



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:05 AM JST

PDB ID : 7DDQ / pdb\_00007ddq  
EMDB ID : EMD-30656  
Title : Structure of RC-LH1-PufX from Rhodobacter veldkampii  
Authors : Bracun, L.; Yamagata, A.; Shirouzu, M.; Liu, L.N.  
Deposited on : 2020-10-29  
Resolution : 2.84 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

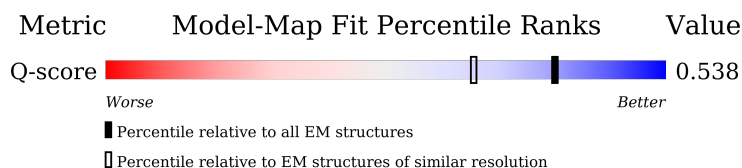
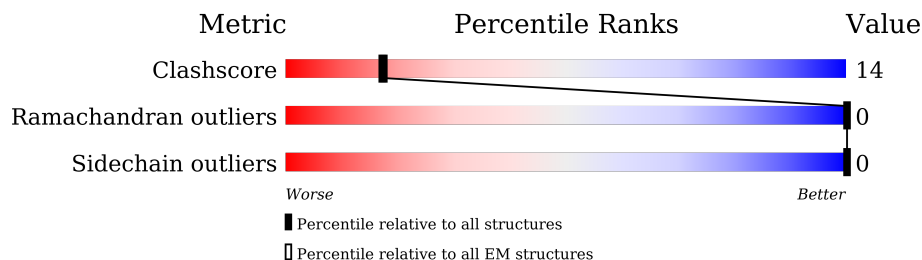
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.84 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.



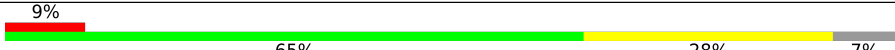
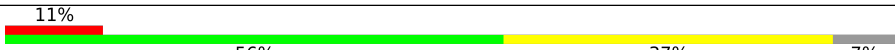
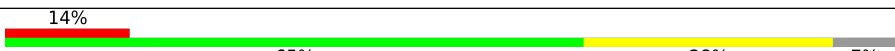
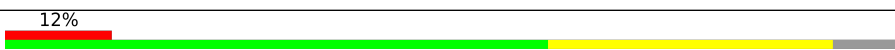
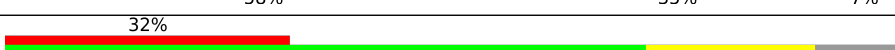
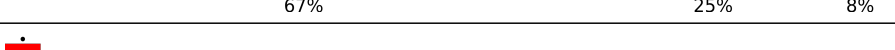
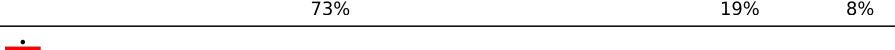
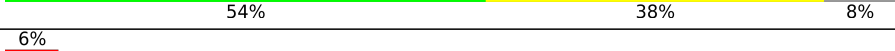
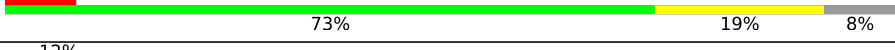
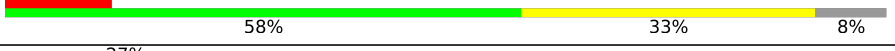
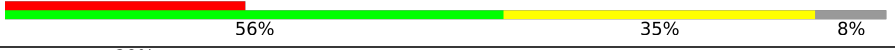
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11884 ( 2.34 - 3.34 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | a     | 57     |                  |
| 1   | b     | 57     |                  |
| 1   | d     | 57     |                  |
| 1   | e     | 57     |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | f     | 57     |    |
| 1   | g     | 57     |    |
| 1   | i     | 57     |    |
| 1   | j     | 57     |    |
| 1   | k     | 57     |    |
| 1   | n     | 57     |    |
| 1   | o     | 57     |    |
| 1   | r     | 57     |    |
| 1   | s     | 57     |    |
| 1   | t     | 57     |    |
| 1   | u     | 57     |    |
| 2   | A     | 48     |    |
| 2   | B     | 48     |  |
| 2   | D     | 48     |  |
| 2   | E     | 48     |  |
| 2   | F     | 48     |  |
| 2   | G     | 48     |  |
| 2   | I     | 48     |  |
| 2   | J     | 48     |  |
| 2   | K     | 48     |  |
| 2   | N     | 48     |  |
| 2   | O     | 48     |  |
| 2   | R     | 48     |  |
| 2   | S     | 48     |  |
| 2   | T     | 48     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | U     | 48     |                  |
| 3   | X     | 83     |                  |
| 4   | L     | 276    |                  |
| 5   | M     | 308    |                  |
| 6   | H     | 252    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 8   | SPO  | s     | 201 | -         | X        | -       | -                |

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 22571 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 Antenna pigment protein alpha chain.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | o     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | t     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | r     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | a     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 373   | 258 | 59 | 54 | 2 |         |       |
| 1   | e     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | b     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | k     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | f     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | u     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 440   | 302 | 71 | 65 | 2 |         |       |
| 1   | s     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | n     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | i     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | j     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | g     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |
| 1   | d     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 305 | 72 | 67 | 2 |         |       |

- Molecule 2 is a protein called Antenna pigment protein beta chain.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | N     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | S     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | O     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | U     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 354   | 237 | 57 | 59 | 1 |         |       |
| 2   | D     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | A     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | J     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | E     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | T     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 354   | 237 | 57 | 59 | 1 |         |       |
| 2   | R     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | K     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | G     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | I     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | F     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |
| 2   | B     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 243 | 58 | 61 | 1 |         |       |

- Molecule 3 is a protein called PufX.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | X     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 610   | 396 | 100 | 110 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | L     | 275      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2188  | 1469 | 350 | 360 | 9 |         |       |

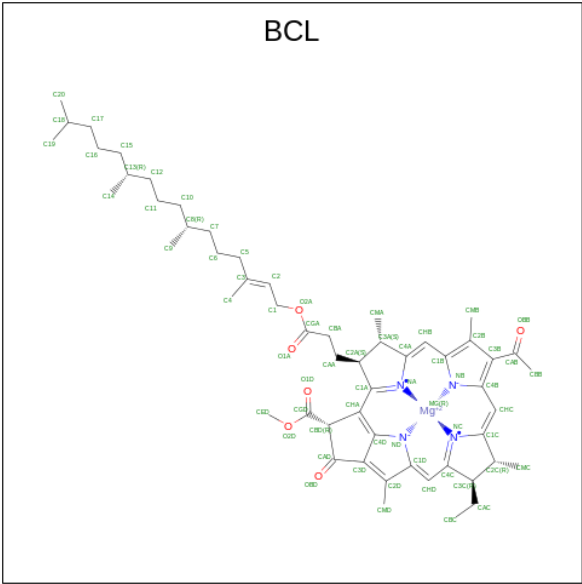
- Molecule 5 is a protein called Reaction center protein M chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | M     | 305      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2420  | 1612 | 393 | 404 | 11 |         |       |

- Molecule 6 is a protein called Photosynthetic reaction center subunit H.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | H     | 250      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1907  | 1223 | 318 | 351 | 15 |         |       |

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 7   | o     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | t     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | t     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | r     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | O     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

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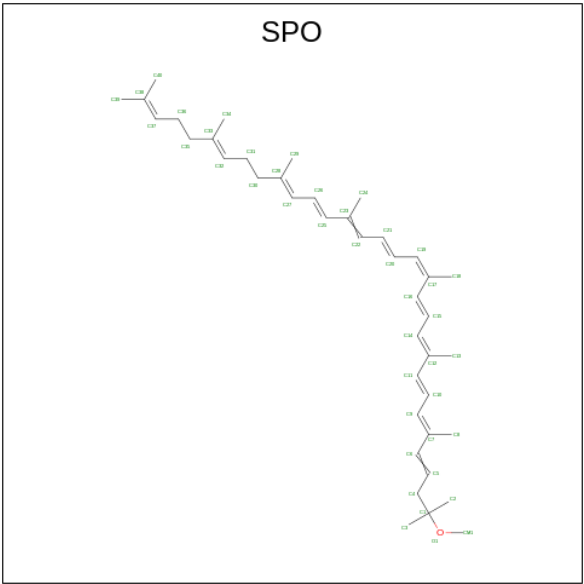
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 7   | e     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | D     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | b     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | b     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | A     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | k     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | E     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | u     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | u     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | s     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | R     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | n     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | K     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | i     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | j     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | j     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | I     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | L     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | M     | 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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 7   | M     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | F     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | F     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

- Molecule 8 is SPHEROIDENE (CCD ID: SPO) (formula: C<sub>41</sub>H<sub>60</sub>O).



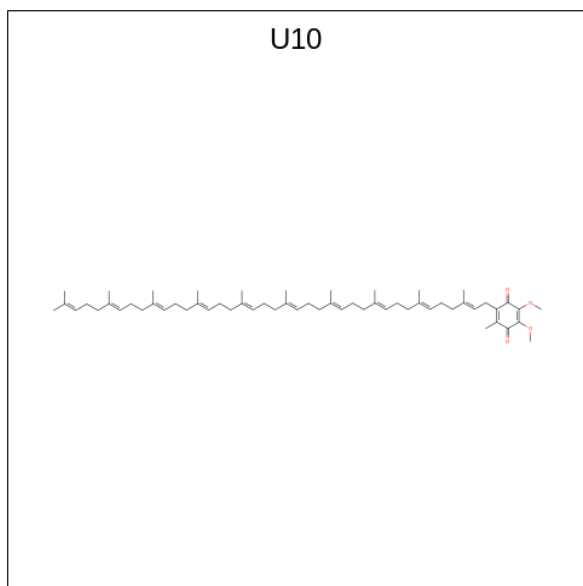
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 8   | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | t     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | r     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | r     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | k     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 8   | E     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | X     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | s     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | j     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | I     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | M     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | g     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | F     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



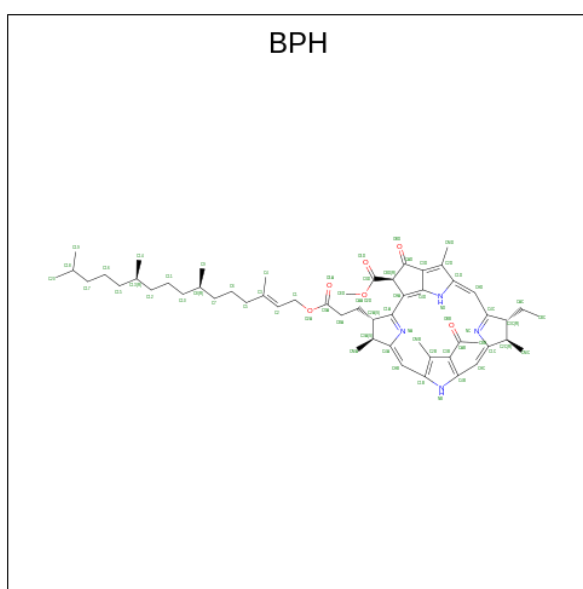
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 9   | a     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 44 | 4 |         |
| 9   | L     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 29 | 4 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 9   | L     | 1        | Total | C  | O | 0       |
|     |       |          | 38    | 34 | 4 |         |
| 9   | L     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 24 | 4 |         |
| 9   | M     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 44 | 4 |         |
| 9   | M     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 14 | 4 |         |

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



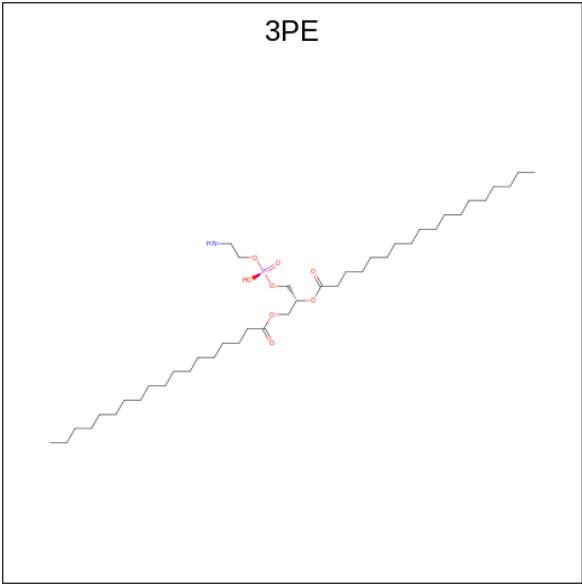
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 10  | L     | 1        | Total | C  | N | O | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |
| 10  | L     | 1        | Total | C  | N | O | 0       |
|     |       |          | 45    | 35 | 4 | 6 |         |
| 10  | M     | 1        | Total | C  | N | O | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 11  | M     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:

C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).

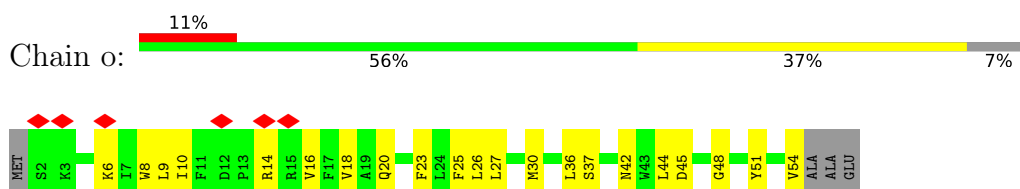


| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 12  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 12  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 12  | d     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 43    | 33 | 1 | 8 | 1 |         |

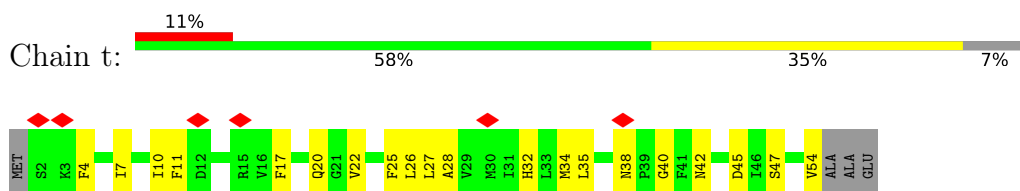
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

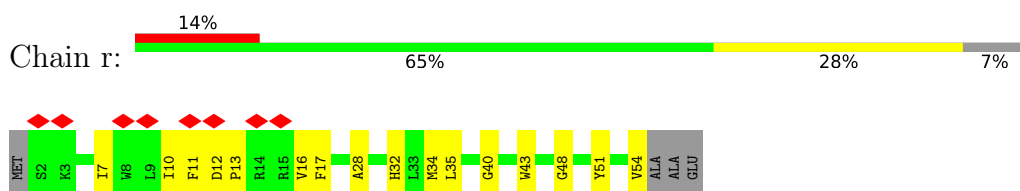
- Molecule 1: Antenna pigment protein alpha chain



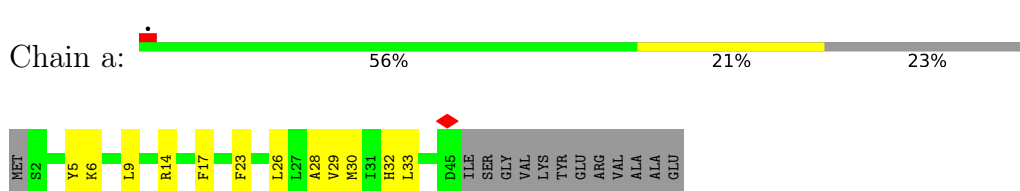
- Molecule 1: Antenna pigment protein alpha chain



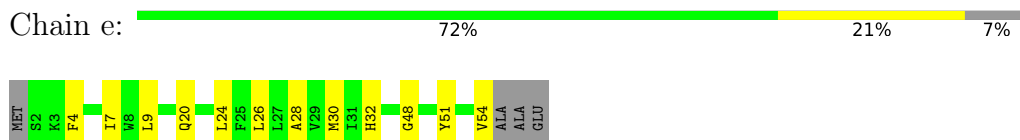
- Molecule 1: Antenna pigment protein alpha chain



- Molecule 1: Antenna pigment protein alpha chain

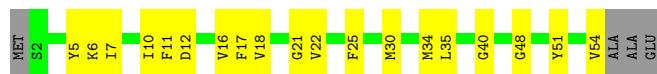


- Molecule 1: Antenna pigment protein alpha chain



- Molecule 1: Antenna pigment protein alpha chain

Chain b:  60% 33% 7%



- Molecule 1: Antenna pigment protein alpha chain

Chain k:  7% 63% 30% 7%



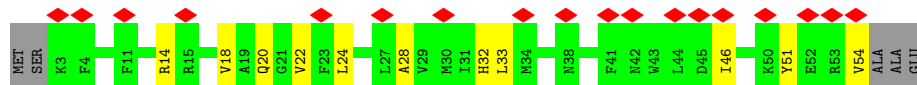
- Molecule 1: Antenna pigment protein alpha chain

Chain f:  67% 26% 7%



- Molecule 1: Antenna pigment protein alpha chain

Chain u:  32% 72% 19% 9%



- Molecule 1: Antenna pigment protein alpha chain

Chain s:  12% 61% 32% 7%



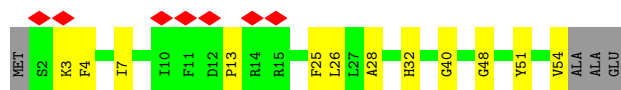
- Molecule 1: Antenna pigment protein alpha chain

Chain n:  9% 65% 28% 7%



- Molecule 1: Antenna pigment protein alpha chain

Chain i:  12% 72% 21% 7%



- Molecule 1: Antenna pigment protein alpha chain



- Molecule 1: Antenna pigment protein alpha chain



- Molecule 1: Antenna pigment protein alpha chain



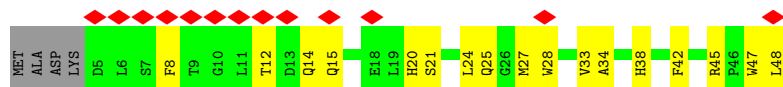
- Molecule 2: Antenna pigment protein beta chain



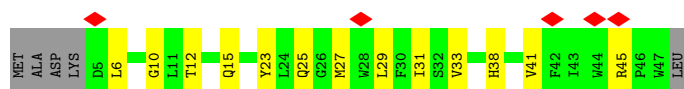
- Molecule 2: Antenna pigment protein beta chain



- Molecule 2: Antenna pigment protein beta chain



- Molecule 2: Antenna pigment protein beta chain



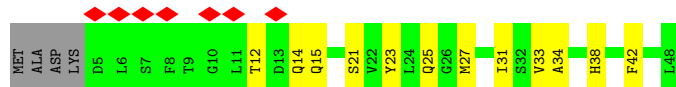
- Molecule 2: Antenna pigment protein beta chain



- Molecule 2: Antenna pigment protein beta chain



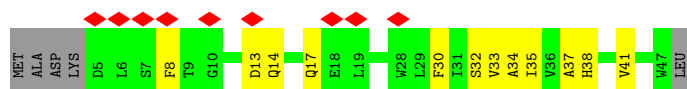
- Molecule 2: Antenna pigment protein beta chain



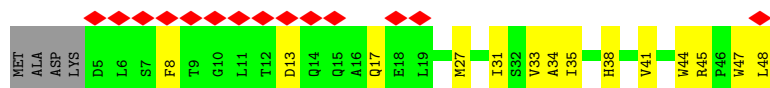
- Molecule 2: Antenna pigment protein beta chain



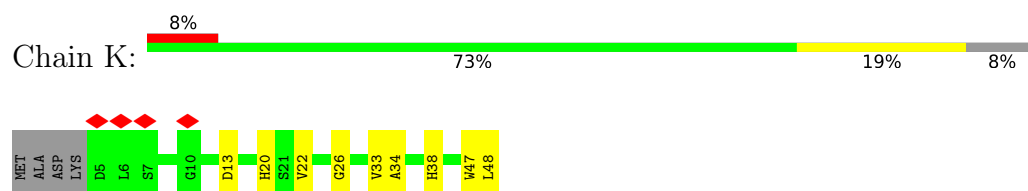
- Molecule 2: Antenna pigment protein beta chain



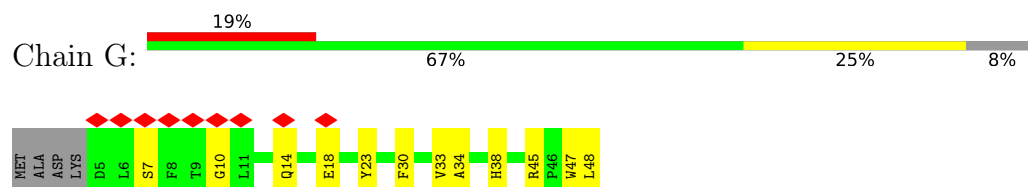
- Molecule 2: Antenna pigment protein beta chain



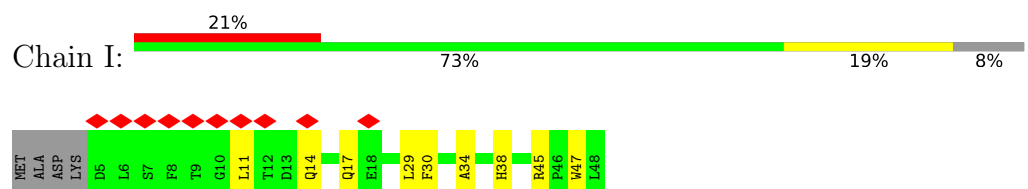
- Molecule 2: Antenna pigment protein beta chain



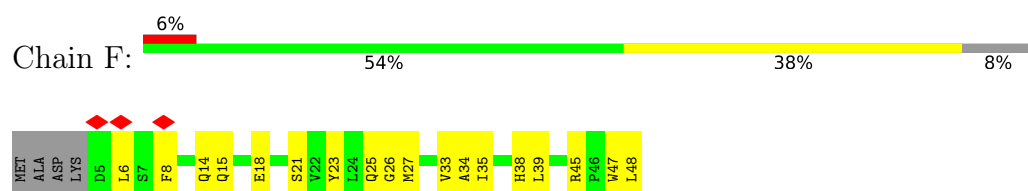
- Molecule 2: Antenna pigment protein beta chain



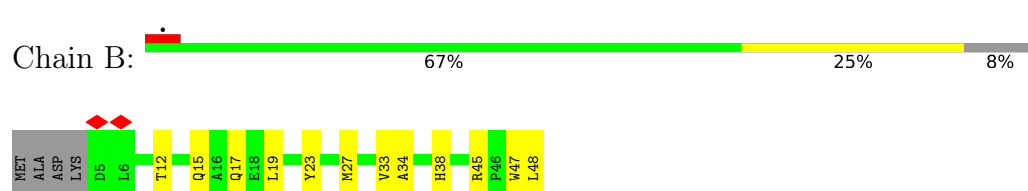
- Molecule 2: Antenna pigment protein beta chain



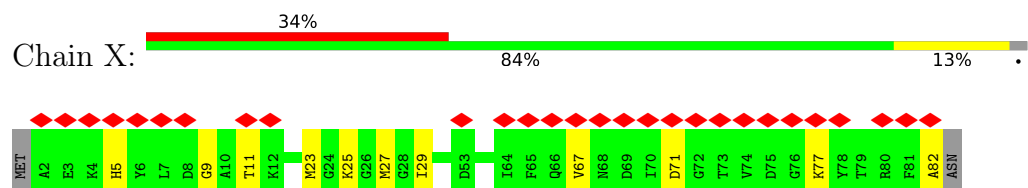
- Molecule 2: Antenna pigment protein beta chain



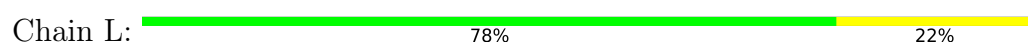
- Molecule 2: Antenna pigment protein beta chain

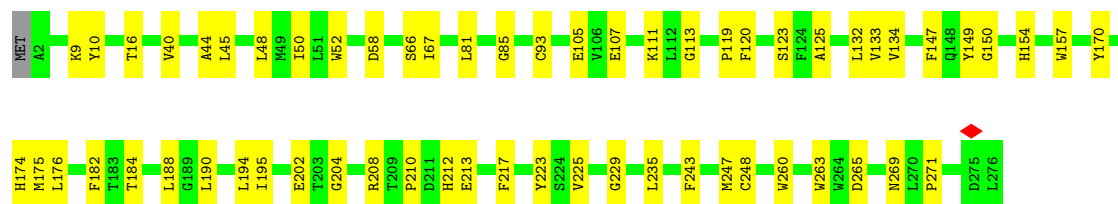


- Molecule 3: PufX

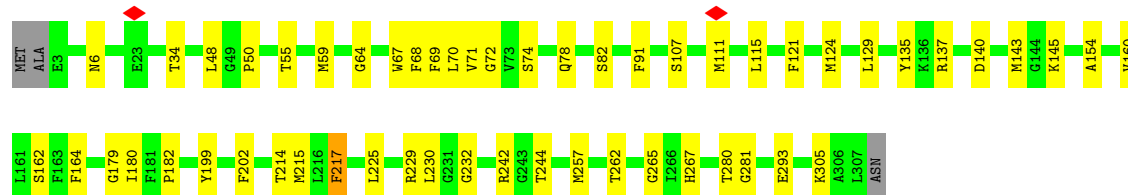
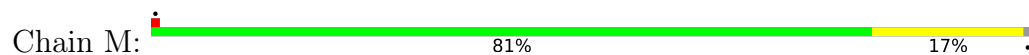


- Molecule 4: Photosynthetic reaction center L subunit

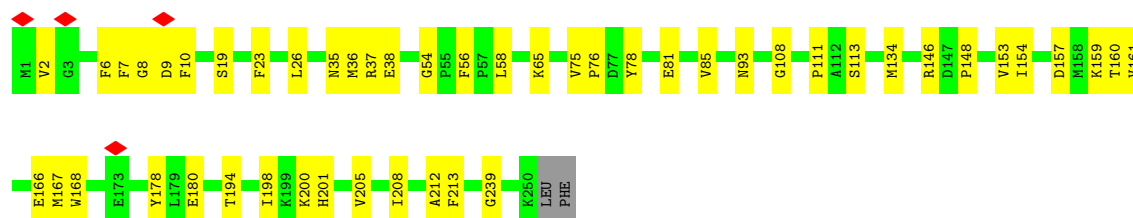
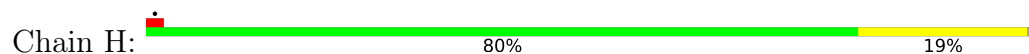




• Molecule 5: Reaction center protein M chain



• Molecule 6: Photosynthetic reaction center subunit H



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 184921                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 48                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.062                                   | Depositor |
| Minimum map value                    | -0.028                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.003                                   | Depositor |
| Recommended contour level            | 0.0157                                  | Depositor |
| Map size ( $\text{\AA}$ )            | 215.8, 215.8, 215.8                     | wwPDB     |
| Map dimensions                       | 260, 260, 260                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.83, 0.83, 0.83                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, U10, SPO, 3PE, FE, BPH

