)     | 39 (100%)  | 0       | 0        | 100         | 100 |
| 7   | D     | 48/64 (75%)     | 46 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 7   | F     | 47/64 (73%)     | 45 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 7   | S     | 49/64 (77%)     | 49 (100%)  | 0       | 0        | 100         | 100 |
| 7   | U     | 49/64 (77%)     | 49 (100%)  | 0       | 0        | 100         | 100 |
| 7   | W     | 52/64 (81%)     | 49 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 7   | Y     | 62/64 (97%)     | 59 (95%)   | 3 (5%)  | 0        | 100         | 100 |
| 8   | E     | 39/47 (83%)     | 39 (100%)  | 0       | 0        | 100         | 100 |
| 8   | G     | 40/47 (85%)     | 40 (100%)  | 0       | 0        | 100         | 100 |
| 8   | T     | 40/47 (85%)     | 40 (100%)  | 0       | 0        | 100         | 100 |
| 8   | V     | 40/47 (85%)     | 40 (100%)  | 0       | 0        | 100         | 100 |
| 8   | X     | 40/47 (85%)     | 39 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 8   | Z     | 39/47 (83%)     | 39 (100%)  | 0       | 0        | 100         | 100 |
| 9   | 3     | 60/66 (91%)     | 60 (100%)  | 0       | 0        | 100         | 100 |
| All | All   | 2514/2833 (89%) | 2465 (98%) | 47 (2%) | 2 (0%)   | 49          | 54  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | Q     | 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%)  | 264 (100%) | 1 (0%)   | 84          | 88  |
| 2   | L     | 223/224 (100%) | 219 (98%)  | 4 (2%)   | 51          | 61  |
| 3   | M     | 252/257 (98%)  | 249 (99%)  | 3 (1%)   | 63          | 72  |
| 4   | H     | 206/206 (100%) | 200 (97%)  | 6 (3%)   | 37          | 44  |
| 5   | 1     | 37/38 (97%)    | 37 (100%)  | 0        | 100         | 100 |
| 5   | 5     | 36/38 (95%)    | 34 (94%)   | 2 (6%)   | 19          | 18  |
| 5   | 7     | 36/38 (95%)    | 35 (97%)   | 1 (3%)   | 38          | 45  |
| 5   | 9     | 37/38 (97%)    | 36 (97%)   | 1 (3%)   | 39          | 47  |
| 5   | A     | 37/38 (97%)    | 36 (97%)   | 1 (3%)   | 39          | 47  |
| 5   | I     | 37/38 (97%)    | 37 (100%)  | 0        | 100         | 100 |
| 5   | K     | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 5   | O     | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 5   | Q     | 37/38 (97%)    | 37 (100%)  | 0        | 100         | 100 |
| 6   | 0     | 35/38 (92%)    | 35 (100%)  | 0        | 100         | 100 |
| 6   | 2     | 34/38 (90%)    | 32 (94%)   | 2 (6%)   | 18          | 16  |
| 6   | 4     | 35/38 (92%)    | 35 (100%)  | 0        | 100         | 100 |
| 6   | 6     | 32/38 (84%)    | 28 (88%)   | 4 (12%)  | 4           | 2   |
| 6   | 8     | 28/38 (74%)    | 27 (96%)   | 1 (4%)   | 31          | 36  |
| 6   | B     | 37/38 (97%)    | 37 (100%)  | 0        | 100         | 100 |
| 6   | J     | 33/38 (87%)    | 33 (100%)  | 0        | 100         | 100 |
| 6   | N     | 32/38 (84%)    | 32 (100%)  | 0        | 100         | 100 |
| 6   | P     | 35/38 (92%)    | 35 (100%)  | 0        | 100         | 100 |
| 6   | R     | 34/38 (90%)    | 34 (100%)  | 0        | 100         | 100 |
| 7   | D     | 43/55 (78%)    | 42 (98%)   | 1 (2%)   | 44          | 53  |
| 7   | F     | 43/55 (78%)    | 43 (100%)  | 0        | 100         | 100 |
| 7   | S     | 43/55 (78%)    | 42 (98%)   | 1 (2%)   | 44          | 53  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 7   | U     | 43/55 (78%)     | 41 (95%)   | 2 (5%)   | 23          | 24  |
| 7   | W     | 45/55 (82%)     | 45 (100%)  | 0        | 100         | 100 |
| 7   | Y     | 55/55 (100%)    | 50 (91%)   | 5 (9%)   | 9           | 5   |
| 8   | E     | 35/40 (88%)     | 34 (97%)   | 1 (3%)   | 37          | 44  |
| 8   | G     | 36/40 (90%)     | 35 (97%)   | 1 (3%)   | 38          | 45  |
| 8   | T     | 36/40 (90%)     | 36 (100%)  | 0        | 100         | 100 |
| 8   | V     | 36/40 (90%)     | 36 (100%)  | 0        | 100         | 100 |
| 8   | X     | 36/40 (90%)     | 36 (100%)  | 0        | 100         | 100 |
| 8   | Z     | 35/40 (88%)     | 34 (97%)   | 1 (3%)   | 37          | 44  |
| 9   | 3     | 48/52 (92%)     | 48 (100%)  | 0        | 100         | 100 |
| All | All   | 2148/2342 (92%) | 2110 (98%) | 38 (2%)  | 51          | 61  |

All (38) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 151 | THR  |
| 2   | L     | 13  | ARG  |
| 2   | L     | 61  | GLU  |
| 2   | L     | 253 | CYS  |
| 2   | L     | 255 | VAL  |
| 3   | M     | 6   | ASN  |
| 3   | M     | 56  | THR  |
| 3   | M     | 216 | PHE  |
| 4   | H     | 75  | THR  |
| 4   | H     | 76  | VAL  |
| 4   | H     | 81  | VAL  |
| 4   | H     | 159 | LEU  |
| 4   | H     | 225 | LEU  |
| 4   | H     | 251 | THR  |
| 5   | A     | 21  | LEU  |
| 7   | D     | 5   | LEU  |
| 8   | E     | 12  | GLU  |
| 8   | G     | 13  | GLU  |
| 7   | S     | 5   | LEU  |
| 7   | U     | 5   | LEU  |
| 7   | U     | 17  | ILE  |
| 7   | Y     | 4   | ASP  |
| 7   | Y     | 5   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | Y     | 24  | PHE  |
| 7   | Y     | 49  | VAL  |
| 7   | Y     | 57  | VAL  |
| 8   | Z     | 13  | GLU  |
| 6   | 2     | 13  | GLN  |
| 6   | 2     | 16  | GLN  |
| 5   | 5     | 6   | HIS  |
| 5   | 5     | 10  | GLN  |
| 6   | 6     | 11  | THR  |
| 6   | 6     | 13  | GLN  |
| 6   | 6     | 33  | VAL  |
| 6   | 6     | 42  | LEU  |
| 5   | 7     | 11  | ILE  |
| 6   | 8     | 17  | GLU  |
| 5   | 9     | 8   | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 322 | GLN  |
| 2   | L     | 150 | HIS  |
| 3   | M     | 6   | ASN  |
| 3   | M     | 74  | ASN  |
| 3   | M     | 85  | GLN  |
| 8   | E     | 24  | GLN  |
| 5   | K     | 6   | HIS  |
| 5   | O     | 10  | GLN  |
| 5   | Q     | 10  | GLN  |
| 6   | R     | 24  | GLN  |
| 8   | V     | 24  | GLN  |
| 8   | Z     | 24  | GLN  |
| 6   | 2     | 13  | GLN  |
| 6   | 8     | 24  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

14 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$ |
| 7   | FME  | U     | 1   | 7    | 8,9,10       | 0.57 | 0           | 8,9,11      | 0.85 | 1 (12%)     |
| 5   | FME  | Q     | 5   | 5    | 8,9,10       | 0.55 | 0           | 8,9,11      | 0.96 | 1 (12%)     |
| 7   | FME  | S     | 1   | 7    | 8,9,10       | 0.56 | 0           | 8,9,11      | 0.89 | 1 (12%)     |
| 7   | FME  | W     | 1   | 7    | 8,9,10       | 0.56 | 0           | 8,9,11      | 0.99 | 1 (12%)     |
| 5   | FME  | I     | 5   | 5    | 8,9,10       | 0.53 | 0           | 8,9,11      | 1.10 | 1 (12%)     |
| 5   | FME  | 5     | 5   | 5    | 8,9,10       | 0.55 | 0           | 8,9,11      | 0.95 | 1 (12%)     |
| 5   | FME  | 9     | 5   | 5    | 8,9,10       | 0.54 | 0           | 8,9,11      | 1.06 | 1 (12%)     |
| 7   | FME  | D     | 1   | 7    | 8,9,10       | 0.54 | 0           | 8,9,11      | 1.04 | 1 (12%)     |
| 4   | FME  | H     | 1   | 4    | 8,9,10       | 0.54 | 0           | 8,9,11      | 0.96 | 1 (12%)     |
| 5   | FME  | O     | 5   | 5    | 8,9,10       | 0.55 | 0           | 8,9,11      | 0.94 | 1 (12%)     |
| 5   | FME  | K     | 5   | 5    | 8,9,10       | 0.53 | 0           | 8,9,11      | 1.18 | 1 (12%)     |
| 5   | FME  | 1     | 5   | 5    | 8,9,10       | 0.54 | 0           | 8,9,11      | 0.92 | 1 (12%)     |
| 7   | FME  | Y     | 1   | 7    | 8,9,10       | 0.55 | 0           | 8,9,11      | 0.93 | 1 (12%)     |
| 5   | FME  | A     | 5   | 5    | 8,9,10       | 0.53 | 0           | 8,9,11      | 1.07 | 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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 7   | FME  | U     | 1   | 7    | -       | 1/7/9/11 | -     |
| 5   | FME  | Q     | 5   | 5    | -       | 3/7/9/11 | -     |
| 7   | FME  | S     | 1   | 7    | -       | 1/7/9/11 | -     |
| 7   | FME  | W     | 1   | 7    | -       | 0/7/9/11 | -     |
| 5   | FME  | I     | 5   | 5    | -       | 0/7/9/11 | -     |
| 5   | FME  | 5     | 5   | 5    | -       | 2/7/9/11 | -     |
| 5   | FME  | 9     | 5   | 5    | -       | 0/7/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 7   | FME  | D     | 1   | 7    | -       | 0/7/9/11 | -     |
| 4   | FME  | H     | 1   | 4    | -       | 3/7/9/11 | -     |
| 5   | FME  | O     | 5   | 5    | -       | 0/7/9/11 | -     |
| 5   | FME  | K     | 5   | 5    | -       | 1/7/9/11 | -     |
| 5   | FME  | 1     | 5   | 5    | -       | 1/7/9/11 | -     |
| 7   | FME  | Y     | 1   | 7    | -       | 1/7/9/11 | -     |
| 5   | FME  | A     | 5   | 5    | -       | 0/7/9/11 | -     |

There are no bond length outliers.

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | D     | 1   | FME  | O-C-CA | -2.76 | 117.68      | 124.77   |
| 5   | K     | 5   | FME  | O-C-CA | -2.75 | 117.69      | 124.77   |
| 5   | I     | 5   | FME  | O-C-CA | -2.75 | 117.70      | 124.77   |
| 5   | 9     | 5   | FME  | O-C-CA | -2.71 | 117.79      | 124.77   |
| 5   | A     | 5   | FME  | O-C-CA | -2.69 | 117.85      | 124.77   |
| 7   | W     | 1   | FME  | O-C-CA | -2.63 | 118.02      | 124.77   |
| 5   | 5     | 5   | FME  | O-C-CA | -2.57 | 118.16      | 124.77   |
| 5   | Q     | 5   | FME  | O-C-CA | -2.55 | 118.22      | 124.77   |
| 5   | O     | 5   | FME  | O-C-CA | -2.53 | 118.27      | 124.77   |
| 7   | Y     | 1   | FME  | O-C-CA | -2.50 | 118.33      | 124.77   |
| 5   | 1     | 5   | FME  | O-C-CA | -2.49 | 118.36      | 124.77   |
| 7   | S     | 1   | FME  | O-C-CA | -2.43 | 118.52      | 124.77   |
| 7   | U     | 1   | FME  | O-C-CA | -2.28 | 118.91      | 124.77   |
| 4   | H     | 1   | FME  | O-C-CA | -2.24 | 119.01      | 124.77   |

There are no chirality outliers.

All (13) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | H     | 1   | 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   | Q     | 5   | FME  | O-C-CA-CB   |
| 7   | S     | 1   | FME  | O1-CN-N-CA  |
| 7   | U     | 1   | FME  | O1-CN-N-CA  |
| 7   | Y     | 1   | FME  | O1-CN-N-CA  |
| 5   | 1     | 5   | FME  | O1-CN-N-CA  |
| 5   | 5     | 5   | FME  | CA-CB-CG-SD |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | H     | 1   | FME  | CB-CA-N-CN  |
| 5   | 5     | 5   | FME  | N-CA-CB-CG  |
| 4   | H     | 1   | FME  | CA-CB-CG-SD |

There are no ring outliers.

7 monomers are involved in 10 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | Q     | 5   | FME  | 3       | 0            |
| 7   | S     | 1   | FME  | 1       | 0            |
| 7   | W     | 1   | FME  | 1       | 0            |
| 7   | D     | 1   | FME  | 1       | 0            |
| 4   | H     | 1   | FME  | 1       | 0            |
| 5   | K     | 5   | FME  | 1       | 0            |
| 7   | Y     | 1   | FME  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 10 are monoatomic - leaving 101 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 | $\# Z  > 2$ |
| 21  | CRT  | K     | 101 | -    | 43,43,43     | 0.67 | 0           | 48,54,54    | 2.31 | 17 (35%)    |
| 16  | BCL  | P     | 102 | -    | 69,74,74     | 1.77 | 18 (26%)    | 79,115,115  | 2.18 | 24 (30%)    |
| 24  | LMT  | 4     | 103 | -    | 36,36,36     | 0.40 | 0           | 47,47,47    | 0.70 | 1 (2%)      |
| 16  | BCL  | B     | 102 | -    | 69,74,74     | 1.78 | 17 (24%)    | 79,115,115  | 2.18 | 25 (31%)    |
| 16  | BCL  | 7     | 102 | -    | 64,69,74     | 1.85 | 17 (26%)    | 73,109,115  | 2.28 | 23 (31%)    |
| 14  | PLM  | C     | 408 | 1    | 10,11,17     | 0.33 | 0           | 9,10,17     | 0.33 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | CRT  | 2     | 103 | -    | 43,43,43     | 0.67 | 0        | 48,54,54    | 2.21 | 18 (37%) |
| 15  | PGV  | D     | 501 | -    | 38,38,50     | 1.02 | 2 (5%)   | 41,44,56    | 1.19 | 3 (7%)   |
| 16  | BCL  | Z     | 102 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.19 | 22 (27%) |
| 21  | CRT  | M     | 407 | -    | 43,43,43     | 0.59 | 0        | 48,54,54    | 2.43 | 17 (35%) |
| 16  | BCL  | 4     | 101 | -    | 69,74,74     | 1.79 | 19 (27%) | 79,115,115  | 2.20 | 24 (30%) |
| 10  | HEM  | C     | 403 | 1    | 50,50,50     | 1.62 | 9 (18%)  | 67,82,82    | 1.61 | 10 (14%) |
| 21  | CRT  | G     | 103 | -    | 43,43,43     | 0.63 | 0        | 48,54,54    | 2.05 | 16 (33%) |
| 24  | LMT  | 2     | 101 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.67 | 1 (2%)   |
| 24  | LMT  | E     | 101 | -    | 36,36,36     | 0.43 | 0        | 47,47,47    | 0.81 | 1 (2%)   |
| 21  | CRT  | Q     | 101 | -    | 43,43,43     | 0.65 | 0        | 48,54,54    | 2.31 | 15 (31%) |
| 21  | CRT  | V     | 103 | -    | 43,43,43     | 0.64 | 0        | 48,54,54    | 2.31 | 19 (39%) |
| 16  | BCL  | I     | 101 | -    | 69,74,74     | 1.80 | 17 (24%) | 79,115,115  | 2.22 | 22 (27%) |
| 13  | Z41  | C     | 407 | -    | 34,34,39     | 0.29 | 0        | 36,36,41    | 0.30 | 0        |
| 24  | LMT  | 2     | 104 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.67 | 1 (2%)   |
| 16  | BCL  | L     | 307 | -    | 69,74,74     | 1.78 | 17 (24%) | 79,115,115  | 2.17 | 20 (25%) |
| 16  | BCL  | J     | 101 | -    | 69,74,74     | 1.77 | 17 (24%) | 79,115,115  | 2.20 | 23 (29%) |
| 24  | LMT  | Z     | 101 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 1.00 | 3 (6%)   |
| 15  | PGV  | L     | 309 | -    | 32,32,50     | 1.14 | 2 (6%)   | 35,38,56    | 1.30 | 3 (8%)   |
| 16  | BCL  | Q     | 102 | -    | 69,74,74     | 1.77 | 18 (26%) | 79,115,115  | 2.24 | 23 (29%) |
| 24  | LMT  | 5     | 101 | -    | 32,32,36     | 0.43 | 0        | 43,43,47    | 1.14 | 3 (6%)   |
| 16  | BCL  | N     | 101 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.19 | 22 (27%) |
| 10  | HEM  | C     | 402 | 1    | 50,50,50     | 1.60 | 9 (18%)  | 67,82,82    | 1.64 | 12 (17%) |
| 16  | BCL  | L     | 301 | -    | 69,74,74     | 1.77 | 17 (24%) | 79,115,115  | 2.22 | 23 (29%) |
| 16  | BCL  | T     | 101 | -    | 69,74,74     | 1.76 | 15 (21%) | 79,115,115  | 2.16 | 20 (25%) |
| 22  | CDL  | D     | 502 | -    | 57,57,99     | 1.11 | 4 (7%)   | 63,69,111   | 1.20 | 5 (7%)   |
| 16  | BCL  | 8     | 102 | -    | 69,74,74     | 1.76 | 16 (23%) | 79,115,115  | 2.20 | 24 (30%) |
| 15  | PGV  | F     | 501 | -    | 35,35,50     | 1.09 | 2 (5%)   | 38,41,56    | 1.16 | 3 (7%)   |
| 24  | LMT  | B     | 101 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.68 | 1 (2%)   |
| 16  | BCL  | X     | 102 | -    | 69,74,74     | 1.77 | 17 (24%) | 79,115,115  | 2.15 | 22 (27%) |
| 16  | BCL  | G     | 102 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.20 | 22 (27%) |
| 16  | BCL  | W     | 101 | -    | 69,74,74     | 1.78 | 19 (27%) | 79,115,115  | 2.24 | 22 (27%) |
| 24  | LMT  | 8     | 101 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.77 | 2 (4%)   |
| 24  | LMT  | G     | 101 | -    | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.68 | 1 (2%)   |
| 16  | BCL  | 2     | 102 | -    | 69,74,74     | 1.77 | 18 (26%) | 79,115,115  | 2.20 | 23 (29%) |
| 21  | CRT  | X     | 103 | -    | 43,43,43     | 0.61 | 0        | 48,54,54    | 2.18 | 17 (35%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 16  | BCL  | M     | 403 | -    | 69,74,74     | 1.77 | 19 (27%) | 79,115,115  | 2.17 | 24 (30%) |
| 17  | BPH  | L     | 302 | -    | 59,70,70     | 0.80 | 3 (5%)   | 59,101,101  | 0.93 | 3 (5%)   |
| 24  | LMT  | P     | 101 | -    | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.61 | 0        |
| 22  | CDL  | M     | 412 | -    | 83,83,99     | 1.04 | 4 (4%)   | 89,95,111   | 1.17 | 6 (6%)   |
| 21  | CRT  | 7     | 101 | -    | 43,43,43     | 0.65 | 0        | 48,54,54    | 1.90 | 10 (20%) |
| 23  | LDA  | O     | 501 | -    | 13,15,15     | 2.18 | 2 (15%)  | 14,17,17    | 0.50 | 0        |
| 15  | PGV  | L     | 306 | -    | 34,34,50     | 1.09 | 2 (5%)   | 37,40,56    | 1.18 | 4 (10%)  |
| 15  | PGV  | L     | 305 | -    | 28,28,50     | 1.21 | 2 (7%)   | 31,34,56    | 1.25 | 3 (9%)   |
| 21  | CRT  | B     | 103 | -    | 43,43,43     | 0.62 | 0        | 48,54,54    | 2.09 | 16 (33%) |
| 16  | BCL  | Y     | 101 | -    | 69,74,74     | 1.78 | 17 (24%) | 79,115,115  | 2.22 | 22 (27%) |
| 22  | CDL  | H     | 302 | -    | 78,78,99     | 1.02 | 4 (5%)   | 84,90,111   | 1.09 | 6 (7%)   |
| 22  | CDL  | M     | 411 | -    | 94,94,99     | 0.95 | 4 (4%)   | 100,106,111 | 1.10 | 7 (7%)   |
| 21  | CRT  | 8     | 103 | -    | 43,43,43     | 0.62 | 0        | 48,54,54    | 2.06 | 15 (31%) |
| 15  | PGV  | M     | 410 | -    | 26,26,50     | 1.29 | 2 (7%)   | 29,31,56    | 1.39 | 6 (20%)  |
| 22  | CDL  | M     | 409 | -    | 38,38,99     | 1.31 | 3 (7%)   | 43,49,111   | 1.18 | 3 (6%)   |
| 23  | LDA  | M     | 413 | -    | 13,15,15     | 2.20 | 2 (15%)  | 14,17,17    | 0.50 | 0        |
| 21  | CRT  | 0     | 103 | -    | 43,43,43     | 0.62 | 0        | 48,54,54    | 2.04 | 16 (33%) |
| 16  | BCL  | 0     | 102 | -    | 69,74,74     | 1.77 | 17 (24%) | 79,115,115  | 2.15 | 23 (29%) |
| 24  | LMT  | G     | 104 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.73 | 1 (2%)   |
| 15  | PGV  | 1     | 401 | -    | 26,26,50     | 1.29 | 2 (7%)   | 29,31,56    | 1.20 | 2 (6%)   |
| 16  | BCL  | 9     | 101 | -    | 69,74,74     | 1.79 | 18 (26%) | 79,115,115  | 2.20 | 23 (29%) |
| 21  | CRT  | 4     | 102 | -    | 43,43,43     | 0.65 | 0        | 48,54,54    | 2.21 | 16 (33%) |
| 18  | UQ8  | L     | 304 | -    | 53,53,53     | 1.23 | 2 (3%)   | 66,67,67    | 1.71 | 16 (24%) |
| 16  | BCL  | M     | 404 | -    | 69,74,74     | 1.80 | 17 (24%) | 79,115,115  | 2.37 | 26 (32%) |
| 17  | BPH  | M     | 405 | -    | 59,70,70     | 0.79 | 4 (6%)   | 59,101,101  | 0.86 | 3 (5%)   |
| 16  | BCL  | U     | 101 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.21 | 20 (25%) |
| 16  | BCL  | S     | 101 | -    | 69,74,74     | 1.78 | 17 (24%) | 79,115,115  | 2.19 | 22 (27%) |
| 16  | BCL  | V     | 102 | -    | 69,74,74     | 1.77 | 16 (23%) | 79,115,115  | 2.15 | 22 (27%) |
| 24  | LMT  | R     | 103 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.71 | 1 (2%)   |
| 18  | UQ8  | L     | 308 | -    | 53,53,53     | 1.26 | 2 (3%)   | 66,67,67    | 1.61 | 16 (24%) |
| 16  | BCL  | 3     | 101 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.27 | 24 (30%) |
| 21  | CRT  | T     | 102 | -    | 43,43,43     | 0.63 | 0        | 48,54,54    | 2.16 | 17 (35%) |
| 16  | BCL  | 6     | 101 | -    | 69,74,74     | 1.77 | 17 (24%) | 79,115,115  | 2.18 | 25 (31%) |
| 16  | BCL  | D     | 503 | -    | 69,74,74     | 1.78 | 17 (24%) | 79,115,115  | 2.25 | 21 (26%) |
| 15  | PGV  | H     | 301 | -    | 35,35,50     | 1.08 | 2 (5%)   | 38,41,56    | 1.23 | 4 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | LMT  | H     | 303 | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.79 | 1 (2%)   |
| 24  | LMT  | V     | 101 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.75 | 0        |
| 15  | PGV  | C     | 409 | -    | 30,30,50     | 1.17 | 2 (6%)   | 33,36,56    | 1.13 | 4 (12%)  |
| 20  | MQ8  | M     | 406 | -    | 54,54,54     | 1.33 | 2 (3%)   | 67,69,69    | 1.51 | 14 (20%) |
| 10  | HEM  | C     | 401 | 1    | 50,50,50     | 1.61 | 9 (18%)  | 67,82,82    | 1.67 | 14 (20%) |
| 16  | BCL  | R     | 101 | -    | 69,74,74     | 1.76 | 17 (24%) | 79,115,115  | 2.16 | 23 (29%) |
| 21  | CRT  | R     | 102 | -    | 43,43,43     | 0.62 | 0        | 48,54,54    | 2.06 | 16 (33%) |
| 15  | PGV  | M     | 408 | -    | 36,36,50     | 1.07 | 2 (5%)   | 39,42,56    | 1.17 | 3 (7%)   |
| 10  | HEM  | C     | 404 | 1    | 50,50,50     | 1.63 | 10 (20%) | 67,82,82    | 1.62 | 11 (16%) |
| 21  | CRT  | N     | 102 | -    | 43,43,43     | 0.61 | 0        | 48,54,54    | 2.13 | 17 (35%) |
| 16  | BCL  | F     | 502 | -    | 69,74,74     | 1.79 | 17 (24%) | 79,115,115  | 2.24 | 22 (27%) |
| 24  | LMT  | M     | 414 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.77 | 0        |
| 24  | LMT  | X     | 101 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.83 | 1 (2%)   |
| 24  | LMT  | O     | 101 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.78 | 1 (2%)   |
| 16  | BCL  | O     | 502 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.26 | 22 (27%) |
| 24  | LMT  | J     | 102 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.75 | 1 (2%)   |
| 24  | LMT  | P     | 103 | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.72 | 1 (2%)   |
| 18  | UQ8  | L     | 303 | -    | 33,33,53     | 1.51 | 2 (6%)   | 42,43,67    | 1.64 | 10 (23%) |
| 16  | BCL  | E     | 102 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.21 | 23 (29%) |
| 21  | CRT  | Z     | 103 | -    | 43,43,43     | 0.62 | 0        | 48,54,54    | 2.12 | 17 (35%) |
| 16  | BCL  | A     | 101 | -    | 69,74,74     | 1.77 | 18 (26%) | 79,115,115  | 2.28 | 22 (27%) |
| 16  | BCL  | K     | 102 | -    | 69,74,74     | 1.78 | 18 (26%) | 79,115,115  | 2.26 | 24 (30%) |
| 21  | CRT  | E     | 103 | -    | 43,43,43     | 0.61 | 0        | 48,54,54    | 2.17 | 17 (35%) |
| 16  | BCL  | 5     | 102 | -    | 69,74,74     | 1.79 | 17 (24%) | 79,115,115  | 2.23 | 23 (29%) |
| 16  | BCL  | 1     | 402 | -    | 69,74,74     | 1.78 | 17 (24%) | 79,115,115  | 2.20 | 24 (30%) |

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   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 21  | CRT  | K     | 101 | -    | -       | 11/51/51/51   | -       |
| 16  | BCL  | P     | 102 | -    | -       | 21/41/137/137 | -       |
| 24  | LMT  | 4     | 103 | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 16  | BCL  | B     | 102 | -    | -       | 17/41/137/137 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 16  | BCL  | 7     | 102 | -    | -       | 12/35/131/137 | -       |
| 14  | PLM  | C     | 408 | 1    | -       | 2/9/9/15      | -       |
| 21  | CRT  | 2     | 103 | -    | -       | 2/51/51/51    | -       |
| 15  | PGV  | D     | 501 | -    | -       | 14/43/43/55   | -       |
| 16  | BCL  | Z     | 102 | -    | -       | 16/41/137/137 | -       |
| 21  | CRT  | M     | 407 | -    | -       | 8/51/51/51    | -       |
| 16  | BCL  | 4     | 101 | -    | -       | 8/41/137/137  | -       |
| 10  | HEM  | C     | 403 | 1    | -       | 4/14/54/54    | -       |
| 21  | CRT  | G     | 103 | -    | -       | 5/51/51/51    | -       |
| 24  | LMT  | 2     | 101 | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 24  | LMT  | E     | 101 | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 21  | CRT  | Q     | 101 | -    | -       | 8/51/51/51    | -       |
| 21  | CRT  | V     | 103 | -    | -       | 5/51/51/51    | -       |
| 16  | BCL  | I     | 101 | -    | -       | 12/41/137/137 | -       |
| 13  | Z41  | C     | 407 | -    | -       | 5/35/35/41    | -       |
| 24  | LMT  | 2     | 104 | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 16  | BCL  | L     | 307 | -    | -       | 12/41/137/137 | -       |
| 16  | BCL  | J     | 101 | -    | -       | 14/41/137/137 | -       |
| 24  | LMT  | Z     | 101 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 15  | PGV  | L     | 309 | -    | -       | 6/37/37/55    | -       |
| 16  | BCL  | Q     | 102 | -    | -       | 11/41/137/137 | -       |
| 24  | LMT  | 5     | 101 | -    | -       | 5/17/57/61    | 0/2/2/2 |
| 16  | BCL  | N     | 101 | -    | -       | 15/41/137/137 | -       |
| 10  | HEM  | C     | 402 | 1    | -       | 7/14/54/54    | -       |
| 16  | BCL  | L     | 301 | -    | -       | 8/41/137/137  | -       |
| 16  | BCL  | T     | 101 | -    | -       | 17/41/137/137 | -       |
| 22  | CDL  | D     | 502 | -    | -       | 21/67/67/110  | -       |
| 16  | BCL  | 8     | 102 | -    | -       | 15/41/137/137 | -       |
| 15  | PGV  | F     | 501 | -    | -       | 4/40/40/55    | -       |
| 24  | LMT  | B     | 101 | -    | -       | 1/21/61/61    | 0/2/2/2 |
| 16  | BCL  | X     | 102 | -    | -       | 16/41/137/137 | -       |
| 16  | BCL  | G     | 102 | -    | -       | 18/41/137/137 | -       |
| 16  | BCL  | W     | 101 | -    | -       | 20/41/137/137 | -       |
| 24  | LMT  | 8     | 101 | -    | -       | 2/21/61/61    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 24  | LMT  | G     | 101 | -    | -       | 5/21/61/61     | 0/2/2/2 |
| 16  | BCL  | 2     | 102 | -    | -       | 14/41/137/137  | -       |
| 21  | CRT  | X     | 103 | -    | -       | 4/51/51/51     | -       |
| 16  | BCL  | M     | 403 | -    | -       | 5/41/137/137   | -       |
| 17  | BPH  | L     | 302 | -    | -       | 3/37/105/105   | 0/5/6/6 |
| 24  | LMT  | P     | 101 | -    | -       | 4/21/61/61     | 0/2/2/2 |
| 22  | CDL  | M     | 412 | -    | -       | 30/93/93/110   | -       |
| 21  | CRT  | 7     | 101 | -    | -       | 5/51/51/51     | -       |
| 23  | LDA  | O     | 501 | -    | -       | 0/13/13/13     | -       |
| 15  | PGV  | L     | 306 | -    | -       | 6/39/39/55     | -       |
| 15  | PGV  | L     | 305 | -    | -       | 14/33/33/55    | -       |
| 21  | CRT  | B     | 103 | -    | -       | 1/51/51/51     | -       |
| 16  | BCL  | Y     | 101 | -    | -       | 18/41/137/137  | -       |
| 22  | CDL  | H     | 302 | -    | -       | 22/89/89/110   | -       |
| 22  | CDL  | M     | 411 | -    | -       | 28/105/105/110 | -       |
| 21  | CRT  | 8     | 103 | -    | -       | 3/51/51/51     | -       |
| 15  | PGV  | M     | 410 | -    | -       | 7/28/28/55     | -       |
| 22  | CDL  | M     | 409 | -    | -       | 18/48/48/110   | -       |
| 23  | LDA  | M     | 413 | -    | -       | 3/13/13/13     | -       |
| 21  | CRT  | 0     | 103 | -    | -       | 2/51/51/51     | -       |
| 16  | BCL  | 0     | 102 | -    | -       | 16/41/137/137  | -       |
| 24  | LMT  | G     | 104 | -    | -       | 2/21/61/61     | 0/2/2/2 |
| 15  | PGV  | 1     | 401 | -    | -       | 12/30/30/55    | -       |
| 16  | BCL  | 9     | 101 | -    | -       | 16/41/137/137  | -       |
| 21  | CRT  | 4     | 102 | -    | -       | 7/51/51/51     | -       |
| 18  | UQ8  | L     | 304 | -    | -       | 14/51/75/75    | 0/1/1/1 |
| 16  | BCL  | M     | 404 | -    | -       | 10/41/137/137  | -       |
| 17  | BPH  | M     | 405 | -    | -       | 4/37/105/105   | 0/5/6/6 |
| 16  | BCL  | U     | 101 | -    | -       | 18/41/137/137  | -       |
| 16  | BCL  | S     | 101 | -    | -       | 11/41/137/137  | -       |
| 16  | BCL  | V     | 102 | -    | -       | 21/41/137/137  | -       |
| 24  | LMT  | R     | 103 | -    | -       | 7/21/61/61     | 0/2/2/2 |
| 18  | UQ8  | L     | 308 | -    | -       | 7/51/75/75     | 0/1/1/1 |
| 16  | BCL  | 3     | 101 | -    | -       | 10/41/137/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 21  | CRT  | T     | 102 | -    | -       | 5/51/51/51    | -       |
| 16  | BCL  | 6     | 101 | -    | -       | 14/41/137/137 | -       |
| 16  | BCL  | D     | 503 | -    | -       | 8/41/137/137  | -       |
| 15  | PGV  | H     | 301 | -    | -       | 15/40/40/55   | -       |
| 24  | LMT  | H     | 303 | -    | -       | 1/21/61/61    | 0/2/2/2 |
| 24  | LMT  | V     | 101 | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 15  | PGV  | C     | 409 | -    | -       | 5/35/35/55    | -       |
| 20  | MQ8  | M     | 406 | -    | -       | 5/47/67/67    | 0/2/2/2 |
| 10  | HEM  | C     | 401 | 1    | -       | 6/14/54/54    | -       |
| 16  | BCL  | R     | 101 | -    | -       | 13/41/137/137 | -       |
| 21  | CRT  | R     | 102 | -    | -       | 2/51/51/51    | -       |
| 15  | PGV  | M     | 408 | -    | -       | 5/41/41/55    | -       |
| 10  | HEM  | C     | 404 | 1    | -       | 6/14/54/54    | -       |
| 21  | CRT  | N     | 102 | -    | -       | 5/51/51/51    | -       |
| 16  | BCL  | F     | 502 | -    | -       | 12/41/137/137 | -       |
| 24  | LMT  | M     | 414 | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 24  | LMT  | X     | 101 | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 24  | LMT  | O     | 101 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 16  | BCL  | O     | 502 | -    | -       | 16/41/137/137 | -       |
| 24  | LMT  | J     | 102 | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 24  | LMT  | P     | 103 | -    | -       | 1/21/61/61    | 0/2/2/2 |
| 18  | UQ8  | L     | 303 | -    | -       | 4/27/51/75    | 0/1/1/1 |
| 16  | BCL  | E     | 102 | -    | -       | 13/41/137/137 | -       |
| 21  | CRT  | Z     | 103 | -    | -       | 8/51/51/51    | -       |
| 16  | BCL  | A     | 101 | -    | -       | 13/41/137/137 | -       |
| 16  | BCL  | K     | 102 | -    | -       | 10/41/137/137 | -       |
| 21  | CRT  | E     | 103 | -    | -       | 0/51/51/51    | -       |
| 16  | BCL  | 5     | 102 | -    | -       | 9/41/137/137  | -       |
| 16  | BCL  | 1     | 402 | -    | -       | 17/41/137/137 | -       |

All (722) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 20  | M     | 406 | MQ8  | C3-C2 | 8.01 | 1.49        | 1.35     |
| 18  | L     | 308 | UQ8  | C6-C1 | 7.75 | 1.49        | 1.35     |
| 18  | L     | 304 | UQ8  | C6-C1 | 7.70 | 1.49        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | L     | 303 | UQ8  | C6-C1   | 7.54  | 1.48        | 1.35     |
| 23  | M     | 413 | LDA  | O1-N1   | -6.81 | 1.25        | 1.42     |
| 23  | O     | 501 | LDA  | O1-N1   | -6.81 | 1.25        | 1.42     |
| 10  | C     | 404 | HEM  | FE-NB   | 5.36  | 2.11        | 1.94     |
| 10  | C     | 403 | HEM  | FE-NB   | 5.33  | 2.11        | 1.94     |
| 10  | C     | 402 | HEM  | FE-NB   | 5.22  | 2.11        | 1.94     |
| 10  | C     | 401 | HEM  | FE-NB   | 5.16  | 2.10        | 1.94     |
| 16  | L     | 301 | BCL  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 16  | N     | 101 | BCL  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 16  | 5     | 102 | BCL  | O2D-CGD | 5.03  | 1.45        | 1.33     |
| 16  | B     | 102 | BCL  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 16  | J     | 101 | BCL  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 16  | 0     | 102 | BCL  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 16  | 7     | 102 | BCL  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 16  | V     | 102 | BCL  | O2D-CGD | 4.99  | 1.45        | 1.33     |
| 16  | G     | 102 | BCL  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 16  | 8     | 102 | BCL  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 16  | 2     | 102 | BCL  | O2D-CGD | 4.98  | 1.45        | 1.33     |
| 16  | 4     | 101 | BCL  | O2D-CGD | 4.97  | 1.45        | 1.33     |
| 16  | E     | 102 | BCL  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 16  | S     | 101 | BCL  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 16  | 1     | 402 | BCL  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 16  | I     | 101 | BCL  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 16  | F     | 502 | BCL  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 16  | 6     | 101 | BCL  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 16  | K     | 102 | BCL  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 16  | X     | 102 | BCL  | O2D-CGD | 4.94  | 1.45        | 1.33     |
| 16  | A     | 101 | BCL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 16  | U     | 101 | BCL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 16  | P     | 102 | BCL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 16  | W     | 101 | BCL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 16  | Q     | 102 | BCL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 16  | D     | 503 | BCL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 16  | Y     | 101 | BCL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 16  | R     | 101 | BCL  | O2D-CGD | 4.92  | 1.45        | 1.33     |
| 16  | T     | 101 | BCL  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 16  | O     | 502 | BCL  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 16  | M     | 404 | BCL  | O2D-CGD | 4.91  | 1.45        | 1.33     |
| 16  | 3     | 101 | BCL  | O2D-CGD | 4.90  | 1.45        | 1.33     |
| 16  | Z     | 102 | BCL  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 16  | 9     | 101 | BCL  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 16  | M     | 404 | BCL  | C3D-C4D | -4.86 | 1.33        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | M     | 403 | BCL  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 22  | M     | 412 | CDL  | OA6-CA5 | 4.85  | 1.45        | 1.35     |
| 16  | L     | 307 | BCL  | C3D-C4D | -4.82 | 1.33        | 1.44     |
| 16  | M     | 403 | BCL  | C3D-C4D | -4.79 | 1.33        | 1.44     |
| 16  | D     | 503 | BCL  | C3D-C4D | -4.79 | 1.33        | 1.44     |
| 16  | 9     | 101 | BCL  | C3D-C4D | -4.75 | 1.33        | 1.44     |
| 20  | M     | 406 | MQ8  | C10-C5  | 4.75  | 1.48        | 1.40     |
| 16  | 7     | 102 | BCL  | C3D-C4D | -4.74 | 1.33        | 1.44     |
| 16  | S     | 101 | BCL  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 16  | O     | 502 | BCL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 16  | U     | 101 | BCL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 16  | W     | 101 | BCL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 16  | K     | 102 | BCL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 16  | A     | 101 | BCL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 16  | F     | 502 | BCL  | C3D-C4D | -4.72 | 1.33        | 1.44     |
| 16  | L     | 301 | BCL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 16  | I     | 101 | BCL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 16  | Q     | 102 | BCL  | C3D-C4D | -4.71 | 1.33        | 1.44     |
| 16  | 5     | 102 | BCL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 16  | G     | 102 | BCL  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 16  | 2     | 102 | BCL  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 16  | L     | 307 | BCL  | O2D-CGD | 4.68  | 1.44        | 1.33     |
| 16  | 0     | 102 | BCL  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 16  | Y     | 101 | BCL  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 16  | 3     | 101 | BCL  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 16  | B     | 102 | BCL  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 16  | 1     | 402 | BCL  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 16  | N     | 101 | BCL  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 16  | R     | 101 | BCL  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 16  | Z     | 102 | BCL  | C3D-C4D | -4.62 | 1.33        | 1.44     |
| 16  | 8     | 102 | BCL  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 16  | 6     | 101 | BCL  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 16  | J     | 101 | BCL  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 16  | X     | 102 | BCL  | C3D-C4D | -4.60 | 1.33        | 1.44     |
| 16  | 4     | 101 | BCL  | C3D-C4D | -4.59 | 1.33        | 1.44     |
| 16  | E     | 102 | BCL  | C3D-C4D | -4.58 | 1.33        | 1.44     |
| 16  | P     | 102 | BCL  | C3D-C4D | -4.58 | 1.33        | 1.44     |
| 16  | T     | 101 | BCL  | C3D-C4D | -4.57 | 1.33        | 1.44     |
| 16  | V     | 102 | BCL  | C3D-C4D | -4.54 | 1.34        | 1.44     |
| 15  | 1     | 401 | PGV  | O01-C1  | 4.44  | 1.46        | 1.34     |
| 22  | M     | 409 | CDL  | OA6-CA5 | 4.37  | 1.46        | 1.34     |
| 22  | M     | 409 | CDL  | OA8-CA7 | 4.37  | 1.46        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 16  | M     | 403 | BCL  | O2A-CGA | 4.36 | 1.46        | 1.33     |
| 16  | 1     | 402 | BCL  | O2A-CGA | 4.35 | 1.46        | 1.33     |
| 22  | M     | 411 | CDL  | OA6-CA5 | 4.33 | 1.46        | 1.34     |
| 16  | Z     | 102 | BCL  | O2A-CGA | 4.30 | 1.45        | 1.33     |
| 16  | 4     | 101 | BCL  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 16  | E     | 102 | BCL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 16  | F     | 502 | BCL  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 16  | 3     | 101 | BCL  | O2A-CGA | 4.27 | 1.45        | 1.33     |
| 16  | V     | 102 | BCL  | O2A-CGA | 4.25 | 1.45        | 1.33     |
| 16  | X     | 102 | BCL  | O2A-CGA | 4.25 | 1.45        | 1.33     |
| 16  | L     | 301 | BCL  | O2A-CGA | 4.24 | 1.45        | 1.33     |
| 16  | I     | 101 | BCL  | O2A-CGA | 4.24 | 1.45        | 1.33     |
| 16  | O     | 502 | BCL  | O2A-CGA | 4.23 | 1.45        | 1.33     |
| 16  | 9     | 101 | BCL  | O2A-CGA | 4.23 | 1.45        | 1.33     |
| 15  | M     | 410 | PGV  | O03-C19 | 4.23 | 1.45        | 1.33     |
| 10  | C     | 402 | HEM  | FE-NC   | 4.23 | 2.09        | 1.95     |
| 22  | M     | 411 | CDL  | OA8-CA7 | 4.23 | 1.45        | 1.33     |
| 15  | 1     | 401 | PGV  | O03-C19 | 4.22 | 1.45        | 1.33     |
| 16  | G     | 102 | BCL  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 16  | S     | 101 | BCL  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 16  | M     | 404 | BCL  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 16  | J     | 101 | BCL  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 16  | U     | 101 | BCL  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 22  | M     | 412 | CDL  | OA8-CA7 | 4.21 | 1.45        | 1.33     |
| 16  | 5     | 102 | BCL  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 16  | 6     | 101 | BCL  | O2A-CGA | 4.20 | 1.45        | 1.33     |
| 16  | K     | 102 | BCL  | O2A-CGA | 4.20 | 1.45        | 1.33     |
| 15  | L     | 309 | PGV  | O03-C19 | 4.20 | 1.45        | 1.33     |
| 16  | R     | 101 | BCL  | O2A-CGA | 4.20 | 1.45        | 1.33     |
| 15  | C     | 409 | PGV  | O03-C19 | 4.20 | 1.45        | 1.33     |
| 15  | L     | 305 | PGV  | O01-C1  | 4.20 | 1.46        | 1.34     |
| 15  | M     | 408 | PGV  | O03-C19 | 4.20 | 1.45        | 1.33     |
| 22  | M     | 412 | CDL  | OB8-CB7 | 4.20 | 1.45        | 1.33     |
| 15  | F     | 501 | PGV  | O03-C19 | 4.19 | 1.45        | 1.33     |
| 15  | L     | 306 | PGV  | O03-C19 | 4.19 | 1.45        | 1.33     |
| 10  | C     | 401 | HEM  | FE-NC   | 4.19 | 2.09        | 1.95     |
| 22  | D     | 502 | CDL  | OB8-CB7 | 4.19 | 1.45        | 1.33     |
| 16  | Q     | 102 | BCL  | O2A-CGA | 4.18 | 1.45        | 1.33     |
| 16  | 7     | 102 | BCL  | O2A-CGA | 4.17 | 1.45        | 1.33     |
| 16  | D     | 503 | BCL  | O2A-CGA | 4.17 | 1.45        | 1.33     |
| 16  | N     | 101 | BCL  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 22  | H     | 302 | CDL  | OA8-CA7 | 4.16 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | P     | 102 | BCL  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 16  | B     | 102 | BCL  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 15  | H     | 301 | PGV  | O03-C19 | 4.15  | 1.45        | 1.33     |
| 16  | T     | 101 | BCL  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 15  | F     | 501 | PGV  | O01-C1  | 4.15  | 1.46        | 1.34     |
| 15  | L     | 309 | PGV  | O01-C1  | 4.15  | 1.46        | 1.34     |
| 16  | O     | 102 | BCL  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 22  | M     | 411 | CDL  | OB8-CB7 | 4.15  | 1.45        | 1.33     |
| 16  | W     | 101 | BCL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 10  | C     | 404 | HEM  | FE-NC   | 4.14  | 2.08        | 1.95     |
| 16  | A     | 101 | BCL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 15  | L     | 305 | PGV  | O03-C19 | 4.12  | 1.45        | 1.33     |
| 22  | H     | 302 | CDL  | OB8-CB7 | 4.11  | 1.45        | 1.33     |
| 16  | Y     | 101 | BCL  | O2A-CGA | 4.11  | 1.45        | 1.33     |
| 22  | D     | 502 | CDL  | OB6-CB5 | 4.11  | 1.45        | 1.34     |
| 22  | D     | 502 | CDL  | OA6-CA5 | 4.11  | 1.45        | 1.34     |
| 16  | 2     | 102 | BCL  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 16  | 8     | 102 | BCL  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 16  | L     | 307 | BCL  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 15  | M     | 408 | PGV  | O01-C1  | 4.09  | 1.45        | 1.34     |
| 10  | C     | 403 | HEM  | FE-NC   | 4.08  | 2.08        | 1.95     |
| 22  | M     | 412 | CDL  | OB6-CB5 | 4.07  | 1.45        | 1.34     |
| 22  | H     | 302 | CDL  | OA6-CA5 | 4.06  | 1.45        | 1.34     |
| 22  | M     | 411 | CDL  | OB6-CB5 | 4.05  | 1.45        | 1.34     |
| 22  | M     | 409 | CDL  | OB6-CB5 | 4.04  | 1.45        | 1.34     |
| 23  | M     | 413 | LDA  | C1-N1   | -4.01 | 1.47        | 1.51     |
| 22  | H     | 302 | CDL  | OB6-CB5 | 4.00  | 1.45        | 1.34     |
| 16  | F     | 502 | BCL  | C3B-C4B | 4.00  | 1.49        | 1.41     |
| 16  | K     | 102 | BCL  | C3B-C4B | 4.00  | 1.49        | 1.41     |
| 15  | H     | 301 | PGV  | O01-C1  | 3.99  | 1.45        | 1.34     |
| 15  | D     | 501 | PGV  | O03-C19 | 3.99  | 1.45        | 1.33     |
| 15  | M     | 410 | PGV  | O01-C1  | 3.99  | 1.45        | 1.34     |
| 16  | 1     | 402 | BCL  | C3B-C4B | 3.98  | 1.49        | 1.41     |
| 15  | L     | 306 | PGV  | O01-C1  | 3.98  | 1.45        | 1.34     |
| 15  | C     | 409 | PGV  | O01-C1  | 3.97  | 1.45        | 1.34     |
| 15  | D     | 501 | PGV  | O01-C1  | 3.97  | 1.45        | 1.34     |
| 16  | 7     | 102 | BCL  | C3B-C4B | 3.94  | 1.48        | 1.41     |
| 16  | S     | 101 | BCL  | C3B-C4B | 3.94  | 1.48        | 1.41     |
| 16  | L     | 307 | BCL  | C3B-C4B | 3.93  | 1.48        | 1.41     |
| 16  | 5     | 102 | BCL  | C3B-C4B | 3.93  | 1.48        | 1.41     |
| 16  | B     | 102 | BCL  | C3B-C4B | 3.92  | 1.48        | 1.41     |
| 16  | W     | 101 | BCL  | C3B-C4B | 3.92  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | M     | 404 | BCL  | C3B-C4B | 3.91  | 1.48        | 1.41     |
| 16  | D     | 503 | BCL  | C3B-C4B | 3.91  | 1.48        | 1.41     |
| 16  | Y     | 101 | BCL  | C3B-C4B | 3.90  | 1.48        | 1.41     |
| 16  | A     | 101 | BCL  | C3B-C4B | 3.90  | 1.48        | 1.41     |
| 16  | T     | 101 | BCL  | C3B-C4B | 3.89  | 1.48        | 1.41     |
| 23  | O     | 501 | LDA  | C1-N1   | -3.89 | 1.47        | 1.51     |
| 16  | L     | 301 | BCL  | C3B-C4B | 3.88  | 1.48        | 1.41     |
| 16  | 3     | 101 | BCL  | C3B-C4B | 3.88  | 1.48        | 1.41     |
| 16  | R     | 101 | BCL  | C3B-C4B | 3.87  | 1.48        | 1.41     |
| 16  | 9     | 101 | BCL  | C3B-C4B | 3.87  | 1.48        | 1.41     |
| 16  | G     | 102 | BCL  | C3B-C4B | 3.87  | 1.48        | 1.41     |
| 16  | O     | 502 | BCL  | C3B-C4B | 3.87  | 1.48        | 1.41     |
| 16  | V     | 102 | BCL  | C3B-C4B | 3.87  | 1.48        | 1.41     |
| 16  | Q     | 102 | BCL  | C3B-C4B | 3.86  | 1.48        | 1.41     |
| 16  | U     | 101 | BCL  | C3B-C4B | 3.85  | 1.48        | 1.41     |
| 16  | E     | 102 | BCL  | C3B-C4B | 3.85  | 1.48        | 1.41     |
| 16  | I     | 101 | BCL  | C3B-C4B | 3.85  | 1.48        | 1.41     |
| 16  | X     | 102 | BCL  | C3B-C4B | 3.85  | 1.48        | 1.41     |
| 16  | P     | 102 | BCL  | C3B-C4B | 3.84  | 1.48        | 1.41     |
| 16  | 8     | 102 | BCL  | C3B-C4B | 3.84  | 1.48        | 1.41     |
| 16  | Z     | 102 | BCL  | C3B-C4B | 3.80  | 1.48        | 1.41     |
| 16  | J     | 101 | BCL  | C3B-C4B | 3.80  | 1.48        | 1.41     |
| 16  | 4     | 101 | BCL  | C3B-C4B | 3.80  | 1.48        | 1.41     |
| 16  | 2     | 102 | BCL  | C3B-C4B | 3.79  | 1.48        | 1.41     |
| 16  | 7     | 102 | BCL  | CHD-C1D | 3.75  | 1.45        | 1.38     |
| 16  | 6     | 101 | BCL  | C3B-C4B | 3.74  | 1.48        | 1.41     |
| 16  | N     | 101 | BCL  | C3B-C4B | 3.73  | 1.48        | 1.41     |
| 16  | 0     | 102 | BCL  | C3B-C4B | 3.71  | 1.48        | 1.41     |
| 16  | M     | 403 | BCL  | C3B-C4B | 3.70  | 1.48        | 1.41     |
| 16  | F     | 502 | BCL  | CHD-C1D | 3.67  | 1.45        | 1.38     |
| 18  | L     | 308 | UQ8  | C4-C3   | 3.65  | 1.49        | 1.36     |
| 16  | I     | 101 | BCL  | CHD-C1D | 3.64  | 1.45        | 1.38     |
| 16  | 5     | 102 | BCL  | CHD-C1D | 3.63  | 1.45        | 1.38     |
| 16  | 9     | 101 | BCL  | CHD-C1D | 3.61  | 1.45        | 1.38     |
| 16  | J     | 101 | BCL  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 16  | W     | 101 | BCL  | CHD-C1D | 3.55  | 1.45        | 1.38     |
| 16  | B     | 102 | BCL  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 16  | A     | 101 | BCL  | CHD-C1D | 3.55  | 1.45        | 1.38     |
| 10  | C     | 404 | HEM  | C1B-NB  | -3.54 | 1.34        | 1.40     |
| 16  | Y     | 101 | BCL  | CHD-C1D | 3.53  | 1.45        | 1.38     |
| 16  | G     | 102 | BCL  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 16  | 6     | 101 | BCL  | OBD-CAD | 3.51  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | C     | 401 | HEM  | C1B-NB  | -3.51 | 1.34        | 1.40     |
| 16  | U     | 101 | BCL  | CHD-C1D | 3.50  | 1.45        | 1.38     |
| 16  | Y     | 101 | BCL  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 16  | S     | 101 | BCL  | CHD-C1D | 3.49  | 1.45        | 1.38     |
| 16  | U     | 101 | BCL  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 16  | E     | 102 | BCL  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 10  | C     | 403 | HEM  | C1B-NB  | -3.48 | 1.34        | 1.40     |
| 16  | 5     | 102 | BCL  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 16  | P     | 102 | BCL  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 16  | 1     | 402 | BCL  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 16  | 3     | 101 | BCL  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 16  | 6     | 101 | BCL  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 16  | 4     | 101 | BCL  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 16  | I     | 101 | BCL  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 16  | W     | 101 | BCL  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 16  | 0     | 102 | BCL  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 16  | M     | 403 | BCL  | CHD-C1D | 3.46  | 1.45        | 1.38     |
| 16  | R     | 101 | BCL  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 16  | D     | 503 | BCL  | CHD-C1D | 3.46  | 1.45        | 1.38     |
| 16  | Q     | 102 | BCL  | CHD-C1D | 3.46  | 1.45        | 1.38     |
| 16  | O     | 502 | BCL  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 16  | 3     | 101 | BCL  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 16  | D     | 503 | BCL  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 16  | 9     | 101 | BCL  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 16  | F     | 502 | BCL  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 16  | 2     | 102 | BCL  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 16  | O     | 502 | BCL  | CHD-C1D | 3.45  | 1.45        | 1.38     |
| 18  | L     | 304 | UQ8  | C4-C3   | 3.44  | 1.48        | 1.36     |
| 16  | 1     | 402 | BCL  | CHD-C1D | 3.44  | 1.45        | 1.38     |
| 16  | T     | 101 | BCL  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 16  | 8     | 102 | BCL  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 16  | L     | 307 | BCL  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 18  | L     | 303 | UQ8  | C4-C3   | 3.43  | 1.48        | 1.36     |
| 16  | Z     | 102 | BCL  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 16  | K     | 102 | BCL  | CHD-C1D | 3.43  | 1.45        | 1.38     |
| 16  | K     | 102 | BCL  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 16  | Q     | 102 | BCL  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 16  | V     | 102 | BCL  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 16  | 7     | 102 | BCL  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 16  | 3     | 101 | BCL  | CHD-C1D | 3.41  | 1.45        | 1.38     |
| 16  | L     | 307 | BCL  | CHD-C1D | 3.41  | 1.45        | 1.38     |
| 16  | M     | 403 | BCL  | CHB-C1B | 3.41  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | X     | 102 | BCL  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 16  | N     | 101 | BCL  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 16  | A     | 101 | BCL  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 16  | S     | 101 | BCL  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 16  | L     | 301 | BCL  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 16  | K     | 102 | BCL  | CHB-C1B | 3.38  | 1.47        | 1.39     |
| 10  | C     | 402 | HEM  | C1B-NB  | -3.38 | 1.34        | 1.40     |
| 16  | S     | 101 | BCL  | CHB-C1B | 3.38  | 1.47        | 1.39     |
| 10  | C     | 403 | HEM  | C4D-ND  | -3.37 | 1.34        | 1.40     |
| 16  | L     | 301 | BCL  | CHD-C1D | 3.37  | 1.45        | 1.38     |
| 16  | X     | 102 | BCL  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 16  | T     | 101 | BCL  | CHB-C1B | 3.36  | 1.47        | 1.39     |
| 16  | I     | 101 | BCL  | CHB-C1B | 3.36  | 1.47        | 1.39     |
| 16  | J     | 101 | BCL  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 16  | 1     | 402 | BCL  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 16  | M     | 403 | BCL  | OBD-CAD | 3.34  | 1.28        | 1.22     |
| 16  | M     | 404 | BCL  | CHC-C4B | 3.34  | 1.46        | 1.39     |
| 16  | Y     | 101 | BCL  | CHB-C1B | 3.34  | 1.46        | 1.39     |
| 16  | R     | 101 | BCL  | CHB-C1B | 3.33  | 1.46        | 1.39     |
| 16  | L     | 307 | BCL  | CHC-C4B | 3.32  | 1.46        | 1.39     |
| 16  | 4     | 101 | BCL  | CHB-C1B | 3.32  | 1.46        | 1.39     |
| 16  | 5     | 102 | BCL  | CHB-C1B | 3.32  | 1.46        | 1.39     |
| 10  | C     | 404 | HEM  | C4D-ND  | -3.31 | 1.34        | 1.40     |
| 16  | 0     | 102 | BCL  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 16  | U     | 101 | BCL  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 16  | L     | 307 | BCL  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 16  | 9     | 101 | BCL  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 16  | M     | 404 | BCL  | CHD-C1D | 3.30  | 1.44        | 1.38     |
| 16  | L     | 301 | BCL  | CHC-C4B | 3.29  | 1.46        | 1.39     |
| 16  | D     | 503 | BCL  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 16  | 7     | 102 | BCL  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 10  | C     | 401 | HEM  | C4D-ND  | -3.28 | 1.34        | 1.40     |
| 16  | B     | 102 | BCL  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 16  | P     | 102 | BCL  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 16  | 2     | 102 | BCL  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 16  | L     | 301 | BCL  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 16  | Z     | 102 | BCL  | CHD-C1D | 3.27  | 1.44        | 1.38     |
| 16  | O     | 502 | BCL  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 16  | F     | 502 | BCL  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 16  | F     | 502 | BCL  | CHC-C4B | 3.26  | 1.46        | 1.39     |
| 16  | Q     | 102 | BCL  | CHB-C1B | 3.26  | 1.46        | 1.39     |
| 16  | E     | 102 | BCL  | CHB-C1B | 3.26  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | Z     | 102 | BCL  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 16  | P     | 102 | BCL  | CHD-C1D | 3.24  | 1.44        | 1.38     |
| 16  | N     | 101 | BCL  | CHD-C1D | 3.24  | 1.44        | 1.38     |
| 16  | G     | 102 | BCL  | CHB-C1B | 3.24  | 1.46        | 1.39     |
| 16  | V     | 102 | BCL  | CHB-C1B | 3.24  | 1.46        | 1.39     |
| 16  | B     | 102 | BCL  | CHD-C1D | 3.24  | 1.44        | 1.38     |
| 16  | 2     | 102 | BCL  | CHD-C1D | 3.24  | 1.44        | 1.38     |
| 16  | N     | 101 | BCL  | CHB-C1B | 3.23  | 1.46        | 1.39     |
| 16  | R     | 101 | BCL  | C1D-ND  | -3.23 | 1.33        | 1.37     |
| 16  | 8     | 102 | BCL  | CHD-C1D | 3.23  | 1.44        | 1.38     |
| 16  | M     | 404 | BCL  | CHB-C1B | 3.23  | 1.46        | 1.39     |
| 10  | C     | 402 | HEM  | C4D-ND  | -3.23 | 1.34        | 1.40     |
| 16  | 1     | 402 | BCL  | CHC-C4B | 3.22  | 1.46        | 1.39     |
| 16  | T     | 101 | BCL  | C1D-ND  | -3.21 | 1.33        | 1.37     |
| 16  | 8     | 102 | BCL  | CHB-C1B | 3.21  | 1.46        | 1.39     |
| 16  | S     | 101 | BCL  | CHC-C4B | 3.21  | 1.46        | 1.39     |
| 16  | V     | 102 | BCL  | C1D-ND  | -3.20 | 1.33        | 1.37     |
| 16  | 7     | 102 | BCL  | CHC-C4B | 3.19  | 1.46        | 1.39     |
| 16  | W     | 101 | BCL  | CHC-C4B | 3.19  | 1.46        | 1.39     |
| 16  | L     | 307 | BCL  | C1D-ND  | -3.19 | 1.33        | 1.37     |
| 16  | M     | 404 | BCL  | C4B-NB  | -3.18 | 1.33        | 1.37     |
| 16  | P     | 102 | BCL  | C1D-ND  | -3.18 | 1.33        | 1.37     |
| 16  | 4     | 101 | BCL  | CHD-C1D | 3.18  | 1.44        | 1.38     |
| 16  | T     | 101 | BCL  | CHD-C1D | 3.18  | 1.44        | 1.38     |
| 16  | W     | 101 | BCL  | CHB-C1B | 3.18  | 1.46        | 1.39     |
| 16  | 4     | 101 | BCL  | C1D-ND  | -3.17 | 1.33        | 1.37     |
| 16  | 8     | 102 | BCL  | CHC-C4B | 3.17  | 1.46        | 1.39     |
| 16  | J     | 101 | BCL  | CHD-C1D | 3.17  | 1.44        | 1.38     |
| 16  | G     | 102 | BCL  | CHD-C1D | 3.17  | 1.44        | 1.38     |
| 16  | A     | 101 | BCL  | CHB-C1B | 3.17  | 1.46        | 1.39     |
| 16  | Y     | 101 | BCL  | CHC-C4B | 3.17  | 1.46        | 1.39     |
| 16  | 0     | 102 | BCL  | CHD-C1D | 3.16  | 1.44        | 1.38     |
| 16  | G     | 102 | BCL  | CHC-C4B | 3.16  | 1.46        | 1.39     |
| 16  | V     | 102 | BCL  | CHD-C1D | 3.16  | 1.44        | 1.38     |
| 16  | E     | 102 | BCL  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 16  | 8     | 102 | BCL  | C1D-ND  | -3.15 | 1.33        | 1.37     |
| 16  | 5     | 102 | BCL  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 16  | M     | 404 | BCL  | OBD-CAD | 3.14  | 1.27        | 1.22     |
| 16  | X     | 102 | BCL  | C1D-ND  | -3.14 | 1.33        | 1.37     |
| 16  | Z     | 102 | BCL  | C1D-ND  | -3.14 | 1.33        | 1.37     |
| 16  | T     | 101 | BCL  | CHC-C4B | 3.14  | 1.46        | 1.39     |
| 16  | R     | 101 | BCL  | CHC-C4B | 3.14  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 17  | M     | 405 | BPH  | C4D-CHA | 3.13  | 1.44        | 1.39     |
| 16  | 9     | 101 | BCL  | CHC-C4B | 3.13  | 1.46        | 1.39     |
| 16  | 2     | 102 | BCL  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 16  | I     | 101 | BCL  | CHC-C4B | 3.13  | 1.46        | 1.39     |
| 16  | X     | 102 | BCL  | CHD-C1D | 3.12  | 1.44        | 1.38     |
| 16  | M     | 403 | BCL  | C3D-C2D | 3.12  | 1.47        | 1.39     |
| 16  | E     | 102 | BCL  | C1D-ND  | -3.12 | 1.33        | 1.37     |
| 16  | 0     | 102 | BCL  | C1D-ND  | -3.12 | 1.33        | 1.37     |
| 16  | B     | 102 | BCL  | CHC-C4B | 3.11  | 1.46        | 1.39     |
| 16  | X     | 102 | BCL  | CHC-C4B | 3.10  | 1.46        | 1.39     |
| 17  | L     | 302 | BPH  | C4D-CHA | 3.10  | 1.44        | 1.39     |
| 16  | 4     | 101 | BCL  | CHC-C4B | 3.10  | 1.46        | 1.39     |
| 16  | V     | 102 | BCL  | CHC-C4B | 3.09  | 1.46        | 1.39     |
| 16  | J     | 101 | BCL  | C1D-ND  | -3.09 | 1.33        | 1.37     |
| 16  | D     | 503 | BCL  | CHC-C4B | 3.09  | 1.46        | 1.39     |
| 16  | B     | 102 | BCL  | C1D-ND  | -3.09 | 1.33        | 1.37     |
| 16  | N     | 101 | BCL  | C1D-ND  | -3.09 | 1.33        | 1.37     |
| 16  | U     | 101 | BCL  | CHC-C4B | 3.09  | 1.46        | 1.39     |
| 16  | R     | 101 | BCL  | CHD-C1D | 3.08  | 1.44        | 1.38     |
| 16  | 2     | 102 | BCL  | CHC-C4B | 3.08  | 1.46        | 1.39     |
| 16  | A     | 101 | BCL  | CHC-C4B | 3.08  | 1.46        | 1.39     |
| 16  | 6     | 101 | BCL  | CHC-C4B | 3.08  | 1.46        | 1.39     |
| 16  | P     | 102 | BCL  | CHC-C4B | 3.08  | 1.46        | 1.39     |
| 16  | 6     | 101 | BCL  | CHD-C1D | 3.08  | 1.44        | 1.38     |
| 16  | 6     | 101 | BCL  | C1D-ND  | -3.06 | 1.33        | 1.37     |
| 16  | J     | 101 | BCL  | CHC-C4B | 3.06  | 1.46        | 1.39     |
| 16  | E     | 102 | BCL  | CHD-C1D | 3.06  | 1.44        | 1.38     |
| 16  | N     | 101 | BCL  | CHC-C4B | 3.05  | 1.46        | 1.39     |
| 16  | Z     | 102 | BCL  | CHC-C4B | 3.05  | 1.46        | 1.39     |
| 16  | P     | 102 | BCL  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 16  | G     | 102 | BCL  | C1D-ND  | -3.04 | 1.33        | 1.37     |
| 16  | L     | 307 | BCL  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 16  | M     | 403 | BCL  | C4B-NB  | -3.03 | 1.33        | 1.37     |
| 16  | 0     | 102 | BCL  | CHC-C4B | 3.03  | 1.46        | 1.39     |
| 16  | K     | 102 | BCL  | CHC-C4B | 3.01  | 1.46        | 1.39     |
| 16  | U     | 101 | BCL  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 16  | 2     | 102 | BCL  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 16  | 1     | 402 | BCL  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 16  | V     | 102 | BCL  | C4B-NB  | -2.99 | 1.33        | 1.37     |
| 16  | V     | 102 | BCL  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 16  | W     | 101 | BCL  | C3D-C2D | 2.99  | 1.47        | 1.39     |
| 16  | I     | 101 | BCL  | C4B-NB  | -2.99 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | N     | 101 | BCL  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 16  | Z     | 102 | BCL  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 16  | 0     | 102 | BCL  | C4B-NB  | -2.98 | 1.33        | 1.37     |
| 16  | 6     | 101 | BCL  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 16  | S     | 101 | BCL  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 16  | 4     | 101 | BCL  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 16  | 5     | 102 | BCL  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 16  | L     | 307 | BCL  | C4B-NB  | -2.97 | 1.34        | 1.37     |
| 16  | O     | 502 | BCL  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 16  | I     | 101 | BCL  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 16  | Q     | 102 | BCL  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 16  | Q     | 102 | BCL  | CHC-C4B | 2.96  | 1.46        | 1.39     |
| 16  | R     | 101 | BCL  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 16  | 3     | 101 | BCL  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 16  | O     | 502 | BCL  | C4B-NB  | -2.96 | 1.34        | 1.37     |
| 16  | 3     | 101 | BCL  | CHC-C4B | 2.95  | 1.46        | 1.39     |
| 16  | D     | 503 | BCL  | C3D-C2D | 2.95  | 1.47        | 1.39     |
| 16  | J     | 101 | BCL  | C3D-C2D | 2.95  | 1.47        | 1.39     |
| 16  | M     | 403 | BCL  | CHC-C4B | 2.95  | 1.46        | 1.39     |
| 16  | O     | 502 | BCL  | CHC-C4B | 2.95  | 1.46        | 1.39     |
| 16  | K     | 102 | BCL  | C3D-C2D | 2.95  | 1.47        | 1.39     |
| 16  | M     | 403 | BCL  | C1D-ND  | -2.94 | 1.34        | 1.37     |
| 16  | 0     | 102 | BCL  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 16  | F     | 502 | BCL  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 16  | X     | 102 | BCL  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 16  | 9     | 101 | BCL  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 16  | 7     | 102 | BCL  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 16  | 8     | 102 | BCL  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 16  | Q     | 102 | BCL  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 16  | Z     | 102 | BCL  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 16  | B     | 102 | BCL  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 16  | Y     | 101 | BCL  | C3D-C2D | 2.91  | 1.46        | 1.39     |
| 16  | G     | 102 | BCL  | C3D-C2D | 2.91  | 1.46        | 1.39     |
| 16  | W     | 101 | BCL  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 16  | B     | 102 | BCL  | C3D-C2D | 2.91  | 1.46        | 1.39     |
| 16  | T     | 101 | BCL  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 16  | K     | 102 | BCL  | C1D-ND  | -2.90 | 1.34        | 1.37     |
| 16  | N     | 101 | BCL  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 16  | E     | 102 | BCL  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 16  | 2     | 102 | BCL  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 16  | E     | 102 | BCL  | C3D-C2D | 2.89  | 1.46        | 1.39     |
| 16  | A     | 101 | BCL  | C3D-C2D | 2.88  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | 9     | 101 | BCL  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 16  | T     | 101 | BCL  | C3D-C2D | 2.86  | 1.46        | 1.39     |
| 16  | I     | 101 | BCL  | CHD-C4C | 2.86  | 1.47        | 1.39     |
| 16  | K     | 102 | BCL  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 16  | 4     | 101 | BCL  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 16  | 9     | 101 | BCL  | C1D-ND  | -2.85 | 1.34        | 1.37     |
| 16  | M     | 404 | BCL  | C1D-ND  | -2.83 | 1.34        | 1.37     |
| 16  | 7     | 102 | BCL  | CHD-C4C | 2.82  | 1.47        | 1.39     |
| 16  | D     | 503 | BCL  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 16  | D     | 503 | BCL  | C1D-ND  | -2.82 | 1.34        | 1.37     |
| 16  | F     | 502 | BCL  | CHD-C4C | 2.82  | 1.47        | 1.39     |
| 16  | M     | 404 | BCL  | C1B-NB  | -2.82 | 1.34        | 1.37     |
| 16  | R     | 101 | BCL  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 16  | S     | 101 | BCL  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 16  | 1     | 402 | BCL  | C1D-ND  | -2.81 | 1.34        | 1.37     |
| 16  | A     | 101 | BCL  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 16  | 3     | 101 | BCL  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 16  | G     | 102 | BCL  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 16  | J     | 101 | BCL  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 16  | 6     | 101 | BCL  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 16  | X     | 102 | BCL  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 16  | U     | 101 | BCL  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 16  | 8     | 102 | BCL  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 16  | L     | 301 | BCL  | C3D-C2D | 2.78  | 1.46        | 1.39     |
| 16  | P     | 102 | BCL  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 16  | 5     | 102 | BCL  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 16  | Y     | 101 | BCL  | CHD-C4C | 2.76  | 1.47        | 1.39     |
| 16  | L     | 301 | BCL  | C1D-ND  | -2.76 | 1.34        | 1.37     |
| 16  | 3     | 101 | BCL  | C1D-ND  | -2.76 | 1.34        | 1.37     |
| 16  | O     | 502 | BCL  | CHD-C4C | 2.76  | 1.47        | 1.39     |
| 16  | 5     | 102 | BCL  | CHD-C4C | 2.76  | 1.46        | 1.39     |
| 16  | 9     | 101 | BCL  | CHD-C4C | 2.76  | 1.46        | 1.39     |
| 16  | W     | 101 | BCL  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 16  | F     | 502 | BCL  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 16  | Q     | 102 | BCL  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 16  | U     | 101 | BCL  | C1D-ND  | -2.74 | 1.34        | 1.37     |
| 16  | L     | 301 | BCL  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 16  | Y     | 101 | BCL  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 16  | I     | 101 | BCL  | C1D-C2D | 2.73  | 1.50        | 1.45     |
| 16  | A     | 101 | BCL  | CHD-C4C | 2.73  | 1.46        | 1.39     |
| 16  | S     | 101 | BCL  | C1D-ND  | -2.73 | 1.34        | 1.37     |
| 10  | C     | 404 | HEM  | C1C-C2C | -2.73 | 1.39        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | M     | 404 | BCL  | C3D-C2D | 2.73  | 1.46        | 1.39     |
| 16  | O     | 502 | BCL  | C1D-ND  | -2.72 | 1.34        | 1.37     |
| 16  | A     | 101 | BCL  | C1D-ND  | -2.72 | 1.34        | 1.37     |
| 16  | K     | 102 | BCL  | CHD-C4C | 2.72  | 1.46        | 1.39     |
| 16  | S     | 101 | BCL  | CHD-C4C | 2.71  | 1.46        | 1.39     |
| 16  | 7     | 102 | BCL  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 16  | 3     | 101 | BCL  | CHD-C4C | 2.69  | 1.46        | 1.39     |
| 16  | W     | 101 | BCL  | CHD-C4C | 2.69  | 1.46        | 1.39     |
| 16  | D     | 503 | BCL  | CHD-C4C | 2.69  | 1.46        | 1.39     |
| 16  | U     | 101 | BCL  | CHD-C4C | 2.68  | 1.46        | 1.39     |
| 16  | Q     | 102 | BCL  | CHD-C4C | 2.68  | 1.46        | 1.39     |
| 16  | 7     | 102 | BCL  | C1D-C2D | 2.67  | 1.50        | 1.45     |
| 16  | Y     | 101 | BCL  | C1D-ND  | -2.67 | 1.34        | 1.37     |
| 16  | 1     | 402 | BCL  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 16  | 1     | 402 | BCL  | CHD-C4C | 2.66  | 1.46        | 1.39     |
| 16  | N     | 101 | BCL  | C1B-NB  | -2.66 | 1.34        | 1.37     |
| 16  | A     | 101 | BCL  | C1D-C2D | 2.65  | 1.50        | 1.45     |
| 16  | F     | 502 | BCL  | C1D-C2D | 2.64  | 1.50        | 1.45     |
| 16  | L     | 307 | BCL  | CHD-C4C | 2.63  | 1.46        | 1.39     |
| 16  | 5     | 102 | BCL  | C1D-C2D | 2.62  | 1.50        | 1.45     |
| 16  | M     | 403 | BCL  | CHD-C4C | 2.61  | 1.46        | 1.39     |
| 16  | I     | 101 | BCL  | C1D-ND  | -2.60 | 1.34        | 1.37     |
| 16  | A     | 101 | BCL  | C1B-NB  | -2.60 | 1.34        | 1.37     |
| 16  | 3     | 101 | BCL  | C1D-C2D | 2.59  | 1.50        | 1.45     |
| 16  | W     | 101 | BCL  | C1D-C2D | 2.59  | 1.50        | 1.45     |
| 16  | W     | 101 | BCL  | C1B-NB  | -2.58 | 1.34        | 1.37     |
| 16  | Q     | 102 | BCL  | C1B-NB  | -2.58 | 1.34        | 1.37     |
| 10  | C     | 401 | HEM  | C1C-C2C | -2.58 | 1.40        | 1.45     |
| 16  | F     | 502 | BCL  | C1D-ND  | -2.58 | 1.34        | 1.37     |
| 16  | 6     | 101 | BCL  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 10  | C     | 403 | HEM  | C1C-C2C | -2.56 | 1.40        | 1.45     |
| 16  | 5     | 102 | BCL  | C1D-ND  | -2.56 | 1.34        | 1.37     |
| 16  | D     | 503 | BCL  | C1B-NB  | -2.56 | 1.34        | 1.37     |
| 16  | 0     | 102 | BCL  | C1B-NB  | -2.55 | 1.34        | 1.37     |
| 16  | O     | 502 | BCL  | C1D-C2D | 2.55  | 1.50        | 1.45     |
| 16  | K     | 102 | BCL  | C1D-C2D | 2.55  | 1.50        | 1.45     |
| 16  | 7     | 102 | BCL  | C1D-ND  | -2.54 | 1.34        | 1.37     |
| 16  | U     | 101 | BCL  | C1D-C2D | 2.54  | 1.50        | 1.45     |
| 16  | S     | 101 | BCL  | C1D-C2D | 2.54  | 1.50        | 1.45     |
| 10  | C     | 401 | HEM  | FE-ND   | -2.54 | 1.87        | 1.94     |
| 16  | 4     | 101 | BCL  | C1B-NB  | -2.53 | 1.34        | 1.37     |
| 16  | 9     | 101 | BCL  | C1D-C2D | 2.53  | 1.50        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | L     | 301 | BCL  | CHD-C4C | 2.53  | 1.46        | 1.39     |
| 16  | 1     | 402 | BCL  | C1B-NB  | -2.52 | 1.34        | 1.37     |
| 16  | S     | 101 | BCL  | C1B-NB  | -2.52 | 1.34        | 1.37     |
| 16  | 4     | 101 | BCL  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 16  | X     | 102 | BCL  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 16  | U     | 101 | BCL  | C1B-NB  | -2.51 | 1.34        | 1.37     |
| 22  | D     | 502 | CDL  | OA8-CA7 | 2.51  | 1.45        | 1.33     |
| 16  | L     | 307 | BCL  | C1B-NB  | -2.51 | 1.34        | 1.37     |
| 16  | Y     | 101 | BCL  | C1D-C2D | 2.51  | 1.50        | 1.45     |
| 16  | M     | 404 | BCL  | CHD-C4C | 2.50  | 1.46        | 1.39     |
| 16  | 1     | 402 | BCL  | C1D-C2D | 2.50  | 1.50        | 1.45     |
| 16  | V     | 102 | BCL  | C1B-NB  | -2.50 | 1.34        | 1.37     |
| 16  | B     | 102 | BCL  | C1B-NB  | -2.50 | 1.34        | 1.37     |
| 16  | J     | 101 | BCL  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 16  | M     | 404 | BCL  | C1D-C2D | 2.49  | 1.50        | 1.45     |
| 16  | G     | 102 | BCL  | C1B-NB  | -2.49 | 1.34        | 1.37     |
| 16  | P     | 102 | BCL  | C1B-NB  | -2.49 | 1.34        | 1.37     |
| 16  | 9     | 101 | BCL  | C1B-NB  | -2.49 | 1.34        | 1.37     |
| 16  | X     | 102 | BCL  | C1B-NB  | -2.49 | 1.34        | 1.37     |
| 16  | 8     | 102 | BCL  | C1B-NB  | -2.49 | 1.34        | 1.37     |
| 16  | Q     | 102 | BCL  | C1D-C2D | 2.48  | 1.50        | 1.45     |
| 16  | T     | 101 | BCL  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 16  | J     | 101 | BCL  | C1B-NB  | -2.47 | 1.34        | 1.37     |
| 16  | 0     | 102 | BCL  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 16  | G     | 102 | BCL  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 16  | P     | 102 | BCL  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 16  | M     | 404 | BCL  | MG-NA   | -2.45 | 2.00        | 2.06     |
| 16  | Z     | 102 | BCL  | CHD-C4C | 2.45  | 1.46        | 1.39     |
| 16  | D     | 503 | BCL  | C1D-C2D | 2.45  | 1.50        | 1.45     |
| 16  | E     | 102 | BCL  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 16  | 4     | 101 | BCL  | MG-NA   | -2.44 | 2.00        | 2.06     |
| 16  | Y     | 101 | BCL  | C1B-NB  | -2.44 | 1.34        | 1.37     |
| 16  | G     | 102 | BCL  | CHD-C4C | 2.44  | 1.46        | 1.39     |
| 16  | 2     | 102 | BCL  | C1B-NB  | -2.43 | 1.34        | 1.37     |
| 16  | Z     | 102 | BCL  | C1B-NB  | -2.43 | 1.34        | 1.37     |
| 16  | K     | 102 | BCL  | MG-NA   | -2.43 | 2.00        | 2.06     |
| 16  | E     | 102 | BCL  | C1B-NB  | -2.43 | 1.34        | 1.37     |
| 16  | 3     | 101 | BCL  | MG-NA   | -2.43 | 2.00        | 2.06     |
| 10  | C     | 402 | HEM  | C1C-C2C | -2.43 | 1.40        | 1.45     |
| 16  | K     | 102 | BCL  | C1B-NB  | -2.43 | 1.34        | 1.37     |
| 16  | L     | 307 | BCL  | MG-NA   | -2.43 | 2.00        | 2.06     |
| 16  | L     | 307 | BCL  | C1D-C2D | 2.42  | 1.50        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | 7     | 102 | BCL  | C1B-NB  | -2.42 | 1.34        | 1.37     |
| 16  | 4     | 101 | BCL  | CHD-C4C | 2.42  | 1.46        | 1.39     |
| 16  | 8     | 102 | BCL  | CHD-C4C | 2.41  | 1.46        | 1.39     |
| 16  | R     | 101 | BCL  | C1B-NB  | -2.41 | 1.34        | 1.37     |
| 16  | 5     | 102 | BCL  | MG-NA   | -2.41 | 2.00        | 2.06     |
| 10  | C     | 402 | HEM  | FE-ND   | -2.41 | 1.87        | 1.94     |
| 10  | C     | 403 | HEM  | FE-ND   | -2.40 | 1.87        | 1.94     |
| 16  | P     | 102 | BCL  | CHD-C4C | 2.40  | 1.45        | 1.39     |
| 16  | 9     | 101 | BCL  | MG-NA   | -2.40 | 2.00        | 2.06     |
| 16  | 8     | 102 | BCL  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 16  | 5     | 102 | BCL  | C1B-NB  | -2.39 | 1.34        | 1.37     |
| 16  | 3     | 101 | BCL  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 16  | M     | 403 | BCL  | MG-NA   | -2.39 | 2.00        | 2.06     |
| 16  | 2     | 102 | BCL  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 16  | 0     | 102 | BCL  | CHD-C4C | 2.38  | 1.45        | 1.39     |
| 16  | B     | 102 | BCL  | CHD-C4C | 2.38  | 1.45        | 1.39     |
| 16  | E     | 102 | BCL  | CHD-C4C | 2.38  | 1.45        | 1.39     |
| 16  | 2     | 102 | BCL  | CHD-C4C | 2.38  | 1.45        | 1.39     |
| 16  | F     | 502 | BCL  | C1B-NB  | -2.38 | 1.34        | 1.37     |
| 16  | O     | 502 | BCL  | C1B-NB  | -2.37 | 1.34        | 1.37     |
| 16  | R     | 101 | BCL  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 16  | V     | 102 | BCL  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 16  | N     | 101 | BCL  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 16  | N     | 101 | BCL  | CHD-C4C | 2.37  | 1.45        | 1.39     |
| 16  | T     | 101 | BCL  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 16  | U     | 101 | BCL  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 16  | T     | 101 | BCL  | CHD-C4C | 2.36  | 1.45        | 1.39     |
| 16  | X     | 102 | BCL  | CHD-C4C | 2.36  | 1.45        | 1.39     |
| 16  | Z     | 102 | BCL  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 16  | 6     | 101 | BCL  | C1B-NB  | -2.36 | 1.34        | 1.37     |
| 16  | Y     | 101 | BCL  | MG-NA   | -2.36 | 2.00        | 2.06     |
| 16  | 6     | 101 | BCL  | CHD-C4C | 2.36  | 1.45        | 1.39     |
| 10  | C     | 404 | HEM  | FE-ND   | -2.35 | 1.87        | 1.94     |
| 16  | J     | 101 | BCL  | CHD-C4C | 2.35  | 1.45        | 1.39     |
| 16  | I     | 101 | BCL  | MG-NC   | -2.35 | 2.00        | 2.06     |
| 16  | V     | 102 | BCL  | CHD-C4C | 2.35  | 1.45        | 1.39     |
| 16  | B     | 102 | BCL  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 16  | 7     | 102 | BCL  | MG-NC   | -2.34 | 2.00        | 2.06     |
| 16  | M     | 403 | BCL  | C1B-NB  | -2.34 | 1.34        | 1.37     |
| 16  | L     | 301 | BCL  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 16  | G     | 102 | BCL  | MG-NA   | -2.33 | 2.00        | 2.06     |
| 16  | M     | 403 | BCL  | C1D-C2D | 2.32  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | R     | 101 | BCL  | CHD-C4C | 2.32  | 1.45        | 1.39     |
| 16  | F     | 502 | BCL  | MG-NC   | -2.32 | 2.00        | 2.06     |
| 16  | I     | 101 | BCL  | MG-NA   | -2.31 | 2.00        | 2.06     |
| 16  | L     | 301 | BCL  | C1D-C2D | 2.31  | 1.49        | 1.45     |
| 10  | C     | 402 | HEM  | C3C-C4C | -2.31 | 1.42        | 1.46     |
| 16  | 6     | 101 | BCL  | MG-NA   | -2.31 | 2.00        | 2.06     |
| 16  | O     | 502 | BCL  | C1B-C2B | 2.30  | 1.48        | 1.43     |
| 16  | I     | 101 | BCL  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 10  | C     | 404 | HEM  | C3C-C4C | -2.29 | 1.42        | 1.46     |
| 16  | 3     | 101 | BCL  | C1B-NB  | -2.28 | 1.34        | 1.37     |
| 16  | 7     | 102 | BCL  | MG-NA   | -2.28 | 2.00        | 2.06     |
| 16  | E     | 102 | BCL  | MG-NA   | -2.28 | 2.00        | 2.06     |
| 16  | K     | 102 | BCL  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 16  | 2     | 102 | BCL  | MG-NA   | -2.28 | 2.00        | 2.06     |
| 17  | M     | 405 | BPH  | C3A-C2A | -2.27 | 1.52        | 1.54     |
| 16  | I     | 101 | BCL  | C1B-NB  | -2.27 | 1.34        | 1.37     |
| 16  | F     | 502 | BCL  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 16  | Y     | 101 | BCL  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 16  | F     | 502 | BCL  | MG-NA   | -2.26 | 2.00        | 2.06     |
| 16  | L     | 307 | BCL  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 16  | 5     | 102 | BCL  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 16  | M     | 404 | BCL  | MG-NC   | -2.26 | 2.00        | 2.06     |
| 16  | L     | 301 | BCL  | C1B-NB  | -2.25 | 1.34        | 1.37     |
| 16  | D     | 503 | BCL  | C1B-C2B | 2.25  | 1.48        | 1.43     |
| 16  | O     | 502 | BCL  | MG-NA   | -2.25 | 2.00        | 2.06     |
| 16  | N     | 101 | BCL  | MG-NA   | -2.24 | 2.00        | 2.06     |
| 10  | C     | 402 | HEM  | C1D-ND  | -2.24 | 1.34        | 1.38     |
| 16  | S     | 101 | BCL  | MG-NA   | -2.23 | 2.01        | 2.06     |
| 16  | 5     | 102 | BCL  | MG-NC   | -2.23 | 2.01        | 2.06     |
| 16  | V     | 102 | BCL  | MG-NA   | -2.23 | 2.01        | 2.06     |
| 16  | 1     | 402 | BCL  | MG-NA   | -2.23 | 2.01        | 2.06     |
| 16  | R     | 101 | BCL  | MG-NA   | -2.22 | 2.01        | 2.06     |
| 16  | 9     | 101 | BCL  | MG-NC   | -2.22 | 2.01        | 2.06     |
| 16  | Z     | 102 | BCL  | MG-NA   | -2.22 | 2.01        | 2.06     |
| 10  | C     | 403 | HEM  | C4B-NB  | -2.22 | 1.34        | 1.38     |
| 16  | W     | 101 | BCL  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 16  | P     | 102 | BCL  | MG-NA   | -2.21 | 2.01        | 2.06     |
| 16  | A     | 101 | BCL  | C1B-C2B | 2.21  | 1.48        | 1.43     |
| 10  | C     | 404 | HEM  | C1D-ND  | -2.21 | 1.34        | 1.38     |
| 16  | X     | 102 | BCL  | MG-NA   | -2.21 | 2.01        | 2.06     |
| 10  | C     | 403 | HEM  | C1D-ND  | -2.21 | 1.34        | 1.38     |
| 16  | 0     | 102 | BCL  | MG-NA   | -2.21 | 2.01        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | G     | 102 | BCL  | MG-NC   | -2.20 | 2.01        | 2.06     |
| 16  | 8     | 102 | BCL  | MG-NA   | -2.20 | 2.01        | 2.06     |
| 16  | Q     | 102 | BCL  | C1B-C2B | 2.20  | 1.48        | 1.43     |
| 16  | 4     | 101 | BCL  | MG-NC   | -2.20 | 2.01        | 2.06     |
| 17  | L     | 302 | BPH  | CBD-CGD | -2.20 | 1.49        | 1.52     |
| 16  | Q     | 102 | BCL  | MG-NA   | -2.19 | 2.01        | 2.06     |
| 10  | C     | 401 | HEM  | C4B-NB  | -2.19 | 1.34        | 1.38     |
| 16  | B     | 102 | BCL  | MG-NA   | -2.19 | 2.01        | 2.06     |
| 10  | C     | 404 | HEM  | C4B-NB  | -2.19 | 1.34        | 1.38     |
| 16  | D     | 503 | BCL  | MG-NC   | -2.19 | 2.01        | 2.06     |
| 16  | 7     | 102 | BCL  | C1B-C2B | 2.19  | 1.48        | 1.43     |
| 16  | D     | 503 | BCL  | MG-NA   | -2.18 | 2.01        | 2.06     |
| 16  | J     | 101 | BCL  | MG-NA   | -2.18 | 2.01        | 2.06     |
| 16  | A     | 101 | BCL  | MG-NA   | -2.18 | 2.01        | 2.06     |
| 10  | C     | 403 | HEM  | C3C-C4C | -2.18 | 1.42        | 1.46     |
| 16  | U     | 101 | BCL  | MG-NA   | -2.17 | 2.01        | 2.06     |
| 16  | M     | 404 | BCL  | C1B-C2B | 2.17  | 1.48        | 1.43     |
| 16  | Y     | 101 | BCL  | MG-NC   | -2.17 | 2.01        | 2.06     |
| 17  | M     | 405 | BPH  | CBD-CGD | -2.16 | 1.49        | 1.52     |
| 16  | 8     | 102 | BCL  | MG-NC   | -2.16 | 2.01        | 2.06     |
| 16  | 9     | 101 | BCL  | C1B-C2B | 2.16  | 1.48        | 1.43     |
| 10  | C     | 402 | HEM  | C4B-NB  | -2.16 | 1.34        | 1.38     |
| 17  | L     | 302 | BPH  | C3A-C2A | -2.16 | 1.52        | 1.54     |
| 16  | M     | 403 | BCL  | C1B-C2B | 2.15  | 1.48        | 1.43     |
| 16  | 6     | 101 | BCL  | MG-NC   | -2.15 | 2.01        | 2.06     |
| 10  | C     | 401 | HEM  | C1D-ND  | -2.15 | 1.34        | 1.38     |
| 16  | 3     | 101 | BCL  | CHC-C1C | -2.14 | 1.32        | 1.37     |
| 16  | 1     | 402 | BCL  | MG-NC   | -2.14 | 2.01        | 2.06     |
| 16  | N     | 101 | BCL  | CHC-C1C | -2.14 | 1.32        | 1.37     |
| 16  | Z     | 102 | BCL  | C1D-C2D | 2.14  | 1.49        | 1.45     |
| 16  | O     | 502 | BCL  | CHC-C1C | -2.14 | 1.32        | 1.37     |
| 16  | G     | 102 | BCL  | CHC-C1C | -2.14 | 1.32        | 1.37     |
| 16  | W     | 101 | BCL  | MG-NA   | -2.13 | 2.01        | 2.06     |
| 16  | G     | 102 | BCL  | C1D-C2D | 2.13  | 1.49        | 1.45     |
| 16  | 0     | 102 | BCL  | CHC-C1C | -2.12 | 1.32        | 1.37     |
| 16  | 1     | 402 | BCL  | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 16  | P     | 102 | BCL  | CHC-C1C | -2.12 | 1.32        | 1.37     |
| 16  | S     | 101 | BCL  | MG-NC   | -2.11 | 2.01        | 2.06     |
| 16  | K     | 102 | BCL  | MG-NC   | -2.11 | 2.01        | 2.06     |
| 16  | N     | 101 | BCL  | MG-NC   | -2.11 | 2.01        | 2.06     |
| 16  | S     | 101 | BCL  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 16  | K     | 102 | BCL  | CHC-C1C | -2.10 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | O     | 502 | BCL  | MG-NC   | -2.10 | 2.01        | 2.06     |
| 16  | P     | 102 | BCL  | MG-NC   | -2.10 | 2.01        | 2.06     |
| 16  | 4     | 101 | BCL  | C1D-C2D | 2.09  | 1.49        | 1.45     |
| 17  | M     | 405 | BPH  | C1B-C2B | 2.09  | 1.41        | 1.39     |
| 16  | 3     | 101 | BCL  | MG-NC   | -2.09 | 2.01        | 2.06     |
| 16  | B     | 102 | BCL  | MG-NC   | -2.09 | 2.01        | 2.06     |
| 16  | B     | 102 | BCL  | CHC-C1C | -2.09 | 1.32        | 1.37     |
| 16  | Z     | 102 | BCL  | MG-NC   | -2.08 | 2.01        | 2.06     |
| 16  | L     | 301 | BCL  | MG-NC   | -2.08 | 2.01        | 2.06     |
| 16  | 4     | 101 | BCL  | CHC-C1C | -2.08 | 1.32        | 1.37     |
| 16  | Z     | 102 | BCL  | CHC-C1C | -2.07 | 1.32        | 1.37     |
| 16  | U     | 101 | BCL  | MG-NC   | -2.07 | 2.01        | 2.06     |
| 16  | U     | 101 | BCL  | CHC-C1C | -2.07 | 1.32        | 1.37     |
| 16  | X     | 102 | BCL  | CHC-C1C | -2.07 | 1.32        | 1.37     |
| 16  | E     | 102 | BCL  | MG-NC   | -2.07 | 2.01        | 2.06     |
| 16  | T     | 101 | BCL  | MG-NA   | -2.07 | 2.01        | 2.06     |
| 16  | Q     | 102 | BCL  | CHC-C1C | -2.07 | 1.32        | 1.37     |
| 16  | 6     | 101 | BCL  | CHC-C1C | -2.07 | 1.32        | 1.37     |
| 16  | M     | 403 | BCL  | CHC-C1C | -2.06 | 1.32        | 1.37     |
| 16  | E     | 102 | BCL  | C1D-C2D | 2.06  | 1.49        | 1.45     |
| 16  | W     | 101 | BCL  | CHC-C1C | -2.06 | 1.32        | 1.37     |
| 16  | J     | 101 | BCL  | CHC-C1C | -2.06 | 1.32        | 1.37     |
| 16  | R     | 101 | BCL  | MG-NC   | -2.06 | 2.01        | 2.06     |
| 16  | 9     | 101 | BCL  | CHC-C1C | -2.06 | 1.32        | 1.37     |
| 16  | 0     | 102 | BCL  | MG-NC   | -2.05 | 2.01        | 2.06     |
| 16  | W     | 101 | BCL  | CHB-C4A | -2.05 | 1.32        | 1.37     |
| 16  | 2     | 102 | BCL  | C1D-C2D | 2.05  | 1.49        | 1.45     |
| 16  | 2     | 102 | BCL  | CHC-C1C | -2.05 | 1.32        | 1.37     |
| 16  | A     | 101 | BCL  | MG-NC   | -2.05 | 2.01        | 2.06     |
| 10  | C     | 404 | HEM  | C1A-C2A | -2.04 | 1.40        | 1.44     |
| 16  | A     | 101 | BCL  | CHB-C4A | -2.04 | 1.32        | 1.37     |
| 16  | L     | 307 | BCL  | MG-NC   | -2.04 | 2.01        | 2.06     |
| 16  | X     | 102 | BCL  | MG-NC   | -2.04 | 2.01        | 2.06     |
| 16  | E     | 102 | BCL  | CHC-C1C | -2.04 | 1.32        | 1.37     |
| 16  | Q     | 102 | BCL  | MG-NC   | -2.04 | 2.01        | 2.06     |
| 10  | C     | 401 | HEM  | C3C-C4C | -2.04 | 1.42        | 1.46     |
| 16  | V     | 102 | BCL  | CHC-C1C | -2.03 | 1.32        | 1.37     |
| 16  | M     | 403 | BCL  | MG-NC   | -2.03 | 2.01        | 2.06     |
| 16  | 2     | 102 | BCL  | MG-NC   | -2.03 | 2.01        | 2.06     |
| 16  | W     | 101 | BCL  | MG-NC   | -2.03 | 2.01        | 2.06     |
| 16  | 4     | 101 | BCL  | C3C-C4C | -2.03 | 1.49        | 1.51     |
| 16  | L     | 301 | BCL  | CHC-C1C | -2.02 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | P     | 102 | BCL  | C1D-C2D | 2.01  | 1.49        | 1.45     |
| 16  | M     | 403 | BCL  | CHB-C4A | -2.01 | 1.32        | 1.37     |
| 16  | R     | 101 | BCL  | CHC-C1C | -2.01 | 1.32        | 1.37     |
| 16  | J     | 101 | BCL  | MG-NC   | -2.00 | 2.01        | 2.06     |
| 16  | N     | 101 | BCL  | C1D-C2D | 2.00  | 1.49        | 1.45     |