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | a     | 0.36         | 0/386       | 0.60        | 0/523       |
| 1   | b     | 0.31         | 0/460       | 0.44        | 0/622       |
| 1   | d     | 0.31         | 0/460       | 0.44        | 0/622       |
| 1   | e     | 0.31         | 0/460       | 0.43        | 0/622       |
| 1   | f     | 0.29         | 0/460       | 0.44        | 0/622       |
| 1   | g     | 0.27         | 0/460       | 0.39        | 0/622       |
| 1   | i     | 0.27         | 0/460       | 0.46        | 0/622       |
| 1   | j     | 0.27         | 0/460       | 0.52        | 0/622       |
| 1   | k     | 0.30         | 0/460       | 0.46        | 0/622       |
| 1   | n     | 0.28         | 0/460       | 0.38        | 0/622       |
| 1   | o     | 0.28         | 0/460       | 0.40        | 0/622       |
| 1   | r     | 0.26         | 0/460       | 0.39        | 0/622       |
| 1   | s     | 0.24         | 0/460       | 0.38        | 0/622       |
| 1   | t     | 0.23         | 0/460       | 0.40        | 0/622       |
| 1   | u     | 0.22         | 0/454       | 0.43        | 0/614       |
| 2   | A     | 0.29         | 0/375       | 0.41        | 0/512       |
| 2   | B     | 0.31         | 0/375       | 0.38        | 0/512       |
| 2   | D     | 0.29         | 0/375       | 0.36        | 0/512       |
| 2   | E     | 0.28         | 0/375       | 0.37        | 0/512       |
| 2   | F     | 0.26         | 0/375       | 0.36        | 0/512       |
| 2   | G     | 0.24         | 0/375       | 0.33        | 0/512       |
| 2   | I     | 0.22         | 0/375       | 0.33        | 0/512       |
| 2   | J     | 0.25         | 0/375       | 0.34        | 0/512       |
| 2   | K     | 0.26         | 0/375       | 0.35        | 0/512       |
| 2   | N     | 0.26         | 0/375       | 0.36        | 0/512       |
| 2   | O     | 0.24         | 0/375       | 0.41        | 0/512       |
| 2   | R     | 0.22         | 0/375       | 0.35        | 0/512       |
| 2   | S     | 0.20         | 0/375       | 0.36        | 0/512       |
| 2   | T     | 0.21         | 0/366       | 0.38        | 0/501       |
| 2   | U     | 0.19         | 0/366       | 0.34        | 0/501       |
| 3   | X     | 0.26         | 0/624       | 0.50        | 0/843       |
| 4   | L     | 0.35         | 0/2272      | 0.48        | 0/3108      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 5   | M     | 0.38         | 0/2507  | 0.50        | 0/3421  |
| 6   | H     | 0.34         | 0/1959  | 0.46        | 0/2664  |
| All | All   | 0.30         | 0/19789 | 0.44        | 0/26917 |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | M     | 0                   | 1                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | M     | 217 | PHE  | Sidechain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | a     | 373   | 0        | 384      | 9       | 0            |
| 1   | b     | 446   | 0        | 462      | 24      | 0            |
| 1   | d     | 446   | 0        | 462      | 13      | 0            |
| 1   | e     | 446   | 0        | 462      | 10      | 0            |
| 1   | f     | 446   | 0        | 462      | 15      | 0            |
| 1   | g     | 446   | 0        | 462      | 10      | 0            |
| 1   | i     | 446   | 0        | 462      | 9       | 0            |
| 1   | j     | 446   | 0        | 462      | 13      | 0            |
| 1   | k     | 446   | 0        | 462      | 15      | 0            |
| 1   | n     | 446   | 0        | 462      | 14      | 0            |
| 1   | o     | 446   | 0        | 462      | 19      | 0            |
| 1   | r     | 446   | 0        | 462      | 15      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | s     | 446   | 0        | 462      | 18      | 0            |
| 1   | t     | 446   | 0        | 462      | 21      | 0            |
| 1   | u     | 440   | 0        | 457      | 9       | 0            |
| 2   | A     | 363   | 0        | 355      | 9       | 0            |
| 2   | B     | 363   | 0        | 355      | 10      | 0            |
| 2   | D     | 363   | 0        | 355      | 9       | 0            |
| 2   | E     | 363   | 0        | 355      | 16      | 0            |
| 2   | F     | 363   | 0        | 355      | 15      | 0            |
| 2   | G     | 363   | 0        | 355      | 9       | 0            |
| 2   | I     | 363   | 0        | 355      | 9       | 0            |
| 2   | J     | 363   | 0        | 355      | 9       | 0            |
| 2   | K     | 363   | 0        | 355      | 8       | 0            |
| 2   | N     | 363   | 0        | 355      | 16      | 0            |
| 2   | O     | 363   | 0        | 355      | 13      | 0            |
| 2   | R     | 363   | 0        | 355      | 14      | 0            |
| 2   | S     | 363   | 0        | 355      | 25      | 0            |
| 2   | T     | 354   | 0        | 344      | 9       | 0            |
| 2   | U     | 354   | 0        | 344      | 14      | 0            |
| 3   | X     | 610   | 0        | 601      | 9       | 0            |
| 4   | L     | 2188  | 0        | 2126     | 46      | 0            |
| 5   | M     | 2420  | 0        | 2363     | 55      | 0            |
| 6   | H     | 1907  | 0        | 1880     | 45      | 0            |
| 7   | A     | 66    | 0        | 74       | 3       | 0            |
| 7   | D     | 66    | 0        | 74       | 2       | 0            |
| 7   | E     | 66    | 0        | 74       | 3       | 0            |
| 7   | F     | 132   | 0        | 148      | 9       | 0            |
| 7   | G     | 66    | 0        | 74       | 2       | 0            |
| 7   | I     | 66    | 0        | 74       | 2       | 0            |
| 7   | K     | 66    | 0        | 74       | 3       | 0            |
| 7   | L     | 66    | 0        | 74       | 3       | 0            |
| 7   | M     | 198   | 0        | 222      | 11      | 0            |
| 7   | N     | 66    | 0        | 74       | 5       | 0            |
| 7   | O     | 66    | 0        | 74       | 3       | 0            |
| 7   | R     | 66    | 0        | 74       | 7       | 0            |
| 7   | S     | 66    | 0        | 74       | 2       | 0            |
| 7   | a     | 66    | 0        | 74       | 2       | 0            |
| 7   | b     | 132   | 0        | 148      | 9       | 0            |
| 7   | d     | 66    | 0        | 74       | 9       | 0            |
| 7   | e     | 66    | 0        | 74       | 5       | 0            |
| 7   | g     | 66    | 0        | 74       | 8       | 0            |
| 7   | i     | 66    | 0        | 74       | 0       | 0            |
| 7   | j     | 132   | 0        | 148      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | k     | 66    | 0        | 74       | 3       | 0            |
| 7   | n     | 66    | 0        | 74       | 5       | 0            |
| 7   | o     | 66    | 0        | 74       | 5       | 0            |
| 7   | r     | 66    | 0        | 74       | 8       | 0            |
| 7   | s     | 66    | 0        | 74       | 5       | 0            |
| 7   | t     | 132   | 0        | 148      | 12      | 0            |
| 7   | u     | 132   | 0        | 148      | 11      | 0            |
| 8   | B     | 42    | 0        | 60       | 11      | 0            |
| 8   | D     | 42    | 0        | 60       | 11      | 0            |
| 8   | E     | 42    | 0        | 60       | 17      | 0            |
| 8   | F     | 42    | 0        | 60       | 12      | 0            |
| 8   | I     | 42    | 0        | 60       | 6       | 0            |
| 8   | M     | 42    | 0        | 60       | 13      | 0            |
| 8   | N     | 42    | 0        | 60       | 12      | 0            |
| 8   | X     | 42    | 0        | 60       | 4       | 0            |
| 8   | g     | 42    | 0        | 60       | 8       | 0            |
| 8   | j     | 42    | 0        | 60       | 7       | 0            |
| 8   | k     | 42    | 0        | 60       | 10      | 0            |
| 8   | r     | 84    | 0        | 120      | 20      | 0            |
| 8   | s     | 42    | 0        | 60       | 16      | 0            |
| 8   | t     | 42    | 0        | 60       | 7       | 0            |
| 9   | L     | 99    | 0        | 117      | 5       | 0            |
| 9   | M     | 66    | 0        | 78       | 6       | 0            |
| 9   | a     | 48    | 0        | 63       | 7       | 0            |
| 10  | L     | 110   | 0        | 113      | 9       | 0            |
| 10  | M     | 65    | 0        | 76       | 12      | 0            |
| 11  | M     | 1     | 0        | 0        | 0       | 0            |
| 12  | H     | 102   | 0        | 164      | 10      | 0            |
| 12  | d     | 43    | 0        | 63       | 2       | 0            |
| All | All   | 22571 | 0        | 23210    | 625     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (625) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 8:r:102:SPO:H21 | 7:O:101:BCL:H11  | 1.53                     | 0.89              |
| 8:t:102:SPO:H19 | 7:t:103:BCL:H11  | 1.58                     | 0.85              |
| 8:t:102:SPO:H37 | 8:t:102:SPO:H301 | 1.59                     | 0.84              |
| 1:s:24:LEU:HD11 | 8:s:201:SPO:H27  | 1.61                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:124:MET:HE3  | 8:M:406:SPO:H351 | 1.62                     | 0.82              |
| 1:o:6:LYS:HA     | 1:o:9:LEU:HD23   | 1.61                     | 0.81              |
| 2:O:12:THR:OG1   | 2:O:15:GLN:OE1   | 2.02                     | 0.78              |
| 1:g:51:TYR:HB2   | 1:g:54:VAL:HA    | 1.65                     | 0.77              |
| 7:d:101:BCL:HHB  | 8:B:101:SPO:H82  | 1.67                     | 0.77              |
| 5:M:179:GLY:HA3  | 5:M:182:PRO:HG2  | 1.67                     | 0.76              |
| 5:M:137:ARG:NH2  | 5:M:140:ASP:OD2  | 2.18                     | 0.76              |
| 1:s:27:LEU:HD11  | 8:s:201:SPO:H83  | 1.67                     | 0.76              |
| 2:T:13:ASP:OD1   | 2:T:17:GLN:NE2   | 2.18                     | 0.75              |
| 1:o:36:LEU:HD11  | 8:N:201:SPO:H41  | 1.65                     | 0.75              |
| 1:a:30:MET:HE3   | 9:a:102:U10:H18  | 1.67                     | 0.75              |
| 2:A:34:ALA:O     | 2:A:38:HIS:ND1   | 2.19                     | 0.74              |
| 2:N:31:ILE:HG12  | 7:N:202:BCL:H12  | 1.70                     | 0.74              |
| 1:o:51:TYR:HB2   | 1:o:54:VAL:HA    | 1.70                     | 0.73              |
| 1:s:48:GLY:HA2   | 1:s:54:VAL:HG23  | 1.70                     | 0.73              |
| 2:R:27:MET:O     | 2:R:31:ILE:HD12  | 1.89                     | 0.72              |
| 5:M:262:THR:HG23 | 5:M:265:GLY:H    | 1.53                     | 0.72              |
| 5:M:91:PHE:H     | 9:M:408:U10:H4M1 | 1.55                     | 0.71              |
| 2:E:23:TYR:HA    | 8:E:201:SPO:H311 | 1.72                     | 0.71              |
| 5:M:262:THR:H    | 6:H:35:ASN:HD22  | 1.39                     | 0.71              |
| 8:N:201:SPO:H27  | 8:N:201:SPO:H241 | 1.72                     | 0.70              |
| 1:f:40:GLY:O     | 2:F:45:ARG:NH1   | 2.24                     | 0.70              |
| 2:R:34:ALA:O     | 2:R:38:HIS:ND1   | 2.21                     | 0.70              |
| 2:F:34:ALA:O     | 2:F:38:HIS:ND1   | 2.24                     | 0.69              |
| 1:t:42:ASN:ND2   | 1:t:45:ASP:OD1   | 2.25                     | 0.69              |
| 8:E:201:SPO:H392 | 1:d:6:LYS:HB3    | 1.74                     | 0.69              |
| 8:M:406:SPO:H241 | 8:M:406:SPO:H27  | 1.75                     | 0.69              |
| 4:L:202:GLU:OE1  | 5:M:145:LYS:NZ   | 2.25                     | 0.69              |
| 5:M:230:LEU:O    | 5:M:232:GLY:N    | 2.25                     | 0.69              |
| 1:b:25:PHE:HA    | 7:b:101:BCL:H12  | 1.75                     | 0.68              |
| 1:f:51:TYR:HB2   | 1:f:54:VAL:HA    | 1.76                     | 0.68              |
| 2:S:34:ALA:O     | 2:S:38:HIS:ND1   | 2.21                     | 0.68              |
| 1:d:51:TYR:HB2   | 1:d:54:VAL:HA    | 1.75                     | 0.68              |
| 2:J:27:MET:HG3   | 8:j:301:SPO:C25  | 2.24                     | 0.67              |
| 2:T:34:ALA:O     | 2:T:38:HIS:ND1   | 2.26                     | 0.67              |
| 1:j:51:TYR:HB2   | 1:j:54:VAL:HA    | 1.76                     | 0.67              |
| 1:t:28:ALA:O     | 1:t:32:HIS:ND1   | 2.22                     | 0.67              |
| 2:I:34:ALA:O     | 2:I:38:HIS:ND1   | 2.25                     | 0.67              |
| 1:b:34:MET:HE1   | 8:B:101:SPO:HM13 | 1.77                     | 0.67              |
| 1:i:4:PHE:O      | 1:i:7:ILE:HG12   | 1.95                     | 0.67              |
| 1:o:44:LEU:HD11  | 8:N:201:SPO:H32A | 1.77                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:188:LEU:HD13 | 5:M:217:PHE:HB2  | 1.78                     | 0.66              |
| 9:a:102:U10:H312 | 1:b:21:GLY:HA3   | 1.77                     | 0.66              |
| 2:O:34:ALA:O     | 2:O:38:HIS:ND1   | 2.21                     | 0.66              |
| 1:t:20:GLN:HE21  | 7:u:101:BCL:H151 | 1.60                     | 0.66              |
| 2:G:34:ALA:O     | 2:G:38:HIS:ND1   | 2.25                     | 0.66              |
| 1:e:28:ALA:O     | 1:e:32:HIS:ND1   | 2.26                     | 0.66              |
| 1:o:25:PHE:HB2   | 7:o:100:BCL:H52  | 1.77                     | 0.66              |
| 5:M:74:SER:O     | 5:M:78:GLN:HG2   | 1.95                     | 0.65              |
| 7:b:101:BCL:CGD  | 7:b:101:BCL:HAA1 | 2.26                     | 0.65              |
| 8:k:102:SPO:H311 | 2:K:26:GLY:HA3   | 1.78                     | 0.65              |
| 8:k:102:SPO:H392 | 2:K:22:VAL:HG11  | 1.77                     | 0.65              |
| 8:D:201:SPO:H343 | 1:b:7:ILE:HG23   | 1.78                     | 0.65              |
| 1:n:30:MET:O     | 1:n:34:MET:HG3   | 1.96                     | 0.65              |
| 8:k:102:SPO:H391 | 1:j:6:LYS:HB2    | 1.79                     | 0.65              |
| 4:L:113:GLY:H    | 6:H:111:PRO:HB3  | 1.62                     | 0.64              |
| 2:U:27:MET:O     | 2:U:31:ILE:HG12  | 1.97                     | 0.64              |
| 2:E:34:ALA:O     | 2:E:38:HIS:ND1   | 2.29                     | 0.64              |
| 9:a:102:U10:H3M2 | 4:L:81:LEU:HD13  | 1.80                     | 0.64              |
| 9:a:102:U10:H311 | 1:b:18:VAL:HA    | 1.80                     | 0.64              |
| 1:j:28:ALA:O     | 1:j:32:HIS:ND1   | 2.31                     | 0.64              |
| 2:N:12:THR:H     | 2:N:15:GLN:HE21  | 1.47                     | 0.63              |
| 7:t:101:BCL:HMB2 | 8:s:201:SPO:H82  | 1.81                     | 0.63              |
| 8:r:102:SPO:H401 | 1:n:7:ILE:HD13   | 1.81                     | 0.63              |
| 1:j:8:TRP:HZ3    | 1:j:16:VAL:HG21  | 1.63                     | 0.63              |
| 2:D:34:ALA:O     | 2:D:38:HIS:ND1   | 2.28                     | 0.62              |
| 7:d:101:BCL:H152 | 8:B:101:SPO:H131 | 1.81                     | 0.62              |
| 2:N:25:GLN:OE1   | 1:k:2:SER:OG     | 2.14                     | 0.62              |
| 1:b:51:TYR:HB2   | 1:b:54:VAL:HA    | 1.82                     | 0.62              |
| 2:O:21:SER:O     | 2:O:25:GLN:NE2   | 2.32                     | 0.62              |
| 1:k:51:TYR:HB2   | 1:k:54:VAL:HG22  | 1.81                     | 0.62              |
| 1:d:28:ALA:O     | 1:d:32:HIS:ND1   | 2.26                     | 0.62              |
| 4:L:50:ILE:HA    | 4:L:67:ILE:HD11  | 1.81                     | 0.62              |
| 2:R:13:ASP:OD1   | 2:R:17:GLN:NE2   | 2.33                     | 0.62              |
| 1:d:32:HIS:HB2   | 8:B:101:SPO:H23  | 1.81                     | 0.61              |
| 1:a:28:ALA:O     | 1:a:32:HIS:ND1   | 2.26                     | 0.61              |
| 1:s:28:ALA:O     | 1:s:32:HIS:ND1   | 2.31                     | 0.61              |
| 4:L:204:GLY:O    | 6:H:65:LYS:NZ    | 2.25                     | 0.61              |
| 7:t:101:BCL:HMB2 | 8:s:201:SPO:H5   | 1.83                     | 0.61              |
| 2:S:23:TYR:OH    | 1:s:20:GLN:NE2   | 2.30                     | 0.61              |
| 1:a:14:ARG:HD2   | 3:X:5:HIS:CG     | 2.36                     | 0.61              |
| 1:r:28:ALA:O     | 1:r:32:HIS:ND1   | 2.33                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:J:34:ALA:O     | 2:J:38:HIS:ND1    | 2.26                     | 0.60              |
| 6:H:154:ILE:HG12 | 6:H:160:THR:HG22  | 1.84                     | 0.60              |
| 1:n:51:TYR:HB2   | 1:n:54:VAL:HA     | 1.81                     | 0.60              |
| 2:J:12:THR:HB    | 2:J:15:GLN:HG3    | 1.82                     | 0.60              |
| 1:g:28:ALA:O     | 1:g:32:HIS:ND1    | 2.32                     | 0.60              |
| 1:t:34:MET:HE2   | 8:t:102:SPO:H21A  | 1.84                     | 0.59              |
| 1:i:51:TYR:HB2   | 1:i:54:VAL:HA     | 1.82                     | 0.59              |
| 2:N:45:ARG:NH1   | 1:n:40:GLY:O      | 2.34                     | 0.59              |
| 4:L:174:HIS:HB2  | 4:L:248:CYS:SG    | 2.42                     | 0.59              |
| 7:L:301:BCL:H193 | 9:M:405:U10:H252  | 1.83                     | 0.59              |
| 10:L:302:BPH:HHc | 10:L:302:BPH:HBB3 | 1.84                     | 0.59              |
| 10:L:306:BPH:HHc | 10:L:306:BPH:HBB3 | 1.85                     | 0.59              |
| 1:u:51:TYR:HB2   | 1:u:54:VAL:HA     | 1.85                     | 0.59              |
| 2:J:12:THR:HG22  | 2:J:14:GLN:H      | 1.67                     | 0.59              |
| 1:f:20:GLN:HG2   | 7:g:101:BCL:H121  | 1.84                     | 0.59              |
| 1:i:3:LYS:HD2    | 1:i:3:LYS:O       | 2.02                     | 0.58              |
| 7:o:100:BCL:HED1 | 2:O:33:VAL:HG12   | 1.84                     | 0.58              |
| 1:n:4:PHE:O      | 1:n:7:ILE:HG12    | 2.04                     | 0.58              |
| 2:G:23:TYR:CE1   | 8:g:102:SPO:H26   | 2.38                     | 0.58              |
| 2:B:34:ALA:O     | 2:B:38:HIS:ND1    | 2.28                     | 0.58              |
| 1:s:51:TYR:HB2   | 1:s:54:VAL:HA     | 1.84                     | 0.58              |
| 1:u:20:GLN:O     | 1:u:24:LEU:HG     | 2.04                     | 0.58              |
| 8:r:103:SPO:C37  | 8:r:103:SPO:H311  | 2.34                     | 0.58              |
| 2:U:45:ARG:HH22  | 1:u:46:ILE:HG21   | 1.68                     | 0.58              |
| 1:g:26:LEU:O     | 1:g:30:MET:HG2    | 2.02                     | 0.58              |
| 5:M:64:GLY:HA3   | 10:M:403:BPH:H5C1 | 1.86                     | 0.58              |
| 1:d:18:VAL:HG11  | 12:d:102:3PE:H222 | 1.84                     | 0.58              |
| 8:r:102:SPO:H25  | 2:O:27:MET:HA     | 1.86                     | 0.58              |
| 8:r:103:SPO:H241 | 8:r:103:SPO:C27   | 2.34                     | 0.58              |
| 1:b:48:GLY:HA2   | 1:b:54:VAL:HG23   | 1.86                     | 0.58              |
| 2:E:27:MET:SD    | 2:E:31:ILE:HD12   | 2.44                     | 0.58              |
| 5:M:202:PHE:HD1  | 5:M:280:THR:HG23  | 1.68                     | 0.58              |
| 1:s:22:VAL:O     | 1:s:26:LEU:HG     | 2.04                     | 0.57              |
| 7:F:103:BCL:H3A  | 7:F:103:BCL:H52   | 1.85                     | 0.57              |
| 7:o:100:BCL:H171 | 8:r:102:SPO:H342  | 1.84                     | 0.57              |
| 1:r:48:GLY:HA2   | 1:r:54:VAL:HG23   | 1.85                     | 0.57              |
| 1:n:48:GLY:HA2   | 1:n:54:VAL:HG23   | 1.86                     | 0.57              |
| 1:r:32:HIS:CG    | 8:r:102:SPO:H6    | 2.40                     | 0.57              |
| 4:L:45:LEU:HD22  | 4:L:93:CYS:SG     | 2.45                     | 0.57              |
| 2:E:21:SER:O     | 2:E:25:GLN:HG3    | 2.05                     | 0.57              |
| 8:E:201:SPO:H362 | 1:d:6:LYS:HB2     | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:U:33:VAL:HG12   | 7:u:101:BCL:HED1  | 1.87                     | 0.57              |
| 1:i:48:GLY:HA2    | 1:i:54:VAL:HG23   | 1.87                     | 0.57              |
| 6:H:153:VAL:HG13  | 6:H:161:VAL:HG23  | 1.86                     | 0.57              |
| 1:o:8:TRP:HZ3     | 1:o:16:VAL:HG21   | 1.70                     | 0.56              |
| 2:U:6:LEU:HD23    | 6:H:154:ILE:HD11  | 1.87                     | 0.56              |
| 1:e:48:GLY:HA2    | 1:e:54:VAL:HG23   | 1.87                     | 0.56              |
| 4:L:9:LYS:NZ      | 6:H:81:GLU:OE1    | 2.29                     | 0.56              |
| 5:M:74:SER:HB2    | 5:M:115:LEU:HD23  | 1.87                     | 0.56              |
| 1:t:47:SER:HB3    | 2:S:47:TRP:O      | 2.06                     | 0.56              |
| 9:a:102:U10:H33   | 7:b:101:BCL:H13   | 1.87                     | 0.56              |
| 2:N:34:ALA:O      | 2:N:38:HIS:ND1    | 2.32                     | 0.56              |
| 1:e:20:GLN:HE21   | 7:F:101:BCL:H121  | 1.69                     | 0.56              |
| 1:e:51:TYR:OH     | 2:D:48:LEU:O      | 2.19                     | 0.56              |
| 2:A:18:GLU:HG2    | 3:X:11:THR:HG23   | 1.87                     | 0.56              |
| 5:M:262:THR:HG22  | 6:H:35:ASN:HD22   | 1.70                     | 0.56              |
| 2:A:30:PHE:HE2    | 7:A:101:BCL:HBA1  | 1.70                     | 0.56              |
| 2:I:14:GLN:HA     | 2:I:17:GLN:NE2    | 2.20                     | 0.56              |
| 10:L:302:BPH:HHC  | 10:L:302:BPH:CBB  | 2.36                     | 0.56              |
| 1:k:3:LYS:HB2     | 1:k:5:TYR:CE1     | 2.41                     | 0.56              |
| 2:F:23:TYR:HD1    | 8:F:102:SPO:H352  | 1.70                     | 0.56              |
| 5:M:199:TYR:CZ    | 5:M:305:LYS:HD2   | 2.40                     | 0.55              |
| 1:f:28:ALA:O      | 1:f:32:HIS:ND1    | 2.34                     | 0.55              |
| 2:T:37:ALA:O      | 2:T:41:VAL:HG23   | 2.06                     | 0.55              |
| 5:M:262:THR:H     | 6:H:35:ASN:ND2    | 2.04                     | 0.55              |
| 4:L:125:ALA:HB2   | 10:L:302:BPH:HAC1 | 1.89                     | 0.55              |
| 2:N:21:SER:O      | 2:N:25:GLN:HG3    | 2.07                     | 0.55              |
| 5:M:244:THR:HG21  | 6:H:113:SER:O     | 2.07                     | 0.55              |
| 1:t:54:VAL:HG23   | 2:S:45:ARG:HH11   | 1.72                     | 0.55              |
| 9:M:405:U10:H221  | 12:H:302:3PE:H352 | 1.89                     | 0.55              |
| 2:F:26:GLY:HA3    | 8:F:102:SPO:H393  | 1.89                     | 0.55              |
| 8:D:201:SPO:H27   | 8:D:201:SPO:H241  | 1.88                     | 0.55              |
| 5:M:69:PHE:HB2    | 10:M:403:BPH:H18  | 1.88                     | 0.55              |
| 2:S:27:MET:HA     | 8:s:201:SPO:H241  | 1.89                     | 0.54              |
| 10:M:403:BPH:H171 | 8:M:406:SPO:H23   | 1.89                     | 0.54              |
| 1:b:40:GLY:O      | 2:B:45:ARG:NH1    | 2.40                     | 0.54              |
| 1:k:33:LEU:HD11   | 8:j:301:SPO:H31   | 1.89                     | 0.54              |
| 1:o:14:ARG:O      | 1:o:18:VAL:HG23   | 2.08                     | 0.54              |
| 3:X:25:LYS:O      | 3:X:29:ILE:HG12   | 2.07                     | 0.54              |
| 2:O:20:HIS:O      | 2:O:24:LEU:HG     | 2.08                     | 0.54              |
| 10:M:403:BPH:HBB3 | 10:M:403:BPH:HHC  | 1.89                     | 0.54              |
| 1:f:20:GLN:NE2    | 7:g:101:BCL:H151  | 2.23                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:L:184:THR:HG21  | 5:M:214:THR:HG23  | 1.88                     | 0.54              |
| 3:X:9:GLY:C       | 3:X:11:THR:H      | 2.16                     | 0.54              |
| 6:H:19:SER:HB3    | 12:H:301:3PE:H3G1 | 1.90                     | 0.54              |
| 9:a:102:U10:H251  | 1:b:22:VAL:HG22   | 1.90                     | 0.53              |
| 2:R:47:TRP:CD1    | 2:R:48:LEU:HG     | 2.43                     | 0.53              |
| 6:H:148:PRO:HG3   | 6:H:198:ILE:HD13  | 1.90                     | 0.53              |
| 1:d:48:GLY:HA2    | 1:d:54:VAL:HG23   | 1.90                     | 0.53              |
| 2:U:38:HIS:HA     | 2:U:41:VAL:HG12   | 1.90                     | 0.53              |
| 7:t:101:BCL:H151  | 1:s:20:GLN:HE21   | 1.74                     | 0.53              |
| 8:D:201:SPO:H343  | 1:b:7:ILE:CG2     | 2.38                     | 0.53              |
| 2:O:42:PHE:HE1    | 2:O:48:LEU:HD23   | 1.74                     | 0.53              |
| 1:b:12:ASP:CB     | 6:H:93:ASN:HD22   | 2.22                     | 0.53              |
| 2:K:47:TRP:CD1    | 2:K:48:LEU:HD12   | 2.44                     | 0.53              |
| 1:t:54:VAL:HB     | 2:S:45:ARG:HD2    | 1.90                     | 0.53              |
| 2:U:12:THR:OG1    | 2:U:15:GLN:HG3    | 2.09                     | 0.53              |
| 2:U:31:ILE:HD12   | 7:u:102:BCL:H11   | 1.90                     | 0.53              |
| 1:s:4:PHE:O       | 1:s:7:ILE:HG12    | 2.09                     | 0.53              |
| 1:i:28:ALA:O      | 1:i:32:HIS:ND1    | 2.33                     | 0.53              |
| 7:M:401:BCL:H111  | 12:H:302:3PE:H3C2 | 1.90                     | 0.53              |
| 1:b:12:ASP:HB2    | 6:H:93:ASN:HD22   | 1.74                     | 0.53              |