All (1287) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | M     | 404 | BCL  | CMD-C2D-C1D | 8.44  | 139.59      | 124.73   |
| 16  | 7     | 102 | BCL  | CMD-C2D-C1D | 8.13  | 139.05      | 124.73   |
| 16  | A     | 101 | BCL  | CMD-C2D-C1D | 8.08  | 138.96      | 124.73   |
| 16  | F     | 502 | BCL  | CMD-C2D-C1D | 8.06  | 138.92      | 124.73   |
| 16  | I     | 101 | BCL  | CMD-C2D-C1D | 8.02  | 138.85      | 124.73   |
| 16  | 5     | 102 | BCL  | CMD-C2D-C1D | 7.94  | 138.71      | 124.73   |
| 16  | O     | 502 | BCL  | CMD-C2D-C1D | 7.88  | 138.60      | 124.73   |
| 16  | L     | 301 | BCL  | CMD-C2D-C1D | 7.85  | 138.54      | 124.73   |
| 16  | 3     | 101 | BCL  | CMD-C2D-C1D | 7.83  | 138.51      | 124.73   |
| 16  | Q     | 102 | BCL  | CMD-C2D-C1D | 7.81  | 138.47      | 124.73   |
| 16  | K     | 102 | BCL  | CMD-C2D-C1D | 7.80  | 138.46      | 124.73   |
| 16  | W     | 101 | BCL  | CMD-C2D-C1D | 7.79  | 138.45      | 124.73   |
| 16  | Y     | 101 | BCL  | CMD-C2D-C1D | 7.78  | 138.43      | 124.73   |
| 16  | 9     | 101 | BCL  | CMD-C2D-C1D | 7.74  | 138.36      | 124.73   |
| 16  | S     | 101 | BCL  | CMD-C2D-C1D | 7.70  | 138.28      | 124.73   |
| 16  | U     | 101 | BCL  | CMD-C2D-C1D | 7.67  | 138.24      | 124.73   |
| 16  | D     | 503 | BCL  | CMD-C2D-C1D | 7.67  | 138.23      | 124.73   |
| 16  | 1     | 402 | BCL  | CMD-C2D-C1D | 7.56  | 138.05      | 124.73   |
| 21  | M     | 407 | CRT  | C37-C36-C35 | -7.26 | 114.71      | 124.91   |
| 16  | L     | 307 | BCL  | CMD-C2D-C1D | 7.25  | 137.50      | 124.73   |
| 21  | Q     | 101 | CRT  | C37-C36-C35 | -7.25 | 114.73      | 124.91   |
| 21  | 4     | 102 | CRT  | C31-C32-C33 | -7.14 | 117.26      | 127.28   |
| 16  | M     | 403 | BCL  | CMD-C2D-C1D | 6.93  | 136.92      | 124.73   |
| 16  | G     | 102 | BCL  | CMD-C2D-C1D | 6.92  | 136.92      | 124.73   |
| 16  | E     | 102 | BCL  | CMD-C2D-C1D | 6.83  | 136.75      | 124.73   |
| 16  | 2     | 102 | BCL  | CMD-C2D-C1D | 6.78  | 136.66      | 124.73   |
| 16  | 8     | 102 | BCL  | CMD-C2D-C1D | 6.77  | 136.65      | 124.73   |
| 16  | Z     | 102 | BCL  | CMD-C2D-C1D | 6.76  | 136.63      | 124.73   |
| 16  | 4     | 101 | BCL  | CMD-C2D-C1D | 6.74  | 136.59      | 124.73   |
| 21  | K     | 101 | CRT  | C4-C5-C6    | -6.72 | 115.48      | 124.91   |
| 16  | W     | 101 | BCL  | C2B-C1B-NB  | 6.71  | 117.28      | 110.33   |
| 16  | B     | 102 | BCL  | CMD-C2D-C1D | 6.69  | 136.51      | 124.73   |
| 16  | A     | 101 | BCL  | C2B-C1B-NB  | 6.69  | 117.27      | 110.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | J     | 101 | BCL  | CMD-C2D-C1D | 6.66  | 136.46      | 124.73   |
| 16  | Z     | 102 | BCL  | C2B-C1B-NB  | 6.66  | 117.23      | 110.33   |
| 16  | 6     | 101 | BCL  | CMD-C2D-C1D | 6.65  | 136.44      | 124.73   |
| 16  | 8     | 102 | BCL  | C2B-C1B-NB  | 6.59  | 117.17      | 110.33   |
| 21  | N     | 102 | CRT  | C37-C36-C35 | -6.58 | 115.67      | 124.91   |
| 16  | F     | 502 | BCL  | C2B-C1B-NB  | 6.58  | 117.15      | 110.33   |
| 16  | N     | 101 | BCL  | CMD-C2D-C1D | 6.58  | 136.31      | 124.73   |
| 16  | B     | 102 | BCL  | C2B-C1B-NB  | 6.58  | 117.15      | 110.33   |
| 16  | E     | 102 | BCL  | C2B-C1B-NB  | 6.57  | 117.14      | 110.33   |
| 16  | V     | 102 | BCL  | C2B-C1B-NB  | 6.55  | 117.11      | 110.33   |
| 16  | P     | 102 | BCL  | C2B-C1B-NB  | 6.55  | 117.11      | 110.33   |
| 16  | P     | 102 | BCL  | CMD-C2D-C1D | 6.52  | 136.22      | 124.73   |
| 16  | 0     | 102 | BCL  | CMD-C2D-C1D | 6.52  | 136.22      | 124.73   |
| 16  | 5     | 102 | BCL  | C2B-C1B-NB  | 6.52  | 117.09      | 110.33   |
| 16  | O     | 502 | BCL  | C2B-C1B-NB  | 6.52  | 117.09      | 110.33   |
| 16  | T     | 101 | BCL  | CMD-C2D-C1D | 6.52  | 136.21      | 124.73   |
| 16  | L     | 301 | BCL  | C2B-C1B-NB  | 6.51  | 117.08      | 110.33   |
| 21  | K     | 101 | CRT  | C37-C36-C35 | -6.51 | 115.77      | 124.91   |
| 16  | Q     | 102 | BCL  | C2B-C1B-NB  | 6.50  | 117.07      | 110.33   |
| 16  | X     | 102 | BCL  | CMD-C2D-C1D | 6.50  | 136.18      | 124.73   |
| 16  | T     | 101 | BCL  | C2B-C1B-NB  | 6.50  | 117.07      | 110.33   |
| 16  | 2     | 102 | BCL  | C2B-C1B-NB  | 6.49  | 117.05      | 110.33   |
| 16  | J     | 101 | BCL  | C2B-C1B-NB  | 6.44  | 117.00      | 110.33   |
| 16  | N     | 101 | BCL  | C2B-C1B-NB  | 6.44  | 117.00      | 110.33   |
| 16  | M     | 404 | BCL  | C2B-C1B-NB  | 6.43  | 117.00      | 110.33   |
| 16  | R     | 101 | BCL  | CMD-C2D-C1D | 6.43  | 136.05      | 124.73   |
| 16  | I     | 101 | BCL  | C2B-C1B-NB  | 6.40  | 116.97      | 110.33   |
| 16  | R     | 101 | BCL  | C2B-C1B-NB  | 6.40  | 116.96      | 110.33   |
| 16  | U     | 101 | BCL  | C2B-C1B-NB  | 6.38  | 116.94      | 110.33   |
| 16  | D     | 503 | BCL  | C2B-C1B-NB  | 6.37  | 116.94      | 110.33   |
| 16  | Y     | 101 | BCL  | C2B-C1B-NB  | 6.37  | 116.93      | 110.33   |
| 16  | S     | 101 | BCL  | C2B-C1B-NB  | 6.37  | 116.93      | 110.33   |
| 16  | G     | 102 | BCL  | C2B-C1B-NB  | 6.37  | 116.93      | 110.33   |
| 16  | 1     | 402 | BCL  | C2B-C1B-NB  | 6.36  | 116.92      | 110.33   |
| 16  | 4     | 101 | BCL  | C2B-C1B-NB  | 6.36  | 116.92      | 110.33   |
| 16  | 9     | 101 | BCL  | C2B-C1B-NB  | 6.35  | 116.91      | 110.33   |
| 21  | G     | 103 | CRT  | C37-C36-C35 | -6.33 | 116.03      | 124.91   |
| 16  | K     | 102 | BCL  | C2B-C1B-NB  | 6.32  | 116.88      | 110.33   |
| 16  | 0     | 102 | BCL  | C2B-C1B-NB  | 6.32  | 116.88      | 110.33   |
| 16  | 3     | 101 | BCL  | C2B-C1B-NB  | 6.30  | 116.86      | 110.33   |
| 21  | B     | 103 | CRT  | C37-C36-C35 | -6.30 | 116.06      | 124.91   |
| 21  | R     | 102 | CRT  | C37-C36-C35 | -6.29 | 116.08      | 124.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | 7     | 102 | BCL  | C2B-C1B-NB  | 6.28  | 116.84      | 110.33   |
| 16  | L     | 307 | BCL  | C2B-C1B-NB  | 6.27  | 116.83      | 110.33   |
| 16  | X     | 102 | BCL  | C2B-C1B-NB  | 6.26  | 116.82      | 110.33   |
| 16  | V     | 102 | BCL  | CMD-C2D-C1D | 6.25  | 135.73      | 124.73   |
| 21  | 8     | 103 | CRT  | C37-C36-C35 | -6.22 | 116.18      | 124.91   |
| 21  | 7     | 101 | CRT  | C37-C36-C35 | -6.22 | 116.18      | 124.91   |
| 16  | M     | 403 | BCL  | C2B-C1B-NB  | 6.17  | 116.73      | 110.33   |
| 16  | 6     | 101 | BCL  | C2B-C1B-NB  | 6.15  | 116.70      | 110.33   |
| 21  | 0     | 103 | CRT  | C37-C36-C35 | -6.13 | 116.31      | 124.91   |
| 21  | X     | 103 | CRT  | C37-C36-C35 | -6.11 | 116.34      | 124.91   |
| 21  | E     | 103 | CRT  | C37-C36-C35 | -6.05 | 116.42      | 124.91   |
| 16  | 3     | 101 | BCL  | CHD-C1D-ND  | -5.93 | 116.46      | 124.80   |
| 16  | M     | 404 | BCL  | CHD-C1D-ND  | -5.91 | 116.49      | 124.80   |
| 16  | A     | 101 | BCL  | CHD-C1D-ND  | -5.91 | 116.49      | 124.80   |
| 16  | 5     | 102 | BCL  | CHD-C1D-ND  | -5.90 | 116.50      | 124.80   |
| 16  | 7     | 102 | BCL  | CHD-C1D-ND  | -5.87 | 116.55      | 124.80   |
| 16  | F     | 502 | BCL  | CHD-C1D-ND  | -5.85 | 116.57      | 124.80   |
| 16  | Y     | 101 | BCL  | CHD-C1D-ND  | -5.83 | 116.60      | 124.80   |
| 16  | K     | 102 | BCL  | CHD-C1D-ND  | -5.82 | 116.61      | 124.80   |
| 16  | I     | 101 | BCL  | CHD-C1D-ND  | -5.81 | 116.62      | 124.80   |
| 16  | D     | 503 | BCL  | CHD-C1D-ND  | -5.81 | 116.63      | 124.80   |
| 21  | V     | 103 | CRT  | C37-C36-C35 | -5.77 | 116.81      | 124.91   |
| 16  | O     | 502 | BCL  | CHD-C1D-ND  | -5.73 | 116.73      | 124.80   |
| 16  | Q     | 102 | BCL  | CHD-C1D-ND  | -5.72 | 116.75      | 124.80   |
| 16  | M     | 403 | BCL  | O2D-CGD-CBD | 5.71  | 121.20      | 111.23   |
| 16  | S     | 101 | BCL  | CHD-C1D-ND  | -5.70 | 116.78      | 124.80   |
| 16  | U     | 101 | BCL  | CHD-C1D-ND  | -5.70 | 116.78      | 124.80   |
| 16  | 1     | 402 | BCL  | CHD-C1D-ND  | -5.69 | 116.79      | 124.80   |
| 16  | 9     | 101 | BCL  | CHD-C1D-ND  | -5.69 | 116.79      | 124.80   |
| 16  | M     | 404 | BCL  | O2D-CGD-CBD | 5.65  | 121.10      | 111.23   |
| 16  | W     | 101 | BCL  | CHD-C1D-ND  | -5.64 | 116.86      | 124.80   |
| 16  | L     | 307 | BCL  | CHD-C1D-ND  | -5.60 | 116.92      | 124.80   |
| 21  | Q     | 101 | CRT  | C3-C1-C2    | 5.52  | 120.52      | 110.43   |
| 21  | V     | 103 | CRT  | C4-C5-C6    | -5.48 | 117.22      | 124.91   |
| 16  | M     | 403 | BCL  | CHD-C1D-ND  | -5.40 | 117.20      | 124.80   |
| 21  | V     | 103 | CRT  | C40-C38-C39 | 5.39  | 120.28      | 110.43   |
| 21  | 2     | 103 | CRT  | C40-C38-C39 | 5.38  | 120.26      | 110.43   |
| 16  | L     | 307 | BCL  | O2D-CGD-CBD | 5.34  | 120.57      | 111.23   |
| 16  | L     | 301 | BCL  | CHD-C1D-ND  | -5.34 | 117.28      | 124.80   |
| 21  | M     | 407 | CRT  | C40-C38-C39 | 5.33  | 120.17      | 110.43   |
| 21  | 2     | 103 | CRT  | C37-C36-C35 | -5.32 | 117.44      | 124.91   |
| 21  | Z     | 103 | CRT  | C37-C36-C35 | -5.24 | 117.55      | 124.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | M     | 404 | BCL  | C3D-C2D-C1D | -5.21 | 98.72       | 105.83   |
| 10  | C     | 402 | HEM  | CHC-C4B-NB  | 5.21  | 130.03      | 124.42   |
| 16  | 4     | 101 | BCL  | CHD-C1D-ND  | -5.19 | 117.50      | 124.80   |
| 22  | M     | 412 | CDL  | OA6-CA5-C11 | 5.19  | 120.34      | 111.09   |
| 16  | D     | 503 | BCL  | O2D-CGD-CBD | 5.19  | 120.30      | 111.23   |
| 21  | M     | 407 | CRT  | C4-C5-C6    | -5.15 | 117.68      | 124.91   |
| 16  | 9     | 101 | BCL  | O2D-CGD-CBD | 5.11  | 120.16      | 111.23   |
| 16  | G     | 102 | BCL  | CHD-C1D-ND  | -5.11 | 117.61      | 124.80   |
| 16  | Z     | 102 | BCL  | CHD-C1D-ND  | -5.10 | 117.63      | 124.80   |
| 10  | C     | 403 | HEM  | CHC-C4B-NB  | 5.08  | 129.89      | 124.42   |
| 21  | T     | 102 | CRT  | C21-C22-C23 | -5.08 | 120.15      | 127.28   |
| 21  | E     | 103 | CRT  | C21-C22-C23 | -5.08 | 120.16      | 127.28   |
| 16  | O     | 502 | BCL  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 16  | W     | 101 | BCL  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 16  | 2     | 102 | BCL  | CHD-C1D-ND  | -5.07 | 117.67      | 124.80   |
| 16  | A     | 101 | BCL  | O2D-CGD-CBD | 5.05  | 120.06      | 111.23   |
| 21  | G     | 103 | CRT  | C4-C5-C6    | -5.04 | 117.84      | 124.91   |
| 16  | 7     | 102 | BCL  | O2D-CGD-CBD | 5.03  | 120.02      | 111.23   |
| 16  | E     | 102 | BCL  | CHD-C1D-ND  | -5.02 | 117.74      | 124.80   |
| 16  | N     | 101 | BCL  | CHD-C1D-ND  | -5.00 | 117.76      | 124.80   |
| 16  | K     | 102 | BCL  | C3D-C2D-C1D | -4.99 | 99.02       | 105.83   |
| 10  | C     | 401 | HEM  | CHC-C4B-NB  | 4.99  | 129.79      | 124.42   |
| 21  | T     | 102 | CRT  | C10-C9-C7   | -4.99 | 120.28      | 127.28   |
| 16  | L     | 301 | BCL  | C3D-C2D-C1D | -4.99 | 99.03       | 105.83   |
| 16  | F     | 502 | BCL  | C3D-C2D-C1D | -4.97 | 99.05       | 105.83   |
| 16  | 1     | 402 | BCL  | O2D-CGD-CBD | 4.97  | 119.92      | 111.23   |
| 16  | O     | 502 | BCL  | C3D-C2D-C1D | -4.97 | 99.05       | 105.83   |
| 16  | F     | 502 | BCL  | O2D-CGD-CBD | 4.96  | 119.91      | 111.23   |
| 16  | D     | 503 | BCL  | C3D-C2D-C1D | -4.96 | 99.06       | 105.83   |
| 16  | Y     | 101 | BCL  | C3D-C2D-C1D | -4.95 | 99.08       | 105.83   |
| 16  | Q     | 102 | BCL  | O2D-CGD-CBD | 4.94  | 119.87      | 111.23   |
| 16  | U     | 101 | BCL  | C3D-C2D-C1D | -4.94 | 99.09       | 105.83   |
| 16  | 3     | 101 | BCL  | C3D-C2D-C1D | -4.94 | 99.09       | 105.83   |
| 16  | J     | 101 | BCL  | CHD-C1D-ND  | -4.94 | 117.85      | 124.80   |
| 21  | Z     | 103 | CRT  | C21-C22-C23 | -4.93 | 120.36      | 127.28   |
| 16  | I     | 101 | BCL  | O2D-CGD-CBD | 4.93  | 119.85      | 111.23   |
| 16  | 8     | 102 | BCL  | CHD-C1D-ND  | -4.93 | 117.87      | 124.80   |
| 16  | W     | 101 | BCL  | C3D-C2D-C1D | -4.93 | 99.11       | 105.83   |
| 16  | 1     | 402 | BCL  | C3D-C2D-C1D | -4.93 | 99.11       | 105.83   |
| 10  | C     | 404 | HEM  | CHC-C4B-NB  | 4.92  | 129.72      | 124.42   |
| 16  | S     | 101 | BCL  | C3D-C2D-C1D | -4.92 | 99.11       | 105.83   |
| 16  | Q     | 102 | BCL  | C3D-C2D-C1D | -4.92 | 99.12       | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | R     | 101 | BCL  | CHD-C1D-ND  | -4.91 | 117.89      | 124.80   |
| 21  | M     | 407 | CRT  | C21-C22-C23 | -4.91 | 120.39      | 127.28   |
| 16  | P     | 102 | BCL  | CHD-C1D-ND  | -4.90 | 117.90      | 124.80   |
| 16  | E     | 102 | BCL  | C3C-C4C-CHD | -4.90 | 113.06      | 123.39   |
| 16  | S     | 101 | BCL  | O2D-CGD-CBD | 4.90  | 119.80      | 111.23   |
| 21  | K     | 101 | CRT  | C3-C1-C2    | 4.90  | 119.38      | 110.43   |
| 16  | 6     | 101 | BCL  | CHD-C1D-ND  | -4.89 | 117.92      | 124.80   |
| 16  | 3     | 101 | BCL  | O2D-CGD-CBD | 4.89  | 119.77      | 111.23   |
| 16  | T     | 101 | BCL  | CHD-C1D-ND  | -4.89 | 117.93      | 124.80   |
| 16  | A     | 101 | BCL  | C3D-C2D-C1D | -4.88 | 99.17       | 105.83   |
| 21  | 2     | 103 | CRT  | C21-C22-C23 | -4.88 | 120.44      | 127.28   |
| 16  | U     | 101 | BCL  | O2D-CGD-CBD | 4.88  | 119.76      | 111.23   |
| 16  | I     | 101 | BCL  | C3D-C2D-C1D | -4.88 | 99.18       | 105.83   |
| 16  | 6     | 101 | BCL  | C3C-C4C-CHD | -4.88 | 113.11      | 123.39   |
| 16  | T     | 101 | BCL  | C3C-C4C-CHD | -4.87 | 113.11      | 123.39   |
| 16  | J     | 101 | BCL  | C3C-C4C-CHD | -4.87 | 113.12      | 123.39   |
| 16  | 7     | 102 | BCL  | C3D-C2D-C1D | -4.86 | 99.20       | 105.83   |
| 16  | K     | 102 | BCL  | O2D-CGD-CBD | 4.86  | 119.72      | 111.23   |
| 16  | 5     | 102 | BCL  | C3D-C2D-C1D | -4.84 | 99.22       | 105.83   |
| 16  | V     | 102 | BCL  | CHD-C1D-ND  | -4.82 | 118.02      | 124.80   |
| 16  | 8     | 102 | BCL  | C3C-C4C-CHD | -4.80 | 113.26      | 123.39   |
| 21  | B     | 103 | CRT  | C21-C22-C23 | -4.80 | 120.54      | 127.28   |
| 16  | X     | 102 | BCL  | C3C-C4C-CHD | -4.80 | 113.27      | 123.39   |
| 16  | 0     | 102 | BCL  | CHD-C1D-ND  | -4.80 | 118.05      | 124.80   |
| 16  | B     | 102 | BCL  | CHD-C1D-ND  | -4.79 | 118.06      | 124.80   |
| 16  | X     | 102 | BCL  | CHD-C1D-ND  | -4.79 | 118.06      | 124.80   |
| 21  | X     | 103 | CRT  | C21-C22-C23 | -4.79 | 120.56      | 127.28   |
| 16  | 2     | 102 | BCL  | C3C-C4C-CHD | -4.78 | 113.32      | 123.39   |
| 16  | 9     | 101 | BCL  | C3D-C2D-C1D | -4.77 | 99.32       | 105.83   |
| 16  | N     | 101 | BCL  | C3C-C4C-CHD | -4.77 | 113.34      | 123.39   |
| 16  | V     | 102 | BCL  | C3C-C4C-CHD | -4.77 | 113.34      | 123.39   |
| 21  | 8     | 103 | CRT  | C21-C22-C23 | -4.76 | 120.60      | 127.28   |
| 16  | B     | 102 | BCL  | C3C-C4C-CHD | -4.76 | 113.35      | 123.39   |
| 16  | 4     | 101 | BCL  | C3C-C4C-CHD | -4.75 | 113.37      | 123.39   |
| 16  | R     | 101 | BCL  | C3C-C4C-CHD | -4.75 | 113.38      | 123.39   |
| 16  | Z     | 102 | BCL  | C3D-C2D-C1D | -4.75 | 99.35       | 105.83   |
| 16  | Z     | 102 | BCL  | C3C-C4C-CHD | -4.75 | 113.38      | 123.39   |
| 16  | 5     | 102 | BCL  | O2D-CGD-CBD | 4.75  | 119.53      | 111.23   |
| 16  | 4     | 101 | BCL  | C3D-C2D-C1D | -4.74 | 99.37       | 105.83   |
| 21  | E     | 103 | CRT  | C4-C5-C6    | -4.73 | 118.28      | 124.91   |
| 16  | 2     | 102 | BCL  | C3D-C2D-C1D | -4.72 | 99.39       | 105.83   |
| 16  | 0     | 102 | BCL  | C3C-C4C-CHD | -4.70 | 113.48      | 123.39   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | P     | 102 | BCL  | C3C-C4C-CHD | -4.69 | 113.50      | 123.39   |
| 16  | E     | 102 | BCL  | C3D-C2D-C1D | -4.68 | 99.44       | 105.83   |
| 18  | L     | 304 | UQ8  | C7-C8-C9    | -4.68 | 118.77      | 126.83   |
| 16  | R     | 101 | BCL  | C3D-C2D-C1D | -4.68 | 99.44       | 105.83   |
| 21  | T     | 102 | CRT  | C37-C36-C35 | -4.68 | 118.34      | 124.91   |
| 16  | N     | 101 | BCL  | C3D-C2D-C1D | -4.68 | 99.45       | 105.83   |
| 16  | X     | 102 | BCL  | C3D-C2D-C1D | -4.67 | 99.46       | 105.83   |
| 21  | N     | 102 | CRT  | C21-C22-C23 | -4.67 | 120.73      | 127.28   |
| 16  | Y     | 101 | BCL  | O2D-CGD-CBD | 4.66  | 119.37      | 111.23   |
| 16  | L     | 307 | BCL  | C3D-C2D-C1D | -4.66 | 99.48       | 105.83   |
| 10  | C     | 401 | HEM  | CHD-C1D-ND  | 4.65  | 129.43      | 124.42   |
| 16  | 8     | 102 | BCL  | C3D-C2D-C1D | -4.65 | 99.48       | 105.83   |
| 16  | 6     | 101 | BCL  | C3D-C2D-C1D | -4.65 | 99.49       | 105.83   |
| 16  | M     | 403 | BCL  | C3D-C2D-C1D | -4.64 | 99.49       | 105.83   |
| 16  | G     | 102 | BCL  | C3C-C4C-CHD | -4.63 | 113.63      | 123.39   |
| 21  | 8     | 103 | CRT  | C4-C5-C6    | -4.62 | 118.42      | 124.91   |
| 21  | R     | 102 | CRT  | C4-C5-C6    | -4.62 | 118.43      | 124.91   |
| 16  | T     | 101 | BCL  | C3D-C2D-C1D | -4.61 | 99.53       | 105.83   |
| 21  | M     | 407 | CRT  | C20-C19-C17 | -4.59 | 120.84      | 127.28   |
| 21  | R     | 102 | CRT  | C21-C22-C23 | -4.59 | 120.85      | 127.28   |
| 16  | J     | 101 | BCL  | C3D-C2D-C1D | -4.57 | 99.59       | 105.83   |
| 16  | G     | 102 | BCL  | C3D-C2D-C1D | -4.56 | 99.61       | 105.83   |
| 16  | M     | 404 | BCL  | C3C-C4C-CHD | -4.56 | 113.79      | 123.39   |
| 16  | V     | 102 | BCL  | C3D-C2D-C1D | -4.55 | 99.62       | 105.83   |
| 16  | 0     | 102 | BCL  | C3D-C2D-C1D | -4.55 | 99.62       | 105.83   |
| 16  | L     | 301 | BCL  | C3C-C4C-CHD | -4.55 | 113.81      | 123.39   |
| 16  | B     | 102 | BCL  | C3D-C2D-C1D | -4.54 | 99.63       | 105.83   |
| 21  | 4     | 102 | CRT  | C37-C36-C35 | -4.54 | 118.54      | 124.91   |
| 21  | K     | 101 | CRT  | C21-C22-C23 | -4.51 | 120.95      | 127.28   |
| 16  | P     | 102 | BCL  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 21  | B     | 103 | CRT  | C4-C5-C6    | -4.46 | 118.65      | 124.91   |
| 21  | V     | 103 | CRT  | C21-C22-C23 | -4.45 | 121.04      | 127.28   |
| 21  | 0     | 103 | CRT  | C21-C22-C23 | -4.44 | 121.05      | 127.28   |
| 21  | 4     | 102 | CRT  | C4-C5-C6    | -4.44 | 118.68      | 124.91   |
| 21  | T     | 102 | CRT  | C5-C6-C7    | -4.42 | 119.21      | 125.89   |
| 21  | Q     | 101 | CRT  | C10-C9-C7   | -4.42 | 121.08      | 127.28   |
| 22  | D     | 502 | CDL  | OB6-CB5-C51 | 4.41  | 121.03      | 111.48   |
| 16  | J     | 101 | BCL  | O2D-CGD-CBD | 4.40  | 118.93      | 111.23   |
| 10  | C     | 404 | HEM  | CHD-C1D-ND  | 4.40  | 129.16      | 124.42   |
| 15  | H     | 301 | PGV  | O01-C1-C2   | 4.39  | 120.97      | 111.48   |
| 16  | E     | 102 | BCL  | C1D-ND-C4D  | -4.35 | 103.26      | 106.31   |
| 15  | L     | 309 | PGV  | O01-C1-C2   | 4.34  | 120.87      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | G     | 103 | CRT  | C21-C22-C23 | -4.31 | 121.24      | 127.28   |
| 21  | O     | 103 | CRT  | C4-C5-C6    | -4.30 | 118.87      | 124.91   |
| 10  | C     | 402 | HEM  | CHD-C1D-ND  | 4.28  | 129.03      | 124.42   |
| 16  | Y     | 101 | BCL  | C1D-ND-C4D  | -4.27 | 103.32      | 106.31   |
| 16  | A     | 101 | BCL  | C1D-ND-C4D  | -4.26 | 103.33      | 106.31   |
| 22  | M     | 411 | CDL  | OA6-CA5-C11 | 4.24  | 120.65      | 111.48   |
| 16  | R     | 101 | BCL  | C1D-ND-C4D  | -4.24 | 103.34      | 106.31   |
| 21  | 2     | 103 | CRT  | C4-C5-C6    | -4.23 | 118.98      | 124.91   |
| 16  | L     | 307 | BCL  | C3C-C4C-CHD | -4.22 | 114.49      | 123.39   |
| 16  | T     | 101 | BCL  | C1D-ND-C4D  | -4.21 | 103.36      | 106.31   |
| 16  | D     | 503 | BCL  | C1D-ND-C4D  | -4.21 | 103.36      | 106.31   |
| 16  | M     | 403 | BCL  | C3C-C4C-CHD | -4.21 | 114.52      | 123.39   |
| 16  | 4     | 101 | BCL  | O2D-CGD-CBD | 4.21  | 118.58      | 111.23   |
| 21  | 4     | 102 | CRT  | C29-C28-C30 | 4.20  | 124.51      | 118.09   |
| 16  | 2     | 102 | BCL  | C1D-ND-C4D  | -4.19 | 103.38      | 106.31   |
| 15  | L     | 306 | PGV  | O01-C1-C2   | 4.17  | 120.50      | 111.48   |
| 16  | U     | 101 | BCL  | C1D-ND-C4D  | -4.17 | 103.39      | 106.31   |
| 16  | Z     | 102 | BCL  | C1D-ND-C4D  | -4.16 | 103.39      | 106.31   |
| 21  | Q     | 101 | CRT  | C5-C6-C7    | -4.15 | 119.62      | 125.89   |
| 16  | R     | 101 | BCL  | C2D-C1D-ND  | 4.15  | 114.23      | 110.13   |
| 16  | N     | 101 | BCL  | C1D-ND-C4D  | -4.14 | 103.40      | 106.31   |
| 15  | L     | 305 | PGV  | O01-C1-C2   | 4.14  | 120.45      | 111.48   |
| 16  | F     | 502 | BCL  | C1D-ND-C4D  | -4.14 | 103.41      | 106.31   |
| 16  | U     | 101 | BCL  | C3B-C4B-NB  | 4.13  | 115.21      | 109.76   |
| 16  | 8     | 102 | BCL  | O2D-CGD-CBD | 4.13  | 118.45      | 111.23   |
| 16  | 8     | 102 | BCL  | C1D-ND-C4D  | -4.13 | 103.41      | 106.31   |
| 10  | C     | 403 | HEM  | CHD-C1D-ND  | 4.13  | 128.87      | 124.42   |
| 16  | K     | 102 | BCL  | C1D-ND-C4D  | -4.13 | 103.41      | 106.31   |
| 16  | 6     | 101 | BCL  | C1D-ND-C4D  | -4.13 | 103.42      | 106.31   |
| 17  | L     | 302 | BPH  | C4D-CHA-CBD | -4.13 | 106.47      | 108.45   |
| 16  | O     | 502 | BCL  | C3C-C4C-CHD | -4.12 | 114.70      | 123.39   |
| 16  | O     | 102 | BCL  | C1D-ND-C4D  | -4.12 | 103.42      | 106.31   |
| 16  | B     | 102 | BCL  | C3B-C4B-NB  | 4.09  | 115.16      | 109.76   |
| 21  | Q     | 101 | CRT  | C21-C22-C23 | -4.09 | 121.54      | 127.28   |
| 16  | G     | 102 | BCL  | C1D-ND-C4D  | -4.09 | 103.44      | 106.31   |
| 16  | Q     | 102 | BCL  | C3C-C4C-CHD | -4.08 | 114.78      | 123.39   |
| 16  | 4     | 101 | BCL  | C1D-ND-C4D  | -4.08 | 103.45      | 106.31   |
| 16  | O     | 102 | BCL  | C3B-C4B-NB  | 4.08  | 115.14      | 109.76   |
| 21  | 7     | 101 | CRT  | C4-C5-C6    | -4.08 | 119.19      | 124.91   |
| 21  | Z     | 103 | CRT  | C5-C6-C7    | -4.07 | 119.75      | 125.89   |
| 16  | B     | 102 | BCL  | C1D-ND-C4D  | -4.07 | 103.46      | 106.31   |
| 16  | E     | 102 | BCL  | C2D-C1D-ND  | 4.07  | 114.15      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | 1     | 402 | BCL  | C1D-ND-C4D  | -4.06 | 103.46      | 106.31   |
| 16  | D     | 503 | BCL  | C3C-C4C-CHD | -4.06 | 114.82      | 123.39   |
| 16  | E     | 102 | BCL  | C3B-C4B-NB  | 4.06  | 115.12      | 109.76   |
| 16  | K     | 102 | BCL  | C3B-C4B-NB  | 4.06  | 115.12      | 109.76   |
| 16  | A     | 101 | BCL  | C3C-C4C-CHD | -4.06 | 114.84      | 123.39   |
| 16  | 3     | 101 | BCL  | C3B-C4B-NB  | 4.05  | 115.11      | 109.76   |
| 16  | P     | 102 | BCL  | C3B-C4B-NB  | 4.05  | 115.10      | 109.76   |
| 16  | P     | 102 | BCL  | C1D-ND-C4D  | -4.05 | 103.47      | 106.31   |
| 15  | M     | 408 | PGV  | O01-C1-C2   | 4.04  | 120.22      | 111.48   |
| 16  | 6     | 101 | BCL  | C3B-C4B-NB  | 4.04  | 115.09      | 109.76   |
| 16  | D     | 503 | BCL  | C3B-C4B-NB  | 4.04  | 115.09      | 109.76   |
| 16  | T     | 101 | BCL  | C2D-C1D-ND  | 4.04  | 114.12      | 110.13   |
| 16  | X     | 102 | BCL  | C1D-ND-C4D  | -4.03 | 103.48      | 106.31   |
| 16  | A     | 101 | BCL  | C3B-C4B-NB  | 4.02  | 115.07      | 109.76   |
| 16  | 4     | 101 | BCL  | C2D-C1D-ND  | 4.02  | 114.11      | 110.13   |
| 16  | L     | 301 | BCL  | C1D-ND-C4D  | -4.02 | 103.49      | 106.31   |
| 16  | 4     | 101 | BCL  | C3B-C4B-NB  | 4.02  | 115.06      | 109.76   |
| 16  | 6     | 101 | BCL  | O2D-CGD-CBD | 4.02  | 118.25      | 111.23   |
| 16  | G     | 102 | BCL  | C3B-C4B-NB  | 4.02  | 115.06      | 109.76   |
| 16  | X     | 102 | BCL  | C3B-C4B-NB  | 4.02  | 115.06      | 109.76   |
| 21  | N     | 102 | CRT  | C4-C5-C6    | -4.02 | 119.28      | 124.91   |
| 16  | O     | 502 | BCL  | C1D-ND-C4D  | -4.01 | 103.50      | 106.31   |
| 16  | 6     | 101 | BCL  | C2D-C1D-ND  | 4.01  | 114.09      | 110.13   |
| 16  | L     | 301 | BCL  | C3B-C4B-NB  | 4.00  | 115.04      | 109.76   |
| 16  | N     | 101 | BCL  | C3B-C4B-NB  | 4.00  | 115.04      | 109.76   |
| 21  | Z     | 103 | CRT  | C10-C9-C7   | -4.00 | 121.67      | 127.28   |
| 16  | 2     | 102 | BCL  | C2D-C1D-ND  | 4.00  | 114.08      | 110.13   |
| 16  | J     | 101 | BCL  | C1D-ND-C4D  | -4.00 | 103.51      | 106.31   |
| 16  | O     | 502 | BCL  | C3B-C4B-NB  | 3.99  | 115.03      | 109.76   |
| 16  | X     | 102 | BCL  | C2D-C1D-ND  | 3.99  | 114.08      | 110.13   |
| 16  | Z     | 102 | BCL  | C2D-C1D-ND  | 3.99  | 114.08      | 110.13   |
| 15  | M     | 410 | PGV  | O01-C1-C2   | 3.99  | 120.11      | 111.48   |
| 16  | 3     | 101 | BCL  | C1D-ND-C4D  | -3.99 | 103.51      | 106.31   |
| 16  | 0     | 102 | BCL  | O2D-CGD-CBD | 3.99  | 118.20      | 111.23   |
| 16  | J     | 101 | BCL  | C3B-C4B-NB  | 3.98  | 115.02      | 109.76   |
| 16  | N     | 101 | BCL  | C2D-C1D-ND  | 3.98  | 114.06      | 110.13   |
| 22  | M     | 409 | CDL  | OB6-CB5-C51 | 3.98  | 120.09      | 111.48   |
| 16  | I     | 101 | BCL  | C1D-ND-C4D  | -3.97 | 103.53      | 106.31   |
| 16  | Q     | 102 | BCL  | C1D-ND-C4D  | -3.97 | 103.53      | 106.31   |
| 16  | 8     | 102 | BCL  | C2D-C1D-ND  | 3.97  | 114.05      | 110.13   |
| 22  | M     | 411 | CDL  | OB6-CB5-C51 | 3.96  | 120.06      | 111.48   |
| 16  | V     | 102 | BCL  | C1D-ND-C4D  | -3.96 | 103.53      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | 5     | 102 | BCL  | C1D-ND-C4D  | -3.96 | 103.53      | 106.31   |
| 16  | Q     | 102 | BCL  | C3B-C4B-NB  | 3.96  | 114.98      | 109.76   |
| 21  | E     | 103 | CRT  | C20-C19-C17 | -3.96 | 121.73      | 127.28   |
| 16  | T     | 101 | BCL  | C1-C2-C3    | -3.95 | 119.72      | 126.20   |
| 16  | V     | 102 | BCL  | C2D-C1D-ND  | 3.95  | 114.03      | 110.13   |
| 21  | X     | 103 | CRT  | C4-C5-C6    | -3.94 | 119.38      | 124.91   |
| 16  | W     | 101 | BCL  | C3C-C4C-CHD | -3.94 | 115.09      | 123.39   |
| 16  | 2     | 102 | BCL  | O2D-CGD-CBD | 3.94  | 118.11      | 111.23   |
| 16  | 3     | 101 | BCL  | C3C-C4C-CHD | -3.94 | 115.09      | 123.39   |
| 16  | N     | 101 | BCL  | O2D-CGD-CBD | 3.93  | 118.11      | 111.23   |
| 16  | Z     | 102 | BCL  | O2D-CGD-CBD | 3.93  | 118.10      | 111.23   |
| 16  | R     | 101 | BCL  | C3B-C4B-NB  | 3.93  | 114.94      | 109.76   |
| 16  | G     | 102 | BCL  | O2D-CGD-CBD | 3.93  | 118.09      | 111.23   |
| 16  | U     | 101 | BCL  | C3C-C4C-CHD | -3.92 | 115.12      | 123.39   |
| 16  | W     | 101 | BCL  | C1D-ND-C4D  | -3.92 | 103.56      | 106.31   |
| 16  | 5     | 102 | BCL  | C3B-C4B-NB  | 3.92  | 114.93      | 109.76   |
| 16  | S     | 101 | BCL  | C1D-ND-C4D  | -3.91 | 103.57      | 106.31   |
| 16  | B     | 102 | BCL  | O2D-CGD-CBD | 3.90  | 118.04      | 111.23   |
| 16  | L     | 307 | BCL  | C1-C2-C3    | -3.89 | 119.82      | 126.20   |
| 16  | R     | 101 | BCL  | O2D-CGD-CBD | 3.89  | 118.04      | 111.23   |
| 15  | D     | 501 | PGV  | O01-C1-C2   | 3.89  | 119.90      | 111.48   |
| 21  | 4     | 102 | CRT  | C21-C22-C23 | -3.89 | 121.82      | 127.28   |
| 16  | L     | 301 | BCL  | C2D-C1D-ND  | 3.87  | 113.96      | 110.13   |
| 16  | 4     | 101 | BCL  | C1-C2-C3    | -3.87 | 119.86      | 126.20   |
| 16  | D     | 503 | BCL  | C2D-C1D-ND  | 3.87  | 113.95      | 110.13   |
| 16  | J     | 101 | BCL  | C2D-C1D-ND  | 3.87  | 113.95      | 110.13   |
| 16  | W     | 101 | BCL  | C3B-C4B-NB  | 3.86  | 114.86      | 109.76   |
| 16  | 0     | 102 | BCL  | C2D-C1D-ND  | 3.86  | 113.95      | 110.13   |
| 16  | P     | 102 | BCL  | C2D-C1D-ND  | 3.86  | 113.94      | 110.13   |
| 21  | X     | 103 | CRT  | C10-C9-C7   | -3.85 | 121.87      | 127.28   |
| 16  | K     | 102 | BCL  | C2D-C1D-ND  | 3.85  | 113.94      | 110.13   |
| 16  | V     | 102 | BCL  | C3B-C4B-NB  | 3.84  | 114.83      | 109.76   |
| 16  | 1     | 402 | BCL  | C2D-C1D-ND  | 3.84  | 113.93      | 110.13   |
| 16  | P     | 102 | BCL  | O2D-CGD-CBD | 3.84  | 117.94      | 111.23   |
| 16  | S     | 101 | BCL  | C3C-C4C-CHD | -3.83 | 115.32      | 123.39   |
| 16  | Z     | 102 | BCL  | C3B-C4B-NB  | 3.82  | 114.81      | 109.76   |
| 16  | Y     | 101 | BCL  | C2D-C1D-ND  | 3.82  | 113.91      | 110.13   |
| 16  | 9     | 101 | BCL  | C1D-ND-C4D  | -3.82 | 103.63      | 106.31   |
| 17  | M     | 405 | BPH  | C4D-CHA-CBD | -3.82 | 106.62      | 108.45   |
| 16  | B     | 102 | BCL  | C2D-C1D-ND  | 3.82  | 113.91      | 110.13   |
| 16  | 1     | 402 | BCL  | C3C-C4C-CHD | -3.82 | 115.34      | 123.39   |
| 16  | Y     | 101 | BCL  | C3B-C4B-NB  | 3.82  | 114.80      | 109.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | O     | 502 | BCL  | C1-C2-C3    | -3.81 | 119.96      | 126.20   |
| 16  | I     | 101 | BCL  | C3B-C4B-NB  | 3.81  | 114.78      | 109.76   |
| 16  | 2     | 102 | BCL  | C3B-C4B-NB  | 3.81  | 114.78      | 109.76   |
| 16  | T     | 101 | BCL  | C3B-C4B-NB  | 3.80  | 114.78      | 109.76   |
| 16  | K     | 102 | BCL  | C3C-C4C-CHD | -3.80 | 115.38      | 123.39   |
| 16  | U     | 101 | BCL  | C2D-C1D-ND  | 3.80  | 113.88      | 110.13   |
| 16  | P     | 102 | BCL  | C1-C2-C3    | -3.80 | 119.98      | 126.20   |
| 21  | 4     | 102 | CRT  | C20-C19-C17 | -3.79 | 121.96      | 127.28   |
| 16  | 9     | 101 | BCL  | C3B-C4B-NB  | 3.78  | 114.75      | 109.76   |
| 16  | F     | 502 | BCL  | C3B-C4B-NB  | 3.78  | 114.74      | 109.76   |
| 16  | V     | 102 | BCL  | O2D-CGD-CBD | 3.77  | 117.83      | 111.23   |
| 16  | Y     | 101 | BCL  | C3C-C4C-CHD | -3.76 | 115.47      | 123.39   |
| 16  | 8     | 102 | BCL  | C3B-C4B-NB  | 3.76  | 114.72      | 109.76   |
| 16  | X     | 102 | BCL  | O2D-CGD-CBD | 3.76  | 117.80      | 111.23   |
| 22  | H     | 302 | CDL  | OA6-CA5-C11 | 3.76  | 119.61      | 111.48   |
| 10  | C     | 401 | HEM  | CHA-C4D-ND  | 3.75  | 129.01      | 124.37   |
| 16  | 3     | 101 | BCL  | C2D-C1D-ND  | 3.75  | 113.84      | 110.13   |
| 16  | 7     | 102 | BCL  | C1D-ND-C4D  | -3.75 | 103.68      | 106.31   |
| 16  | K     | 102 | BCL  | C1-C2-C3    | -3.75 | 120.06      | 126.20   |
| 21  | X     | 103 | CRT  | C5-C6-C7    | -3.75 | 120.23      | 125.89   |
| 16  | Y     | 101 | BCL  | C1-C2-C3    | -3.73 | 120.08      | 126.20   |
| 16  | 1     | 402 | BCL  | C3B-C4B-NB  | 3.73  | 114.69      | 109.76   |
| 16  | G     | 102 | BCL  | C2D-C1D-ND  | 3.73  | 113.82      | 110.13   |
| 15  | 1     | 401 | PGV  | O01-C1-C2   | 3.72  | 119.53      | 111.48   |
| 16  | T     | 101 | BCL  | O2D-CGD-CBD | 3.72  | 117.73      | 111.23   |
| 16  | A     | 101 | BCL  | C2D-C1D-ND  | 3.71  | 113.80      | 110.13   |
| 16  | O     | 502 | BCL  | C2D-C1D-ND  | 3.71  | 113.80      | 110.13   |
| 22  | H     | 302 | CDL  | OB6-CB5-C51 | 3.71  | 119.51      | 111.48   |
| 16  | F     | 502 | BCL  | C2D-C1D-ND  | 3.71  | 113.80      | 110.13   |
| 16  | Q     | 102 | BCL  | C2D-C1D-ND  | 3.70  | 113.79      | 110.13   |
| 21  | N     | 102 | CRT  | C10-C9-C7   | -3.70 | 122.09      | 127.28   |
| 16  | L     | 307 | BCL  | C1D-ND-C4D  | -3.70 | 103.72      | 106.31   |
| 16  | M     | 404 | BCL  | C1D-ND-C4D  | -3.70 | 103.72      | 106.31   |
| 21  | N     | 102 | CRT  | C20-C19-C17 | -3.69 | 122.11      | 127.28   |
| 16  | M     | 403 | BCL  | C3B-C4B-NB  | 3.68  | 114.61      | 109.76   |
| 22  | D     | 502 | CDL  | OA6-CA5-C11 | 3.67  | 119.42      | 111.48   |
| 10  | C     | 401 | HEM  | CHB-C1B-NB  | 3.67  | 128.91      | 124.37   |
| 16  | W     | 101 | BCL  | C2D-C1D-ND  | 3.67  | 113.76      | 110.13   |
| 16  | S     | 101 | BCL  | C2D-C1D-ND  | 3.66  | 113.75      | 110.13   |
| 16  | N     | 101 | BCL  | C1-C2-C3    | -3.66 | 120.21      | 126.20   |
| 21  | Q     | 101 | CRT  | C20-C19-C17 | -3.66 | 122.15      | 127.28   |
| 22  | M     | 412 | CDL  | OB6-CB5-C51 | 3.66  | 119.39      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | V     | 102 | BCL  | C1-C2-C3    | -3.65 | 120.21      | 126.20   |
| 16  | 7     | 102 | BCL  | C1-C2-C3    | -3.65 | 120.22      | 126.20   |
| 16  | S     | 101 | BCL  | C3B-C4B-NB  | 3.65  | 114.57      | 109.76   |
| 16  | E     | 102 | BCL  | O2D-CGD-CBD | 3.65  | 117.60      | 111.23   |
| 15  | F     | 501 | PGV  | O01-C1-C2   | 3.64  | 119.36      | 111.48   |
| 16  | M     | 404 | BCL  | O2D-CGD-O1D | -3.64 | 116.76      | 123.85   |
| 10  | C     | 403 | HEM  | CHA-C4D-ND  | 3.64  | 128.87      | 124.37   |
| 21  | X     | 103 | CRT  | C20-C19-C17 | -3.64 | 122.17      | 127.28   |
| 15  | C     | 409 | PGV  | O01-C1-C2   | 3.64  | 119.35      | 111.48   |
| 16  | M     | 404 | BCL  | C2D-C1D-ND  | 3.64  | 113.73      | 110.13   |
| 21  | 7     | 101 | CRT  | C20-C19-C17 | -3.63 | 122.19      | 127.28   |
| 16  | 7     | 102 | BCL  | C3B-C4B-NB  | 3.59  | 114.50      | 109.76   |
| 22  | M     | 412 | CDL  | CA4-OA6-CA5 | -3.59 | 111.51      | 117.85   |
| 16  | L     | 307 | BCL  | C3D-C4D-ND  | 3.58  | 115.81      | 109.99   |
| 16  | F     | 502 | BCL  | C3C-C4C-CHD | -3.58 | 115.84      | 123.39   |
| 16  | 8     | 102 | BCL  | C1-C2-C3    | -3.58 | 120.33      | 126.20   |
| 16  | L     | 301 | BCL  | O2D-CGD-CBD | 3.57  | 117.48      | 111.23   |
| 16  | Y     | 101 | BCL  | C3D-C4D-ND  | 3.57  | 115.79      | 109.99   |
| 16  | M     | 403 | BCL  | C1-C2-C3    | -3.57 | 120.34      | 126.20   |
| 16  | A     | 101 | BCL  | C3D-C4D-ND  | 3.57  | 115.79      | 109.99   |
| 16  | R     | 101 | BCL  | C1-C2-C3    | -3.56 | 120.36      | 126.20   |
| 16  | I     | 101 | BCL  | C3D-C4D-ND  | 3.55  | 115.76      | 109.99   |
| 16  | U     | 101 | BCL  | C3D-C4D-ND  | 3.55  | 115.76      | 109.99   |
| 16  | M     | 404 | BCL  | C3B-C4B-NB  | 3.55  | 114.44      | 109.76   |
| 21  | 8     | 103 | CRT  | C20-C19-C17 | -3.54 | 122.31      | 127.28   |
| 16  | 5     | 102 | BCL  | C2D-C1D-ND  | 3.54  | 113.63      | 110.13   |
| 18  | L     | 304 | UQ8  | C12-C13-C14 | -3.54 | 119.52      | 127.62   |
| 16  | 9     | 101 | BCL  | C3C-C4C-CHD | -3.54 | 115.93      | 123.39   |
| 16  | I     | 101 | BCL  | C2D-C1D-ND  | 3.53  | 113.62      | 110.13   |
| 16  | P     | 102 | BCL  | C3D-C4D-ND  | 3.52  | 115.71      | 109.99   |
| 16  | K     | 102 | BCL  | C3D-C4D-ND  | 3.52  | 115.71      | 109.99   |
| 16  | X     | 102 | BCL  | C1-C2-C3    | -3.52 | 120.44      | 126.20   |
| 16  | 0     | 102 | BCL  | C1-C2-C3    | -3.51 | 120.45      | 126.20   |
| 16  | M     | 403 | BCL  | C1D-ND-C4D  | -3.51 | 103.85      | 106.31   |
| 16  | 2     | 102 | BCL  | C1-C2-C3    | -3.51 | 120.45      | 126.20   |
| 16  | F     | 502 | BCL  | C3D-C4D-ND  | 3.50  | 115.68      | 109.99   |
| 16  | D     | 503 | BCL  | C3D-C4D-ND  | 3.50  | 115.68      | 109.99   |
| 16  | 9     | 101 | BCL  | C3D-C4D-ND  | 3.50  | 115.67      | 109.99   |
| 16  | 9     | 101 | BCL  | C2D-C1D-ND  | 3.49  | 113.58      | 110.13   |
| 16  | 5     | 102 | BCL  | C3D-C4D-ND  | 3.49  | 115.67      | 109.99   |
| 16  | O     | 502 | BCL  | C3D-C4D-ND  | 3.49  | 115.66      | 109.99   |
| 16  | Z     | 102 | BCL  | C3D-C4D-ND  | 3.49  | 115.66      | 109.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | G     | 102 | BCL  | C3D-C4D-ND  | 3.49  | 115.66      | 109.99   |
| 24  | 5     | 101 | LMT  | C1-O1'-C1'  | -3.49 | 107.72      | 113.68   |
| 16  | M     | 403 | BCL  | C3D-C4D-ND  | 3.49  | 115.65      | 109.99   |
| 16  | E     | 102 | BCL  | C3D-C4D-ND  | 3.47  | 115.63      | 109.99   |
| 21  | T     | 102 | CRT  | C32-C31-C30 | -3.47 | 113.14      | 123.20   |
| 16  | 2     | 102 | BCL  | C3D-C4D-ND  | 3.47  | 115.63      | 109.99   |
| 21  | M     | 407 | CRT  | C32-C31-C30 | -3.47 | 113.14      | 123.20   |
| 21  | Q     | 101 | CRT  | C32-C31-C30 | -3.47 | 113.14      | 123.20   |
| 16  | L     | 307 | BCL  | C2D-C1D-ND  | 3.47  | 113.56      | 110.13   |
| 21  | G     | 103 | CRT  | C20-C19-C17 | -3.46 | 122.42      | 127.28   |
| 16  | 0     | 102 | BCL  | C3D-C4D-ND  | 3.46  | 115.62      | 109.99   |
| 16  | Q     | 102 | BCL  | C3D-C4D-ND  | 3.46  | 115.61      | 109.99   |
| 16  | W     | 101 | BCL  | C3D-C4D-ND  | 3.46  | 115.61      | 109.99   |
| 16  | 1     | 402 | BCL  | C3D-C4D-ND  | 3.45  | 115.60      | 109.99   |
| 16  | 5     | 102 | BCL  | C3C-C4C-CHD | -3.45 | 116.12      | 123.39   |
| 16  | S     | 101 | BCL  | C3D-C4D-ND  | 3.45  | 115.59      | 109.99   |
| 16  | L     | 307 | BCL  | C3B-C4B-NB  | 3.45  | 114.31      | 109.76   |
| 16  | N     | 101 | BCL  | C3D-C4D-ND  | 3.44  | 115.58      | 109.99   |
| 16  | 3     | 101 | BCL  | C3D-C4D-ND  | 3.44  | 115.58      | 109.99   |
| 21  | Z     | 103 | CRT  | C20-C19-C17 | -3.44 | 122.45      | 127.28   |
| 10  | C     | 404 | HEM  | CHB-C1B-NB  | 3.44  | 128.62      | 124.37   |
| 16  | 8     | 102 | BCL  | C3D-C4D-ND  | 3.43  | 115.56      | 109.99   |
| 16  | M     | 404 | BCL  | O2A-CGA-CBA | 3.43  | 122.29      | 111.83   |
| 21  | T     | 102 | CRT  | C20-C19-C17 | -3.42 | 122.48      | 127.28   |
| 21  | K     | 101 | CRT  | C20-C19-C17 | -3.42 | 122.48      | 127.28   |
| 16  | B     | 102 | BCL  | C3D-C4D-ND  | 3.42  | 115.55      | 109.99   |
| 16  | 7     | 102 | BCL  | C3D-C4D-ND  | 3.42  | 115.54      | 109.99   |
| 16  | 7     | 102 | BCL  | C2D-C1D-ND  | 3.41  | 113.50      | 110.13   |
| 22  | M     | 411 | CDL  | OB8-CB7-C71 | 3.40  | 122.21      | 111.83   |
| 16  | R     | 101 | BCL  | C3D-C4D-ND  | 3.39  | 115.50      | 109.99   |
| 16  | M     | 403 | BCL  | C2D-C1D-ND  | 3.39  | 113.48      | 110.13   |
| 21  | X     | 103 | CRT  | C32-C31-C30 | -3.39 | 113.38      | 123.20   |
| 16  | J     | 101 | BCL  | C3D-C4D-ND  | 3.39  | 115.50      | 109.99   |
| 16  | 4     | 101 | BCL  | C3D-C4D-ND  | 3.39  | 115.49      | 109.99   |
| 16  | T     | 101 | BCL  | C3D-C4D-ND  | 3.39  | 115.49      | 109.99   |
| 18  | L     | 308 | UQ8  | C7-C8-C9    | -3.38 | 121.00      | 126.83   |
| 16  | W     | 101 | BCL  | C1-C2-C3    | -3.38 | 120.67      | 126.20   |
| 15  | D     | 501 | PGV  | C02-O01-C1  | -3.37 | 109.72      | 117.80   |
| 18  | L     | 304 | UQ8  | C37-C38-C39 | -3.37 | 119.91      | 127.62   |
| 16  | 6     | 101 | BCL  | C1-C2-C3    | -3.37 | 120.67      | 126.20   |
| 16  | 6     | 101 | BCL  | C3D-C4D-ND  | 3.37  | 115.47      | 109.99   |
| 16  | A     | 101 | BCL  | C1-C2-C3    | -3.37 | 120.68      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | M     | 407 | CRT  | C10-C9-C7   | -3.37 | 122.56      | 127.28   |
| 16  | L     | 301 | BCL  | O2A-CGA-CBA | 3.36  | 122.09      | 111.83   |
| 10  | C     | 402 | HEM  | CHB-C1B-NB  | 3.36  | 128.52      | 124.37   |
| 16  | V     | 102 | BCL  | C3D-C4D-ND  | 3.34  | 115.42      | 109.99   |
| 16  | I     | 101 | BCL  | C1-C2-C3    | -3.34 | 120.72      | 126.20   |
| 16  | I     | 101 | BCL  | C3C-C4C-CHD | -3.33 | 116.36      | 123.39   |
| 15  | F     | 501 | PGV  | O03-C19-C20 | 3.33  | 122.00      | 111.83   |
| 21  | N     | 102 | CRT  | C5-C6-C7    | -3.33 | 120.86      | 125.89   |
| 16  | D     | 503 | BCL  | C1-C2-C3    | -3.32 | 120.75      | 126.20   |
| 16  | G     | 102 | BCL  | C1-C2-C3    | -3.32 | 120.75      | 126.20   |
| 16  | X     | 102 | BCL  | C3D-C4D-ND  | 3.32  | 115.38      | 109.99   |
| 18  | L     | 304 | UQ8  | C27-C28-C29 | -3.31 | 120.04      | 127.62   |
| 18  | L     | 303 | UQ8  | C12-C13-C14 | -3.31 | 120.05      | 127.62   |
| 20  | M     | 406 | MQ8  | C34-C33-C35 | 3.30  | 120.96      | 115.23   |
| 10  | C     | 402 | HEM  | C1B-NB-C4B  | 3.30  | 109.11      | 105.21   |
| 21  | 2     | 103 | CRT  | C20-C19-C17 | -3.29 | 122.66      | 127.28   |
| 21  | 7     | 101 | CRT  | C10-C9-C7   | -3.29 | 122.66      | 127.28   |
| 21  | B     | 103 | CRT  | C32-C31-C30 | -3.29 | 113.68      | 123.20   |
| 16  | B     | 102 | BCL  | C1-C2-C3    | -3.29 | 120.81      | 126.20   |
| 21  | 7     | 101 | CRT  | C21-C22-C23 | -3.28 | 122.67      | 127.28   |
| 16  | M     | 404 | BCL  | C3D-C4D-ND  | 3.28  | 115.32      | 109.99   |
| 21  | M     | 407 | CRT  | O2-C38-C40  | -3.28 | 86.40       | 108.97   |
| 20  | M     | 406 | MQ8  | C36-C37-C38 | -3.28 | 120.12      | 127.62   |
| 21  | M     | 407 | CRT  | C14-C15-C16 | -3.28 | 113.70      | 123.20   |
| 10  | C     | 404 | HEM  | CHA-C4D-ND  | 3.27  | 128.42      | 124.37   |
| 21  | N     | 102 | CRT  | C32-C31-C30 | -3.26 | 113.76      | 123.20   |
| 21  | 2     | 103 | CRT  | C10-C9-C7   | -3.25 | 122.72      | 127.28   |
| 18  | L     | 304 | UQ8  | C40-C39-C41 | 3.25  | 120.87      | 115.23   |
| 16  | J     | 101 | BCL  | C1-C2-C3    | -3.25 | 120.88      | 126.20   |
| 16  | L     | 301 | BCL  | C3D-C4D-ND  | 3.24  | 115.25      | 109.99   |
| 10  | C     | 402 | HEM  | CHA-C4D-ND  | 3.22  | 128.35      | 124.37   |
| 10  | C     | 403 | HEM  | C1B-NB-C4B  | 3.22  | 109.02      | 105.21   |
| 16  | 5     | 102 | BCL  | C1-C2-C3    | -3.22 | 120.92      | 126.20   |
| 21  | 0     | 103 | CRT  | C32-C31-C30 | -3.21 | 113.89      | 123.20   |
| 10  | C     | 401 | HEM  | C1B-NB-C4B  | 3.20  | 109.00      | 105.21   |
| 21  | Z     | 103 | CRT  | C14-C15-C16 | -3.20 | 113.92      | 123.20   |
| 16  | 7     | 102 | BCL  | C3C-C4C-CHD | -3.19 | 116.66      | 123.39   |
| 10  | C     | 404 | HEM  | C1B-NB-C4B  | 3.18  | 108.98      | 105.21   |
| 21  | E     | 103 | CRT  | C32-C31-C30 | -3.18 | 113.98      | 123.20   |
| 21  | G     | 103 | CRT  | C32-C31-C30 | -3.18 | 113.98      | 123.20   |
| 18  | L     | 303 | UQ8  | C1M-C1-C6   | -3.17 | 119.23      | 124.45   |
| 18  | L     | 303 | UQ8  | C7-C8-C9    | -3.17 | 121.37      | 126.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | 8     | 103 | CRT  | C32-C31-C30 | -3.16 | 114.03      | 123.20   |
| 21  | V     | 103 | CRT  | O2-C38-C39  | -3.15 | 87.28       | 108.97   |
| 18  | L     | 308 | UQ8  | C30-C29-C31 | 3.15  | 120.69      | 115.23   |
| 21  | Z     | 103 | CRT  | C31-C32-C33 | -3.15 | 122.86      | 127.28   |
| 16  | 0     | 102 | BCL  | C4-C3-C5    | 3.15  | 120.69      | 115.23   |
| 21  | Z     | 103 | CRT  | C26-C27-C28 | -3.14 | 122.88      | 127.28   |
| 18  | L     | 304 | UQ8  | C22-C23-C24 | -3.13 | 120.45      | 127.62   |
| 16  | Z     | 102 | BCL  | O2A-CGA-CBA | 3.13  | 121.36      | 111.83   |
| 21  | 4     | 102 | CRT  | C36-C35-C33 | -3.12 | 121.17      | 125.89   |
| 16  | Z     | 102 | BCL  | C1-C2-C3    | -3.12 | 121.08      | 126.20   |
| 16  | Q     | 102 | BCL  | C4-C3-C5    | 3.12  | 120.65      | 115.23   |
| 21  | 7     | 101 | CRT  | C5-C6-C7    | -3.11 | 121.19      | 125.89   |
| 24  | X     | 101 | LMT  | C1B-O1B-C4' | -3.11 | 110.61      | 117.98   |
| 21  | 8     | 103 | CRT  | C10-C9-C7   | -3.11 | 122.92      | 127.28   |
| 18  | L     | 303 | UQ8  | C15-C14-C16 | 3.10  | 120.62      | 115.23   |
| 16  | L     | 307 | BCL  | CHC-C4B-NB  | -3.10 | 119.39      | 124.05   |
| 16  | Q     | 102 | BCL  | C1-C2-C3    | -3.10 | 121.11      | 126.20   |
| 21  | G     | 103 | CRT  | C14-C15-C16 | -3.10 | 114.23      | 123.20   |
| 21  | 2     | 103 | CRT  | O2-C38-C40  | -3.08 | 87.77       | 108.97   |
| 21  | 4     | 102 | CRT  | C10-C9-C7   | -3.08 | 122.95      | 127.28   |
| 18  | L     | 303 | UQ8  | C7-C6-C1    | -3.08 | 119.61      | 124.89   |
| 21  | T     | 102 | CRT  | C14-C15-C16 | -3.08 | 114.28      | 123.20   |
| 15  | M     | 410 | PGV  | O03-C19-C20 | 3.07  | 121.20      | 111.83   |
| 16  | 2     | 102 | BCL  | O2A-CGA-CBA | 3.07  | 121.20      | 111.83   |
| 18  | L     | 308 | UQ8  | C32-C33-C34 | -3.07 | 120.60      | 127.62   |
| 21  | B     | 103 | CRT  | C20-C19-C17 | -3.07 | 122.98      | 127.28   |
| 16  | D     | 503 | BCL  | C4-C3-C5    | 3.06  | 120.55      | 115.23   |
| 16  | E     | 102 | BCL  | O2A-CGA-CBA | 3.05  | 121.14      | 111.83   |
| 16  | T     | 101 | BCL  | C1C-NC-C4C  | -3.05 | 105.29      | 106.68   |
| 21  | Q     | 101 | CRT  | C15-C14-C12 | -3.05 | 123.01      | 127.28   |
| 16  | S     | 101 | BCL  | C1-C2-C3    | -3.05 | 121.21      | 126.20   |
| 16  | K     | 102 | BCL  | C4-C3-C5    | 3.04  | 120.51      | 115.23   |
| 21  | K     | 101 | CRT  | C10-C9-C7   | -3.04 | 123.02      | 127.28   |
| 16  | E     | 102 | BCL  | C1C-NC-C4C  | -3.03 | 105.30      | 106.68   |
| 16  | F     | 502 | BCL  | C1-C2-C3    | -3.03 | 121.23      | 126.20   |
| 16  | R     | 101 | BCL  | C4-C3-C5    | 3.03  | 120.49      | 115.23   |
| 21  | E     | 103 | CRT  | C9-C10-C11  | -3.02 | 114.44      | 123.20   |
| 16  | 1     | 402 | BCL  | C1-C2-C3    | -3.02 | 121.25      | 126.20   |
| 20  | M     | 406 | MQ8  | C29-C28-C30 | 3.02  | 120.47      | 115.23   |
| 16  | 8     | 102 | BCL  | O2A-CGA-CBA | 3.02  | 121.04      | 111.83   |
| 16  | 3     | 101 | BCL  | C1C-NC-C4C  | -3.02 | 105.30      | 106.68   |
| 21  | 2     | 103 | CRT  | O2-C38-C39  | -3.02 | 88.22       | 108.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | M     | 406 | MQ8  | C16-C17-C18 | -3.01 | 120.73      | 127.62   |
| 16  | P     | 102 | BCL  | CHB-C4A-NA  | 3.01  | 128.74      | 124.40   |
| 21  | V     | 103 | CRT  | C14-C15-C16 | -3.01 | 114.48      | 123.20   |
| 16  | J     | 101 | BCL  | C1C-NC-C4C  | -3.01 | 105.31      | 106.68   |
| 21  | R     | 102 | CRT  | C32-C31-C30 | -3.01 | 114.49      | 123.20   |
| 16  | N     | 101 | BCL  | O2A-CGA-CBA | 3.00  | 120.99      | 111.83   |
| 16  | L     | 301 | BCL  | CED-O2D-CGD | 3.00  | 122.72      | 115.92   |
| 21  | 2     | 103 | CRT  | C32-C31-C30 | -3.00 | 114.52      | 123.20   |
| 16  | X     | 102 | BCL  | C1C-NC-C4C  | -2.99 | 105.31      | 106.68   |
| 21  | V     | 103 | CRT  | C20-C19-C17 | -2.99 | 123.09      | 127.28   |
| 24  | E     | 101 | LMT  | C1B-O1B-C4' | -2.99 | 110.89      | 117.98   |
| 16  | 6     | 101 | BCL  | O2A-CGA-CBA | 2.99  | 120.94      | 111.83   |
| 22  | H     | 302 | CDL  | OA8-CA7-C31 | 2.97  | 120.90      | 111.83   |
| 21  | V     | 103 | CRT  | C32-C31-C30 | -2.97 | 114.60      | 123.20   |
| 21  | K     | 101 | CRT  | C21-C20-C19 | -2.97 | 117.45      | 123.52   |
| 15  | M     | 408 | PGV  | C02-O01-C1  | -2.96 | 110.71      | 117.80   |
| 15  | L     | 309 | PGV  | O03-C19-C20 | 2.96  | 120.86      | 111.83   |
| 16  | G     | 102 | BCL  | O2A-CGA-CBA | 2.96  | 120.86      | 111.83   |
| 16  | M     | 404 | BCL  | C4A-NA-C1A  | 2.95  | 108.03      | 106.68   |
| 16  | V     | 102 | BCL  | C1C-NC-C4C  | -2.95 | 105.33      | 106.68   |
| 18  | L     | 308 | UQ8  | C7-C6-C1    | -2.95 | 119.83      | 124.89   |
| 21  | X     | 103 | CRT  | C21-C20-C19 | -2.95 | 117.48      | 123.52   |
| 16  | J     | 101 | BCL  | O2A-CGA-CBA | 2.95  | 120.83      | 111.83   |
| 16  | 4     | 101 | BCL  | CHB-C4A-NA  | 2.95  | 128.66      | 124.40   |
| 15  | L     | 309 | PGV  | C02-O01-C1  | -2.95 | 110.74      | 117.80   |
| 16  | S     | 101 | BCL  | C4-C3-C5    | 2.95  | 120.34      | 115.23   |
| 16  | A     | 101 | BCL  | CHC-C1C-NC  | 2.95  | 128.65      | 124.40   |
| 16  | B     | 102 | BCL  | O2A-CGA-CBA | 2.95  | 120.82      | 111.83   |
| 16  | 2     | 102 | BCL  | C4-C3-C5    | 2.95  | 120.34      | 115.23   |
| 16  | 3     | 101 | BCL  | C4-C3-C5    | 2.94  | 120.33      | 115.23   |
| 16  | B     | 102 | BCL  | CHB-C4A-NA  | 2.93  | 128.63      | 124.40   |
| 21  | V     | 103 | CRT  | O2-C38-C40  | -2.93 | 88.81       | 108.97   |
| 16  | V     | 102 | BCL  | O2A-CGA-CBA | 2.93  | 120.77      | 111.83   |
| 16  | Z     | 102 | BCL  | C1C-NC-C4C  | -2.93 | 105.34      | 106.68   |
| 16  | B     | 102 | BCL  | C4-C3-C5    | 2.91  | 120.28      | 115.23   |
| 16  | F     | 502 | BCL  | C4-C3-C5    | 2.91  | 120.28      | 115.23   |
| 21  | Z     | 103 | CRT  | C4-C5-C6    | -2.90 | 120.84      | 124.91   |
| 21  | 0     | 103 | CRT  | C14-C15-C16 | -2.90 | 114.80      | 123.20   |
| 18  | L     | 308 | UQ8  | C40-C39-C41 | 2.90  | 120.26      | 115.23   |
| 16  | E     | 102 | BCL  | CHB-C4A-NA  | 2.90  | 128.58      | 124.40   |
| 18  | L     | 304 | UQ8  | C35-C34-C36 | 2.89  | 120.25      | 115.23   |
| 22  | H     | 302 | CDL  | OB8-CB7-C71 | 2.89  | 120.65      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | Q     | 102 | BCL  | CHC-C1C-NC  | 2.89  | 128.57      | 124.40   |
| 21  | E     | 103 | CRT  | C14-C15-C16 | -2.89 | 114.83      | 123.20   |
| 22  | M     | 409 | CDL  | OA8-CA7-C31 | 2.89  | 119.92      | 111.15   |
| 16  | E     | 102 | BCL  | C1-C2-C3    | -2.89 | 121.47      | 126.20   |
| 16  | P     | 102 | BCL  | C4-C3-C5    | 2.89  | 120.24      | 115.23   |
| 16  | R     | 101 | BCL  | C1C-NC-C4C  | -2.88 | 105.36      | 106.68   |
| 21  | T     | 102 | CRT  | C21-C20-C19 | -2.88 | 117.62      | 123.52   |
| 21  | 7     | 101 | CRT  | C32-C31-C30 | -2.88 | 114.86      | 123.20   |
| 15  | H     | 301 | PGV  | O03-C19-C20 | 2.88  | 120.61      | 111.83   |
| 10  | C     | 401 | HEM  | C3B-C4B-NB  | -2.88 | 107.40      | 109.47   |
| 16  | O     | 502 | BCL  | CHC-C1C-NC  | 2.87  | 128.54      | 124.40   |
| 16  | J     | 101 | BCL  | C4-C3-C5    | 2.87  | 120.21      | 115.23   |
| 16  | A     | 101 | BCL  | C4-C3-C5    | 2.87  | 120.21      | 115.23   |
| 16  | 8     | 102 | BCL  | CHB-C4A-NA  | 2.87  | 128.54      | 124.40   |
| 21  | K     | 101 | CRT  | C32-C31-C30 | -2.86 | 114.91      | 123.20   |
| 20  | M     | 406 | MQ8  | C26-C27-C28 | -2.86 | 121.08      | 127.62   |
| 16  | N     | 101 | BCL  | CHB-C4A-NA  | 2.86  | 128.53      | 124.40   |
| 16  | P     | 102 | BCL  | O2A-CGA-CBA | 2.86  | 120.54      | 111.83   |
| 16  | Y     | 101 | BCL  | O2A-CGA-CBA | 2.85  | 120.52      | 111.83   |
| 16  | K     | 102 | BCL  | CHC-C1C-NC  | 2.85  | 128.51      | 124.40   |
| 16  | 0     | 102 | BCL  | C1C-NC-C4C  | -2.85 | 105.38      | 106.68   |
| 16  | 3     | 101 | BCL  | C1-C2-C3    | -2.84 | 121.54      | 126.20   |
| 21  | Z     | 103 | CRT  | C36-C35-C33 | -2.84 | 121.60      | 125.89   |
| 18  | L     | 304 | UQ8  | C32-C33-C34 | -2.84 | 121.13      | 127.62   |
| 16  | 0     | 102 | BCL  | CHB-C4A-NA  | 2.84  | 128.50      | 124.40   |
| 16  | 6     | 101 | BCL  | CHB-C4A-NA  | 2.83  | 128.49      | 124.40   |
| 16  | 4     | 101 | BCL  | O2A-CGA-CBA | 2.83  | 120.47      | 111.83   |
| 21  | 0     | 103 | CRT  | C27-C26-C25 | -2.83 | 115.00      | 123.20   |
| 16  | V     | 102 | BCL  | CHB-C4A-NA  | 2.83  | 128.48      | 124.40   |
| 21  | R     | 102 | CRT  | C21-C20-C19 | -2.83 | 117.73      | 123.52   |
| 21  | 0     | 103 | CRT  | C21-C20-C19 | -2.83 | 117.74      | 123.52   |
| 21  | R     | 102 | CRT  | C14-C15-C16 | -2.82 | 115.02      | 123.20   |
| 16  | U     | 101 | BCL  | C1-C2-C3    | -2.82 | 121.57      | 126.20   |
| 16  | 8     | 102 | BCL  | C4-C3-C5    | 2.82  | 120.13      | 115.23   |
| 16  | G     | 102 | BCL  | C4-C3-C5    | 2.82  | 120.12      | 115.23   |
| 16  | 5     | 102 | BCL  | C4-C3-C5    | 2.82  | 120.12      | 115.23   |
| 15  | 1     | 401 | PGV  | O03-C19-C20 | 2.81  | 120.42      | 111.83   |
| 16  | 3     | 101 | BCL  | CHC-C1C-NC  | 2.81  | 128.46      | 124.40   |
| 10  | C     | 402 | HEM  | CHD-C4C-NC  | 2.81  | 127.51      | 124.45   |
| 16  | W     | 101 | BCL  | C4-C3-C5    | 2.81  | 120.11      | 115.23   |
| 21  | B     | 103 | CRT  | C14-C15-C16 | -2.81 | 115.06      | 123.20   |
| 15  | L     | 306 | PGV  | O03-C19-C20 | 2.81  | 120.40      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | 8     | 102 | BCL  | C2A-C1A-CHA | -2.81 | 118.99      | 123.87   |
| 16  | L     | 307 | BCL  | O2A-CGA-CBA | 2.81  | 120.39      | 111.83   |
| 18  | L     | 308 | UQ8  | C17-C18-C19 | -2.81 | 121.20      | 127.62   |
| 18  | L     | 308 | UQ8  | C20-C19-C21 | 2.81  | 120.10      | 115.23   |
| 16  | J     | 101 | BCL  | CHB-C4A-NA  | 2.80  | 128.45      | 124.40   |
| 16  | 2     | 102 | BCL  | CHB-C4A-NA  | 2.80  | 128.44      | 124.40   |
| 21  | M     | 407 | CRT  | C34-C33-C35 | 2.80  | 122.37      | 118.09   |
| 21  | B     | 103 | CRT  | C21-C20-C19 | -2.80 | 117.80      | 123.52   |
| 16  | U     | 101 | BCL  | O2A-CGA-CBA | 2.79  | 120.35      | 111.83   |
| 16  | 6     | 101 | BCL  | C1C-NC-C4C  | -2.79 | 105.41      | 106.68   |
| 17  | M     | 405 | BPH  | C2B-C1B-NB  | -2.79 | 107.41      | 109.43   |
| 24  | B     | 101 | LMT  | C1B-O1B-C4' | -2.79 | 111.36      | 117.98   |
| 18  | L     | 304 | UQ8  | C15-C14-C16 | 2.79  | 120.06      | 115.23   |
| 21  | E     | 103 | CRT  | C13-C12-C11 | 2.78  | 122.34      | 118.09   |
| 16  | 5     | 102 | BCL  | CHC-C1C-NC  | 2.78  | 128.42      | 124.40   |
| 16  | G     | 102 | BCL  | CHB-C4A-NA  | 2.78  | 128.41      | 124.40   |
| 21  | R     | 102 | CRT  | C20-C19-C17 | -2.78 | 123.38      | 127.28   |
| 16  | M     | 404 | BCL  | CAA-C2A-C3A | -2.78 | 105.49      | 113.00   |
| 16  | M     | 403 | BCL  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 16  | L     | 307 | BCL  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 16  | U     | 101 | BCL  | CHC-C1C-NC  | 2.77  | 128.40      | 124.40   |
| 18  | L     | 304 | UQ8  | C7-C6-C1    | -2.77 | 120.15      | 124.89   |
| 21  | Z     | 103 | CRT  | C32-C31-C30 | -2.77 | 115.18      | 123.20   |
| 21  | B     | 103 | CRT  | C9-C10-C11  | -2.77 | 115.19      | 123.20   |
| 16  | P     | 102 | BCL  | C2A-C1A-CHA | -2.76 | 119.07      | 123.87   |
| 16  | T     | 101 | BCL  | CHB-C4A-NA  | 2.76  | 128.39      | 124.40   |
| 21  | M     | 407 | CRT  | C35-C33-C32 | -2.76 | 114.67      | 119.01   |
| 16  | 6     | 101 | BCL  | C4-C3-C5    | 2.76  | 120.02      | 115.23   |
| 16  | 4     | 101 | BCL  | C4A-NA-C1A  | 2.76  | 107.94      | 106.68   |
| 16  | B     | 102 | BCL  | C2A-C1A-CHA | -2.76 | 119.08      | 123.87   |
| 10  | C     | 403 | HEM  | CHB-C1B-NB  | 2.75  | 127.77      | 124.37   |
| 21  | M     | 407 | CRT  | O2-C38-C39  | -2.75 | 90.06       | 108.97   |
| 10  | C     | 404 | HEM  | CHD-C1D-C2D | -2.75 | 120.69      | 125.03   |
| 16  | L     | 301 | BCL  | C4-C3-C5    | 2.75  | 120.00      | 115.23   |
| 16  | U     | 101 | BCL  | C4-C3-C5    | 2.75  | 119.99      | 115.23   |
| 16  | T     | 101 | BCL  | C2A-C1A-CHA | -2.75 | 119.10      | 123.87   |
| 16  | W     | 101 | BCL  | CHC-C1C-NC  | 2.74  | 128.36      | 124.40   |
| 18  | L     | 308 | UQ8  | C35-C34-C36 | 2.74  | 119.99      | 115.23   |
| 10  | C     | 404 | HEM  | CHD-C4C-NC  | 2.74  | 127.44      | 124.45   |
| 16  | K     | 102 | BCL  | CHC-C4B-NB  | -2.74 | 119.94      | 124.05   |
| 16  | M     | 403 | BCL  | CHC-C1C-NC  | 2.74  | 128.35      | 124.40   |
| 21  | X     | 103 | CRT  | C27-C26-C25 | -2.74 | 115.27      | 123.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | L     | 308 | UQ8  | C1M-C1-C6   | -2.73 | 119.96      | 124.45   |
| 16  | 6     | 101 | BCL  | C2A-C1A-CHA | -2.73 | 119.12      | 123.87   |
| 16  | K     | 102 | BCL  | O2A-CGA-CBA | 2.73  | 120.17      | 111.83   |
| 16  | F     | 502 | BCL  | CHC-C1C-NC  | 2.73  | 128.34      | 124.40   |
| 16  | I     | 101 | BCL  | C4-C3-C5    | 2.73  | 119.96      | 115.23   |
| 16  | 2     | 102 | BCL  | C2A-C1A-CHA | -2.73 | 119.13      | 123.87   |
| 16  | 0     | 102 | BCL  | C2A-C1A-CHA | -2.73 | 119.13      | 123.87   |
| 21  | K     | 101 | CRT  | C15-C14-C12 | -2.73 | 123.45      | 127.28   |
| 17  | L     | 302 | BPH  | C2B-C1B-NB  | -2.72 | 107.47      | 109.43   |
| 16  | O     | 502 | BCL  | O2A-CGA-CBA | 2.72  | 120.11      | 111.83   |
| 24  | 5     | 101 | LMT  | O1'-C1'-C2' | 2.71  | 112.39      | 108.27   |
| 16  | D     | 503 | BCL  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 16  | 2     | 102 | BCL  | C1C-NC-C4C  | -2.71 | 105.44      | 106.68   |
| 16  | 9     | 101 | BCL  | O2A-CGA-CBA | 2.71  | 120.09      | 111.83   |
| 16  | Z     | 102 | BCL  | C2A-C1A-CHA | -2.71 | 119.17      | 123.87   |
| 21  | R     | 102 | CRT  | C9-C10-C11  | -2.71 | 115.36      | 123.20   |
| 24  | R     | 103 | LMT  | C1B-O1B-C4' | -2.70 | 111.57      | 117.98   |
| 16  | E     | 102 | BCL  | C4-C3-C5    | 2.70  | 119.92      | 115.23   |
| 16  | L     | 301 | BCL  | C1-C2-C3    | -2.70 | 121.77      | 126.20   |
| 21  | G     | 103 | CRT  | C13-C12-C11 | 2.70  | 122.22      | 118.09   |
| 16  | X     | 102 | BCL  | O2A-CGA-CBA | 2.70  | 120.07      | 111.83   |
| 22  | M     | 411 | CDL  | OA8-CA7-C31 | 2.69  | 120.05      | 111.83   |
| 16  | D     | 503 | BCL  | CHC-C1C-NC  | 2.69  | 128.28      | 124.40   |
| 21  | X     | 103 | CRT  | C14-C15-C16 | -2.69 | 115.40      | 123.20   |
| 21  | 4     | 102 | CRT  | C30-C28-C27 | -2.69 | 114.78      | 119.01   |
| 16  | M     | 403 | BCL  | C1C-NC-C4C  | -2.69 | 105.45      | 106.68   |
| 21  | B     | 103 | CRT  | C5-C6-C7    | -2.69 | 121.83      | 125.89   |
| 16  | W     | 101 | BCL  | O2D-CGD-O1D | -2.69 | 118.62      | 123.85   |
| 20  | M     | 406 | MQ8  | C41-C42-C43 | -2.68 | 121.48      | 127.62   |
| 16  | 3     | 101 | BCL  | CHC-C4B-NB  | -2.68 | 120.03      | 124.05   |
| 16  | M     | 404 | BCL  | C1D-CHD-C4C | -2.68 | 120.16      | 126.62   |
| 16  | X     | 102 | BCL  | CHB-C4A-NA  | 2.68  | 128.27      | 124.40   |
| 21  | Q     | 101 | CRT  | C34-C33-C35 | 2.68  | 122.18      | 118.09   |
| 20  | M     | 406 | MQ8  | C21-C22-C23 | -2.68 | 121.50      | 127.62   |
| 24  | P     | 103 | LMT  | C1B-O1B-C4' | -2.67 | 111.64      | 117.98   |
| 21  | 0     | 103 | CRT  | C9-C10-C11  | -2.67 | 115.47      | 123.20   |
| 24  | J     | 102 | LMT  | C1B-O1B-C4' | -2.67 | 111.66      | 117.98   |
| 16  | Z     | 102 | BCL  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 16  | S     | 101 | BCL  | O2D-CGD-O1D | -2.66 | 118.67      | 123.85   |
| 24  | G     | 101 | LMT  | C1B-O1B-C4' | -2.66 | 111.67      | 117.98   |
| 16  | 7     | 102 | BCL  | O2A-CGA-CBA | 2.66  | 119.95      | 111.83   |
| 16  | M     | 404 | BCL  | CHC-C4B-NB  | -2.66 | 120.06      | 124.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | 9     | 101 | BCL  | CHC-C4B-NB  | -2.66 | 120.07      | 124.05   |
| 18  | L     | 303 | UQ8  | C10-C9-C11  | 2.65  | 119.84      | 115.23   |
| 10  | C     | 401 | HEM  | CHD-C1D-C2D | -2.65 | 120.84      | 125.03   |
| 16  | R     | 101 | BCL  | CHB-C4A-NA  | 2.65  | 128.22      | 124.40   |
| 16  | E     | 102 | BCL  | C2A-C1A-CHA | -2.65 | 119.28      | 123.87   |
| 21  | Z     | 103 | CRT  | C13-C12-C11 | 2.65  | 122.13      | 118.09   |
| 16  | 9     | 101 | BCL  | C1-C2-C3    | -2.64 | 121.86      | 126.20   |
| 21  | Q     | 101 | CRT  | C4-C5-C6    | -2.64 | 121.20      | 124.91   |
| 16  | 3     | 101 | BCL  | O2A-CGA-CBA | 2.64  | 119.87      | 111.83   |
| 16  | Y     | 101 | BCL  | CHC-C1C-NC  | 2.64  | 128.20      | 124.40   |
| 16  | X     | 102 | BCL  | C4-C3-C5    | 2.64  | 119.80      | 115.23   |
| 16  | A     | 101 | BCL  | CHC-C4B-NB  | -2.63 | 120.10      | 124.05   |
| 16  | 1     | 402 | BCL  | CHC-C4B-NB  | -2.63 | 120.10      | 124.05   |
| 16  | A     | 101 | BCL  | O2D-CGD-O1D | -2.63 | 118.72      | 123.85   |
| 16  | X     | 102 | BCL  | CHC-C1C-NC  | 2.63  | 128.20      | 124.40   |
| 16  | Y     | 101 | BCL  | C4-C3-C5    | 2.63  | 119.80      | 115.23   |
| 21  | V     | 103 | CRT  | C9-C10-C11  | -2.63 | 115.58      | 123.20   |
| 16  | 7     | 102 | BCL  | C4-C3-C5    | 2.63  | 119.80      | 115.23   |
| 16  | X     | 102 | BCL  | C2A-C1A-CHA | -2.63 | 119.30      | 123.87   |
| 15  | L     | 305 | PGV  | O03-C19-C20 | 2.63  | 119.86      | 111.83   |
| 21  | T     | 102 | CRT  | C27-C26-C25 | -2.63 | 115.58      | 123.20   |
| 21  | K     | 101 | CRT  | C14-C15-C16 | -2.63 | 115.58      | 123.20   |
| 21  | G     | 103 | CRT  | C10-C9-C7   | -2.63 | 123.59      | 127.28   |
| 16  | S     | 101 | BCL  | CHC-C1C-NC  | 2.63  | 128.19      | 124.40   |
| 16  | 9     | 101 | BCL  | C4-C3-C5    | 2.63  | 119.79      | 115.23   |
| 20  | M     | 406 | MQ8  | C14-C13-C15 | 2.62  | 119.78      | 115.23   |
| 21  | Q     | 101 | CRT  | C27-C26-C25 | -2.62 | 115.60      | 123.20   |
| 21  | 2     | 103 | CRT  | C5-C6-C7    | -2.62 | 121.93      | 125.89   |
| 16  | B     | 102 | BCL  | CHC-C1C-NC  | 2.62  | 128.18      | 124.40   |
| 16  | N     | 101 | BCL  | C4-C3-C5    | 2.62  | 119.77      | 115.23   |
| 15  | D     | 501 | PGV  | O03-C19-C20 | 2.62  | 119.82      | 111.83   |
| 16  | M     | 404 | BCL  | CMD-C2D-C3D | -2.62 | 121.68      | 127.69   |
| 16  | G     | 102 | BCL  | C2A-C1A-CHA | -2.62 | 119.32      | 123.87   |
| 16  | I     | 101 | BCL  | CHC-C1C-NC  | 2.62  | 128.18      | 124.40   |
| 16  | P     | 102 | BCL  | CHC-C1C-NC  | 2.61  | 128.17      | 124.40   |
| 22  | M     | 412 | CDL  | OB8-CB7-C71 | 2.61  | 119.81      | 111.83   |
| 16  | J     | 101 | BCL  | C2A-C1A-CHA | -2.61 | 119.33      | 123.87   |
| 21  | E     | 103 | CRT  | C21-C20-C19 | -2.61 | 118.18      | 123.52   |
| 16  | 3     | 101 | BCL  | C1D-CHD-C4C | -2.61 | 120.33      | 126.62   |
| 16  | N     | 101 | BCL  | C1C-NC-C4C  | -2.61 | 105.49      | 106.68   |
| 16  | Z     | 102 | BCL  | CHC-C1C-NC  | 2.61  | 128.16      | 124.40   |
| 16  | Q     | 102 | BCL  | CHC-C4B-NB  | -2.61 | 120.14      | 124.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | 7     | 102 | BCL  | CHC-C1C-NC  | 2.61  | 128.16      | 124.40   |
| 21  | B     | 103 | CRT  | C13-C12-C11 | 2.60  | 122.06      | 118.09   |
| 24  | Z     | 101 | LMT  | O1'-C1'-C2' | 2.60  | 112.22      | 108.27   |
| 16  | P     | 102 | BCL  | C1C-NC-C4C  | -2.60 | 105.49      | 106.68   |
| 16  | D     | 503 | BCL  | O2A-CGA-CBA | 2.60  | 119.75      | 111.83   |
| 21  | E     | 103 | CRT  | C26-C27-C28 | -2.60 | 123.64      | 127.28   |
| 10  | C     | 402 | HEM  | CHD-C1D-C2D | -2.59 | 120.93      | 125.03   |
| 16  | M     | 403 | BCL  | C4-C3-C5    | 2.59  | 119.73      | 115.23   |
| 16  | R     | 101 | BCL  | C2A-C1A-CHA | -2.59 | 119.37      | 123.87   |
| 22  | D     | 502 | CDL  | OB8-CB7-C71 | 2.59  | 119.74      | 111.83   |
| 21  | 4     | 102 | CRT  | C5-C6-C7    | -2.59 | 121.98      | 125.89   |
| 16  | R     | 101 | BCL  | CHC-C1C-NC  | 2.59  | 128.14      | 124.40   |
| 21  | Z     | 103 | CRT  | C21-C20-C19 | -2.59 | 118.22      | 123.52   |
| 16  | 7     | 102 | BCL  | CMD-C2D-C3D | -2.59 | 121.76      | 127.69   |
| 16  | T     | 101 | BCL  | C4-C3-C5    | 2.59  | 119.72      | 115.23   |
| 16  | 9     | 101 | BCL  | CHC-C1C-NC  | 2.59  | 128.13      | 124.40   |
| 21  | M     | 407 | CRT  | C9-C10-C11  | -2.58 | 115.71      | 123.20   |
| 16  | W     | 101 | BCL  | CMB-C2B-C3B | 2.58  | 133.82      | 125.67   |
| 16  | M     | 403 | BCL  | C1D-CHD-C4C | -2.58 | 120.39      | 126.62   |
| 21  | T     | 102 | CRT  | C36-C35-C33 | -2.58 | 121.99      | 125.89   |
| 16  | V     | 102 | BCL  | CHC-C1C-NC  | 2.58  | 128.13      | 124.40   |
| 16  | F     | 502 | BCL  | CHC-C4B-NB  | -2.58 | 120.18      | 124.05   |
| 20  | M     | 406 | MQ8  | C45-C43-C44 | 2.58  | 119.70      | 115.23   |
| 16  | 1     | 402 | BCL  | CHC-C1C-NC  | 2.58  | 128.12      | 124.40   |
| 21  | 2     | 103 | CRT  | C26-C27-C28 | -2.58 | 123.66      | 127.28   |
| 21  | K     | 101 | CRT  | C26-C27-C28 | -2.58 | 123.67      | 127.28   |
| 15  | C     | 409 | PGV  | O03-C19-C20 | 2.58  | 119.69      | 111.83   |
| 20  | M     | 406 | MQ8  | C24-C23-C25 | 2.58  | 119.70      | 115.23   |
| 21  | 2     | 103 | CRT  | C14-C15-C16 | -2.57 | 115.75      | 123.20   |
| 21  | X     | 103 | CRT  | C29-C28-C30 | 2.57  | 122.01      | 118.09   |
| 21  | X     | 103 | CRT  | C34-C33-C35 | 2.57  | 122.01      | 118.09   |
| 18  | L     | 304 | UQ8  | C25-C24-C26 | 2.57  | 119.69      | 115.23   |
| 18  | L     | 303 | UQ8  | C17-C18-C19 | -2.57 | 121.75      | 127.62   |
| 21  | T     | 102 | CRT  | C4-C5-C6    | -2.57 | 121.31      | 124.91   |
| 21  | V     | 103 | CRT  | C21-C20-C19 | -2.56 | 118.27      | 123.52   |
| 21  | R     | 102 | CRT  | C18-C17-C16 | 2.56  | 122.00      | 118.09   |
| 22  | M     | 409 | CDL  | CB4-OB6-CB5 | -2.55 | 111.68      | 117.80   |
| 16  | W     | 101 | BCL  | O2A-CGA-CBA | 2.55  | 119.62      | 111.83   |
| 16  | 1     | 402 | BCL  | O2A-CGA-CBA | 2.55  | 119.62      | 111.83   |
| 21  | R     | 102 | CRT  | C27-C26-C25 | -2.55 | 115.80      | 123.20   |
| 16  | O     | 502 | BCL  | C4-C3-C5    | 2.55  | 119.66      | 115.23   |
| 16  | L     | 301 | BCL  | CHB-C4A-NA  | 2.55  | 128.08      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | M     | 408 | PGV  | O03-C19-C20 | 2.55  | 119.60      | 111.83   |
| 18  | L     | 308 | UQ8  | C22-C23-C24 | -2.54 | 121.80      | 127.62   |
| 15  | C     | 409 | PGV  | C02-O01-C1  | -2.54 | 111.71      | 117.80   |
| 16  | Z     | 102 | BCL  | C4-C3-C5    | 2.54  | 119.64      | 115.23   |
| 16  | J     | 101 | BCL  | CHC-C1C-NC  | 2.54  | 128.07      | 124.40   |
| 16  | A     | 101 | BCL  | CMD-C2D-C3D | -2.54 | 121.87      | 127.69   |
| 10  | C     | 402 | HEM  | C3B-C4B-NB  | -2.54 | 107.65      | 109.47   |
| 16  | Y     | 101 | BCL  | CHC-C4B-NB  | -2.54 | 120.24      | 124.05   |
| 16  | 9     | 101 | BCL  | O2D-CGD-O1D | -2.54 | 118.91      | 123.85   |
| 21  | E     | 103 | CRT  | C34-C33-C35 | 2.53  | 121.96      | 118.09   |
| 16  | R     | 101 | BCL  | O2A-CGA-CBA | 2.53  | 119.56      | 111.83   |
| 16  | 4     | 101 | BCL  | C4-C3-C5    | 2.53  | 119.62      | 115.23   |
| 16  | M     | 404 | BCL  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 16  | U     | 101 | BCL  | O2D-CGD-O1D | -2.53 | 118.92      | 123.85   |
| 16  | 8     | 102 | BCL  | C1C-NC-C4C  | -2.53 | 105.53      | 106.68   |
| 16  | W     | 101 | BCL  | CHC-C4B-NB  | -2.53 | 120.26      | 124.05   |
| 16  | Q     | 102 | BCL  | CMB-C2B-C3B | 2.53  | 133.64      | 125.67   |
| 21  | T     | 102 | CRT  | C13-C12-C11 | 2.53  | 121.95      | 118.09   |
| 16  | N     | 101 | BCL  | C2A-C1A-CHA | -2.53 | 119.48      | 123.87   |
| 15  | L     | 306 | PGV  | C02-O01-C1  | -2.52 | 111.75      | 117.80   |
| 16  | G     | 102 | BCL  | CHC-C4B-NB  | -2.52 | 120.26      | 124.05   |
| 21  | R     | 102 | CRT  | C34-C33-C35 | 2.52  | 121.94      | 118.09   |
| 21  | 4     | 102 | CRT  | C27-C26-C25 | -2.52 | 115.89      | 123.20   |
| 24  | 2     | 104 | LMT  | C1B-O1B-C4' | -2.52 | 112.00      | 117.98   |
| 21  | N     | 102 | CRT  | C34-C33-C35 | 2.52  | 121.94      | 118.09   |
| 16  | 5     | 102 | BCL  | CHC-C4B-NB  | -2.52 | 120.27      | 124.05   |
| 16  | A     | 101 | BCL  | O2A-CGA-CBA | 2.52  | 119.52      | 111.83   |
| 16  | L     | 301 | BCL  | CHC-C1C-NC  | 2.52  | 128.03      | 124.40   |
| 21  | 0     | 103 | CRT  | C20-C19-C17 | -2.52 | 123.75      | 127.28   |
| 16  | 0     | 102 | BCL  | CHC-C1C-NC  | 2.52  | 128.03      | 124.40   |
| 16  | M     | 404 | BCL  | C6-C5-C3    | -2.52 | 107.34      | 113.47   |
| 16  | 4     | 101 | BCL  | CHC-C4B-NB  | -2.52 | 120.28      | 124.05   |
| 21  | G     | 103 | CRT  | C9-C10-C11  | -2.51 | 115.91      | 123.20   |
| 16  | B     | 102 | BCL  | CHC-C4B-NB  | -2.51 | 120.28      | 124.05   |
| 16  | O     | 502 | BCL  | O2D-CGD-O1D | -2.51 | 118.96      | 123.85   |
| 21  | T     | 102 | CRT  | C29-C28-C30 | 2.51  | 121.92      | 118.09   |
| 21  | 0     | 103 | CRT  | C13-C12-C11 | 2.51  | 121.92      | 118.09   |
| 16  | V     | 102 | BCL  | C2A-C1A-CHA | -2.51 | 119.52      | 123.87   |
| 21  | M     | 407 | CRT  | C13-C12-C11 | 2.50  | 121.91      | 118.09   |
| 16  | V     | 102 | BCL  | C4-C3-C5    | 2.50  | 119.57      | 115.23   |
| 16  | E     | 102 | BCL  | CHC-C4B-NB  | -2.50 | 120.29      | 124.05   |
| 21  | N     | 102 | CRT  | C27-C26-C25 | -2.50 | 115.95      | 123.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | 3     | 101 | BCL  | C4A-NA-C1A  | 2.50  | 107.82      | 106.68   |
| 18  | L     | 308 | UQ8  | C25-C24-C26 | 2.50  | 119.57      | 115.23   |
| 16  | T     | 101 | BCL  | CHC-C1C-NC  | 2.50  | 128.01      | 124.40   |
| 15  | L     | 305 | PGV  | C02-O01-C1  | -2.50 | 111.81      | 117.80   |
| 16  | 1     | 402 | BCL  | CMB-C2B-C3B | 2.50  | 133.55      | 125.67   |
| 16  | I     | 101 | BCL  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 21  | B     | 103 | CRT  | C34-C33-C35 | 2.50  | 121.90      | 118.09   |
| 16  | 8     | 102 | BCL  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |
| 16  | N     | 101 | BCL  | CHC-C1C-NC  | 2.50  | 128.00      | 124.40   |
| 21  | V     | 103 | CRT  | C18-C17-C16 | 2.50  | 121.90      | 118.09   |
| 16  | J     | 101 | BCL  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |
| 21  | N     | 102 | CRT  | C29-C28-C30 | 2.50  | 121.90      | 118.09   |
| 21  | G     | 103 | CRT  | C26-C27-C28 | -2.49 | 123.78      | 127.28   |
| 21  | Q     | 101 | CRT  | C35-C33-C32 | -2.49 | 115.09      | 119.01   |
| 16  | D     | 503 | BCL  | CHC-C4B-NB  | -2.49 | 120.31      | 124.05   |
| 16  | I     | 101 | BCL  | CMD-C2D-C3D | -2.49 | 121.98      | 127.69   |
| 21  | E     | 103 | CRT  | C29-C28-C30 | 2.49  | 121.89      | 118.09   |
| 16  | A     | 101 | BCL  | CMB-C2B-C3B | 2.49  | 133.52      | 125.67   |
| 16  | B     | 102 | BCL  | C1C-NC-C4C  | -2.49 | 105.55      | 106.68   |
| 16  | N     | 101 | BCL  | CHC-C4B-NB  | -2.48 | 120.32      | 124.05   |
| 16  | 6     | 101 | BCL  | CHC-C1C-NC  | 2.48  | 127.98      | 124.40   |
| 16  | 2     | 102 | BCL  | CHC-C1C-NC  | 2.48  | 127.98      | 124.40   |
| 21  | V     | 103 | CRT  | C13-C12-C11 | 2.48  | 121.88      | 118.09   |
| 16  | M     | 403 | BCL  | O2A-CGA-CBA | 2.48  | 119.40      | 111.83   |
| 16  | M     | 404 | BCL  | CMB-C2B-C3B | 2.48  | 133.49      | 125.67   |
| 21  | 8     | 103 | CRT  | C15-C14-C12 | -2.48 | 123.80      | 127.28   |
| 16  | 5     | 102 | BCL  | CMB-C2B-C3B | 2.48  | 133.49      | 125.67   |
| 16  | 8     | 102 | BCL  | CHC-C1C-NC  | 2.48  | 127.97      | 124.40   |
| 16  | U     | 101 | BCL  | CHC-C4B-NB  | -2.47 | 120.34      | 124.05   |
| 21  | X     | 103 | CRT  | C26-C27-C28 | -2.47 | 123.81      | 127.28   |
| 16  | K     | 102 | BCL  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 16  | E     | 102 | BCL  | CHC-C1C-NC  | 2.47  | 127.96      | 124.40   |
| 24  | 0     | 101 | LMT  | C1B-O1B-C4' | -2.47 | 112.12      | 117.98   |
| 21  | E     | 103 | CRT  | C27-C26-C25 | -2.47 | 116.05      | 123.20   |
| 16  | F     | 502 | BCL  | CMD-C2D-C3D | -2.47 | 122.03      | 127.69   |
| 21  | 2     | 103 | CRT  | C13-C12-C11 | 2.47  | 121.86      | 118.09   |
| 16  | O     | 502 | BCL  | CHC-C4B-NB  | -2.46 | 120.35      | 124.05   |
| 21  | N     | 102 | CRT  | C21-C20-C19 | -2.46 | 118.48      | 123.52   |
| 20  | M     | 406 | MQ8  | C19-C18-C20 | 2.46  | 119.50      | 115.23   |
| 21  | V     | 103 | CRT  | C10-C9-C7   | -2.46 | 123.83      | 127.28   |
| 16  | I     | 101 | BCL  | O2A-CGA-CBA | 2.46  | 119.33      | 111.83   |
| 22  | D     | 502 | CDL  | CB4-OB6-CB5 | -2.46 | 111.91      | 117.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | L     | 303 | UQ8  | C20-C19-C21 | 2.46  | 119.50      | 115.23   |
| 16  | D     | 503 | BCL  | CMB-C2B-C3B | 2.46  | 133.41      | 125.67   |
| 16  | 7     | 102 | BCL  | CHC-C4B-NB  | -2.45 | 120.37      | 124.05   |
| 18  | L     | 304 | UQ8  | C17-C18-C19 | -2.45 | 122.01      | 127.62   |
| 18  | L     | 308 | UQ8  | C37-C38-C39 | -2.45 | 122.01      | 127.62   |
| 16  | S     | 101 | BCL  | CMB-C2B-C3B | 2.45  | 133.40      | 125.67   |
| 16  | Q     | 102 | BCL  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 16  | 5     | 102 | BCL  | CMD-C2D-C3D | -2.45 | 122.07      | 127.69   |
| 16  | R     | 101 | BCL  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 16  | I     | 101 | BCL  | CHC-C4B-NB  | -2.45 | 120.38      | 124.05   |
| 18  | L     | 304 | UQ8  | C20-C19-C21 | 2.45  | 119.47      | 115.23   |
| 16  | F     | 502 | BCL  | CMB-C2B-C3B | 2.45  | 133.38      | 125.67   |
| 16  | S     | 101 | BCL  | CHC-C4B-NB  | -2.44 | 120.38      | 124.05   |
| 21  | G     | 103 | CRT  | C34-C33-C35 | 2.44  | 121.82      | 118.09   |
| 10  | C     | 403 | HEM  | CHD-C4C-NC  | 2.44  | 127.11      | 124.45   |
| 24  | 4     | 103 | LMT  | C1B-O1B-C4' | -2.44 | 112.20      | 117.98   |
| 21  | 0     | 103 | CRT  | C18-C17-C16 | 2.44  | 121.81      | 118.09   |
| 16  | I     | 101 | BCL  | O2D-CGD-O1D | -2.44 | 119.11      | 123.85   |
| 21  | V     | 103 | CRT  | C26-C27-C28 | -2.44 | 123.86      | 127.28   |
| 16  | L     | 301 | BCL  | O2A-CGA-O1A | -2.43 | 117.54      | 123.63   |
| 16  | Q     | 102 | BCL  | O2A-CGA-CBA | 2.43  | 119.25      | 111.83   |
| 16  | 6     | 101 | BCL  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |
| 21  | 0     | 103 | CRT  | C29-C28-C30 | 2.43  | 121.80      | 118.09   |
| 16  | X     | 102 | BCL  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |
| 16  | 1     | 402 | BCL  | O2D-CGD-O1D | -2.42 | 119.13      | 123.85   |
| 16  | 4     | 101 | BCL  | C2A-C1A-CHA | -2.42 | 119.66      | 123.87   |
| 16  | 4     | 101 | BCL  | CHC-C1C-NC  | 2.42  | 127.89      | 124.40   |
| 16  | 3     | 101 | BCL  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 16  | X     | 102 | BCL  | C1D-CHD-C4C | -2.42 | 120.79      | 126.62   |
| 16  | T     | 101 | BCL  | CMB-C2B-C3B | 2.42  | 133.29      | 125.67   |
| 16  | K     | 102 | BCL  | CMB-C2B-C3B | 2.42  | 133.29      | 125.67   |
| 10  | C     | 402 | HEM  | CBA-CAA-C2A | -2.41 | 105.86      | 112.53   |
| 16  | M     | 404 | BCL  | C1C-NC-C4C  | -2.41 | 105.58      | 106.68   |
| 20  | M     | 406 | MQ8  | C39-C38-C40 | 2.41  | 119.41      | 115.23   |
| 16  | G     | 102 | BCL  | CHC-C1C-NC  | 2.41  | 127.87      | 124.40   |
| 21  | N     | 102 | CRT  | C15-C14-C12 | -2.41 | 123.91      | 127.28   |
| 16  | Z     | 102 | BCL  | CMB-C2B-C3B | 2.40  | 133.25      | 125.67   |
| 16  | 2     | 102 | BCL  | O2D-CGD-O1D | -2.40 | 119.17      | 123.85   |
| 16  | 7     | 102 | BCL  | O2D-CGD-O1D | -2.40 | 119.17      | 123.85   |
| 16  | L     | 301 | BCL  | C1D-CHD-C4C | -2.40 | 120.83      | 126.62   |
| 16  | L     | 307 | BCL  | C4-C3-C5    | 2.40  | 119.39      | 115.23   |
| 18  | L     | 308 | UQ8  | C46-C44-C45 | 2.40  | 120.11      | 114.59   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | P     | 102 | BCL  | CHC-C4B-NB  | -2.40 | 120.45      | 124.05   |
| 21  | Z     | 103 | CRT  | C9-C10-C11  | -2.40 | 116.25      | 123.20   |
| 16  | 4     | 101 | BCL  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 21  | 2     | 103 | CRT  | C21-C20-C19 | -2.39 | 118.62      | 123.52   |
| 16  | M     | 404 | BCL  | O2A-CGA-O1A | -2.39 | 117.64      | 123.63   |
| 21  | B     | 103 | CRT  | C18-C17-C16 | 2.39  | 121.74      | 118.09   |
| 18  | L     | 304 | UQ8  | C46-C44-C45 | 2.39  | 120.10      | 114.59   |
| 16  | L     | 307 | BCL  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 21  | V     | 103 | CRT  | C27-C26-C25 | -2.39 | 116.27      | 123.20   |
| 16  | Z     | 102 | BCL  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 10  | C     | 403 | HEM  | CHD-C1D-C2D | -2.39 | 121.25      | 125.03   |
| 16  | 9     | 101 | BCL  | CMB-C2B-C3B | 2.39  | 133.20      | 125.67   |
| 16  | F     | 502 | BCL  | O2A-CGA-CBA | 2.39  | 119.11      | 111.83   |
| 16  | A     | 101 | BCL  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |
| 16  | V     | 102 | BCL  | O2D-CGD-O1D | -2.39 | 119.20      | 123.85   |
| 16  | Y     | 101 | BCL  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |
| 18  | L     | 303 | UQ8  | C25-C24-C26 | 2.38  | 120.08      | 114.59   |
| 10  | C     | 401 | HEM  | CHD-C4C-NC  | 2.38  | 127.05      | 124.45   |
| 16  | 1     | 402 | BCL  | C4-C3-C5    | 2.38  | 119.36      | 115.23   |
| 24  | 5     | 101 | LMT  | O1B-C4'-C3' | 2.38  | 113.28      | 107.23   |
| 16  | F     | 502 | BCL  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 16  | P     | 102 | BCL  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 21  | X     | 103 | CRT  | C15-C14-C12 | -2.38 | 123.94      | 127.28   |
| 21  | 8     | 103 | CRT  | C27-C26-C25 | -2.38 | 116.31      | 123.20   |
| 16  | 9     | 101 | BCL  | C1D-CHD-C4C | -2.38 | 120.89      | 126.62   |
| 21  | V     | 103 | CRT  | C34-C33-C35 | 2.38  | 121.72      | 118.09   |
| 16  | B     | 102 | BCL  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 21  | B     | 103 | CRT  | C10-C9-C7   | -2.37 | 123.95      | 127.28   |
| 24  | 8     | 101 | LMT  | C1B-O1B-C4' | -2.37 | 112.35      | 117.98   |
| 16  | E     | 102 | BCL  | C1D-CHD-C4C | -2.37 | 120.90      | 126.62   |
| 16  | N     | 101 | BCL  | C1D-CHD-C4C | -2.37 | 120.90      | 126.62   |
| 16  | O     | 502 | BCL  | CMB-C2B-C3B | 2.37  | 133.15      | 125.67   |
| 16  | 5     | 102 | BCL  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 16  | 5     | 102 | BCL  | O2A-CGA-CBA | 2.37  | 119.06      | 111.83   |
| 16  | B     | 102 | BCL  | CMB-C2B-C3B | 2.37  | 133.14      | 125.67   |
| 16  | S     | 101 | BCL  | O2A-CGA-CBA | 2.36  | 119.05      | 111.83   |
| 21  | R     | 102 | CRT  | C29-C28-C30 | 2.36  | 121.70      | 118.09   |
| 16  | Z     | 102 | BCL  | C1D-CHD-C4C | -2.36 | 120.92      | 126.62   |
| 16  | 0     | 102 | BCL  | C1D-CHD-C4C | -2.36 | 120.92      | 126.62   |
| 10  | C     | 403 | HEM  | C3B-C4B-NB  | -2.36 | 107.77      | 109.47   |
| 16  | K     | 102 | BCL  | C1C-NC-C4C  | -2.36 | 105.60      | 106.68   |
| 16  | N     | 101 | BCL  | CMB-C2B-C3B | 2.36  | 133.11      | 125.67   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | 6     | 101 | BCL  | C1D-CHD-C4C | -2.36 | 120.93      | 126.62   |
| 16  | L     | 301 | BCL  | CHC-C4B-NB  | -2.36 | 120.51      | 124.05   |
| 21  | E     | 103 | CRT  | C5-C6-C7    | -2.35 | 122.33      | 125.89   |
| 16  | B     | 102 | BCL  | C1D-CHD-C4C | -2.35 | 120.95      | 126.62   |
| 16  | R     | 101 | BCL  | CHC-C4B-NB  | -2.35 | 120.52      | 124.05   |
| 16  | T     | 101 | BCL  | CHC-C4B-NB  | -2.35 | 120.53      | 124.05   |
| 16  | M     | 404 | BCL  | CHC-C1C-NC  | 2.35  | 127.79      | 124.40   |
| 21  | B     | 103 | CRT  | C27-C26-C25 | -2.35 | 116.40      | 123.20   |
| 21  | T     | 102 | CRT  | C26-C27-C28 | -2.35 | 123.99      | 127.28   |
| 16  | 9     | 101 | BCL  | CHB-C4A-NA  | 2.35  | 127.78      | 124.40   |
| 21  | V     | 103 | CRT  | C29-C28-C30 | 2.34  | 121.67      | 118.09   |
| 16  | 9     | 101 | BCL  | CMD-C2D-C3D | -2.34 | 122.32      | 127.69   |
| 16  | J     | 101 | BCL  | C1D-CHD-C4C | -2.34 | 120.98      | 126.62   |
| 16  | R     | 101 | BCL  | CMB-C2B-C3B | 2.34  | 133.04      | 125.67   |
| 16  | T     | 101 | BCL  | C1D-CHD-C4C | -2.34 | 120.98      | 126.62   |
| 21  | 7     | 101 | CRT  | C27-C26-C25 | -2.34 | 116.43      | 123.20   |
| 16  | L     | 307 | BCL  | CMB-C2B-C3B | 2.34  | 133.03      | 125.67   |
| 16  | 7     | 102 | BCL  | CMB-C2B-C3B | 2.33  | 133.03      | 125.67   |
| 16  | M     | 403 | BCL  | CHC-C4B-NB  | -2.33 | 120.55      | 124.05   |
| 21  | R     | 102 | CRT  | C13-C12-C11 | 2.33  | 121.65      | 118.09   |
| 21  | N     | 102 | CRT  | C14-C15-C16 | -2.33 | 116.44      | 123.20   |
| 21  | 8     | 103 | CRT  | C5-C6-C7    | -2.33 | 122.37      | 125.89   |
| 21  | G     | 103 | CRT  | C29-C28-C30 | 2.33  | 121.65      | 118.09   |
| 16  | O     | 502 | BCL  | CMD-C2D-C3D | -2.33 | 122.35      | 127.69   |
| 16  | V     | 102 | BCL  | C1D-CHD-C4C | -2.33 | 121.01      | 126.62   |
| 21  | T     | 102 | CRT  | C18-C17-C16 | 2.33  | 121.64      | 118.09   |
| 16  | 3     | 101 | BCL  | O2D-CGD-O1D | -2.33 | 119.32      | 123.85   |
| 24  | Z     | 101 | LMT  | C1-O1'-C1'  | -2.32 | 109.71      | 113.68   |
| 16  | A     | 101 | BCL  | C2A-C1A-CHA | -2.32 | 119.84      | 123.87   |
| 21  | B     | 103 | CRT  | C26-C27-C28 | -2.32 | 124.02      | 127.28   |
| 15  | M     | 410 | PGV  | C02-O01-C1  | -2.32 | 112.24      | 117.80   |
| 21  | 0     | 103 | CRT  | C34-C33-C35 | 2.32  | 121.63      | 118.09   |
| 16  | 4     | 101 | BCL  | C1D-CHD-C4C | -2.32 | 121.02      | 126.62   |
| 21  | R     | 102 | CRT  | C10-C9-C7   | -2.32 | 124.02      | 127.28   |
| 16  | K     | 102 | BCL  | C2A-C1A-CHA | -2.32 | 119.84      | 123.87   |
| 21  | B     | 103 | CRT  | C29-C28-C30 | 2.32  | 121.63      | 118.09   |
| 16  | T     | 101 | BCL  | O2D-CGD-O1D | -2.32 | 119.34      | 123.85   |
| 16  | 4     | 101 | BCL  | CHB-C1B-NB  | -2.31 | 120.58      | 124.05   |
| 16  | B     | 102 | BCL  | C4D-CHA-C1A | -2.31 | 118.48      | 121.24   |
| 16  | L     | 301 | BCL  | CMB-C2B-C3B | 2.31  | 132.96      | 125.67   |
| 16  | Y     | 101 | BCL  | CMB-C2B-C3B | 2.31  | 132.96      | 125.67   |
| 16  | 3     | 101 | BCL  | CMD-C2D-C3D | -2.31 | 122.39      | 127.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | E     | 103 | CRT  | C10-C9-C7   | -2.31 | 124.04      | 127.28   |
| 16  | G     | 102 | BCL  | C1D-CHD-C4C | -2.31 | 121.06      | 126.62   |
| 16  | S     | 101 | BCL  | C1D-CHD-C4C | -2.31 | 121.06      | 126.62   |
| 16  | E     | 102 | BCL  | CMB-C2B-C3B | 2.31  | 132.94      | 125.67   |
| 16  | 8     | 102 | BCL  | CMB-C2B-C3B | 2.31  | 132.94      | 125.67   |
| 15  | M     | 410 | PGV  | O14-P-O13   | 2.30  | 119.81      | 110.83   |
| 16  | X     | 102 | BCL  | CHC-C4B-NB  | -2.30 | 120.59      | 124.05   |
| 16  | Q     | 102 | BCL  | CMD-C2D-C3D | -2.30 | 122.41      | 127.69   |
| 16  | 8     | 102 | BCL  | C1D-CHD-C4C | -2.30 | 121.06      | 126.62   |
| 21  | 4     | 102 | CRT  | C14-C15-C16 | -2.30 | 116.53      | 123.20   |
| 10  | C     | 401 | HEM  | CHB-C1B-C2B | -2.30 | 120.41      | 126.95   |
| 16  | 5     | 102 | BCL  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 16  | M     | 404 | BCL  | C4-C3-C2    | -2.30 | 117.72      | 123.63   |
| 16  | V     | 102 | BCL  | CHC-C4B-NB  | -2.30 | 120.60      | 124.05   |
| 24  | H     | 303 | LMT  | C1B-O1B-C4' | -2.30 | 112.53      | 117.98   |
| 21  | 8     | 103 | CRT  | C29-C28-C30 | 2.30  | 121.60      | 118.09   |
| 16  | 2     | 102 | BCL  | CMB-C2B-C3B | 2.30  | 132.92      | 125.67   |
| 16  | O     | 502 | BCL  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 16  | 5     | 102 | BCL  | C1D-CHD-C4C | -2.30 | 121.08      | 126.62   |
| 22  | H     | 302 | CDL  | CA4-OA6-CA5 | -2.30 | 112.30      | 117.80   |
| 18  | L     | 304 | UQ8  | C1M-C1-C6   | -2.30 | 120.67      | 124.45   |
| 16  | L     | 301 | BCL  | CMD-C2D-C3D | -2.30 | 122.42      | 127.69   |
| 16  | F     | 502 | BCL  | CHB-C4A-NA  | 2.30  | 127.71      | 124.40   |
| 16  | 7     | 102 | BCL  | CHB-C4A-NA  | 2.30  | 127.71      | 124.40   |
| 16  | 1     | 402 | BCL  | C6-C5-C3    | -2.29 | 107.88      | 113.47   |
| 16  | J     | 101 | BCL  | CHC-C4B-NB  | -2.29 | 120.61      | 124.05   |
| 18  | L     | 308 | UQ8  | C10-C9-C11  | 2.29  | 119.21      | 115.23   |
| 16  | K     | 102 | BCL  | CHB-C4A-NA  | 2.29  | 127.71      | 124.40   |
| 21  | 8     | 103 | CRT  | C34-C33-C35 | 2.29  | 121.59      | 118.09   |
| 16  | Z     | 102 | BCL  | CHC-C4B-NB  | -2.29 | 120.61      | 124.05   |
| 16  | 0     | 102 | BCL  | O2D-CGD-O1D | -2.29 | 119.40      | 123.85   |
| 16  | W     | 101 | BCL  | CMD-C2D-C3D | -2.29 | 122.44      | 127.69   |
| 16  | G     | 102 | BCL  | CMB-C2B-C3B | 2.29  | 132.88      | 125.67   |
| 21  | 7     | 101 | CRT  | C15-C14-C12 | -2.28 | 124.07      | 127.28   |
| 16  | V     | 102 | BCL  | CMB-C2B-C3B | 2.28  | 132.87      | 125.67   |
| 20  | M     | 406 | MQ8  | C50-C48-C49 | 2.28  | 119.84      | 114.59   |
| 16  | G     | 102 | BCL  | O2D-CGD-O1D | -2.28 | 119.41      | 123.85   |
| 16  | M     | 403 | BCL  | CMB-C2B-C3B | 2.27  | 132.84      | 125.67   |
| 16  | U     | 101 | BCL  | CMB-C2B-C3B | 2.27  | 132.84      | 125.67   |
| 21  | 2     | 103 | CRT  | C34-C33-C35 | 2.27  | 121.56      | 118.09   |
| 21  | 0     | 103 | CRT  | C10-C9-C7   | -2.27 | 124.09      | 127.28   |
| 16  | Q     | 102 | BCL  | CHB-C4A-NA  | 2.27  | 127.68      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | N     | 102 | CRT  | C26-C27-C28 | -2.27 | 124.09      | 127.28   |
| 21  | 0     | 103 | CRT  | C26-C27-C28 | -2.27 | 124.09      | 127.28   |
| 16  | I     | 101 | BCL  | CMB-C2B-C3B | 2.27  | 132.83      | 125.67   |
| 21  | K     | 101 | CRT  | C34-C33-C35 | 2.27  | 121.55      | 118.09   |
| 16  | 7     | 102 | BCL  | C1D-CHD-C4C | -2.27 | 121.15      | 126.62   |
| 16  | K     | 102 | BCL  | C1D-CHD-C4C | -2.27 | 121.15      | 126.62   |
| 16  | 6     | 101 | BCL  | C4D-CHA-C1A | -2.27 | 118.54      | 121.24   |
| 16  | Y     | 101 | BCL  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 21  | R     | 102 | CRT  | C26-C27-C28 | -2.27 | 124.10      | 127.28   |
| 21  | M     | 407 | CRT  | C27-C26-C25 | -2.26 | 116.64      | 123.20   |
| 16  | J     | 101 | BCL  | CMB-C2B-C3B | 2.26  | 132.80      | 125.67   |
| 16  | R     | 101 | BCL  | C1D-CHD-C4C | -2.26 | 121.17      | 126.62   |
| 16  | 8     | 102 | BCL  | C4D-CHA-C1A | -2.26 | 118.55      | 121.24   |
| 16  | U     | 101 | BCL  | C2A-C1A-CHA | -2.26 | 119.95      | 123.87   |
| 16  | P     | 102 | BCL  | CMB-C2B-C3B | 2.25  | 132.78      | 125.67   |
| 16  | 2     | 102 | BCL  | C1D-CHD-C4C | -2.25 | 121.18      | 126.62   |
| 10  | C     | 404 | HEM  | C3B-C4B-NB  | -2.25 | 107.85      | 109.47   |
| 16  | K     | 102 | BCL  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 15  | H     | 301 | PGV  | C02-O01-C1  | -2.25 | 112.42      | 117.80   |
| 16  | P     | 102 | BCL  | C1-O2A-CGA  | 2.25  | 122.08      | 116.65   |
| 21  | 2     | 103 | CRT  | C9-C10-C11  | -2.24 | 116.70      | 123.20   |
| 16  | 4     | 101 | BCL  | CMB-C2B-C3B | 2.24  | 132.74      | 125.67   |
| 21  | G     | 103 | CRT  | C21-C20-C19 | -2.24 | 118.93      | 123.52   |
| 21  | T     | 102 | CRT  | C34-C33-C35 | 2.24  | 121.51      | 118.09   |
| 21  | G     | 103 | CRT  | C27-C26-C25 | -2.24 | 116.72      | 123.20   |
| 20  | M     | 406 | MQ8  | C31-C32-C33 | -2.24 | 122.50      | 127.62   |
| 16  | G     | 102 | BCL  | CHB-C1B-NB  | -2.24 | 120.69      | 124.05   |
| 16  | 6     | 101 | BCL  | CHB-C1B-NB  | -2.23 | 120.70      | 124.05   |
| 16  | S     | 101 | BCL  | CHB-C4A-NA  | 2.23  | 127.62      | 124.40   |
| 16  | I     | 101 | BCL  | C2A-C1A-CHA | -2.23 | 120.00      | 123.87   |
| 16  | 6     | 101 | BCL  | CHC-C4B-NB  | -2.23 | 120.70      | 124.05   |
| 16  | 8     | 102 | BCL  | CHC-C4B-NB  | -2.23 | 120.71      | 124.05   |
| 16  | 0     | 102 | BCL  | CHC-C4B-NB  | -2.23 | 120.71      | 124.05   |
| 21  | 4     | 102 | CRT  | C31-C30-C28 | 2.23  | 132.47      | 126.36   |
| 16  | 9     | 101 | BCL  | C1C-NC-C4C  | -2.23 | 105.66      | 106.68   |
| 21  | K     | 101 | CRT  | C18-C17-C16 | 2.23  | 121.49      | 118.09   |
| 16  | Q     | 102 | BCL  | C2A-C1A-CHA | -2.23 | 120.00      | 123.87   |
| 16  | P     | 102 | BCL  | C1D-CHD-C4C | -2.22 | 121.26      | 126.62   |
| 16  | 1     | 402 | BCL  | C1D-CHD-C4C | -2.22 | 121.26      | 126.62   |
| 21  | 7     | 101 | CRT  | C29-C28-C30 | 2.22  | 121.48      | 118.09   |
| 16  | Q     | 102 | BCL  | C1D-CHD-C4C | -2.22 | 121.27      | 126.62   |
| 21  | 2     | 103 | CRT  | C29-C28-C30 | 2.22  | 121.48      | 118.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | T     | 102 | CRT  | C8-C7-C9    | -2.22 | 119.22      | 122.82   |
| 16  | S     | 101 | BCL  | CMD-C2D-C3D | -2.22 | 122.61      | 127.69   |
| 21  | V     | 103 | CRT  | C31-C32-C33 | -2.22 | 124.17      | 127.28   |
| 16  | 2     | 102 | BCL  | CHC-C4B-NB  | -2.22 | 120.72      | 124.05   |
| 16  | L     | 301 | BCL  | C2A-C1A-CHA | -2.22 | 120.02      | 123.87   |
| 16  | Y     | 101 | BCL  | CHB-C4A-NA  | 2.21  | 127.60      | 124.40   |
| 21  | 0     | 103 | CRT  | C5-C6-C7    | -2.21 | 122.55      | 125.89   |
| 21  | 8     | 103 | CRT  | C14-C15-C16 | -2.21 | 116.79      | 123.20   |
| 22  | M     | 412 | CDL  | OA8-CA7-C31 | 2.21  | 118.58      | 111.83   |
| 16  | F     | 502 | BCL  | C1D-CHD-C4C | -2.21 | 121.29      | 126.62   |
| 16  | X     | 102 | BCL  | CMB-C2B-C3B | 2.21  | 132.63      | 125.67   |
| 16  | N     | 101 | BCL  | O2D-CGD-O1D | -2.21 | 119.55      | 123.85   |
| 21  | G     | 103 | CRT  | C18-C17-C16 | 2.20  | 121.45      | 118.09   |
| 16  | M     | 403 | BCL  | C1-O2A-CGA  | 2.20  | 121.98      | 116.65   |
| 16  | Q     | 102 | BCL  | CHB-C1B-C2B | -2.20 | 121.04      | 127.43   |
| 10  | C     | 401 | HEM  | CHA-C4D-C3D | -2.20 | 121.17      | 125.23   |
| 16  | U     | 101 | BCL  | CHB-C4A-NA  | 2.20  | 127.57      | 124.40   |
| 21  | 8     | 103 | CRT  | C26-C27-C28 | -2.20 | 124.20      | 127.28   |
| 16  | 3     | 101 | BCL  | CMB-C2B-C3B | 2.19  | 132.59      | 125.67   |
| 16  | 1     | 402 | BCL  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 21  | 8     | 103 | CRT  | C21-C20-C19 | -2.19 | 119.04      | 123.52   |
| 21  | K     | 101 | CRT  | C1-C4-C5    | 2.19  | 118.67      | 112.98   |
| 22  | M     | 411 | CDL  | OB8-CB7-OB9 | -2.19 | 118.15      | 123.63   |
| 16  | U     | 101 | BCL  | CMD-C2D-C3D | -2.19 | 122.67      | 127.69   |
| 18  | L     | 304 | UQ8  | C30-C29-C31 | 2.19  | 119.03      | 115.23   |
| 16  | 9     | 101 | BCL  | C2A-C1A-CHA | -2.19 | 120.07      | 123.87   |
| 16  | V     | 102 | BCL  | C1-O2A-CGA  | 2.19  | 121.94      | 116.65   |
| 16  | L     | 307 | BCL  | C1D-CHD-C4C | -2.18 | 121.36      | 126.62   |
| 16  | 0     | 102 | BCL  | CMB-C2B-C3B | 2.18  | 132.54      | 125.67   |
| 21  | Z     | 103 | CRT  | C18-C17-C16 | 2.17  | 121.41      | 118.09   |
| 16  | D     | 503 | BCL  | CMD-C2D-C3D | -2.17 | 122.71      | 127.69   |
| 21  | Z     | 103 | CRT  | C27-C26-C25 | -2.17 | 116.91      | 123.20   |
| 16  | G     | 102 | BCL  | C1C-NC-C4C  | -2.17 | 105.69      | 106.68   |
| 21  | X     | 103 | CRT  | C13-C12-C11 | 2.17  | 121.40      | 118.09   |
| 16  | D     | 503 | BCL  | C2A-C1A-CHA | -2.17 | 120.11      | 123.87   |
| 16  | 7     | 102 | BCL  | C2A-C1A-CHA | -2.17 | 120.11      | 123.87   |
| 16  | 1     | 402 | BCL  | C2A-C1A-CHA | -2.17 | 120.11      | 123.87   |
| 21  | X     | 103 | CRT  | C9-C10-C11  | -2.16 | 116.93      | 123.20   |
| 10  | C     | 403 | HEM  | C1A-CHA-C4D | -2.16 | 121.16      | 126.25   |
| 16  | B     | 102 | BCL  | C1-O2A-CGA  | 2.16  | 121.89      | 116.65   |
| 10  | C     | 401 | HEM  | C1A-CHA-C4D | -2.16 | 121.16      | 126.25   |
| 22  | M     | 412 | CDL  | CB4-OB6-CB5 | -2.16 | 112.63      | 117.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | Q     | 102 | BCL  | C1C-NC-C4C  | -2.16 | 105.69      | 106.68   |
| 16  | A     | 101 | BCL  | CHB-C1B-C2B | -2.16 | 121.16      | 127.43   |
| 17  | L     | 302 | BPH  | CMA-C3A-C4A | -2.16 | 109.97      | 114.61   |
| 10  | C     | 401 | HEM  | CBA-CAA-C2A | -2.16 | 106.57      | 112.53   |
| 16  | 2     | 102 | BCL  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 16  | B     | 102 | BCL  | CED-O2D-CGD | 2.15  | 120.80      | 115.92   |
| 15  | H     | 301 | PGV  | O01-C1-O02  | -2.15 | 118.68      | 123.70   |
| 21  | 4     | 102 | CRT  | C9-C10-C11  | -2.15 | 116.97      | 123.20   |
| 16  | X     | 102 | BCL  | CHB-C1B-NB  | -2.15 | 120.83      | 124.05   |
| 16  | F     | 502 | BCL  | C2A-C1A-CHA | -2.15 | 120.14      | 123.87   |
| 16  | P     | 102 | BCL  | CHB-C1B-NB  | -2.14 | 120.83      | 124.05   |
| 16  | 0     | 102 | BCL  | CHB-C1B-NB  | -2.14 | 120.83      | 124.05   |
| 16  | 7     | 102 | BCL  | CHD-C1D-C2D | 2.14  | 129.94      | 125.49   |
| 22  | M     | 411 | CDL  | CB4-OB6-CB5 | -2.14 | 112.68      | 117.80   |
| 16  | S     | 101 | BCL  | CHB-C1B-C2B | -2.14 | 121.22      | 127.43   |
| 16  | Y     | 101 | BCL  | C1D-CHD-C4C | -2.14 | 121.47      | 126.62   |
| 16  | I     | 101 | BCL  | C1D-CHD-C4C | -2.14 | 121.47      | 126.62   |
| 10  | C     | 403 | HEM  | CHA-C4D-C3D | -2.14 | 121.29      | 125.23   |
| 24  | Z     | 101 | LMT  | O5'-C5'-C4' | 2.13  | 114.14      | 109.72   |
| 16  | O     | 502 | BCL  | C1D-CHD-C4C | -2.13 | 121.47      | 126.62   |
| 16  | W     | 101 | BCL  | CHB-C4A-NA  | 2.13  | 127.48      | 124.40   |
| 22  | M     | 411 | CDL  | CB6-CB4-CB3 | -2.13 | 106.81      | 111.78   |
| 16  | O     | 502 | BCL  | C2A-C1A-CHA | -2.13 | 120.17      | 123.87   |
| 16  | W     | 101 | BCL  | C1D-CHD-C4C | -2.13 | 121.49      | 126.62   |
| 16  | 5     | 102 | BCL  | C2A-C1A-CHA | -2.13 | 120.18      | 123.87   |
| 15  | F     | 501 | PGV  | O03-C19-O04 | -2.13 | 118.31      | 123.63   |
| 16  | F     | 502 | BCL  | CHB-C1B-C2B | -2.13 | 121.26      | 127.43   |
| 16  | M     | 403 | BCL  | CHB-C1B-C2B | -2.12 | 121.26      | 127.43   |
| 16  | P     | 102 | BCL  | C4D-CHA-C1A | -2.12 | 118.71      | 121.24   |
| 24  | 2     | 101 | LMT  | C1B-O1B-C4' | -2.12 | 112.95      | 117.98   |
| 16  | L     | 301 | BCL  | C4D-CHA-C1A | -2.12 | 118.72      | 121.24   |
| 15  | M     | 410 | PGV  | O03-C19-O04 | -2.12 | 118.33      | 123.63   |
| 16  | 6     | 101 | BCL  | CMB-C2B-C3B | 2.12  | 132.35      | 125.67   |
| 21  | X     | 103 | CRT  | C18-C17-C16 | 2.12  | 121.32      | 118.09   |
| 16  | 6     | 101 | BCL  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 16  | M     | 403 | BCL  | O1D-CGD-CBD | -2.12 | 120.34      | 124.52   |
| 16  | 4     | 101 | BCL  | C1C-NC-C4C  | -2.12 | 105.71      | 106.68   |
| 21  | E     | 103 | CRT  | C18-C17-C16 | 2.11  | 121.32      | 118.09   |
| 16  | Y     | 101 | BCL  | C2A-C1A-CHA | -2.11 | 120.20      | 123.87   |
| 16  | 1     | 402 | BCL  | CMD-C2D-C3D | -2.11 | 122.84      | 127.69   |
| 16  | 1     | 402 | BCL  | CHB-C1B-C2B | -2.11 | 121.29      | 127.43   |
| 16  | W     | 101 | BCL  | C2A-C1A-CHA | -2.11 | 120.20      | 123.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | R     | 102 | CRT  | C5-C6-C7    | -2.11 | 122.70      | 125.89   |
| 16  | W     | 101 | BCL  | CHB-C1B-C2B | -2.11 | 121.31      | 127.43   |
| 15  | M     | 410 | PGV  | O01-C1-O02  | -2.11 | 118.78      | 123.70   |
| 17  | M     | 405 | BPH  | CMA-C3A-C4A | -2.11 | 110.07      | 114.61   |
| 21  | M     | 407 | CRT  | C30-C28-C27 | -2.11 | 115.70      | 119.01   |
| 16  | E     | 102 | BCL  | O2D-CGD-O1D | -2.10 | 119.75      | 123.85   |
| 18  | L     | 308 | UQ8  | C32-C31-C29 | -2.10 | 106.22      | 113.19   |
| 16  | O     | 502 | BCL  | CHB-C1B-C2B | -2.10 | 121.32      | 127.43   |
| 16  | E     | 102 | BCL  | CHB-C1B-NB  | -2.10 | 120.90      | 124.05   |
| 10  | C     | 401 | HEM  | CBD-CAD-C3D | -2.10 | 106.72      | 112.53   |
| 16  | D     | 503 | BCL  | CHB-C4A-NA  | 2.10  | 127.43      | 124.40   |
| 16  | M     | 404 | BCL  | CGD-CBD-CAD | -2.10 | 104.06      | 110.85   |
| 16  | E     | 102 | BCL  | C4A-NA-C1A  | 2.10  | 107.64      | 106.68   |
| 16  | M     | 403 | BCL  | CHB-C4A-NA  | 2.09  | 127.42      | 124.40   |
| 21  | Q     | 101 | CRT  | C21-C20-C19 | -2.09 | 119.23      | 123.52   |
| 16  | 5     | 102 | BCL  | CHD-C1D-C2D | 2.09  | 129.84      | 125.49   |
| 16  | S     | 101 | BCL  | C2A-C1A-CHA | -2.09 | 120.24      | 123.87   |
| 22  | D     | 502 | CDL  | OB6-CB5-OB7 | -2.09 | 118.82      | 123.70   |
| 10  | C     | 402 | HEM  | CAD-CBD-CGD | -2.09 | 108.13      | 113.67   |
| 16  | 7     | 102 | BCL  | CHB-C1B-C2B | -2.09 | 121.37      | 127.43   |
| 21  | N     | 102 | CRT  | C18-C17-C16 | 2.08  | 121.27      | 118.09   |
| 16  | M     | 403 | BCL  | C2A-C1A-CHA | -2.08 | 120.26      | 123.87   |
| 21  | 2     | 103 | CRT  | C27-C26-C25 | -2.08 | 117.19      | 123.20   |
| 22  | H     | 302 | CDL  | OA8-CA7-OA9 | -2.07 | 118.44      | 123.63   |
| 21  | Q     | 101 | CRT  | C29-C28-C30 | 2.07  | 121.26      | 118.09   |
| 21  | K     | 101 | CRT  | C27-C26-C25 | -2.07 | 117.19      | 123.20   |
| 15  | C     | 409 | PGV  | O01-C1-O02  | -2.07 | 118.86      | 123.70   |
| 16  | K     | 102 | BCL  | C4A-NA-C1A  | 2.07  | 107.62      | 106.68   |
| 16  | N     | 101 | BCL  | C4A-NA-C1A  | 2.07  | 107.62      | 106.68   |
| 21  | E     | 103 | CRT  | C11-C12-C14 | -2.07 | 115.75      | 119.01   |
| 21  | G     | 103 | CRT  | C35-C33-C32 | -2.07 | 115.75      | 119.01   |
| 16  | L     | 307 | BCL  | C1-O2A-CGA  | 2.06  | 121.64      | 116.65   |
| 16  | 3     | 101 | BCL  | C2A-C1A-CHA | -2.06 | 120.29      | 123.87   |
| 16  | 5     | 102 | BCL  | CHB-C1B-C2B | -2.06 | 121.45      | 127.43   |
| 16  | 2     | 102 | BCL  | C4D-CHA-C1A | -2.06 | 118.79      | 121.24   |
| 16  | 0     | 102 | BCL  | O2A-CGA-CBA | 2.06  | 118.11      | 111.83   |
| 16  | R     | 101 | BCL  | CHB-C1B-NB  | -2.06 | 120.96      | 124.05   |
| 21  | Q     | 101 | CRT  | C14-C15-C16 | -2.06 | 117.24      | 123.20   |
| 16  | J     | 101 | BCL  | CHB-C1B-NB  | -2.06 | 120.97      | 124.05   |
| 16  | M     | 404 | BCL  | CHD-C1D-C2D | 2.06  | 129.76      | 125.49   |
| 18  | L     | 303 | UQ8  | C22-C23-C24 | -2.05 | 120.79      | 127.64   |
| 16  | I     | 101 | BCL  | CHD-C1D-C2D | 2.05  | 129.75      | 125.49   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | B     | 102 | BCL  | CHB-C1B-NB  | -2.05 | 120.98      | 124.05   |
| 21  | 4     | 102 | CRT  | C32-C31-C30 | 2.05  | 129.13      | 123.20   |
| 16  | 4     | 101 | BCL  | C4D-CHA-C1A | -2.04 | 118.81      | 121.24   |
| 16  | 9     | 101 | BCL  | CHB-C1B-C2B | -2.04 | 121.50      | 127.43   |
| 21  | 8     | 103 | CRT  | C18-C17-C16 | 2.04  | 121.21      | 118.09   |
| 24  | G     | 104 | LMT  | C1B-O1B-C4' | -2.04 | 113.14      | 117.98   |
| 16  | 8     | 102 | BCL  | CHB-C1B-NB  | -2.04 | 120.99      | 124.05   |
| 16  | L     | 307 | BCL  | CMD-C2D-C3D | -2.04 | 123.02      | 127.69   |
| 18  | L     | 308 | UQ8  | C12-C13-C14 | -2.04 | 122.96      | 127.62   |
| 10  | C     | 404 | HEM  | CHB-C1B-C2B | -2.04 | 121.16      | 126.95   |
| 16  | 6     | 101 | BCL  | C6-C5-C3    | -2.03 | 108.51      | 113.47   |
| 24  | 8     | 101 | LMT  | C1-O1'-C1'  | -2.03 | 110.21      | 113.68   |
| 21  | K     | 101 | CRT  | C29-C28-C30 | 2.03  | 121.19      | 118.09   |
| 16  | Z     | 102 | BCL  | CHB-C1B-C2B | -2.03 | 121.54      | 127.43   |
| 16  | A     | 101 | BCL  | CHD-C1D-C2D | 2.03  | 129.70      | 125.49   |
| 16  | 3     | 101 | BCL  | CHD-C1D-C2D | 2.03  | 129.70      | 125.49   |
| 21  | M     | 407 | CRT  | C18-C17-C16 | 2.02  | 121.18      | 118.09   |
| 16  | R     | 101 | BCL  | C4D-CHA-C1A | -2.02 | 118.83      | 121.24   |
| 16  | D     | 503 | BCL  | CHB-C1B-C2B | -2.02 | 121.56      | 127.43   |
| 10  | C     | 404 | HEM  | CHA-C4D-C3D | -2.02 | 121.50      | 125.23   |
| 10  | C     | 404 | HEM  | C1A-CHA-C4D | -2.02 | 121.49      | 126.25   |
| 10  | C     | 402 | HEM  | C1A-CHA-C4D | -2.02 | 121.50      | 126.25   |
| 15  | L     | 306 | PGV  | O01-C1-O02  | -2.02 | 118.99      | 123.70   |
| 21  | Z     | 103 | CRT  | C29-C28-C30 | 2.02  | 121.17      | 118.09   |
| 16  | Y     | 101 | BCL  | CHB-C1B-C2B | -2.02 | 121.57      | 127.43   |
| 10  | C     | 401 | HEM  | C4D-ND-C1D  | 2.02  | 107.59      | 105.21   |
| 21  | N     | 102 | CRT  | C9-C10-C11  | -2.01 | 117.36      | 123.20   |
| 21  | K     | 101 | CRT  | C9-C10-C11  | -2.01 | 117.37      | 123.20   |
| 16  | J     | 101 | BCL  | C4D-CHA-C1A | -2.01 | 118.84      | 121.24   |
| 16  | 8     | 102 | BCL  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 16  | K     | 102 | BCL  | CHB-C1B-C2B | -2.01 | 121.58      | 127.43   |
| 21  | N     | 102 | CRT  | C35-C33-C32 | -2.01 | 115.84      | 119.01   |
| 16  | 0     | 102 | BCL  | C4D-CHA-C1A | -2.01 | 118.85      | 121.24   |
| 10  | C     | 402 | HEM  | CHA-C1A-NA  | 2.01  | 127.50      | 123.86   |
| 16  | 1     | 402 | BCL  | C1-O2A-CGA  | 2.00  | 121.50      | 116.65   |
| 21  | 4     | 102 | CRT  | C13-C12-C11 | 2.00  | 121.15      | 118.09   |