| 4:L:16:THR:HA     | 4:L:107:GLU:HG2   | 1.91                     | 0.52              |
| 1:a:6:LYS:HA      | 1:a:9:LEU:HD23    | 1.90                     | 0.52              |
| 1:a:17:PHE:HD1    | 3:X:23:MET:HE3    | 1.74                     | 0.52              |
| 2:O:47:TRP:CD1    | 2:O:48:LEU:HD22   | 2.45                     | 0.52              |
| 2:U:45:ARG:HH12   | 1:u:46:ILE:HD13   | 1.74                     | 0.52              |
| 1:f:17:PHE:CD2    | 8:F:102:SPO:H351  | 2.44                     | 0.52              |
| 1:f:20:GLN:HE21   | 7:g:101:BCL:H151  | 1.74                     | 0.52              |
| 2:K:34:ALA:O      | 2:K:38:HIS:ND1    | 2.33                     | 0.52              |
| 7:M:402:BCL:H43   | 7:M:407:BCL:HBC3  | 1.91                     | 0.52              |
| 1:t:11:PHE:CE1    | 1:u:14:ARG:HG2    | 2.45                     | 0.52              |
| 7:t:103:BCL:HBA2  | 2:T:30:PHE:HE1    | 1.74                     | 0.52              |
| 10:M:403:BPH:HBC3 | 10:M:403:BPH:HHD  | 1.91                     | 0.52              |
| 2:E:35:ILE:O      | 2:E:39:LEU:HG     | 2.09                     | 0.52              |
| 4:L:81:LEU:HA     | 4:L:85:GLY:HA3    | 1.91                     | 0.52              |
| 2:S:30:PHE:HB3    | 8:s:201:SPO:H242  | 1.92                     | 0.52              |
| 2:N:14:GLN:O      | 2:N:17:GLN:HB2    | 2.10                     | 0.51              |
| 1:e:9:LEU:HD22    | 2:E:7:SER:HB3     | 1.92                     | 0.51              |
| 7:e:100:BCL:HED1  | 2:E:33:VAL:HG12   | 1.92                     | 0.51              |
| 1:k:27:LEU:HD11   | 8:k:102:SPO:H5    | 1.92                     | 0.51              |
| 4:L:120:PHE:O     | 4:L:123:SER:OG    | 2.24                     | 0.51              |
| 2:S:27:MET:HE2    | 8:s:201:SPO:H25   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:17:PHE:HZ     | 8:B:101:SPO:H342  | 1.74                     | 0.51              |
| 2:J:33:VAL:HG12   | 7:j:302:BCL:HED1  | 1.91                     | 0.51              |
| 2:N:12:THR:N      | 2:N:15:GLN:HE21   | 2.07                     | 0.51              |
| 1:i:40:GLY:O      | 2:I:45:ARG:NH2    | 2.43                     | 0.51              |
| 1:g:48:GLY:HA2    | 1:g:54:VAL:HG23   | 1.93                     | 0.51              |
| 2:N:30:PHE:HE1    | 7:N:202:BCL:HBA1  | 1.74                     | 0.51              |
| 2:T:32:SER:HA     | 2:T:35:ILE:HG12   | 1.92                     | 0.51              |
| 2:F:33:VAL:HG12   | 7:F:101:BCL:HED1  | 1.92                     | 0.51              |
| 8:F:102:SPO:H402  | 8:F:102:SPO:H32   | 1.91                     | 0.51              |
| 7:r:101:BCL:HED1  | 2:R:33:VAL:HG12   | 1.93                     | 0.51              |
| 2:O:47:TRP:NE1    | 2:O:48:LEU:HD22   | 2.26                     | 0.51              |
| 2:F:35:ILE:O      | 2:F:39:LEU:HG     | 2.11                     | 0.51              |
| 2:B:12:THR:OG1    | 2:B:15:GLN:HG3    | 2.10                     | 0.51              |
| 8:E:201:SPO:H9    | 7:F:101:BCL:HBA2  | 1.93                     | 0.51              |
| 2:U:6:LEU:HD21    | 6:H:201:HIS:HD2   | 1.74                     | 0.51              |
| 6:H:208:ILE:HG13  | 6:H:212:ALA:HB3   | 1.93                     | 0.50              |
| 1:j:23:PHE:HZ     | 8:j:301:SPO:H132  | 1.77                     | 0.50              |
| 4:L:170:TYR:O     | 4:L:260:TRP:HB3   | 2.11                     | 0.50              |
| 5:M:72:GLY:HA3    | 8:M:406:SPO:H31   | 1.94                     | 0.50              |
| 7:k:101:BCL:HED1  | 2:K:33:VAL:HG12   | 1.93                     | 0.50              |
| 7:g:101:BCL:H161  | 8:g:102:SPO:H361  | 1.93                     | 0.50              |
| 2:U:25:GLN:O      | 2:U:29:LEU:HG     | 2.11                     | 0.50              |
| 1:k:6:LYS:NZ      | 2:K:13:ASP:OD2    | 2.37                     | 0.50              |
| 4:L:265:ASP:O     | 4:L:269:ASN:HB2   | 2.11                     | 0.50              |
| 1:o:37:SER:OG     | 5:M:82:SER:HA     | 2.12                     | 0.50              |
| 4:L:9:LYS:HB3     | 6:H:85:VAL:HG11   | 1.93                     | 0.50              |
| 6:H:168:TRP:HB2   | 6:H:178:TYR:HB2   | 1.94                     | 0.50              |
| 1:e:24:LEU:HD11   | 8:E:201:SPO:H21   | 1.93                     | 0.50              |
| 4:L:176:LEU:HB2   | 9:L:304:U10:H112  | 1.94                     | 0.50              |
| 1:d:32:HIS:CB     | 8:B:101:SPO:H23   | 2.41                     | 0.50              |
| 4:L:210:PRO:HA    | 4:L:213:GLU:HG2   | 1.94                     | 0.50              |
| 10:L:302:BPH:HMA2 | 5:M:215:MET:HE1   | 1.94                     | 0.50              |
| 10:L:306:BPH:HMC1 | 10:M:403:BPH:HMA1 | 1.93                     | 0.50              |
| 1:j:4:PHE:O       | 1:j:7:ILE:HG12    | 2.12                     | 0.49              |
| 5:M:180:ILE:HG12  | 8:M:406:SPO:H133  | 1.93                     | 0.49              |
| 2:N:11:LEU:HA     | 2:N:15:GLN:HE21   | 1.77                     | 0.49              |
| 7:n:100:BCL:H203  | 2:K:20:HIS:HE1    | 1.78                     | 0.49              |
| 7:t:101:BCL:H151  | 1:s:20:GLN:NE2    | 2.27                     | 0.49              |
| 5:M:180:ILE:HD11  | 7:M:407:BCL:H172  | 1.93                     | 0.49              |
| 8:r:103:SPO:H352  | 8:r:103:SPO:H292  | 1.94                     | 0.49              |
| 1:e:4:PHE:O       | 1:e:7:ILE:HG12    | 2.11                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:H:205:VAL:HG21 | 6:H:213:PHE:HZ   | 1.78                     | 0.49              |
| 7:d:101:BCL:H111 | 8:B:101:SPO:H131 | 1.93                     | 0.49              |
| 7:o:100:BCL:H101 | 7:o:100:BCL:H142 | 1.94                     | 0.49              |
| 1:t:7:ILE:HD11   | 7:u:101:BCL:H203 | 1.94                     | 0.49              |
| 2:G:47:TRP:CD1   | 2:G:48:LEU:HG    | 2.47                     | 0.49              |
| 4:L:40:VAL:HG21  | 9:M:405:U10:H371 | 1.93                     | 0.49              |
| 5:M:124:MET:HB2  | 8:M:406:SPO:H312 | 1.95                     | 0.49              |
| 1:o:10:ILE:HG23  | 2:O:8:PHE:HD2    | 1.78                     | 0.49              |
| 1:k:22:VAL:HG21  | 5:M:59:MET:HG2   | 1.95                     | 0.49              |
| 2:T:14:GLN:HA    | 2:T:17:GLN:OE1   | 2.12                     | 0.49              |
| 1:j:31:ILE:HA    | 1:j:34:MET:HE2   | 1.94                     | 0.49              |
| 1:t:25:PHE:CE2   | 1:s:23:PHE:HE1   | 2.31                     | 0.49              |
| 8:E:201:SPO:H15  | 7:E:202:BCL:O1A  | 2.13                     | 0.49              |
| 1:d:25:PHE:HB2   | 7:d:101:BCL:H52  | 1.94                     | 0.49              |
| 8:D:201:SPO:H392 | 1:b:6:LYS:HB3    | 1.95                     | 0.48              |
| 2:J:21:SER:O     | 2:J:25:GLN:HG3   | 2.13                     | 0.48              |
| 2:F:27:MET:HG3   | 8:F:102:SPO:C21  | 2.42                     | 0.48              |
| 2:S:11:LEU:HD21  | 2:S:19:LEU:HD12  | 1.95                     | 0.48              |
| 2:E:23:TYR:CA    | 8:E:201:SPO:H311 | 2.42                     | 0.48              |
| 6:H:8:GLY:O      | 6:H:9:ASP:HB2    | 2.13                     | 0.48              |
| 2:B:23:TYR:CE1   | 2:B:27:MET:HE3   | 2.48                     | 0.48              |
| 8:F:102:SPO:H241 | 8:F:102:SPO:C28  | 2.43                     | 0.48              |
| 7:G:101:BCL:CHB  | 7:G:101:BCL:H101 | 2.43                     | 0.48              |
| 4:L:111:LYS:O    | 6:H:111:PRO:HG3  | 2.14                     | 0.48              |
| 1:o:27:LEU:HD11  | 8:r:102:SPO:H81  | 1.96                     | 0.48              |
| 8:N:201:SPO:HM11 | 1:n:35:LEU:HG    | 1.95                     | 0.48              |
| 2:I:29:LEU:HD23  | 8:I:102:SPO:H37  | 1.94                     | 0.48              |
| 5:M:281:GLY:O    | 7:M:402:BCL:HED3 | 2.13                     | 0.48              |
| 6:H:146:ARG:CZ   | 6:H:200:LYS:HG3  | 2.43                     | 0.48              |
| 1:b:51:TYR:HB2   | 1:b:54:VAL:CA    | 2.44                     | 0.48              |
| 1:s:29:VAL:O     | 1:s:33:LEU:HG    | 2.14                     | 0.48              |
| 4:L:10:TYR:OH    | 5:M:244:THR:HG22 | 2.13                     | 0.48              |
| 4:L:133:VAL:HG23 | 4:L:134:VAL:HG23 | 1.96                     | 0.48              |
| 1:f:48:GLY:HA2   | 1:f:54:VAL:HG23  | 1.96                     | 0.47              |
| 2:E:22:VAL:HG12  | 8:E:201:SPO:H342 | 1.96                     | 0.47              |
| 8:I:102:SPO:H291 | 8:I:102:SPO:H393 | 1.96                     | 0.47              |
| 2:S:27:MET:HA    | 8:s:201:SPO:C24  | 2.44                     | 0.47              |
| 1:r:12:ASP:O     | 1:r:16:VAL:HG23  | 2.13                     | 0.47              |
| 8:X:201:SPO:H362 | 8:X:201:SPO:H341 | 1.45                     | 0.47              |
| 5:M:135:TYR:CE2  | 5:M:145:LYS:HG2  | 2.49                     | 0.47              |
| 2:F:21:SER:O     | 2:F:25:GLN:HG3   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:r:103:SPO:H11   | 7:s:202:BCL:HBA2 | 1.96                     | 0.47              |
| 1:u:18:VAL:O      | 1:u:22:VAL:HG23  | 2.15                     | 0.47              |
| 2:S:5:ASP:OD1     | 1:s:9:LEU:HB3    | 2.15                     | 0.47              |
| 8:s:201:SPO:H312  | 8:s:201:SPO:H291 | 1.55                     | 0.47              |
| 6:H:111:PRO:HB2   | 6:H:239:GLY:HA2  | 1.97                     | 0.47              |
| 7:t:101:BCL:CMB   | 8:s:201:SPO:H82  | 2.43                     | 0.47              |
| 1:r:40:GLY:O      | 2:R:45:ARG:NH1   | 2.48                     | 0.47              |
| 1:f:34:MET:HG3    | 6:H:7:PHE:CD1    | 2.49                     | 0.47              |
| 1:i:54:VAL:CG1    | 2:G:45:ARG:HG3   | 2.44                     | 0.47              |
| 7:N:202:BCL:H3A   | 7:N:202:BCL:H52  | 1.96                     | 0.47              |
| 2:A:47:TRP:HZ2    | 7:A:101:BCL:H152 | 1.80                     | 0.47              |
| 1:f:6:LYS:HG2     | 1:f:9:LEU:HD12   | 1.96                     | 0.47              |
| 2:E:27:MET:HG2    | 8:E:201:SPO:H20  | 1.97                     | 0.47              |
| 10:L:302:BPH:H9C3 | 7:M:401:BCL:H193 | 1.96                     | 0.47              |
| 1:o:48:GLY:HA2    | 1:o:54:VAL:HG23  | 1.96                     | 0.47              |
| 2:N:12:THR:HG23   | 2:N:15:GLN:NE2   | 2.30                     | 0.47              |
| 7:t:101:BCL:HED1  | 2:T:33:VAL:HG12  | 1.96                     | 0.47              |
| 8:r:102:SPO:H19   | 7:O:101:BCL:C1   | 2.45                     | 0.47              |
| 3:X:71:ASP:OD2    | 3:X:71:ASP:N     | 2.46                     | 0.47              |
| 4:L:44:ALA:O      | 4:L:48:LEU:HB2   | 2.14                     | 0.47              |
| 4:L:208:ARG:HG3   | 5:M:143:MET:HG2  | 1.96                     | 0.47              |
| 1:t:54:VAL:HB     | 2:S:45:ARG:CD    | 2.45                     | 0.47              |
| 2:U:23:TYR:OH     | 1:u:20:GLN:OE1   | 2.24                     | 0.47              |
| 8:E:201:SPO:H241  | 8:E:201:SPO:H26  | 1.44                     | 0.47              |
| 2:D:21:SER:O      | 2:D:25:GLN:HG3   | 2.15                     | 0.47              |
| 1:k:48:GLY:HA2    | 1:k:54:VAL:HG23  | 1.96                     | 0.47              |
| 8:E:201:SPO:H362  | 1:d:6:LYS:CB     | 2.45                     | 0.47              |
| 8:s:201:SPO:HM13  | 8:s:201:SPO:H23  | 1.51                     | 0.47              |
| 8:I:102:SPO:H241  | 8:I:102:SPO:H26  | 1.71                     | 0.47              |
| 7:g:101:BCL:H51   | 7:g:101:BCL:H11  | 1.70                     | 0.47              |
| 1:f:5:TYR:OH      | 1:f:6:LYS:HE2    | 2.15                     | 0.46              |
| 5:M:68:PHE:CE2    | 8:M:406:SPO:H82  | 2.50                     | 0.46              |
| 5:M:265:GLY:HA3   | 6:H:35:ASN:ND2   | 2.30                     | 0.46              |
| 12:H:301:3PE:H322 | 12:H:301:3PE:H31 | 1.79                     | 0.46              |
| 1:o:42:ASN:HD22   | 1:o:45:ASP:HB2   | 1.79                     | 0.46              |
| 8:r:103:SPO:H22   | 2:R:27:MET:HG3   | 1.97                     | 0.46              |
| 8:E:201:SPO:C15   | 7:E:202:BCL:H11  | 2.45                     | 0.46              |
| 2:K:48:LEU:HD22   | 7:K:101:BCL:H171 | 1.97                     | 0.46              |
| 1:r:7:ILE:HA      | 1:r:10:ILE:HD13  | 1.96                     | 0.46              |
| 1:n:3:LYS:HD3     | 1:n:5:TYR:HE1    | 1.80                     | 0.46              |
| 2:G:7:SER:HB3     | 2:G:10:GLY:H     | 1.80                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:L:271:PRO:HD3  | 9:L:305:U10:H8    | 1.97                     | 0.46              |
| 6:H:134:MET:SD   | 6:H:167:MET:HE3   | 2.55                     | 0.46              |
| 1:t:17:PHE:HD2   | 1:s:11:PHE:CZ     | 2.33                     | 0.46              |
| 1:e:26:LEU:O     | 1:e:30:MET:HG2    | 2.16                     | 0.46              |
| 1:g:42:ASN:ND2   | 1:g:45:ASP:OD2    | 2.49                     | 0.46              |
| 2:S:30:PHE:HE2   | 7:S:101:BCL:HBA2  | 1.81                     | 0.46              |
| 1:b:54:VAL:CG1   | 2:A:45:ARG:HD3    | 2.46                     | 0.46              |
| 4:L:150:GLY:O    | 4:L:154:HIS:ND1   | 2.49                     | 0.46              |
| 4:L:182:PHE:CD2  | 10:M:403:BPH:HBB1 | 2.51                     | 0.46              |
| 4:L:194:LEU:HD21 | 4:L:213:GLU:HB2   | 1.98                     | 0.46              |
| 8:M:406:SPO:H311 | 8:M:406:SPO:H291  | 1.77                     | 0.46              |
| 6:H:157:ASP:O    | 6:H:159:LYS:N     | 2.48                     | 0.46              |
| 2:B:19:LEU:HG    | 8:B:101:SPO:H341  | 1.98                     | 0.46              |
| 2:B:23:TYR:HE1   | 2:B:27:MET:HE3    | 1.81                     | 0.46              |
| 2:B:47:TRP:CD1   | 2:B:48:LEU:HD22   | 2.51                     | 0.46              |
| 8:F:102:SPO:H32  | 8:F:102:SPO:C38   | 2.46                     | 0.46              |
| 2:S:25:GLN:O     | 2:S:29:LEU:HG     | 2.15                     | 0.46              |
| 8:M:406:SPO:H21A | 8:M:406:SPO:H5    | 1.42                     | 0.46              |
| 4:L:105:GLU:HB3  | 4:L:119:PRO:HG3   | 1.97                     | 0.46              |
| 1:g:6:LYS:HA     | 1:g:9:LEU:HD23    | 1.98                     | 0.46              |
| 1:o:42:ASN:ND2   | 1:o:45:ASP:HB2    | 2.31                     | 0.46              |
| 7:N:202:BCL:H141 | 7:N:202:BCL:H192  | 1.98                     | 0.46              |
| 2:N:48:LEU:HD12  | 7:N:202:BCL:H162  | 1.97                     | 0.45              |
| 2:S:33:VAL:HG12  | 7:s:202:BCL:HED1  | 1.99                     | 0.45              |
| 2:N:11:LEU:HA    | 2:N:15:GLN:NE2    | 2.31                     | 0.45              |
| 5:M:160:VAL:HA   | 5:M:164:PHE:HB2   | 1.97                     | 0.45              |
| 1:j:35:LEU:HD11  | 7:j:303:BCL:HHD   | 1.99                     | 0.45              |
| 1:t:35:LEU:HD11  | 7:t:103:BCL:HHD   | 1.98                     | 0.45              |
| 5:M:111:MET:HE3  | 5:M:111:MET:HA    | 1.98                     | 0.45              |
| 2:N:33:VAL:HG12  | 7:n:100:BCL:HED1  | 1.98                     | 0.45              |
| 8:N:201:SPO:H21  | 8:N:201:SPO:H25   | 1.80                     | 0.45              |
| 1:r:51:TYR:HB2   | 1:r:54:VAL:HA     | 1.98                     | 0.45              |
| 1:b:5:TYR:CE2    | 2:B:17:GLN:HG3    | 2.51                     | 0.45              |
| 1:b:35:LEU:HD11  | 7:b:102:BCL:HHD   | 1.99                     | 0.45              |
| 5:M:257:MET:HB2  | 9:M:405:U10:H23   | 1.98                     | 0.45              |
| 7:K:101:BCL:H112 | 7:K:101:BCL:C2B   | 2.46                     | 0.45              |
| 1:k:6:LYS:HA     | 1:k:9:LEU:HD23    | 1.97                     | 0.45              |
| 1:f:54:VAL:HG11  | 2:E:45:ARG:HB3    | 1.98                     | 0.45              |
| 2:E:12:THR:OG1   | 2:E:15:GLN:HG3    | 2.17                     | 0.45              |
| 8:j:301:SPO:H361 | 8:j:301:SPO:H341  | 1.81                     | 0.45              |
| 1:f:45:ASP:O     | 1:f:49:VAL:HG23   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:L:301:BCL:CGA  | 7:M:401:BCL:HBC1  | 2.47                     | 0.45              |
| 7:r:101:BCL:HHD  | 2:R:41:VAL:HG21   | 1.99                     | 0.45              |
| 8:s:201:SPO:HM12 | 8:s:201:SPO:H32A  | 1.49                     | 0.45              |
| 2:I:30:PHE:HA    | 8:I:102:SPO:H342  | 1.97                     | 0.45              |
| 4:L:223:TYR:HE2  | 4:L:225:VAL:HG22  | 1.82                     | 0.45              |
| 6:H:108:GLY:O    | 6:H:113:SER:HA    | 2.17                     | 0.45              |
| 1:g:4:PHE:O      | 1:g:7:ILE:HG12    | 2.17                     | 0.45              |
| 1:o:6:LYS:O      | 1:o:9:LEU:HB2     | 2.16                     | 0.45              |
| 7:k:101:BCL:H62  | 7:k:101:BCL:H41   | 1.73                     | 0.45              |
| 2:J:27:MET:HG2   | 2:J:31:ILE:CD1    | 2.47                     | 0.45              |
| 7:u:102:BCL:H171 | 7:u:102:BCL:H13   | 1.60                     | 0.45              |
| 4:L:223:TYR:CE2  | 4:L:225:VAL:HG22  | 2.52                     | 0.45              |
| 5:M:162:SER:HB2  | 8:M:406:SPO:C27   | 2.47                     | 0.45              |
| 1:g:25:PHE:HB2   | 7:g:101:BCL:H51   | 1.99                     | 0.45              |
| 8:N:201:SPO:HM12 | 1:n:31:ILE:HG23   | 1.99                     | 0.44              |
| 1:t:17:PHE:HD2   | 1:s:11:PHE:HZ     | 1.64                     | 0.44              |
| 5:M:34:THR:HG22  | 5:M:50:PRO:HD3    | 1.99                     | 0.44              |
| 5:M:107:SER:O    | 5:M:107:SER:OG    | 2.28                     | 0.44              |
| 8:N:201:SPO:H23  | 1:n:31:ILE:HA     | 1.99                     | 0.44              |
| 7:t:103:BCL:C1B  | 7:t:103:BCL:H101  | 2.47                     | 0.44              |
| 8:D:201:SPO:H393 | 1:b:10:ILE:HD11   | 1.98                     | 0.44              |
| 7:k:101:BCL:HHC  | 7:k:101:BCL:OBB   | 2.16                     | 0.44              |
| 4:L:182:PHE:HB3  | 10:M:403:BPH:HBB2 | 1.99                     | 0.44              |
| 8:X:201:SPO:H291 | 8:X:201:SPO:H312  | 1.51                     | 0.44              |
| 5:M:121:PHE:CD1  | 8:M:406:SPO:H393  | 2.53                     | 0.44              |
| 8:t:102:SPO:H22A | 8:t:102:SPO:HM12  | 1.69                     | 0.44              |
| 2:D:23:TYR:CE1   | 8:D:201:SPO:H25   | 2.52                     | 0.44              |
| 2:R:47:TRP:CE2   | 7:R:101:BCL:H2C   | 2.53                     | 0.44              |
| 7:F:101:BCL:H141 | 7:F:101:BCL:H162  | 1.73                     | 0.44              |
| 1:i:13:PRO:HG2   | 2:I:11:LEU:HD11   | 1.99                     | 0.44              |
| 7:I:101:BCL:H62  | 7:I:101:BCL:H41   | 1.86                     | 0.44              |
| 4:L:175:MET:SD   | 7:M:407:BCL:HED3  | 2.57                     | 0.44              |
| 6:H:7:PHE:HB2    | 6:H:10:PHE:HB3    | 1.99                     | 0.44              |
| 7:t:101:BCL:H121 | 1:s:20:GLN:HG3    | 1.98                     | 0.44              |
| 9:M:405:U10:H201 | 12:H:302:3PE:H371 | 1.99                     | 0.44              |
| 2:F:6:LEU:HD11   | 2:F:8:PHE:CE1     | 2.53                     | 0.44              |
| 7:o:100:BCL:H151 | 8:N:201:SPO:H22   | 1.99                     | 0.44              |
| 2:S:21:SER:O     | 2:S:25:GLN:HG3    | 2.18                     | 0.44              |
| 1:u:28:ALA:O     | 1:u:32:HIS:ND1    | 2.45                     | 0.44              |
| 8:D:201:SPO:H10  | 8:D:201:SPO:H81   | 1.88                     | 0.44              |
| 4:L:195:ILE:HG21 | 5:M:267:HIS:ND1   | 2.33                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:6:PHE:N       | 6:H:10:PHE:O      | 2.51                     | 0.44              |
| 7:d:101:BCL:H62   | 7:d:101:BCL:H41   | 1.41                     | 0.44              |
| 1:a:29:VAL:O      | 1:a:33:LEU:HG     | 2.18                     | 0.43              |
| 1:j:54:VAL:HG11   | 2:I:45:ARG:HB3    | 2.00                     | 0.43              |
| 5:M:293:GLU:OE1   | 6:H:2:VAL:HG11    | 2.18                     | 0.43              |
| 1:o:16:VAL:O      | 1:o:20:GLN:HG3    | 2.18                     | 0.43              |
| 8:r:102:SPO:H81   | 8:r:102:SPO:H10   | 1.58                     | 0.43              |
| 2:G:45:ARG:NH1    | 1:g:40:GLY:O      | 2.44                     | 0.43              |
| 8:j:301:SPO:H22   | 8:j:301:SPO:H26   | 1.80                     | 0.43              |
| 7:j:303:BCL:H72   | 7:j:303:BCL:CHB   | 2.48                     | 0.43              |
| 5:M:154:ALA:HB2   | 10:M:403:BPH:HAC1 | 2.00                     | 0.43              |
| 1:o:23:PHE:HE2    | 8:r:102:SPO:H182  | 1.83                     | 0.43              |
| 2:S:23:TYR:HE1    | 2:S:27:MET:HE3    | 1.84                     | 0.43              |
| 1:r:13:PRO:O      | 1:r:17:PHE:HD2    | 2.00                     | 0.43              |
| 5:M:262:THR:HG22  | 6:H:35:ASN:ND2    | 2.32                     | 0.43              |
| 12:H:301:3PE:H342 | 12:H:301:3PE:H371 | 1.45                     | 0.43              |
| 2:N:48:LEU:HD23   | 2:N:48:LEU:HA     | 1.87                     | 0.43              |
| 8:N:201:SPO:HM12  | 8:N:201:SPO:H22A  | 1.40                     | 0.43              |
| 8:N:201:SPO:H21A  | 8:N:201:SPO:H5    | 1.23                     | 0.43              |
| 1:r:12:ASP:OD1    | 1:r:13:PRO:HD2    | 2.17                     | 0.43              |
| 1:k:4:PHE:O       | 1:k:7:ILE:HG12    | 2.18                     | 0.43              |
| 8:k:102:SPO:H33   | 1:n:32:HIS:HB2    | 2.00                     | 0.43              |
| 8:s:201:SPO:H15   | 8:s:201:SPO:H19   | 1.42                     | 0.43              |
| 1:g:32:HIS:CG     | 8:F:102:SPO:H42   | 2.54                     | 0.43              |
| 1:o:27:LEU:HD11   | 8:r:102:SPO:C8    | 2.49                     | 0.43              |
| 1:r:43:TRP:CE3    | 7:r:101:BCL:HBC2  | 2.53                     | 0.43              |
| 7:L:301:BCL:HHC   | 7:L:301:BCL:OBB   | 2.18                     | 0.43              |
| 5:M:67:TRP:O      | 5:M:71:VAL:HG23   | 2.18                     | 0.43              |
| 8:N:201:SPO:H241  | 8:N:201:SPO:C27   | 2.44                     | 0.43              |
| 1:t:4:PHE:O       | 1:t:7:ILE:HG12    | 2.19                     | 0.43              |
| 2:D:19:LEU:HD21   | 1:d:13:PRO:HG3    | 2.01                     | 0.43              |
| 8:k:102:SPO:H10   | 7:n:100:BCL:H3A   | 1.99                     | 0.43              |
| 8:I:102:SPO:HM13  | 8:I:102:SPO:H23   | 1.60                     | 0.43              |
| 6:H:58:LEU:HD23   | 6:H:78:TYR:HE1    | 1.84                     | 0.43              |
| 1:i:25:PHE:HD2    | 1:i:26:LEU:HD12   | 1.83                     | 0.43              |
| 2:F:47:TRP:CD1    | 2:F:48:LEU:HD22   | 2.54                     | 0.43              |
| 7:e:100:BCL:H141  | 7:e:100:BCL:H162  | 1.56                     | 0.43              |
| 2:T:8:PHE:HZ      | 6:H:201:HIS:ND1   | 2.16                     | 0.43              |
| 12:H:302:3PE:H3E2 | 12:H:302:3PE:H3H2 | 1.51                     | 0.43              |
| 7:b:101:BCL:HED1  | 2:B:33:VAL:HG12   | 2.00                     | 0.43              |
| 8:t:102:SPO:H11   | 7:u:101:BCL:H3A   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:f:17:PHE:CG    | 8:F:102:SPO:H351  | 2.53                     | 0.43              |
| 7:R:101:BCL:H71  | 7:R:101:BCL:H112  | 1.89                     | 0.43              |
| 4:L:66:SER:HA    | 4:L:149:TYR:O     | 2.19                     | 0.43              |
| 1:e:20:GLN:NE2   | 7:F:101:BCL:H151  | 2.34                     | 0.42              |
| 7:u:102:BCL:H162 | 7:u:102:BCL:H192  | 1.71                     | 0.42              |
| 3:X:77:LYS:HD2   | 3:X:82:ALA:O      | 2.18                     | 0.42              |
| 8:g:102:SPO:H32  | 8:g:102:SPO:H241  | 2.00                     | 0.42              |
| 1:r:34:MET:HE2   | 1:r:34:MET:HB3    | 1.85                     | 0.42              |
| 7:r:101:BCL:H18  | 8:r:103:SPO:H403  | 2.02                     | 0.42              |
| 7:a:101:BCL:H61  | 2:A:33:VAL:HG11   | 1.99                     | 0.42              |
| 8:D:201:SPO:HM12 | 8:D:201:SPO:H22A  | 1.85                     | 0.42              |
| 7:b:101:BCL:OBB  | 7:b:101:BCL:HHC   | 2.19                     | 0.42              |
| 1:k:29:VAL:HG11  | 5:M:121:PHE:CE2   | 2.54                     | 0.42              |
| 2:G:33:VAL:HG12  | 7:g:101:BCL:HED1  | 2.01                     | 0.42              |
| 7:F:101:BCL:H51  | 7:F:101:BCL:H11   | 1.76                     | 0.42              |
| 2:S:23:TYR:CE1   | 2:S:27:MET:HE3    | 2.55                     | 0.42              |
| 8:r:103:SPO:HM12 | 1:s:32:HIS:HB3    | 2.01                     | 0.42              |
| 7:e:100:BCL:HHC  | 7:e:100:BCL:OBB   | 2.19                     | 0.42              |
| 2:F:26:GLY:C     | 8:F:102:SPO:H27   | 2.44                     | 0.42              |
| 2:B:27:MET:HB2   | 8:B:101:SPO:H243  | 2.01                     | 0.42              |
| 1:k:18:VAL:HG11  | 5:M:55:THR:HG23   | 2.02                     | 0.42              |
| 7:u:102:BCL:H91  | 7:u:102:BCL:H193  | 2.01                     | 0.42              |
| 8:M:406:SPO:H341 | 8:M:406:SPO:H362  | 1.49                     | 0.42              |
| 6:H:26:LEU:HB2   | 12:H:301:3PE:H382 | 2.00                     | 0.42              |
| 7:s:202:BCL:H162 | 7:s:202:BCL:H192  | 1.76                     | 0.42              |
| 6:H:54:GLY:HA3   | 12:H:302:3PE:HN3  | 1.83                     | 0.42              |
| 8:r:103:SPO:H15  | 8:r:103:SPO:H131  | 1.93                     | 0.42              |
| 7:a:101:BCL:HHD  | 2:A:41:VAL:HG21   | 2.02                     | 0.42              |
| 7:u:102:BCL:H62  | 7:u:102:BCL:H41   | 1.89                     | 0.42              |
| 3:X:67:VAL:HG23  | 4:L:58:ASP:HB2    | 2.01                     | 0.42              |
| 7:s:202:BCL:OBB  | 7:s:202:BCL:HHC   | 2.19                     | 0.42              |
| 2:R:47:TRP:CD2   | 7:R:101:BCL:H2C   | 2.55                     | 0.42              |
| 6:H:205:VAL:HG21 | 6:H:213:PHE:CZ    | 2.55                     | 0.42              |
| 8:F:102:SPO:H20  | 8:F:102:SPO:H181  | 1.67                     | 0.42              |
| 2:S:24:LEU:O     | 2:S:28:TRP:CD1    | 2.73                     | 0.42              |
| 2:S:30:PHE:HB3   | 8:s:201:SPO:C24   | 2.49                     | 0.42              |
| 1:e:24:LEU:CD1   | 8:E:201:SPO:H21   | 2.48                     | 0.42              |
| 8:E:201:SPO:HM12 | 8:E:201:SPO:H22A  | 1.77                     | 0.42              |
| 1:j:13:PRO:HA    | 1:j:16:VAL:HG22   | 2.01                     | 0.42              |
| 4:L:190:LEU:HD22 | 4:L:217:PHE:HZ    | 1.84                     | 0.42              |
| 5:M:59:MET:HB3   | 5:M:129:LEU:HD13  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:g:102:SPO:HM12 | 8:g:102:SPO:H32A | 1.48                     | 0.42              |
| 8:N:201:SPO:H33  | 8:N:201:SPO:HM13 | 1.46                     | 0.42              |
| 1:t:10:ILE:HD11  | 2:U:15:GLN:OE1   | 2.19                     | 0.42              |
| 7:r:101:BCL:H61  | 7:r:101:BCL:H41  | 1.83                     | 0.42              |
| 8:r:103:SPO:H352 | 8:r:103:SPO:C29  | 2.49                     | 0.42              |
| 1:a:23:PHE:HB2   | 7:b:101:BCL:H162 | 2.02                     | 0.42              |
| 7:e:100:BCL:HED1 | 2:E:33:VAL:CG1   | 2.50                     | 0.42              |
| 2:D:38:HIS:CE1   | 7:D:202:BCL:H91  | 2.55                     | 0.42              |
| 2:R:47:TRP:HZ2   | 7:R:101:BCL:H143 | 1.84                     | 0.42              |
| 5:M:6:ASN:ND2    | 6:H:194:THR:HG22 | 2.35                     | 0.42              |
| 2:O:24:LEU:O     | 2:O:28:TRP:CD1   | 2.73                     | 0.42              |
| 2:D:33:VAL:HG12  | 7:d:101:BCL:HED1 | 2.02                     | 0.42              |
| 1:k:34:MET:HE1   | 8:k:102:SPO:O1   | 2.20                     | 0.42              |
| 7:d:101:BCL:H152 | 7:d:101:BCL:H111 | 1.66                     | 0.42              |
| 2:U:6:LEU:HD21   | 6:H:201:HIS:CD2  | 2.53                     | 0.41              |
| 2:D:41:VAL:HG21  | 7:d:101:BCL:HHD  | 2.02                     | 0.41              |
| 1:b:11:PHE:HB3   | 1:b:16:VAL:HG21  | 2.02                     | 0.41              |
| 1:b:30:MET:O     | 1:b:34:MET:HG3   | 2.20                     | 0.41              |
| 7:b:101:BCL:H61  | 7:b:101:BCL:H41  | 1.92                     | 0.41              |
| 2:R:31:ILE:O     | 2:R:35:ILE:HG13  | 2.19                     | 0.41              |
| 1:t:34:MET:HE3   | 1:t:34:MET:HB3   | 2.00                     | 0.41              |
| 8:r:103:SPO:HM12 | 8:r:103:SPO:H32A | 1.51                     | 0.41              |
| 7:O:101:BCL:C1B  | 7:O:101:BCL:H112 | 2.51                     | 0.41              |
| 1:j:22:VAL:O     | 1:j:26:LEU:HG    | 2.19                     | 0.41              |
| 9:L:304:U10:H222 | 9:L:304:U10:H201 | 1.82                     | 0.41              |
| 8:t:102:SPO:HM13 | 1:u:33:LEU:HD21  | 2.02                     | 0.41              |
| 7:r:101:BCL:HBC3 | 2:R:44:TRP:CZ3   | 2.56                     | 0.41              |
| 2:O:14:GLN:HG2   | 2:O:15:GLN:N     | 2.35                     | 0.41              |
| 2:G:14:GLN:O     | 2:G:18:GLU:HG3   | 2.20                     | 0.41              |
| 4:L:243:PHE:O    | 4:L:247:MET:HG2  | 2.20                     | 0.41              |
| 8:g:102:SPO:H31  | 8:g:102:SPO:H5   | 1.25                     | 0.41              |
| 2:F:33:VAL:CG1   | 7:F:101:BCL:HED1 | 2.49                     | 0.41              |
| 7:t:103:BCL:H72  | 7:t:103:BCL:CHB  | 2.50                     | 0.41              |
| 2:S:11:LEU:HD12  | 2:R:8:PHE:HZ     | 1.85                     | 0.41              |
| 1:a:26:LEU:HD23  | 1:a:26:LEU:HA    | 1.92                     | 0.41              |
| 7:R:101:BCL:H101 | 7:R:101:BCL:CHB  | 2.51                     | 0.41              |
| 4:L:263:TRP:HE1  | 9:L:304:U10:H252 | 1.85                     | 0.41              |
| 5:M:229:ARG:H    | 5:M:229:ARG:HG3  | 1.70                     | 0.41              |
| 6:H:36:MET:HE1   | 6:H:56:PHE:O     | 2.21                     | 0.41              |
| 1:d:26:LEU:HD23  | 1:d:26:LEU:HA    | 1.87                     | 0.41              |
| 1:t:22:VAL:O     | 1:t:26:LEU:HG    | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:5:TYR:CE1    | 2:A:17:GLN:HG3   | 2.54                     | 0.41              |
| 1:b:11:PHE:HB3   | 1:b:16:VAL:CG2   | 2.51                     | 0.41              |
| 7:b:101:BCL:H51  | 7:b:101:BCL:H11  | 1.80                     | 0.41              |
| 7:u:102:BCL:H51  | 7:u:102:BCL:HAA1 | 2.02                     | 0.41              |
| 1:n:28:ALA:O     | 1:n:32:HIS:ND1   | 2.34                     | 0.41              |
| 2:G:30:PHE:CG    | 8:g:102:SPO:H22  | 2.55                     | 0.41              |
| 7:G:101:BCL:H112 | 7:G:101:BCL:H71  | 1.69                     | 0.41              |
| 8:M:406:SPO:H21  | 8:M:406:SPO:H25  | 1.86                     | 0.41              |
| 2:S:23:TYR:HA    | 8:s:201:SPO:H342 | 2.02                     | 0.41              |
| 2:J:23:TYR:HA    | 8:j:301:SPO:H343 | 2.01                     | 0.41              |
| 2:E:19:LEU:CD1   | 8:E:201:SPO:H352 | 2.51                     | 0.41              |
| 7:n:100:BCL:H61  | 7:n:100:BCL:H41  | 1.72                     | 0.41              |
| 7:j:303:BCL:C2B  | 7:j:303:BCL:H112 | 2.51                     | 0.41              |
| 4:L:147:PHE:HB3  | 4:L:157:TRP:CD2  | 2.55                     | 0.41              |
| 4:L:225:VAL:HG12 | 4:L:229:GLY:HA3  | 2.02                     | 0.41              |
| 2:F:14:GLN:NE2   | 2:F:15:GLN:HG3   | 2.35                     | 0.41              |
| 8:F:102:SPO:H32A | 8:F:102:SPO:HM12 | 1.84                     | 0.41              |
| 1:o:20:GLN:HE21  | 7:r:101:BCL:H121 | 1.85                     | 0.41              |
| 2:S:35:ILE:O     | 2:S:39:LEU:HD23  | 2.21                     | 0.41              |
| 7:u:102:BCL:H62  | 7:u:102:BCL:H92  | 1.83                     | 0.41              |
| 1:s:43:TRP:CD2   | 7:s:202:BCL:H2C  | 2.55                     | 0.41              |
| 8:s:201:SPO:H10  | 8:s:201:SPO:H81  | 1.62                     | 0.41              |
| 1:j:48:GLY:HA2   | 1:j:54:VAL:HG23  | 2.02                     | 0.41              |
| 5:M:70:LEU:HD22  | 5:M:115:LEU:HD11 | 2.02                     | 0.41              |
| 5:M:242:ARG:NH1  | 6:H:38:GLU:OE2   | 2.54                     | 0.41              |
| 7:M:402:BCL:H102 | 7:M:407:BCL:HBB2 | 2.02                     | 0.41              |
| 2:N:24:LEU:HD12  | 2:N:27:MET:HE2   | 2.02                     | 0.41              |
| 9:a:102:U10:H1M3 | 9:a:102:U10:H71  | 1.89                     | 0.41              |
| 1:b:34:MET:HE1   | 8:B:101:SPO:CM1  | 2.47                     | 0.41              |
| 9:L:303:U10:H172 | 9:L:303:U10:H151 | 1.75                     | 0.41              |
| 5:M:179:GLY:CA   | 5:M:182:PRO:HG2  | 2.43                     | 0.41              |
| 7:M:402:BCL:H203 | 7:M:407:BCL:H142 | 2.02                     | 0.41              |
| 1:d:4:PHE:O      | 1:d:7:ILE:HG12   | 2.20                     | 0.41              |
| 8:B:101:SPO:H341 | 8:B:101:SPO:H362 | 1.84                     | 0.41              |
| 1:t:27:LEU:HD11  | 8:t:102:SPO:C8   | 2.51                     | 0.41              |
| 1:t:54:VAL:HG23  | 2:S:45:ARG:NH1   | 2.34                     | 0.41              |
| 8:D:201:SPO:H301 | 8:D:201:SPO:H26  | 1.60                     | 0.41              |
| 8:k:102:SPO:H33  | 1:n:32:HIS:CB    | 2.51                     | 0.41              |
| 2:E:30:PHE:CG    | 8:E:201:SPO:H22  | 2.56                     | 0.41              |
| 3:X:27:MET:HE3   | 3:X:27:MET:HB2   | 1.87                     | 0.41              |
| 8:X:201:SPO:H33  | 8:X:201:SPO:H5   | 1.77                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:L:235:LEU:HD23  | 5:M:225:LEU:HD12  | 2.03                     | 0.41              |
| 10:L:302:BPH:H141 | 7:M:401:BCL:HBB3  | 2.03                     | 0.41              |
| 10:L:306:BPH:HMA1 | 5:M:48:LEU:HB3    | 2.03                     | 0.41              |
| 2:F:47:TRP:CE2    | 7:F:103:BCL:H2C   | 2.56                     | 0.41              |
| 1:r:11:PHE:HB3    | 1:r:16:VAL:CG2    | 2.50                     | 0.41              |
| 1:r:54:VAL:HG11   | 2:O:45:ARG:HB3    | 2.02                     | 0.41              |
| 7:e:100:BCL:HBB2  | 8:D:201:SPO:H22A  | 2.03                     | 0.41              |
| 7:R:101:BCL:H111  | 7:R:101:BCL:H152  | 1.93                     | 0.41              |
| 6:H:75:VAL:HA     | 6:H:76:PRO:C      | 2.46                     | 0.41              |
| 8:D:201:SPO:H341  | 8:D:201:SPO:H361  | 1.42                     | 0.40              |
| 2:A:22:VAL:HG12   | 8:X:201:SPO:H293  | 2.04                     | 0.40              |
| 1:k:33:LEU:HD23   | 1:k:33:LEU:HA     | 1.94                     | 0.40              |
| 1:f:7:ILE:HG21    | 8:g:102:SPO:H401  | 2.02                     | 0.40              |
| 8:E:201:SPO:H5    | 8:E:201:SPO:H31   | 1.66                     | 0.40              |
| 2:I:47:TRP:CD2    | 7:I:101:BCL:H2C   | 2.56                     | 0.40              |
| 7:g:101:BCL:OBB   | 7:g:101:BCL:HHC   | 2.21                     | 0.40              |
| 8:g:102:SPO:H23   | 8:g:102:SPO:HM13  | 1.58                     | 0.40              |
| 7:d:101:BCL:H62   | 7:d:101:BCL:H102  | 1.85                     | 0.40              |
| 7:j:302:BCL:OBB   | 7:j:302:BCL:HHC   | 2.22                     | 0.40              |
| 4:L:132:LEU:HD23  | 4:L:132:LEU:HA    | 1.91                     | 0.40              |
| 6:H:166:GLU:HB3   | 6:H:180:GLU:HB3   | 2.03                     | 0.40              |
| 12:d:102:3PE:H341 | 12:d:102:3PE:H371 | 1.91                     | 0.40              |
| 2:S:39:LEU:HD13   | 7:S:101:BCL:H201  | 2.02                     | 0.40              |
| 2:U:10:GLY:HA3    | 2:T:8:PHE:CE1     | 2.56                     | 0.40              |
| 7:A:101:BCL:H3A   | 7:A:101:BCL:H52   | 2.03                     | 0.40              |
| 1:k:35:LEU:HD11   | 7:K:101:BCL:HHD   | 2.03                     | 0.40              |
| 8:k:102:SPO:H22A  | 7:n:100:BCL:HBB2  | 2.02                     | 0.40              |
| 2:J:42:PHE:CG     | 7:j:303:BCL:H18   | 2.56                     | 0.40              |
| 2:I:29:LEU:HD23   | 8:I:102:SPO:C37   | 2.52                     | 0.40              |
| 5:M:68:PHE:HD2    | 10:M:403:BPH:H161 | 1.86                     | 0.40              |
| 10:M:403:BPH:C2B  | 7:M:407:BCL:H2    | 2.51                     | 0.40              |
| 10:M:403:BPH:H162 | 10:M:403:BPH:H121 | 1.79                     | 0.40              |
| 6:H:23:PHE:CD1    | 12:H:301:3PE:H381 | 2.56                     | 0.40              |
| 1:r:11:PHE:HB3    | 1:r:16:VAL:HG21   | 2.03                     | 0.40              |
| 1:r:35:LEU:HD11   | 7:R:101:BCL:HHD   | 2.03                     | 0.40              |
| 2:D:38:HIS:ND1    | 7:D:202:BCL:H91   | 2.36                     | 0.40              |
| 1:b:34:MET:HE3    | 4:L:52:TRP:CZ3    | 2.56                     | 0.40              |
| 1:j:34:MET:SD     | 8:j:301:SPO:H23   | 2.61                     | 0.40              |
| 4:L:208:ARG:HD3   | 4:L:212:HIS:CD2   | 2.57                     | 0.40              |
| 6:H:37:ARG:HG2    | 6:H:76:PRO:HD3    | 2.03                     | 0.40              |
| 1:o:26:LEU:O      | 1:o:30:MET:HG2    | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:38:ASN:C     | 1:t:40:GLY:H     | 2.29                     | 0.40              |
| 7:r:101:BCL:OBB  | 7:r:101:BCL:HHC  | 2.22                     | 0.40              |
| 8:k:102:SPO:H341 | 8:k:102:SPO:H361 | 1.91                     | 0.40              |
| 2:E:47:TRP:CE2   | 7:E:202:BCL:H2C  | 2.57                     | 0.40              |
| 1:n:52:GLU:O     | 1:n:53:ARG:HB2   | 2.22                     | 0.40              |
| 2:F:14:GLN:O     | 2:F:18:GLU:HG3   | 2.22                     | 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   | a     | 42/57 (74%) | 41 (98%) | 1 (2%)  | 0        | 100         | 100 |
| 1   | b     | 51/57 (90%) | 46 (90%) | 5 (10%) | 0        | 100         | 100 |
| 1   | d     | 51/57 (90%) | 48 (94%) | 3 (6%)  | 0        | 100         | 100 |
| 1   | e     | 51/57 (90%) | 47 (92%) | 4 (8%)  | 0        | 100         | 100 |
| 1   | f     | 51/57 (90%) | 47 (92%) | 4 (8%)  | 0        | 100         | 100 |
| 1   | g     | 51/57 (90%) | 48 (94%) | 3 (6%)  | 0        | 100         | 100 |
| 1   | i     | 51/57 (90%) | 46 (90%) | 5 (10%) | 0        | 100         | 100 |
| 1   | j     | 51/57 (90%) | 47 (92%) | 4 (8%)  | 0        | 100         | 100 |
| 1   | k     | 51/57 (90%) | 46 (90%) | 5 (10%) | 0        | 100         | 100 |
| 1   | n     | 51/57 (90%) | 46 (90%) | 5 (10%) | 0        | 100         | 100 |
| 1   | o     | 51/57 (90%) | 47 (92%) | 4 (8%)  | 0        | 100         | 100 |
| 1   | r     | 51/57 (90%) | 46 (90%) | 5 (10%) | 0        | 100         | 100 |
| 1   | s     | 51/57 (90%) | 47 (92%) | 4 (8%)  | 0        | 100         | 100 |
| 1   | t     | 51/57 (90%) | 47 (92%) | 4 (8%)  | 0        | 100         | 100 |
| 1   | u     | 50/57 (88%) | 45 (90%) | 5 (10%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | A     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | B     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | D     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | E     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | F     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | G     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | I     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | J     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | K     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | N     | 42/48 (88%)     | 41 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 2   | O     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | R     | 42/48 (88%)     | 41 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 2   | S     | 42/48 (88%)     | 42 (100%)  | 0        | 0        | 100         | 100 |
| 2   | T     | 41/48 (85%)     | 40 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 2   | U     | 41/48 (85%)     | 40 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 3   | X     | 79/83 (95%)     | 72 (91%)   | 7 (9%)   | 0        | 100         | 100 |
| 4   | L     | 273/276 (99%)   | 265 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 5   | M     | 303/308 (98%)   | 291 (96%)  | 12 (4%)  | 0        | 100         | 100 |
| 6   | H     | 248/252 (98%)   | 233 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| All | All   | 2286/2494 (92%) | 2179 (95%) | 107 (5%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed    | Rotameric | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1   | a     | 40/50 (80%) | 40 (100%) | 0        | 100         | 100 |
| 1   | b     | 48/50 (96%) | 48 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | d     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | e     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | f     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | g     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | i     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | j     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | k     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | n     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | o     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | r     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | s     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | t     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 1   | u     | 47/50 (94%)    | 47 (100%)  | 0        | 100         | 100 |
| 2   | A     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | B     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | D     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | E     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | F     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | G     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | I     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | J     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | K     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | N     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | O     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | R     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | S     | 38/41 (93%)    | 38 (100%)  | 0        | 100         | 100 |
| 2   | T     | 37/41 (90%)    | 37 (100%)  | 0        | 100         | 100 |
| 2   | U     | 37/41 (90%)    | 37 (100%)  | 0        | 100         | 100 |
| 3   | X     | 60/62 (97%)    | 60 (100%)  | 0        | 100         | 100 |
| 4   | L     | 219/220 (100%) | 219 (100%) | 0        | 100         | 100 |
| 5   | M     | 241/243 (99%)  | 241 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 6   | H     | 202/204 (99%)   | 202 (100%)  | 0        | 100         | 100 |
| All | All   | 2001/2094 (96%) | 2001 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | o     | 38  | ASN  |
| 2   | N     | 15  | GLN  |
| 1   | t     | 20  | GLN  |
| 1   | t     | 42  | ASN  |
| 1   | r     | 20  | GLN  |
| 1   | r     | 38  | ASN  |
| 2   | O     | 25  | GLN  |
| 1   | a     | 42  | ASN  |
| 2   | U     | 14  | GLN  |
| 1   | e     | 20  | GLN  |
| 2   | D     | 14  | GLN  |
| 2   | A     | 17  | GLN  |
| 3   | X     | 5   | HIS  |
| 1   | s     | 20  | GLN  |
| 2   | R     | 14  | GLN  |
| 1   | n     | 38  | ASN  |
| 1   | j     | 20  | GLN  |
| 2   | I     | 14  | GLN  |
| 2   | I     | 17  | GLN  |
| 4   | L     | 68  | ASN  |
| 4   | L     | 160 | ASN  |
| 4   | L     | 200 | ASN  |
| 5   | M     | 78  | GLN  |
| 6   | H     | 5   | ASN  |
| 6   | H     | 32  | GLN  |
| 6   | H     | 35  | ASN  |
| 6   | H     | 61  | GLN  |
| 6   | H     | 93  | ASN  |
| 1   | g     | 20  | GLN  |
| 2   | F     | 17  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 62 ligands modelled in this entry, 1 is monoatomic - leaving 61 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 | $\# Z  > 2$ |
| 7   | BCL  | r     | 101 | 1    | 69,74,74     | 1.17 | 6 (8%)      | 83,115,115  | 1.59 | 16 (19%)    |
| 7   | BCL  | k     | 101 | 1    | 69,74,74     | 1.15 | 8 (11%)     | 83,115,115  | 1.58 | 16 (19%)    |
| 7   | BCL  | a     | 101 | 1    | 69,74,74     | 1.14 | 6 (8%)      | 83,115,115  | 1.59 | 14 (16%)    |
| 7   | BCL  | o     | 100 | 1    | 69,74,74     | 1.26 | 8 (11%)     | 83,115,115  | 1.63 | 13 (15%)    |
| 7   | BCL  | M     | 407 | -    | 69,74,74     | 1.21 | 8 (11%)     | 83,115,115  | 1.42 | 12 (14%)    |
| 8   | SPO  | k     | 102 | -    | 40,41,41     | 2.24 | 12 (30%)    | 47,50,50    | 5.30 | 21 (44%)    |
| 9   | U10  | L     | 303 | -    | 33,33,63     | 2.76 | 10 (30%)    | 40,43,79    | 1.64 | 9 (22%)     |
| 8   | SPO  | r     | 103 | -    | 40,41,41     | 2.35 | 12 (30%)    | 47,50,50    | 5.14 | 16 (34%)    |
| 8   | SPO  | s     | 201 | -    | 40,41,41     | 2.31 | 12 (30%)    | 47,50,50    | 5.51 | 25 (53%)    |
| 7   | BCL  | b     | 101 | -    | 69,74,74     | 1.21 | 6 (8%)      | 83,115,115  | 1.79 | 20 (24%)    |
| 7   | BCL  | F     | 101 | 1    | 69,74,74     | 1.25 | 9 (13%)     | 83,115,115  | 1.64 | 17 (20%)    |
| 12  | 3PE  | H     | 301 | -    | 50,50,50     | 0.93 | 3 (6%)      | 53,55,55    | 1.15 | 2 (3%)      |
| 8   | SPO  | M     | 406 | -    | 40,41,41     | 2.26 | 13 (32%)    | 47,50,50    | 4.07 | 20 (42%)    |
| 8   | SPO  | r     | 102 | -    | 40,41,41     | 2.29 | 12 (30%)    | 47,50,50    | 5.28 | 24 (51%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | 3PE  | d     | 102 | -    | 42,42,50     | 1.00 | 2 (4%)   | 45,47,55    | 2.33 | 7 (15%)  |
| 10  | BPH  | L     | 302 | -    | 59,70,70     | 1.09 | 6 (10%)  | 61,101,101  | 1.87 | 11 (18%) |
| 7   | BCL  | e     | 100 | 1    | 69,74,74     | 1.23 | 8 (11%)  | 83,115,115  | 1.73 | 17 (20%) |
| 7   | BCL  | g     | 101 | 1    | 69,74,74     | 1.18 | 7 (10%)  | 83,115,115  | 1.57 | 15 (18%) |
| 7   | BCL  | b     | 102 | 2    | 69,74,74     | 1.12 | 7 (10%)  | 83,115,115  | 1.49 | 11 (13%) |
| 7   | BCL  | u     | 101 | 1    | 69,74,74     | 1.10 | 6 (8%)   | 83,115,115  | 1.56 | 15 (18%) |
| 8   | SPO  | B     | 101 | -    | 40,41,41     | 2.20 | 11 (27%) | 47,50,50    | 3.96 | 21 (44%) |
| 8   | SPO  | D     | 201 | -    | 40,41,41     | 2.19 | 11 (27%) | 47,50,50    | 5.18 | 18 (38%) |
| 7   | BCL  | n     | 100 | 1    | 69,74,74     | 1.16 | 7 (10%)  | 83,115,115  | 1.63 | 17 (20%) |
| 7   | BCL  | S     | 101 | 2    | 69,74,74     | 1.09 | 6 (8%)   | 83,115,115  | 1.48 | 11 (13%) |
| 7   | BCL  | D     | 202 | 2    | 69,74,74     | 1.14 | 7 (10%)  | 83,115,115  | 1.49 | 14 (16%) |
| 7   | BCL  | I     | 101 | 2    | 69,74,74     | 1.11 | 5 (7%)   | 83,115,115  | 1.47 | 13 (15%) |
| 7   | BCL  | N     | 202 | 2    | 69,74,74     | 1.14 | 5 (7%)   | 83,115,115  | 1.68 | 16 (19%) |
| 9   | U10  | M     | 405 | -    | 48,48,63     | 2.70 | 14 (29%) | 58,61,79    | 1.72 | 14 (24%) |
| 7   | BCL  | u     | 102 | 2    | 69,74,74     | 1.11 | 4 (5%)   | 83,115,115  | 1.68 | 9 (10%)  |
| 8   | SPO  | g     | 102 | -    | 40,41,41     | 2.40 | 12 (30%) | 47,50,50    | 5.01 | 24 (51%) |
| 8   | SPO  | N     | 201 | -    | 40,41,41     | 2.21 | 12 (30%) | 47,50,50    | 5.19 | 22 (46%) |
| 7   | BCL  | M     | 402 | 5    | 69,74,74     | 1.16 | 6 (8%)   | 83,115,115  | 1.75 | 16 (19%) |
| 8   | SPO  | F     | 102 | -    | 40,41,41     | 2.26 | 12 (30%) | 47,50,50    | 3.91 | 18 (38%) |
| 7   | BCL  | t     | 103 | 2    | 69,74,74     | 1.13 | 6 (8%)   | 83,115,115  | 1.40 | 10 (12%) |
| 9   | U10  | L     | 304 | -    | 38,38,63     | 2.69 | 12 (31%) | 46,49,79    | 1.71 | 13 (28%) |
| 10  | BPH  | L     | 306 | -    | 39,50,70     | 1.19 | 3 (7%)   | 37,77,101   | 2.30 | 9 (24%)  |
| 7   | BCL  | s     | 202 | 1    | 69,74,74     | 1.13 | 6 (8%)   | 83,115,115  | 1.55 | 13 (15%) |
| 7   | BCL  | G     | 101 | 2    | 69,74,74     | 1.08 | 6 (8%)   | 83,115,115  | 1.47 | 14 (16%) |
| 9   | U10  | a     | 102 | -    | 48,48,63     | 2.70 | 13 (27%) | 58,61,79    | 1.71 | 16 (27%) |
| 7   | BCL  | t     | 101 | 1    | 69,74,74     | 1.10 | 5 (7%)   | 83,115,115  | 1.58 | 15 (18%) |
| 8   | SPO  | t     | 102 | -    | 40,41,41     | 2.37 | 12 (30%) | 47,50,50    | 4.36 | 24 (51%) |
| 7   | BCL  | R     | 101 | 2    | 69,74,74     | 1.09 | 6 (8%)   | 83,115,115  | 1.41 | 11 (13%) |
| 7   | BCL  | M     | 401 | 4    | 69,74,74     | 1.12 | 7 (10%)  | 83,115,115  | 1.51 | 12 (14%) |
| 7   | BCL  | i     | 100 | 1    | 69,74,74     | 1.19 | 8 (11%)  | 83,115,115  | 1.54 | 15 (18%) |
| 12  | 3PE  | H     | 302 | -    | 50,50,50     | 0.95 | 2 (4%)   | 53,55,55    | 1.16 | 3 (5%)   |
| 7   | BCL  | j     | 302 | 1    | 69,74,74     | 1.14 | 7 (10%)  | 83,115,115  | 1.59 | 16 (19%) |
| 9   | U10  | M     | 408 | -    | 18,18,63     | 2.86 | 8 (44%)  | 22,25,79    | 1.49 | 3 (13%)  |
| 8   | SPO  | I     | 102 | -    | 40,41,41     | 2.33 | 12 (30%) | 47,50,50    | 4.92 | 19 (40%) |
| 7   | BCL  | F     | 103 | 2    | 69,74,74     | 1.13 | 7 (10%)  | 83,115,115  | 1.63 | 16 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | BCL  | d     | 101 | 1    | 69,74,74     | 1.21 | 8 (11%)  | 83,115,115  | 1.63 | 16 (19%) |
| 8   | SPO  | E     | 201 | -    | 40,41,41     | 2.24 | 10 (25%) | 47,50,50    | 5.37 | 24 (51%) |
| 7   | BCL  | K     | 101 | 2    | 69,74,74     | 1.12 | 5 (7%)   | 83,115,115  | 1.48 | 12 (14%) |
| 8   | SPO  | X     | 201 | -    | 40,41,41     | 2.23 | 12 (30%) | 47,50,50    | 3.47 | 17 (36%) |
| 8   | SPO  | j     | 301 | -    | 40,41,41     | 2.21 | 12 (30%) | 47,50,50    | 4.04 | 18 (38%) |
| 9   | U10  | L     | 305 | -    | 28,28,63     | 2.68 | 10 (35%) | 34,37,79    | 1.45 | 5 (14%)  |
| 10  | BPH  | M     | 403 | -    | 59,70,70     | 1.20 | 5 (8%)   | 61,101,101  | 2.14 | 9 (14%)  |
| 7   | BCL  | j     | 303 | 2    | 69,74,74     | 1.15 | 6 (8%)   | 83,115,115  | 1.51 | 14 (16%) |
| 7   | BCL  | E     | 202 | 2    | 69,74,74     | 1.12 | 7 (10%)  | 83,115,115  | 1.57 | 13 (15%) |
| 7   | BCL  | A     | 101 | 2    | 69,74,74     | 1.20 | 7 (10%)  | 83,115,115  | 1.49 | 12 (14%) |
| 7   | BCL  | L     | 301 | 4    | 69,74,74     | 1.19 | 8 (11%)  | 83,115,115  | 1.48 | 13 (15%) |
| 7   | BCL  | O     | 101 | 2    | 69,74,74     | 1.09 | 5 (7%)   | 83,115,115  | 1.47 | 13 (15%) |