There are no chirality outliers.

All (924) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | C     | 401 | HEM  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | C     | 402 | HEM  | C2B-C3B-CAB-CBB |
| 10  | C     | 402 | HEM  | C2C-C3C-CAC-CBC |
| 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  | C4B-C3B-CAB-CBB |
| 14  | C     | 408 | PLM  | O2-C1-C2-C3     |
| 15  | C     | 409 | PGV  | C03-O11-P-O12   |
| 15  | C     | 409 | PGV  | C03-O11-P-O13   |
| 15  | C     | 409 | PGV  | C03-O11-P-O14   |
| 15  | L     | 305 | PGV  | C03-O11-P-O12   |
| 15  | L     | 305 | PGV  | C04-O12-P-O11   |
| 15  | L     | 305 | PGV  | C04-O12-P-O13   |
| 15  | L     | 305 | PGV  | O12-C04-C05-C06 |
| 15  | M     | 408 | PGV  | C03-O11-P-O14   |
| 15  | H     | 301 | PGV  | C04-O12-P-O11   |
| 15  | D     | 501 | PGV  | C03-O11-P-O12   |
| 15  | D     | 501 | PGV  | C03-O11-P-O13   |
| 15  | D     | 501 | PGV  | C03-O11-P-O14   |
| 15  | F     | 501 | PGV  | C04-O12-P-O13   |
| 15  | 1     | 401 | PGV  | C03-O11-P-O12   |
| 15  | 1     | 401 | PGV  | C2-C1-O01-C02   |
| 16  | M     | 404 | BCL  | CAD-CBD-CGD-O1D |
| 16  | M     | 404 | BCL  | CAD-CBD-CGD-O2D |
| 16  | A     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 16  | A     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 16  | B     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 16  | B     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 16  | B     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 16  | D     | 503 | BCL  | C2C-C3C-CAC-CBC |
| 16  | D     | 503 | BCL  | C4C-C3C-CAC-CBC |
| 16  | G     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | O     | 502 | BCL  | C2C-C3C-CAC-CBC |
| 16  | O     | 502 | BCL  | C4C-C3C-CAC-CBC |
| 16  | Q     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 16  | Q     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 16  | T     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 16  | T     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 16  | U     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 16  | U     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 16  | U     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 16  | U     | 101 | BCL  | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | V     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 16  | W     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 16  | W     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 16  | W     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 16  | W     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 16  | Y     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 16  | Y     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | Z     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 16  | Z     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 16  | 1     | 402 | BCL  | C1A-C2A-CAA-CBA |
| 16  | 1     | 402 | BCL  | C3A-C2A-CAA-CBA |
| 16  | 2     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 16  | 3     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 16  | 7     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 16  | 7     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 16  | 7     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | 8     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 16  | 9     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 16  | 9     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 16  | 0     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 16  | 0     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 18  | L     | 303 | UQ8  | C14-C16-C17-C18 |
| 21  | M     | 407 | CRT  | C32-C33-C35-C36 |
| 21  | M     | 407 | CRT  | C34-C33-C35-C36 |
| 21  | M     | 407 | CRT  | C35-C36-C37-C38 |
| 21  | M     | 407 | CRT  | C36-C37-C38-C39 |
| 21  | M     | 407 | CRT  | C36-C37-C38-O2  |
| 21  | G     | 103 | CRT  | C36-C37-C38-C39 |
| 21  | G     | 103 | CRT  | C36-C37-C38-C40 |
| 21  | G     | 103 | CRT  | C36-C37-C38-O2  |
| 21  | K     | 101 | CRT  | C1-C4-C5-C6     |
| 21  | N     | 102 | CRT  | C15-C16-C17-C19 |
| 21  | Q     | 101 | CRT  | C2-C1-O1-C1M    |
| 21  | Q     | 101 | CRT  | C10-C11-C12-C14 |
| 21  | T     | 102 | CRT  | O1-C1-C4-C5     |
| 21  | T     | 102 | CRT  | C2-C1-C4-C5     |
| 21  | T     | 102 | CRT  | C3-C1-C4-C5     |
| 21  | T     | 102 | CRT  | C5-C6-C7-C8     |
| 21  | T     | 102 | CRT  | C5-C6-C7-C9     |
| 21  | V     | 103 | CRT  | O1-C1-C4-C5     |
| 21  | V     | 103 | CRT  | C2-C1-C4-C5     |
| 21  | V     | 103 | CRT  | C3-C1-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | V     | 103 | CRT  | C36-C37-C38-C39 |
| 21  | X     | 103 | CRT  | C10-C11-C12-C13 |
| 21  | X     | 103 | CRT  | C10-C11-C12-C14 |
| 21  | Z     | 103 | CRT  | C32-C33-C35-C36 |
| 21  | Z     | 103 | CRT  | C34-C33-C35-C36 |
| 21  | Z     | 103 | CRT  | C36-C37-C38-C39 |
| 21  | Z     | 103 | CRT  | C36-C37-C38-C40 |
| 21  | Z     | 103 | CRT  | C36-C37-C38-O2  |
| 21  | 2     | 103 | CRT  | C36-C37-C38-C40 |
| 21  | 4     | 102 | CRT  | C10-C11-C12-C14 |
| 21  | 4     | 102 | CRT  | C15-C16-C17-C19 |
| 22  | M     | 409 | CDL  | CA2-OA2-PA1-OA3 |
| 22  | M     | 409 | CDL  | CA2-OA2-PA1-OA4 |
| 22  | M     | 409 | CDL  | CA2-OA2-PA1-OA5 |
| 22  | M     | 409 | CDL  | CA3-OA5-PA1-OA2 |
| 22  | M     | 409 | CDL  | CA3-OA5-PA1-OA4 |
| 22  | M     | 409 | CDL  | CB2-OB2-PB2-OB4 |
| 22  | M     | 409 | CDL  | CB2-OB2-PB2-OB5 |
| 22  | M     | 409 | CDL  | OB6-CB4-CB6-OB8 |
| 22  | M     | 411 | CDL  | CA2-OA2-PA1-OA4 |
| 22  | M     | 411 | CDL  | CA2-OA2-PA1-OA5 |
| 22  | M     | 411 | CDL  | CA3-OA5-PA1-OA3 |
| 22  | M     | 411 | CDL  | CB3-OB5-PB2-OB3 |
| 22  | M     | 412 | CDL  | CA3-OA5-PA1-OA2 |
| 22  | M     | 412 | CDL  | CA3-OA5-PA1-OA4 |
| 22  | M     | 412 | CDL  | CB2-OB2-PB2-OB5 |
| 22  | M     | 412 | CDL  | CB3-OB5-PB2-OB2 |
| 22  | M     | 412 | CDL  | CB3-OB5-PB2-OB3 |
| 22  | H     | 302 | CDL  | O1-C1-CB2-OB2   |
| 22  | H     | 302 | CDL  | CA2-C1-CB2-OB2  |
| 22  | H     | 302 | CDL  | CA3-OA5-PA1-OA3 |
| 22  | H     | 302 | CDL  | CB2-OB2-PB2-OB4 |
| 22  | H     | 302 | CDL  | CB2-OB2-PB2-OB5 |
| 22  | D     | 502 | CDL  | CA2-C1-CB2-OB2  |
| 22  | D     | 502 | CDL  | CA2-OA2-PA1-OA4 |
| 22  | D     | 502 | CDL  | CA2-OA2-PA1-OA5 |
| 22  | D     | 502 | CDL  | CA3-OA5-PA1-OA2 |
| 22  | D     | 502 | CDL  | OA5-CA3-CA4-OA6 |
| 22  | D     | 502 | CDL  | C11-CA5-OA6-CA4 |
| 24  | 5     | 101 | LMT  | C3'-C4'-O1B-C1B |
| 16  | G     | 102 | BCL  | CBD-CGD-O2D-CED |
| 16  | T     | 101 | BCL  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | 0     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 15  | 1     | 401 | PGV  | O02-C1-O01-C02  |
| 22  | D     | 502 | CDL  | OA7-CA5-OA6-CA4 |
| 16  | E     | 102 | BCL  | C3-C5-C6-C7     |
| 16  | 4     | 101 | BCL  | C3-C5-C6-C7     |
| 17  | M     | 405 | BPH  | C3-C5-C6-C7     |
| 16  | K     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 16  | T     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 16  | 0     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 16  | I     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | Q     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | R     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | S     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | 3     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | I     | 101 | BCL  | C2-C3-C5-C6     |
| 16  | Q     | 102 | BCL  | C2-C3-C5-C6     |
| 16  | S     | 101 | BCL  | C2-C3-C5-C6     |
| 16  | M     | 404 | BCL  | C3-C5-C6-C7     |
| 16  | G     | 102 | BCL  | C3-C5-C6-C7     |
| 16  | I     | 101 | BCL  | C3-C5-C6-C7     |
| 16  | Y     | 101 | BCL  | C3-C5-C6-C7     |
| 16  | 6     | 101 | BCL  | C3-C5-C6-C7     |
| 16  | 9     | 101 | BCL  | C3-C5-C6-C7     |
| 15  | 1     | 401 | PGV  | C20-C19-O03-C01 |
| 16  | K     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 16  | Z     | 102 | BCL  | C3-C5-C6-C7     |
| 16  | X     | 102 | BCL  | CBD-CGD-O2D-CED |
| 16  | 2     | 102 | BCL  | CBD-CGD-O2D-CED |
| 16  | 0     | 102 | BCL  | CBD-CGD-O2D-CED |
| 22  | H     | 302 | CDL  | O1-C1-CA2-OA2   |
| 22  | D     | 502 | CDL  | O1-C1-CB2-OB2   |
| 16  | N     | 101 | BCL  | CBD-CGD-O2D-CED |
| 15  | D     | 501 | PGV  | C2-C1-O01-C02   |
| 16  | G     | 102 | BCL  | O1D-CGD-O2D-CED |
| 16  | A     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | F     | 502 | BCL  | C4-C3-C5-C6     |
| 16  | 1     | 402 | BCL  | C4-C3-C5-C6     |
| 17  | M     | 405 | BPH  | C4-C3-C5-C6     |
| 16  | F     | 502 | BCL  | C2-C3-C5-C6     |
| 16  | R     | 101 | BCL  | C2-C3-C5-C6     |
| 16  | 3     | 101 | BCL  | C2-C3-C5-C6     |
| 17  | M     | 405 | BPH  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | L     | 304 | UQ8  | C13-C14-C16-C17 |
| 18  | L     | 303 | UQ8  | C19-C21-C22-C23 |
| 18  | L     | 304 | UQ8  | C14-C16-C17-C18 |
| 18  | L     | 308 | UQ8  | C14-C16-C17-C18 |
| 24  | R     | 103 | LMT  | O5'-C1'-O1'-C1  |
| 16  | L     | 307 | BCL  | CBD-CGD-O2D-CED |
| 16  | V     | 102 | BCL  | CBD-CGD-O2D-CED |
| 15  | 1     | 401 | PGV  | O04-C19-O03-C01 |
| 15  | D     | 501 | PGV  | O02-C1-O01-C02  |
| 16  | U     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 16  | W     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 18  | L     | 304 | UQ8  | C15-C14-C16-C17 |
| 16  | 0     | 102 | BCL  | C2-C3-C5-C6     |
| 16  | L     | 307 | BCL  | C11-C10-C8-C9   |
| 16  | B     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | E     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | I     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | J     | 101 | BCL  | C6-C7-C8-C9     |
| 16  | J     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | N     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | P     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | R     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | T     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | V     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | X     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | Z     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | 2     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | 6     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | 9     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | 0     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | L     | 305 | PGV  | O12-C04-C05-O05 |
| 22  | M     | 409 | CDL  | O1-C1-CB2-OB2   |
| 22  | M     | 412 | CDL  | O1-C1-CB2-OB2   |
| 24  | Z     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 21  | K     | 101 | CRT  | C5-C6-C7-C8     |
| 21  | N     | 102 | CRT  | C10-C11-C12-C13 |
| 21  | N     | 102 | CRT  | C15-C16-C17-C18 |
| 21  | Q     | 101 | CRT  | C10-C11-C12-C13 |
| 21  | 4     | 102 | CRT  | C10-C11-C12-C13 |
| 21  | 4     | 102 | CRT  | C15-C16-C17-C18 |
| 21  | 7     | 101 | CRT  | C10-C11-C12-C13 |
| 21  | K     | 101 | CRT  | C5-C6-C7-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | W     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 16  | B     | 102 | BCL  | CBD-CGD-O2D-CED |
| 16  | E     | 102 | BCL  | C13-C15-C16-C17 |
| 16  | F     | 502 | BCL  | C13-C15-C16-C17 |
| 24  | X     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 16  | L     | 301 | BCL  | C15-C16-C17-C18 |
| 16  | Y     | 101 | BCL  | CBD-CGD-O2D-CED |
| 16  | A     | 101 | BCL  | C6-C7-C8-C10    |
| 16  | K     | 102 | BCL  | C6-C7-C8-C10    |
| 16  | 1     | 402 | BCL  | C11-C10-C8-C7   |
| 16  | 8     | 102 | BCL  | C12-C13-C15-C16 |
| 22  | M     | 412 | CDL  | C71-CB7-OB8-CB6 |
| 16  | 0     | 102 | BCL  | C4-C3-C5-C6     |
| 18  | L     | 308 | UQ8  | C19-C21-C22-C23 |
| 16  | D     | 503 | BCL  | C3-C5-C6-C7     |
| 16  | Z     | 102 | BCL  | C15-C16-C17-C18 |
| 16  | 1     | 402 | BCL  | C13-C15-C16-C17 |
| 15  | L     | 306 | PGV  | C1-C2-C3-C4     |
| 16  | O     | 502 | BCL  | C8-C10-C11-C12  |
| 16  | P     | 102 | BCL  | C13-C15-C16-C17 |
| 16  | T     | 101 | BCL  | C5-C6-C7-C8     |
| 16  | U     | 101 | BCL  | C10-C11-C12-C13 |
| 16  | 9     | 101 | BCL  | C5-C6-C7-C8     |
| 16  | E     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 16  | N     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 16  | 6     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 16  | J     | 101 | BCL  | C5-C6-C7-C8     |
| 16  | Y     | 101 | BCL  | C5-C6-C7-C8     |
| 16  | Z     | 102 | BCL  | C8-C10-C11-C12  |
| 16  | Z     | 102 | BCL  | C10-C11-C12-C13 |
| 22  | H     | 302 | CDL  | CA5-C11-C12-C13 |
| 16  | E     | 102 | BCL  | C10-C11-C12-C13 |
| 16  | N     | 101 | BCL  | C5-C6-C7-C8     |
| 16  | P     | 102 | BCL  | C8-C10-C11-C12  |
| 16  | 6     | 101 | BCL  | C10-C11-C12-C13 |
| 16  | U     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 22  | D     | 502 | CDL  | CA5-C11-C12-C13 |
| 16  | X     | 102 | BCL  | O1D-CGD-O2D-CED |
| 16  | 2     | 102 | BCL  | O1D-CGD-O2D-CED |
| 16  | 1     | 402 | BCL  | C3-C5-C6-C7     |
| 24  | 4     | 103 | LMT  | C5'-C4'-O1B-C1B |
| 16  | V     | 102 | BCL  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | J     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 16  | 7     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 16  | P     | 102 | BCL  | CBD-CGD-O2D-CED |
| 16  | 0     | 102 | BCL  | O1D-CGD-O2D-CED |
| 16  | Q     | 102 | BCL  | C3-C5-C6-C7     |
| 16  | G     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 16  | Z     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 16  | O     | 502 | BCL  | CBA-CGA-O2A-C1  |
| 16  | I     | 101 | BCL  | C13-C15-C16-C17 |
| 16  | 1     | 402 | BCL  | C15-C16-C17-C18 |
| 16  | 8     | 102 | BCL  | C5-C6-C7-C8     |
| 16  | I     | 101 | BCL  | C5-C6-C7-C8     |
| 16  | P     | 102 | BCL  | C15-C16-C17-C18 |
| 16  | 2     | 102 | BCL  | C15-C16-C17-C18 |
| 17  | L     | 302 | BPH  | C15-C16-C17-C18 |
| 16  | N     | 101 | BCL  | O1D-CGD-O2D-CED |
| 16  | G     | 102 | BCL  | C5-C6-C7-C8     |
| 16  | 2     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | A     | 101 | BCL  | C2-C3-C5-C6     |
| 16  | 1     | 402 | BCL  | C2-C3-C5-C6     |
| 15  | H     | 301 | PGV  | C2-C1-O01-C02   |
| 15  | H     | 301 | PGV  | O02-C1-O01-C02  |
| 24  | 4     | 103 | LMT  | C3'-C4'-O1B-C1B |
| 16  | M     | 404 | BCL  | CBA-CGA-O2A-C1  |
| 16  | E     | 102 | BCL  | C15-C16-C17-C18 |
| 21  | M     | 407 | CRT  | C5-C6-C7-C8     |
| 21  | X     | 103 | CRT  | C15-C16-C17-C18 |
| 21  | 7     | 101 | CRT  | C15-C16-C17-C18 |
| 21  | 7     | 101 | CRT  | C10-C11-C12-C14 |
| 16  | J     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 15  | H     | 301 | PGV  | C04-C05-C06-O06 |
| 15  | D     | 501 | PGV  | C04-C05-C06-O06 |
| 22  | M     | 412 | CDL  | OB9-CB7-OB8-CB6 |
| 16  | R     | 101 | BCL  | C3-C5-C6-C7     |
| 16  | 2     | 102 | BCL  | C5-C6-C7-C8     |
| 16  | 9     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 16  | G     | 102 | BCL  | C15-C16-C17-C18 |
| 16  | 3     | 101 | BCL  | C5-C6-C7-C8     |
| 16  | N     | 101 | BCL  | C16-C17-C18-C19 |
| 16  | 7     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 13  | C     | 407 | Z41  | C11-C10-C9-C8   |
| 22  | M     | 411 | CDL  | C42-C43-C44-C45 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | M     | 413 | LDA  | C4-C5-C6-C7     |
| 24  | 2     | 104 | LMT  | C6-C7-C8-C9     |
| 16  | V     | 102 | BCL  | O1D-CGD-O2D-CED |
| 16  | E     | 102 | BCL  | C5-C6-C7-C8     |
| 22  | H     | 302 | CDL  | C59-C60-C61-C62 |
| 15  | D     | 501 | PGV  | O05-C05-C06-O06 |
| 16  | 2     | 102 | BCL  | C13-C15-C16-C17 |
| 16  | E     | 102 | BCL  | C6-C7-C8-C10    |
| 16  | S     | 101 | BCL  | C6-C7-C8-C10    |
| 16  | U     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | X     | 102 | BCL  | C6-C7-C8-C10    |
| 24  | Z     | 101 | LMT  | C6-C7-C8-C9     |
| 16  | O     | 502 | BCL  | O1A-CGA-O2A-C1  |
| 16  | B     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 16  | J     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 16  | O     | 502 | BCL  | C3A-C2A-CAA-CBA |
| 16  | V     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 16  | 2     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 16  | 3     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 16  | 8     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 24  | M     | 414 | LMT  | O5'-C5'-C6'-O6' |
| 24  | X     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 13  | C     | 407 | Z41  | C10-C11-C12-C13 |
| 22  | H     | 302 | CDL  | C12-C13-C14-C15 |
| 24  | 2     | 104 | LMT  | C5-C6-C7-C8     |
| 24  | Z     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 16  | L     | 307 | BCL  | O1D-CGD-O2D-CED |
| 16  | N     | 101 | BCL  | C16-C17-C18-C20 |
| 24  | P     | 101 | LMT  | C2-C3-C4-C5     |
| 24  | V     | 101 | LMT  | O1'-C1-C2-C3    |
| 16  | 2     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 16  | M     | 404 | BCL  | O1A-CGA-O2A-C1  |
| 16  | 9     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 16  | U     | 101 | BCL  | C5-C6-C7-C8     |
| 16  | X     | 102 | BCL  | C10-C11-C12-C13 |
| 16  | 2     | 102 | BCL  | C2-C3-C5-C6     |
| 24  | 0     | 101 | LMT  | C3'-C4'-O1B-C1B |
| 22  | M     | 412 | CDL  | C51-CB5-OB6-CB4 |
| 16  | Z     | 102 | BCL  | C13-C15-C16-C17 |
| 21  | K     | 101 | CRT  | C10-C11-C12-C13 |
| 21  | Q     | 101 | CRT  | C15-C16-C17-C18 |
| 21  | 0     | 103 | CRT  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | M     | 407 | CRT  | C1-C4-C5-C6     |
| 16  | 3     | 101 | BCL  | C3-C5-C6-C7     |
| 15  | H     | 301 | PGV  | C3-C4-C5-C6     |
| 22  | M     | 412 | CDL  | C41-C42-C43-C44 |
| 24  | H     | 303 | LMT  | C6-C7-C8-C9     |
| 16  | M     | 404 | BCL  | C4-C3-C5-C6     |
| 16  | B     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | U     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | W     | 101 | BCL  | C4-C3-C5-C6     |
| 18  | L     | 304 | UQ8  | C30-C29-C31-C32 |
| 16  | W     | 101 | BCL  | C2-C3-C5-C6     |
| 16  | B     | 102 | BCL  | C5-C6-C7-C8     |
| 16  | Z     | 102 | BCL  | C5-C6-C7-C8     |
| 22  | M     | 411 | CDL  | C55-C56-C57-C58 |
| 15  | M     | 408 | PGV  | O01-C02-C03-O11 |
| 24  | G     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 20  | M     | 406 | MQ8  | C28-C30-C31-C32 |
| 16  | 0     | 102 | BCL  | C8-C10-C11-C12  |
| 10  | C     | 401 | HEM  | C4B-C3B-CAB-CBB |
| 10  | C     | 402 | HEM  | C4B-C3B-CAB-CBB |
| 10  | C     | 402 | HEM  | C4C-C3C-CAC-CBC |
| 24  | E     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 15  | M     | 410 | PGV  | C21-C22-C23-C24 |
| 15  | H     | 301 | PGV  | C1-C2-C3-C4     |
| 24  | B     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 22  | M     | 412 | CDL  | OB6-CB4-CB6-OB8 |
| 15  | M     | 410 | PGV  | C20-C19-O03-C01 |
| 16  | 1     | 402 | BCL  | CBA-CGA-O2A-C1  |
| 24  | V     | 101 | LMT  | C6-C7-C8-C9     |
| 24  | V     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 24  | 0     | 101 | LMT  | C5'-C4'-O1B-C1B |
| 16  | J     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 16  | K     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 16  | Y     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 16  | 8     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 16  | 0     | 102 | BCL  | C5-C6-C7-C8     |
| 24  | V     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 15  | D     | 501 | PGV  | C22-C23-C24-C25 |
| 16  | B     | 102 | BCL  | O1D-CGD-O2D-CED |
| 16  | U     | 101 | BCL  | C3-C5-C6-C7     |
| 16  | 8     | 102 | BCL  | C3-C5-C6-C7     |
| 16  | J     | 101 | BCL  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | O     | 502 | BCL  | C1A-C2A-CAA-CBA |
| 16  | T     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 16  | V     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 16  | Y     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 24  | R     | 103 | LMT  | O5'-C5'-C6'-O6' |
| 22  | H     | 302 | CDL  | OA5-CA3-CA4-CA6 |
| 22  | D     | 502 | CDL  | OA5-CA3-CA4-CA6 |
| 24  | P     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 22  | M     | 412 | CDL  | C58-C59-C60-C61 |
| 16  | S     | 101 | BCL  | C3-C5-C6-C7     |
| 16  | A     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | E     | 102 | BCL  | C11-C10-C8-C7   |
| 16  | V     | 102 | BCL  | C6-C7-C8-C10    |
| 16  | Z     | 102 | BCL  | C6-C7-C8-C10    |
| 16  | 0     | 102 | BCL  | C11-C10-C8-C7   |
| 24  | R     | 103 | LMT  | C2-C3-C4-C5     |
| 16  | 1     | 402 | BCL  | C8-C10-C11-C12  |
| 16  | T     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 16  | V     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 16  | X     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 16  | 3     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 16  | 7     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 21  | K     | 101 | CRT  | C2-C1-C4-C5     |
| 21  | K     | 101 | CRT  | C3-C1-C4-C5     |
| 21  | N     | 102 | CRT  | C36-C37-C38-C39 |
| 21  | Q     | 101 | CRT  | C2-C1-C4-C5     |
| 21  | V     | 103 | CRT  | C36-C37-C38-C40 |
| 21  | Z     | 103 | CRT  | C2-C1-C4-C5     |
| 21  | 2     | 103 | CRT  | C36-C37-C38-C39 |
| 16  | D     | 503 | BCL  | C15-C16-C17-C18 |
| 16  | O     | 502 | BCL  | C4-C3-C5-C6     |
| 18  | L     | 304 | UQ8  | C12-C11-C9-C10  |
| 16  | U     | 101 | BCL  | C2-C3-C5-C6     |
| 18  | L     | 304 | UQ8  | C28-C29-C31-C32 |
| 18  | L     | 304 | UQ8  | C12-C11-C9-C8   |
| 24  | 2     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 16  | A     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | K     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | K     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | N     | 101 | BCL  | C6-C7-C8-C9     |
| 16  | Z     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | 9     | 101 | BCL  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | X     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 22  | M     | 412 | CDL  | C31-CA7-OA8-CA6 |
| 24  | G     | 101 | LMT  | C3'-C4'-O1B-C1B |
| 16  | M     | 404 | BCL  | CBD-CGD-O2D-CED |
| 22  | D     | 502 | CDL  | C56-C57-C58-C59 |
| 15  | D     | 501 | PGV  | O03-C01-C02-C03 |
| 15  | H     | 301 | PGV  | C4-C5-C6-C7     |
| 22  | M     | 412 | CDL  | C57-C58-C59-C60 |
| 24  | V     | 101 | LMT  | C5-C6-C7-C8     |
| 22  | H     | 302 | CDL  | C54-C55-C56-C57 |
| 16  | J     | 101 | BCL  | C8-C10-C11-C12  |
| 16  | K     | 102 | BCL  | C15-C16-C17-C18 |
| 16  | Y     | 101 | BCL  | O1D-CGD-O2D-CED |
| 16  | L     | 307 | BCL  | CBA-CGA-O2A-C1  |
| 16  | F     | 502 | BCL  | C16-C17-C18-C19 |
| 16  | T     | 101 | BCL  | C16-C17-C18-C19 |
| 16  | 1     | 402 | BCL  | O1A-CGA-O2A-C1  |
| 24  | P     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 16  | O     | 502 | BCL  | C2-C3-C5-C6     |
| 15  | M     | 410 | PGV  | C22-C23-C24-C25 |
| 24  | R     | 103 | LMT  | O5B-C5B-C6B-O6B |
| 24  | 0     | 101 | LMT  | O5B-C5B-C6B-O6B |
| 16  | 4     | 101 | BCL  | C15-C16-C17-C18 |
| 24  | 2     | 104 | LMT  | O5'-C5'-C6'-O6' |
| 22  | M     | 411 | CDL  | CA5-C11-C12-C13 |
| 22  | M     | 412 | CDL  | OA9-CA7-OA8-CA6 |
| 16  | 0     | 102 | BCL  | C15-C16-C17-C18 |
| 16  | P     | 102 | BCL  | O1D-CGD-O2D-CED |
| 24  | G     | 101 | LMT  | C5'-C4'-O1B-C1B |
| 22  | M     | 412 | CDL  | C71-C72-C73-C74 |
| 24  | V     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 15  | D     | 501 | PGV  | C24-C25-C26-C27 |
| 18  | L     | 304 | UQ8  | C40-C39-C41-C42 |
| 16  | M     | 404 | BCL  | C2-C3-C5-C6     |
| 16  | 9     | 101 | BCL  | C2-C3-C5-C6     |
| 13  | C     | 407 | Z41  | C25-C26-C27-C28 |
| 22  | M     | 411 | CDL  | C16-C17-C18-C19 |
| 15  | L     | 305 | PGV  | O03-C01-C02-O01 |
| 24  | 0     | 101 | LMT  | C4-C5-C6-C7     |
| 20  | M     | 406 | MQ8  | C38-C40-C41-C42 |
| 22  | M     | 412 | CDL  | C53-C54-C55-C56 |
| 16  | P     | 102 | BCL  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | G     | 103 | CRT  | C39-C38-O2-C2M  |
| 21  | G     | 103 | CRT  | C40-C38-O2-C2M  |
| 21  | K     | 101 | CRT  | C3-C1-O1-C1M    |
| 21  | Q     | 101 | CRT  | C3-C1-O1-C1M    |
| 16  | T     | 101 | BCL  | CBD-CGD-O2D-CED |
| 15  | M     | 410 | PGV  | O04-C19-O03-C01 |
| 16  | 7     | 102 | BCL  | C5-C6-C7-C8     |
| 16  | 1     | 402 | BCL  | C16-C17-C18-C19 |
| 16  | 2     | 102 | BCL  | C16-C17-C18-C19 |
| 16  | N     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | 4     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | 9     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | 6     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 16  | W     | 101 | BCL  | C13-C15-C16-C17 |
| 22  | M     | 412 | CDL  | OB7-CB5-OB6-CB4 |
| 15  | H     | 301 | PGV  | O05-C05-C06-O06 |
| 16  | E     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | F     | 502 | BCL  | C11-C10-C8-C9   |
| 16  | T     | 101 | BCL  | C14-C13-C15-C16 |
| 16  | W     | 101 | BCL  | C15-C16-C17-C18 |
| 16  | 8     | 102 | BCL  | C13-C15-C16-C17 |
| 10  | C     | 402 | HEM  | C3D-CAD-CBD-CGD |
| 24  | 5     | 101 | LMT  | C2'-C1'-O1'-C1  |
| 15  | M     | 408 | PGV  | C01-C02-C03-O11 |
| 22  | M     | 411 | CDL  | OA5-CA3-CA4-CA6 |
| 16  | L     | 307 | BCL  | C11-C10-C8-C7   |
| 16  | B     | 102 | BCL  | C11-C10-C8-C7   |
| 16  | D     | 503 | BCL  | C6-C7-C8-C10    |
| 16  | F     | 502 | BCL  | C11-C10-C8-C7   |
| 16  | G     | 102 | BCL  | C6-C7-C8-C10    |
| 16  | J     | 101 | BCL  | C6-C7-C8-C10    |
| 16  | K     | 102 | BCL  | C11-C10-C8-C7   |
| 16  | N     | 101 | BCL  | C6-C7-C8-C10    |
| 16  | N     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | Q     | 102 | BCL  | C12-C13-C15-C16 |
| 16  | S     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | T     | 101 | BCL  | C12-C13-C15-C16 |
| 16  | U     | 101 | BCL  | C6-C7-C8-C10    |
| 16  | W     | 101 | BCL  | C6-C7-C8-C10    |
| 16  | Z     | 102 | BCL  | C11-C10-C8-C7   |
| 16  | 7     | 102 | BCL  | C6-C7-C8-C10    |
| 16  | 9     | 101 | BCL  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | M     | 412 | CDL  | O1-C1-CA2-OA2   |
| 16  | Y     | 101 | BCL  | C8-C10-C11-C12  |
| 24  | V     | 101 | LMT  | O5B-C1B-O1B-C4' |
| 16  | L     | 307 | BCL  | O1A-CGA-O2A-C1  |
| 16  | G     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | V     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | 7     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | F     | 502 | BCL  | C15-C16-C17-C18 |
| 16  | B     | 102 | BCL  | C2-C3-C5-C6     |
| 16  | N     | 101 | BCL  | C2-C3-C5-C6     |
| 22  | M     | 412 | CDL  | C72-C73-C74-C75 |
| 21  | R     | 102 | CRT  | C15-C16-C17-C18 |
| 15  | M     | 410 | PGV  | C19-C20-C21-C22 |
| 16  | B     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 18  | L     | 308 | UQ8  | C39-C41-C42-C43 |
| 16  | F     | 502 | BCL  | C16-C17-C18-C20 |
| 16  | T     | 101 | BCL  | C16-C17-C18-C20 |
| 22  | M     | 409 | CDL  | CB3-CB4-CB6-OB8 |
| 16  | E     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | V     | 102 | BCL  | C2-C3-C5-C6     |
| 13  | C     | 407 | Z41  | O2-C17-C18-O3   |
| 22  | M     | 411 | CDL  | OA5-CA3-CA4-OA6 |
| 15  | L     | 309 | PGV  | C19-C20-C21-C22 |
| 22  | M     | 411 | CDL  | CB7-C71-C72-C73 |
| 22  | H     | 302 | CDL  | C17-C18-C19-C20 |
| 16  | W     | 101 | BCL  | C5-C6-C7-C8     |
| 15  | D     | 501 | PGV  | O03-C01-C02-O01 |
| 22  | D     | 502 | CDL  | OB6-CB4-CB6-OB8 |
| 24  | M     | 414 | LMT  | C5'-C4'-O1B-C1B |
| 24  | M     | 414 | LMT  | C3'-C4'-O1B-C1B |
| 24  | R     | 103 | LMT  | O1'-C1-C2-C3    |
| 16  | G     | 102 | BCL  | C2-C3-C5-C6     |
| 22  | M     | 412 | CDL  | C56-C57-C58-C59 |
| 24  | M     | 414 | LMT  | C4B-C5B-C6B-O6B |
| 16  | Q     | 102 | BCL  | C14-C13-C15-C16 |
| 16  | W     | 101 | BCL  | C6-C7-C8-C9     |
| 24  | 5     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 24  | 0     | 101 | LMT  | C11-C10-C9-C8   |
| 16  | A     | 101 | BCL  | C16-C17-C18-C19 |
| 24  | Z     | 101 | LMT  | C1-C2-C3-C4     |
| 16  | M     | 403 | BCL  | C4C-C3C-CAC-CBC |
| 16  | X     | 102 | BCL  | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | 4     | 101 | BCL  | C2-C3-C5-C6     |
| 16  | 1     | 402 | BCL  | C16-C17-C18-C20 |
| 16  | 2     | 102 | BCL  | C16-C17-C18-C20 |
| 22  | H     | 302 | CDL  | CB2-C1-CA2-OA2  |
| 22  | M     | 409 | CDL  | OB5-CB3-CB4-CB6 |
| 22  | D     | 502 | CDL  | OB5-CB3-CB4-CB6 |
| 16  | 3     | 101 | BCL  | C10-C11-C12-C13 |
| 16  | I     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | P     | 102 | BCL  | C6-C7-C8-C10    |
| 16  | P     | 102 | BCL  | C11-C10-C8-C7   |
| 16  | R     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | T     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | W     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | X     | 102 | BCL  | C11-C12-C13-C15 |
| 16  | 1     | 402 | BCL  | C6-C7-C8-C10    |
| 16  | 2     | 102 | BCL  | C11-C10-C8-C7   |
| 16  | 6     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | 9     | 101 | BCL  | C11-C10-C8-C7   |
| 21  | 7     | 101 | CRT  | C1-C4-C5-C6     |
| 21  | M     | 407 | CRT  | C5-C6-C7-C9     |
| 21  | N     | 102 | CRT  | C10-C11-C12-C14 |
| 21  | 7     | 101 | CRT  | C15-C16-C17-C19 |
| 16  | P     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 15  | D     | 501 | PGV  | C31-C32-C33-C34 |
| 16  | W     | 101 | BCL  | C16-C17-C18-C19 |
| 16  | Y     | 101 | BCL  | C4-C3-C5-C6     |
| 10  | C     | 401 | HEM  | C2C-C3C-CAC-CBC |
| 10  | C     | 403 | HEM  | C2C-C3C-CAC-CBC |
| 10  | C     | 404 | HEM  | C2C-C3C-CAC-CBC |
| 16  | E     | 102 | BCL  | C2-C3-C5-C6     |
| 16  | 7     | 102 | BCL  | C2-C3-C5-C6     |
| 16  | 6     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 13  | C     | 407 | Z41  | C12-C13-C14-C15 |
| 18  | L     | 308 | UQ8  | C5-C4-O4-C4M    |
| 16  | B     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 16  | T     | 101 | BCL  | C3-C5-C6-C7     |
| 22  | M     | 411 | CDL  | C54-C55-C56-C57 |
| 16  | T     | 101 | BCL  | O1D-CGD-O2D-CED |
| 22  | M     | 409 | CDL  | OB5-CB3-CB4-OB6 |
| 16  | 5     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | Y     | 101 | BCL  | C10-C11-C12-C13 |
| 22  | H     | 302 | CDL  | OB6-CB4-CB6-OB8 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | M     | 403 | BCL  | C11-C10-C8-C9   |
| 16  | D     | 503 | BCL  | C11-C10-C8-C9   |
| 16  | S     | 101 | BCL  | C11-C10-C8-C9   |
| 24  | 5     | 101 | LMT  | C4-C5-C6-C7     |
| 15  | L     | 306 | PGV  | C21-C22-C23-C24 |
| 16  | L     | 307 | BCL  | C5-C6-C7-C8     |
| 16  | A     | 101 | BCL  | C13-C15-C16-C17 |
| 16  | G     | 102 | BCL  | C13-C15-C16-C17 |
| 22  | M     | 412 | CDL  | C38-C39-C40-C41 |
| 16  | 0     | 102 | BCL  | C16-C17-C18-C19 |
| 16  | P     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 16  | N     | 101 | BCL  | C15-C16-C17-C18 |
| 24  | V     | 101 | LMT  | C2B-C1B-O1B-C4' |
| 24  | 8     | 101 | LMT  | C1-C2-C3-C4     |
| 22  | H     | 302 | CDL  | C71-CB7-OB8-CB6 |
| 16  | Z     | 102 | BCL  | C4-C3-C5-C6     |
| 16  | 8     | 102 | BCL  | C4-C3-C5-C6     |
| 21  | Q     | 101 | CRT  | C15-C16-C17-C19 |
| 21  | R     | 102 | CRT  | C15-C16-C17-C19 |
| 21  | X     | 103 | CRT  | C15-C16-C17-C19 |
| 23  | M     | 413 | LDA  | C5-C6-C7-C8     |
| 15  | L     | 306 | PGV  | C01-C02-C03-O11 |
| 16  | M     | 403 | BCL  | C6-C7-C8-C10    |
| 16  | F     | 502 | BCL  | C6-C7-C8-C10    |
| 16  | G     | 102 | BCL  | C11-C10-C8-C7   |
| 16  | W     | 101 | BCL  | C12-C13-C15-C16 |
| 16  | Y     | 101 | BCL  | C6-C7-C8-C10    |
| 16  | 6     | 101 | BCL  | C6-C7-C8-C10    |
| 16  | 8     | 102 | BCL  | C11-C12-C13-C15 |
| 16  | 9     | 101 | BCL  | C11-C12-C13-C15 |
| 16  | R     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 21  | Z     | 103 | CRT  | C3-C1-C4-C5     |
| 16  | V     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 16  | 5     | 102 | BCL  | C10-C11-C12-C13 |
| 24  | G     | 104 | LMT  | C4-C5-C6-C7     |
| 15  | L     | 306 | PGV  | O01-C02-C03-O11 |
| 15  | L     | 309 | PGV  | O01-C02-C03-O11 |
| 22  | M     | 412 | CDL  | OB5-CB3-CB4-OB6 |
| 22  | D     | 502 | CDL  | OB5-CB3-CB4-OB6 |
| 16  | U     | 101 | BCL  | C6-C7-C8-C9     |
| 16  | W     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | 1     | 402 | BCL  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | V     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 22  | M     | 409 | CDL  | OA6-CA4-CA6-OA8 |
| 24  | M     | 414 | LMT  | O5B-C5B-C6B-O6B |
| 16  | A     | 101 | BCL  | C16-C17-C18-C20 |
| 15  | L     | 305 | PGV  | O03-C01-C02-C03 |
| 22  | M     | 412 | CDL  | CB3-CB4-CB6-OB8 |
| 16  | 5     | 102 | BCL  | C2-C3-C5-C6     |
| 22  | H     | 302 | CDL  | OB9-CB7-OB8-CB6 |
| 15  | L     | 309 | PGV  | C20-C19-O03-C01 |
| 15  | C     | 409 | PGV  | C04-O12-P-O13   |
| 15  | L     | 305 | PGV  | C03-O11-P-O13   |
| 15  | M     | 408 | PGV  | C03-O11-P-O12   |
| 15  | H     | 301 | PGV  | C04-O12-P-O13   |
| 15  | 1     | 401 | PGV  | C03-O11-P-O13   |
| 21  | 8     | 103 | CRT  | C11-C10-C9-C7   |
| 22  | M     | 409 | CDL  | CB3-OB5-PB2-OB4 |
| 22  | M     | 411 | CDL  | CB2-OB2-PB2-OB3 |
| 22  | M     | 412 | CDL  | CB2-OB2-PB2-OB3 |
| 22  | D     | 502 | CDL  | CA3-OA5-PA1-OA3 |
| 22  | D     | 502 | CDL  | CB2-OB2-PB2-OB3 |
| 16  | 4     | 101 | BCL  | C16-C17-C18-C19 |
| 18  | L     | 304 | UQ8  | C25-C24-C26-C27 |
| 16  | Y     | 101 | BCL  | C2-C3-C5-C6     |
| 18  | L     | 304 | UQ8  | C38-C39-C41-C42 |
| 24  | M     | 414 | LMT  | O1'-C1-C2-C3    |
| 16  | P     | 102 | BCL  | C3-C5-C6-C7     |
| 16  | P     | 102 | BCL  | C10-C11-C12-C13 |
| 22  | M     | 412 | CDL  | C78-C79-C80-C81 |
| 15  | 1     | 401 | PGV  | C04-O12-P-O13   |
| 15  | 1     | 401 | PGV  | C03-C02-O01-C1  |
| 21  | 4     | 102 | CRT  | C28-C30-C31-C32 |
| 22  | H     | 302 | CDL  | C78-C79-C80-C81 |
| 16  | W     | 101 | BCL  | C16-C17-C18-C20 |
| 15  | L     | 309 | PGV  | C01-C02-C03-O11 |
| 16  | V     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 16  | D     | 503 | BCL  | C6-C7-C8-C9     |
| 16  | F     | 502 | BCL  | C6-C7-C8-C9     |
| 16  | P     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | 5     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | 5     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | 8     | 102 | BCL  | C11-C12-C13-C14 |
| 16  | 8     | 102 | BCL  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | 5     | 102 | BCL  | C11-C10-C8-C7   |
| 23  | M     | 413 | LDA  | C1-C2-C3-C4     |
| 15  | H     | 301 | PGV  | O01-C02-C03-O11 |
| 22  | H     | 302 | CDL  | OA5-CA3-CA4-OA6 |
| 15  | D     | 501 | PGV  | C25-C26-C27-C28 |
| 24  | R     | 103 | LMT  | C5-C6-C7-C8     |
| 16  | 9     | 101 | BCL  | C10-C11-C12-C13 |
| 16  | X     | 102 | BCL  | C15-C16-C17-C18 |
| 15  | L     | 306 | PGV  | C22-C23-C24-C25 |
| 24  | G     | 104 | LMT  | C11-C10-C9-C8   |
| 16  | Y     | 101 | BCL  | C16-C17-C18-C20 |
| 16  | 4     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 16  | L     | 301 | BCL  | C3-C5-C6-C7     |
| 16  | B     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 22  | M     | 412 | CDL  | C31-C32-C33-C34 |
| 16  | O     | 502 | BCL  | O1D-CGD-O2D-CED |
| 21  | 8     | 103 | CRT  | C1-C4-C5-C6     |
| 16  | P     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 16  | V     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 20  | M     | 406 | MQ8  | C24-C23-C25-C26 |
| 16  | M     | 403 | BCL  | C10-C11-C12-C13 |
| 16  | Z     | 102 | BCL  | C2-C3-C5-C6     |
| 16  | 6     | 101 | BCL  | C6-C7-C8-C9     |
| 15  | L     | 309 | PGV  | O04-C19-O03-C01 |
| 15  | H     | 301 | PGV  | C6-C7-C8-C9     |
| 24  | 8     | 101 | LMT  | C3-C4-C5-C6     |
| 16  | S     | 101 | BCL  | C5-C6-C7-C8     |
| 16  | J     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 10  | C     | 404 | HEM  | C4C-C3C-CAC-CBC |
| 16  | 7     | 102 | BCL  | C11-C10-C8-C7   |
| 16  | Y     | 101 | BCL  | C16-C17-C18-C19 |
| 16  | R     | 101 | BCL  | O1D-CGD-O2D-CED |
| 22  | M     | 411 | CDL  | C35-C36-C37-C38 |
| 24  | R     | 103 | LMT  | C3-C4-C5-C6     |
| 22  | H     | 302 | CDL  | C13-C14-C15-C16 |
| 21  | 4     | 102 | CRT  | C31-C32-C33-C34 |
| 15  | F     | 501 | PGV  | C1-C2-C3-C4     |
| 15  | H     | 301 | PGV  | C23-C24-C25-C26 |
| 22  | H     | 302 | CDL  | C18-C19-C20-C21 |
| 16  | Q     | 102 | BCL  | C13-C15-C16-C17 |
| 16  | 5     | 102 | BCL  | C8-C10-C11-C12  |
| 16  | K     | 102 | BCL  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | L     | 303 | UQ8  | C15-C14-C16-C17 |
| 18  | L     | 304 | UQ8  | C23-C24-C26-C27 |
| 24  | J     | 102 | LMT  | C6-C7-C8-C9     |
| 22  | M     | 409 | CDL  | CA2-C1-CB2-OB2  |
| 16  | R     | 101 | BCL  | C13-C15-C16-C17 |
| 18  | L     | 304 | UQ8  | C2-C3-O3-C3M    |
| 15  | L     | 309 | PGV  | O03-C01-C02-C03 |
| 16  | P     | 102 | BCL  | C5-C6-C7-C8     |
| 16  | 8     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 16  | M     | 403 | BCL  | C6-C7-C8-C9     |
| 16  | A     | 101 | BCL  | C6-C7-C8-C9     |
| 16  | N     | 101 | BCL  | C11-C12-C13-C14 |
| 16  | O     | 502 | BCL  | C11-C10-C8-C9   |
| 16  | Q     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | V     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | W     | 101 | BCL  | C14-C13-C15-C16 |
| 16  | 9     | 101 | BCL  | C11-C12-C13-C14 |
| 16  | 0     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | O     | 502 | BCL  | CBD-CGD-O2D-CED |
| 16  | K     | 102 | BCL  | C2-C3-C5-C6     |
| 16  | B     | 102 | BCL  | C13-C15-C16-C17 |
| 16  | B     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 16  | 4     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 16  | V     | 102 | BCL  | C8-C10-C11-C12  |
| 16  | G     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 16  | P     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 21  | 4     | 102 | CRT  | C31-C32-C33-C35 |
| 16  | 3     | 101 | BCL  | C15-C16-C17-C18 |
| 16  | P     | 102 | BCL  | C4-C3-C5-C6     |
| 15  | H     | 301 | PGV  | C01-C02-C03-O11 |
| 16  | Q     | 102 | BCL  | C11-C10-C8-C7   |
| 24  | Z     | 101 | LMT  | C7-C8-C9-C10    |
| 16  | G     | 102 | BCL  | C16-C17-C18-C19 |
| 22  | D     | 502 | CDL  | CB5-C51-C52-C53 |
| 10  | C     | 401 | HEM  | CAA-CBA-CGA-O2A |
| 21  | K     | 101 | CRT  | C36-C37-C38-C39 |
| 21  | Q     | 101 | CRT  | C3-C1-C4-C5     |
| 21  | 8     | 103 | CRT  | C2-C1-C4-C5     |
| 16  | Y     | 101 | BCL  | C13-C15-C16-C17 |
| 16  | X     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 10  | C     | 401 | HEM  | CAA-CBA-CGA-O1A |
| 22  | M     | 412 | CDL  | CA2-C1-CB2-OB2  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | B     | 103 | CRT  | C5-C6-C7-C8     |
| 16  | 6     | 101 | BCL  | C4-C3-C5-C6     |
| 16  | E     | 102 | BCL  | C8-C10-C11-C12  |
| 16  | 6     | 101 | BCL  | C2-C3-C5-C6     |
| 16  | 7     | 102 | BCL  | C2-C1-O2A-CGA   |
| 16  | S     | 101 | BCL  | C8-C10-C11-C12  |
| 16  | L     | 301 | BCL  | C11-C10-C8-C9   |
| 16  | Y     | 101 | BCL  | C11-C10-C8-C9   |
| 24  | P     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 16  | 6     | 101 | BCL  | C13-C15-C16-C17 |
| 22  | M     | 411 | CDL  | C43-C44-C45-C46 |
| 16  | X     | 102 | BCL  | C4-C3-C5-C6     |
| 18  | L     | 308 | UQ8  | C35-C34-C36-C37 |
| 22  | M     | 411 | CDL  | C1-CA2-OA2-PA1  |
| 16  | 8     | 102 | BCL  | C2-C3-C5-C6     |
| 16  | 8     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 22  | M     | 411 | CDL  | C15-C16-C17-C18 |
| 22  | M     | 412 | CDL  | CA3-CA4-CA6-OA8 |
| 22  | D     | 502 | CDL  | CA3-CA4-CA6-OA8 |
| 24  | G     | 101 | LMT  | C3-C4-C5-C6     |
| 22  | D     | 502 | CDL  | C12-C13-C14-C15 |
| 16  | U     | 101 | BCL  | C15-C16-C17-C18 |
| 15  | 1     | 401 | PGV  | O01-C02-C03-O11 |
| 18  | L     | 304 | UQ8  | C20-C19-C21-C22 |
| 15  | L     | 305 | PGV  | C4-C5-C6-C7     |
| 16  | I     | 101 | BCL  | C16-C17-C18-C19 |
| 16  | R     | 101 | BCL  | C16-C17-C18-C19 |
| 16  | 3     | 101 | BCL  | C16-C17-C18-C19 |
| 16  | 6     | 101 | BCL  | C16-C17-C18-C20 |
| 15  | C     | 409 | PGV  | C4-C5-C6-C7     |
| 16  | A     | 101 | BCL  | O1D-CGD-O2D-CED |
| 20  | M     | 406 | MQ8  | C19-C18-C20-C21 |
| 22  | M     | 411 | CDL  | OA6-CA4-CA6-OA8 |
| 16  | X     | 102 | BCL  | C2-C3-C5-C6     |
| 18  | L     | 308 | UQ8  | C33-C34-C36-C37 |
| 22  | M     | 409 | CDL  | C1-CB2-OB2-PB2  |
| 16  | L     | 301 | BCL  | C11-C10-C8-C7   |
| 16  | V     | 102 | BCL  | C5-C6-C7-C8     |
| 16  | G     | 102 | BCL  | C11-C10-C8-C9   |
| 16  | J     | 101 | BCL  | C14-C13-C15-C16 |
| 16  | S     | 101 | BCL  | C6-C7-C8-C9     |
| 16  | F     | 502 | BCL  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | O     | 502 | BCL  | C2-C1-O2A-CGA   |
| 16  | P     | 102 | BCL  | C2-C1-O2A-CGA   |
| 22  | M     | 411 | CDL  | OA9-CA7-OA8-CA6 |
| 16  | I     | 101 | BCL  | O1D-CGD-O2D-CED |
| 16  | P     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 16  | 8     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 15  | L     | 305 | PGV  | C5-C6-C7-C8     |
| 24  | 5     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 22  | M     | 411 | CDL  | C31-CA7-OA8-CA6 |
| 15  | H     | 301 | PGV  | O01-C1-C2-C3    |
| 17  | L     | 302 | BPH  | O2A-C1-C2-C3    |
| 22  | M     | 409 | CDL  | CA3-CA4-OA6-CA5 |
| 16  | S     | 101 | BCL  | C16-C17-C18-C20 |
| 22  | M     | 411 | CDL  | CA7-C31-C32-C33 |
| 24  | G     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 16  | Z     | 102 | BCL  | O1D-CGD-O2D-CED |
| 16  | G     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 22  | D     | 502 | CDL  | CB3-CB4-CB6-OB8 |
| 10  | C     | 401 | HEM  | C4C-C3C-CAC-CBC |
| 10  | C     | 403 | HEM  | C4C-C3C-CAC-CBC |
| 16  | A     | 101 | BCL  | CBD-CGD-O2D-CED |
| 16  | G     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 16  | 5     | 102 | BCL  | C16-C17-C18-C19 |
| 16  | F     | 502 | BCL  | C10-C11-C12-C13 |
| 22  | M     | 411 | CDL  | C77-C78-C79-C80 |
| 15  | F     | 501 | PGV  | O03-C01-C02-O01 |
| 16  | Q     | 102 | BCL  | C6-C7-C8-C9     |
| 16  | R     | 101 | BCL  | C6-C7-C8-C9     |
| 16  | U     | 101 | BCL  | C11-C10-C8-C9   |
| 16  | X     | 102 | BCL  | C11-C12-C13-C14 |
| 16  | 1     | 402 | BCL  | C6-C7-C8-C9     |
| 21  | 0     | 103 | CRT  | C5-C6-C7-C9     |
| 22  | D     | 502 | CDL  | C53-C54-C55-C56 |
| 18  | L     | 308 | UQ8  | C3-C4-O4-C4M    |
| 21  | K     | 101 | CRT  | O1-C1-C4-C5     |
| 21  | Z     | 103 | CRT  | O1-C1-C4-C5     |
| 24  | P     | 103 | LMT  | C4-C5-C6-C7     |
| 16  | U     | 101 | BCL  | C16-C17-C18-C19 |
| 16  | L     | 307 | BCL  | C6-C7-C8-C10    |
| 16  | M     | 404 | BCL  | C6-C7-C8-C10    |
| 16  | J     | 101 | BCL  | C11-C10-C8-C7   |
| 16  | S     | 101 | BCL  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | L     | 307 | BCL  | C16-C17-C18-C20 |
| 16  | 6     | 101 | BCL  | C16-C17-C18-C19 |
| 18  | L     | 303 | UQ8  | C13-C14-C16-C17 |
| 21  | K     | 101 | CRT  | C39-C38-O2-C2M  |
| 15  | M     | 408 | PGV  | C27-C28-C29-C30 |
| 16  | R     | 101 | BCL  | CBD-CGD-O2D-CED |
| 24  | J     | 102 | LMT  | C4'-C5'-C6'-O6' |
| 10  | C     | 402 | HEM  | CAD-CBD-CGD-O1D |
| 24  | 2     | 101 | LMT  | O1'-C1-C2-C3    |
| 15  | D     | 501 | PGV  | C20-C21-C22-C23 |
| 16  | Y     | 101 | BCL  | C6-C7-C8-C9     |
| 22  | M     | 409 | CDL  | CA3-CA4-CA6-OA8 |
| 22  | M     | 411 | CDL  | CA3-CA4-CA6-OA8 |
| 16  | I     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 16  | R     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 16  | X     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 16  | L     | 307 | BCL  | CAA-CBA-CGA-O2A |
| 22  | H     | 302 | CDL  | C12-C11-CA5-OA6 |
| 21  | K     | 101 | CRT  | C10-C11-C12-C14 |
| 16  | V     | 102 | BCL  | C16-C17-C18-C20 |
| 10  | C     | 404 | HEM  | CAA-CBA-CGA-O2A |
| 15  | M     | 410 | PGV  | O01-C1-C2-C3    |
| 15  | 1     | 401 | PGV  | O01-C1-C2-C3    |
| 16  | 9     | 101 | BCL  | O1D-CGD-O2D-CED |
| 24  | J     | 102 | LMT  | C4-C5-C6-C7     |
| 16  | M     | 404 | BCL  | C2-C1-O2A-CGA   |
| 16  | I     | 101 | BCL  | C2-C1-O2A-CGA   |
| 16  | L     | 307 | BCL  | C12-C13-C15-C16 |
| 16  | J     | 101 | BCL  | C12-C13-C15-C16 |
| 16  | V     | 102 | BCL  | C11-C12-C13-C15 |
| 16  | B     | 102 | BCL  | C16-C17-C18-C20 |
| 16  | I     | 101 | BCL  | CBD-CGD-O2D-CED |
| 18  | L     | 304 | UQ8  | C4-C3-O3-C3M    |
| 17  | M     | 405 | BPH  | C5-C6-C7-C8     |
| 16  | N     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 16  | 5     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 16  | 0     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 15  | L     | 305 | PGV  | C20-C19-O03-C01 |
| 16  | P     | 102 | BCL  | CAA-CBA-CGA-O1A |
| 16  | O     | 502 | BCL  | C2A-CAA-CBA-CGA |
| 22  | M     | 412 | CDL  | C72-C71-CB7-OB8 |
| 24  | E     | 101 | LMT  | C3'-C4'-O1B-C1B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | L     | 305 | PGV  | C02-C03-O11-P   |
| 15  | H     | 301 | PGV  | C02-C03-O11-P   |
| 10  | C     | 402 | HEM  | CAD-CBD-CGD-O2D |
| 16  | G     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 16  | X     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 20  | M     | 406 | MQ8  | C22-C23-C25-C26 |
| 24  | V     | 101 | LMT  | C4-C5-C6-C7     |
| 22  | M     | 411 | CDL  | C80-C81-C82-C83 |
| 15  | F     | 501 | PGV  | C22-C23-C24-C25 |
| 16  | 4     | 101 | BCL  | C5-C6-C7-C8     |
| 22  | M     | 411 | CDL  | C71-CB7-OB8-CB6 |
| 16  | O     | 502 | BCL  | C14-C13-C15-C16 |
| 16  | X     | 102 | BCL  | C11-C10-C8-C9   |
| 15  | M     | 410 | PGV  | O02-C1-C2-C3    |
| 15  | 1     | 401 | PGV  | O02-C1-C2-C3    |
| 24  | X     | 101 | LMT  | C3'-C4'-O1B-C1B |
| 16  | L     | 301 | BCL  | O1A-CGA-O2A-C1  |
| 15  | L     | 305 | PGV  | C2-C3-C4-C5     |
| 15  | L     | 306 | PGV  | C4-C5-C6-C7     |
| 15  | 1     | 401 | PGV  | O03-C19-C20-C21 |
| 16  | T     | 101 | BCL  | C13-C15-C16-C17 |
| 17  | L     | 302 | BPH  | C8-C10-C11-C12  |
| 22  | M     | 411 | CDL  | C71-C72-C73-C74 |
| 16  | L     | 307 | BCL  | CAA-CBA-CGA-O1A |
| 10  | C     | 404 | HEM  | CAA-CBA-CGA-O1A |
| 16  | V     | 102 | BCL  | CAA-CBA-CGA-O1A |
| 22  | H     | 302 | CDL  | C12-C11-CA5-OA7 |
| 16  | O     | 502 | BCL  | C15-C16-C17-C18 |
| 16  | R     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 14  | C     | 408 | PLM  | C2-C3-C4-C5     |
| 16  | L     | 301 | BCL  | C2-C1-O2A-CGA   |
| 16  | D     | 503 | BCL  | C2-C1-O2A-CGA   |
| 16  | U     | 101 | BCL  | C2-C1-O2A-CGA   |
| 16  | W     | 101 | BCL  | C2-C1-O2A-CGA   |
| 16  | 1     | 402 | BCL  | C2-C1-O2A-CGA   |
| 22  | M     | 411 | CDL  | C36-C37-C38-C39 |
| 24  | M     | 414 | LMT  | O5B-C1B-O1B-C4' |
| 16  | L     | 301 | BCL  | C2A-CAA-CBA-CGA |
| 15  | L     | 305 | PGV  | O04-C19-O03-C01 |
| 16  | L     | 301 | BCL  | CBA-CGA-O2A-C1  |
| 22  | M     | 411 | CDL  | C52-C53-C54-C55 |