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   | BCL  | r     | 101 | 1    | -       | 5/41/137/137  | -       |
| 7   | BCL  | k     | 101 | 1    | -       | 3/41/137/137  | -       |
| 7   | BCL  | a     | 101 | 1    | -       | 5/41/137/137  | -       |
| 7   | BCL  | o     | 100 | 1    | -       | 10/41/137/137 | -       |
| 7   | BCL  | M     | 407 | -    | -       | 5/41/137/137  | -       |
| 8   | SPO  | k     | 102 | -    | -       | 21/47/47/47   | -       |
| 9   | U10  | L     | 303 | -    | -       | 12/27/51/87   | 0/1/1/1 |
| 8   | SPO  | r     | 103 | -    | -       | 18/47/47/47   | -       |
| 8   | SPO  | s     | 201 | -    | -       | 21/47/47/47   | -       |
| 7   | BCL  | b     | 101 | -    | -       | 10/41/137/137 | -       |
| 7   | BCL  | F     | 101 | 1    | -       | 3/41/137/137  | -       |
| 12  | 3PE  | H     | 301 | -    | -       | 26/54/54/54   | -       |
| 8   | SPO  | M     | 406 | -    | -       | 21/47/47/47   | -       |
| 8   | SPO  | r     | 102 | -    | -       | 16/47/47/47   | -       |
| 12  | 3PE  | d     | 102 | -    | -       | 19/46/46/54   | -       |
| 10  | BPH  | L     | 302 | -    | -       | 4/37/105/105  | 0/5/6/6 |
| 7   | BCL  | e     | 100 | 1    | -       | 3/41/137/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 7   | BCL  | g     | 101 | 1    | -       | 1/41/137/137  | -       |
| 7   | BCL  | b     | 102 | 2    | -       | 5/41/137/137  | -       |
| 7   | BCL  | u     | 101 | 1    | -       | 3/41/137/137  | -       |
| 8   | SPO  | B     | 101 | -    | -       | 14/47/47/47   | -       |
| 8   | SPO  | D     | 201 | -    | -       | 15/47/47/47   | -       |
| 7   | BCL  | n     | 100 | 1    | -       | 6/41/137/137  | -       |
| 7   | BCL  | S     | 101 | 2    | -       | 4/41/137/137  | -       |
| 7   | BCL  | D     | 202 | 2    | -       | 6/41/137/137  | -       |
| 7   | BCL  | I     | 101 | 2    | -       | 10/41/137/137 | -       |
| 7   | BCL  | N     | 202 | 2    | -       | 7/41/137/137  | -       |
| 9   | U10  | M     | 405 | -    | -       | 12/45/69/87   | 0/1/1/1 |
| 7   | BCL  | u     | 102 | 2    | -       | 8/41/137/137  | -       |
| 8   | SPO  | g     | 102 | -    | -       | 19/47/47/47   | -       |
| 8   | SPO  | N     | 201 | -    | -       | 16/47/47/47   | -       |
| 7   | BCL  | M     | 402 | 5    | -       | 7/41/137/137  | -       |
| 8   | SPO  | F     | 102 | -    | -       | 17/47/47/47   | -       |
| 7   | BCL  | t     | 103 | 2    | -       | 6/41/137/137  | -       |
| 9   | U10  | L     | 304 | -    | -       | 15/33/57/87   | 0/1/1/1 |
| 10  | BPH  | L     | 306 | -    | -       | 2/13/81/105   | 0/5/6/6 |
| 7   | BCL  | s     | 202 | 1    | -       | 4/41/137/137  | -       |
| 7   | BCL  | G     | 101 | 2    | -       | 8/41/137/137  | -       |
| 9   | U10  | a     | 102 | -    | -       | 12/45/69/87   | 0/1/1/1 |
| 7   | BCL  | t     | 101 | 1    | -       | 4/41/137/137  | -       |
| 8   | SPO  | t     | 102 | -    | -       | 13/47/47/47   | -       |
| 7   | BCL  | R     | 101 | 2    | -       | 10/41/137/137 | -       |
| 7   | BCL  | M     | 401 | 4    | -       | 2/41/137/137  | -       |
| 7   | BCL  | i     | 100 | 1    | -       | 3/41/137/137  | -       |
| 12  | 3PE  | H     | 302 | -    | -       | 31/54/54/54   | -       |
| 7   | BCL  | j     | 302 | 1    | -       | 4/41/137/137  | -       |
| 9   | U10  | M     | 408 | -    | -       | 6/9/33/87     | 0/1/1/1 |
| 8   | SPO  | I     | 102 | -    | -       | 13/47/47/47   | -       |
| 7   | BCL  | F     | 103 | 2    | -       | 7/41/137/137  | -       |
| 7   | BCL  | d     | 101 | 1    | -       | 4/41/137/137  | -       |
| 8   | SPO  | E     | 201 | -    | -       | 17/47/47/47   | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 7   | BCL  | K     | 101 | 2    | -       | 8/41/137/137  | -       |
| 8   | SPO  | X     | 201 | -    | -       | 14/47/47/47   | -       |
| 8   | SPO  | j     | 301 | -    | -       | 19/47/47/47   | -       |
| 9   | U10  | L     | 305 | -    | -       | 9/21/45/87    | 0/1/1/1 |
| 10  | BPH  | M     | 403 | -    | -       | 8/37/105/105  | 0/5/6/6 |
| 7   | BCL  | j     | 303 | 2    | -       | 9/41/137/137  | -       |
| 7   | BCL  | E     | 202 | 2    | -       | 5/41/137/137  | -       |
| 7   | BCL  | A     | 101 | 2    | -       | 10/41/137/137 | -       |
| 7   | BCL  | L     | 301 | 4    | -       | 5/41/137/137  | -       |
| 7   | BCL  | O     | 101 | 2    | -       | 11/41/137/137 | -       |

All (488) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | L     | 303 | U10  | C8-C9   | 6.23  | 1.47        | 1.33     |
| 9   | L     | 303 | U10  | C13-C14 | 6.17  | 1.47        | 1.33     |
| 9   | L     | 304 | U10  | C13-C14 | 6.14  | 1.47        | 1.33     |
| 9   | M     | 405 | U10  | C8-C9   | 6.05  | 1.47        | 1.33     |
| 9   | L     | 303 | U10  | C18-C19 | 6.02  | 1.47        | 1.33     |
| 9   | L     | 304 | U10  | C23-C24 | 6.00  | 1.47        | 1.33     |
| 9   | L     | 305 | U10  | C13-C14 | 5.98  | 1.47        | 1.33     |
| 9   | M     | 405 | U10  | C23-C24 | 5.98  | 1.47        | 1.33     |
| 9   | M     | 405 | U10  | C33-C34 | 5.96  | 1.47        | 1.33     |
| 9   | L     | 305 | U10  | C8-C9   | 5.94  | 1.47        | 1.33     |
| 9   | a     | 102 | U10  | C18-C19 | 5.94  | 1.47        | 1.33     |
| 9   | L     | 304 | U10  | C8-C9   | 5.93  | 1.47        | 1.33     |
| 9   | M     | 408 | U10  | O4-C4   | -5.84 | 1.22        | 1.36     |
| 9   | a     | 102 | U10  | C13-C14 | 5.84  | 1.47        | 1.33     |
| 9   | a     | 102 | U10  | O4-C4   | -5.81 | 1.22        | 1.36     |
| 9   | a     | 102 | U10  | C23-C24 | 5.79  | 1.46        | 1.33     |
| 9   | L     | 304 | U10  | C18-C19 | 5.78  | 1.46        | 1.33     |
| 9   | a     | 102 | U10  | C33-C34 | 5.77  | 1.46        | 1.33     |
| 9   | a     | 102 | U10  | C28-C29 | 5.76  | 1.46        | 1.33     |
| 9   | M     | 405 | U10  | O3-C3   | -5.76 | 1.22        | 1.36     |
| 9   | a     | 102 | U10  | C8-C9   | 5.72  | 1.46        | 1.33     |
| 9   | L     | 303 | U10  | O4-C4   | -5.71 | 1.22        | 1.36     |
| 9   | a     | 102 | U10  | O3-C3   | -5.70 | 1.22        | 1.36     |
| 9   | M     | 405 | U10  | C28-C29 | 5.67  | 1.46        | 1.33     |
| 9   | M     | 405 | U10  | C18-C19 | 5.61  | 1.46        | 1.33     |
| 9   | M     | 405 | U10  | C13-C14 | 5.60  | 1.46        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | M     | 408 | U10  | O3-C3   | -5.58 | 1.23        | 1.36     |
| 9   | L     | 304 | U10  | O3-C3   | -5.54 | 1.23        | 1.36     |
| 9   | L     | 303 | U10  | O3-C3   | -5.41 | 1.23        | 1.36     |
| 9   | L     | 304 | U10  | O4-C4   | -5.37 | 1.23        | 1.36     |
| 9   | L     | 305 | U10  | O4-C4   | -5.36 | 1.23        | 1.36     |
| 9   | M     | 405 | U10  | O4-C4   | -5.35 | 1.23        | 1.36     |
| 9   | L     | 305 | U10  | O3-C3   | -5.34 | 1.23        | 1.36     |
| 9   | L     | 304 | U10  | C28-C29 | 5.32  | 1.47        | 1.32     |
| 9   | L     | 303 | U10  | C23-C24 | 5.23  | 1.47        | 1.32     |
| 9   | M     | 408 | U10  | C8-C9   | 5.22  | 1.47        | 1.32     |
| 9   | a     | 102 | U10  | C38-C39 | 5.22  | 1.47        | 1.32     |
| 9   | M     | 405 | U10  | C38-C39 | 5.16  | 1.47        | 1.32     |
| 9   | L     | 305 | U10  | C18-C19 | 5.12  | 1.47        | 1.32     |
| 8   | r     | 103 | SPO  | C25-C23 | 5.03  | 1.56        | 1.45     |
| 8   | g     | 102 | SPO  | C16-C17 | 4.96  | 1.56        | 1.45     |
| 8   | E     | 201 | SPO  | C16-C17 | 4.85  | 1.56        | 1.45     |
| 8   | N     | 201 | SPO  | C25-C23 | 4.81  | 1.56        | 1.45     |
| 8   | I     | 102 | SPO  | C16-C17 | 4.80  | 1.56        | 1.45     |
| 8   | M     | 406 | SPO  | C16-C17 | 4.80  | 1.56        | 1.45     |
| 8   | t     | 102 | SPO  | C16-C17 | 4.76  | 1.56        | 1.45     |
| 8   | t     | 102 | SPO  | C11-C12 | 4.70  | 1.56        | 1.45     |
| 8   | M     | 406 | SPO  | C25-C23 | 4.70  | 1.56        | 1.45     |
| 8   | F     | 102 | SPO  | C25-C23 | 4.69  | 1.56        | 1.45     |
| 8   | g     | 102 | SPO  | C11-C12 | 4.68  | 1.56        | 1.45     |
| 8   | B     | 101 | SPO  | C16-C17 | 4.66  | 1.56        | 1.45     |
| 7   | u     | 102 | BCL  | MG-NA   | 4.65  | 2.17        | 2.06     |
| 8   | B     | 101 | SPO  | C11-C12 | 4.62  | 1.55        | 1.45     |
| 8   | X     | 201 | SPO  | C16-C17 | 4.61  | 1.55        | 1.45     |
| 8   | r     | 103 | SPO  | C16-C17 | 4.60  | 1.55        | 1.45     |
| 8   | s     | 201 | SPO  | C25-C23 | 4.59  | 1.55        | 1.45     |
| 7   | t     | 103 | BCL  | MG-NA   | 4.57  | 2.17        | 2.06     |
| 8   | E     | 201 | SPO  | C11-C12 | 4.57  | 1.55        | 1.45     |
| 8   | r     | 102 | SPO  | C16-C17 | 4.56  | 1.55        | 1.45     |
| 8   | k     | 102 | SPO  | C25-C23 | 4.55  | 1.55        | 1.45     |
| 7   | M     | 407 | BCL  | MG-NA   | 4.49  | 2.16        | 2.06     |
| 7   | u     | 101 | BCL  | MG-NA   | 4.46  | 2.16        | 2.06     |
| 7   | k     | 101 | BCL  | MG-NA   | 4.44  | 2.16        | 2.06     |
| 8   | D     | 201 | SPO  | C16-C17 | 4.41  | 1.55        | 1.45     |
| 8   | E     | 201 | SPO  | C15-C14 | 4.40  | 1.57        | 1.43     |
| 8   | D     | 201 | SPO  | C25-C23 | 4.40  | 1.55        | 1.45     |
| 7   | a     | 101 | BCL  | MG-NA   | 4.39  | 2.16        | 2.06     |
| 8   | t     | 102 | SPO  | C25-C23 | 4.39  | 1.55        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 8   | I     | 102 | SPO  | C25-C23 | 4.39 | 1.55        | 1.45     |
| 8   | t     | 102 | SPO  | C6-C7   | 4.38 | 1.55        | 1.45     |
| 7   | j     | 303 | BCL  | MG-NA   | 4.38 | 2.16        | 2.06     |
| 7   | N     | 202 | BCL  | MG-NA   | 4.35 | 2.16        | 2.06     |
| 7   | F     | 103 | BCL  | MG-NA   | 4.34 | 2.16        | 2.06     |
| 8   | s     | 201 | SPO  | C16-C17 | 4.34 | 1.55        | 1.45     |
| 8   | M     | 406 | SPO  | C15-C14 | 4.33 | 1.56        | 1.43     |
| 7   | t     | 101 | BCL  | MG-NA   | 4.33 | 2.16        | 2.06     |
| 8   | r     | 103 | SPO  | C11-C12 | 4.33 | 1.55        | 1.45     |
| 7   | A     | 101 | BCL  | MG-NA   | 4.32 | 2.16        | 2.06     |
| 8   | I     | 102 | SPO  | C6-C7   | 4.32 | 1.55        | 1.45     |
| 7   | E     | 202 | BCL  | MG-NA   | 4.31 | 2.16        | 2.06     |
| 8   | j     | 301 | SPO  | C25-C23 | 4.29 | 1.55        | 1.45     |
| 8   | X     | 201 | SPO  | C25-C23 | 4.28 | 1.55        | 1.45     |
| 8   | F     | 102 | SPO  | C16-C17 | 4.28 | 1.55        | 1.45     |
| 8   | k     | 102 | SPO  | C11-C12 | 4.28 | 1.55        | 1.45     |
| 8   | s     | 201 | SPO  | C11-C12 | 4.28 | 1.55        | 1.45     |
| 7   | b     | 101 | BCL  | MG-NA   | 4.27 | 2.16        | 2.06     |
| 7   | r     | 101 | BCL  | MG-NA   | 4.27 | 2.16        | 2.06     |
| 7   | I     | 101 | BCL  | MG-NA   | 4.27 | 2.16        | 2.06     |
| 8   | k     | 102 | SPO  | C16-C17 | 4.24 | 1.55        | 1.45     |
| 7   | d     | 101 | BCL  | MG-NA   | 4.23 | 2.16        | 2.06     |
| 8   | I     | 102 | SPO  | C11-C12 | 4.23 | 1.55        | 1.45     |
| 8   | D     | 201 | SPO  | C11-C12 | 4.21 | 1.55        | 1.45     |
| 8   | X     | 201 | SPO  | C11-C12 | 4.20 | 1.55        | 1.45     |
| 8   | g     | 102 | SPO  | C15-C14 | 4.20 | 1.56        | 1.43     |
| 8   | r     | 102 | SPO  | C11-C12 | 4.20 | 1.55        | 1.45     |
| 7   | R     | 101 | BCL  | MG-NA   | 4.19 | 2.16        | 2.06     |
| 8   | g     | 102 | SPO  | C25-C23 | 4.19 | 1.54        | 1.45     |
| 8   | g     | 102 | SPO  | C6-C7   | 4.18 | 1.54        | 1.45     |
| 8   | E     | 201 | SPO  | C20-C19 | 4.17 | 1.56        | 1.43     |
| 7   | K     | 101 | BCL  | MG-NA   | 4.17 | 2.16        | 2.06     |
| 8   | k     | 102 | SPO  | C6-C7   | 4.15 | 1.54        | 1.45     |
| 7   | S     | 101 | BCL  | MG-NA   | 4.14 | 2.16        | 2.06     |
| 7   | G     | 101 | BCL  | MG-NA   | 4.14 | 2.16        | 2.06     |
| 8   | X     | 201 | SPO  | C6-C7   | 4.14 | 1.54        | 1.45     |
| 7   | j     | 302 | BCL  | MG-NA   | 4.14 | 2.16        | 2.06     |
| 8   | r     | 102 | SPO  | C25-C23 | 4.13 | 1.54        | 1.45     |
| 7   | e     | 100 | BCL  | MG-NA   | 4.13 | 2.16        | 2.06     |
| 8   | t     | 102 | SPO  | C10-C9  | 4.13 | 1.56        | 1.43     |
| 7   | n     | 100 | BCL  | MG-NA   | 4.12 | 2.16        | 2.06     |
| 7   | b     | 102 | BCL  | MG-NA   | 4.12 | 2.16        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | F     | 101 | BCL  | MG-NA   | 4.12  | 2.16        | 2.06     |
| 7   | M     | 401 | BCL  | MG-NA   | 4.11  | 2.16        | 2.06     |
| 7   | i     | 100 | BCL  | MG-NA   | 4.10  | 2.16        | 2.06     |
| 8   | r     | 103 | SPO  | C6-C7   | 4.08  | 1.54        | 1.45     |
| 8   | F     | 102 | SPO  | C11-C12 | 4.07  | 1.54        | 1.45     |
| 8   | r     | 103 | SPO  | C26-C27 | 4.07  | 1.56        | 1.43     |
| 8   | g     | 102 | SPO  | C26-C27 | 4.07  | 1.56        | 1.43     |
| 7   | s     | 202 | BCL  | MG-NA   | 4.07  | 2.15        | 2.06     |
| 8   | s     | 201 | SPO  | C6-C7   | 4.07  | 1.54        | 1.45     |
| 8   | g     | 102 | SPO  | C20-C19 | 4.07  | 1.56        | 1.43     |
| 7   | M     | 402 | BCL  | MG-NA   | 4.04  | 2.15        | 2.06     |
| 8   | t     | 102 | SPO  | C26-C27 | 4.04  | 1.56        | 1.43     |
| 7   | g     | 101 | BCL  | MG-NA   | 4.04  | 2.15        | 2.06     |
| 8   | j     | 301 | SPO  | C6-C7   | 4.03  | 1.54        | 1.45     |
| 8   | t     | 102 | SPO  | C15-C14 | 4.03  | 1.55        | 1.43     |
| 8   | g     | 102 | SPO  | C21-C22 | 4.02  | 1.55        | 1.43     |
| 8   | D     | 201 | SPO  | C6-C7   | 4.00  | 1.54        | 1.45     |
| 8   | B     | 101 | SPO  | C6-C7   | 4.00  | 1.54        | 1.45     |
| 7   | O     | 101 | BCL  | MG-NA   | 4.00  | 2.15        | 2.06     |
| 8   | M     | 406 | SPO  | C11-C12 | 4.00  | 1.54        | 1.45     |
| 10  | M     | 403 | BPH  | CBD-CGD | -3.99 | 1.47        | 1.52     |
| 8   | s     | 201 | SPO  | C4-C5   | 3.98  | 1.56        | 1.50     |
| 8   | N     | 201 | SPO  | C6-C7   | 3.97  | 1.54        | 1.45     |
| 8   | X     | 201 | SPO  | C15-C14 | 3.96  | 1.55        | 1.43     |
| 8   | I     | 102 | SPO  | C15-C14 | 3.95  | 1.55        | 1.43     |
| 8   | r     | 102 | SPO  | C15-C14 | 3.95  | 1.55        | 1.43     |
| 8   | r     | 102 | SPO  | C21-C22 | 3.94  | 1.55        | 1.43     |
| 8   | E     | 201 | SPO  | C21-C22 | 3.93  | 1.55        | 1.43     |
| 8   | N     | 201 | SPO  | C11-C12 | 3.93  | 1.54        | 1.45     |
| 8   | F     | 102 | SPO  | C26-C27 | 3.93  | 1.55        | 1.43     |
| 7   | o     | 100 | BCL  | MG-NA   | 3.92  | 2.15        | 2.06     |
| 7   | D     | 202 | BCL  | MG-NA   | 3.91  | 2.15        | 2.06     |
| 8   | g     | 102 | SPO  | C10-C9  | 3.90  | 1.55        | 1.43     |
| 9   | a     | 102 | U10  | C4-C5   | -3.89 | 1.37        | 1.48     |
| 8   | r     | 102 | SPO  | C10-C9  | 3.89  | 1.55        | 1.43     |
| 8   | B     | 101 | SPO  | C10-C9  | 3.89  | 1.55        | 1.43     |
| 8   | r     | 103 | SPO  | C15-C14 | 3.88  | 1.55        | 1.43     |
| 8   | F     | 102 | SPO  | C10-C9  | 3.88  | 1.55        | 1.43     |
| 8   | r     | 102 | SPO  | C26-C27 | 3.88  | 1.55        | 1.43     |
| 8   | r     | 102 | SPO  | C6-C7   | 3.88  | 1.54        | 1.45     |
| 8   | I     | 102 | SPO  | C26-C27 | 3.87  | 1.55        | 1.43     |
| 8   | k     | 102 | SPO  | C10-C9  | 3.87  | 1.55        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8   | t     | 102 | SPO  | C21-C22 | 3.87  | 1.55        | 1.43     |
| 7   | L     | 301 | BCL  | MG-NA   | 3.86  | 2.15        | 2.06     |
| 8   | F     | 102 | SPO  | C6-C7   | 3.85  | 1.54        | 1.45     |
| 8   | N     | 201 | SPO  | C16-C17 | 3.85  | 1.54        | 1.45     |
| 8   | j     | 301 | SPO  | C16-C17 | 3.83  | 1.54        | 1.45     |
| 8   | j     | 301 | SPO  | C10-C9  | 3.83  | 1.55        | 1.43     |
| 8   | s     | 201 | SPO  | C26-C27 | 3.83  | 1.55        | 1.43     |
| 8   | s     | 201 | SPO  | C10-C9  | 3.82  | 1.55        | 1.43     |
| 8   | N     | 201 | SPO  | C10-C9  | 3.82  | 1.55        | 1.43     |
| 8   | I     | 102 | SPO  | C10-C9  | 3.82  | 1.55        | 1.43     |
| 8   | D     | 201 | SPO  | C15-C14 | 3.81  | 1.55        | 1.43     |
| 8   | r     | 103 | SPO  | C10-C9  | 3.81  | 1.55        | 1.43     |
| 8   | E     | 201 | SPO  | C25-C23 | 3.79  | 1.54        | 1.45     |
| 8   | k     | 102 | SPO  | C26-C27 | 3.79  | 1.55        | 1.43     |
| 8   | j     | 301 | SPO  | C26-C27 | 3.78  | 1.55        | 1.43     |
| 8   | g     | 102 | SPO  | C4-C5   | 3.78  | 1.56        | 1.50     |
| 8   | M     | 406 | SPO  | C20-C19 | 3.77  | 1.55        | 1.43     |
| 8   | D     | 201 | SPO  | C10-C9  | 3.77  | 1.55        | 1.43     |
| 8   | I     | 102 | SPO  | C21-C22 | 3.77  | 1.55        | 1.43     |
| 8   | s     | 201 | SPO  | C15-C14 | 3.77  | 1.55        | 1.43     |
| 8   | j     | 301 | SPO  | C21-C22 | 3.76  | 1.55        | 1.43     |
| 7   | L     | 301 | BCL  | O1A-CGA | -3.75 | 1.11        | 1.22     |
| 8   | B     | 101 | SPO  | C21-C22 | 3.75  | 1.55        | 1.43     |
| 8   | E     | 201 | SPO  | C10-C9  | 3.74  | 1.55        | 1.43     |
| 8   | X     | 201 | SPO  | C20-C19 | 3.72  | 1.55        | 1.43     |
| 8   | B     | 101 | SPO  | C26-C27 | 3.72  | 1.55        | 1.43     |
| 8   | j     | 301 | SPO  | C11-C12 | 3.72  | 1.53        | 1.45     |
| 8   | B     | 101 | SPO  | C15-C14 | 3.72  | 1.55        | 1.43     |
| 8   | k     | 102 | SPO  | C15-C14 | 3.72  | 1.55        | 1.43     |
| 8   | B     | 101 | SPO  | C25-C23 | 3.71  | 1.53        | 1.45     |
| 8   | I     | 102 | SPO  | C4-C5   | 3.71  | 1.56        | 1.50     |
| 8   | t     | 102 | SPO  | C20-C19 | 3.71  | 1.54        | 1.43     |
| 8   | M     | 406 | SPO  | C10-C9  | 3.68  | 1.54        | 1.43     |
| 8   | X     | 201 | SPO  | C26-C27 | 3.68  | 1.54        | 1.43     |
| 8   | r     | 102 | SPO  | C20-C19 | 3.67  | 1.54        | 1.43     |
| 8   | N     | 201 | SPO  | C26-C27 | 3.66  | 1.54        | 1.43     |
| 9   | L     | 303 | U10  | C3-C2   | -3.66 | 1.38        | 1.48     |
| 8   | I     | 102 | SPO  | C20-C19 | 3.65  | 1.54        | 1.43     |
| 8   | B     | 101 | SPO  | C20-C19 | 3.63  | 1.54        | 1.43     |
| 8   | r     | 103 | SPO  | C20-C19 | 3.62  | 1.54        | 1.43     |
| 8   | r     | 103 | SPO  | C21-C22 | 3.62  | 1.54        | 1.43     |
| 9   | M     | 405 | U10  | C3-C2   | -3.62 | 1.38        | 1.48     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8   | j     | 301 | SPO  | C20-C19 | 3.62  | 1.54        | 1.43     |
| 8   | M     | 406 | SPO  | C26-C27 | 3.61  | 1.54        | 1.43     |
| 9   | a     | 102 | U10  | C3-C2   | -3.61 | 1.38        | 1.48     |
| 8   | N     | 201 | SPO  | C21-C22 | 3.60  | 1.54        | 1.43     |
| 8   | X     | 201 | SPO  | C10-C9  | 3.59  | 1.54        | 1.43     |
| 8   | F     | 102 | SPO  | C15-C14 | 3.58  | 1.54        | 1.43     |
| 8   | D     | 201 | SPO  | C20-C19 | 3.57  | 1.54        | 1.43     |
| 8   | s     | 201 | SPO  | C21-C22 | 3.57  | 1.54        | 1.43     |
| 8   | E     | 201 | SPO  | C26-C27 | 3.56  | 1.54        | 1.43     |
| 8   | X     | 201 | SPO  | C21-C22 | 3.55  | 1.54        | 1.43     |
| 8   | N     | 201 | SPO  | C4-C5   | 3.55  | 1.55        | 1.50     |
| 10  | L     | 306 | BPH  | CBD-CGD | -3.55 | 1.47        | 1.52     |
| 8   | F     | 102 | SPO  | C21-C22 | 3.55  | 1.54        | 1.43     |
| 8   | F     | 102 | SPO  | C20-C19 | 3.55  | 1.54        | 1.43     |
| 8   | E     | 201 | SPO  | C6-C7   | 3.55  | 1.53        | 1.45     |
| 8   | j     | 301 | SPO  | C15-C14 | 3.55  | 1.54        | 1.43     |
| 9   | M     | 408 | U10  | C4-C5   | -3.54 | 1.38        | 1.48     |
| 8   | k     | 102 | SPO  | C20-C19 | 3.54  | 1.54        | 1.43     |
| 8   | D     | 201 | SPO  | C21-C22 | 3.54  | 1.54        | 1.43     |
| 8   | D     | 201 | SPO  | C26-C27 | 3.53  | 1.54        | 1.43     |
| 8   | M     | 406 | SPO  | C6-C7   | 3.51  | 1.53        | 1.45     |
| 9   | M     | 405 | U10  | C4-C5   | -3.50 | 1.38        | 1.48     |
| 8   | t     | 102 | SPO  | C4-C5   | 3.50  | 1.55        | 1.50     |
| 8   | k     | 102 | SPO  | C21-C22 | 3.49  | 1.54        | 1.43     |
| 9   | M     | 408 | U10  | C3-C2   | -3.48 | 1.38        | 1.48     |
| 9   | L     | 304 | U10  | C4-C5   | -3.47 | 1.38        | 1.48     |
| 7   | b     | 101 | BCL  | O1A-CGA | -3.45 | 1.12        | 1.22     |
| 10  | L     | 302 | BPH  | CBD-CGD | -3.44 | 1.47        | 1.52     |
| 7   | M     | 402 | BCL  | O1A-CGA | -3.43 | 1.12        | 1.22     |
| 8   | N     | 201 | SPO  | C20-C19 | 3.42  | 1.54        | 1.43     |
| 8   | M     | 406 | SPO  | C21-C22 | 3.39  | 1.54        | 1.43     |
| 8   | N     | 201 | SPO  | C15-C14 | 3.39  | 1.53        | 1.43     |
| 8   | r     | 103 | SPO  | C4-C5   | 3.36  | 1.55        | 1.50     |
| 8   | r     | 102 | SPO  | C4-C5   | 3.36  | 1.55        | 1.50     |
| 8   | s     | 201 | SPO  | C20-C19 | 3.35  | 1.53        | 1.43     |
| 8   | X     | 201 | SPO  | C4-C5   | 3.30  | 1.55        | 1.50     |
| 8   | B     | 101 | SPO  | C4-C5   | 3.28  | 1.55        | 1.50     |
| 7   | t     | 103 | BCL  | MG-NC   | 3.22  | 2.13        | 2.06     |
| 8   | k     | 102 | SPO  | C4-C5   | 3.21  | 1.55        | 1.50     |
| 12  | d     | 102 | 3PE  | O21-C2  | -3.21 | 1.38        | 1.46     |
| 8   | E     | 201 | SPO  | C4-C5   | 3.21  | 1.55        | 1.50     |
| 10  | M     | 403 | BPH  | C3D-CAD | -3.20 | 1.40        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8   | j     | 301 | SPO  | C4-C5   | 3.19  | 1.55        | 1.50     |
| 8   | F     | 102 | SPO  | C4-C5   | 3.18  | 1.55        | 1.50     |
| 9   | L     | 305 | U10  | C3-C2   | -3.16 | 1.39        | 1.48     |
| 7   | F     | 101 | BCL  | O1A-CGA | -3.16 | 1.13        | 1.22     |
| 9   | L     | 305 | U10  | C4-C5   | -3.13 | 1.39        | 1.48     |
| 8   | D     | 201 | SPO  | C4-C5   | 3.09  | 1.55        | 1.50     |
| 7   | o     | 100 | BCL  | O1A-CGA | -3.08 | 1.13        | 1.22     |
| 7   | u     | 102 | BCL  | MG-NC   | 3.08  | 2.13        | 2.06     |
| 9   | L     | 303 | U10  | C4-C5   | -3.06 | 1.40        | 1.48     |
| 8   | M     | 406 | SPO  | C4-C5   | 3.04  | 1.55        | 1.50     |
| 9   | L     | 304 | U10  | C3-C2   | -3.02 | 1.40        | 1.48     |
| 7   | n     | 100 | BCL  | O1A-CGA | -3.01 | 1.13        | 1.22     |
| 12  | H     | 302 | 3PE  | O21-C2  | -2.99 | 1.39        | 1.46     |
| 7   | o     | 100 | BCL  | C3C-C4C | -2.98 | 1.47        | 1.51     |
| 9   | M     | 405 | U10  | C6-C5   | -2.98 | 1.38        | 1.46     |
| 7   | u     | 101 | BCL  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 7   | M     | 407 | BCL  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 9   | M     | 408 | U10  | C6-C5   | -2.92 | 1.38        | 1.46     |
| 7   | e     | 100 | BCL  | O2A-CGA | -2.89 | 1.24        | 1.33     |
| 7   | D     | 202 | BCL  | C3D-C4D | -2.87 | 1.37        | 1.44     |
| 10  | L     | 306 | BPH  | C3D-CAD | -2.86 | 1.41        | 1.47     |
| 7   | e     | 100 | BCL  | O1A-CGA | -2.86 | 1.14        | 1.22     |
| 7   | d     | 101 | BCL  | C3C-C4C | -2.85 | 1.48        | 1.51     |
| 7   | r     | 101 | BCL  | O1A-CGA | -2.84 | 1.14        | 1.22     |
| 7   | M     | 402 | BCL  | C3D-C4D | -2.84 | 1.37        | 1.44     |
| 7   | j     | 303 | BCL  | C3D-C4D | -2.84 | 1.37        | 1.44     |
| 10  | L     | 302 | BPH  | C3D-CAD | -2.83 | 1.41        | 1.47     |
| 9   | L     | 303 | U10  | C6-C5   | -2.81 | 1.38        | 1.46     |
| 7   | t     | 101 | BCL  | MG-NC   | 2.81  | 2.12        | 2.06     |
| 7   | i     | 100 | BCL  | O1A-CGA | -2.80 | 1.14        | 1.22     |
| 7   | d     | 101 | BCL  | O1A-CGA | -2.80 | 1.14        | 1.22     |
| 7   | K     | 101 | BCL  | C1D-C2D | -2.79 | 1.39        | 1.45     |
| 7   | F     | 101 | BCL  | O2A-CGA | -2.79 | 1.25        | 1.33     |
| 9   | a     | 102 | U10  | C6-C5   | -2.78 | 1.38        | 1.46     |
| 7   | M     | 401 | BCL  | MG-NC   | 2.77  | 2.12        | 2.06     |
| 7   | o     | 100 | BCL  | C3B-C4B | 2.77  | 1.46        | 1.41     |
| 7   | N     | 202 | BCL  | C3D-C4D | -2.76 | 1.37        | 1.44     |
| 7   | N     | 202 | BCL  | C1D-C2D | -2.75 | 1.39        | 1.45     |
| 7   | a     | 101 | BCL  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 7   | b     | 102 | BCL  | C3D-C4D | -2.74 | 1.38        | 1.44     |
| 7   | r     | 101 | BCL  | C3B-C4B | 2.74  | 1.46        | 1.41     |
| 9   | L     | 305 | U10  | C6-C5   | -2.74 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | j     | 303 | BCL  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 7   | A     | 101 | BCL  | C3D-C4D | -2.73 | 1.38        | 1.44     |
| 10  | M     | 403 | BPH  | O1A-CGA | -2.73 | 1.14        | 1.22     |
| 7   | R     | 101 | BCL  | MG-NC   | 2.73  | 2.12        | 2.06     |
| 7   | M     | 407 | BCL  | C3D-C4D | -2.73 | 1.38        | 1.44     |
| 7   | K     | 101 | BCL  | C3D-C4D | -2.72 | 1.38        | 1.44     |
| 7   | k     | 101 | BCL  | O1A-CGA | -2.71 | 1.14        | 1.22     |
| 7   | F     | 103 | BCL  | C3D-C4D | -2.71 | 1.38        | 1.44     |
| 9   | M     | 405 | U10  | C1-C2   | -2.71 | 1.37        | 1.47     |
| 7   | E     | 202 | BCL  | C3D-C4D | -2.71 | 1.38        | 1.44     |
| 7   | I     | 101 | BCL  | C3D-C4D | -2.70 | 1.38        | 1.44     |
| 7   | b     | 101 | BCL  | C1D-C2D | -2.69 | 1.40        | 1.45     |
| 7   | g     | 101 | BCL  | O1A-CGA | -2.69 | 1.14        | 1.22     |
| 9   | L     | 303 | U10  | C1-C2   | -2.69 | 1.37        | 1.47     |
| 7   | G     | 101 | BCL  | C3D-C4D | -2.68 | 1.38        | 1.44     |
| 7   | O     | 101 | BCL  | C3D-C4D | -2.68 | 1.38        | 1.44     |
| 7   | F     | 101 | BCL  | C3D-C4D | -2.67 | 1.38        | 1.44     |
| 7   | M     | 401 | BCL  | CHD-C1D | 2.66  | 1.43        | 1.38     |
| 7   | o     | 100 | BCL  | C3D-C4D | -2.66 | 1.38        | 1.44     |
| 7   | N     | 202 | BCL  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 7   | G     | 101 | BCL  | MG-NC   | 2.64  | 2.12        | 2.06     |
| 7   | e     | 100 | BCL  | C3D-C4D | -2.63 | 1.38        | 1.44     |
| 7   | A     | 101 | BCL  | C3C-C4C | -2.63 | 1.48        | 1.51     |
| 7   | r     | 101 | BCL  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 7   | d     | 101 | BCL  | C3B-C4B | 2.62  | 1.45        | 1.41     |
| 7   | j     | 302 | BCL  | C3D-C4D | -2.62 | 1.38        | 1.44     |
| 7   | S     | 101 | BCL  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 7   | d     | 101 | BCL  | C1D-C2D | -2.61 | 1.40        | 1.45     |
| 7   | e     | 100 | BCL  | C1D-C2D | -2.61 | 1.40        | 1.45     |
| 7   | k     | 101 | BCL  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 7   | i     | 100 | BCL  | C3D-C4D | -2.61 | 1.38        | 1.44     |
| 7   | L     | 301 | BCL  | C3D-C4D | -2.60 | 1.38        | 1.44     |
| 7   | M     | 401 | BCL  | O1A-CGA | -2.60 | 1.14        | 1.22     |
| 7   | n     | 100 | BCL  | O2A-CGA | -2.60 | 1.25        | 1.33     |
| 12  | H     | 302 | 3PE  | O31-C31 | 2.59  | 1.40        | 1.33     |
| 8   | r     | 102 | SPO  | C35-C33 | 2.58  | 1.56        | 1.51     |
| 7   | s     | 202 | BCL  | C3B-C4B | 2.58  | 1.45        | 1.41     |
| 9   | L     | 304 | U10  | C6-C5   | -2.57 | 1.39        | 1.46     |
| 8   | F     | 102 | SPO  | C30-C28 | 2.57  | 1.56        | 1.51     |
| 7   | s     | 202 | BCL  | MG-NC   | 2.57  | 2.12        | 2.06     |
| 7   | g     | 101 | BCL  | C3D-C4D | -2.57 | 1.38        | 1.44     |
| 7   | O     | 101 | BCL  | MG-NC   | 2.56  | 2.12        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | d     | 102 | 3PE  | O31-C31 | 2.56  | 1.40        | 1.33     |
| 7   | a     | 101 | BCL  | C3D-C4D | -2.56 | 1.38        | 1.44     |
| 7   | d     | 101 | BCL  | O2A-CGA | -2.56 | 1.25        | 1.33     |
| 10  | L     | 302 | BPH  | C3B-C4B | 2.55  | 1.45        | 1.41     |
| 7   | R     | 101 | BCL  | C3D-C4D | -2.54 | 1.38        | 1.44     |
| 7   | A     | 101 | BCL  | O1A-CGA | -2.54 | 1.15        | 1.22     |
| 7   | A     | 101 | BCL  | MG-NC   | 2.54  | 2.12        | 2.06     |
| 7   | A     | 101 | BCL  | C1D-C2D | -2.54 | 1.40        | 1.45     |
| 8   | t     | 102 | SPO  | C30-C28 | 2.53  | 1.56        | 1.51     |
| 7   | b     | 101 | BCL  | MG-NC   | 2.53  | 2.12        | 2.06     |
| 7   | F     | 101 | BCL  | C3B-C4B | 2.53  | 1.45        | 1.41     |
| 7   | e     | 100 | BCL  | MG-NC   | 2.53  | 2.12        | 2.06     |
| 7   | S     | 101 | BCL  | C3D-C4D | -2.53 | 1.38        | 1.44     |
| 7   | b     | 101 | BCL  | C3D-C4D | -2.53 | 1.38        | 1.44     |
| 7   | t     | 103 | BCL  | C3D-C4D | -2.53 | 1.38        | 1.44     |
| 7   | e     | 100 | BCL  | C3C-C4C | -2.52 | 1.48        | 1.51     |
| 7   | s     | 202 | BCL  | O1A-CGA | -2.51 | 1.15        | 1.22     |
| 7   | k     | 101 | BCL  | C3D-C4D | -2.50 | 1.38        | 1.44     |
| 8   | g     | 102 | SPO  | C30-C28 | 2.50  | 1.56        | 1.51     |
| 9   | L     | 305 | U10  | C1-C2   | -2.50 | 1.38        | 1.47     |
| 7   | g     | 101 | BCL  | MG-NC   | 2.50  | 2.12        | 2.06     |
| 7   | a     | 101 | BCL  | C3B-C4B | 2.50  | 1.45        | 1.41     |
| 7   | d     | 101 | BCL  | C3D-C4D | -2.50 | 1.38        | 1.44     |
| 12  | H     | 301 | 3PE  | O21-C2  | -2.49 | 1.40        | 1.46     |
| 7   | i     | 100 | BCL  | MG-NC   | 2.49  | 2.12        | 2.06     |
| 7   | n     | 100 | BCL  | C3D-C4D | -2.49 | 1.38        | 1.44     |
| 9   | M     | 408 | U10  | C1-C2   | -2.49 | 1.38        | 1.47     |
| 7   | I     | 101 | BCL  | MG-NC   | 2.48  | 2.12        | 2.06     |
| 7   | o     | 100 | BCL  | C1D-C2D | -2.48 | 1.40        | 1.45     |
| 7   | F     | 103 | BCL  | MG-NC   | 2.47  | 2.12        | 2.06     |
| 8   | I     | 102 | SPO  | C30-C28 | 2.47  | 1.56        | 1.51     |
| 8   | r     | 102 | SPO  | C30-C28 | 2.47  | 1.56        | 1.51     |
| 7   | L     | 301 | BCL  | C3B-C4B | 2.47  | 1.45        | 1.41     |
| 7   | t     | 103 | BCL  | C1D-C2D | -2.46 | 1.40        | 1.45     |
| 7   | M     | 407 | BCL  | C1D-C2D | -2.46 | 1.40        | 1.45     |
| 7   | g     | 101 | BCL  | O2A-CGA | -2.46 | 1.26        | 1.33     |
| 7   | F     | 101 | BCL  | MG-NC   | 2.46  | 2.12        | 2.06     |
| 7   | F     | 103 | BCL  | C1D-C2D | -2.45 | 1.40        | 1.45     |
| 7   | F     | 103 | BCL  | C3B-C4B | 2.45  | 1.45        | 1.41     |
| 7   | j     | 302 | BCL  | C3C-C4C | -2.45 | 1.48        | 1.51     |
| 7   | E     | 202 | BCL  | O1A-CGA | -2.45 | 1.15        | 1.22     |
| 7   | i     | 100 | BCL  | O2A-CGA | -2.44 | 1.26        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | n     | 100 | BCL  | C3B-C4B | 2.44  | 1.45        | 1.41     |
| 8   | F     | 102 | SPO  | C35-C33 | 2.43  | 1.56        | 1.51     |
| 7   | r     | 101 | BCL  | C3D-C4D | -2.43 | 1.38        | 1.44     |
| 8   | j     | 301 | SPO  | C30-C28 | 2.43  | 1.56        | 1.51     |
| 7   | D     | 202 | BCL  | C3B-C4B | 2.42  | 1.45        | 1.41     |
| 7   | t     | 103 | BCL  | C3B-C4B | 2.42  | 1.45        | 1.41     |
| 8   | r     | 103 | SPO  | C35-C33 | 2.41  | 1.56        | 1.51     |
| 8   | M     | 406 | SPO  | C30-C28 | 2.41  | 1.56        | 1.51     |
| 7   | n     | 100 | BCL  | MG-NC   | 2.41  | 2.12        | 2.06     |
| 8   | M     | 406 | SPO  | C9-C7   | -2.41 | 1.32        | 1.35     |
| 7   | D     | 202 | BCL  | O1A-CGA | -2.41 | 1.15        | 1.22     |
| 7   | K     | 101 | BCL  | MG-NC   | 2.40  | 2.12        | 2.06     |
| 7   | b     | 102 | BCL  | MG-NC   | 2.40  | 2.12        | 2.06     |
| 7   | E     | 202 | BCL  | C3B-C4B | 2.40  | 1.45        | 1.41     |
| 8   | s     | 201 | SPO  | C30-C28 | 2.40  | 1.56        | 1.51     |
| 7   | M     | 402 | BCL  | CHD-C1D | 2.39  | 1.43        | 1.38     |
| 7   | i     | 100 | BCL  | C3B-C4B | 2.39  | 1.45        | 1.41     |
| 7   | M     | 407 | BCL  | C3B-C4B | 2.39  | 1.45        | 1.41     |
| 7   | M     | 401 | BCL  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 9   | M     | 405 | U10  | C6-C1   | 2.37  | 1.39        | 1.35     |
| 7   | L     | 301 | BCL  | C1D-C2D | -2.37 | 1.40        | 1.45     |
| 9   | L     | 304 | U10  | C1-C2   | -2.37 | 1.38        | 1.47     |
| 7   | M     | 407 | BCL  | CHD-C1D | 2.37  | 1.43        | 1.38     |
| 7   | o     | 100 | BCL  | MG-NC   | 2.37  | 2.11        | 2.06     |
| 7   | I     | 101 | BCL  | C3B-C4B | 2.37  | 1.45        | 1.41     |
| 7   | E     | 202 | BCL  | MG-NC   | 2.36  | 2.11        | 2.06     |
| 7   | R     | 101 | BCL  | C3B-C4B | 2.36  | 1.45        | 1.41     |
| 8   | g     | 102 | SPO  | C35-C33 | 2.36  | 1.56        | 1.51     |
| 9   | L     | 305 | U10  | C6-C1   | 2.35  | 1.39        | 1.35     |
| 7   | n     | 100 | BCL  | C1D-C2D | -2.35 | 1.40        | 1.45     |
| 12  | H     | 301 | 3PE  | O31-C31 | 2.35  | 1.40        | 1.33     |
| 7   | j     | 302 | BCL  | MG-NC   | 2.35  | 2.11        | 2.06     |
| 7   | d     | 101 | BCL  | MG-NC   | 2.35  | 2.11        | 2.06     |
| 7   | t     | 101 | BCL  | C3B-C4B | 2.34  | 1.45        | 1.41     |
| 7   | j     | 302 | BCL  | C3B-C4B | 2.34  | 1.45        | 1.41     |
| 8   | t     | 102 | SPO  | C35-C33 | 2.34  | 1.56        | 1.51     |
| 7   | u     | 101 | BCL  | C3B-C4B | 2.33  | 1.45        | 1.41     |
| 10  | L     | 302 | BPH  | C2C-C3C | -2.33 | 1.52        | 1.54     |
| 7   | e     | 100 | BCL  | C3B-C4B | 2.32  | 1.45        | 1.41     |
| 9   | M     | 408 | U10  | C6-C1   | 2.32  | 1.39        | 1.35     |
| 7   | u     | 101 | BCL  | CHD-C1D | 2.31  | 1.42        | 1.38     |
| 7   | i     | 100 | BCL  | C3C-C4C | -2.31 | 1.48        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | b     | 102 | BCL  | O1A-CGA | -2.31 | 1.15        | 1.22     |
| 7   | M     | 407 | BCL  | O1A-CGA | -2.30 | 1.15        | 1.22     |
| 8   | r     | 103 | SPO  | C30-C28 | 2.30  | 1.56        | 1.51     |
| 7   | t     | 101 | BCL  | C3D-C4D | -2.30 | 1.39        | 1.44     |
| 7   | j     | 303 | BCL  | C3B-C4B | 2.30  | 1.45        | 1.41     |
| 8   | k     | 102 | SPO  | C30-C28 | 2.29  | 1.56        | 1.51     |
| 8   | s     | 201 | SPO  | C35-C33 | 2.29  | 1.56        | 1.51     |
| 7   | s     | 202 | BCL  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 8   | B     | 101 | SPO  | C35-C33 | 2.28  | 1.56        | 1.51     |
| 7   | g     | 101 | BCL  | C3B-C4B | 2.27  | 1.45        | 1.41     |
| 8   | I     | 102 | SPO  | C35-C33 | 2.26  | 1.56        | 1.51     |
| 7   | b     | 101 | BCL  | C3B-C4B | 2.26  | 1.45        | 1.41     |
| 7   | D     | 202 | BCL  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 7   | b     | 102 | BCL  | C1D-C2D | -2.25 | 1.40        | 1.45     |
| 12  | H     | 301 | 3PE  | O21-C21 | 2.25  | 1.40        | 1.34     |
| 7   | k     | 101 | BCL  | C3B-C4B | 2.25  | 1.45        | 1.41     |
| 7   | D     | 202 | BCL  | C1D-C2D | -2.24 | 1.40        | 1.45     |
| 7   | F     | 101 | BCL  | C1D-C2D | -2.23 | 1.40        | 1.45     |
| 7   | k     | 101 | BCL  | O2A-CGA | -2.23 | 1.26        | 1.33     |
| 7   | M     | 401 | BCL  | C3B-C4B | 2.22  | 1.45        | 1.41     |
| 7   | O     | 101 | BCL  | C3B-C4B | 2.22  | 1.45        | 1.41     |
| 9   | a     | 102 | U10  | C1-C2   | -2.21 | 1.39        | 1.47     |
| 8   | N     | 201 | SPO  | C30-C28 | 2.21  | 1.55        | 1.51     |
| 7   | s     | 202 | BCL  | C1D-C2D | -2.20 | 1.41        | 1.45     |
| 7   | b     | 102 | BCL  | C4B-NB  | -2.20 | 1.35        | 1.37     |
| 7   | j     | 302 | BCL  | C1D-C2D | -2.20 | 1.41        | 1.45     |
| 7   | k     | 101 | BCL  | C1D-C2D | -2.20 | 1.41        | 1.45     |
| 7   | K     | 101 | BCL  | C3C-C4C | -2.20 | 1.48        | 1.51     |
| 7   | F     | 103 | BCL  | O1A-CGA | -2.19 | 1.16        | 1.22     |
| 7   | M     | 407 | BCL  | O2A-CGA | -2.19 | 1.26        | 1.33     |
| 7   | j     | 303 | BCL  | C1D-C2D | -2.19 | 1.41        | 1.45     |
| 8   | j     | 301 | SPO  | C35-C33 | 2.19  | 1.55        | 1.51     |
| 7   | j     | 303 | BCL  | CHD-C1D | 2.18  | 1.42        | 1.38     |
| 7   | a     | 101 | BCL  | C1D-C2D | -2.18 | 1.41        | 1.45     |
| 8   | k     | 102 | SPO  | C35-C33 | 2.18  | 1.55        | 1.51     |
| 7   | r     | 101 | BCL  | C1D-C2D | -2.18 | 1.41        | 1.45     |
| 10  | M     | 403 | BPH  | O2A-CGA | -2.18 | 1.26        | 1.33     |
| 7   | S     | 101 | BCL  | C3B-C4B | 2.17  | 1.45        | 1.41     |
| 7   | i     | 100 | BCL  | C1D-C2D | -2.17 | 1.41        | 1.45     |
| 10  | L     | 302 | BPH  | C3D-C4D | -2.17 | 1.38        | 1.41     |
| 7   | b     | 102 | BCL  | C3C-C4C | -2.17 | 1.48        | 1.51     |
| 7   | S     | 101 | BCL  | O1A-CGA | -2.17 | 1.16        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | u     | 102 | BCL  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 7   | t     | 101 | BCL  | CHD-C1D | 2.16  | 1.42        | 1.38     |
| 7   | E     | 202 | BCL  | CHD-C1D | 2.16  | 1.42        | 1.38     |
| 10  | L     | 306 | BPH  | C3B-C4B | 2.16  | 1.45        | 1.41     |
| 7   | a     | 101 | BCL  | O1A-CGA | -2.16 | 1.16        | 1.22     |
| 8   | D     | 201 | SPO  | C30-C28 | 2.16  | 1.55        | 1.51     |
| 7   | g     | 101 | BCL  | C1D-C2D | -2.15 | 1.41        | 1.45     |
| 7   | u     | 102 | BCL  | CHD-C1D | 2.14  | 1.42        | 1.38     |
| 7   | F     | 101 | BCL  | CHD-C1D | 2.13  | 1.42        | 1.38     |
| 7   | M     | 402 | BCL  | C4B-NB  | -2.13 | 1.35        | 1.37     |
| 9   | L     | 304 | U10  | C6-C1   | 2.13  | 1.39        | 1.35     |
| 7   | R     | 101 | BCL  | C1D-C2D | -2.13 | 1.41        | 1.45     |
| 7   | M     | 402 | BCL  | C3B-C4B | 2.12  | 1.45        | 1.41     |
| 7   | R     | 101 | BCL  | O1A-CGA | -2.12 | 1.16        | 1.22     |
| 7   | j     | 302 | BCL  | O1A-CGA | -2.12 | 1.16        | 1.22     |
| 7   | o     | 100 | BCL  | O2A-CGA | -2.12 | 1.27        | 1.33     |
| 7   | u     | 101 | BCL  | O1A-CGA | -2.12 | 1.16        | 1.22     |
| 7   | I     | 101 | BCL  | C1D-C2D | -2.11 | 1.41        | 1.45     |
| 8   | N     | 201 | SPO  | C35-C33 | 2.11  | 1.55        | 1.51     |
| 8   | X     | 201 | SPO  | C30-C28 | 2.10  | 1.55        | 1.51     |
| 7   | M     | 401 | BCL  | C1D-C2D | -2.10 | 1.41        | 1.45     |
| 7   | G     | 101 | BCL  | CHD-C1D | 2.08  | 1.42        | 1.38     |
| 7   | G     | 101 | BCL  | C1D-C2D | -2.08 | 1.41        | 1.45     |
| 7   | L     | 301 | BCL  | MG-NC   | 2.08  | 2.11        | 2.06     |
| 7   | N     | 202 | BCL  | C3B-C4B | 2.07  | 1.44        | 1.41     |
| 7   | A     | 101 | BCL  | C3B-C4B | 2.06  | 1.44        | 1.41     |
| 7   | F     | 101 | BCL  | C3C-C4C | -2.06 | 1.49        | 1.51     |
| 7   | S     | 101 | BCL  | C1D-C2D | -2.06 | 1.41        | 1.45     |
| 8   | X     | 201 | SPO  | C35-C33 | 2.05  | 1.55        | 1.51     |
| 7   | O     | 101 | BCL  | CHD-C1D | 2.05  | 1.42        | 1.38     |
| 7   | F     | 103 | BCL  | CHD-C1D | 2.05  | 1.42        | 1.38     |
| 7   | L     | 301 | BCL  | O2A-CGA | -2.05 | 1.27        | 1.33     |
| 10  | L     | 302 | BPH  | C1C-C2C | -2.05 | 1.47        | 1.51     |
| 7   | t     | 103 | BCL  | CHD-C1D | 2.04  | 1.42        | 1.38     |
| 7   | k     | 101 | BCL  | CHD-C1D | 2.04  | 1.42        | 1.38     |
| 8   | M     | 406 | SPO  | C35-C33 | 2.04  | 1.55        | 1.51     |
| 7   | u     | 101 | BCL  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 7   | G     | 101 | BCL  | C3B-C4B | 2.02  | 1.44        | 1.41     |
| 10  | M     | 403 | BPH  | C3B-CAB | -2.02 | 1.43        | 1.49     |
| 7   | L     | 301 | BCL  | C4B-NB  | -2.02 | 1.35        | 1.37     |
| 7   | D     | 202 | BCL  | CHD-C1D | 2.01  | 1.42        | 1.38     |
| 7   | E     | 202 | BCL  | C1D-C2D | -2.00 | 1.41        | 1.45     |