There are no ring outliers.

97 monomers are involved in 428 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | K     | 101 | CRT  | 9       | 0            |
| 16  | P     | 102 | BCL  | 8       | 0            |
| 24  | 4     | 103 | LMT  | 2       | 0            |
| 16  | B     | 102 | BCL  | 8       | 0            |
| 16  | 7     | 102 | BCL  | 6       | 0            |
| 14  | C     | 408 | PLM  | 3       | 0            |
| 21  | 2     | 103 | CRT  | 7       | 0            |
| 15  | D     | 501 | PGV  | 4       | 0            |
| 16  | Z     | 102 | BCL  | 8       | 0            |
| 21  | M     | 407 | CRT  | 5       | 0            |
| 16  | 4     | 101 | BCL  | 6       | 0            |
| 10  | C     | 403 | HEM  | 4       | 0            |
| 21  | G     | 103 | CRT  | 7       | 0            |
| 24  | 2     | 101 | LMT  | 1       | 0            |
| 24  | E     | 101 | LMT  | 2       | 0            |
| 21  | Q     | 101 | CRT  | 8       | 0            |
| 21  | V     | 103 | CRT  | 3       | 0            |
| 16  | I     | 101 | BCL  | 5       | 0            |
| 24  | 2     | 104 | LMT  | 3       | 0            |
| 16  | L     | 307 | BCL  | 7       | 0            |
| 16  | J     | 101 | BCL  | 5       | 0            |
| 24  | Z     | 101 | LMT  | 2       | 0            |
| 15  | L     | 309 | PGV  | 4       | 0            |
| 16  | Q     | 102 | BCL  | 4       | 0            |
| 24  | 5     | 101 | LMT  | 1       | 0            |
| 16  | N     | 101 | BCL  | 7       | 0            |
| 10  | C     | 402 | HEM  | 7       | 0            |
| 16  | L     | 301 | BCL  | 1       | 0            |
| 16  | T     | 101 | BCL  | 10      | 0            |
| 22  | D     | 502 | CDL  | 3       | 0            |
| 16  | 8     | 102 | BCL  | 4       | 0            |
| 15  | F     | 501 | PGV  | 3       | 0            |
| 24  | B     | 101 | LMT  | 3       | 0            |
| 16  | X     | 102 | BCL  | 7       | 0            |
| 16  | G     | 102 | BCL  | 5       | 0            |
| 16  | W     | 101 | BCL  | 2       | 0            |
| 24  | 8     | 101 | LMT  | 4       | 0            |
| 24  | G     | 101 | LMT  | 2       | 0            |
| 16  | 2     | 102 | BCL  | 10      | 0            |
| 21  | X     | 103 | CRT  | 9       | 0            |
| 16  | M     | 403 | BCL  | 2       | 0            |
| 17  | L     | 302 | BPH  | 5       | 0            |

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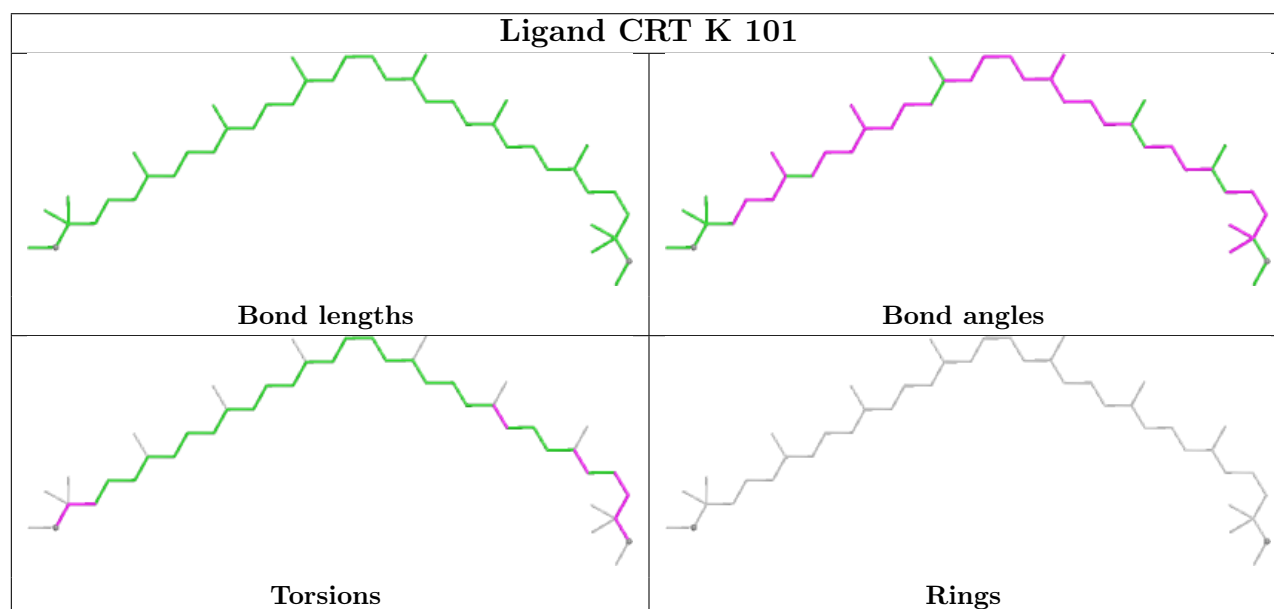
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | P     | 101 | LMT  | 2       | 0            |
| 22  | M     | 412 | CDL  | 7       | 0            |
| 21  | 7     | 101 | CRT  | 10      | 0            |
| 23  | O     | 501 | LDA  | 1       | 0            |
| 15  | L     | 306 | PGV  | 3       | 0            |
| 15  | L     | 305 | PGV  | 4       | 0            |
| 21  | B     | 103 | CRT  | 5       | 0            |
| 16  | Y     | 101 | BCL  | 3       | 0            |
| 22  | H     | 302 | CDL  | 2       | 0            |
| 22  | M     | 411 | CDL  | 5       | 0            |
| 21  | 8     | 103 | CRT  | 7       | 0            |
| 15  | M     | 410 | PGV  | 3       | 0            |
| 22  | M     | 409 | CDL  | 1       | 0            |
| 21  | 0     | 103 | CRT  | 4       | 0            |
| 16  | 0     | 102 | BCL  | 8       | 0            |
| 24  | G     | 104 | LMT  | 4       | 0            |
| 15  | 1     | 401 | PGV  | 3       | 0            |
| 16  | 9     | 101 | BCL  | 4       | 0            |
| 21  | 4     | 102 | CRT  | 11      | 0            |
| 18  | L     | 304 | UQ8  | 12      | 0            |
| 16  | M     | 404 | BCL  | 6       | 0            |
| 17  | M     | 405 | BPH  | 7       | 0            |
| 16  | U     | 101 | BCL  | 5       | 0            |
| 16  | S     | 101 | BCL  | 6       | 0            |
| 16  | V     | 102 | BCL  | 8       | 0            |
| 24  | R     | 103 | LMT  | 2       | 0            |
| 18  | L     | 308 | UQ8  | 9       | 0            |
| 16  | 3     | 101 | BCL  | 6       | 0            |
| 21  | T     | 102 | CRT  | 7       | 0            |
| 16  | 6     | 101 | BCL  | 6       | 0            |
| 16  | D     | 503 | BCL  | 4       | 0            |
| 15  | H     | 301 | PGV  | 3       | 0            |
| 24  | H     | 303 | LMT  | 3       | 0            |
| 24  | V     | 101 | LMT  | 2       | 0            |
| 15  | C     | 409 | PGV  | 2       | 0            |
| 20  | M     | 406 | MQ8  | 4       | 0            |
| 10  | C     | 401 | HEM  | 7       | 0            |
| 16  | R     | 101 | BCL  | 7       | 0            |
| 21  | R     | 102 | CRT  | 5       | 0            |
| 10  | C     | 404 | HEM  | 4       | 0            |
| 21  | N     | 102 | CRT  | 1       | 0            |
| 16  | F     | 502 | BCL  | 1       | 0            |

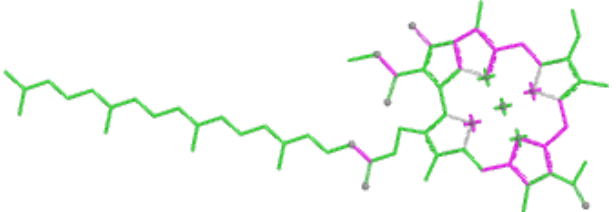
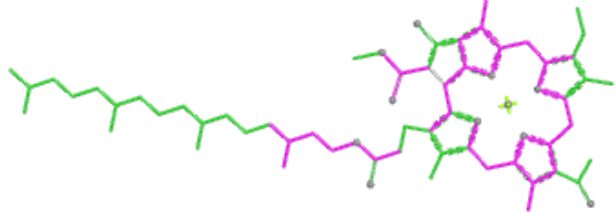
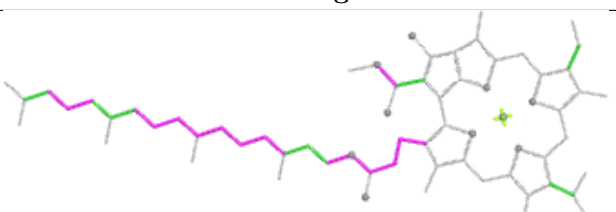
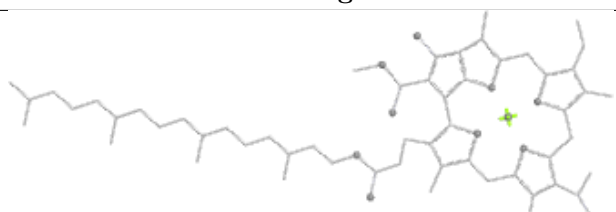
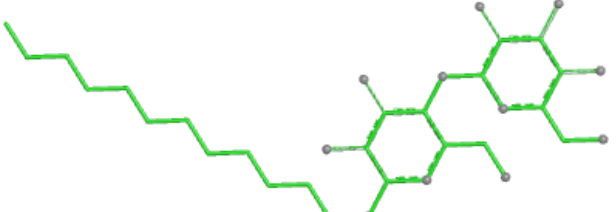
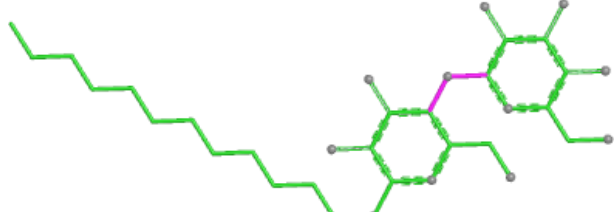
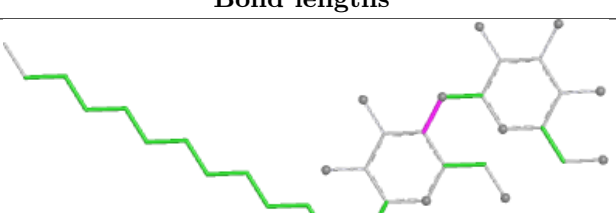
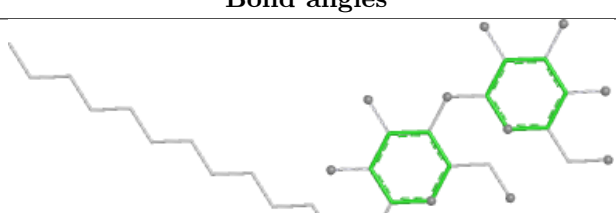
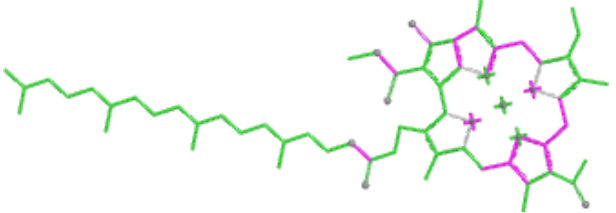
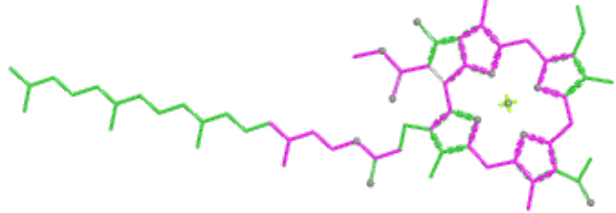
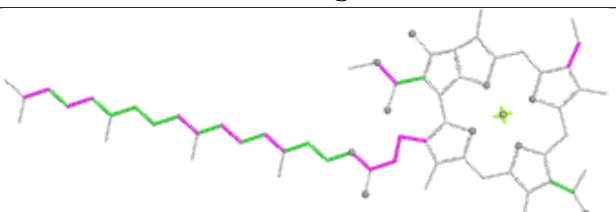
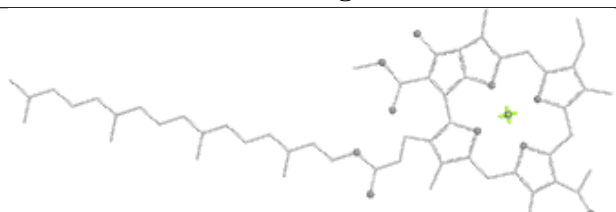
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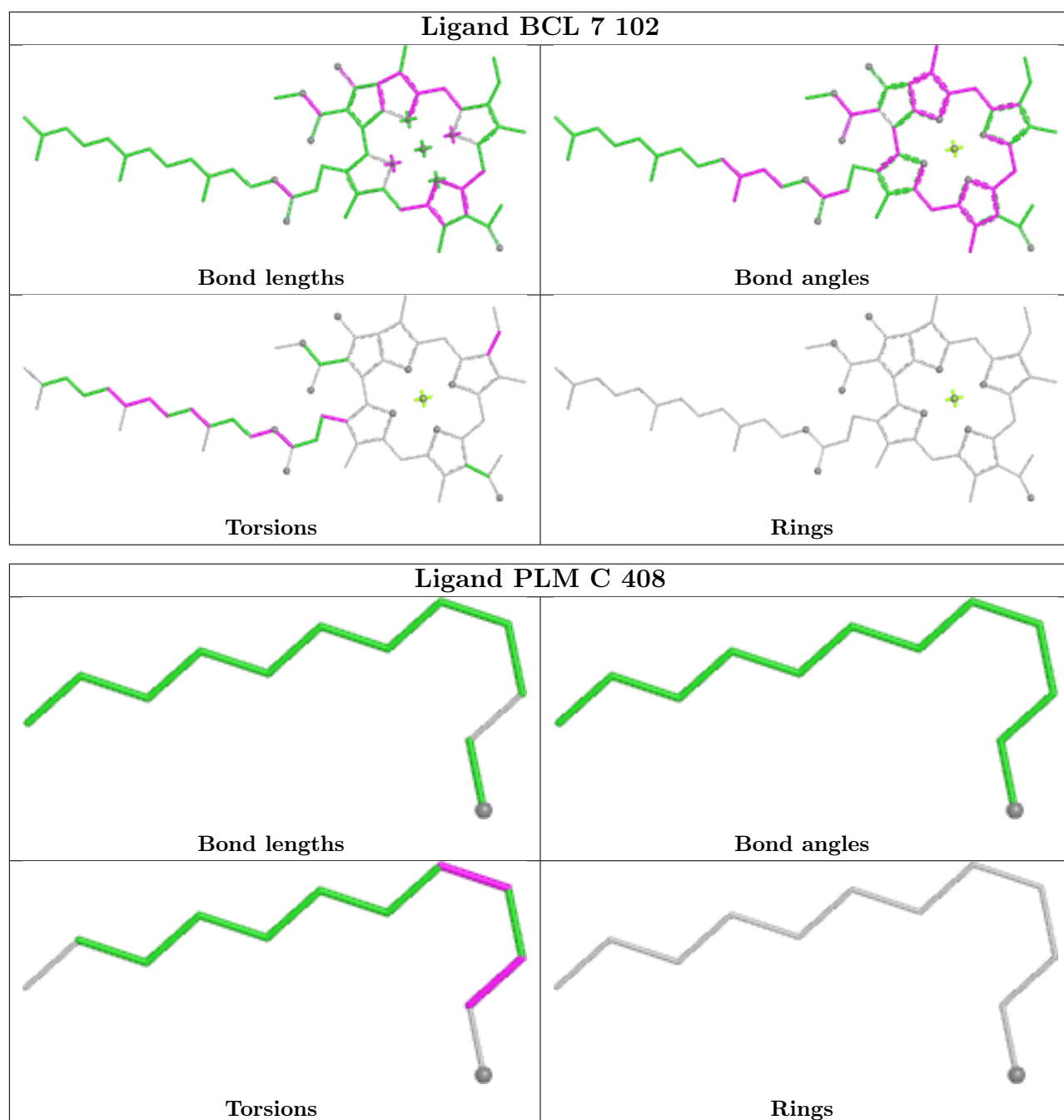
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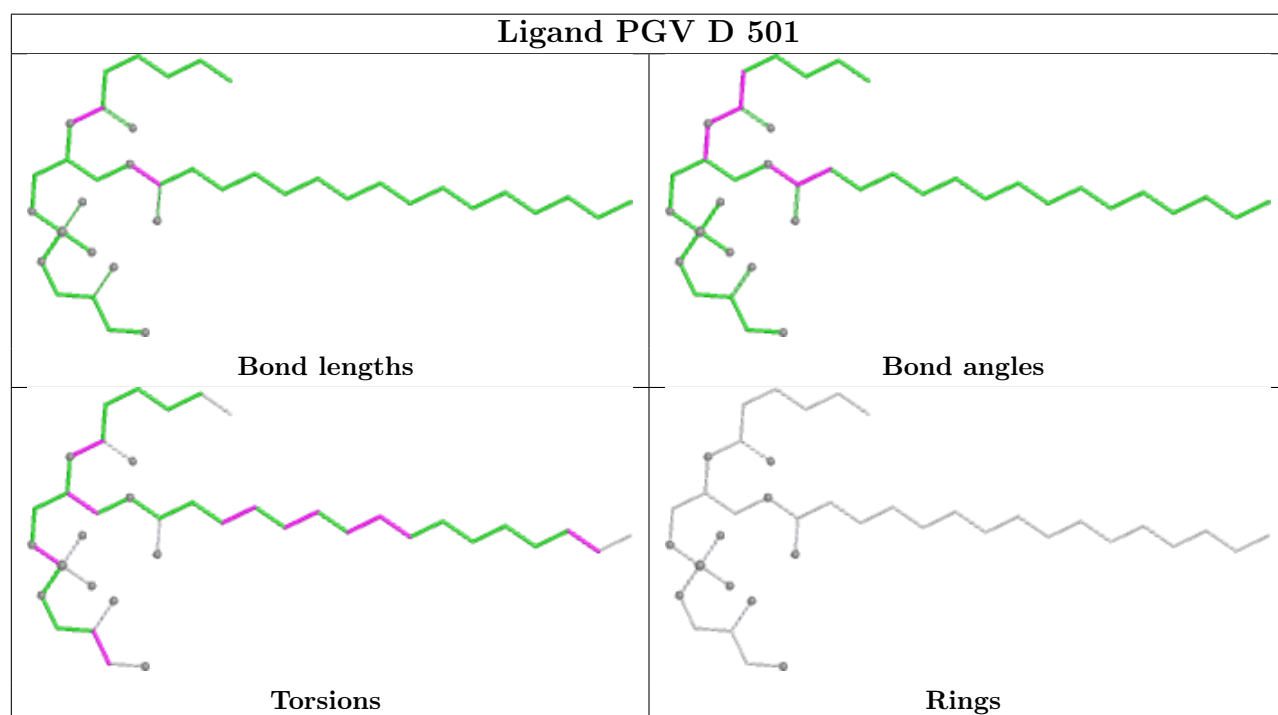
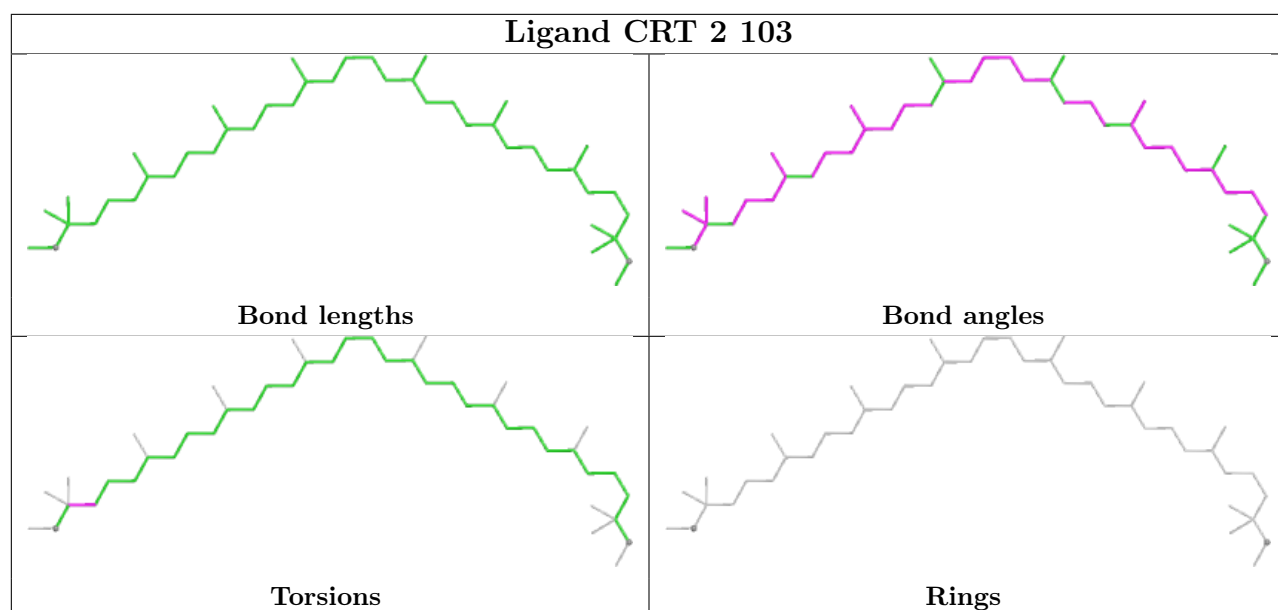
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | M     | 414 | LMT  | 2       | 0            |
| 24  | O     | 101 | LMT  | 3       | 0            |
| 16  | O     | 502 | BCL  | 3       | 0            |
| 24  | J     | 102 | LMT  | 2       | 0            |
| 24  | P     | 103 | LMT  | 3       | 0            |
| 18  | L     | 303 | UQ8  | 4       | 0            |
| 16  | E     | 102 | BCL  | 7       | 0            |
| 21  | Z     | 103 | CRT  | 6       | 0            |
| 16  | A     | 101 | BCL  | 1       | 0            |
| 16  | K     | 102 | BCL  | 6       | 0            |
| 21  | E     | 103 | CRT  | 4       | 0            |
| 16  | 5     | 102 | BCL  | 6       | 0            |
| 16  | 1     | 402 | BCL  | 3       | 0            |

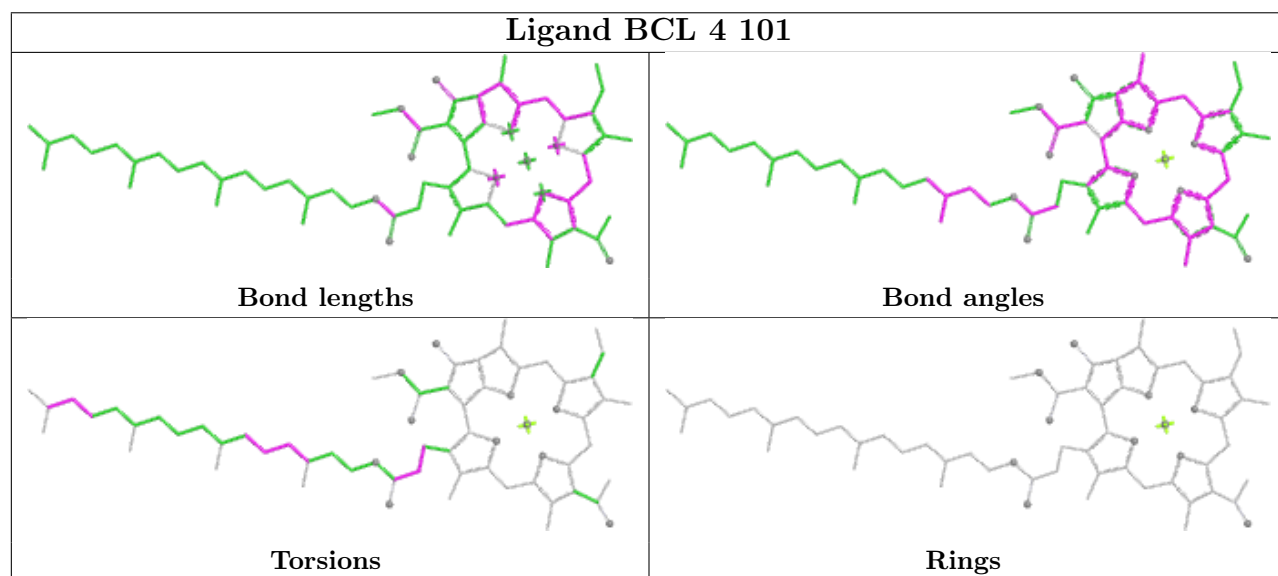
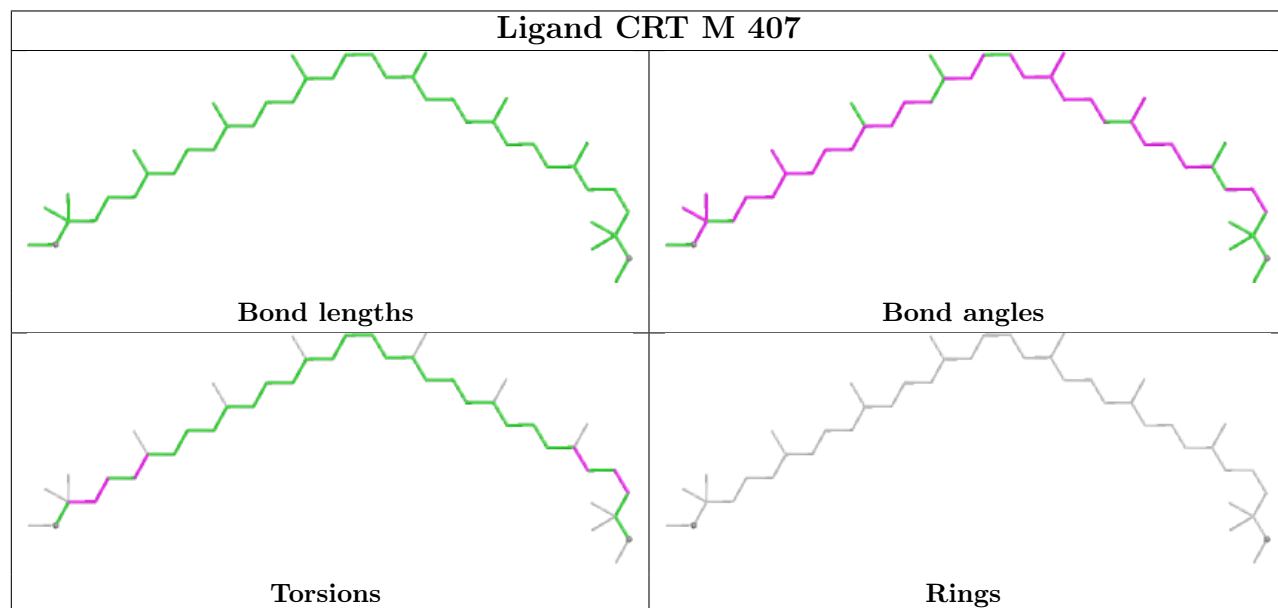
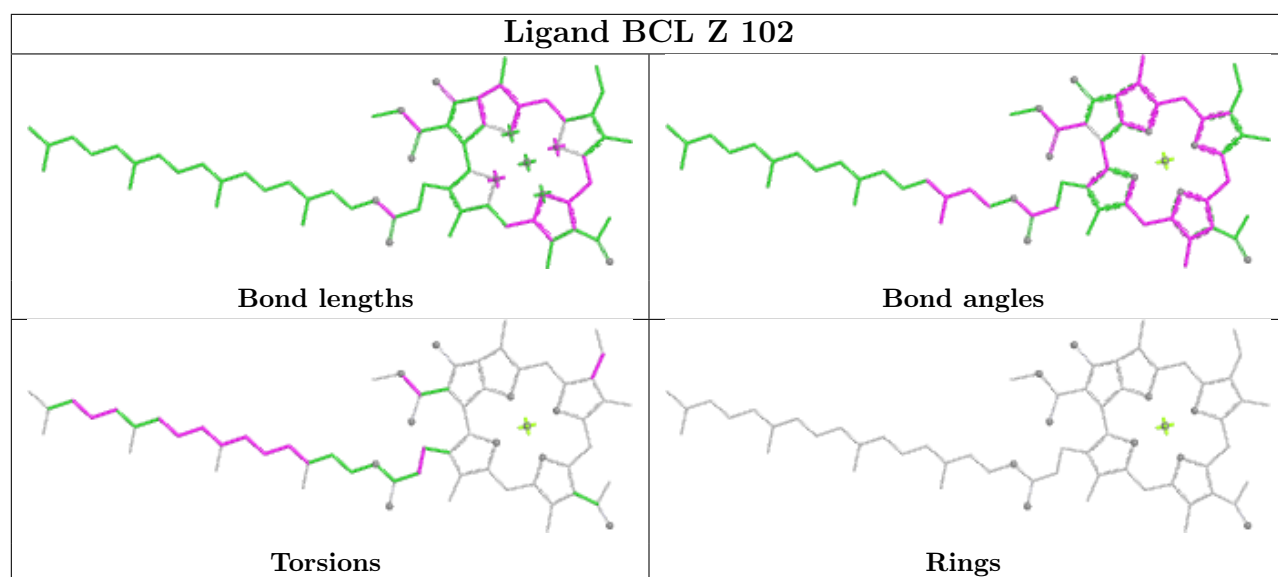
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

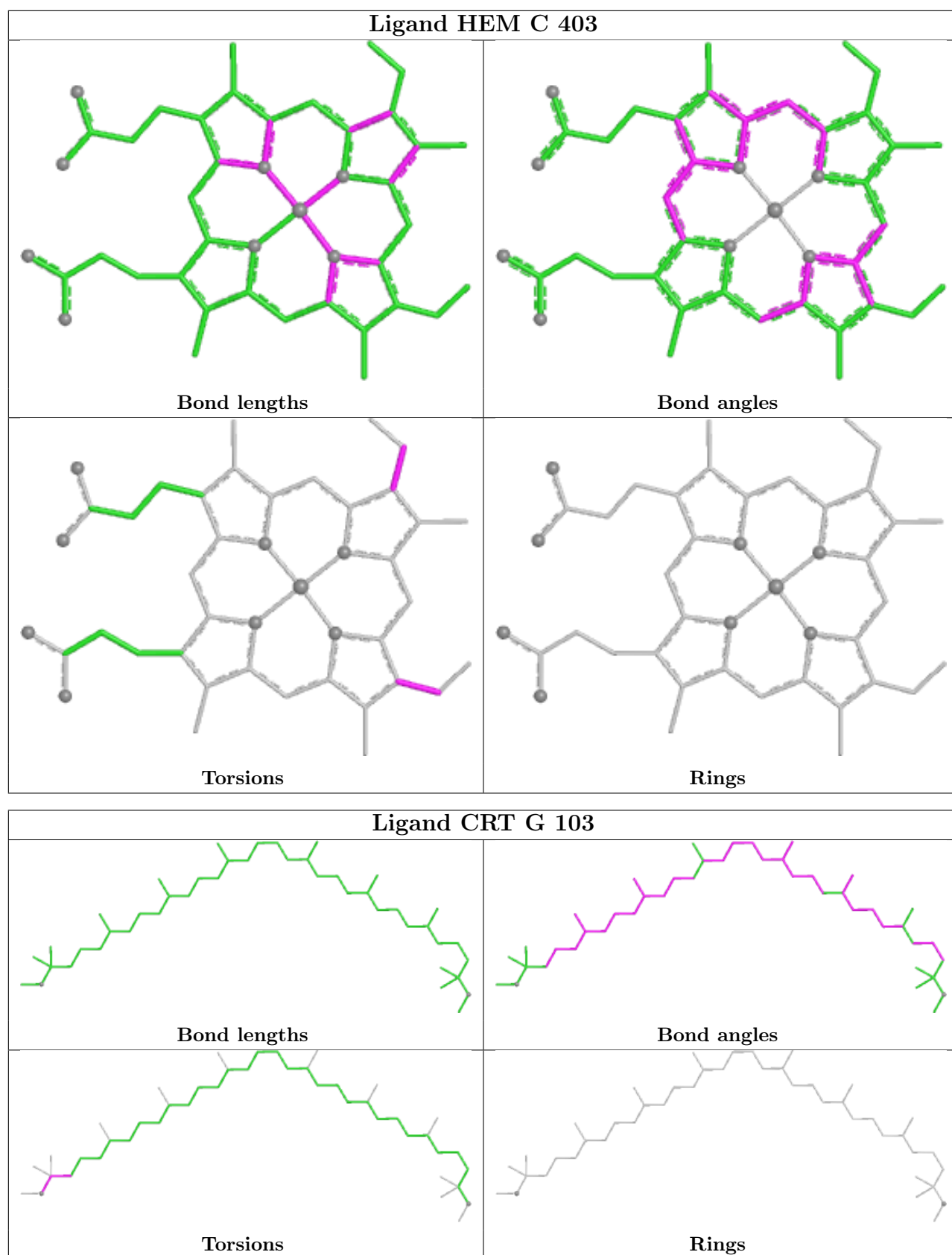


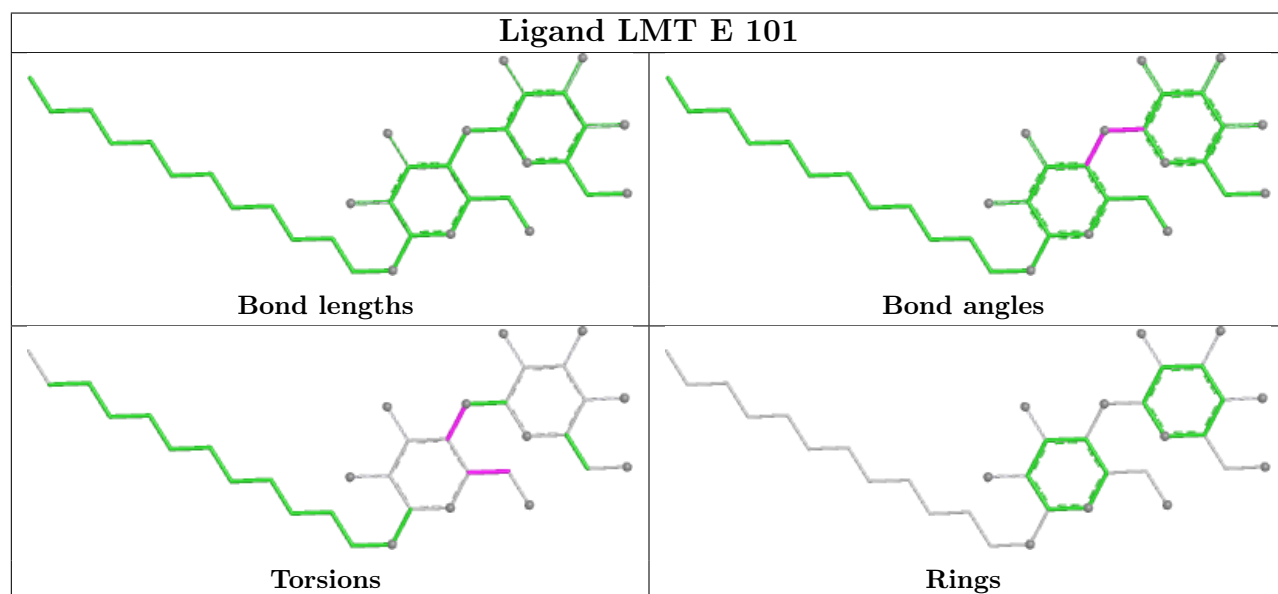
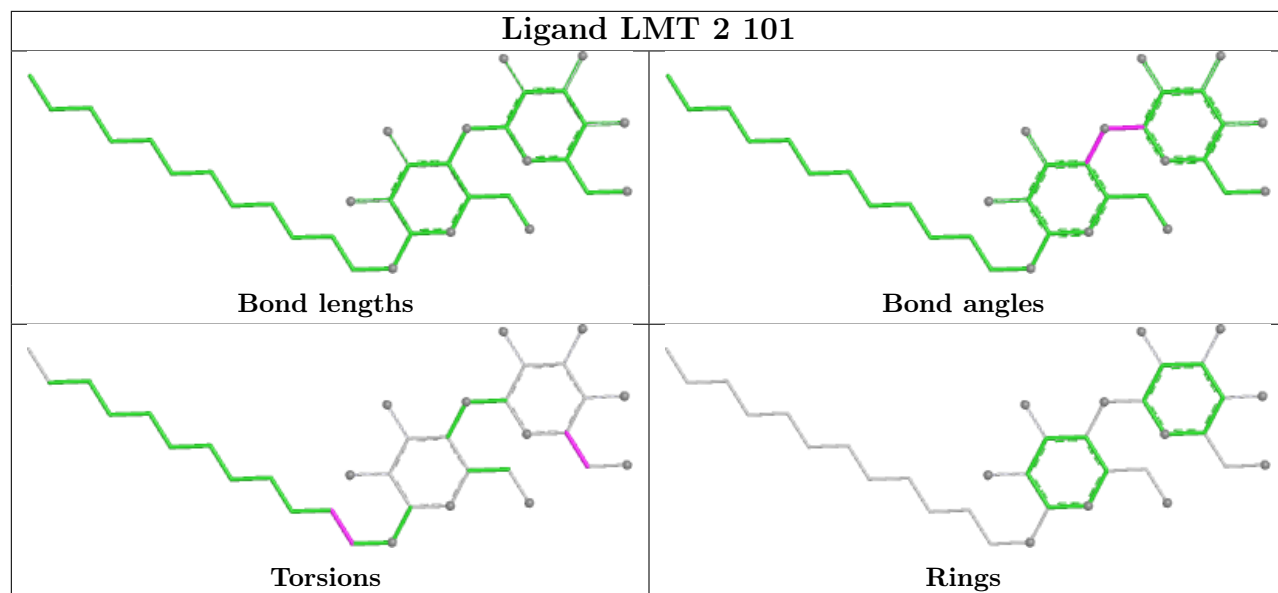
| Ligand BCL P 102                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMT 4 103                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCL B 102                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

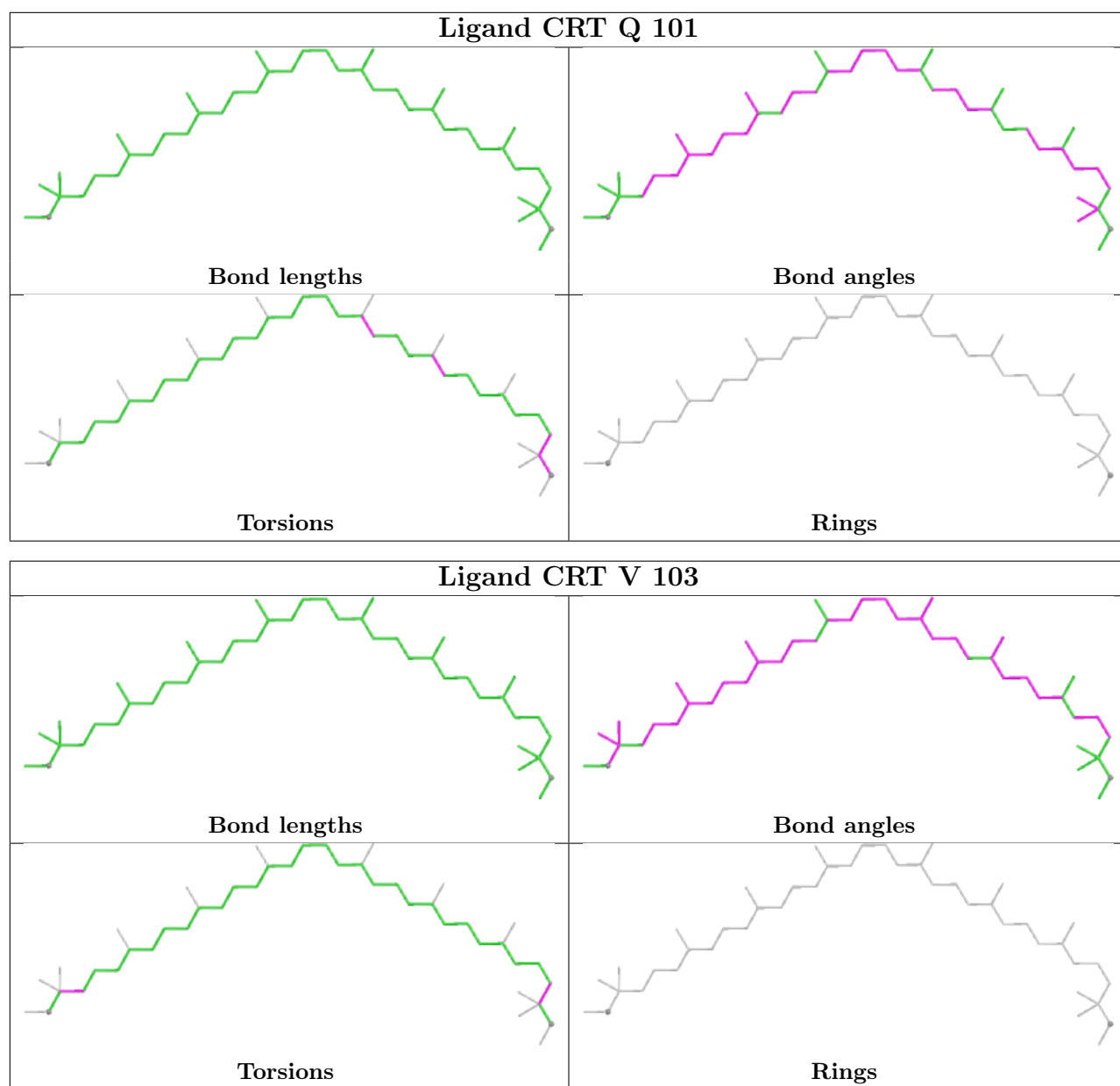


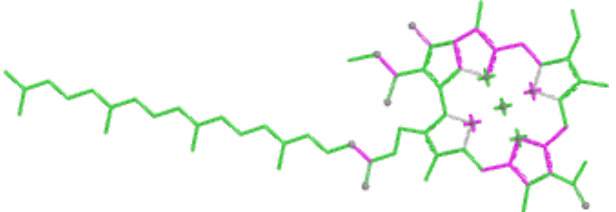
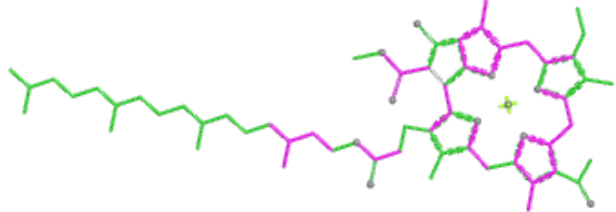
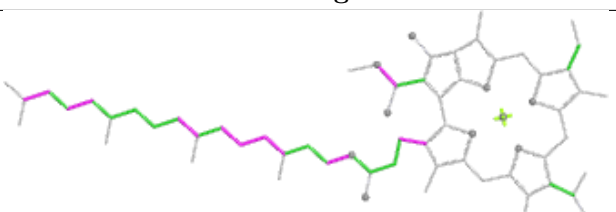
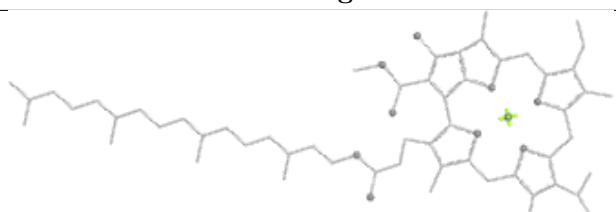
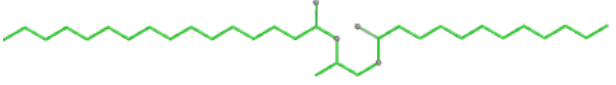
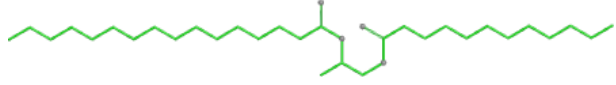
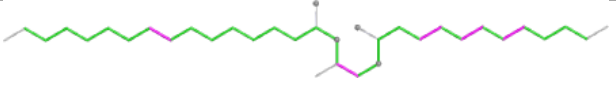
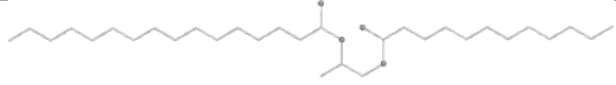
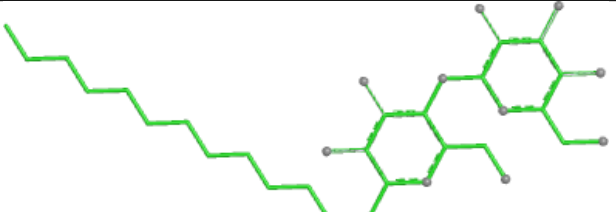
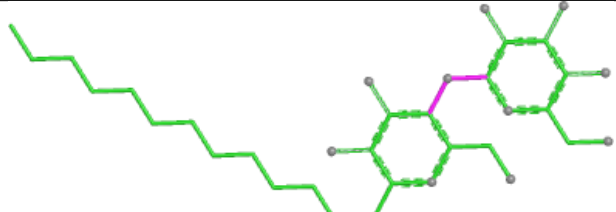
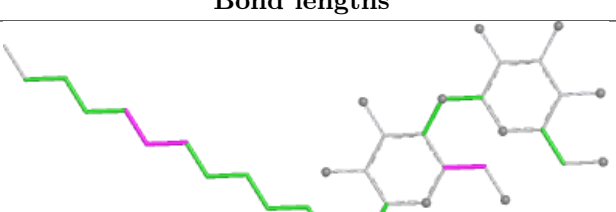
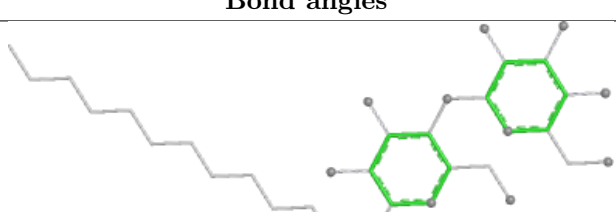


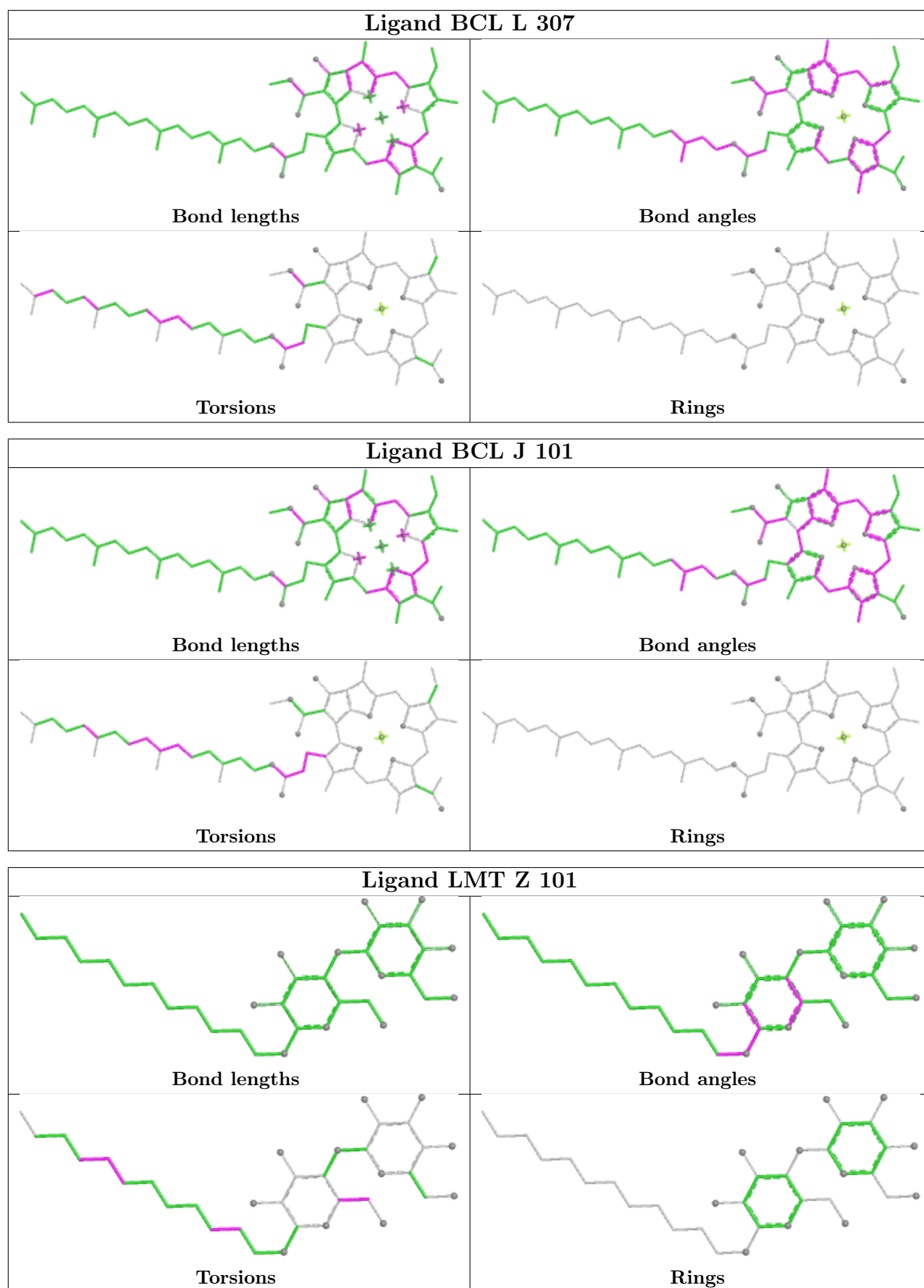


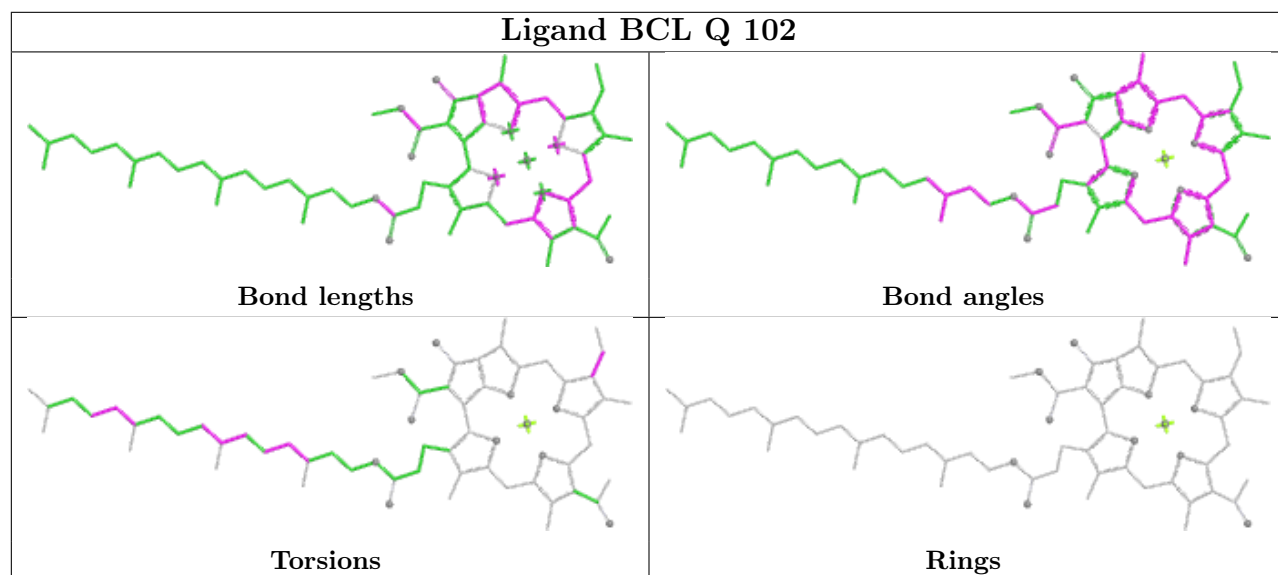
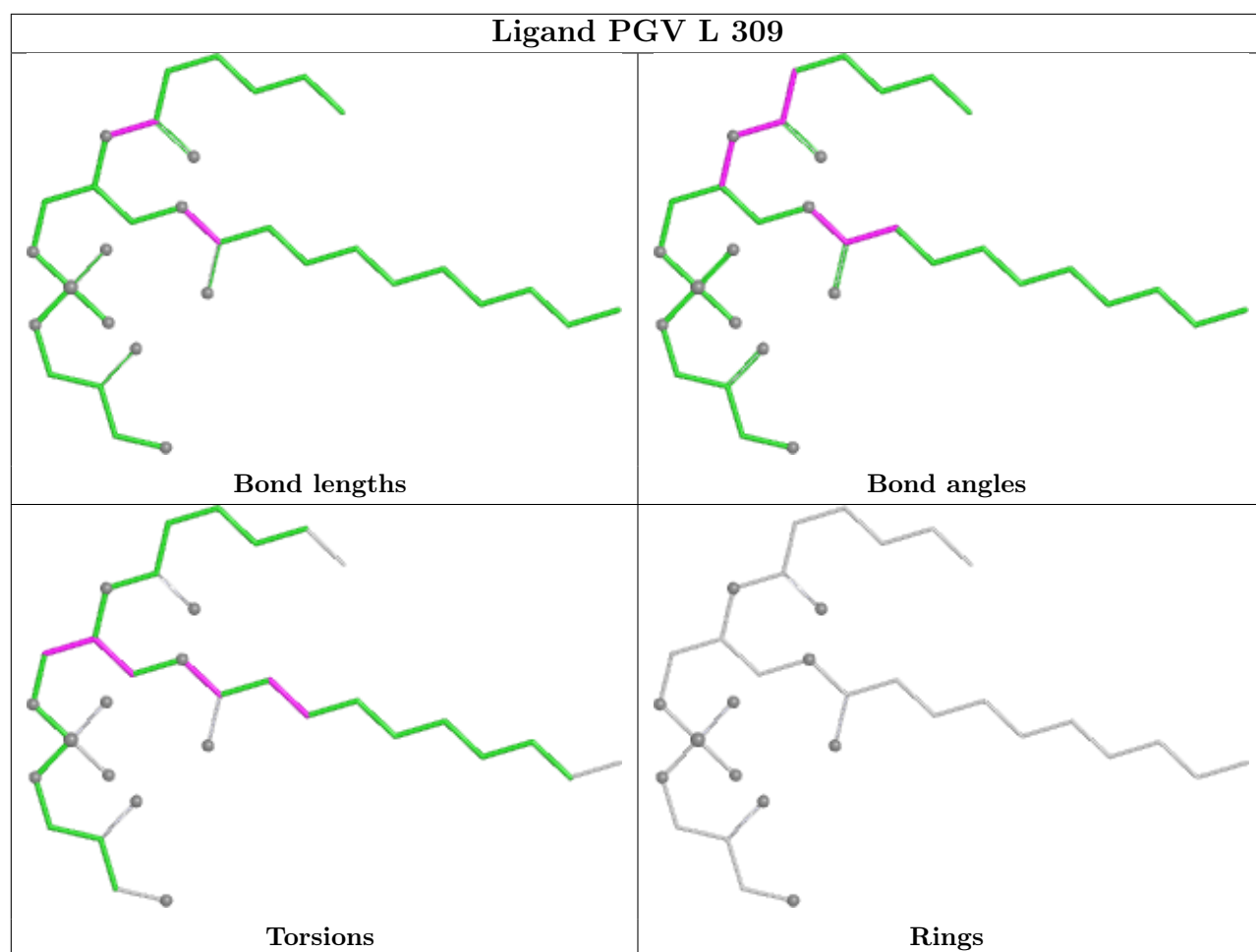


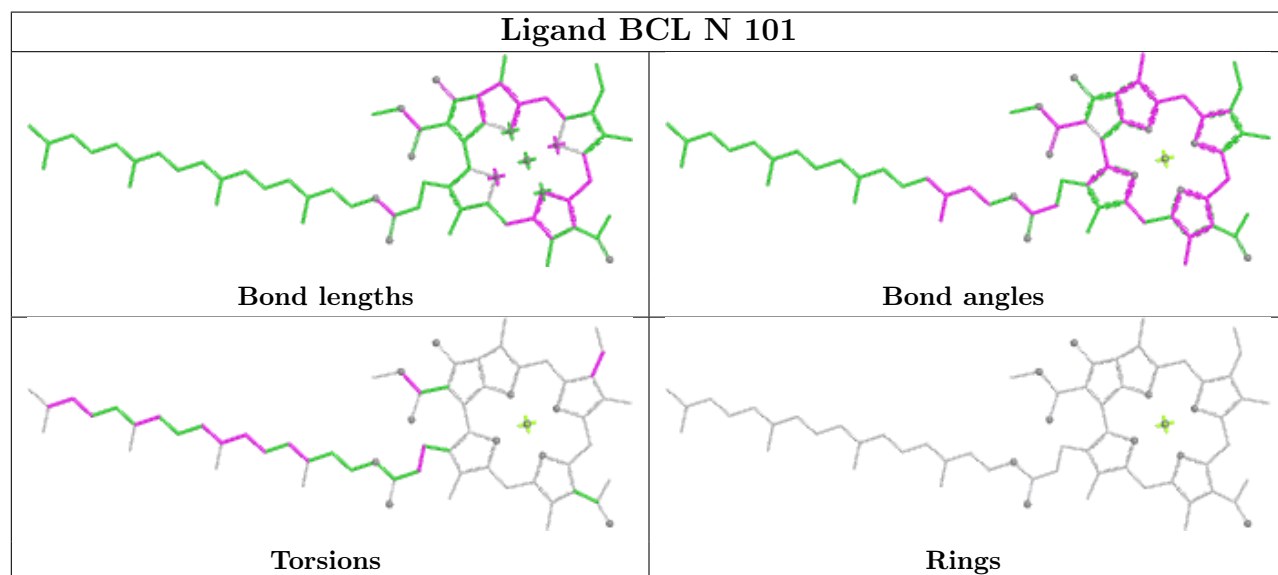
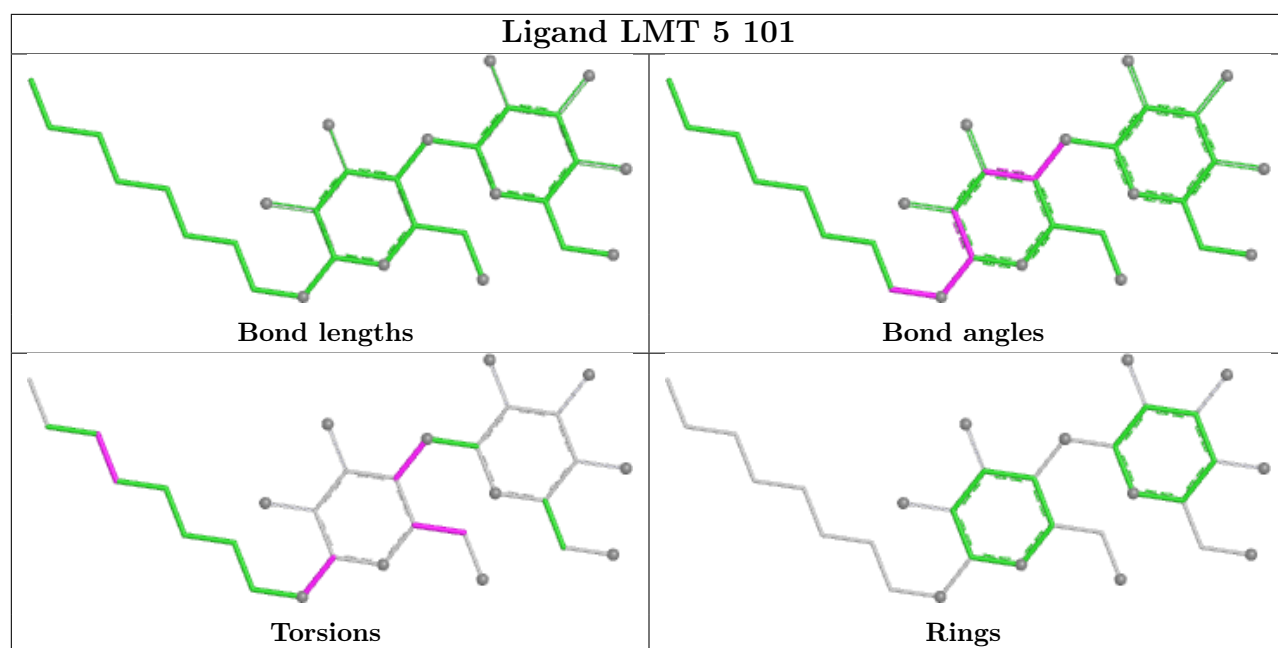


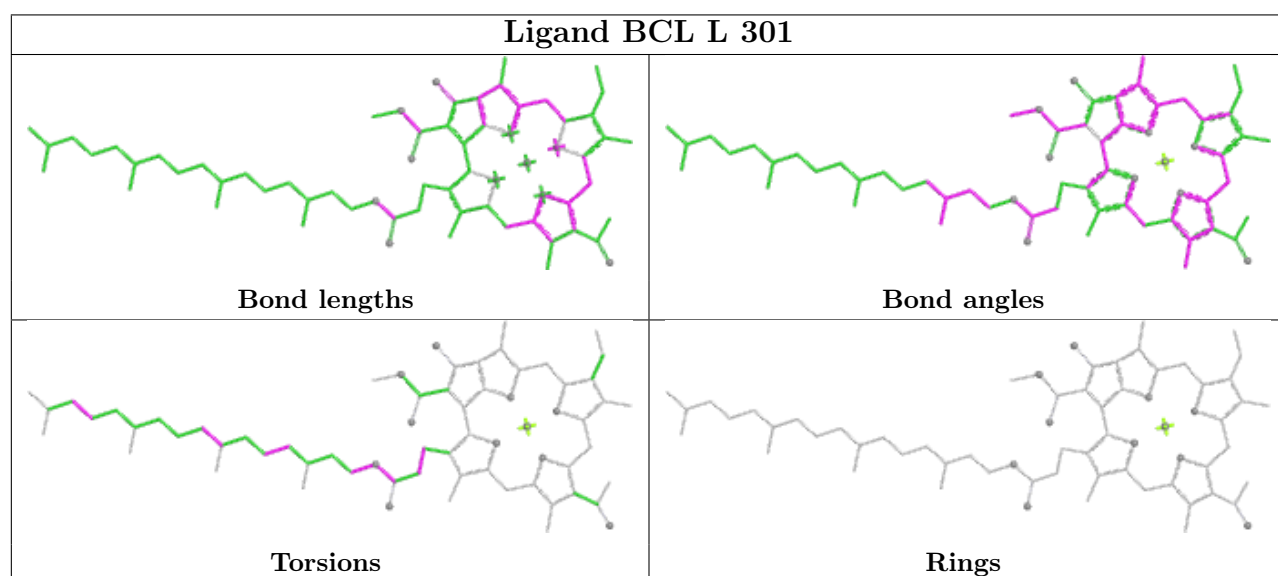
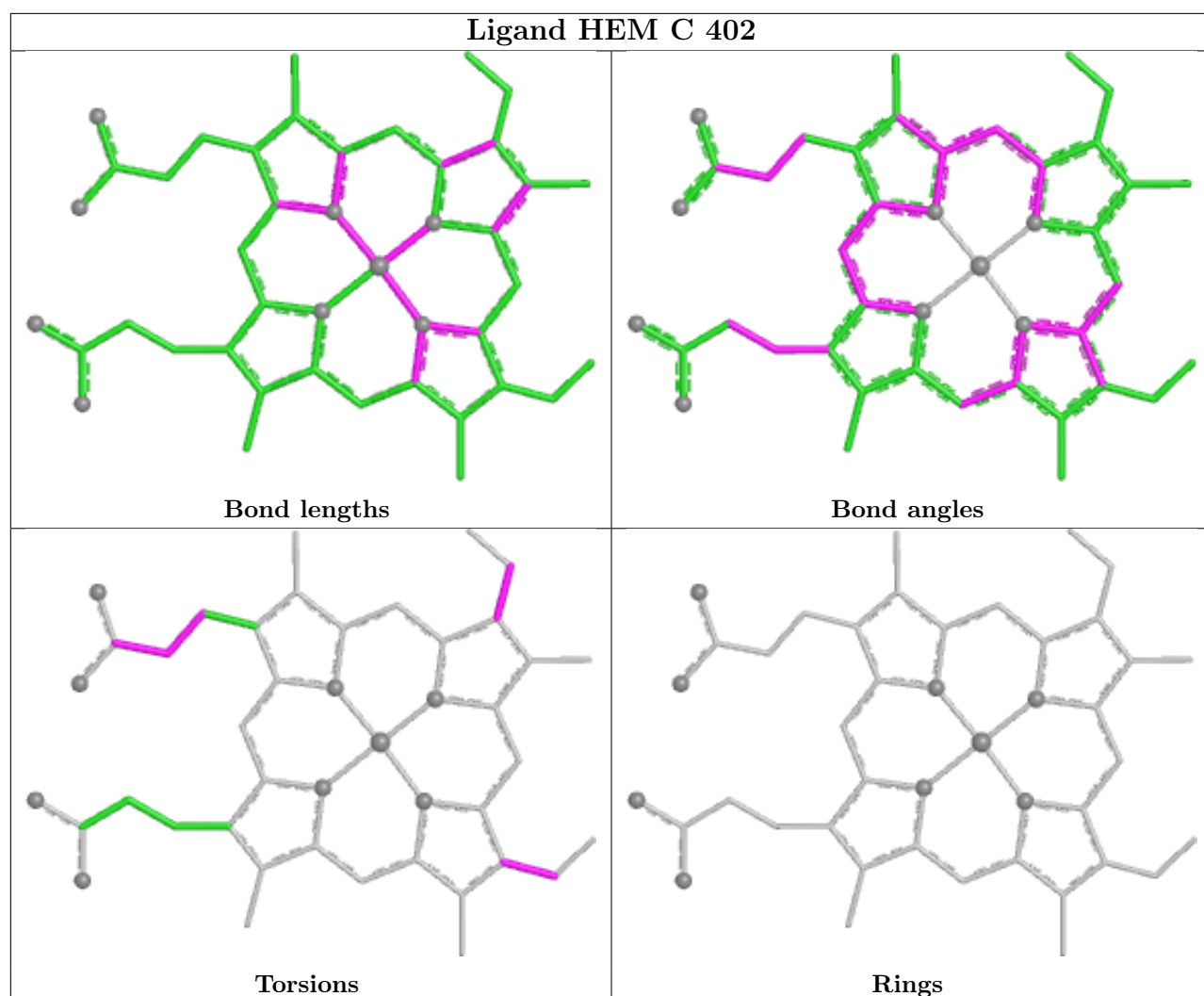


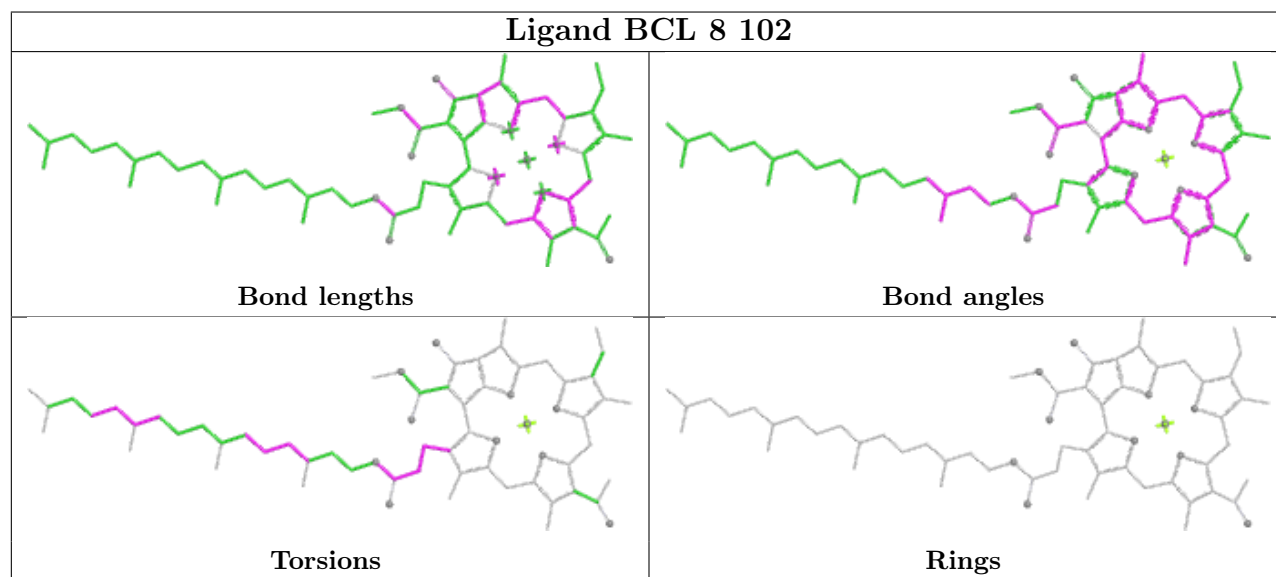
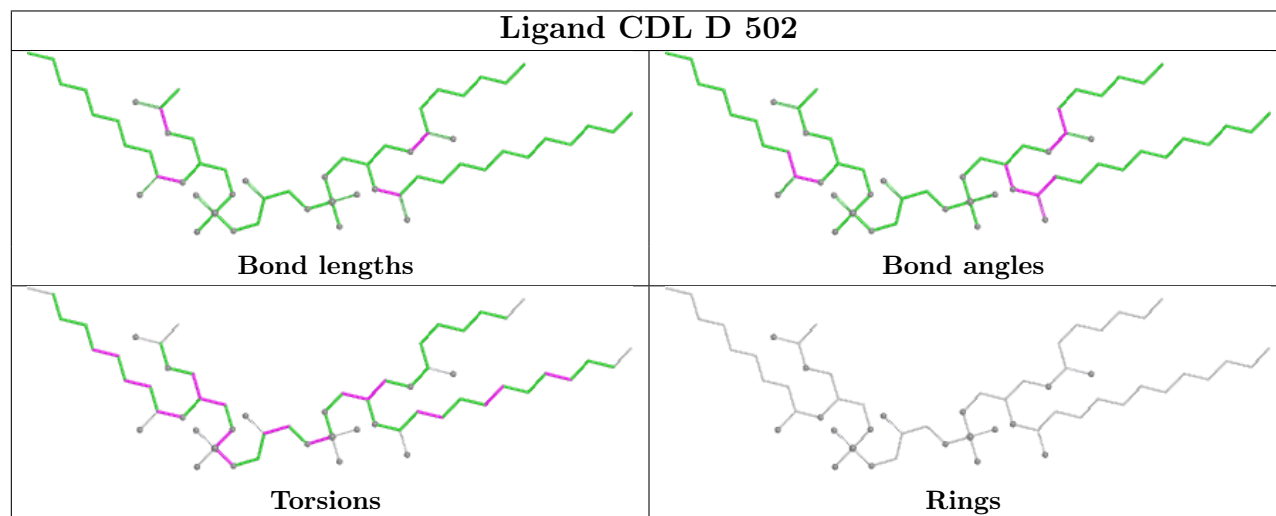
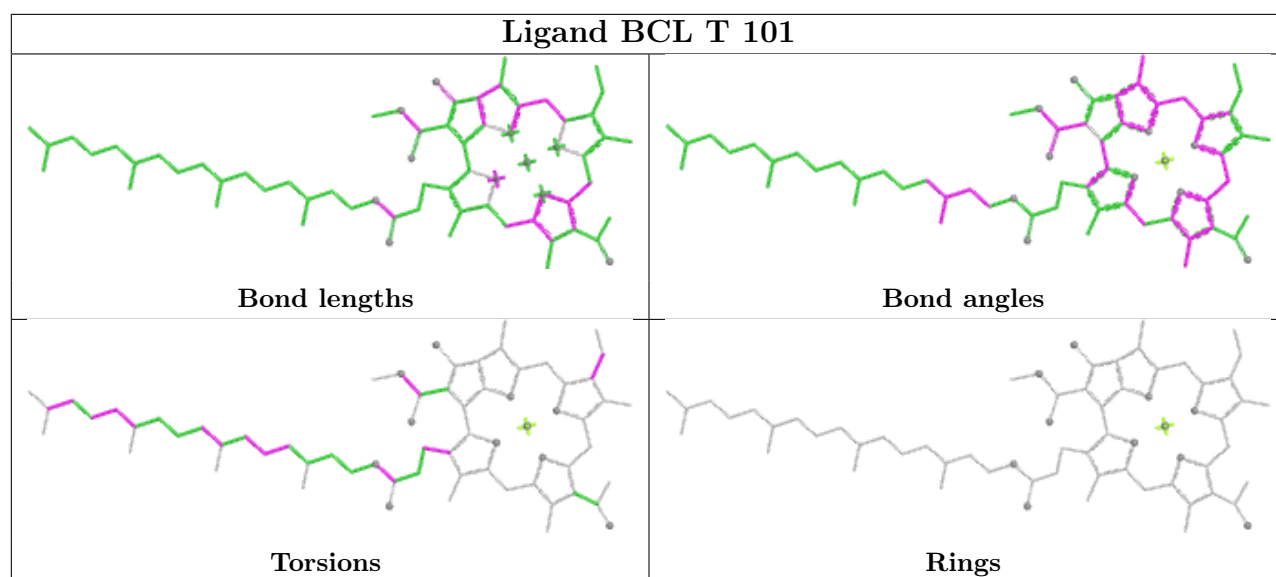
| Ligand BCL I 101                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand Z41 C 407                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMT 2 104                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

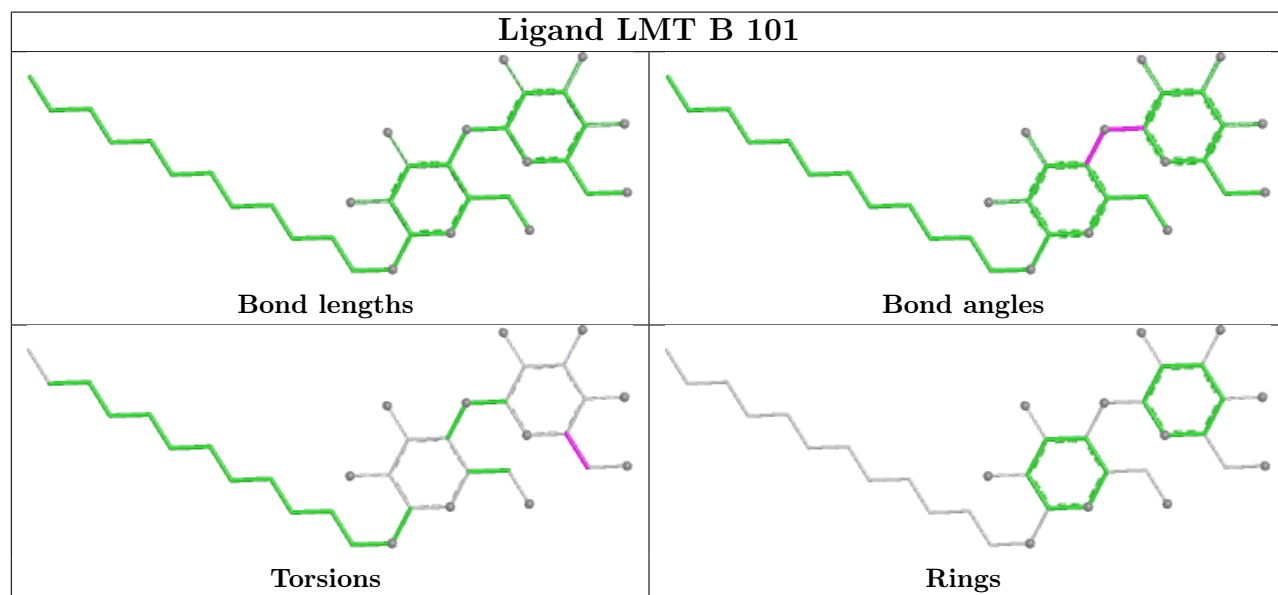
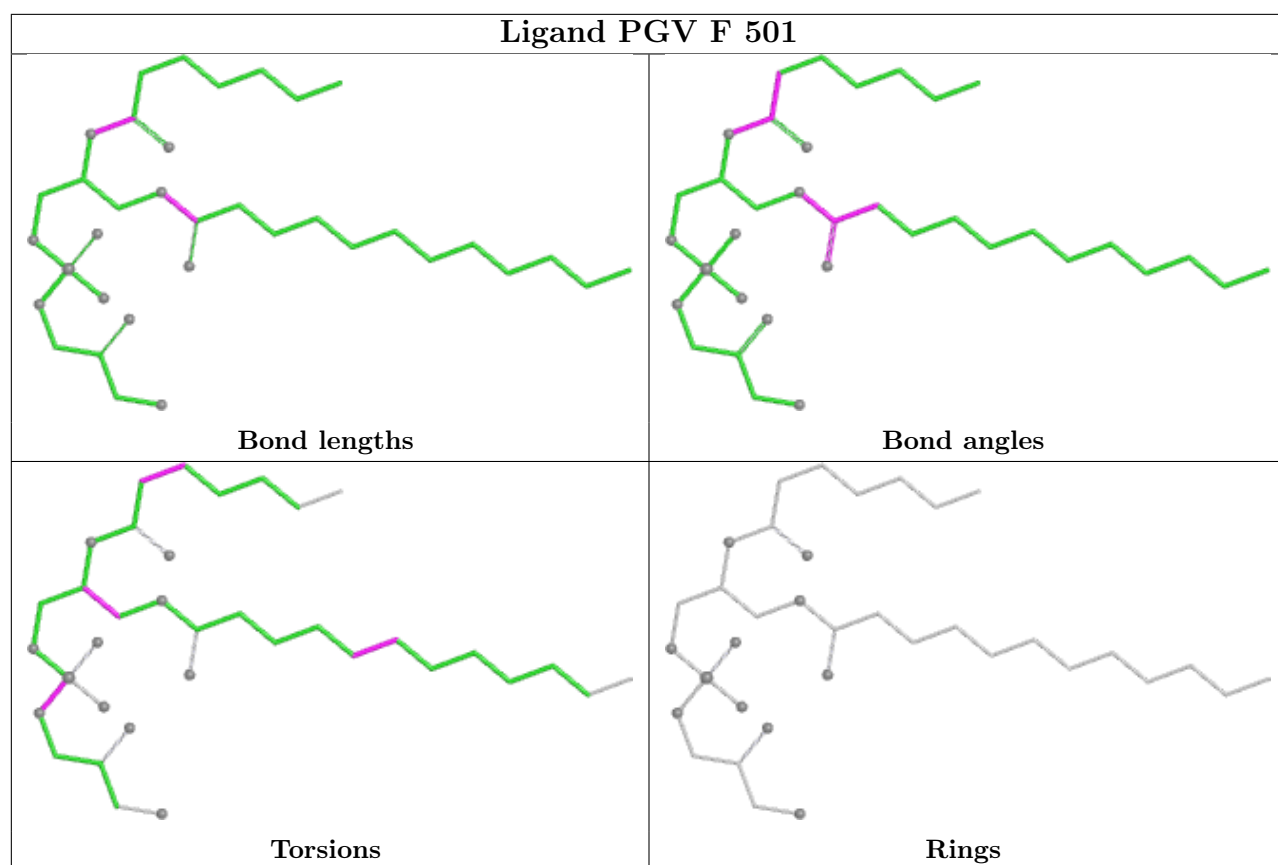


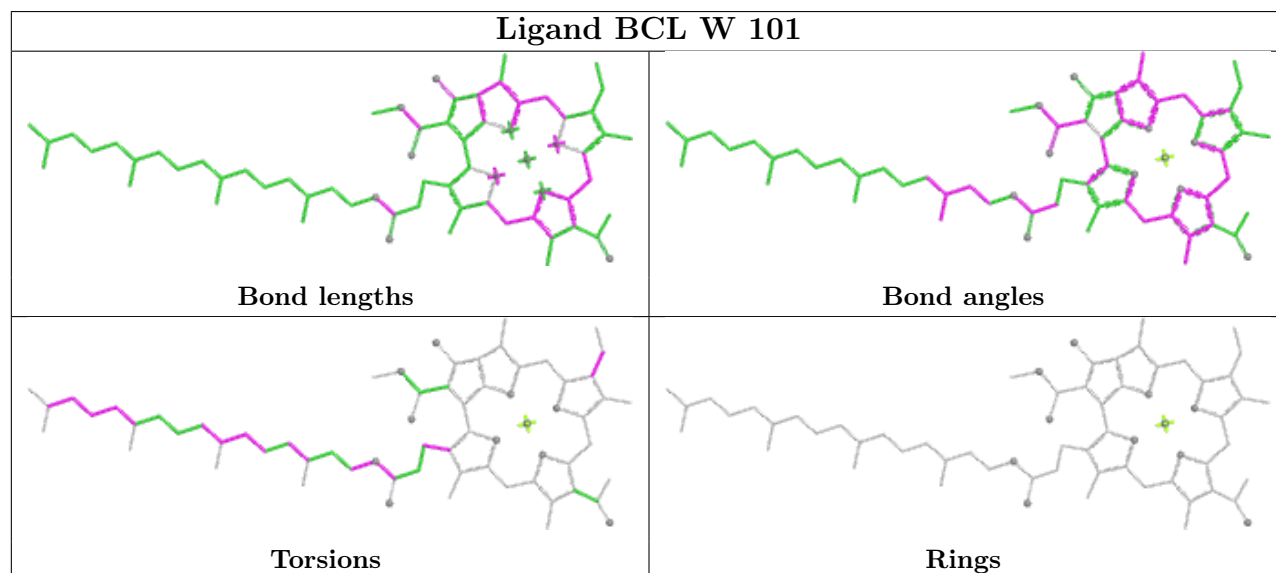
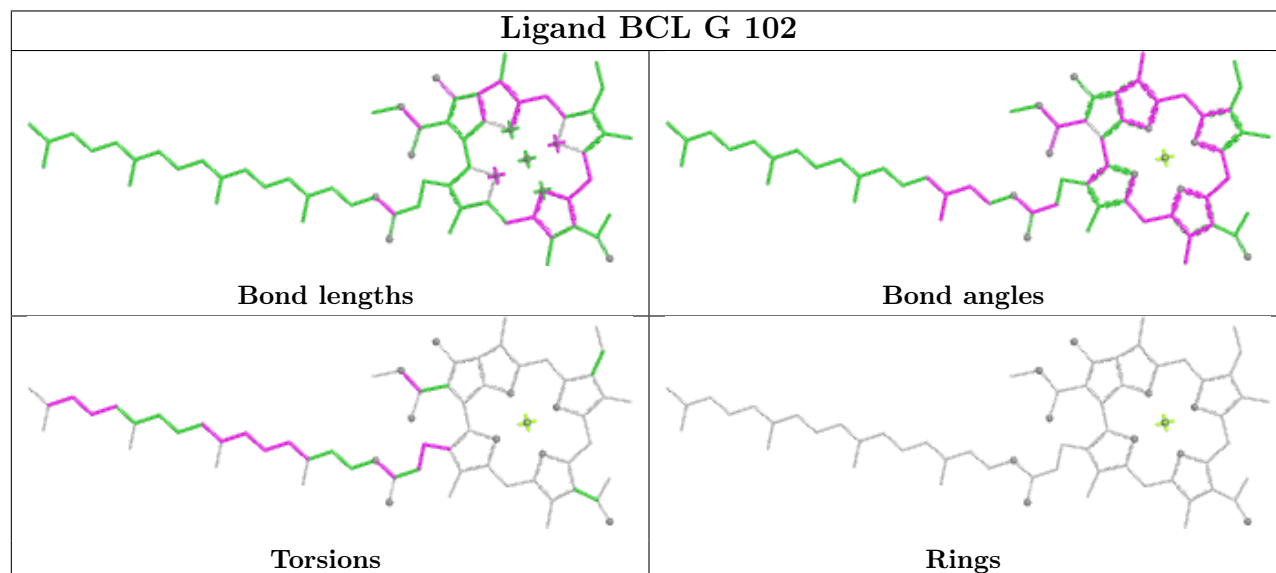
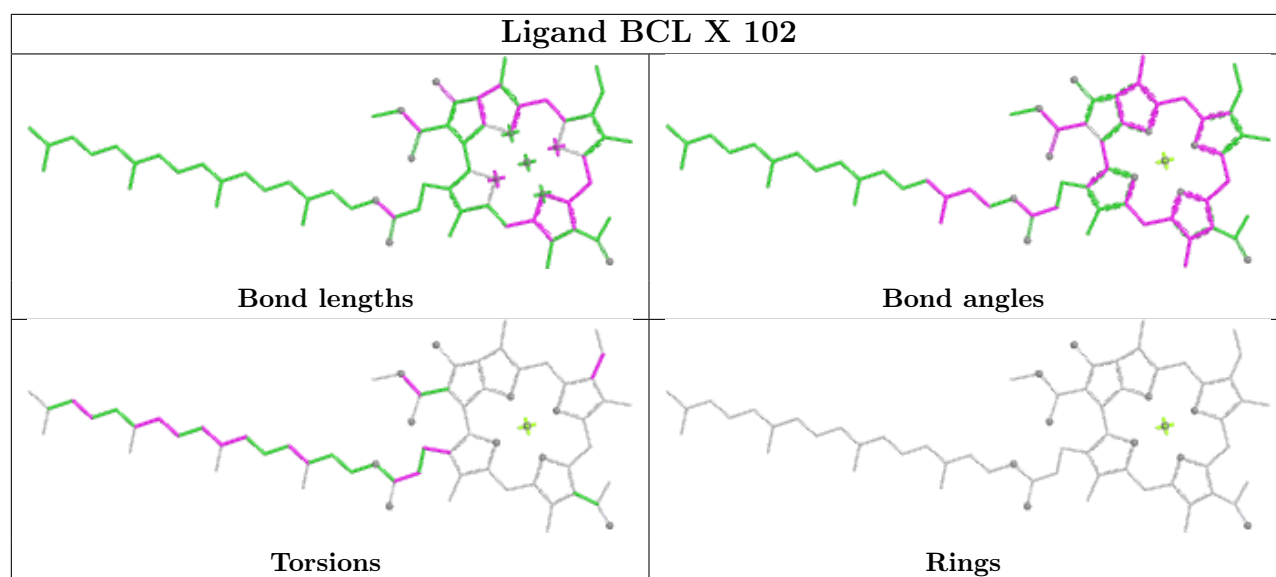


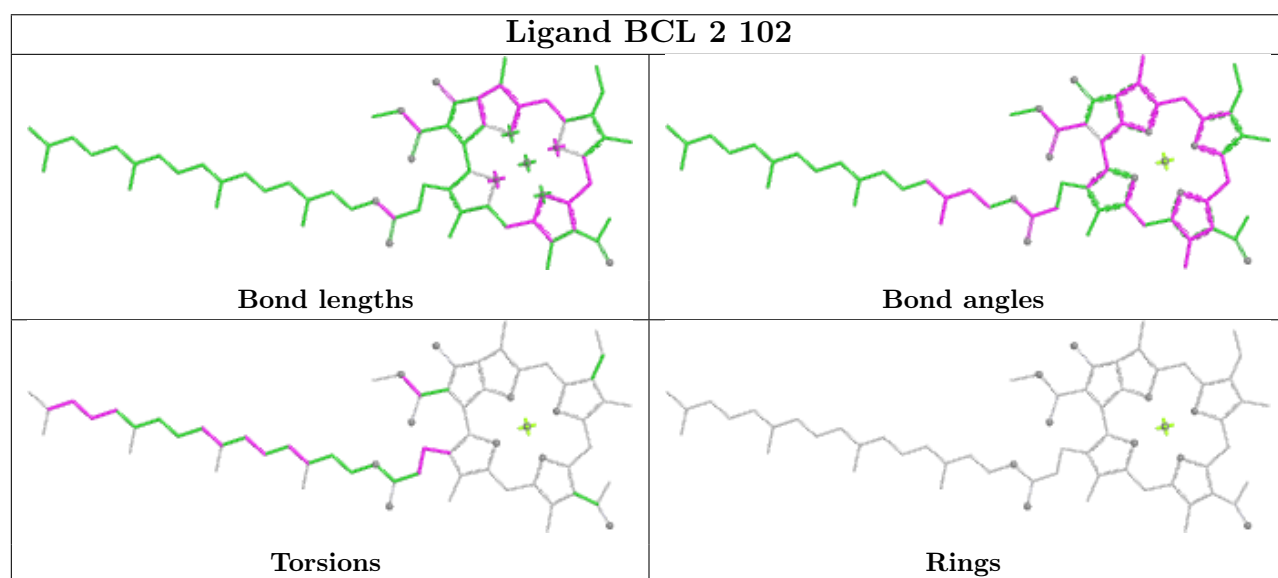
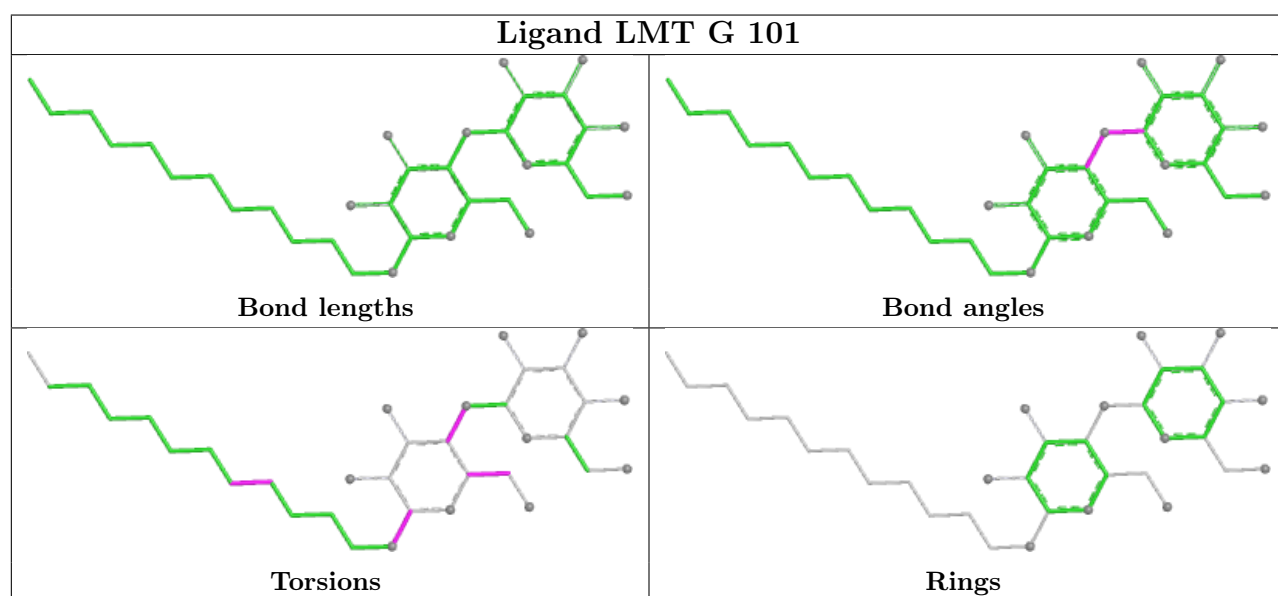
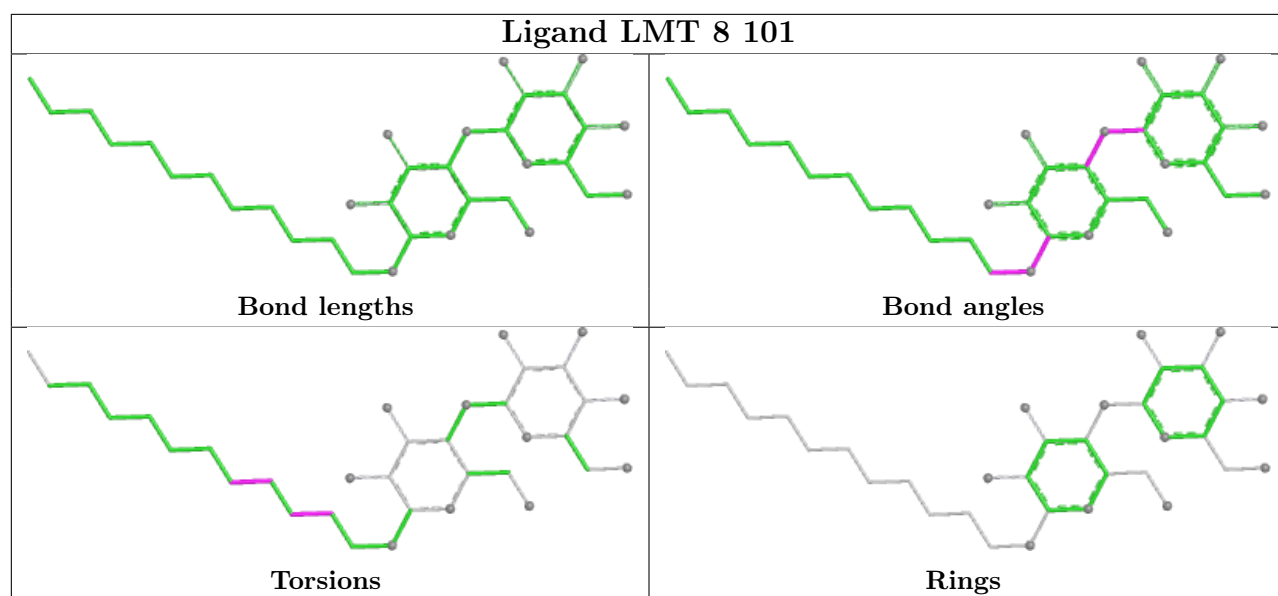


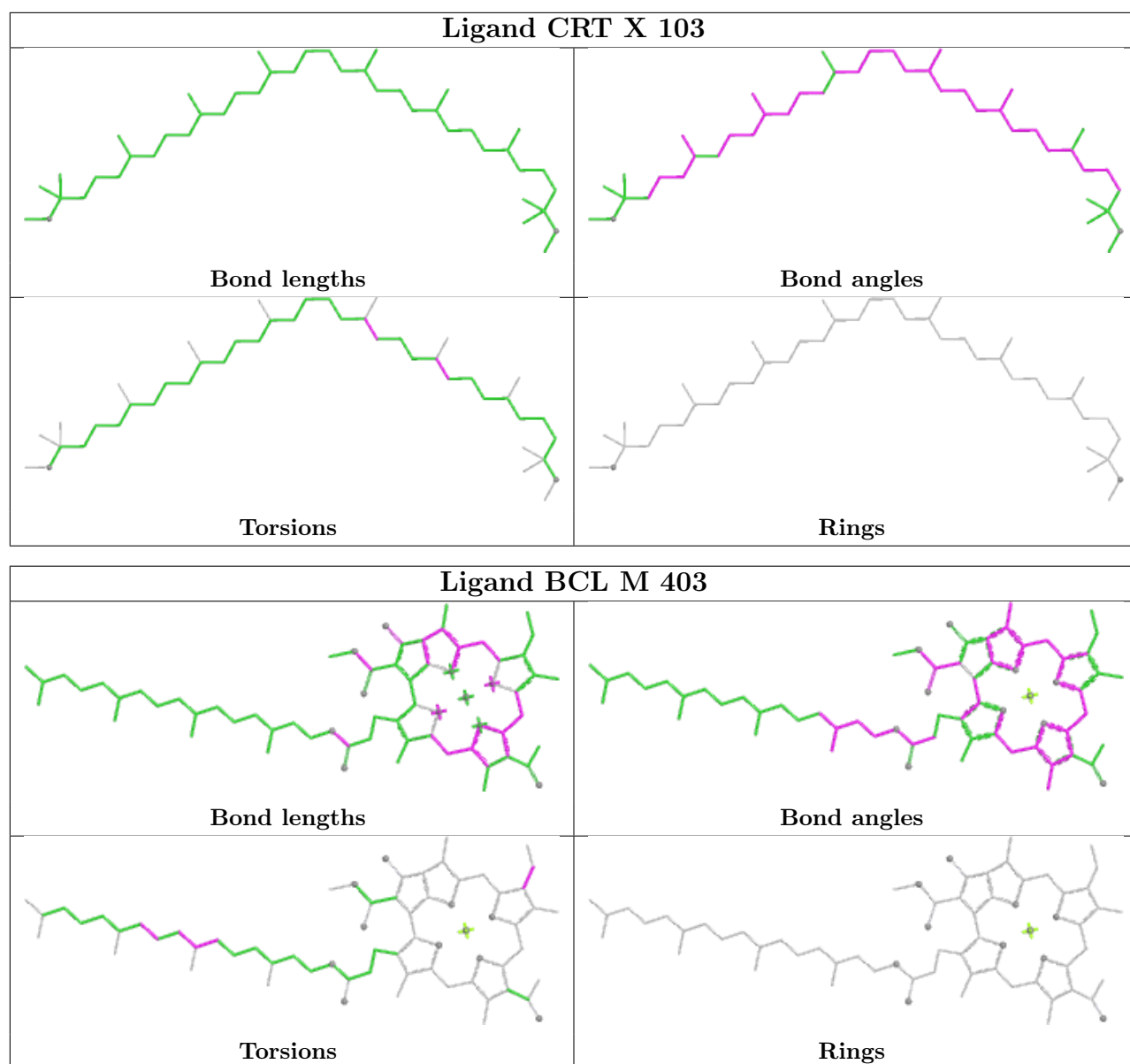


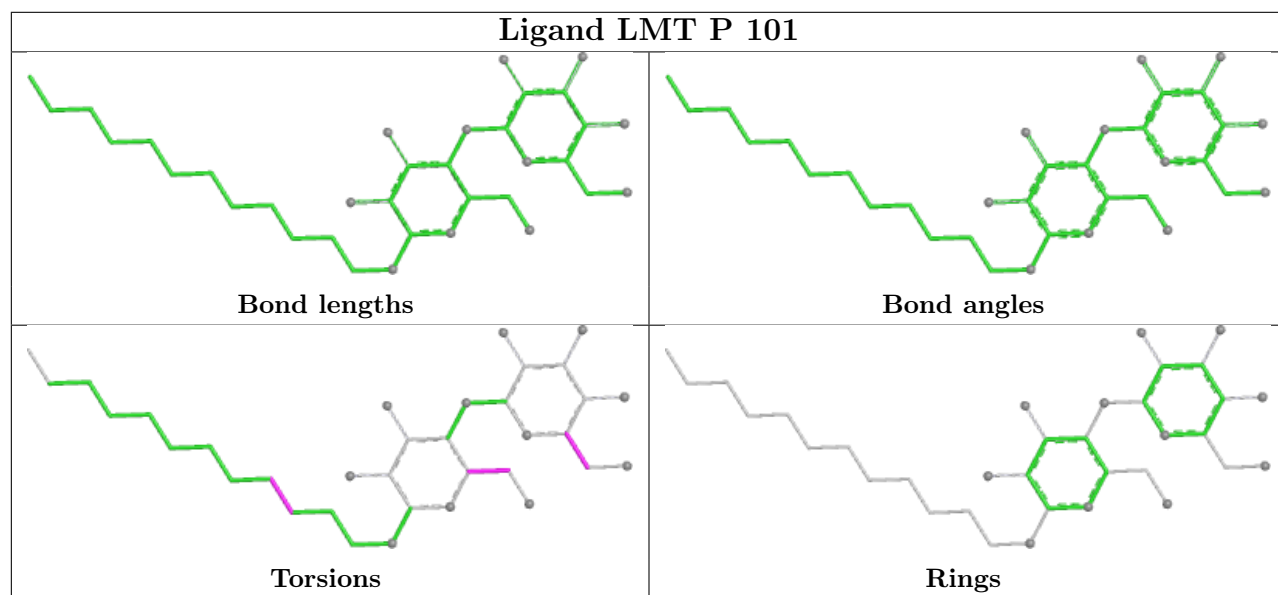
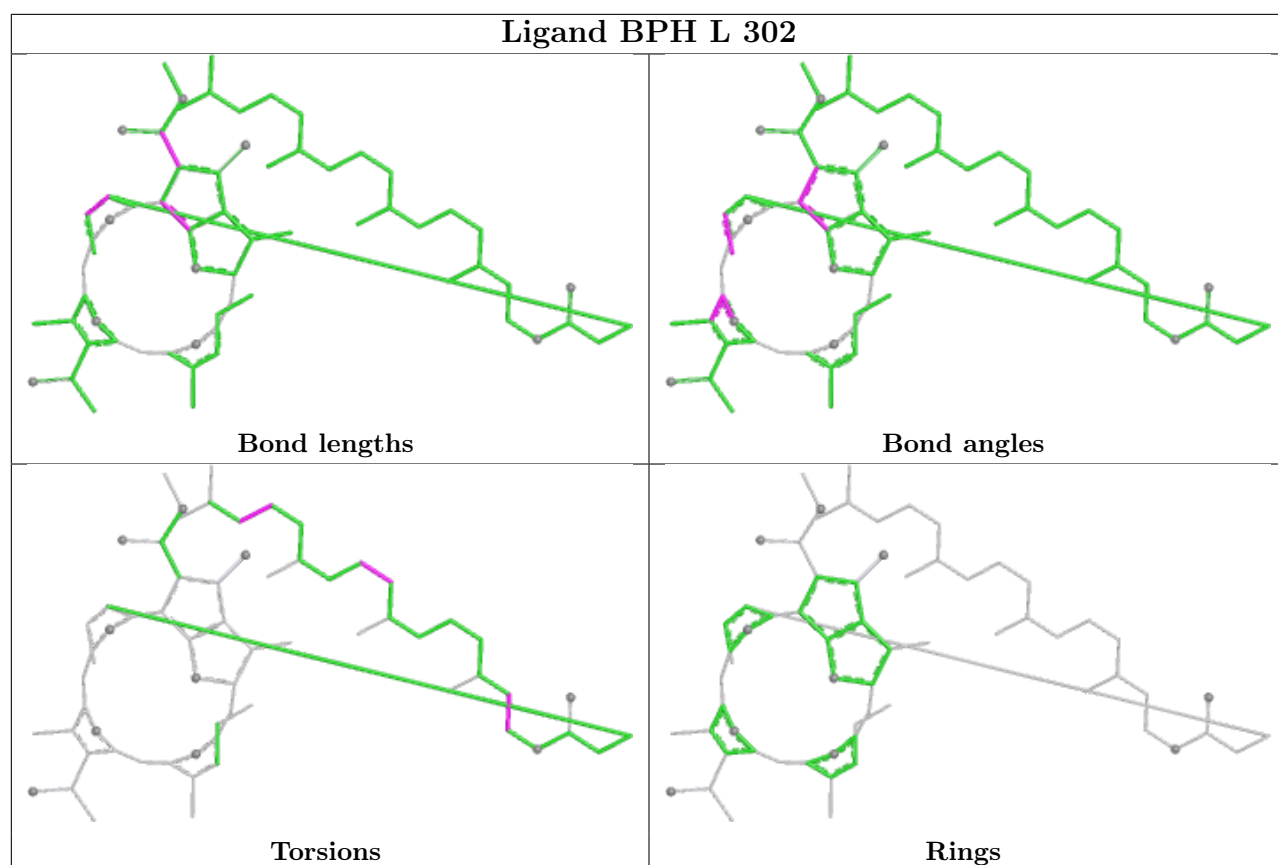


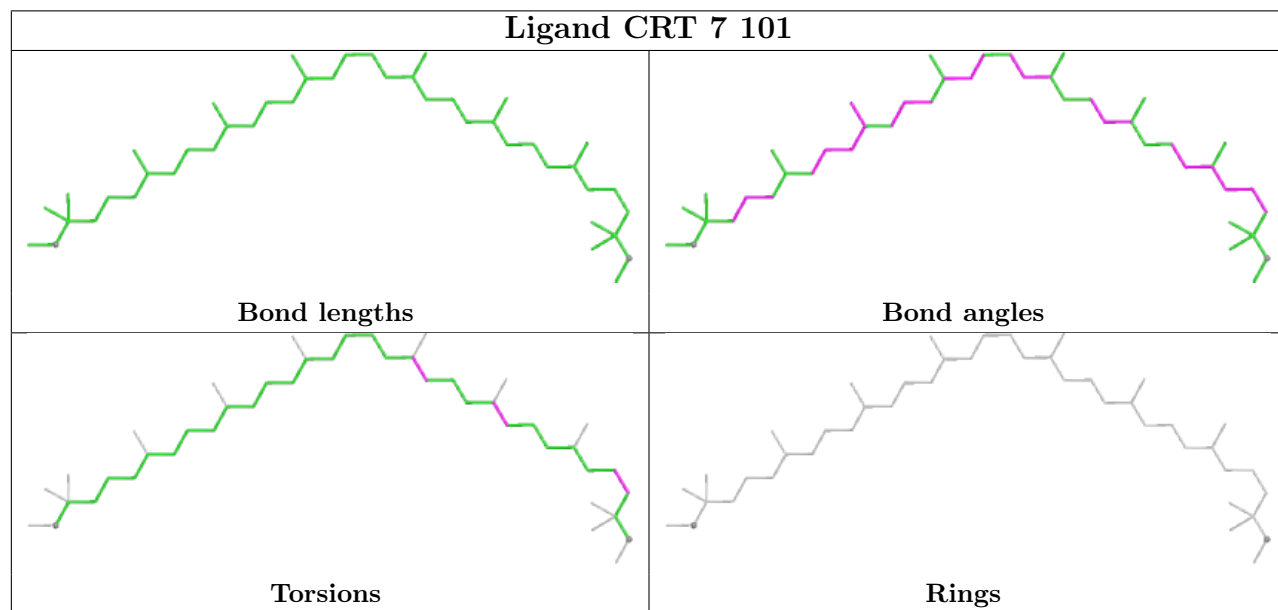
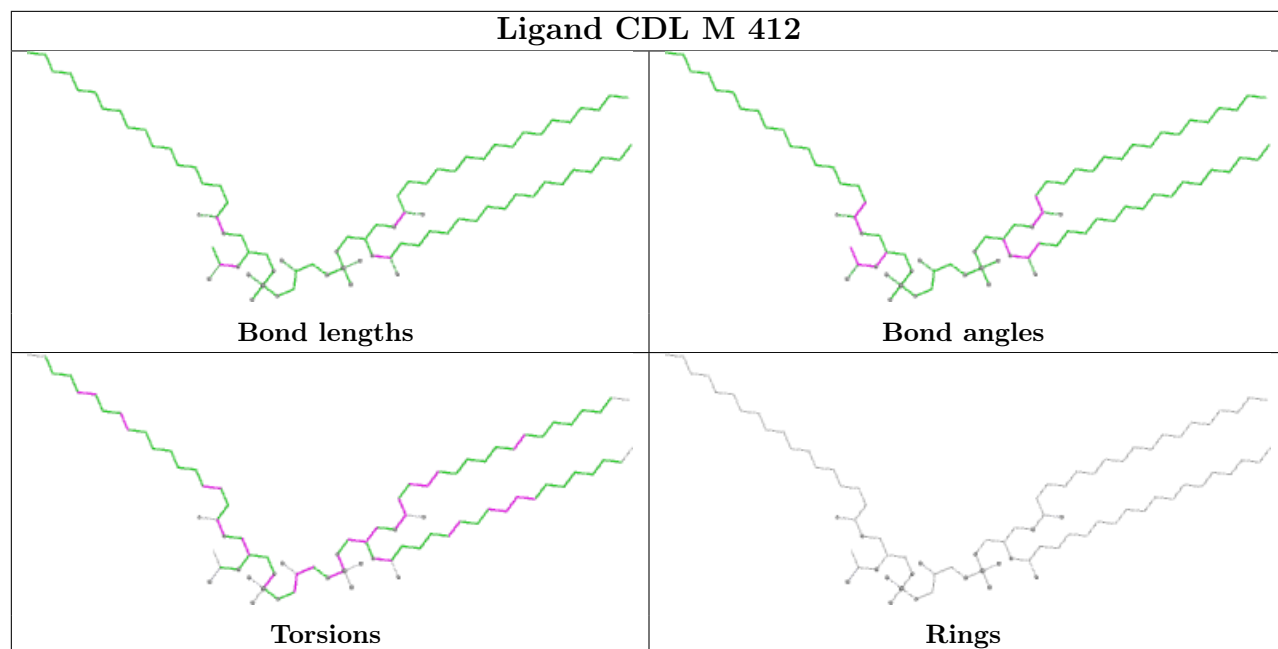


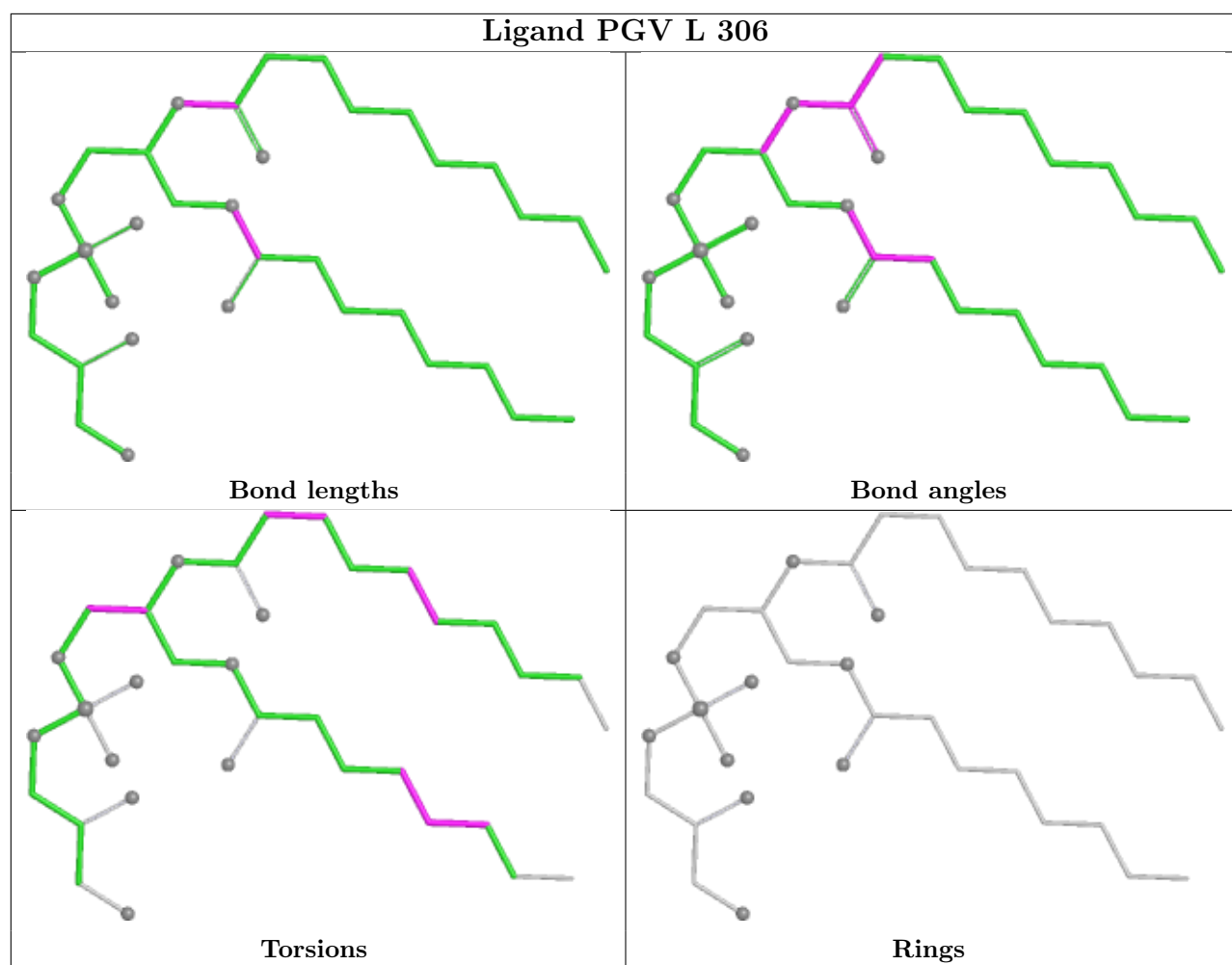


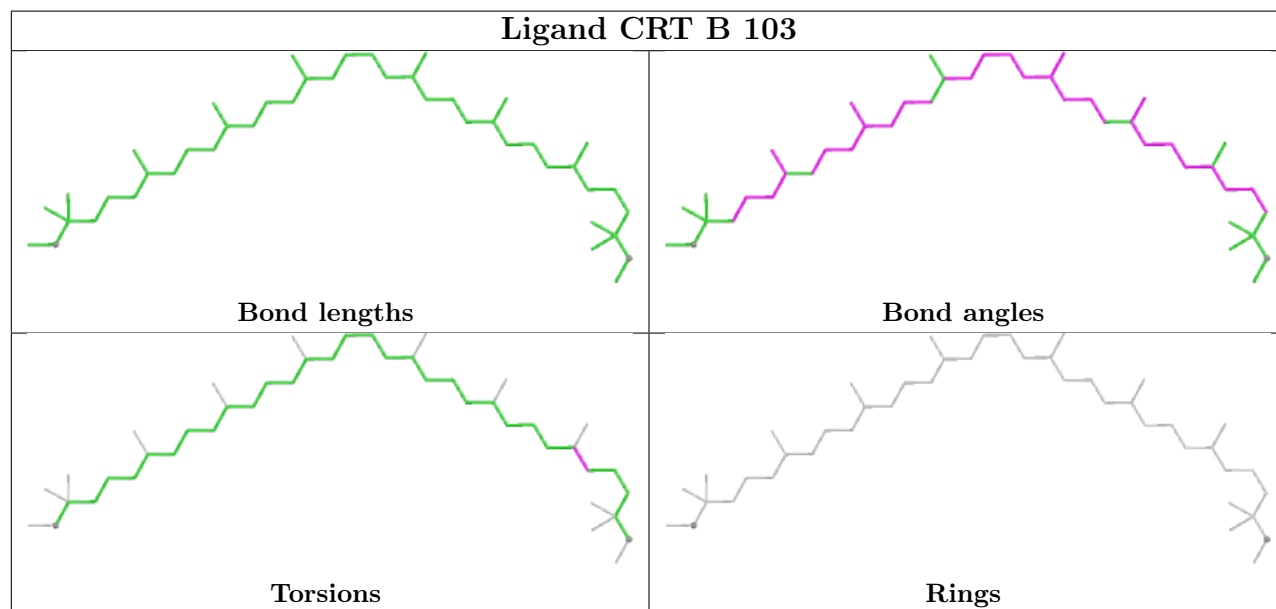
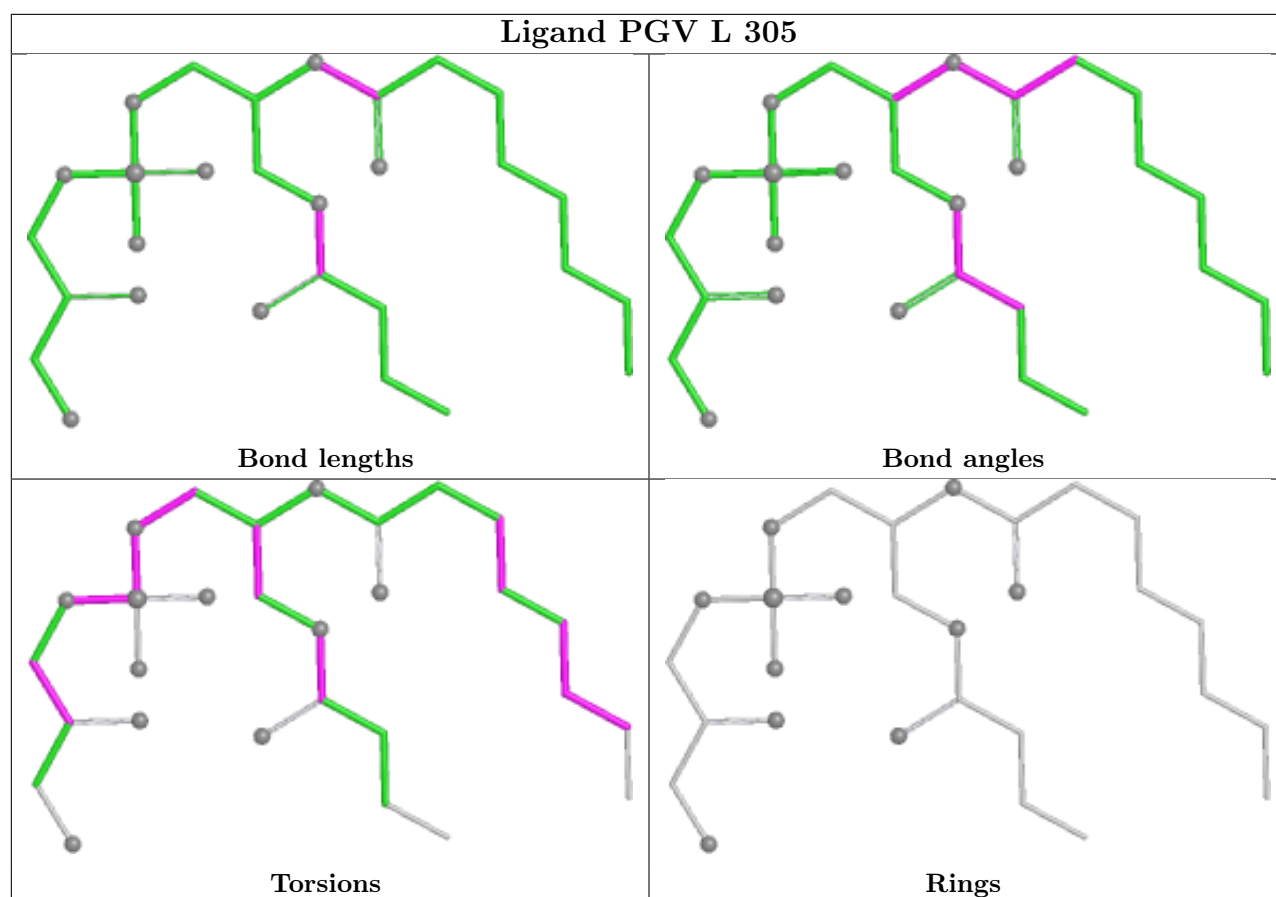


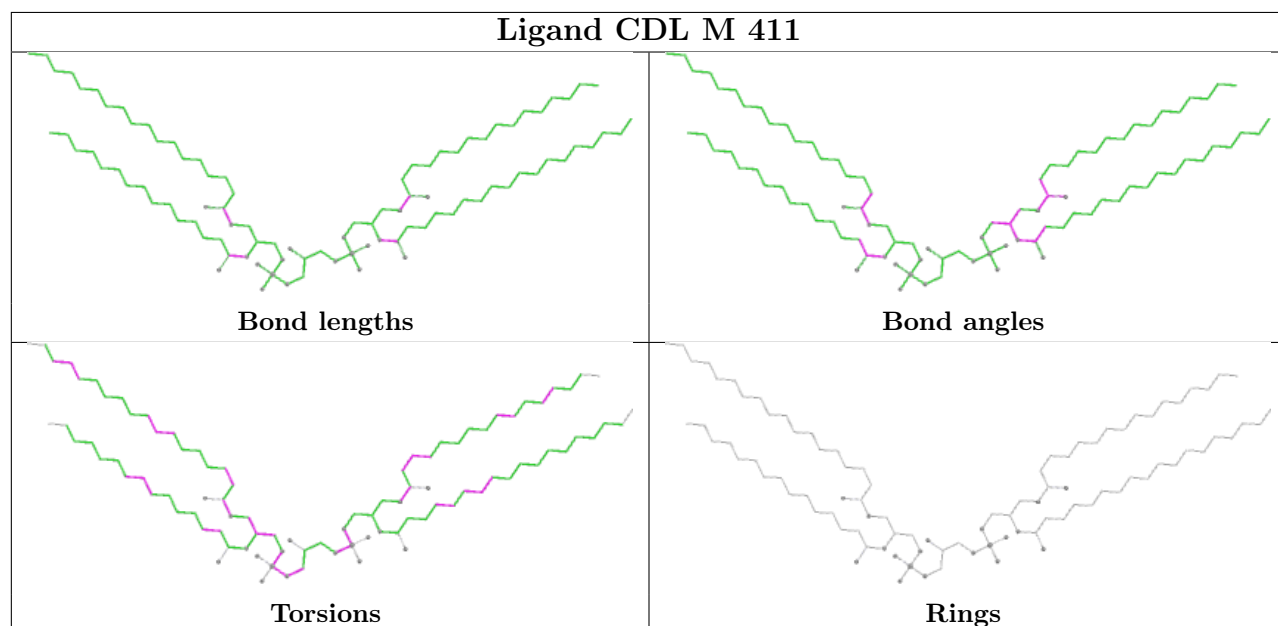
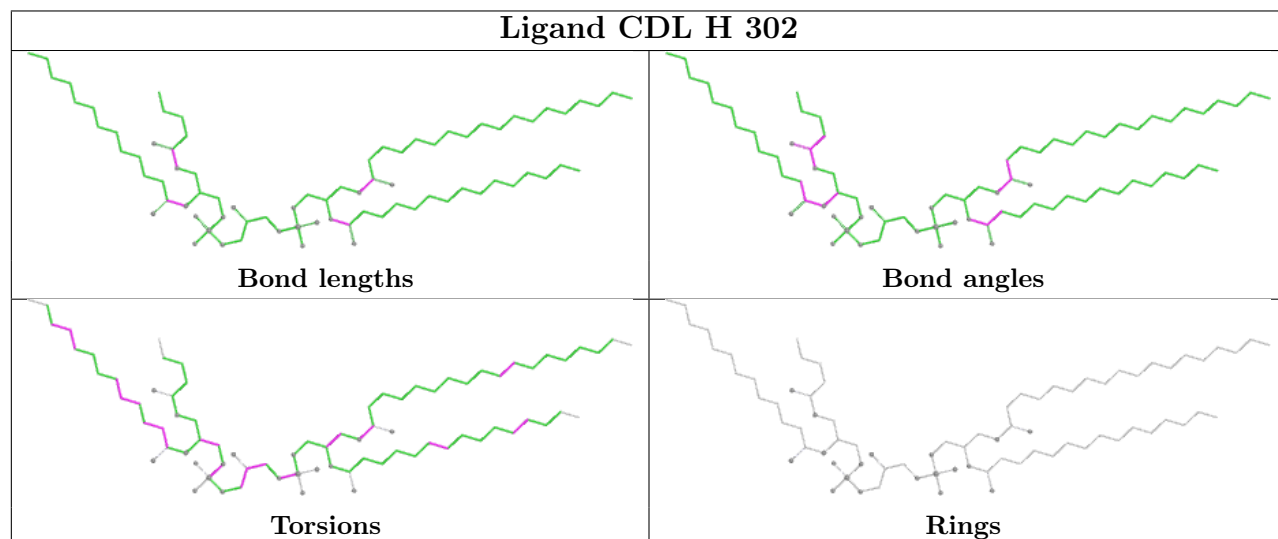
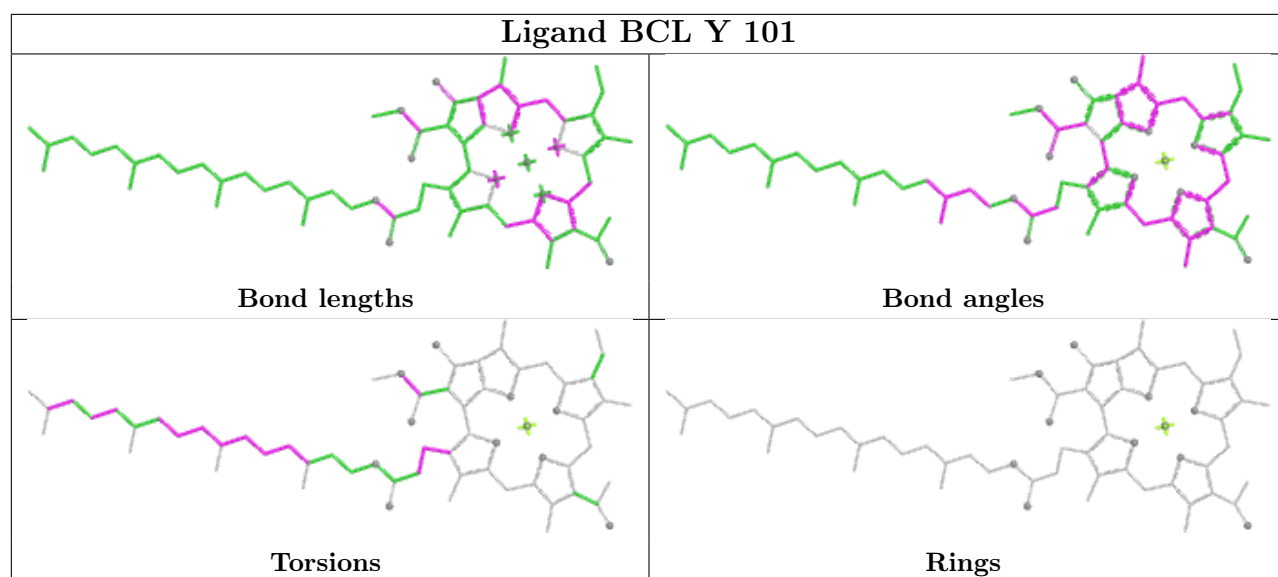


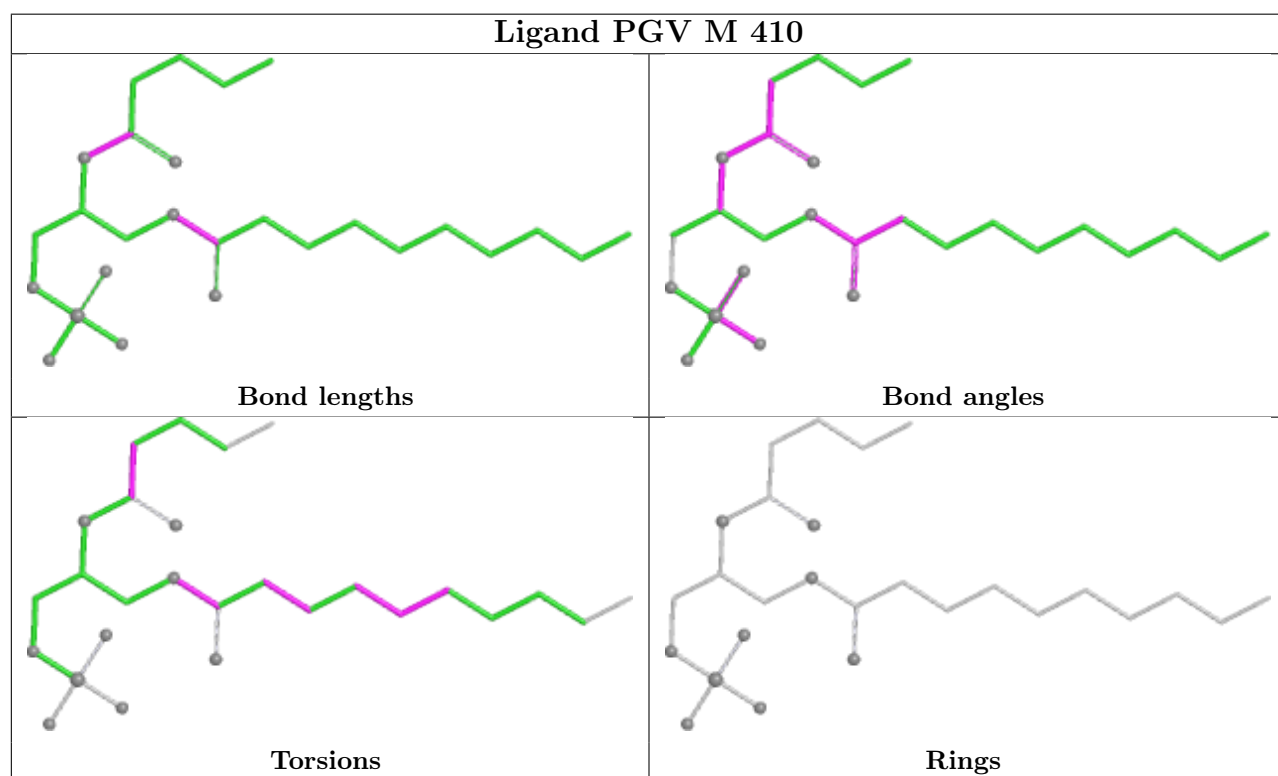
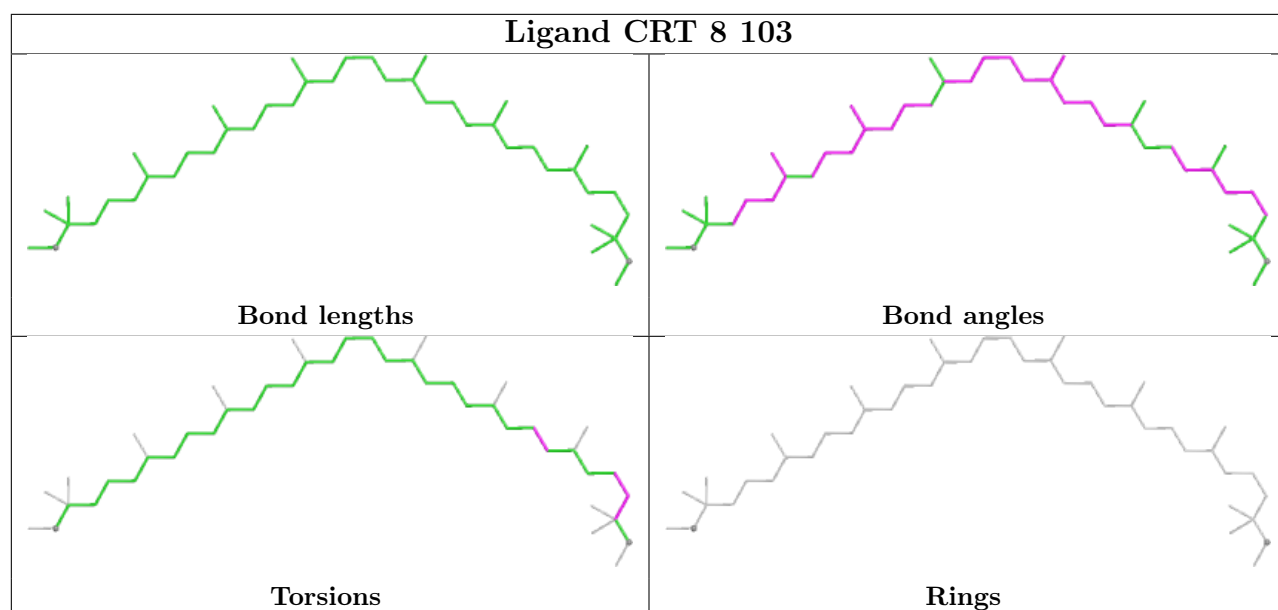