All (889) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 8   | N     | 201 | SPO  | C3-C1-C4    | -23.58 | 74.66       | 110.86   |
| 8   | r     | 102 | SPO  | C2-C1-C4    | -22.57 | 76.21       | 110.86   |
| 8   | g     | 102 | SPO  | C2-C1-C4    | -22.55 | 76.24       | 110.86   |
| 8   | E     | 201 | SPO  | C2-C1-C4    | -21.70 | 77.55       | 110.86   |
| 8   | k     | 102 | SPO  | C3-C1-C4    | -21.57 | 77.74       | 110.86   |
| 8   | r     | 103 | SPO  | C3-C1-C4    | -21.37 | 78.05       | 110.86   |
| 8   | I     | 102 | SPO  | C2-C1-C4    | -20.80 | 78.92       | 110.86   |
| 8   | k     | 102 | SPO  | C2-C1-C4    | -20.65 | 79.15       | 110.86   |
| 8   | D     | 201 | SPO  | C3-C1-C4    | -20.64 | 79.17       | 110.86   |
| 8   | D     | 201 | SPO  | C2-C1-C4    | -20.58 | 79.26       | 110.86   |
| 8   | s     | 201 | SPO  | C3-C1-C4    | -19.82 | 80.43       | 110.86   |
| 8   | E     | 201 | SPO  | C3-C1-C4    | -19.63 | 80.73       | 110.86   |
| 8   | r     | 103 | SPO  | C2-C1-C4    | -19.49 | 80.93       | 110.86   |
| 8   | I     | 102 | SPO  | C3-C1-C4    | -18.19 | 82.93       | 110.86   |
| 8   | s     | 201 | SPO  | C2-C1-C4    | -18.18 | 82.94       | 110.86   |
| 8   | r     | 102 | SPO  | C3-C1-C4    | -17.28 | 84.32       | 110.86   |
| 8   | M     | 406 | SPO  | C3-C1-C2    | 16.99  | 142.32      | 110.37   |
| 8   | t     | 102 | SPO  | C3-C1-C2    | 16.77  | 141.91      | 110.37   |
| 8   | F     | 102 | SPO  | C3-C1-C2    | 16.11  | 140.67      | 110.37   |
| 8   | X     | 201 | SPO  | C3-C1-C2    | 16.05  | 140.56      | 110.37   |
| 8   | g     | 102 | SPO  | C3-C1-C4    | -15.92 | 86.41       | 110.86   |
| 8   | N     | 201 | SPO  | C2-C1-C4    | -15.60 | 86.91       | 110.86   |
| 8   | j     | 301 | SPO  | C3-C1-C2    | 15.23  | 139.01      | 110.37   |
| 8   | s     | 201 | SPO  | C3-C1-C2    | 14.66  | 137.95      | 110.37   |
| 8   | B     | 101 | SPO  | C3-C1-C2    | 13.95  | 136.61      | 110.37   |
| 8   | r     | 103 | SPO  | C3-C1-C2    | 13.83  | 136.38      | 110.37   |
| 8   | N     | 201 | SPO  | C3-C1-C2    | 13.54  | 135.83      | 110.37   |
| 8   | I     | 102 | SPO  | C3-C1-C2    | 13.40  | 135.57      | 110.37   |
| 8   | r     | 102 | SPO  | C3-C1-C2    | 12.41  | 133.71      | 110.37   |
| 8   | g     | 102 | SPO  | C3-C1-C2    | 12.36  | 133.61      | 110.37   |
| 10  | M     | 403 | BPH  | C4D-CHA-CBD | -11.57 | 103.28      | 108.52   |
| 8   | j     | 301 | SPO  | C2-C1-C4    | -11.21 | 93.65       | 110.86   |
| 8   | F     | 102 | SPO  | C3-C1-C4    | -10.88 | 94.15       | 110.86   |
| 8   | B     | 101 | SPO  | C2-C1-C4    | -10.57 | 94.64       | 110.86   |
| 8   | s     | 201 | SPO  | C10-C9-C7   | -10.43 | 112.42      | 127.31   |
| 8   | t     | 102 | SPO  | C3-C1-C4    | -10.20 | 95.20       | 110.86   |
| 8   | t     | 102 | SPO  | C2-C1-C4    | -10.17 | 95.24       | 110.86   |
| 8   | D     | 201 | SPO  | C3-C1-C2    | 10.13  | 129.43      | 110.37   |
| 8   | X     | 201 | SPO  | C2-C1-C4    | -10.07 | 95.40       | 110.86   |
| 10  | L     | 302 | BPH  | C4D-CHA-CBD | -9.98  | 104.00      | 108.52   |
| 8   | D     | 201 | SPO  | C5-C6-C7    | -9.95  | 110.85      | 125.89   |
| 8   | s     | 201 | SPO  | C15-C14-C12 | -9.70  | 113.46      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | L     | 306 | BPH  | C4D-CHA-CBD | -9.67 | 104.14      | 108.52   |
| 8   | j     | 301 | SPO  | C5-C6-C7    | -9.67 | 111.28      | 125.89   |
| 8   | E     | 201 | SPO  | C3-C1-C2    | 9.55  | 128.33      | 110.37   |
| 8   | M     | 406 | SPO  | C5-C6-C7    | -9.53 | 111.49      | 125.89   |
| 8   | t     | 102 | SPO  | C21-C22-C23 | -9.51 | 113.74      | 127.31   |
| 8   | j     | 301 | SPO  | C3-C1-C4    | -9.51 | 96.26       | 110.86   |
| 8   | k     | 102 | SPO  | C3-C1-C2    | 9.45  | 128.15      | 110.37   |
| 8   | M     | 406 | SPO  | C2-C1-C4    | -9.44 | 96.36       | 110.86   |
| 8   | F     | 102 | SPO  | C2-C1-C4    | -9.21 | 96.72       | 110.86   |
| 8   | k     | 102 | SPO  | C5-C6-C7    | -8.82 | 112.56      | 125.89   |
| 8   | r     | 102 | SPO  | C10-C9-C7   | -8.22 | 115.58      | 127.31   |
| 8   | j     | 301 | SPO  | C15-C14-C12 | -8.17 | 115.65      | 127.31   |
| 8   | E     | 201 | SPO  | C5-C6-C7    | -8.16 | 113.56      | 125.89   |
| 8   | M     | 406 | SPO  | C3-C1-C4    | -8.02 | 98.55       | 110.86   |
| 8   | r     | 102 | SPO  | C5-C6-C7    | -7.96 | 113.86      | 125.89   |
| 8   | B     | 101 | SPO  | C3-C1-C4    | -7.79 | 98.90       | 110.86   |
| 8   | X     | 201 | SPO  | C3-C1-C4    | -7.75 | 98.96       | 110.86   |
| 8   | B     | 101 | SPO  | C11-C12-C14 | 7.45  | 130.38      | 118.94   |
| 8   | s     | 201 | SPO  | C5-C6-C7    | -7.17 | 115.05      | 125.89   |
| 12  | d     | 102 | 3PE  | O11-P-O14   | -7.13 | 81.21       | 109.07   |
| 8   | F     | 102 | SPO  | C20-C19-C17 | -7.09 | 117.19      | 127.31   |
| 8   | t     | 102 | SPO  | C15-C14-C12 | -7.05 | 117.24      | 127.31   |
| 8   | N     | 201 | SPO  | C20-C19-C17 | -6.95 | 117.39      | 127.31   |
| 8   | k     | 102 | SPO  | C20-C19-C17 | -6.93 | 117.42      | 127.31   |
| 7   | u     | 102 | BCL  | C1-C2-C3    | 6.82  | 137.84      | 126.04   |
| 12  | d     | 102 | 3PE  | O12-P-O11   | -6.82 | 76.07       | 107.75   |
| 8   | B     | 101 | SPO  | C21-C22-C23 | -6.73 | 117.71      | 127.31   |
| 8   | F     | 102 | SPO  | C15-C14-C12 | -6.58 | 117.93      | 127.31   |
| 8   | E     | 201 | SPO  | C20-C19-C17 | -6.54 | 117.98      | 127.31   |
| 12  | d     | 102 | 3PE  | O13-P-O14   | -6.50 | 83.67       | 109.07   |
| 8   | B     | 101 | SPO  | C13-C12-C14 | -6.37 | 114.00      | 122.92   |
| 7   | b     | 101 | BCL  | C1-O2A-CGA  | 6.37  | 133.14      | 116.44   |
| 8   | B     | 101 | SPO  | C10-C11-C12 | -6.35 | 108.57      | 126.42   |
| 8   | B     | 101 | SPO  | C20-C19-C17 | -6.20 | 118.47      | 127.31   |
| 8   | r     | 103 | SPO  | C24-C23-C22 | -6.05 | 114.44      | 122.92   |
| 12  | d     | 102 | 3PE  | O12-P-O13   | -6.05 | 79.66       | 107.75   |
| 7   | M     | 401 | BCL  | CHD-C1D-ND  | -6.03 | 118.91      | 124.45   |
| 7   | M     | 402 | BCL  | CHD-C1D-ND  | -5.87 | 119.06      | 124.45   |
| 7   | j     | 302 | BCL  | CHD-C1D-ND  | -5.81 | 119.12      | 124.45   |
| 7   | o     | 100 | BCL  | C1-C2-C3    | -5.77 | 116.07      | 126.04   |
| 8   | I     | 102 | SPO  | C20-C19-C17 | -5.73 | 119.14      | 127.31   |
| 7   | u     | 101 | BCL  | CHD-C1D-ND  | -5.72 | 119.19      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | t     | 102 | SPO  | C5-C6-C7    | -5.71 | 117.26      | 125.89   |
| 8   | g     | 102 | SPO  | C5-C6-C7    | -5.67 | 117.32      | 125.89   |
| 7   | M     | 402 | BCL  | C4D-CHA-C1A | 5.67  | 128.15      | 121.25   |
| 8   | M     | 406 | SPO  | C10-C9-C7   | -5.64 | 119.26      | 127.31   |
| 7   | M     | 402 | BCL  | C16-C15-C13 | 5.61  | 134.05      | 115.92   |
| 7   | F     | 101 | BCL  | CHD-C1D-ND  | -5.59 | 119.32      | 124.45   |
| 7   | d     | 101 | BCL  | CHD-C1D-ND  | -5.54 | 119.36      | 124.45   |
| 7   | E     | 202 | BCL  | C4D-CHA-C1A | 5.52  | 127.96      | 121.25   |
| 7   | n     | 100 | BCL  | CHD-C1D-ND  | -5.50 | 119.40      | 124.45   |
| 7   | a     | 101 | BCL  | C4D-CHA-C1A | 5.45  | 127.89      | 121.25   |
| 8   | k     | 102 | SPO  | C21-C22-C23 | -5.44 | 119.55      | 127.31   |
| 7   | t     | 101 | BCL  | CHD-C1D-ND  | -5.42 | 119.47      | 124.45   |
| 7   | K     | 101 | BCL  | C4D-CHA-C1A | 5.40  | 127.82      | 121.25   |
| 7   | s     | 202 | BCL  | CHD-C1D-ND  | -5.39 | 119.50      | 124.45   |
| 7   | k     | 101 | BCL  | CHD-C1D-ND  | -5.37 | 119.52      | 124.45   |
| 7   | E     | 202 | BCL  | CHD-C1D-ND  | -5.36 | 119.53      | 124.45   |
| 7   | L     | 301 | BCL  | CHD-C1D-ND  | -5.36 | 119.53      | 124.45   |
| 7   | u     | 102 | BCL  | CHD-C1D-ND  | -5.34 | 119.55      | 124.45   |
| 7   | F     | 103 | BCL  | C4D-CHA-C1A | 5.33  | 127.74      | 121.25   |
| 8   | t     | 102 | SPO  | C26-C25-C23 | -5.33 | 111.44      | 126.42   |
| 7   | O     | 101 | BCL  | C4D-CHA-C1A | 5.32  | 127.72      | 121.25   |
| 7   | b     | 102 | BCL  | C4D-CHA-C1A | 5.32  | 127.72      | 121.25   |
| 7   | o     | 100 | BCL  | C4D-CHA-C1A | 5.30  | 127.70      | 121.25   |
| 7   | r     | 101 | BCL  | CHD-C1D-ND  | -5.30 | 119.58      | 124.45   |
| 7   | j     | 303 | BCL  | C4D-CHA-C1A | 5.30  | 127.70      | 121.25   |
| 7   | I     | 101 | BCL  | C4D-CHA-C1A | 5.30  | 127.69      | 121.25   |
| 7   | o     | 100 | BCL  | CHD-C1D-ND  | -5.29 | 119.59      | 124.45   |
| 7   | e     | 100 | BCL  | CHD-C1D-ND  | -5.29 | 119.60      | 124.45   |
| 8   | E     | 201 | SPO  | C6-C7-C9    | 5.28  | 127.05      | 118.94   |
| 7   | t     | 103 | BCL  | C4D-CHA-C1A | 5.28  | 127.67      | 121.25   |
| 7   | O     | 101 | BCL  | CHD-C1D-ND  | -5.28 | 119.60      | 124.45   |
| 7   | i     | 100 | BCL  | CHD-C1D-ND  | -5.27 | 119.61      | 124.45   |
| 7   | R     | 101 | BCL  | CHD-C1D-ND  | -5.26 | 119.62      | 124.45   |
| 7   | g     | 101 | BCL  | CHD-C1D-ND  | -5.25 | 119.63      | 124.45   |
| 8   | F     | 102 | SPO  | C21-C22-C23 | -5.25 | 119.81      | 127.31   |
| 7   | R     | 101 | BCL  | C4D-CHA-C1A | 5.24  | 127.63      | 121.25   |
| 7   | L     | 301 | BCL  | C4D-CHA-C1A | 5.24  | 127.62      | 121.25   |
| 7   | N     | 202 | BCL  | C4D-CHA-C1A | 5.23  | 127.61      | 121.25   |
| 8   | r     | 102 | SPO  | C15-C14-C12 | -5.22 | 119.86      | 127.31   |
| 7   | n     | 100 | BCL  | C4D-CHA-C1A | 5.21  | 127.59      | 121.25   |
| 7   | a     | 101 | BCL  | CHD-C1D-ND  | -5.20 | 119.67      | 124.45   |
| 7   | u     | 102 | BCL  | C4D-CHA-C1A | 5.19  | 127.56      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | A     | 101 | BCL  | C4D-CHA-C1A | 5.18  | 127.55      | 121.25   |
| 7   | D     | 202 | BCL  | C4D-CHA-C1A | 5.18  | 127.55      | 121.25   |
| 7   | S     | 101 | BCL  | CHD-C1D-ND  | -5.18 | 119.70      | 124.45   |
| 8   | N     | 201 | SPO  | C21-C22-C23 | -5.17 | 119.93      | 127.31   |
| 7   | G     | 101 | BCL  | C4D-CHA-C1A | 5.17  | 127.55      | 121.25   |
| 7   | D     | 202 | BCL  | CHD-C1D-ND  | -5.16 | 119.71      | 124.45   |
| 7   | S     | 101 | BCL  | C4D-CHA-C1A | 5.13  | 127.50      | 121.25   |
| 7   | b     | 102 | BCL  | CHD-C1D-ND  | -5.13 | 119.74      | 124.45   |
| 7   | t     | 101 | BCL  | C4D-CHA-C1A | 5.12  | 127.48      | 121.25   |
| 7   | G     | 101 | BCL  | CHD-C1D-ND  | -5.11 | 119.76      | 124.45   |
| 8   | M     | 406 | SPO  | C21-C20-C19 | -5.10 | 113.02      | 123.47   |
| 7   | j     | 302 | BCL  | C4D-CHA-C1A | 5.10  | 127.46      | 121.25   |
| 7   | b     | 101 | BCL  | C4D-CHA-C1A | 5.09  | 127.45      | 121.25   |
| 7   | I     | 101 | BCL  | CHD-C1D-ND  | -5.09 | 119.78      | 124.45   |
| 7   | g     | 101 | BCL  | C4D-CHA-C1A | 5.09  | 127.44      | 121.25   |
| 7   | F     | 103 | BCL  | CHD-C1D-ND  | -5.08 | 119.78      | 124.45   |
| 7   | b     | 101 | BCL  | CHD-C1D-ND  | -5.07 | 119.79      | 124.45   |
| 9   | L     | 303 | U10  | C7-C8-C9    | -5.07 | 118.34      | 126.79   |
| 7   | F     | 101 | BCL  | C4D-CHA-C1A | 5.07  | 127.42      | 121.25   |
| 8   | t     | 102 | SPO  | C10-C9-C7   | -5.05 | 120.10      | 127.31   |
| 8   | s     | 201 | SPO  | C15-C16-C17 | -5.03 | 112.29      | 126.42   |
| 7   | d     | 101 | BCL  | C4D-CHA-C1A | 5.02  | 127.36      | 121.25   |
| 7   | k     | 101 | BCL  | C4D-CHA-C1A | 5.02  | 127.36      | 121.25   |
| 7   | e     | 100 | BCL  | C4D-CHA-C1A | 4.98  | 127.31      | 121.25   |
| 7   | j     | 303 | BCL  | CHD-C1D-ND  | -4.98 | 119.88      | 124.45   |
| 7   | r     | 101 | BCL  | C4D-CHA-C1A | 4.97  | 127.29      | 121.25   |
| 7   | u     | 101 | BCL  | C4D-CHA-C1A | 4.97  | 127.29      | 121.25   |
| 8   | D     | 201 | SPO  | C20-C19-C17 | -4.95 | 120.24      | 127.31   |
| 8   | g     | 102 | SPO  | C21-C20-C19 | -4.93 | 113.37      | 123.47   |
| 7   | M     | 401 | BCL  | C4D-CHA-C1A | 4.92  | 127.23      | 121.25   |
| 8   | E     | 201 | SPO  | C26-C25-C23 | -4.91 | 112.62      | 126.42   |
| 7   | A     | 101 | BCL  | CHD-C1D-ND  | -4.84 | 120.01      | 124.45   |
| 7   | N     | 202 | BCL  | CHD-C1D-ND  | -4.83 | 120.02      | 124.45   |
| 7   | K     | 101 | BCL  | CHD-C1D-ND  | -4.82 | 120.02      | 124.45   |
| 7   | i     | 100 | BCL  | C4D-CHA-C1A | 4.77  | 127.06      | 121.25   |
| 10  | L     | 306 | BPH  | C4D-ND-C1D  | -4.77 | 103.97      | 108.83   |
| 8   | E     | 201 | SPO  | C31-C32-C33 | -4.75 | 116.22      | 127.66   |
| 7   | N     | 202 | BCL  | C1-O2A-CGA  | 4.75  | 128.90      | 116.44   |
| 10  | M     | 403 | BPH  | C4D-ND-C1D  | -4.74 | 104.01      | 108.83   |
| 8   | B     | 101 | SPO  | C15-C14-C12 | 4.70  | 134.02      | 127.31   |
| 7   | s     | 202 | BCL  | C4D-CHA-C1A | 4.70  | 126.97      | 121.25   |
| 7   | M     | 407 | BCL  | C4D-CHA-C1A | 4.68  | 126.94      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | t     | 103 | BCL  | CHD-C1D-ND  | -4.67 | 120.16      | 124.45   |
| 8   | s     | 201 | SPO  | C10-C11-C12 | -4.64 | 113.38      | 126.42   |
| 8   | N     | 201 | SPO  | C24-C23-C25 | 4.60  | 125.33      | 118.08   |
| 8   | M     | 406 | SPO  | C9-C10-C11  | -4.54 | 109.04      | 123.22   |
| 7   | M     | 407 | BCL  | CHD-C1D-ND  | -4.50 | 120.32      | 124.45   |
| 8   | N     | 201 | SPO  | C24-C23-C22 | -4.48 | 116.64      | 122.92   |
| 10  | L     | 302 | BPH  | C4D-ND-C1D  | -4.48 | 104.28      | 108.83   |
| 8   | g     | 102 | SPO  | C25-C23-C22 | 4.45  | 125.77      | 118.94   |
| 8   | s     | 201 | SPO  | C8-C7-C9    | -4.45 | 116.70      | 122.92   |
| 8   | r     | 103 | SPO  | C5-C6-C7    | -4.42 | 119.21      | 125.89   |
| 8   | D     | 201 | SPO  | C10-C9-C7   | -4.41 | 121.01      | 127.31   |
| 8   | E     | 201 | SPO  | C25-C23-C22 | 4.40  | 125.69      | 118.94   |
| 8   | M     | 406 | SPO  | C24-C23-C22 | -4.39 | 116.78      | 122.92   |
| 8   | j     | 301 | SPO  | C14-C15-C16 | -4.39 | 109.53      | 123.22   |
| 8   | D     | 201 | SPO  | O1-C1-C2    | -4.38 | 78.82       | 108.97   |
| 7   | E     | 202 | BCL  | C1-C2-C3    | 4.37  | 133.60      | 126.04   |
| 7   | u     | 102 | BCL  | C4A-NA-C1A  | 4.37  | 108.67      | 106.71   |
| 8   | g     | 102 | SPO  | O1-C1-C2    | -4.37 | 78.95       | 108.97   |
| 8   | E     | 201 | SPO  | O1-C1-C2    | -4.36 | 78.97       | 108.97   |
| 8   | t     | 102 | SPO  | C20-C19-C17 | -4.36 | 121.09      | 127.31   |
| 8   | r     | 103 | SPO  | C10-C9-C7   | -4.33 | 121.13      | 127.31   |
| 8   | t     | 102 | SPO  | C21-C20-C19 | -4.33 | 114.61      | 123.47   |
| 8   | j     | 301 | SPO  | C20-C19-C17 | -4.32 | 121.15      | 127.31   |
| 7   | N     | 202 | BCL  | C16-C15-C13 | 4.31  | 129.85      | 115.92   |
| 8   | E     | 201 | SPO  | C16-C17-C19 | 4.31  | 125.55      | 118.94   |
| 8   | k     | 102 | SPO  | O1-C1-C2    | -4.29 | 79.47       | 108.97   |
| 8   | E     | 201 | SPO  | C9-C10-C11  | -4.28 | 109.87      | 123.22   |
| 12  | H     | 302 | 3PE  | O21-C21-C22 | 4.26  | 120.69      | 111.50   |
| 8   | k     | 102 | SPO  | C15-C14-C12 | -4.26 | 121.23      | 127.31   |
| 8   | s     | 201 | SPO  | C24-C23-C22 | -4.22 | 117.01      | 122.92   |
| 7   | F     | 103 | BCL  | C11-C10-C8  | -4.21 | 102.30      | 115.92   |
| 7   | e     | 100 | BCL  | C17-C16-C15 | 4.20  | 132.56      | 113.24   |
| 7   | M     | 401 | BCL  | C1D-ND-C4D  | -4.19 | 103.36      | 106.33   |
| 8   | F     | 102 | SPO  | C24-C23-C22 | -4.16 | 117.09      | 122.92   |
| 9   | M     | 405 | U10  | C20-C19-C21 | 4.15  | 122.26      | 115.27   |
| 8   | t     | 102 | SPO  | C25-C23-C22 | 4.12  | 125.26      | 118.94   |
| 8   | k     | 102 | SPO  | O1-C1-C3    | -4.12 | 80.67       | 108.97   |
| 7   | M     | 402 | BCL  | C4A-NA-C1A  | 4.11  | 108.56      | 106.71   |
| 8   | X     | 201 | SPO  | C5-C6-C7    | -4.11 | 119.68      | 125.89   |
| 8   | r     | 102 | SPO  | O1-C1-C2    | -4.10 | 80.76       | 108.97   |
| 8   | D     | 201 | SPO  | O1-C1-C3    | -4.10 | 80.79       | 108.97   |
| 7   | e     | 100 | BCL  | C4A-NA-C1A  | 4.09  | 108.54      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | E     | 201 | SPO  | O1-C1-C3    | -4.07 | 81.01       | 108.97   |
| 8   | M     | 406 | SPO  | C21-C22-C23 | -4.06 | 121.52      | 127.31   |
| 12  | H     | 301 | 3PE  | O21-C21-C22 | 4.03  | 120.18      | 111.50   |
| 8   | g     | 102 | SPO  | C24-C23-C22 | -4.01 | 117.30      | 122.92   |
| 7   | u     | 101 | BCL  | C1D-ND-C4D  | -3.99 | 103.50      | 106.33   |
| 8   | D     | 201 | SPO  | C24-C23-C25 | 3.99  | 124.36      | 118.08   |
| 8   | E     | 201 | SPO  | C15-C16-C17 | -3.95 | 115.32      | 126.42   |
| 8   | r     | 102 | SPO  | C6-C7-C9    | 3.95  | 125.00      | 118.94   |
| 8   | r     | 103 | SPO  | O1-C1-C3    | -3.94 | 81.88       | 108.97   |
| 8   | M     | 406 | SPO  | C15-C14-C12 | -3.92 | 121.71      | 127.31   |
| 10  | M     | 403 | BPH  | C1-C2-C3    | 3.91  | 132.80      | 126.04   |
| 8   | r     | 102 | SPO  | C15-C16-C17 | -3.90 | 115.45      | 126.42   |
| 8   | r     | 102 | SPO  | O1-C1-C3    | -3.90 | 82.16       | 108.97   |
| 8   | N     | 201 | SPO  | O1-C1-C3    | -3.89 | 82.22       | 108.97   |
| 8   | N     | 201 | SPO  | O1-C1-C2    | -3.88 | 82.28       | 108.97   |
| 7   | d     | 101 | BCL  | C1D-ND-C4D  | -3.87 | 103.59      | 106.33   |
| 7   | k     | 101 | BCL  | C4A-NA-C1A  | 3.86  | 108.44      | 106.71   |
| 8   | I     | 102 | SPO  | O1-C1-C2    | -3.86 | 82.45       | 108.97   |
| 8   | s     | 201 | SPO  | O1-C1-C3    | -3.84 | 82.58       | 108.97   |
| 8   | M     | 406 | SPO  | C24-C23-C25 | 3.84  | 124.12      | 118.08   |
| 7   | s     | 202 | BCL  | C1D-ND-C4D  | -3.83 | 103.61      | 106.33   |
| 9   | L     | 304 | U10  | C22-C23-C24 | -3.83 | 118.43      | 127.66   |
| 8   | g     | 102 | SPO  | C20-C21-C22 | 3.83  | 131.32      | 123.47   |
| 8   | g     | 102 | SPO  | C15-C16-C17 | -3.83 | 115.66      | 126.42   |
| 7   | b     | 101 | BCL  | O2D-CGD-CBD | 3.83  | 118.07      | 111.27   |
| 8   | t     | 102 | SPO  | C24-C23-C22 | -3.83 | 117.56      | 122.92   |
| 8   | r     | 103 | SPO  | C24-C23-C25 | 3.82  | 124.10      | 118.08   |
| 8   | B     | 101 | SPO  | C26-C25-C23 | -3.81 | 115.71      | 126.42   |
| 7   | N     | 202 | BCL  | C17-C16-C15 | 3.80  | 130.70      | 113.24   |
| 7   | o     | 100 | BCL  | C1D-ND-C4D  | -3.80 | 103.64      | 106.33   |
| 7   | j     | 302 | BCL  | C1D-ND-C4D  | -3.78 | 103.65      | 106.33   |
| 8   | s     | 201 | SPO  | O1-C1-C2    | -3.77 | 83.06       | 108.97   |
| 8   | t     | 102 | SPO  | C13-C12-C14 | -3.77 | 117.65      | 122.92   |
| 7   | A     | 101 | BCL  | C4A-NA-C1A  | 3.75  | 108.39      | 106.71   |
| 8   | r     | 102 | SPO  | C21-C20-C19 | -3.75 | 115.80      | 123.47   |
| 7   | t     | 101 | BCL  | C1D-ND-C4D  | -3.75 | 103.67      | 106.33   |
| 7   | F     | 101 | BCL  | C1D-ND-C4D  | -3.74 | 103.68      | 106.33   |
| 10  | M     | 403 | BPH  | C17-C16-C15 | 3.73  | 130.37      | 113.24   |
| 7   | r     | 101 | BCL  | C1D-ND-C4D  | -3.71 | 103.70      | 106.33   |
| 7   | a     | 101 | BCL  | C16-C15-C13 | 3.70  | 127.89      | 115.92   |
| 7   | e     | 100 | BCL  | C1D-ND-C4D  | -3.69 | 103.71      | 106.33   |
| 8   | g     | 102 | SPO  | C21-C22-C23 | 3.67  | 132.55      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | I     | 102 | SPO  | C21-C22-C23 | -3.67 | 122.07      | 127.31   |
| 8   | X     | 201 | SPO  | C20-C19-C17 | -3.67 | 122.07      | 127.31   |
| 8   | j     | 301 | SPO  | C21-C20-C19 | -3.66 | 115.97      | 123.47   |
| 7   | u     | 102 | BCL  | C1D-ND-C4D  | -3.65 | 103.74      | 106.33   |
| 7   | i     | 100 | BCL  | C1D-ND-C4D  | -3.65 | 103.74      | 106.33   |
| 8   | r     | 103 | SPO  | C20-C21-C22 | -3.65 | 116.00      | 123.47   |
| 8   | k     | 102 | SPO  | C31-C32-C33 | -3.63 | 118.93      | 127.66   |
| 7   | n     | 100 | BCL  | C1D-ND-C4D  | -3.63 | 103.76      | 106.33   |
| 9   | L     | 304 | U10  | C7-C8-C9    | -3.62 | 120.76      | 126.79   |
| 7   | K     | 101 | BCL  | C4A-NA-C1A  | 3.62  | 108.33      | 106.71   |
| 7   | b     | 102 | BCL  | C4A-NA-C1A  | 3.62  | 108.33      | 106.71   |
| 8   | E     | 201 | SPO  | C8-C7-C9    | -3.60 | 117.88      | 122.92   |
| 8   | s     | 201 | SPO  | C6-C7-C9    | 3.60  | 124.46      | 118.94   |
| 7   | g     | 101 | BCL  | C1D-ND-C4D  | -3.60 | 103.78      | 106.33   |
| 7   | E     | 202 | BCL  | C4A-NA-C1A  | 3.59  | 108.32      | 106.71   |
| 7   | k     | 101 | BCL  | C1D-ND-C4D  | -3.57 | 103.80      | 106.33   |
| 8   | r     | 103 | SPO  | O1-C1-C2    | -3.57 | 84.41       | 108.97   |
| 8   | D     | 201 | SPO  | C31-C32-C33 | -3.57 | 119.06      | 127.66   |
| 12  | d     | 102 | 3PE  | O21-C21-C22 | 3.57  | 119.19      | 111.50   |
| 12  | d     | 102 | 3PE  | O12-P-O14   | 3.55  | 129.81      | 112.24   |
| 7   | g     | 101 | BCL  | C4A-NA-C1A  | 3.55  | 108.30      | 106.71   |
| 8   | s     | 201 | SPO  | C25-C23-C22 | 3.55  | 124.39      | 118.94   |
| 8   | F     | 102 | SPO  | C10-C9-C7   | -3.55 | 122.25      | 127.31   |
| 9   | L     | 304 | U10  | C25-C24-C26 | 3.54  | 121.23      | 115.27   |
| 9   | a     | 102 | U10  | C27-C28-C29 | -3.53 | 119.16      | 127.66   |
| 9   | L     | 304 | U10  | C17-C18-C19 | -3.52 | 119.19      | 127.66   |
| 7   | F     | 103 | BCL  | C4A-NA-C1A  | 3.51  | 108.28      | 106.71   |
| 9   | M     | 405 | U10  | C35-C34-C36 | 3.51  | 121.18      | 115.27   |
| 7   | d     | 101 | BCL  | C4A-NA-C1A  | 3.51  | 108.28      | 106.71   |
| 8   | E     | 201 | SPO  | C21-C20-C19 | -3.49 | 116.33      | 123.47   |
| 8   | I     | 102 | SPO  | O1-C1-C3    | -3.48 | 85.04       | 108.97   |
| 7   | F     | 101 | BCL  | C4A-NA-C1A  | 3.47  | 108.27      | 106.71   |
| 8   | I     | 102 | SPO  | C5-C6-C7    | -3.46 | 120.66      | 125.89   |
| 8   | F     | 102 | SPO  | C24-C23-C25 | 3.46  | 123.52      | 118.08   |
| 8   | r     | 103 | SPO  | C15-C14-C12 | -3.43 | 122.42      | 127.31   |
| 7   | a     | 101 | BCL  | C4A-NA-C1A  | 3.42  | 108.25      | 106.71   |
| 7   | O     | 101 | BCL  | C1C-NC-C4C  | 3.42  | 108.24      | 106.71   |
| 8   | k     | 102 | SPO  | C14-C15-C16 | -3.40 | 112.62      | 123.22   |
| 9   | M     | 405 | U10  | C12-C13-C14 | -3.40 | 119.48      | 127.66   |
| 8   | M     | 406 | SPO  | C13-C12-C11 | -3.39 | 112.74      | 118.08   |
| 8   | E     | 201 | SPO  | C34-C33-C35 | 3.37  | 120.94      | 115.27   |
| 8   | D     | 201 | SPO  | C20-C21-C22 | -3.37 | 116.58      | 123.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | M     | 402 | BCL  | C1D-ND-C4D  | -3.36 | 103.95      | 106.33   |
| 7   | I     | 101 | BCL  | C1D-ND-C4D  | -3.35 | 103.95      | 106.33   |
| 8   | I     | 102 | SPO  | C26-C25-C23 | -3.35 | 117.01      | 126.42   |
| 10  | L     | 302 | BPH  | C3D-C4D-ND  | 3.34  | 112.28      | 107.72   |
| 8   | D     | 201 | SPO  | C25-C23-C22 | -3.34 | 113.82      | 118.94   |
| 10  | L     | 306 | BPH  | C3D-C4D-ND  | 3.33  | 112.25      | 107.72   |
| 7   | a     | 101 | BCL  | C1D-ND-C4D  | -3.32 | 103.97      | 106.33   |
| 7   | b     | 101 | BCL  | CHA-C1A-NA  | -3.32 | 118.79      | 126.40   |
| 7   | u     | 102 | BCL  | CAB-C3B-C2B | 3.32  | 133.31      | 128.34   |
| 7   | S     | 101 | BCL  | C1D-ND-C4D  | -3.31 | 103.98      | 106.33   |
| 10  | L     | 302 | BPH  | OBD-CAD-CBD | -3.30 | 120.98      | 125.82   |
| 8   | N     | 201 | SPO  | C14-C15-C16 | -3.29 | 112.94      | 123.22   |
| 8   | k     | 102 | SPO  | C24-C23-C22 | -3.29 | 118.31      | 122.92   |
| 8   | N     | 201 | SPO  | C13-C12-C11 | 3.29  | 123.26      | 118.08   |
| 8   | r     | 102 | SPO  | C10-C11-C12 | -3.28 | 117.19      | 126.42   |
| 7   | M     | 402 | BCL  | C1-O2A-CGA  | 3.28  | 125.05      | 116.44   |
| 8   | M     | 406 | SPO  | C11-C12-C14 | 3.27  | 123.97      | 118.94   |
| 7   | j     | 303 | BCL  | C1D-ND-C4D  | -3.27 | 104.01      | 106.33   |
| 8   | g     | 102 | SPO  | O1-C1-C3    | -3.27 | 86.49       | 108.97   |
| 7   | r     | 101 | BCL  | C4A-NA-C1A  | 3.27  | 108.17      | 106.71   |
| 9   | a     | 102 | U10  | C1M-C1-C6   | -3.26 | 119.08      | 124.40   |
| 8   | N     | 201 | SPO  | C31-C32-C33 | -3.25 | 119.83      | 127.66   |
| 7   | s     | 202 | BCL  | CAB-C3B-C2B | 3.25  | 133.21      | 128.34   |
| 7   | A     | 101 | BCL  | C1D-ND-C4D  | -3.24 | 104.03      | 106.33   |
| 7   | n     | 100 | BCL  | C4A-NA-C1A  | 3.24  | 108.16      | 106.71   |
| 10  | M     | 403 | BPH  | C3D-C4D-ND  | 3.23  | 112.12      | 107.72   |
| 7   | N     | 202 | BCL  | C1D-ND-C4D  | -3.22 | 104.04      | 106.33   |
| 8   | B     | 101 | SPO  | C29-C28-C30 | 3.22  | 120.69      | 115.27   |
| 7   | t     | 103 | BCL  | CHA-C1A-NA  | -3.22 | 119.03      | 126.40   |
| 10  | L     | 306 | BPH  | O2D-CGD-CBD | 3.21  | 115.07      | 111.00   |
| 9   | a     | 102 | U10  | C17-C18-C19 | -3.20 | 119.95      | 127.66   |
| 9   | a     | 102 | U10  | C15-C14-C16 | 3.20  | 120.65      | 115.27   |
| 7   | b     | 101 | BCL  | C16-C15-C13 | 3.19  | 126.24      | 115.92   |
| 7   | S     | 101 | BCL  | C4A-NA-C1A  | 3.19  | 108.14      | 106.71   |
| 7   | d     | 101 | BCL  | O2D-CGD-CBD | 3.19  | 116.93      | 111.27   |
| 7   | G     | 101 | BCL  | C1D-ND-C4D  | -3.18 | 104.08      | 106.33   |
| 7   | t     | 101 | BCL  | C4A-NA-C1A  | 3.17  | 108.13      | 106.71   |
| 7   | D     | 202 | BCL  | C1D-ND-C4D  | -3.17 | 104.08      | 106.33   |
| 7   | M     | 407 | BCL  | CHA-C1A-NA  | -3.16 | 119.16      | 126.40   |
| 7   | D     | 202 | BCL  | C4A-NA-C1A  | 3.16  | 108.13      | 106.71   |
| 8   | g     | 102 | SPO  | C15-C14-C12 | 3.16  | 131.81      | 127.31   |
| 8   | N     | 201 | SPO  | C34-C33-C35 | 3.16  | 120.58      | 115.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | b     | 102 | BCL  | CAB-C3B-C2B | 3.15  | 133.06      | 128.34   |
| 7   | R     | 101 | BCL  | C1D-ND-C4D  | -3.15 | 104.09      | 106.33   |
| 7   | t     | 101 | BCL  | CHA-C1A-NA  | -3.15 | 119.19      | 126.40   |
| 7   | i     | 100 | BCL  | C1C-NC-C4C  | 3.15  | 108.12      | 106.71   |
| 7   | b     | 102 | BCL  | C1D-ND-C4D  | -3.14 | 104.10      | 106.33   |
| 8   | g     | 102 | SPO  | C29-C28-C30 | 3.14  | 120.56      | 115.27   |
| 10  | M     | 403 | BPH  | OBD-CAD-CBD | -3.14 | 121.21      | 125.82   |
| 7   | b     | 101 | BCL  | C1D-ND-C4D  | -3.14 | 104.11      | 106.33   |
| 8   | B     | 101 | SPO  | C18-C17-C19 | -3.13 | 118.53      | 122.92   |
| 7   | L     | 301 | BCL  | C1D-ND-C4D  | -3.13 | 104.11      | 106.33   |
| 9   | M     | 405 | U10  | C17-C18-C19 | -3.12 | 120.14      | 127.66   |
| 7   | u     | 101 | BCL  | CHA-C1A-NA  | -3.12 | 119.26      | 126.40   |
| 9   | M     | 405 | U10  | C27-C28-C29 | -3.12 | 120.16      | 127.66   |
| 8   | r     | 102 | SPO  | C26-C25-C23 | -3.11 | 117.67      | 126.42   |
| 7   | M     | 402 | BCL  | CHA-C1A-NA  | -3.11 | 119.27      | 126.40   |
| 8   | g     | 102 | SPO  | C11-C12-C14 | -3.10 | 114.18      | 118.94   |
| 9   | a     | 102 | U10  | C10-C9-C11  | 3.10  | 120.49      | 115.27   |
| 8   | N     | 201 | SPO  | C11-C12-C14 | -3.09 | 114.20      | 118.94   |
| 7   | o     | 100 | BCL  | CHA-C1A-NA  | -3.09 | 119.32      | 126.40   |
| 8   | B     | 101 | SPO  | C14-C15-C16 | -3.09 | 113.58      | 123.22   |
| 8   | r     | 102 | SPO  | C29-C28-C30 | 3.08  | 120.45      | 115.27   |
| 8   | s     | 201 | SPO  | C13-C12-C14 | -3.08 | 118.61      | 122.92   |
| 7   | F     | 103 | BCL  | C1D-ND-C4D  | -3.07 | 104.15      | 106.33   |
| 7   | E     | 202 | BCL  | C1D-ND-C4D  | -3.06 | 104.16      | 106.33   |
| 7   | G     | 101 | BCL  | C1C-NC-C4C  | 3.06  | 108.08      | 106.71   |
| 7   | t     | 103 | BCL  | C1D-ND-C4D  | -3.06 | 104.16      | 106.33   |
| 7   | N     | 202 | BCL  | CHA-C1A-NA  | -3.05 | 119.41      | 126.40   |
| 8   | k     | 102 | SPO  | C13-C12-C11 | 3.05  | 122.88      | 118.08   |
| 7   | N     | 202 | BCL  | C4A-NA-C1A  | 3.04  | 108.07      | 106.71   |
| 7   | r     | 101 | BCL  | C1C-NC-C4C  | 3.04  | 108.07      | 106.71   |
| 7   | O     | 101 | BCL  | C1D-ND-C4D  | -3.04 | 104.18      | 106.33   |
| 9   | a     | 102 | U10  | C20-C19-C21 | 3.03  | 120.38      | 115.27   |
| 8   | N     | 201 | SPO  | C29-C28-C30 | 3.03  | 120.37      | 115.27   |
| 7   | d     | 101 | BCL  | CHA-C1A-NA  | -3.03 | 119.47      | 126.40   |
| 9   | M     | 405 | U10  | C22-C23-C24 | -3.03 | 120.37      | 127.66   |
| 7   | M     | 407 | BCL  | C2A-C1A-CHA | 3.03  | 129.15      | 123.86   |
| 7   | M     | 407 | BCL  | C1C-NC-C4C  | 3.03  | 108.07      | 106.71   |
| 7   | o     | 100 | BCL  | C1C-NC-C4C  | 3.02  | 108.06      | 106.71   |
| 7   | a     | 101 | BCL  | CHA-C1A-NA  | -3.02 | 119.49      | 126.40   |
| 7   | n     | 100 | BCL  | CHA-C1A-NA  | -3.02 | 119.49      | 126.40   |
| 7   | M     | 401 | BCL  | CHA-C1A-NA  | -3.01 | 119.50      | 126.40   |
| 7   | j     | 302 | BCL  | CHA-C1A-NA  | -3.01 | 119.51      | 126.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | e     | 100 | BCL  | CED-O2D-CGD | -3.01 | 109.14      | 115.94   |
| 8   | k     | 102 | SPO  | C34-C33-C35 | 3.01  | 120.33      | 115.27   |
| 7   | L     | 301 | BCL  | C4A-NA-C1A  | 3.01  | 108.06      | 106.71   |
| 8   | t     | 102 | SPO  | C34-C33-C35 | 3.00  | 120.33      | 115.27   |
| 8   | s     | 201 | SPO  | C18-C17-C16 | 3.00  | 122.81      | 118.08   |
| 7   | G     | 101 | BCL  | CHA-C1A-NA  | -3.00 | 119.53      | 126.40   |
| 8   | N     | 201 | SPO  | C5-C6-C7    | -3.00 | 121.36      | 125.89   |
| 7   | e     | 100 | BCL  | C1C-NC-C4C  | 3.00  | 108.05      | 106.71   |
| 7   | j     | 302 | BCL  | C4A-NA-C1A  | 3.00  | 108.05      | 106.71   |
| 8   | D     | 201 | SPO  | C14-C15-C16 | -2.99 | 113.89      | 123.22   |
| 7   | F     | 103 | BCL  | CHA-C1A-NA  | -2.99 | 119.56      | 126.40   |
| 8   | r     | 103 | SPO  | C29-C28-C30 | 2.99  | 120.30      | 115.27   |
| 8   | k     | 102 | SPO  | C24-C23-C25 | 2.98  | 122.78      | 118.08   |
| 7   | r     | 101 | BCL  | CHA-C1A-NA  | -2.98 | 119.56      | 126.40   |
| 7   | k     | 101 | BCL  | CAB-C3B-C2B | 2.98  | 132.81      | 128.34   |
| 8   | X     | 201 | SPO  | C31-C32-C33 | -2.98 | 120.48      | 127.66   |
| 7   | j     | 303 | BCL  | CHA-C1A-NA  | -2.98 | 119.57      | 126.40   |
| 7   | L     | 301 | BCL  | CHA-C1A-NA  | -2.98 | 119.57      | 126.40   |
| 8   | E     | 201 | SPO  | C20-C21-C22 | 2.98  | 129.57      | 123.47   |
| 7   | S     | 101 | BCL  | CAB-C3B-C2B | 2.98  | 132.80      | 128.34   |
| 7   | j     | 302 | BCL  | O2D-CGD-CBD | 2.98  | 116.56      | 111.27   |
| 7   | i     | 100 | BCL  | CHA-C1A-NA  | -2.97 | 119.60      | 126.40   |