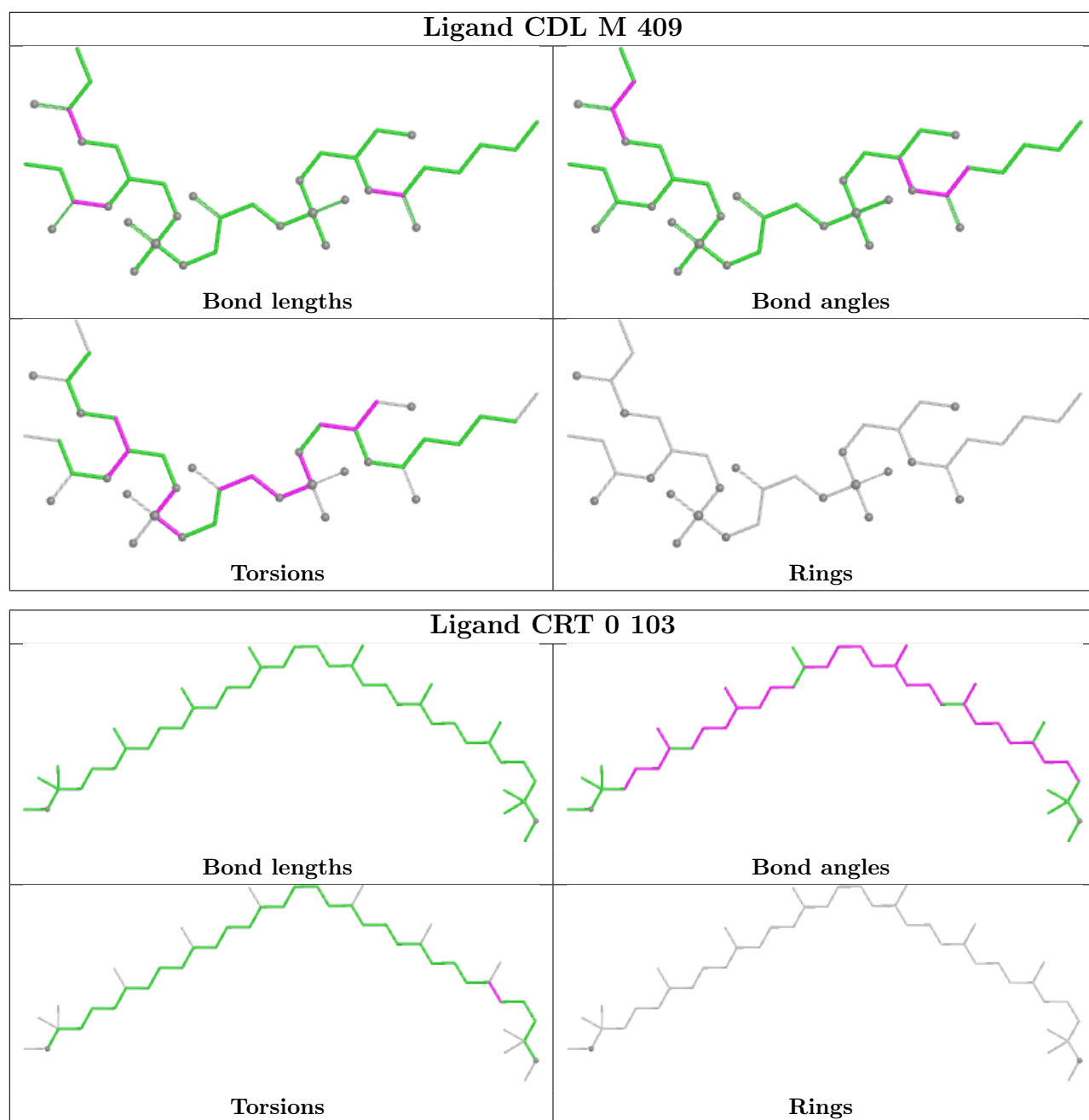


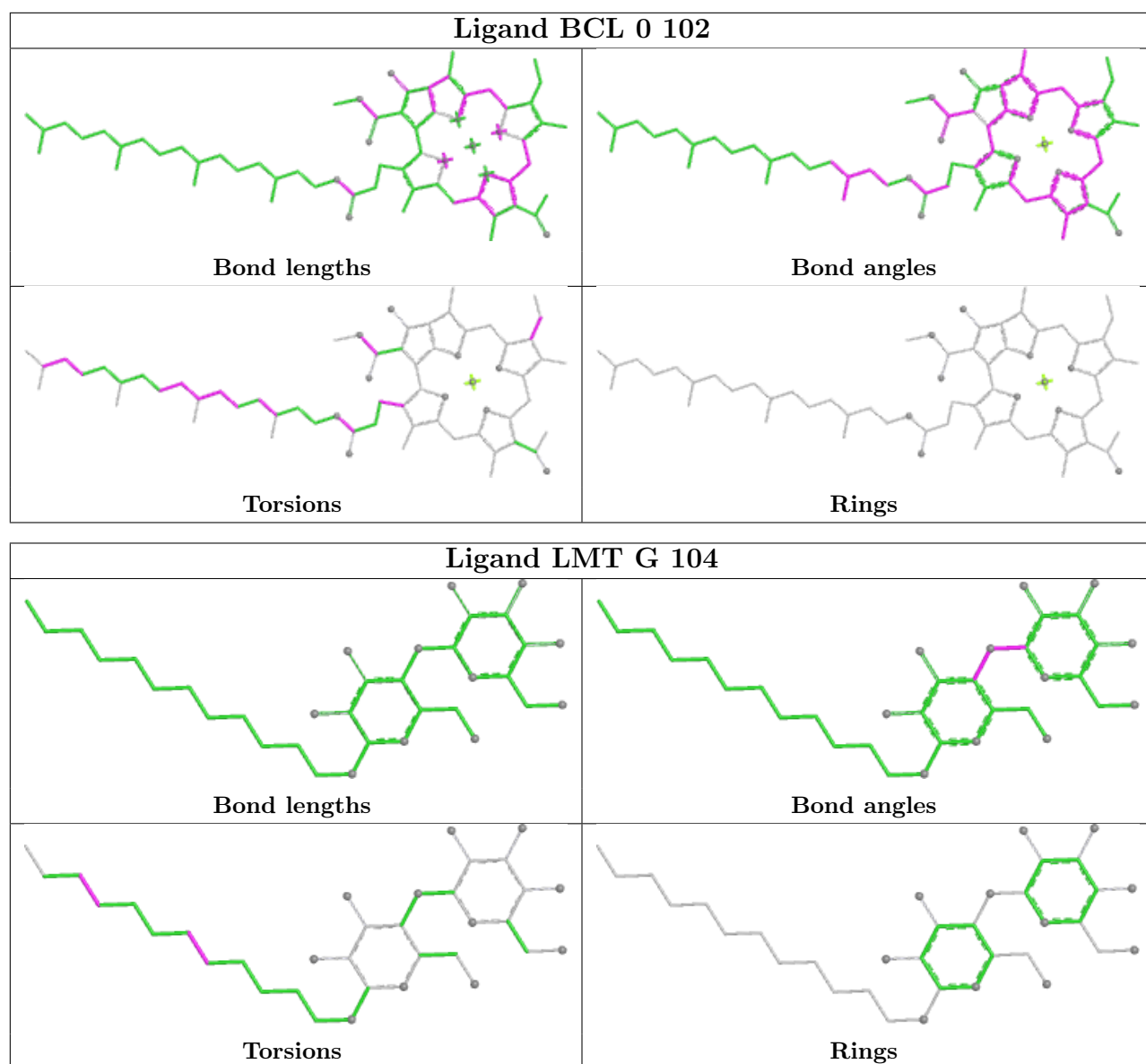


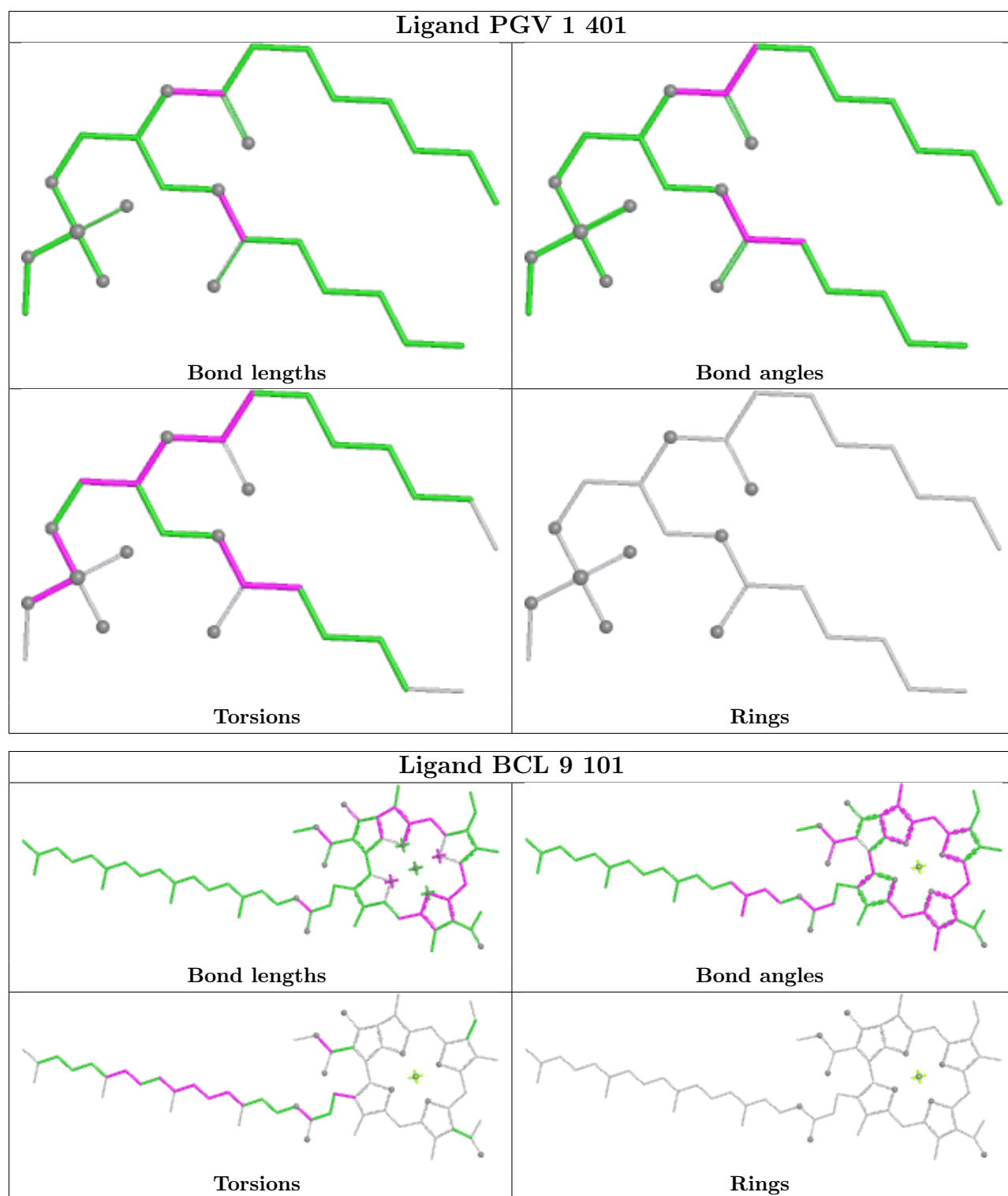


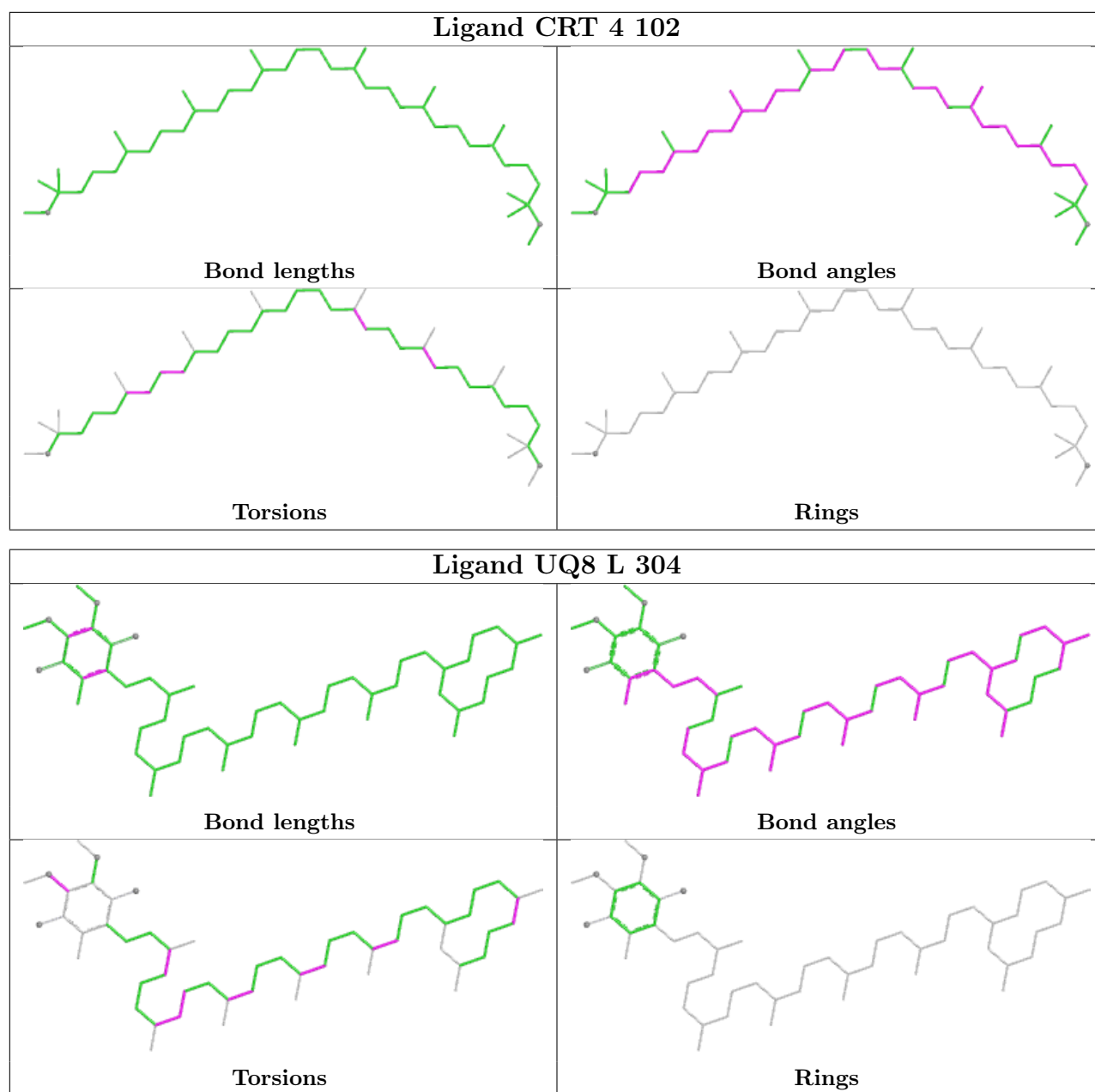


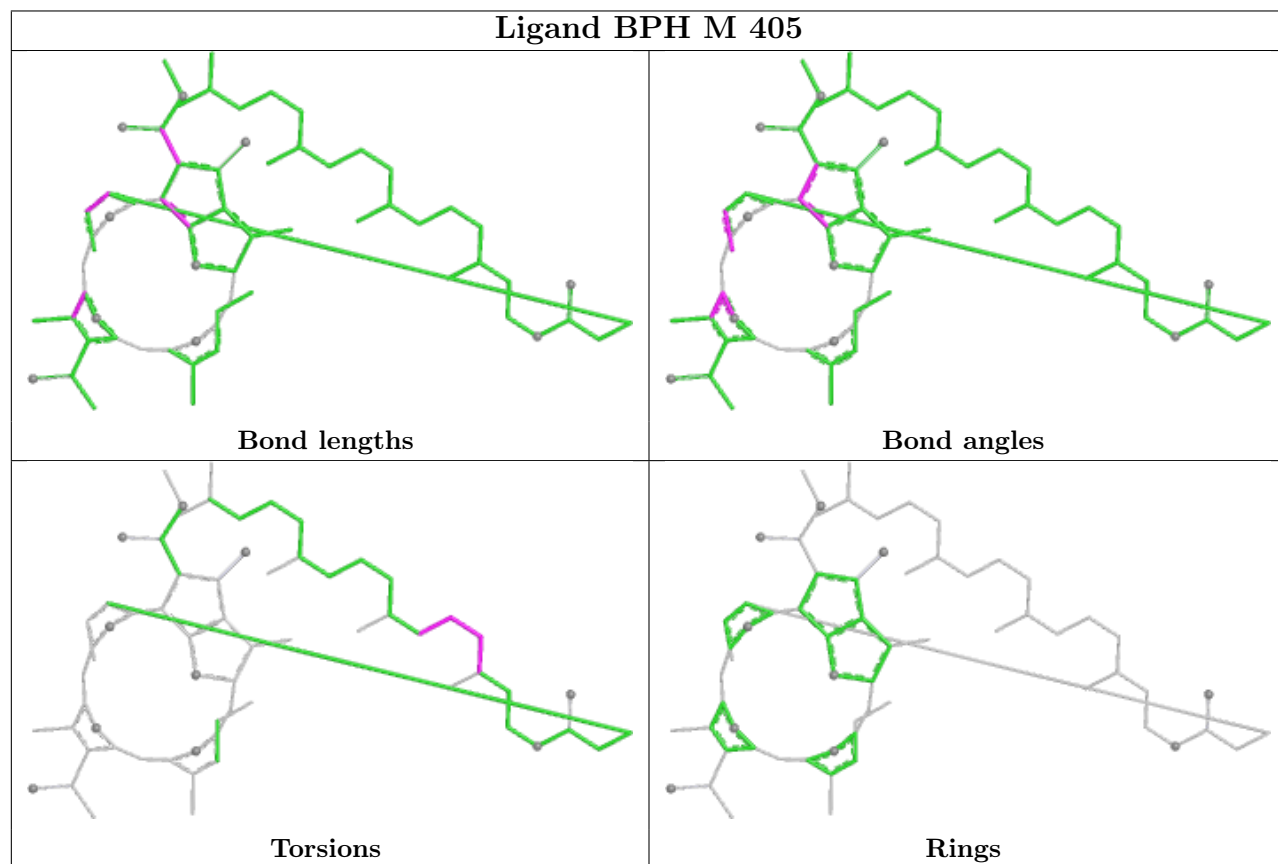
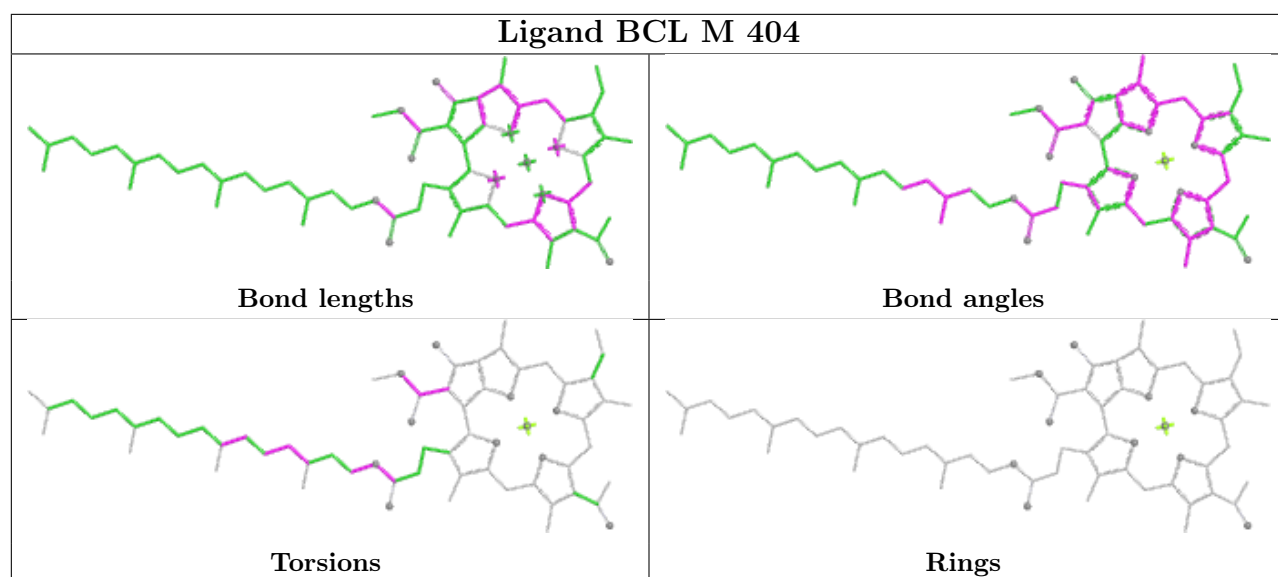


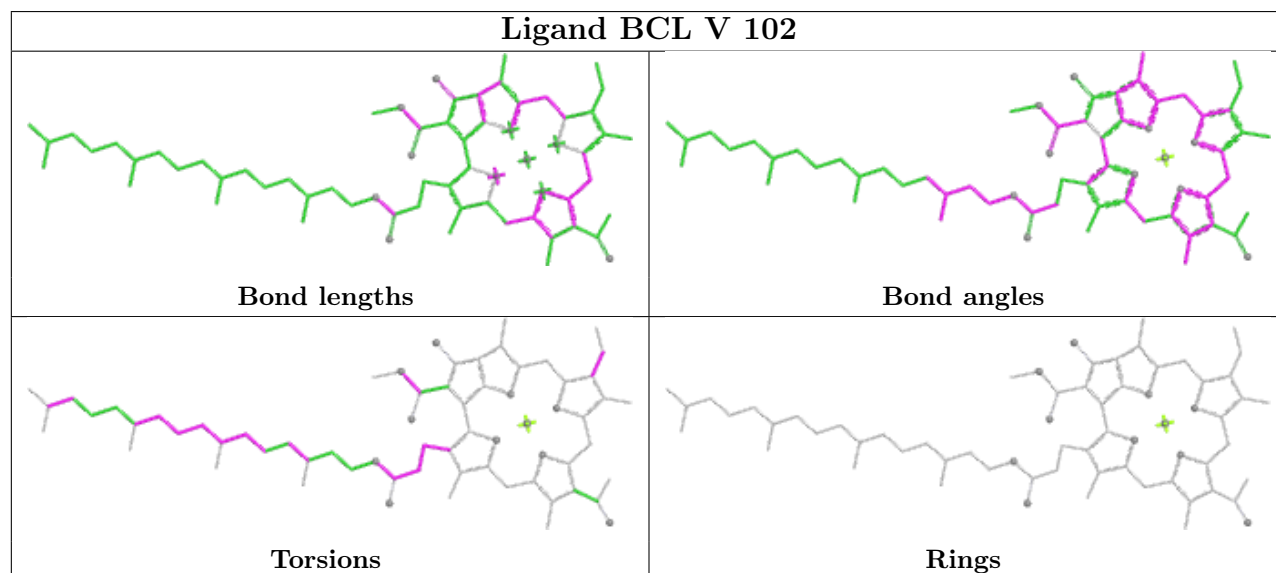
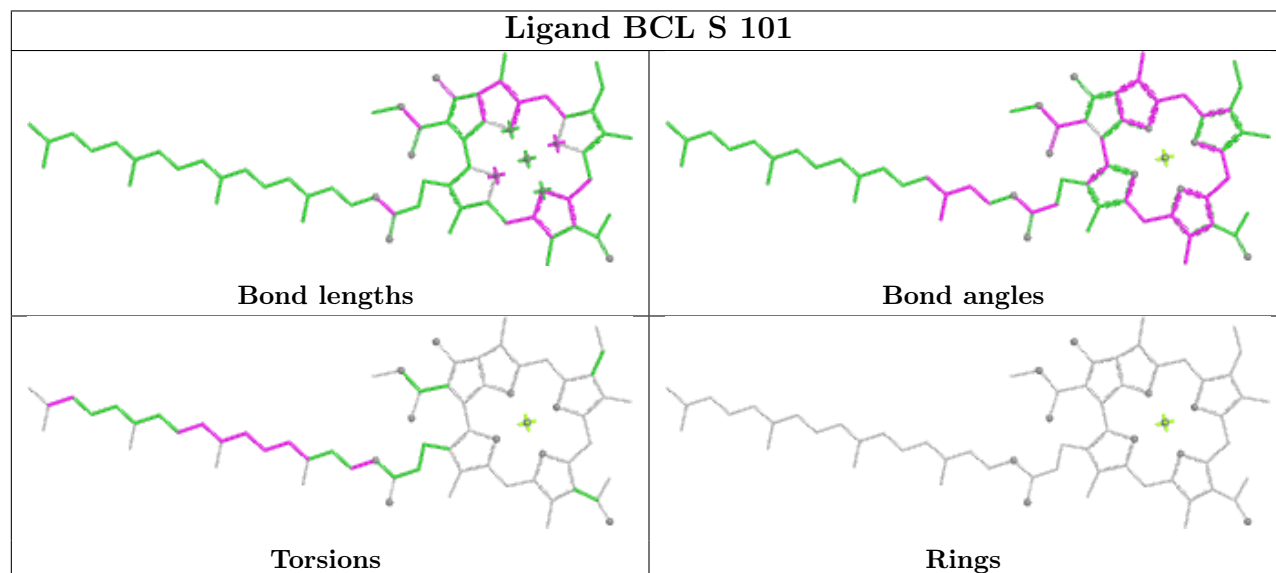
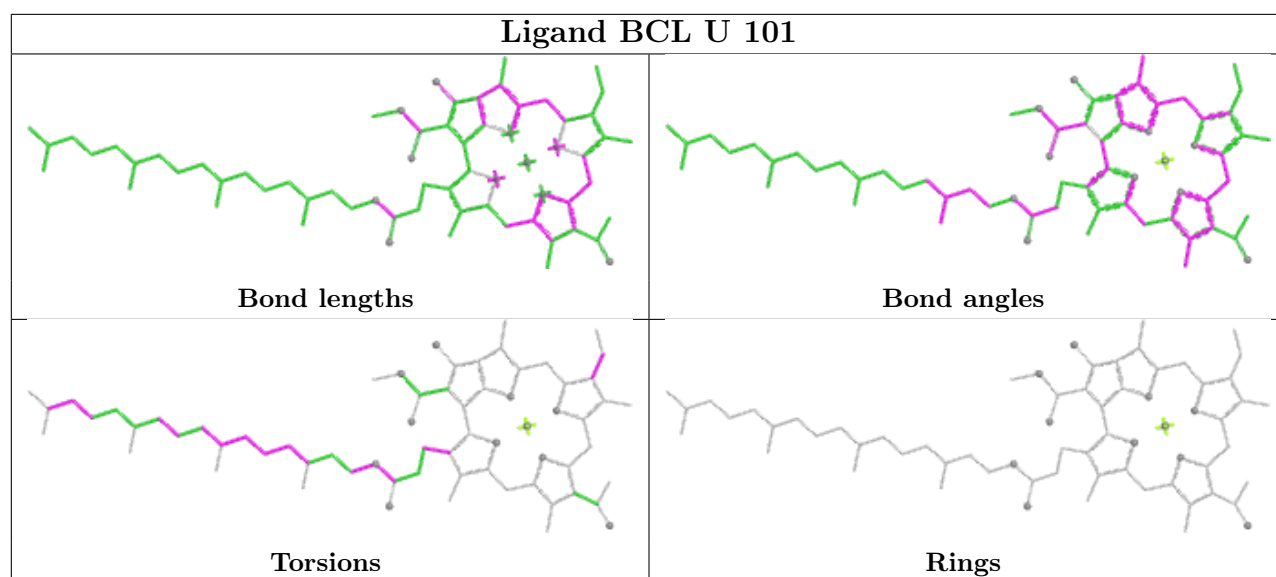


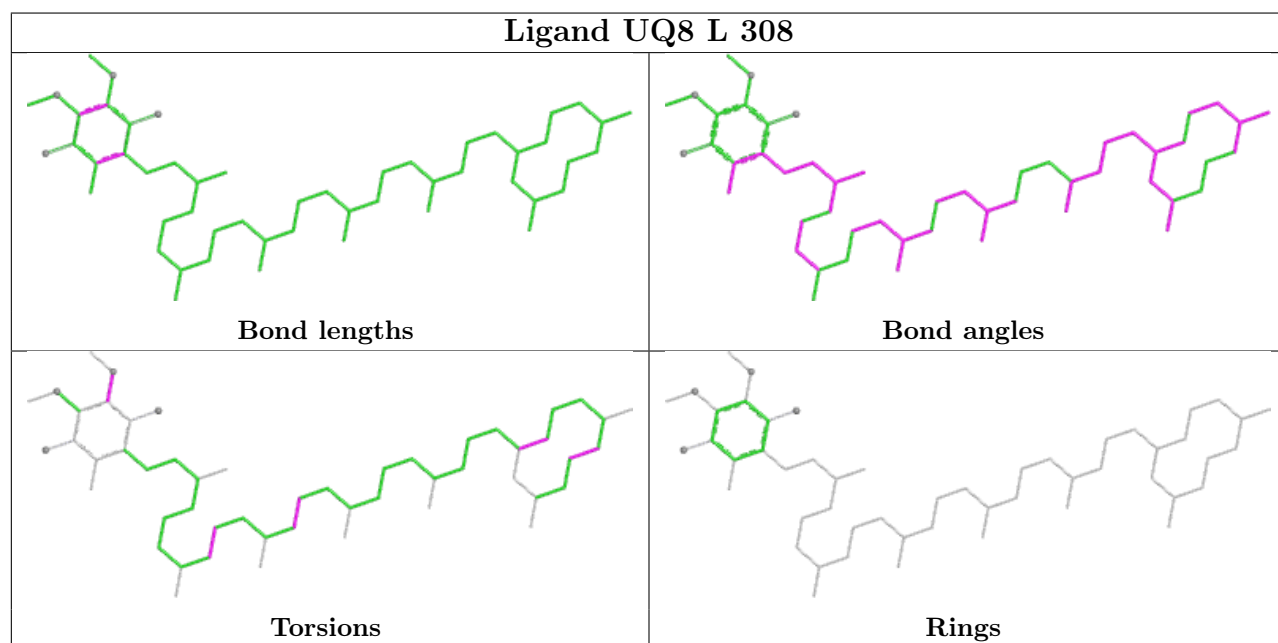
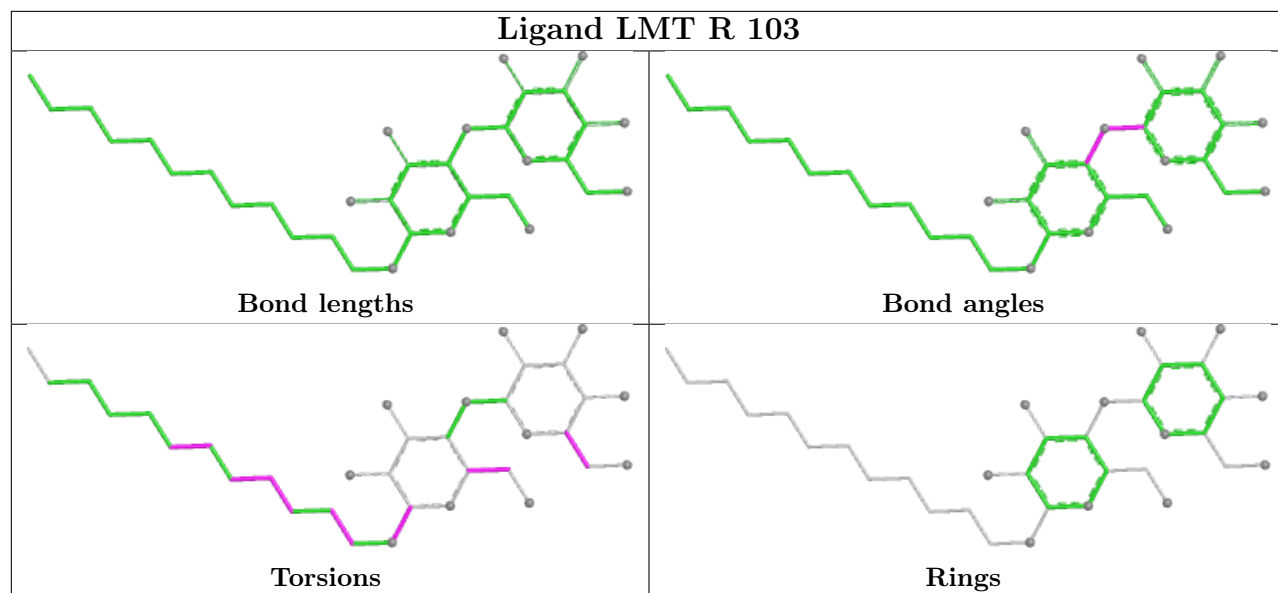


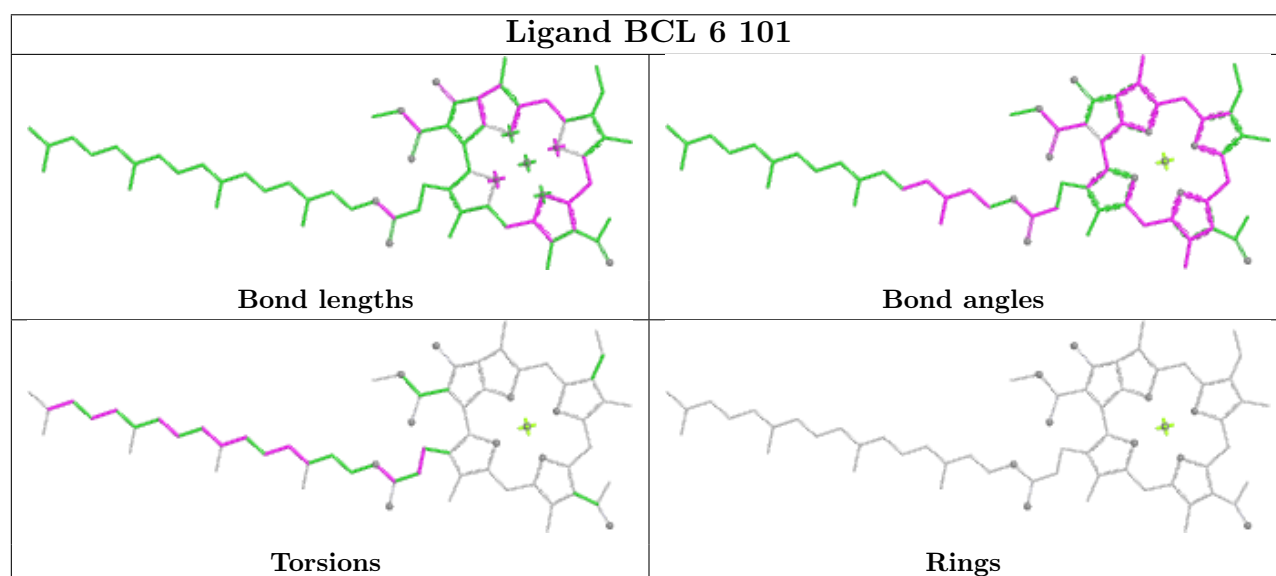
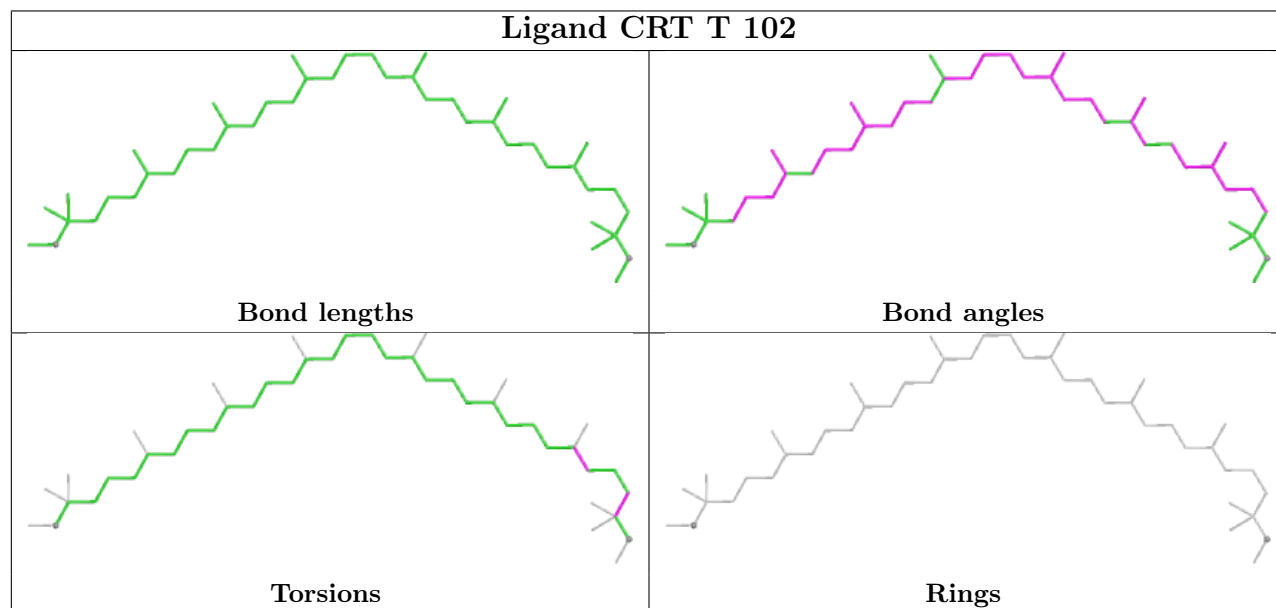
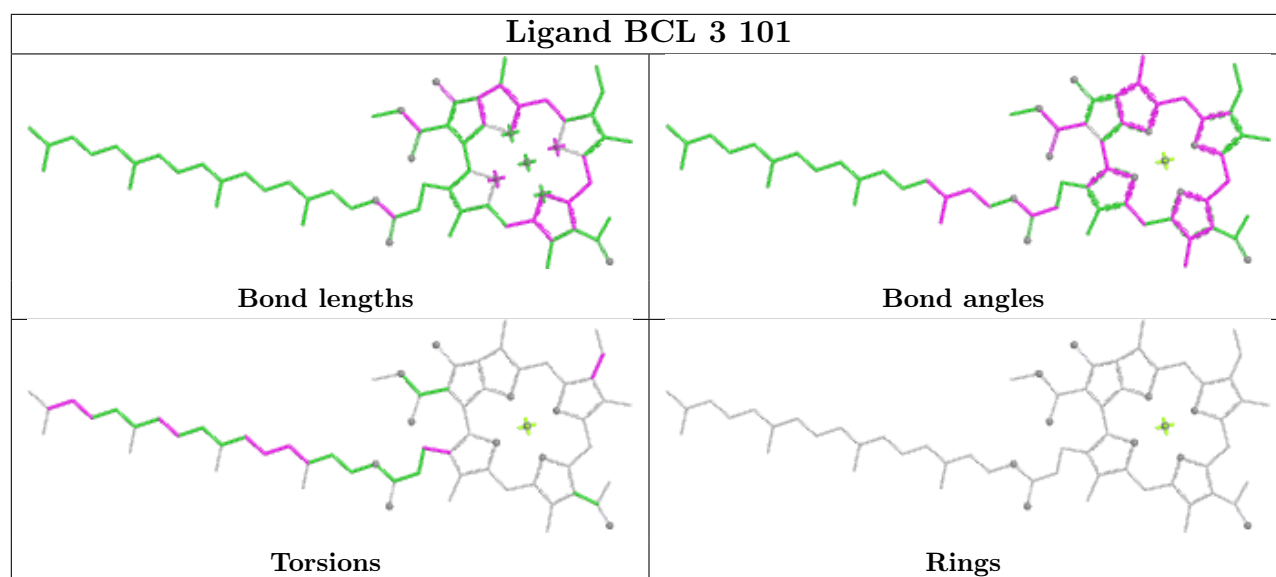


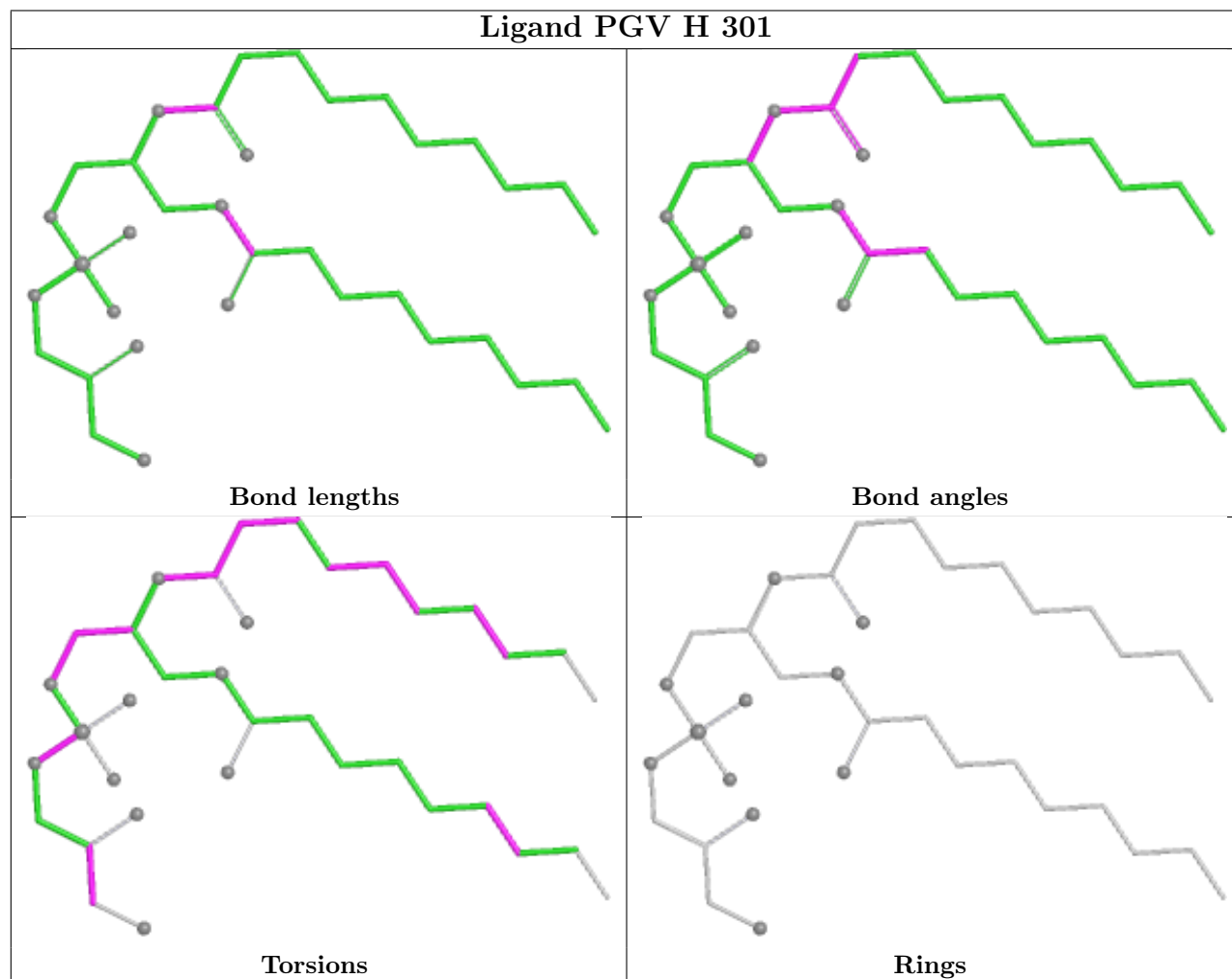
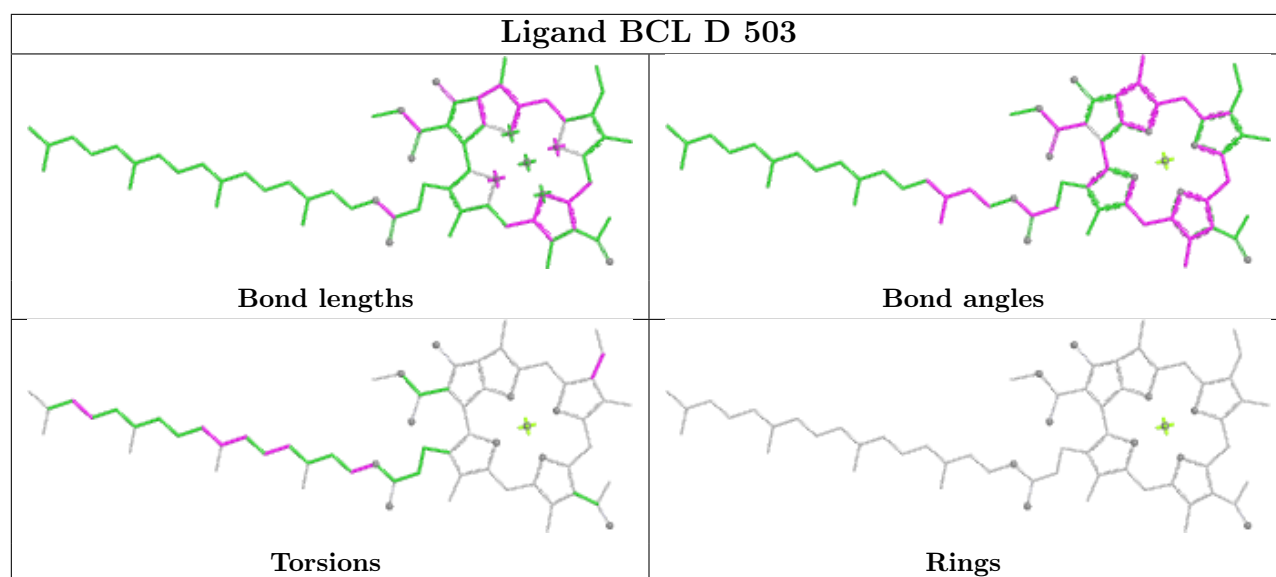


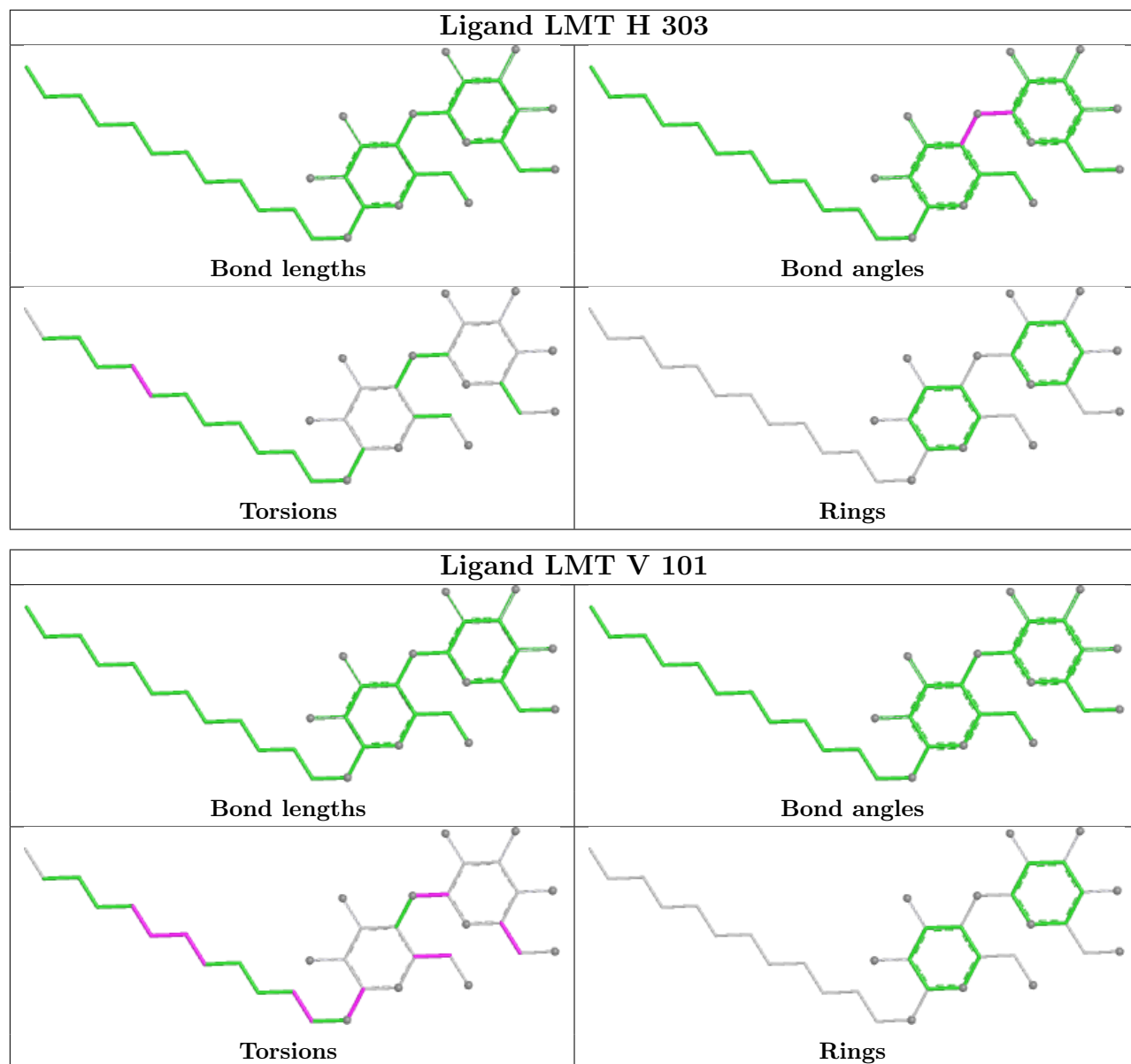


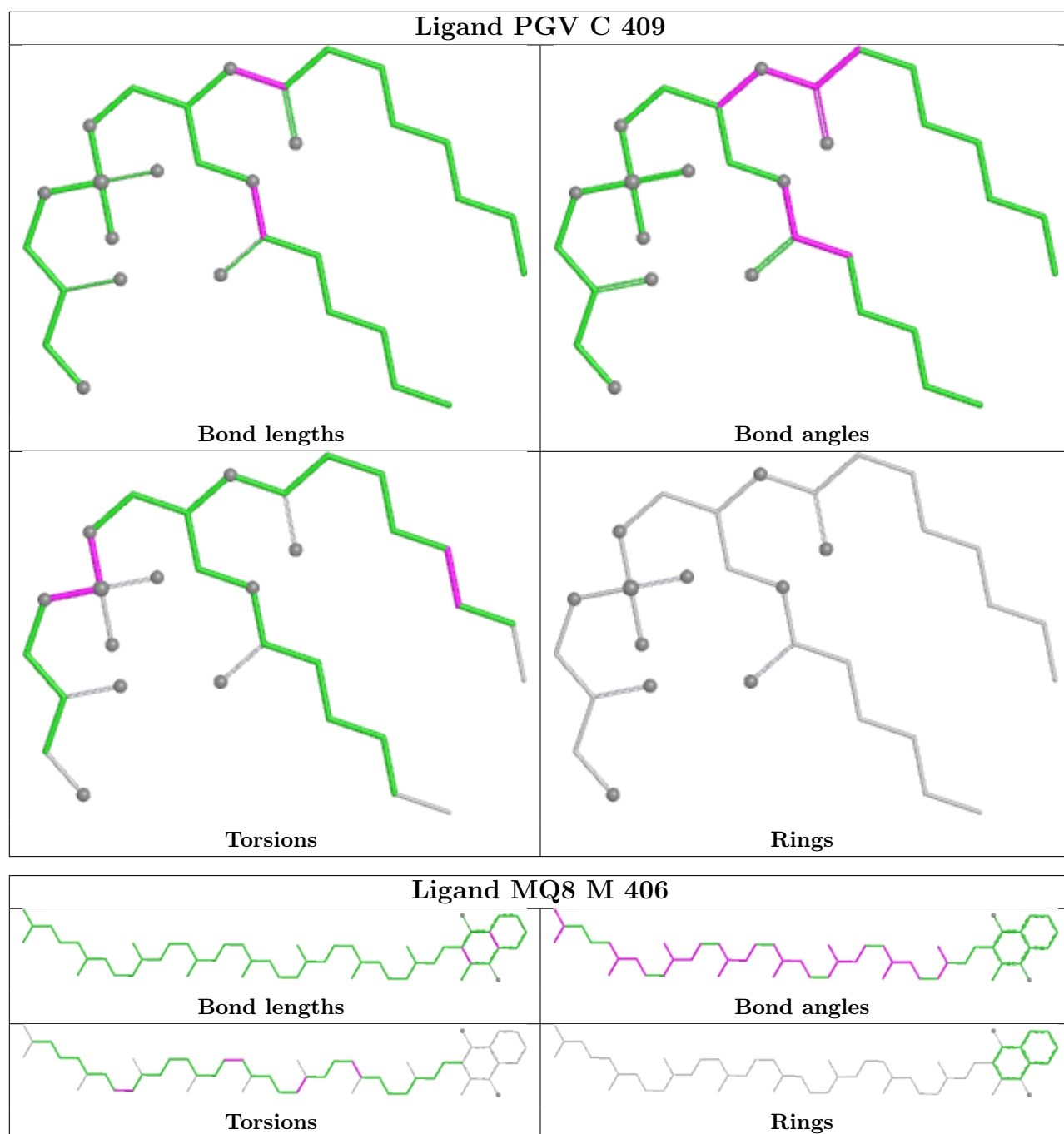


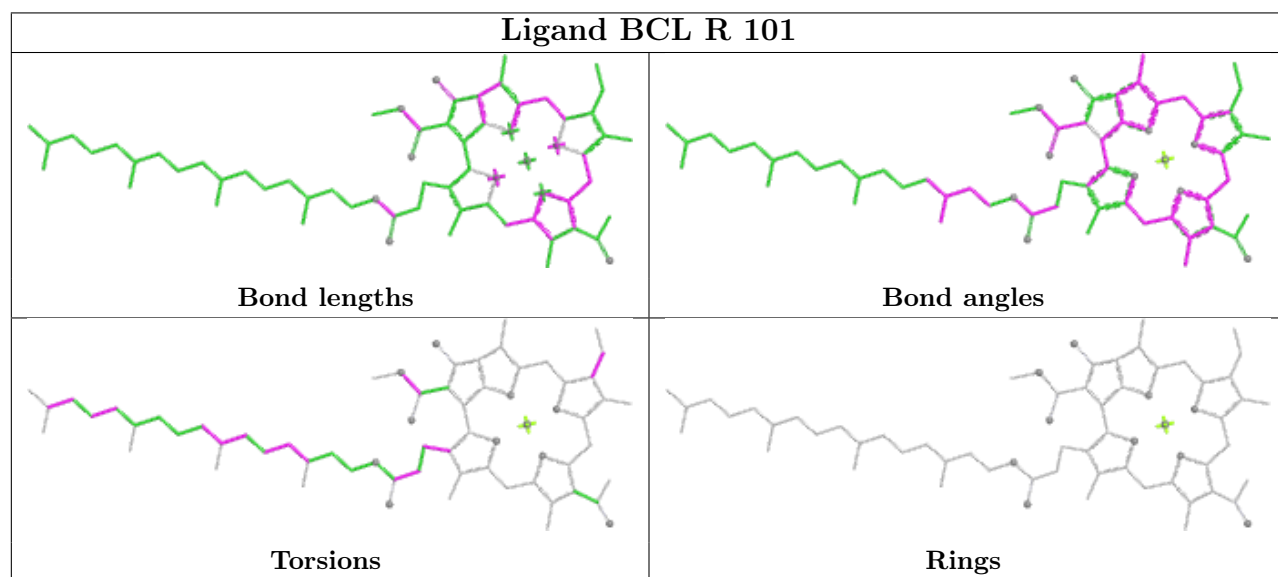
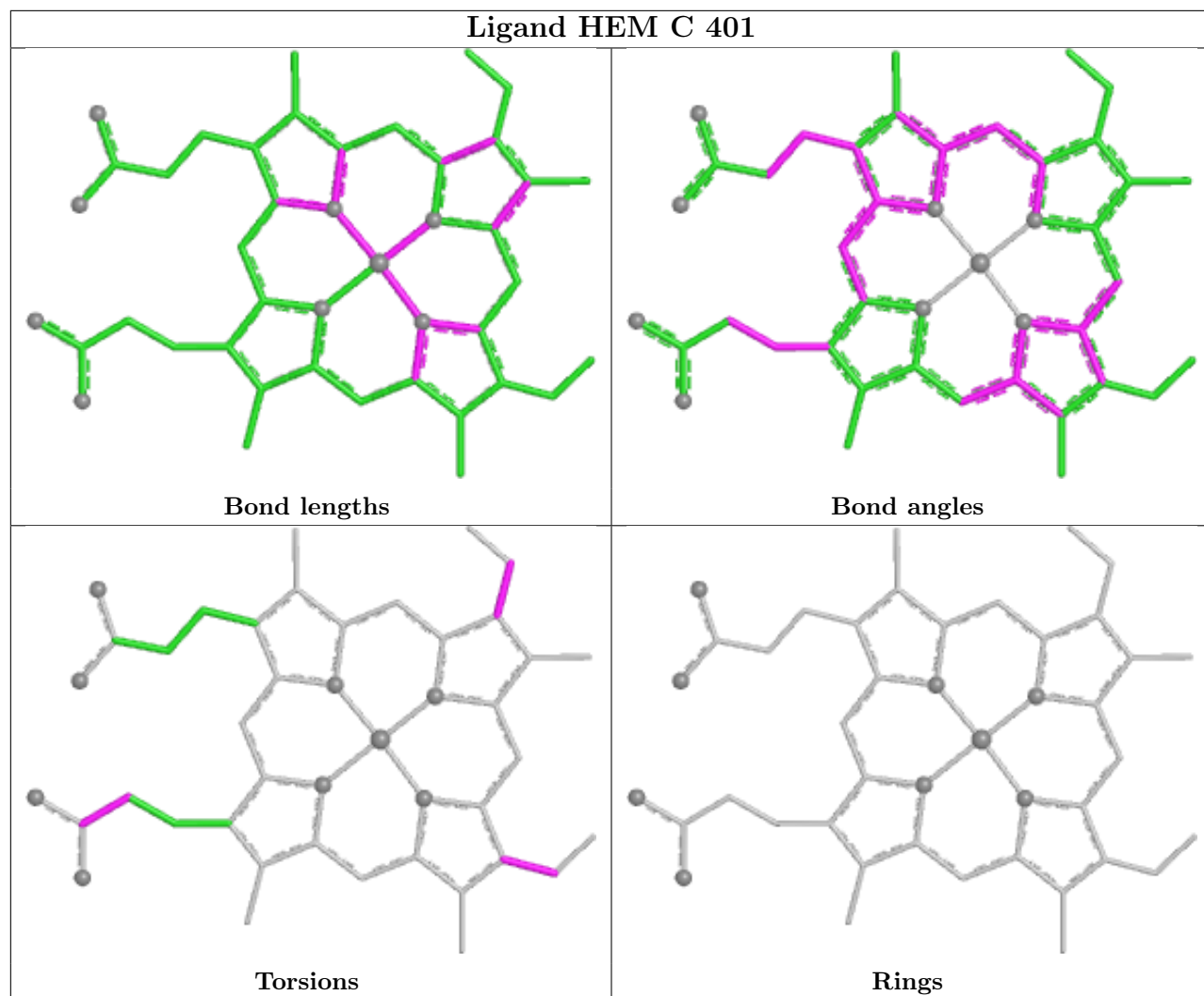


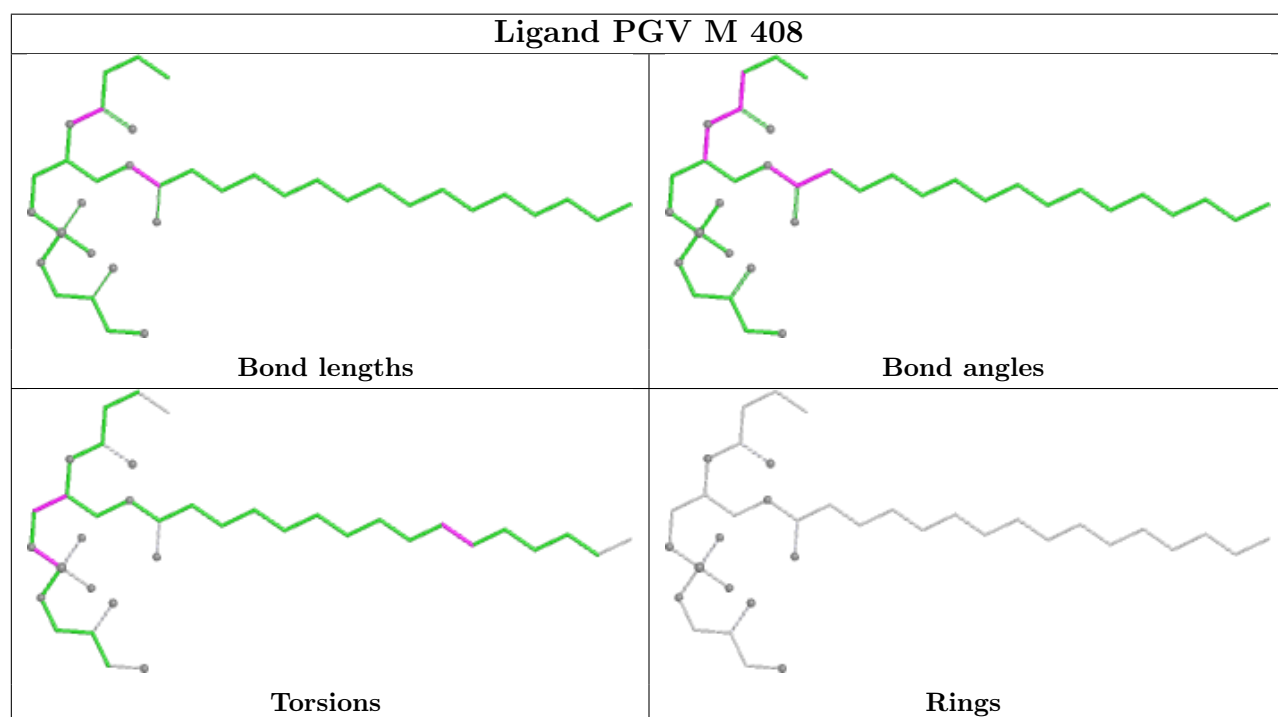
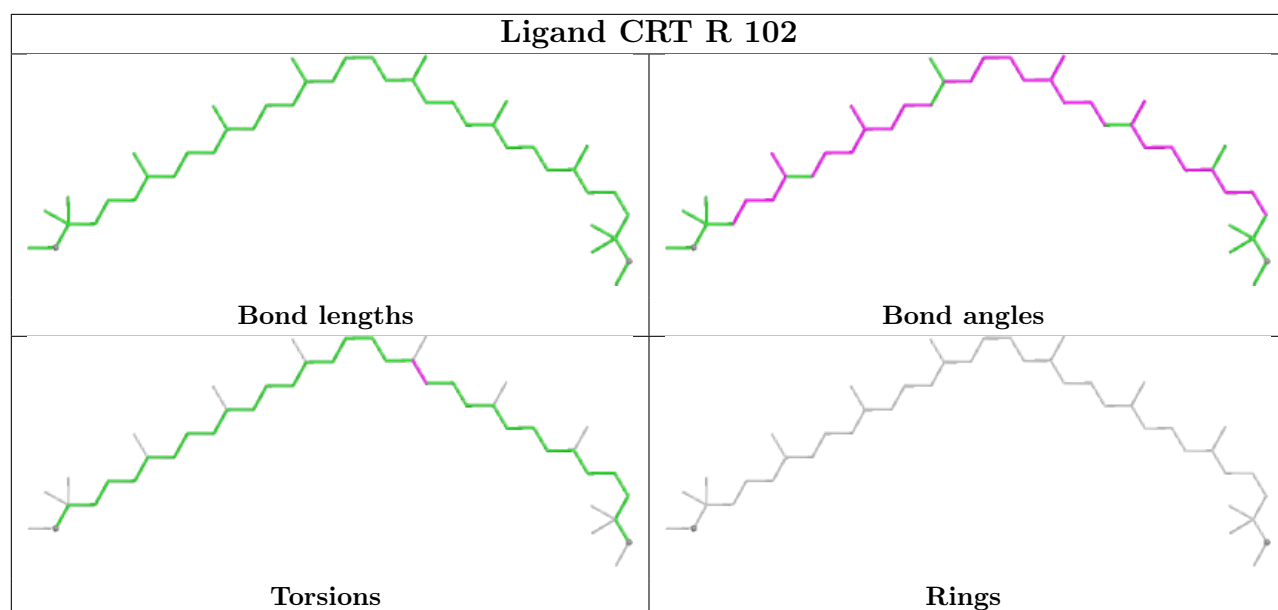


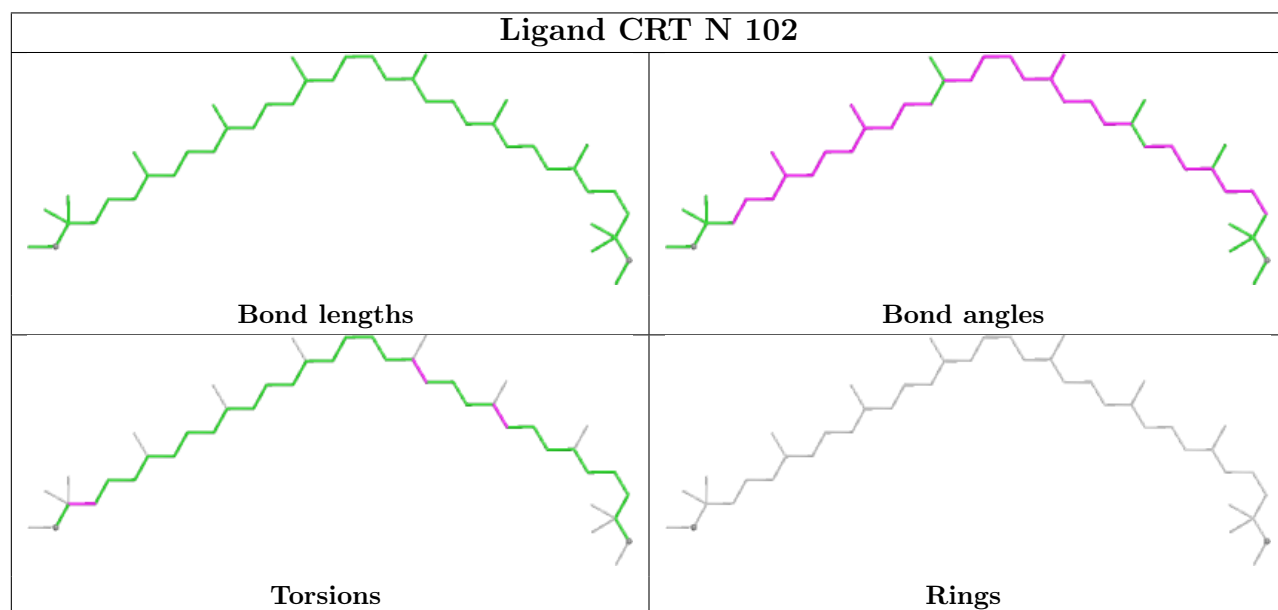
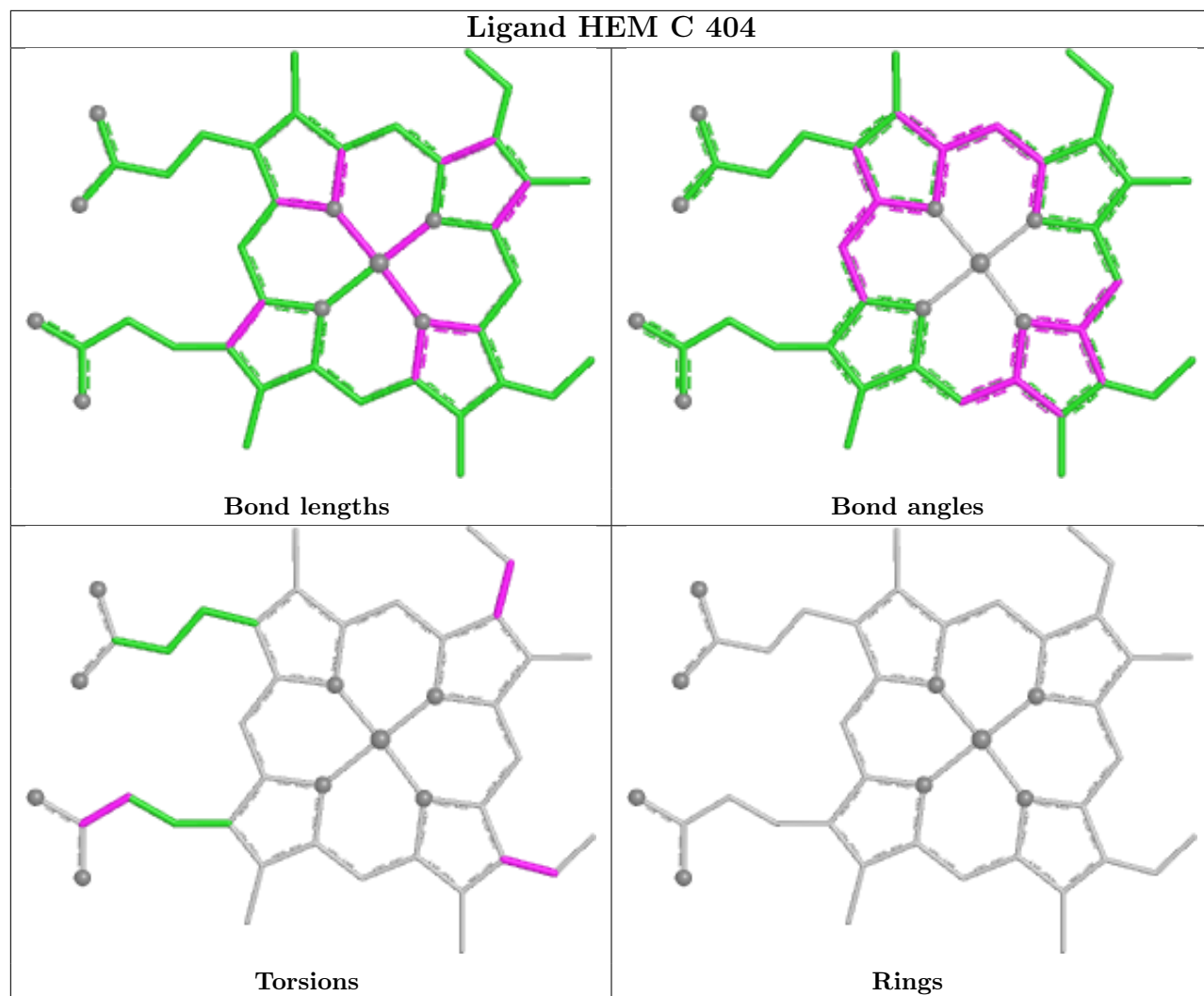


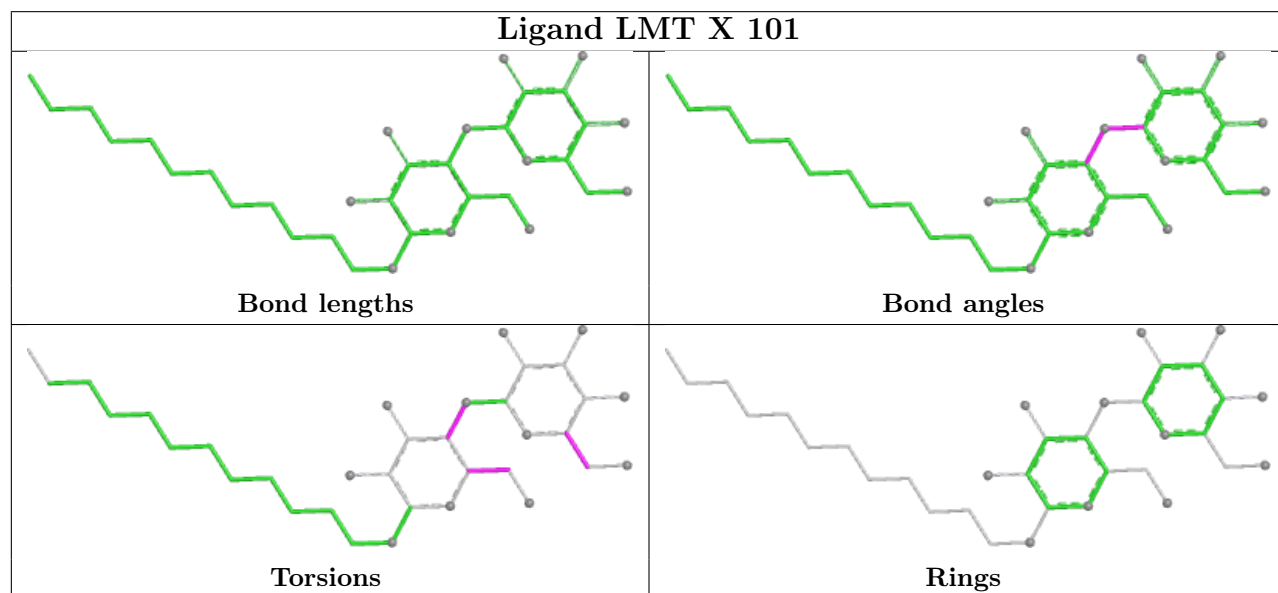
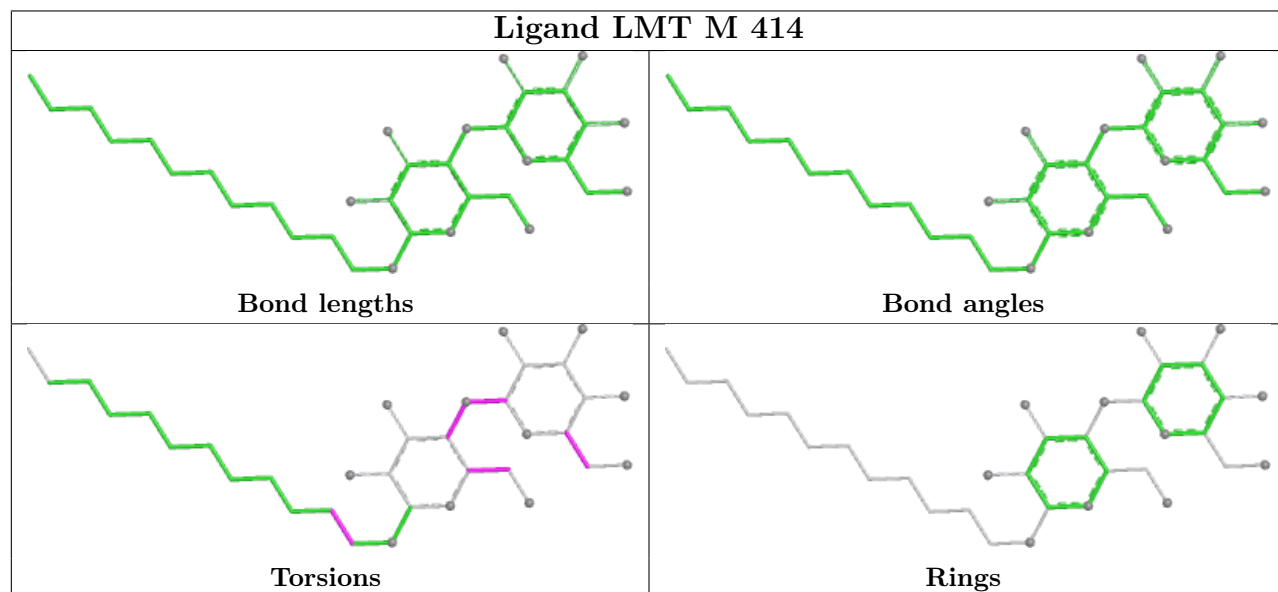
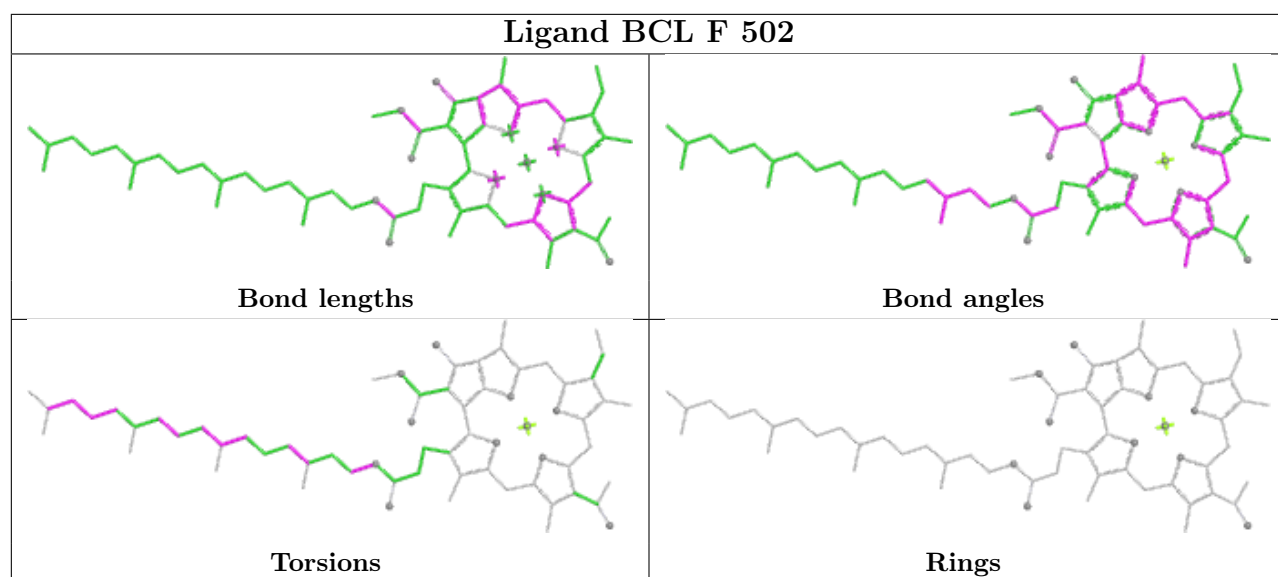


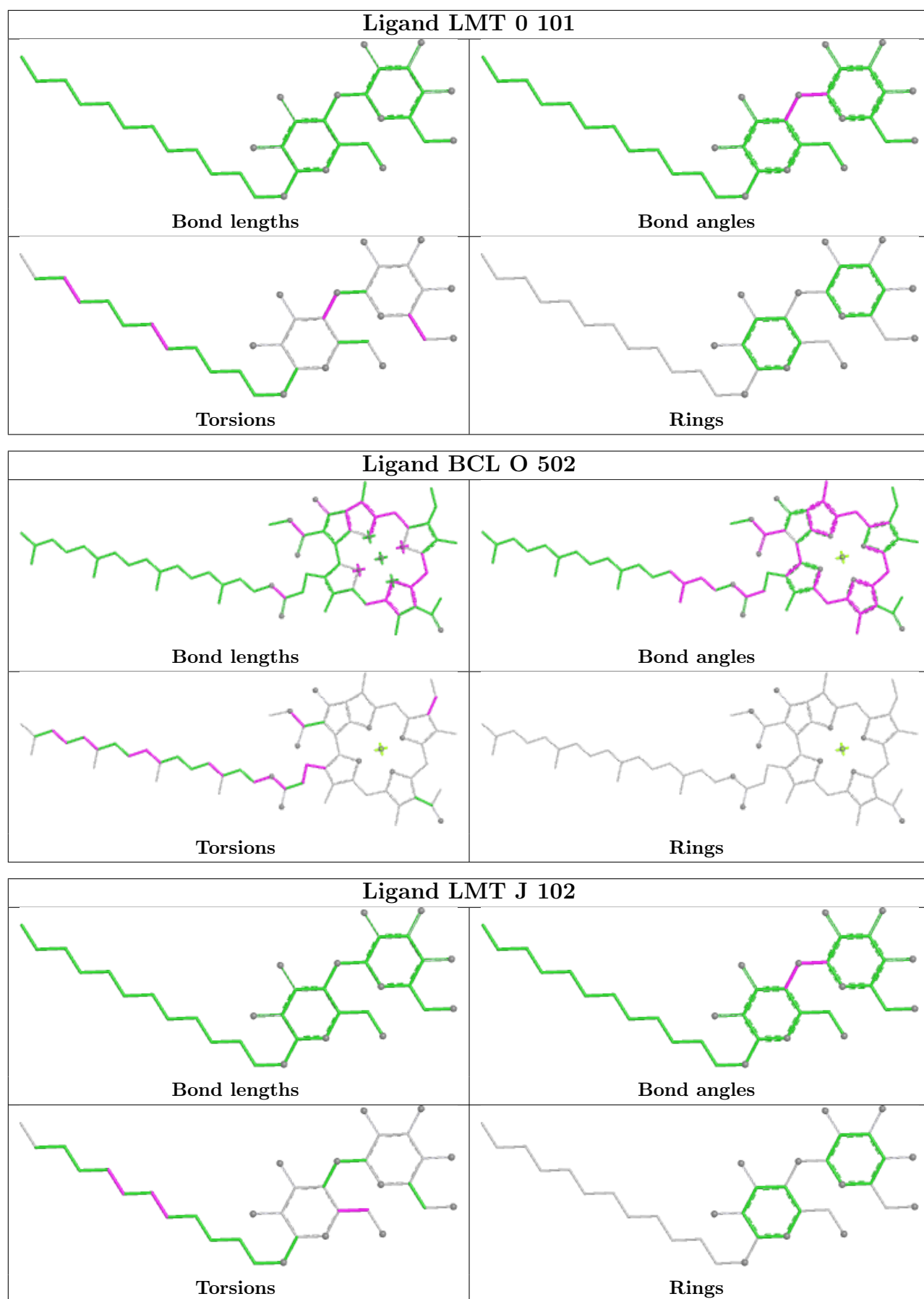


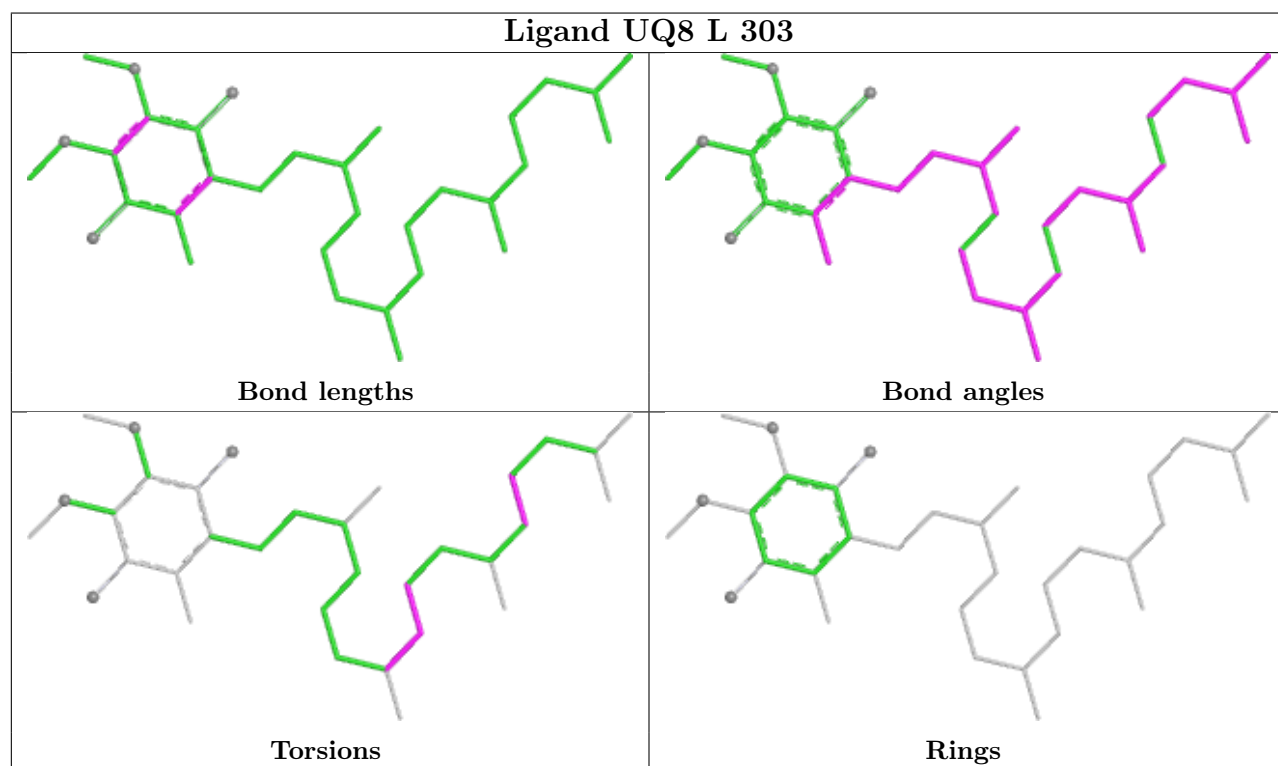
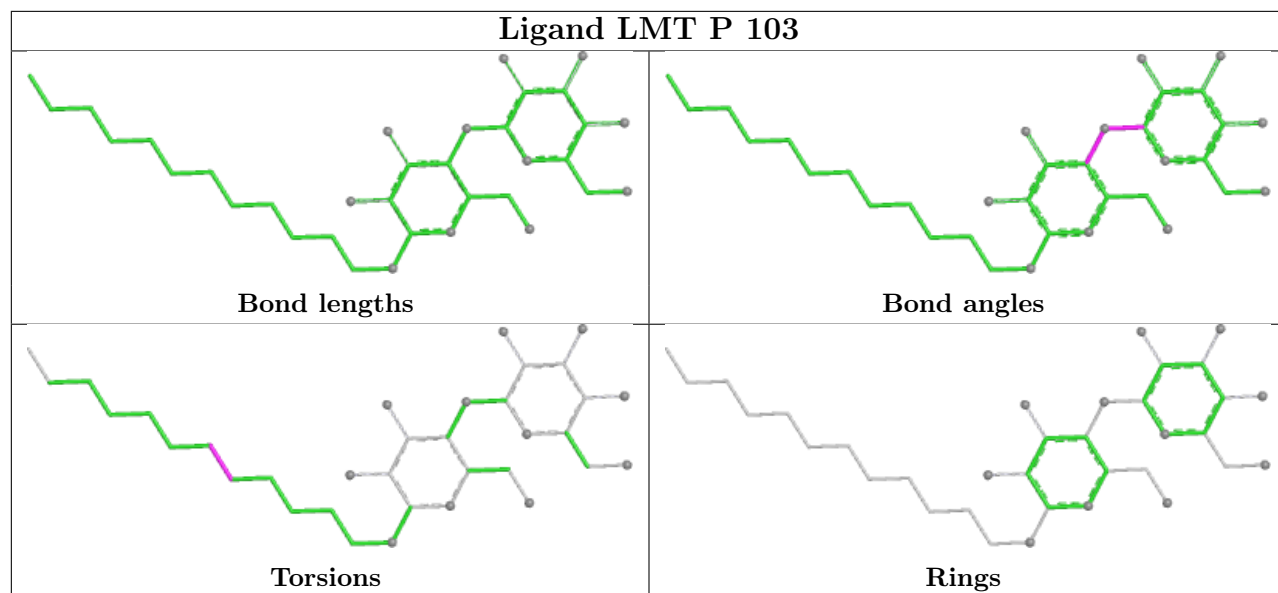


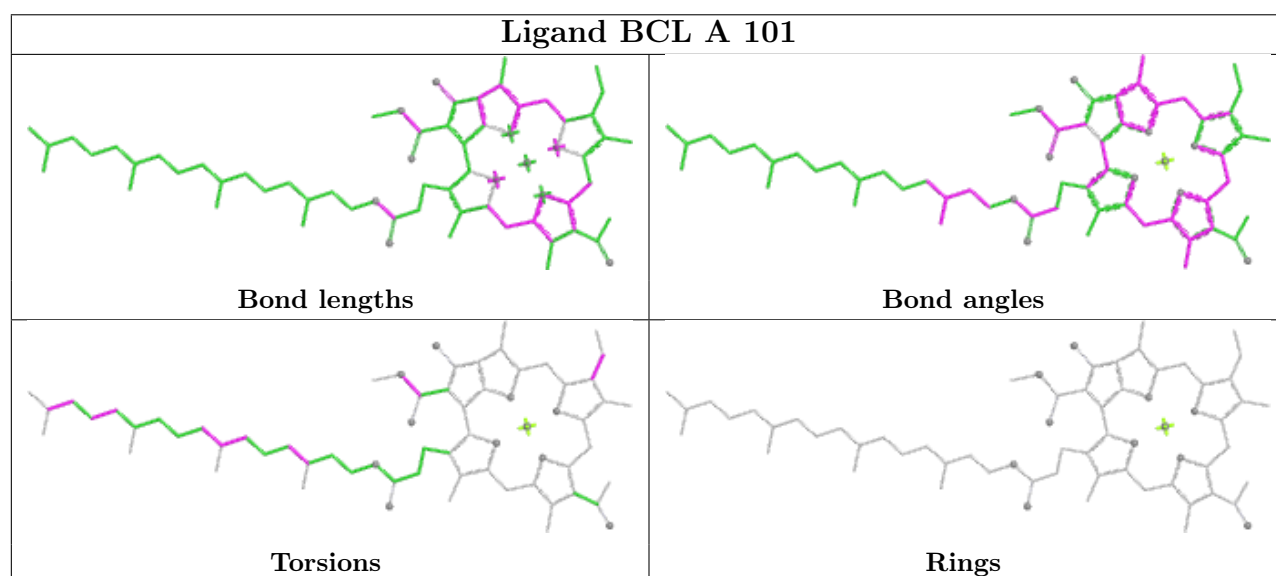
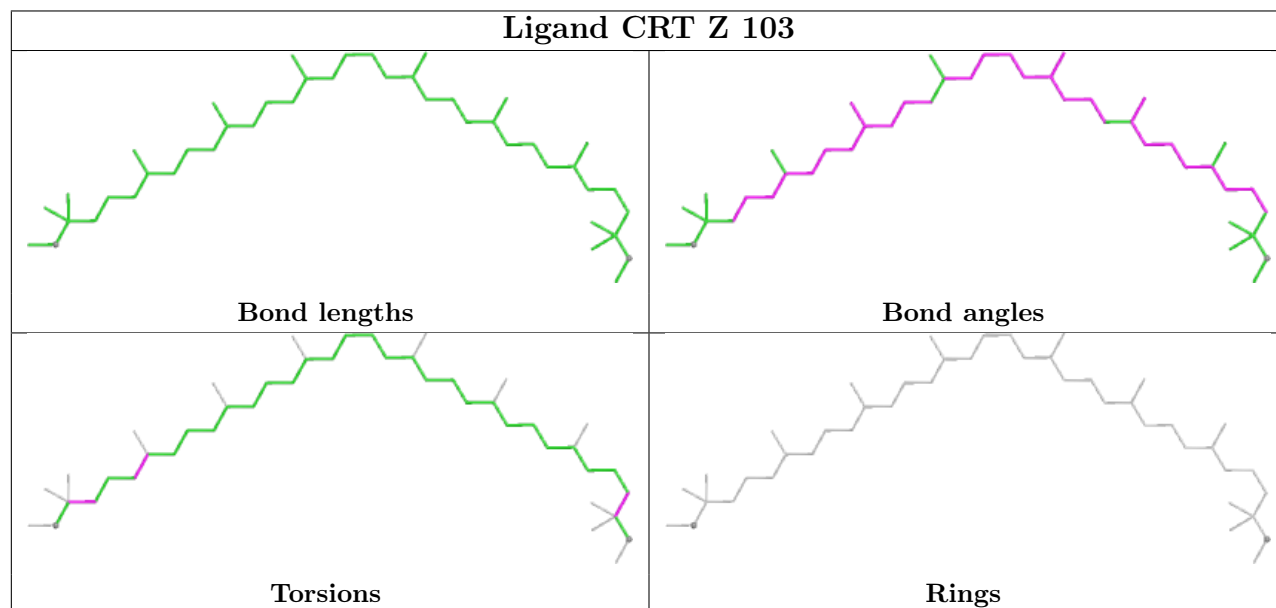
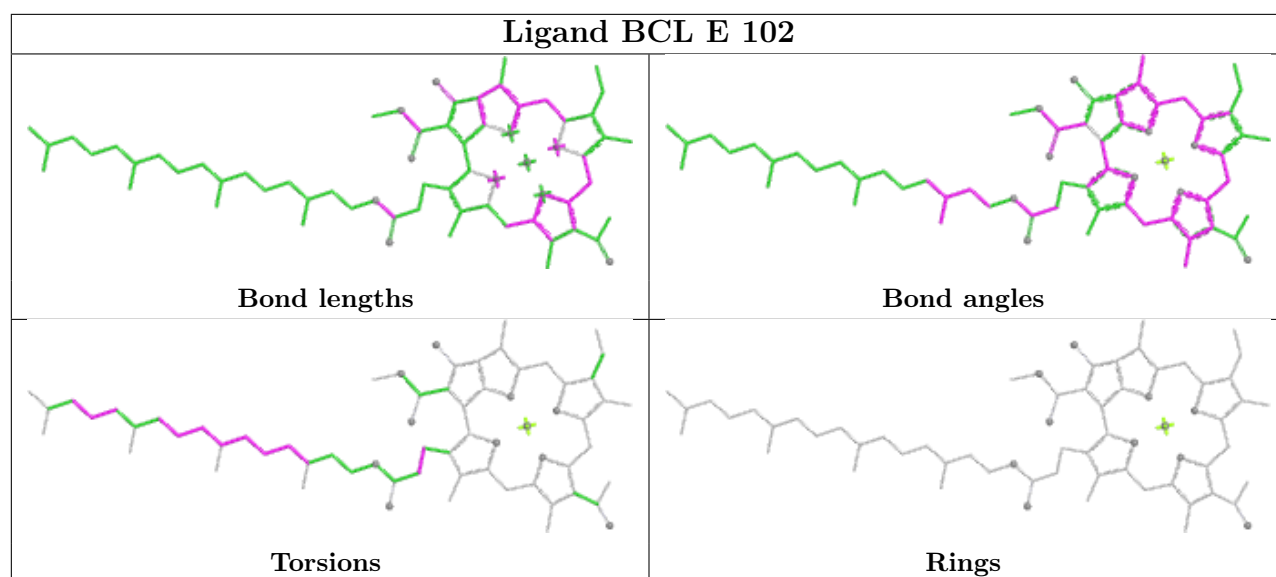


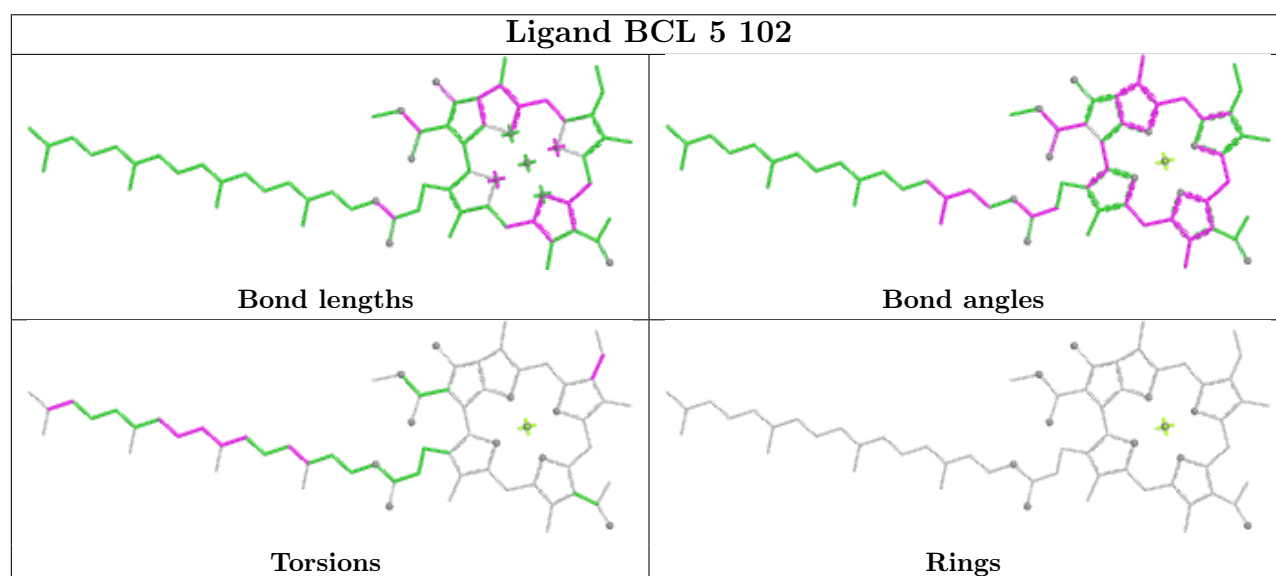
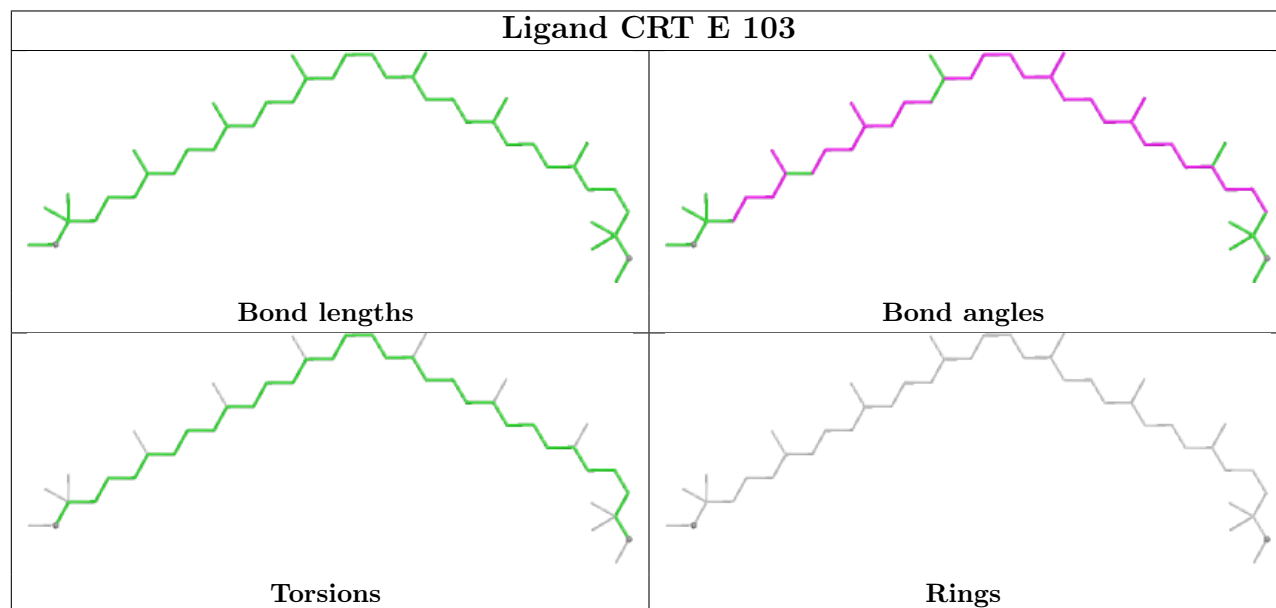
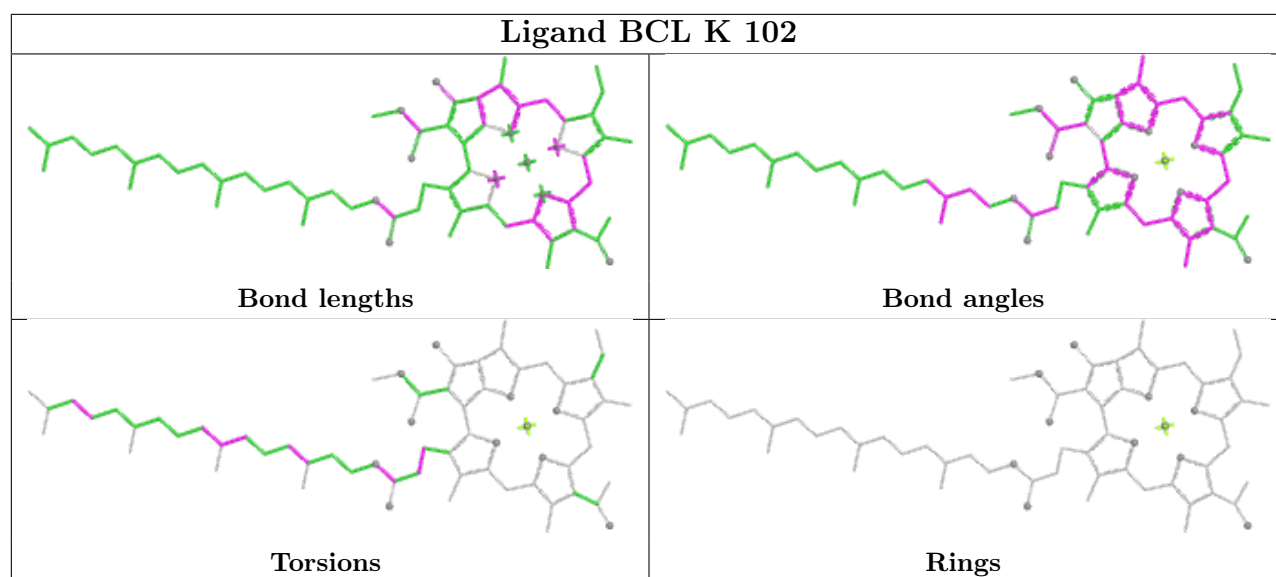


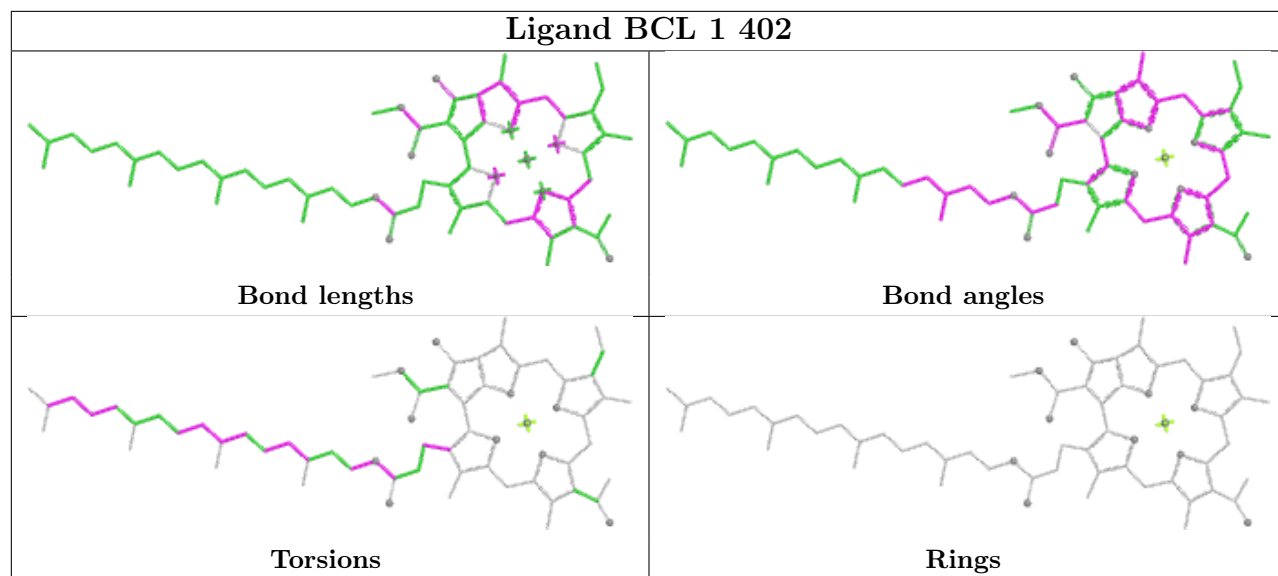












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

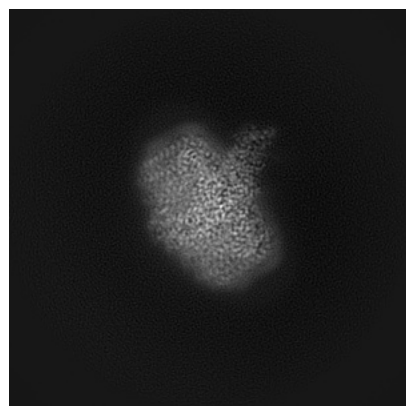
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37466. These allow visual inspection of the internal detail of the map and identification of artifacts.

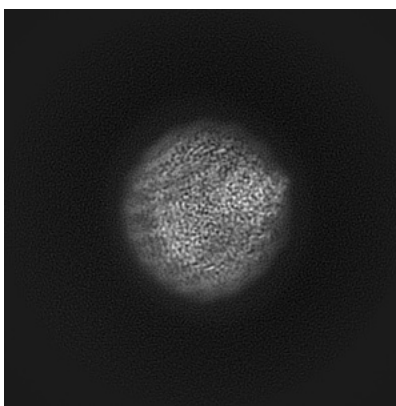
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

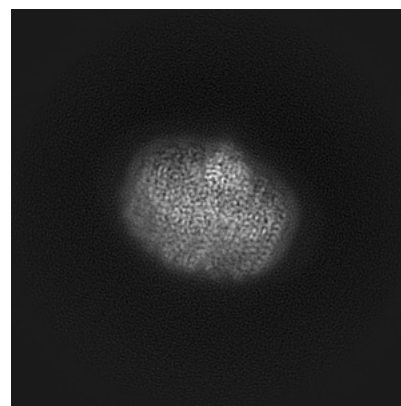
#### 6.1.1 Primary map



X

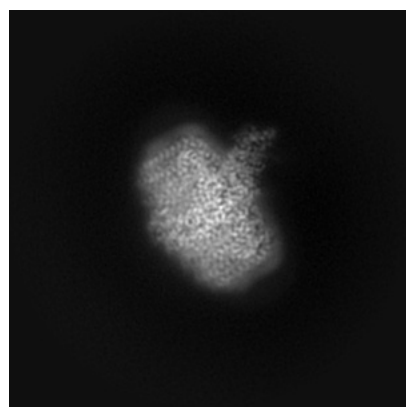


Y

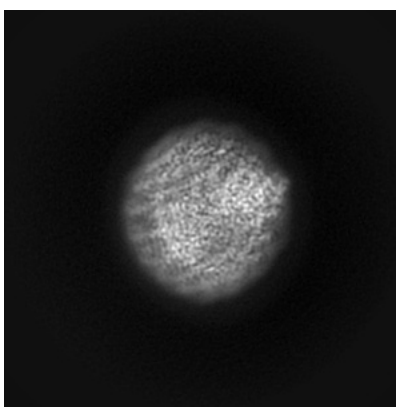


Z

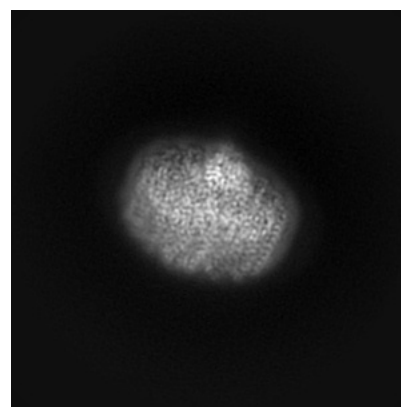
#### 6.1.2 Raw map



X



Y

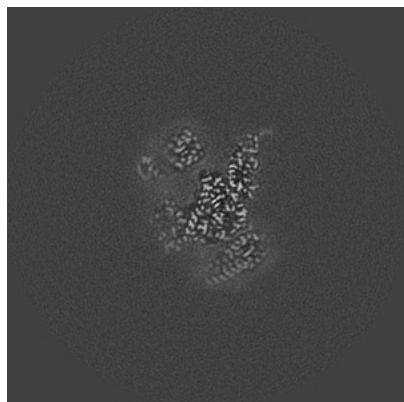


Z

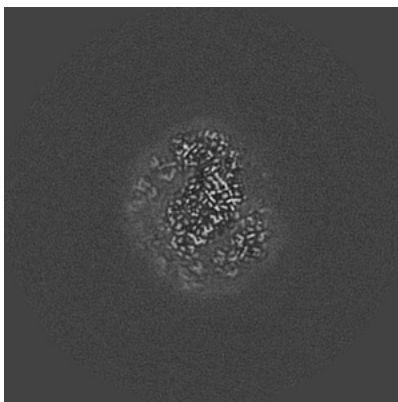
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

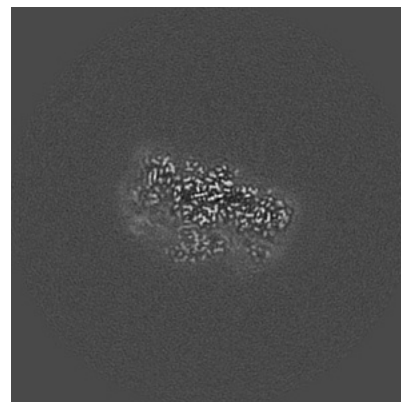
### 6.2.1 Primary map



X Index: 180

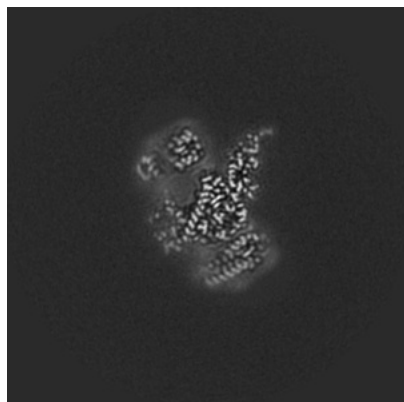


Y Index: 180

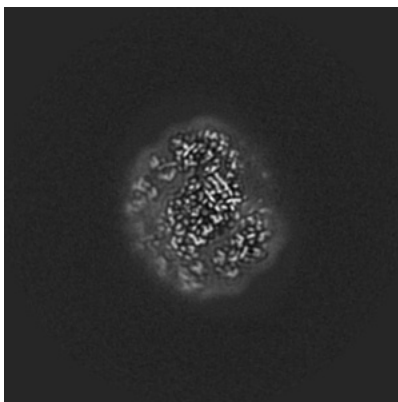


Z Index: 180

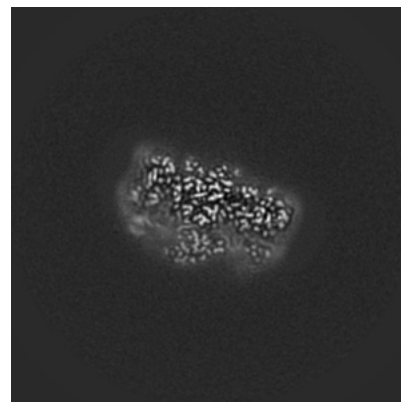
### 6.2.2 Raw map



X Index: 180



Y Index: 180

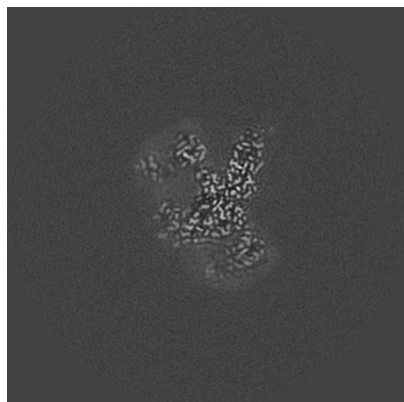


Z Index: 180

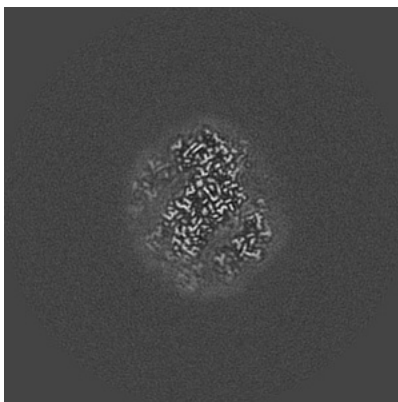
The images above show central slices of the map in three orthogonal directions.

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

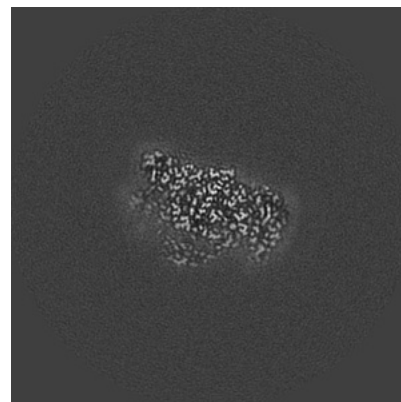
### 6.3.1 Primary map



X Index: 184

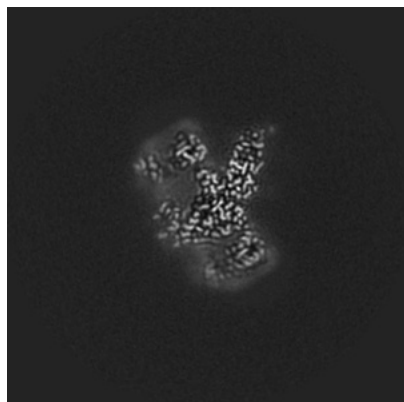


Y Index: 178

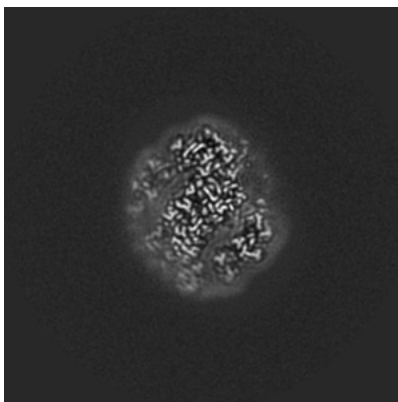


Z Index: 173

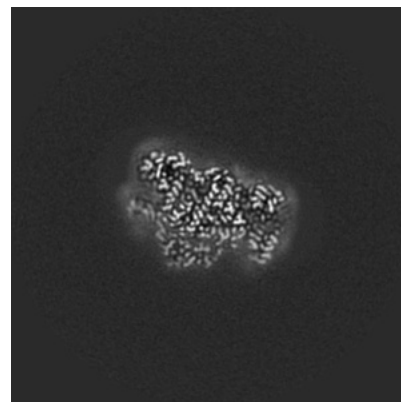
### 6.3.2 Raw map



X Index: 184



Y Index: 178

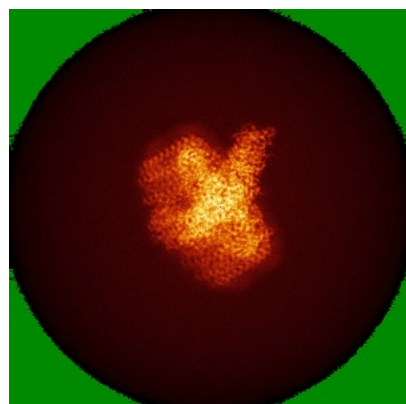


Z Index: 169

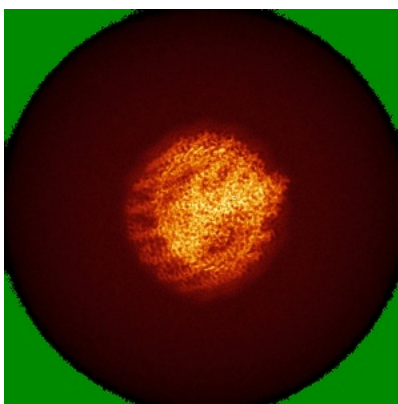
The images above show the largest variance slices of the map in three orthogonal directions.

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

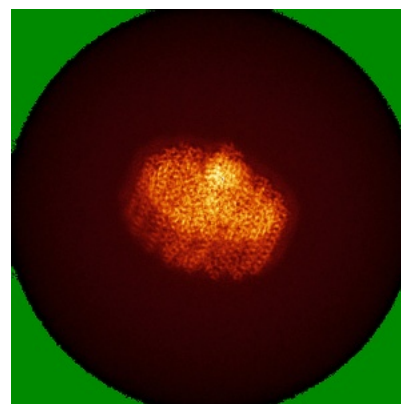
### 6.4.1 Primary map



X

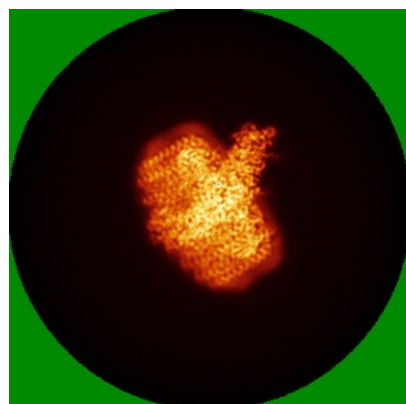


Y

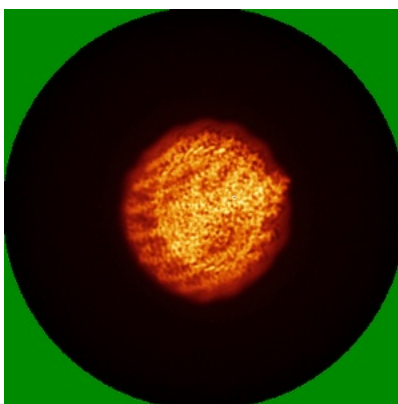


Z

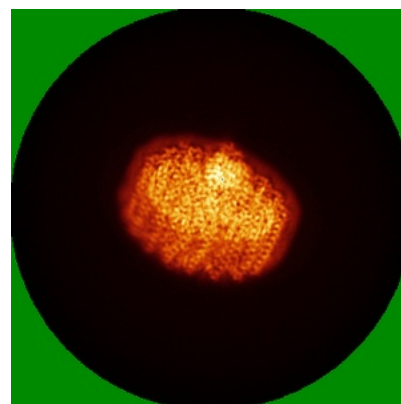
### 6.4.2 Raw map



X



Y

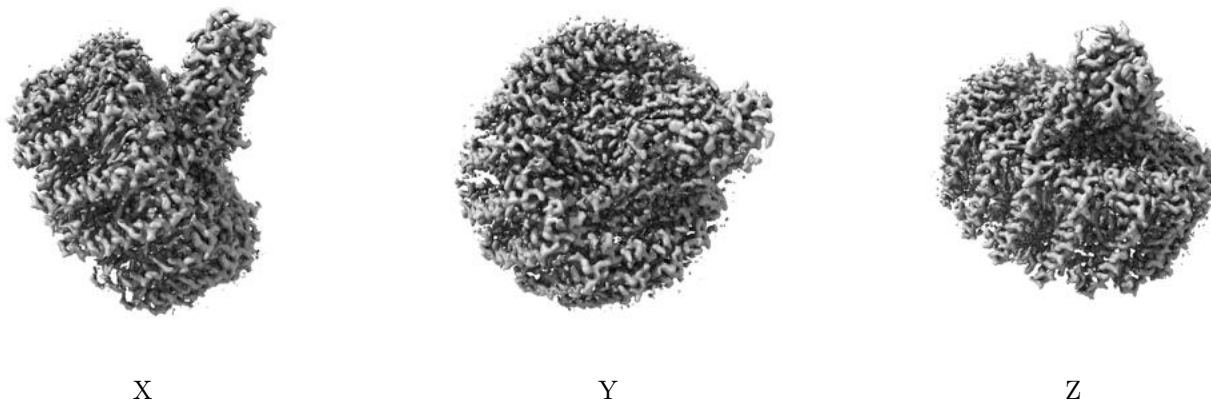


Z

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.

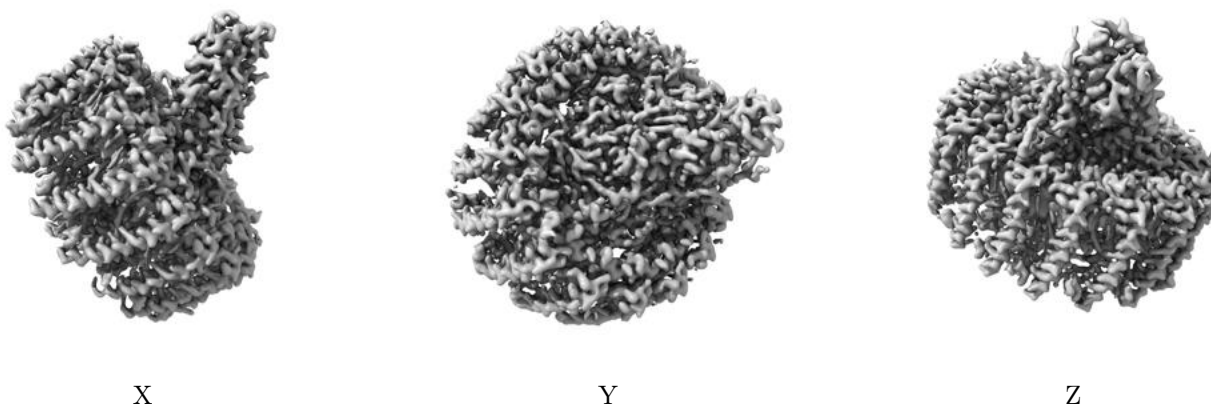
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

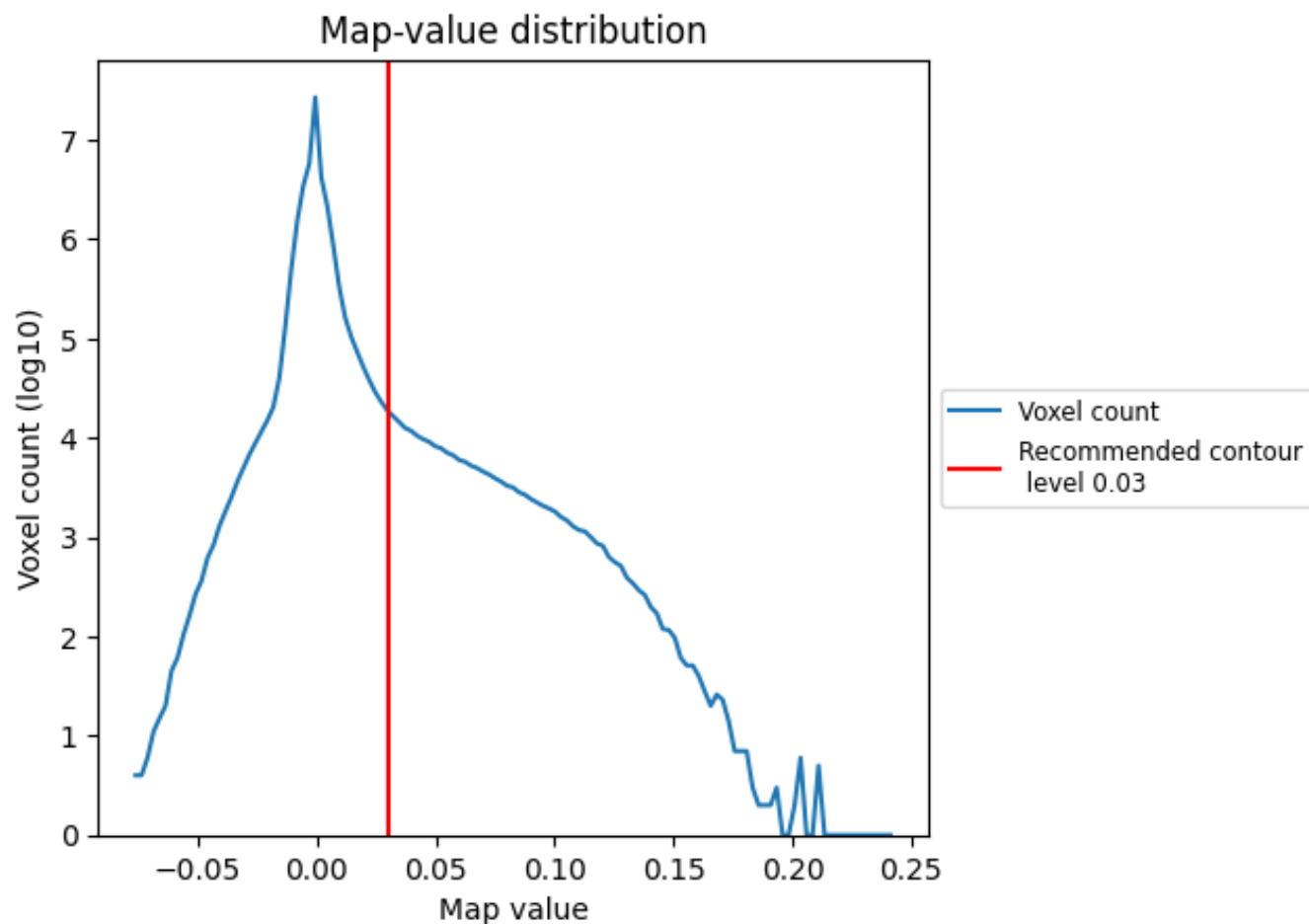
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

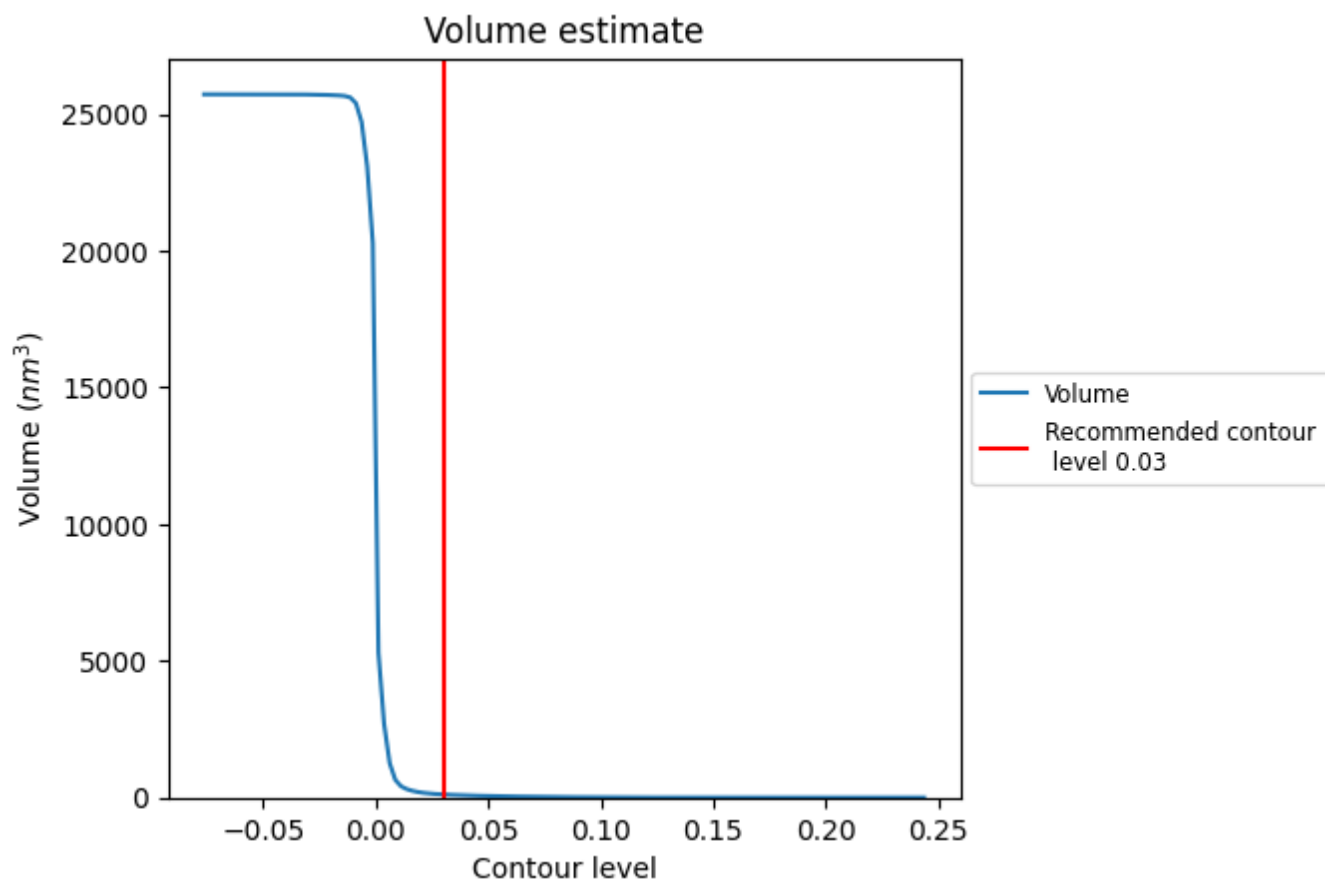
This section contains the results of statistical analysis of the map.

### 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.

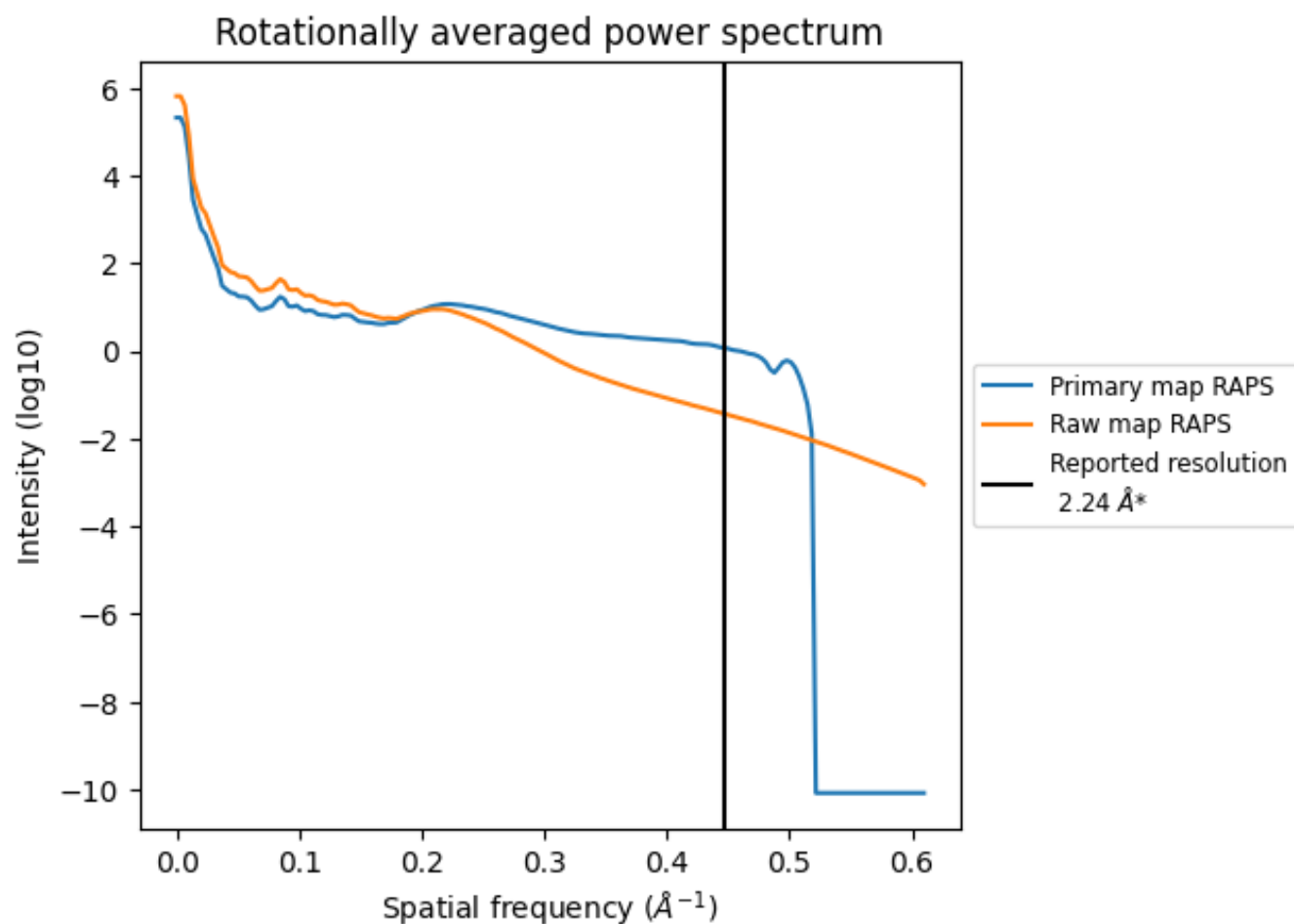
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113  $\text{nm}^3$ ; this corresponds to an approximate mass of 102 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 ⓘ

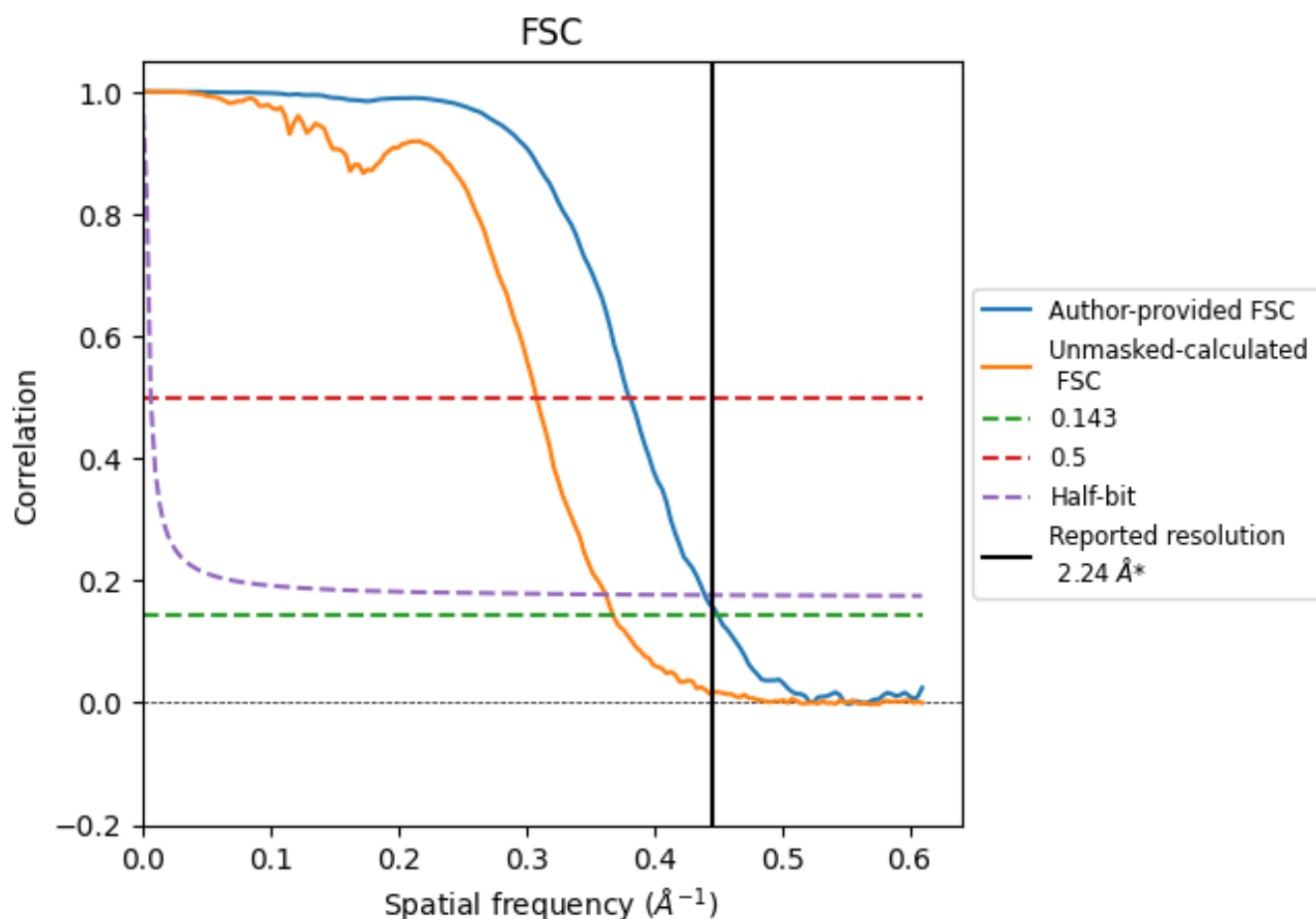


\*Reported resolution corresponds to spatial frequency of 0.446 Å<sup>-1</sup>

## 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](#)

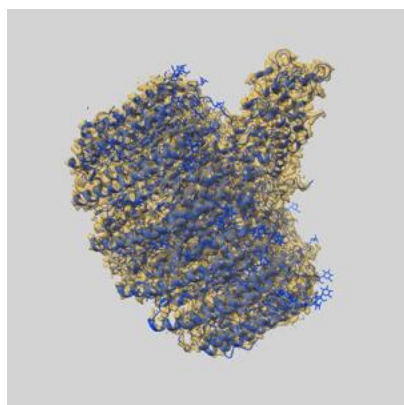
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.24                               | -    | -        |
| Author-provided FSC curve | 2.22                               | 2.63 | 2.27     |
| Unmasked-calculated*      | 2.72                               | 3.24 | 2.76     |

\*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 2.72 differs from the reported value 2.24 by more than 10 %

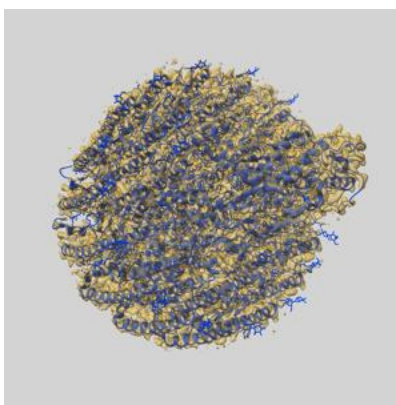
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37466 and PDB model 8WDV. Per-residue inclusion information can be found in section [3](#) on page [22](#).

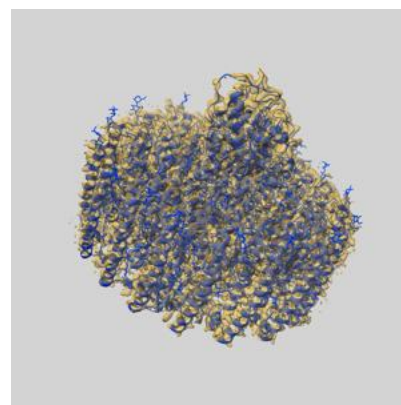
### 9.1 Map-model overlay [i](#)



X



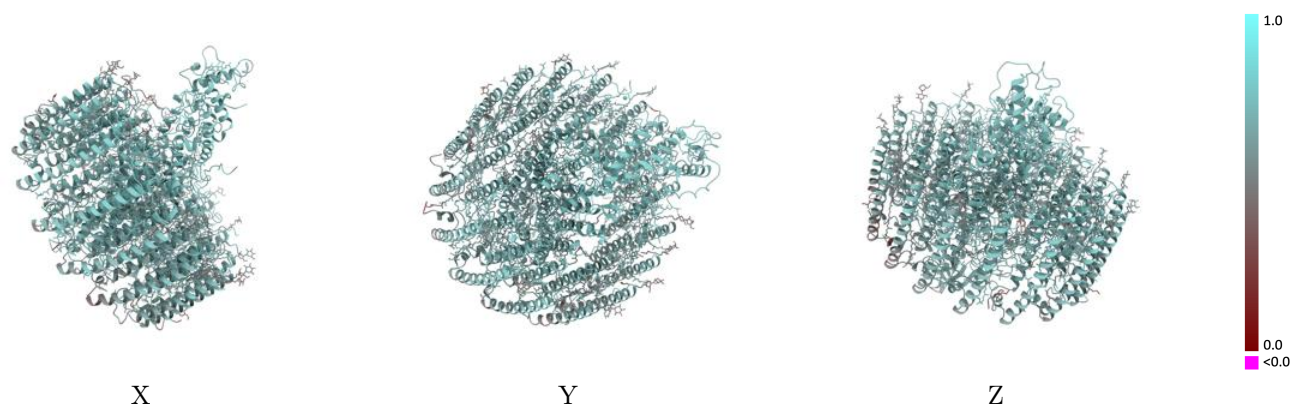
Y



Z

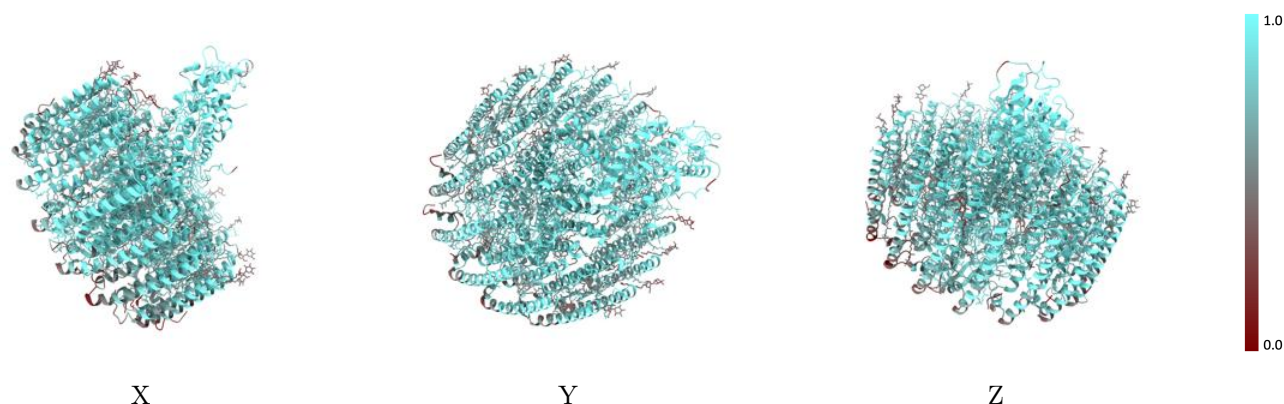
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



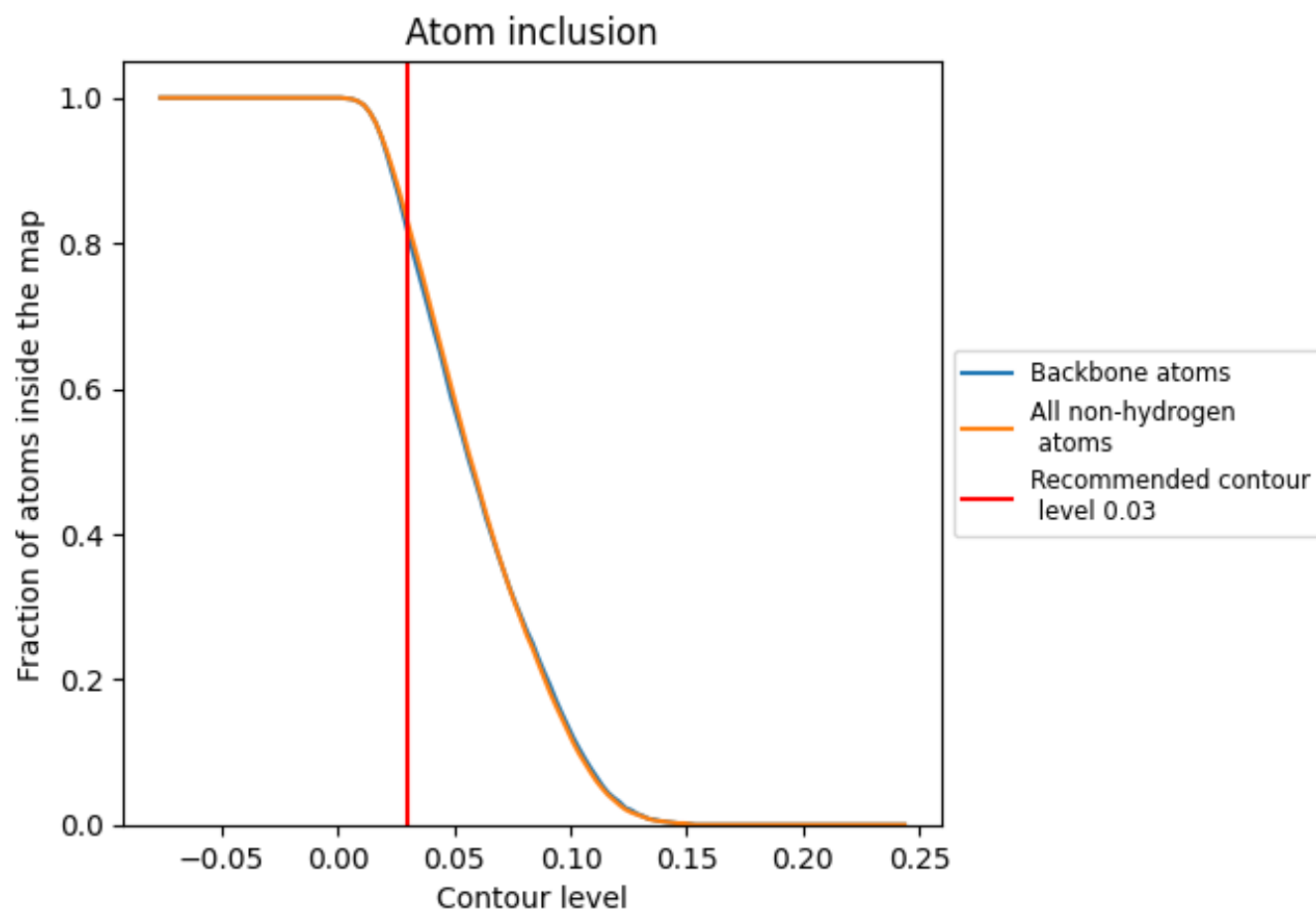
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 83% 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 (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8290   |  0.6580   |
| 0     |  0.7650   |  0.6280   |
| 1     |  0.8150   |  0.6430   |
| 2     |  0.6960   |  0.6040   |
| 3     |  0.8110   |  0.6480   |
| 4     |  0.6440   |  0.5770   |
| 5     |  0.7650   |  0.6040   |
| 6     |  0.6760   |  0.5750   |
| 7     |  0.7660   |  0.6160   |
| 8     |  0.7020   |  0.5930   |
| 9     |  0.8460   |  0.6580   |
| A     |  0.8940   |  0.6750   |
| B     |  0.7940   |  0.6350   |
| C     |  0.9510   |  0.7090   |
| D     |  0.7750  |  0.6370  |
| E     |  0.7850 |  0.6330 |
| F     |  0.7180 |  0.6200 |
| G     |  0.6630 |  0.5930 |
| H     |  0.7680 |  0.6550 |
| I     |  0.8100 |  0.6400 |
| J     |  0.7160 |  0.6030 |
| K     |  0.7400 |  0.6140 |
| L     |  0.9290 |  0.7070 |
| M     |  0.9120 |  0.7000 |
| N     |  0.7460 |  0.6180 |
| O     |  0.8540 |  0.6600 |
| P     |  0.7610 |  0.6250 |
| Q     |  0.9020 |  0.6800 |
| R     |  0.8250 |  0.6570 |
| S     |  0.8850 |  0.6740 |
| T     |  0.8640 |  0.6690 |
| U     |  0.8740 |  0.6720 |
| V     |  0.8140 |  0.6490 |
| W     |  0.8130 |  0.6500 |
| X     |  0.7960 |  0.6420 |



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*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Y     |  0.7380 |  0.6250 |
| Z     |  0.7910 |  0.6290 |