| 9   | M     | 408 | U10  | C6-C1-C2    | 2.97  | 121.53      | 119.18   |
| 7   | M     | 407 | BCL  | C1D-ND-C4D  | -2.97 | 104.23      | 106.33   |
| 8   | j     | 301 | SPO  | C31-C32-C33 | -2.97 | 120.52      | 127.66   |
| 7   | k     | 101 | BCL  | O2D-CGD-CBD | 2.97  | 116.54      | 111.27   |
| 7   | K     | 101 | BCL  | C1D-ND-C4D  | -2.96 | 104.23      | 106.33   |
| 8   | B     | 101 | SPO  | C9-C10-C11  | 2.96  | 132.46      | 123.22   |
| 8   | B     | 101 | SPO  | C25-C23-C22 | 2.96  | 123.48      | 118.94   |
| 8   | j     | 301 | SPO  | C29-C28-C30 | 2.96  | 120.25      | 115.27   |
| 7   | j     | 303 | BCL  | C4A-NA-C1A  | 2.96  | 108.04      | 106.71   |
| 8   | k     | 102 | SPO  | C29-C28-C30 | 2.96  | 120.25      | 115.27   |
| 7   | s     | 202 | BCL  | C4A-NA-C1A  | 2.95  | 108.03      | 106.71   |
| 7   | g     | 101 | BCL  | CHA-C1A-NA  | -2.95 | 119.65      | 126.40   |
| 7   | a     | 101 | BCL  | C1C-NC-C4C  | 2.94  | 108.03      | 106.71   |
| 7   | F     | 101 | BCL  | CHC-C4B-NB  | -2.94 | 121.14      | 124.26   |
| 7   | S     | 101 | BCL  | CHA-C1A-NA  | -2.94 | 119.67      | 126.40   |
| 7   | b     | 102 | BCL  | CHA-C1A-NA  | -2.93 | 119.68      | 126.40   |
| 7   | E     | 202 | BCL  | CHA-C1A-NA  | -2.93 | 119.68      | 126.40   |
| 7   | K     | 101 | BCL  | CHA-C1A-NA  | -2.93 | 119.69      | 126.40   |
| 7   | s     | 202 | BCL  | CHA-C1A-NA  | -2.92 | 119.70      | 126.40   |
| 9   | a     | 102 | U10  | C30-C29-C31 | 2.92  | 120.19      | 115.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | d     | 101 | BCL  | CMB-C2B-C1B | -2.92 | 120.92      | 125.37   |
| 12  | H     | 301 | 3PE  | O31-C31-C32 | 2.91  | 121.05      | 111.91   |
| 8   | r     | 102 | SPO  | C8-C7-C9    | -2.91 | 118.84      | 122.92   |
| 7   | O     | 101 | BCL  | CHA-C1A-NA  | -2.91 | 119.74      | 126.40   |
| 9   | L     | 304 | U10  | C15-C14-C16 | 2.91  | 120.16      | 115.27   |
| 7   | e     | 100 | BCL  | CHA-C1A-NA  | -2.90 | 119.75      | 126.40   |
| 7   | R     | 101 | BCL  | CHA-C1A-NA  | -2.90 | 119.75      | 126.40   |
| 7   | I     | 101 | BCL  | CHA-C1A-NA  | -2.90 | 119.77      | 126.40   |
| 7   | k     | 101 | BCL  | CHA-C1A-NA  | -2.89 | 119.78      | 126.40   |
| 7   | F     | 101 | BCL  | O2D-CGD-CBD | 2.89  | 116.40      | 111.27   |
| 9   | L     | 303 | U10  | C6-C1-C2    | 2.89  | 121.46      | 119.18   |
| 7   | j     | 303 | BCL  | C1C-NC-C4C  | 2.88  | 108.00      | 106.71   |
| 7   | r     | 101 | BCL  | C11-C10-C8  | -2.88 | 106.61      | 115.92   |
| 8   | E     | 201 | SPO  | C10-C9-C7   | 2.88  | 131.42      | 127.31   |
| 7   | F     | 101 | BCL  | CHA-C1A-NA  | -2.88 | 119.81      | 126.40   |
| 9   | L     | 305 | U10  | C12-C13-C14 | -2.88 | 120.73      | 127.66   |
| 7   | b     | 101 | BCL  | CED-O2D-CGD | -2.88 | 109.43      | 115.94   |
| 8   | F     | 102 | SPO  | C15-C16-C17 | -2.88 | 118.34      | 126.42   |
| 8   | I     | 102 | SPO  | C29-C28-C30 | 2.88  | 120.11      | 115.27   |
| 9   | M     | 405 | U10  | C30-C29-C31 | 2.87  | 120.10      | 115.27   |
| 7   | I     | 101 | BCL  | C4A-NA-C1A  | 2.87  | 108.00      | 106.71   |
| 7   | o     | 100 | BCL  | CHC-C4B-NB  | -2.87 | 121.22      | 124.26   |
| 7   | u     | 102 | BCL  | CHA-C1A-NA  | -2.86 | 119.84      | 126.40   |
| 7   | u     | 101 | BCL  | C2A-C1A-CHA | 2.86  | 128.87      | 123.86   |
| 9   | L     | 304 | U10  | C20-C19-C21 | 2.86  | 120.08      | 115.27   |
| 7   | K     | 101 | BCL  | C1-C2-C3    | 2.86  | 130.98      | 126.04   |
| 8   | E     | 201 | SPO  | C24-C23-C22 | -2.85 | 118.93      | 122.92   |
| 8   | D     | 201 | SPO  | C29-C28-C30 | 2.85  | 120.07      | 115.27   |
| 7   | M     | 401 | BCL  | C2A-C1A-CHA | 2.85  | 128.84      | 123.86   |
| 7   | A     | 101 | BCL  | CHA-C1A-NA  | -2.85 | 119.88      | 126.40   |
| 7   | F     | 101 | BCL  | C1C-NC-C4C  | 2.85  | 107.99      | 106.71   |
| 7   | e     | 100 | BCL  | CAB-C3B-C2B | 2.85  | 132.60      | 128.34   |
| 12  | H     | 302 | 3PE  | O31-C31-C32 | 2.85  | 120.84      | 111.91   |
| 8   | g     | 102 | SPO  | C31-C32-C33 | -2.84 | 120.81      | 127.66   |
| 7   | o     | 100 | BCL  | C2A-C1A-CHA | 2.84  | 128.83      | 123.86   |
| 9   | a     | 102 | U10  | C12-C13-C14 | -2.84 | 120.83      | 127.66   |
| 7   | F     | 101 | BCL  | CED-O2D-CGD | -2.84 | 109.52      | 115.94   |
| 8   | B     | 101 | SPO  | C20-C21-C22 | -2.83 | 117.67      | 123.47   |
| 7   | e     | 100 | BCL  | O2D-CGD-CBD | 2.82  | 116.29      | 111.27   |
| 7   | G     | 101 | BCL  | C2A-C1A-CHA | 2.82  | 128.79      | 123.86   |
| 7   | j     | 302 | BCL  | CAB-C3B-C2B | 2.82  | 132.56      | 128.34   |
| 10  | M     | 403 | BPH  | OBB-CAB-C3B | 2.82  | 124.99      | 119.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | M     | 405 | U10  | C25-C24-C26 | 2.82  | 120.01      | 115.27   |
| 10  | L     | 306 | BPH  | OBD-CAD-CBD | -2.81 | 121.69      | 125.82   |
| 8   | N     | 201 | SPO  | C20-C21-C22 | -2.80 | 117.73      | 123.47   |
| 8   | j     | 301 | SPO  | C34-C33-C35 | 2.80  | 119.98      | 115.27   |
| 8   | s     | 201 | SPO  | C16-C17-C19 | -2.80 | 114.64      | 118.94   |
| 7   | j     | 303 | BCL  | C1-C2-C3    | 2.80  | 130.89      | 126.04   |
| 7   | i     | 100 | BCL  | O2D-CGD-CBD | 2.80  | 116.24      | 111.27   |
| 7   | D     | 202 | BCL  | CHA-C1A-NA  | -2.79 | 120.00      | 126.40   |
| 7   | r     | 101 | BCL  | CHC-C4B-NB  | -2.79 | 121.30      | 124.26   |
| 7   | t     | 101 | BCL  | C2A-C1A-CHA | 2.79  | 128.74      | 123.86   |
| 8   | M     | 406 | SPO  | C8-C7-C9    | -2.79 | 119.01      | 122.92   |
| 8   | B     | 101 | SPO  | C34-C33-C32 | -2.79 | 116.52      | 123.68   |
| 7   | e     | 100 | BCL  | CHC-C4B-NB  | -2.79 | 121.30      | 124.26   |
| 7   | M     | 402 | BCL  | CHC-C4B-NB  | -2.79 | 121.31      | 124.26   |
| 7   | u     | 101 | BCL  | CAB-C3B-C2B | 2.78  | 132.50      | 128.34   |
| 8   | B     | 101 | SPO  | C24-C23-C22 | -2.77 | 119.04      | 122.92   |
| 7   | b     | 101 | BCL  | CAB-C3B-C2B | 2.77  | 132.49      | 128.34   |
| 7   | s     | 202 | BCL  | C2A-C1A-CHA | 2.77  | 128.71      | 123.86   |
| 7   | n     | 100 | BCL  | O2D-CGD-CBD | 2.77  | 116.19      | 111.27   |
| 7   | g     | 101 | BCL  | CED-O2D-CGD | -2.77 | 109.67      | 115.94   |
| 9   | L     | 303 | U10  | C17-C18-C19 | -2.76 | 121.00      | 127.66   |
| 7   | d     | 101 | BCL  | CHC-C4B-NB  | -2.76 | 121.33      | 124.26   |
| 7   | L     | 301 | BCL  | CAB-C3B-C2B | 2.76  | 132.47      | 128.34   |
| 7   | e     | 100 | BCL  | O2D-CGD-O1D | -2.76 | 118.45      | 123.84   |
| 8   | s     | 201 | SPO  | C11-C12-C14 | 2.75  | 123.16      | 118.94   |
| 7   | u     | 101 | BCL  | C4A-NA-C1A  | 2.75  | 107.94      | 106.71   |
| 7   | u     | 101 | BCL  | C17-C16-C15 | 2.75  | 125.88      | 113.24   |
| 7   | L     | 301 | BCL  | C1C-NC-C4C  | 2.75  | 107.94      | 106.71   |
| 7   | i     | 100 | BCL  | CHC-C4B-NB  | -2.75 | 121.35      | 124.26   |
| 7   | I     | 101 | BCL  | CAB-C3B-C2B | 2.75  | 132.46      | 128.34   |
| 7   | o     | 100 | BCL  | CMB-C2B-C1B | -2.74 | 121.19      | 125.37   |
| 7   | s     | 202 | BCL  | O2D-CGD-CBD | 2.73  | 116.12      | 111.27   |
| 8   | r     | 102 | SPO  | C25-C23-C22 | -2.73 | 114.75      | 118.94   |
| 7   | g     | 101 | BCL  | CHC-C4B-NB  | -2.73 | 121.37      | 124.26   |
| 9   | a     | 102 | U10  | C35-C34-C36 | 2.73  | 119.86      | 115.27   |
| 7   | s     | 202 | BCL  | CHC-C4B-NB  | -2.73 | 121.37      | 124.26   |
| 8   | B     | 101 | SPO  | C34-C33-C35 | 2.72  | 119.85      | 115.27   |
| 7   | b     | 101 | BCL  | C2A-C1A-CHA | 2.72  | 128.62      | 123.86   |
| 9   | L     | 303 | U10  | C20-C19-C21 | 2.72  | 119.85      | 115.27   |
| 7   | D     | 202 | BCL  | CHC-C4B-NB  | -2.72 | 121.38      | 124.26   |
| 7   | j     | 302 | BCL  | CHC-C4B-NB  | -2.72 | 121.38      | 124.26   |
| 8   | X     | 201 | SPO  | C10-C9-C7   | -2.71 | 123.44      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | r     | 103 | SPO  | C10-C11-C12 | -2.70 | 118.83      | 126.42   |
| 9   | M     | 405 | U10  | C10-C9-C11  | 2.69  | 119.80      | 115.27   |
| 7   | i     | 100 | BCL  | CAB-C3B-C2B | 2.69  | 132.37      | 128.34   |
| 8   | M     | 406 | SPO  | C6-C7-C9    | 2.68  | 123.06      | 118.94   |
| 10  | L     | 306 | BPH  | C2D-C1D-ND  | 2.68  | 111.38      | 109.53   |
| 9   | L     | 303 | U10  | C15-C14-C16 | 2.68  | 119.78      | 115.27   |
| 7   | E     | 202 | BCL  | C1C-NC-C4C  | 2.68  | 107.91      | 106.71   |
| 8   | I     | 102 | SPO  | C34-C33-C35 | 2.67  | 119.77      | 115.27   |
| 7   | M     | 407 | BCL  | CHC-C4B-NB  | -2.67 | 121.43      | 124.26   |
| 8   | X     | 201 | SPO  | C27-C26-C25 | -2.67 | 114.88      | 123.22   |
| 7   | b     | 101 | BCL  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 7   | R     | 101 | BCL  | CAB-C3B-C2B | 2.67  | 132.34      | 128.34   |
| 7   | F     | 103 | BCL  | C6-C7-C8    | 2.67  | 124.55      | 115.92   |
| 7   | i     | 100 | BCL  | CMB-C2B-C1B | -2.67 | 121.31      | 125.37   |
| 8   | X     | 201 | SPO  | C9-C10-C11  | -2.67 | 114.89      | 123.22   |
| 7   | F     | 101 | BCL  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 7   | A     | 101 | BCL  | C1C-NC-C4C  | 2.67  | 107.91      | 106.71   |
| 8   | E     | 201 | SPO  | C18-C17-C19 | -2.67 | 119.19      | 122.92   |
| 7   | k     | 101 | BCL  | CHC-C4B-NB  | -2.67 | 121.44      | 124.26   |
| 9   | L     | 305 | U10  | C21-C19-C20 | 2.66  | 120.48      | 114.60   |
| 7   | e     | 100 | BCL  | C2A-C1A-CHA | 2.66  | 128.51      | 123.86   |
| 7   | b     | 102 | BCL  | C1C-NC-C4C  | 2.66  | 107.90      | 106.71   |
| 8   | M     | 406 | SPO  | C29-C28-C30 | 2.66  | 119.74      | 115.27   |
| 7   | n     | 100 | BCL  | CHC-C4B-NB  | -2.66 | 121.45      | 124.26   |
| 7   | F     | 101 | BCL  | C17-C16-C15 | 2.65  | 125.42      | 113.24   |
| 9   | L     | 305 | U10  | C10-C9-C11  | 2.65  | 119.73      | 115.27   |
| 7   | G     | 101 | BCL  | CAB-C3B-C2B | 2.65  | 132.31      | 128.34   |
| 7   | b     | 101 | BCL  | C4A-NA-C1A  | 2.65  | 107.90      | 106.71   |
| 7   | F     | 101 | BCL  | CMB-C2B-C1B | -2.64 | 121.34      | 125.37   |
| 7   | M     | 402 | BCL  | CAB-C3B-C2B | 2.64  | 132.30      | 128.34   |
| 8   | F     | 102 | SPO  | C31-C32-C33 | -2.64 | 121.31      | 127.66   |
| 9   | L     | 303 | U10  | O5-C5-C6    | -2.63 | 116.93      | 121.55   |
| 7   | j     | 303 | BCL  | CAB-C3B-C2B | 2.63  | 132.27      | 128.34   |
| 9   | M     | 405 | U10  | C15-C14-C16 | 2.63  | 119.69      | 115.27   |
| 9   | L     | 304 | U10  | C12-C13-C14 | -2.62 | 121.34      | 127.66   |
| 7   | g     | 101 | BCL  | C2A-C1A-CHA | 2.62  | 128.45      | 123.86   |
| 7   | a     | 101 | BCL  | C1-C2-C3    | 2.62  | 130.58      | 126.04   |
| 10  | L     | 302 | BPH  | OBB-CAB-CBB | -2.62 | 114.27      | 120.17   |
| 7   | G     | 101 | BCL  | CHC-C4B-NB  | -2.62 | 121.48      | 124.26   |
| 8   | r     | 102 | SPO  | C20-C19-C17 | -2.61 | 123.58      | 127.31   |
| 8   | r     | 103 | SPO  | C20-C19-C17 | -2.61 | 123.58      | 127.31   |
| 7   | t     | 101 | BCL  | CHC-C4B-NB  | -2.61 | 121.49      | 124.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | d     | 102 | 3PE  | O31-C31-C32 | 2.61  | 120.10      | 111.91   |
| 8   | j     | 301 | SPO  | C8-C7-C6    | 2.61  | 122.19      | 118.08   |
| 8   | k     | 102 | SPO  | C18-C17-C19 | -2.60 | 119.27      | 122.92   |
| 7   | d     | 101 | BCL  | CED-O2D-CGD | -2.60 | 110.05      | 115.94   |
| 7   | F     | 103 | BCL  | CHC-C4B-NB  | -2.60 | 121.50      | 124.26   |
| 7   | g     | 101 | BCL  | CAB-C3B-C2B | 2.60  | 132.24      | 128.34   |
| 7   | n     | 100 | BCL  | C11-C10-C8  | -2.60 | 107.51      | 115.92   |
| 8   | M     | 406 | SPO  | C31-C32-C33 | -2.60 | 121.40      | 127.66   |
| 7   | k     | 101 | BCL  | CED-O2D-CGD | -2.60 | 110.06      | 115.94   |
| 7   | t     | 101 | BCL  | CAB-C3B-C2B | 2.59  | 132.22      | 128.34   |
| 7   | d     | 101 | BCL  | C2A-C1A-CHA | 2.59  | 128.39      | 123.86   |
| 8   | F     | 102 | SPO  | C29-C28-C30 | 2.59  | 119.63      | 115.27   |
| 8   | g     | 102 | SPO  | C13-C12-C11 | 2.59  | 122.16      | 118.08   |
| 9   | a     | 102 | U10  | C25-C24-C26 | 2.59  | 119.62      | 115.27   |
| 7   | n     | 100 | BCL  | C2A-C1A-CHA | 2.58  | 128.38      | 123.86   |
| 7   | L     | 301 | BCL  | C2A-C1A-CHA | 2.58  | 128.37      | 123.86   |
| 8   | F     | 102 | SPO  | C36-C37-C38 | -2.58 | 118.93      | 127.75   |
| 8   | X     | 201 | SPO  | C34-C33-C35 | 2.58  | 119.61      | 115.27   |
| 8   | r     | 102 | SPO  | C21-C22-C23 | 2.58  | 130.99      | 127.31   |
| 8   | F     | 102 | SPO  | C34-C33-C35 | 2.58  | 119.60      | 115.27   |
| 7   | n     | 100 | BCL  | CMB-C2B-C1B | -2.58 | 121.45      | 125.37   |
| 8   | t     | 102 | SPO  | C27-C26-C25 | 2.57  | 131.25      | 123.22   |
| 7   | a     | 101 | BCL  | C2A-C1A-CHA | 2.57  | 128.36      | 123.86   |
| 7   | F     | 101 | BCL  | C1-C2-C3    | -2.57 | 121.60      | 126.04   |
| 7   | b     | 101 | BCL  | CHC-C4B-NB  | -2.57 | 121.54      | 124.26   |
| 7   | R     | 101 | BCL  | C4A-NA-C1A  | 2.57  | 107.86      | 106.71   |
| 7   | R     | 101 | BCL  | C2A-C1A-CHA | 2.57  | 128.35      | 123.86   |
| 7   | F     | 103 | BCL  | C1-C2-C3    | 2.57  | 130.48      | 126.04   |
| 7   | O     | 101 | BCL  | C2A-C1A-CHA | 2.57  | 128.35      | 123.86   |
| 8   | N     | 201 | SPO  | C1-C4-C5    | 2.57  | 119.86      | 113.06   |
| 7   | d     | 101 | BCL  | OBB-CAB-CBB | -2.56 | 114.05      | 119.73   |
| 8   | t     | 102 | SPO  | C40-C38-C39 | 2.56  | 120.27      | 114.60   |
| 7   | g     | 101 | BCL  | CMB-C2B-C1B | -2.56 | 121.47      | 125.37   |
| 7   | D     | 202 | BCL  | CMB-C2B-C1B | -2.56 | 121.47      | 125.37   |
| 8   | g     | 102 | SPO  | C34-C33-C35 | 2.56  | 119.58      | 115.27   |
| 7   | n     | 100 | BCL  | CAB-C3B-C2B | 2.56  | 132.17      | 128.34   |
| 7   | b     | 101 | BCL  | CMB-C2B-C1B | -2.56 | 121.47      | 125.37   |
| 7   | S     | 101 | BCL  | C1C-NC-C4C  | 2.56  | 107.86      | 106.71   |
| 9   | M     | 408 | U10  | C7-C6-C5    | -2.56 | 115.40      | 118.48   |
| 7   | E     | 202 | BCL  | CHC-C4B-NB  | -2.55 | 121.55      | 124.26   |
| 7   | R     | 101 | BCL  | CHC-C4B-NB  | -2.55 | 121.56      | 124.26   |
| 8   | D     | 201 | SPO  | C9-C10-C11  | -2.55 | 115.26      | 123.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | M     | 402 | BCL  | C2A-C1A-CHA | 2.55  | 128.31      | 123.86   |
| 7   | I     | 101 | BCL  | C1-C2-C3    | 2.55  | 130.45      | 126.04   |
| 7   | F     | 101 | BCL  | C2A-C1A-CHA | 2.54  | 128.31      | 123.86   |
| 7   | n     | 100 | BCL  | C1C-NC-C4C  | 2.54  | 107.85      | 106.71   |
| 9   | L     | 304 | U10  | C1M-C1-C6   | -2.54 | 120.26      | 124.40   |
| 7   | u     | 101 | BCL  | C1C-NC-C4C  | 2.54  | 107.85      | 106.71   |
| 9   | a     | 102 | U10  | C41-C39-C40 | 2.54  | 120.21      | 114.60   |
| 9   | L     | 304 | U10  | C10-C9-C11  | 2.54  | 119.54      | 115.27   |
| 8   | s     | 201 | SPO  | C20-C19-C17 | -2.54 | 123.69      | 127.31   |
| 7   | k     | 101 | BCL  | O2D-CGD-O1D | -2.53 | 118.89      | 123.84   |
| 8   | k     | 102 | SPO  | C40-C38-C39 | 2.53  | 120.19      | 114.60   |
| 7   | g     | 101 | BCL  | C1C-NC-C4C  | 2.52  | 107.84      | 106.71   |
| 7   | r     | 101 | BCL  | C2A-C1A-CHA | 2.52  | 128.27      | 123.86   |
| 10  | M     | 403 | BPH  | C2D-C1D-ND  | 2.52  | 111.27      | 109.53   |
| 7   | r     | 101 | BCL  | O2D-CGD-CBD | 2.52  | 115.74      | 111.27   |
| 7   | n     | 100 | BCL  | OBb-CAB-CBB | -2.52 | 114.15      | 119.73   |
| 7   | e     | 100 | BCL  | OBb-CAB-CBB | -2.51 | 114.16      | 119.73   |
| 7   | t     | 101 | BCL  | O2D-CGD-CBD | 2.51  | 115.73      | 111.27   |
| 9   | M     | 405 | U10  | C41-C39-C40 | 2.51  | 120.14      | 114.60   |
| 7   | A     | 101 | BCL  | CBA-CAA-C2A | -2.50 | 106.47      | 113.86   |
| 7   | M     | 402 | BCL  | OBb-CAB-CBB | -2.50 | 114.19      | 119.73   |
| 7   | k     | 101 | BCL  | C2A-C1A-CHA | 2.50  | 128.23      | 123.86   |
| 8   | N     | 201 | SPO  | C40-C38-C39 | 2.50  | 120.12      | 114.60   |
| 7   | N     | 202 | BCL  | O2A-CGA-O1A | 2.50  | 129.90      | 123.59   |
| 7   | A     | 101 | BCL  | CHC-C4B-NB  | -2.50 | 121.61      | 124.26   |
| 7   | K     | 101 | BCL  | CAB-C3B-C2B | 2.50  | 132.08      | 128.34   |
| 7   | M     | 407 | BCL  | CMB-C2B-C1B | -2.50 | 121.57      | 125.37   |
| 7   | D     | 202 | BCL  | C1-C2-C3    | 2.49  | 130.35      | 126.04   |
| 7   | A     | 101 | BCL  | C2A-C1A-CHA | 2.49  | 128.21      | 123.86   |
| 9   | L     | 305 | U10  | C15-C14-C16 | 2.49  | 119.46      | 115.27   |
| 7   | e     | 100 | BCL  | C16-C15-C13 | -2.48 | 107.89      | 115.92   |
| 8   | X     | 201 | SPO  | C21-C22-C23 | -2.48 | 123.77      | 127.31   |
| 7   | M     | 401 | BCL  | C1-O2A-CGA  | 2.48  | 122.95      | 116.44   |
| 7   | S     | 101 | BCL  | CHC-C4B-NB  | -2.48 | 121.63      | 124.26   |
| 8   | j     | 301 | SPO  | C10-C9-C7   | -2.48 | 123.77      | 127.31   |
| 7   | r     | 101 | BCL  | CAB-C3B-C2B | 2.48  | 132.06      | 128.34   |
| 7   | N     | 202 | BCL  | C2A-C1A-CHA | 2.48  | 128.20      | 123.86   |
| 7   | g     | 101 | BCL  | O2D-CGD-CBD | 2.48  | 115.67      | 111.27   |
| 7   | I     | 101 | BCL  | C2A-C1A-CHA | 2.48  | 128.19      | 123.86   |
| 7   | i     | 100 | BCL  | C4A-NA-C1A  | 2.48  | 107.82      | 106.71   |
| 7   | j     | 302 | BCL  | CMB-C2B-C1B | -2.47 | 121.60      | 125.37   |
| 8   | g     | 102 | SPO  | C9-C10-C11  | -2.47 | 115.50      | 123.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | j     | 301 | SPO  | C40-C38-C39 | 2.47  | 120.07      | 114.60   |
| 10  | L     | 302 | BPH  | O2D-CGD-CBD | 2.47  | 114.12      | 111.00   |
| 7   | d     | 101 | BCL  | C4B-C3B-C2B | -2.47 | 104.39      | 108.36   |
| 7   | t     | 103 | BCL  | C4A-NA-C1A  | 2.47  | 107.81      | 106.71   |
| 7   | d     | 101 | BCL  | O2D-CGD-O1D | -2.47 | 119.02      | 123.84   |
| 7   | K     | 101 | BCL  | C2A-C1A-CHA | 2.47  | 128.17      | 123.86   |
| 7   | I     | 101 | BCL  | CHC-C4B-NB  | -2.46 | 121.65      | 124.26   |
| 7   | F     | 103 | BCL  | CAB-C3B-C2B | 2.46  | 132.02      | 128.34   |
| 7   | O     | 101 | BCL  | CHC-C4B-NB  | -2.46 | 121.66      | 124.26   |
| 8   | g     | 102 | SPO  | C40-C38-C39 | 2.45  | 120.03      | 114.60   |
| 7   | e     | 100 | BCL  | CMB-C2B-C1B | -2.45 | 121.63      | 125.37   |
| 7   | E     | 202 | BCL  | CAB-C3B-C2B | 2.45  | 132.01      | 128.34   |
| 9   | a     | 102 | U10  | C32-C33-C34 | -2.45 | 121.75      | 127.66   |
| 7   | t     | 103 | BCL  | C2A-C1A-CHA | 2.45  | 128.15      | 123.86   |
| 7   | k     | 101 | BCL  | OBb-CAB-CBB | -2.45 | 114.30      | 119.73   |
| 8   | I     | 102 | SPO  | C20-C21-C22 | -2.45 | 118.46      | 123.47   |
| 7   | D     | 202 | BCL  | CAB-C3B-C2B | 2.45  | 132.01      | 128.34   |
| 8   | t     | 102 | SPO  | C29-C28-C30 | 2.45  | 119.39      | 115.27   |
| 8   | t     | 102 | SPO  | C31-C32-C33 | -2.45 | 121.77      | 127.66   |
| 7   | L     | 301 | BCL  | CHC-C4B-NB  | -2.44 | 121.67      | 124.26   |
| 8   | r     | 102 | SPO  | C34-C33-C35 | 2.44  | 119.38      | 115.27   |
| 8   | j     | 301 | SPO  | C9-C10-C11  | -2.44 | 115.60      | 123.22   |
| 7   | d     | 101 | BCL  | C1C-NC-C4C  | 2.44  | 107.80      | 106.71   |
| 9   | L     | 303 | U10  | C26-C24-C25 | 2.43  | 119.97      | 114.60   |
| 9   | M     | 405 | U10  | C32-C33-C34 | -2.43 | 121.80      | 127.66   |
| 8   | s     | 201 | SPO  | C40-C38-C39 | 2.43  | 119.97      | 114.60   |
| 8   | X     | 201 | SPO  | C40-C38-C39 | 2.43  | 119.97      | 114.60   |
| 7   | F     | 103 | BCL  | C1C-NC-C4C  | 2.42  | 107.80      | 106.71   |
| 7   | o     | 100 | BCL  | C4B-C3B-C2B | -2.42 | 104.46      | 108.36   |
| 7   | j     | 302 | BCL  | C2A-C1A-CHA | 2.42  | 128.09      | 123.86   |
| 7   | u     | 101 | BCL  | CHC-C4B-NB  | -2.42 | 121.69      | 124.26   |
| 10  | L     | 302 | BPH  | CMB-C2B-C3B | 2.42  | 129.20      | 124.68   |
| 7   | n     | 100 | BCL  | CED-O2D-CGD | -2.42 | 110.47      | 115.94   |
| 7   | i     | 100 | BCL  | C2A-C1A-CHA | 2.42  | 128.08      | 123.86   |
| 7   | M     | 401 | BCL  | CHC-C4B-NB  | -2.41 | 121.70      | 124.26   |
| 7   | d     | 101 | BCL  | CAB-C3B-C2B | 2.41  | 131.95      | 128.34   |
| 7   | b     | 101 | BCL  | OBb-CAB-CBB | -2.41 | 114.39      | 119.73   |
| 8   | k     | 102 | SPO  | C21-C20-C19 | -2.41 | 118.54      | 123.47   |
| 7   | j     | 303 | BCL  | C2A-C1A-CHA | 2.41  | 128.07      | 123.86   |
| 7   | M     | 407 | BCL  | OBb-CAB-CBB | -2.40 | 114.40      | 119.73   |
| 8   | E     | 201 | SPO  | C29-C28-C30 | 2.40  | 119.31      | 115.27   |
| 7   | i     | 100 | BCL  | CED-O2D-CGD | -2.40 | 110.50      | 115.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | b     | 101 | BCL  | CAA-C2A-C1A | 2.40  | 119.85      | 111.97   |
| 7   | t     | 103 | BCL  | CAB-C3B-C2B | 2.40  | 131.94      | 128.34   |
| 9   | M     | 408 | U10  | C11-C9-C10  | 2.40  | 119.91      | 114.60   |
| 7   | K     | 101 | BCL  | CHC-C4B-NB  | -2.40 | 121.72      | 124.26   |
| 7   | I     | 101 | BCL  | C1C-NC-C4C  | 2.40  | 107.78      | 106.71   |
| 7   | j     | 303 | BCL  | CHC-C4B-NB  | -2.40 | 121.72      | 124.26   |
| 7   | b     | 101 | BCL  | C1-C2-C3    | -2.40 | 121.90      | 126.04   |
| 7   | N     | 202 | BCL  | CAB-C3B-C2B | 2.40  | 131.93      | 128.34   |
| 7   | M     | 407 | BCL  | C4A-NA-C1A  | 2.40  | 107.78      | 106.71   |
| 10  | L     | 306 | BPH  | CMD-C2D-C3D | 2.40  | 129.16      | 124.68   |
| 7   | u     | 102 | BCL  | C2A-C1A-CHA | 2.39  | 128.05      | 123.86   |
| 7   | F     | 103 | BCL  | C2A-C1A-CHA | 2.39  | 128.04      | 123.86   |
| 7   | k     | 101 | BCL  | C6-C7-C8    | -2.39 | 108.19      | 115.92   |
| 7   | s     | 202 | BCL  | CMB-C2B-C1B | -2.39 | 121.73      | 125.37   |
| 8   | t     | 102 | SPO  | C10-C11-C12 | -2.39 | 119.71      | 126.42   |
| 7   | N     | 202 | BCL  | CHC-C4B-NB  | -2.39 | 121.73      | 124.26   |
| 7   | b     | 102 | BCL  | CHC-C4B-NB  | -2.38 | 121.73      | 124.26   |
| 7   | n     | 100 | BCL  | O2D-CGD-O1D | -2.38 | 119.18      | 123.84   |
| 8   | I     | 102 | SPO  | C18-C17-C19 | -2.38 | 119.59      | 122.92   |
| 7   | t     | 103 | BCL  | CHC-C4B-NB  | -2.38 | 121.74      | 124.26   |
| 7   | r     | 101 | BCL  | O2D-CGD-O1D | -2.38 | 119.19      | 123.84   |
| 8   | r     | 103 | SPO  | C40-C38-C39 | 2.37  | 119.85      | 114.60   |
| 7   | D     | 202 | BCL  | C2A-C1A-CHA | 2.37  | 128.01      | 123.86   |
| 7   | r     | 101 | BCL  | CMB-C2B-C1B | -2.37 | 121.76      | 125.37   |
| 7   | u     | 101 | BCL  | O2D-CGD-CBD | 2.37  | 115.48      | 111.27   |
| 7   | s     | 202 | BCL  | OBB-CAB-CBB | -2.37 | 114.49      | 119.73   |
| 7   | j     | 302 | BCL  | C16-C15-C13 | 2.36  | 123.55      | 115.92   |
| 7   | b     | 102 | BCL  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 7   | s     | 202 | BCL  | C4B-C3B-C2B | -2.36 | 104.56      | 108.36   |
| 7   | t     | 101 | BCL  | C1C-NC-C4C  | 2.36  | 107.77      | 106.71   |
| 8   | X     | 201 | SPO  | C14-C15-C16 | -2.36 | 115.86      | 123.22   |
| 7   | n     | 100 | BCL  | C4B-C3B-C2B | -2.35 | 104.58      | 108.36   |
| 8   | s     | 201 | SPO  | C36-C37-C38 | -2.35 | 119.72      | 127.75   |
| 7   | D     | 202 | BCL  | C1C-NC-C4C  | 2.34  | 107.76      | 106.71   |
| 8   | F     | 102 | SPO  | C40-C38-C39 | 2.34  | 119.77      | 114.60   |
| 8   | N     | 201 | SPO  | C6-C7-C9    | -2.34 | 115.35      | 118.94   |
| 7   | M     | 407 | BCL  | CAB-C3B-C2B | 2.34  | 131.84      | 128.34   |
| 10  | L     | 306 | BPH  | CMB-C2B-C3B | 2.34  | 129.05      | 124.68   |
| 9   | M     | 405 | U10  | C4M-O4-C4   | 2.34  | 124.74      | 116.47   |
| 9   | L     | 305 | U10  | C7-C8-C9    | -2.33 | 122.91      | 126.79   |
| 7   | a     | 101 | BCL  | CHC-C4B-NB  | -2.33 | 121.79      | 124.26   |
| 7   | t     | 103 | BCL  | C1C-NC-C4C  | 2.32  | 107.75      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | O     | 101 | BCL  | C4A-NA-C1A  | 2.32  | 107.75      | 106.71   |
| 7   | i     | 100 | BCL  | C4B-C3B-C2B | -2.32 | 104.62      | 108.36   |
| 7   | e     | 100 | BCL  | C4B-C3B-C2B | -2.32 | 104.63      | 108.36   |
| 7   | g     | 101 | BCL  | O2D-CGD-O1D | -2.32 | 119.31      | 123.84   |
| 7   | r     | 101 | BCL  | C4B-C3B-C2B | -2.31 | 104.64      | 108.36   |
| 8   | r     | 102 | SPO  | C40-C38-C39 | 2.31  | 119.71      | 114.60   |
| 7   | g     | 101 | BCL  | OBb-CAB-CBB | -2.31 | 114.61      | 119.73   |
| 8   | F     | 102 | SPO  | C18-C17-C19 | -2.31 | 119.68      | 122.92   |
| 8   | r     | 102 | SPO  | C11-C12-C14 | 2.31  | 122.49      | 118.94   |
| 7   | N     | 202 | BCL  | C1C-NC-C4C  | 2.31  | 107.74      | 106.71   |
| 7   | M     | 402 | BCL  | CED-O2D-CGD | 2.31  | 121.16      | 115.94   |
| 7   | O     | 101 | BCL  | C1-C2-C3    | 2.31  | 130.03      | 126.04   |
| 7   | j     | 302 | BCL  | CED-O2D-CGD | -2.31 | 110.72      | 115.94   |
| 7   | u     | 102 | BCL  | CHC-C4B-NB  | -2.30 | 121.82      | 124.26   |
| 7   | F     | 101 | BCL  | OBb-CAB-CBB | -2.30 | 114.63      | 119.73   |
| 7   | F     | 101 | BCL  | C4B-C3B-C2B | -2.30 | 104.66      | 108.36   |
| 9   | L     | 303 | U10  | C12-C13-C14 | -2.30 | 122.12      | 127.66   |
| 7   | E     | 202 | BCL  | C2A-C1A-CHA | 2.30  | 127.88      | 123.86   |
| 8   | I     | 102 | SPO  | C24-C23-C22 | -2.29 | 119.71      | 122.92   |
| 7   | k     | 101 | BCL  | C4B-C3B-C2B | -2.29 | 104.67      | 108.36   |
| 7   | j     | 302 | BCL  | C4B-C3B-C2B | -2.29 | 104.67      | 108.36   |
| 7   | i     | 100 | BCL  | OBb-CAB-CBB | -2.29 | 114.65      | 119.73   |
| 7   | r     | 101 | BCL  | OBb-CAB-CBB | -2.29 | 114.66      | 119.73   |
| 7   | N     | 202 | BCL  | OBb-CAB-CBB | -2.29 | 114.66      | 119.73   |
| 7   | g     | 101 | BCL  | C4B-C3B-C2B | -2.29 | 104.68      | 108.36   |
| 7   | b     | 101 | BCL  | C4B-C3B-C2B | -2.29 | 104.68      | 108.36   |
| 7   | D     | 202 | BCL  | O2D-CGD-O1D | -2.28 | 119.37      | 123.84   |
| 10  | L     | 306 | BPH  | CBA-CAA-C2A | 2.28  | 120.48      | 113.81   |
| 7   | i     | 100 | BCL  | O2D-CGD-O1D | -2.28 | 119.38      | 123.84   |
| 7   | L     | 301 | BCL  | C4B-C3B-C2B | -2.28 | 104.70      | 108.36   |
| 7   | M     | 401 | BCL  | C11-C12-C13 | -2.28 | 108.56      | 115.92   |
| 7   | o     | 100 | BCL  | CAB-C3B-C2B | 2.27  | 131.74      | 128.34   |
| 8   | D     | 201 | SPO  | C26-C25-C23 | 2.27  | 132.79      | 126.42   |
| 7   | S     | 101 | BCL  | C2A-C1A-CHA | 2.27  | 127.82      | 123.86   |
| 8   | I     | 102 | SPO  | C13-C12-C11 | 2.27  | 121.65      | 118.08   |
| 9   | L     | 304 | U10  | C31-C29-C30 | 2.27  | 119.61      | 114.60   |
| 7   | M     | 402 | BCL  | C4B-C3B-C2B | -2.27 | 104.72      | 108.36   |
| 7   | L     | 301 | BCL  | OBb-CAB-CBB | -2.26 | 114.71      | 119.73   |
| 7   | t     | 101 | BCL  | C4B-C3B-C2B | -2.26 | 104.72      | 108.36   |
| 8   | g     | 102 | SPO  | C8-C7-C6    | 2.26  | 121.64      | 118.08   |
| 8   | X     | 201 | SPO  | O1-C1-C3    | -2.26 | 93.41       | 108.97   |
| 10  | L     | 302 | BPH  | CMD-C2D-C3D | 2.26  | 128.91      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | G     | 101 | BCL  | C4A-NA-C1A  | 2.26  | 107.72      | 106.71   |
| 9   | a     | 102 | U10  | C7-C8-C9    | -2.26 | 123.03      | 126.79   |
| 7   | t     | 101 | BCL  | CMB-C2B-C1B | -2.26 | 121.93      | 125.37   |
| 7   | D     | 202 | BCL  | C4B-C3B-C2B | -2.25 | 104.73      | 108.36   |
| 10  | L     | 302 | BPH  | CAC-C3C-C2C | -2.25 | 108.63      | 114.26   |
| 7   | O     | 101 | BCL  | CAB-C3B-C2B | 2.25  | 131.71      | 128.34   |
| 8   | I     | 102 | SPO  | C8-C7-C6    | 2.25  | 121.62      | 118.08   |
| 7   | F     | 103 | BCL  | C4B-C3B-C2B | -2.25 | 104.75      | 108.36   |
| 8   | F     | 102 | SPO  | C13-C12-C11 | 2.24  | 121.61      | 118.08   |
| 8   | t     | 102 | SPO  | C18-C17-C19 | -2.24 | 119.78      | 122.92   |
| 7   | t     | 101 | BCL  | OBB-CAB-CBB | -2.24 | 114.77      | 119.73   |
| 7   | j     | 303 | BCL  | CMB-C2B-C1B | -2.23 | 121.97      | 125.37   |
| 7   | d     | 101 | BCL  | C2D-C1D-ND  | 2.23  | 111.75      | 110.10   |
| 7   | k     | 101 | BCL  | CMB-C2B-C1B | -2.23 | 121.97      | 125.37   |
| 7   | j     | 302 | BCL  | OBB-CAB-CBB | -2.23 | 114.79      | 119.73   |
| 7   | F     | 103 | BCL  | CMB-C2B-C1B | -2.23 | 121.98      | 125.37   |
| 7   | I     | 101 | BCL  | OBB-CAB-CBB | -2.23 | 114.80      | 119.73   |
| 9   | L     | 303 | U10  | C22-C23-C24 | -2.22 | 120.15      | 127.75   |
| 8   | g     | 102 | SPO  | C36-C37-C38 | -2.22 | 120.16      | 127.75   |
| 7   | O     | 101 | BCL  | CMB-C2B-C1B | -2.22 | 121.99      | 125.37   |
| 8   | t     | 102 | SPO  | C6-C7-C9    | 2.22  | 122.34      | 118.94   |
| 7   | o     | 100 | BCL  | OBB-CAB-CBB | -2.22 | 114.82      | 119.73   |
| 7   | K     | 101 | BCL  | O2D-CGD-O1D | -2.21 | 119.52      | 123.84   |
| 7   | E     | 202 | BCL  | C4B-C3B-C2B | -2.21 | 104.80      | 108.36   |
| 7   | E     | 202 | BCL  | CMB-C2B-C1B | -2.21 | 122.01      | 125.37   |
| 8   | N     | 201 | SPO  | C36-C37-C38 | -2.21 | 120.20      | 127.75   |
| 9   | a     | 102 | U10  | C37-C38-C39 | -2.21 | 120.21      | 127.75   |
| 10  | M     | 403 | BPH  | CMD-C2D-C3D | 2.20  | 128.80      | 124.68   |
| 7   | E     | 202 | BCL  | OBB-CAB-CBB | -2.20 | 114.85      | 119.73   |
| 8   | j     | 301 | SPO  | C20-C21-C22 | 2.20  | 127.99      | 123.47   |
| 7   | M     | 402 | BCL  | C6-C7-C8    | -2.20 | 108.80      | 115.92   |
| 7   | a     | 101 | BCL  | CMB-C2B-C1B | -2.20 | 122.02      | 125.37   |
| 8   | D     | 201 | SPO  | C13-C12-C11 | 2.20  | 121.54      | 118.08   |
| 7   | I     | 101 | BCL  | CMB-C2B-C1B | -2.19 | 122.03      | 125.37   |
| 7   | a     | 101 | BCL  | C4B-C3B-C2B | -2.19 | 104.84      | 108.36   |
| 7   | K     | 101 | BCL  | C1C-NC-C4C  | 2.18  | 107.69      | 106.71   |
| 7   | D     | 202 | BCL  | OBB-CAB-CBB | -2.18 | 114.90      | 119.73   |
| 7   | I     | 101 | BCL  | C4B-C3B-C2B | -2.18 | 104.86      | 108.36   |
| 7   | G     | 101 | BCL  | O2D-CGD-O1D | -2.17 | 119.59      | 123.84   |
| 7   | k     | 101 | BCL  | C1C-NC-C4C  | 2.17  | 107.68      | 106.71   |
| 7   | L     | 301 | BCL  | CMB-C2B-C1B | -2.17 | 122.06      | 125.37   |
| 8   | j     | 301 | SPO  | C36-C37-C38 | -2.17 | 120.35      | 127.75   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | j     | 303 | BCL  | OBB-CAB-CBB | -2.16 | 114.94      | 119.73   |
| 8   | X     | 201 | SPO  | C36-C37-C38 | -2.16 | 120.37      | 127.75   |
| 9   | L     | 304 | U10  | C25-C24-C23 | -2.16 | 118.15      | 123.68   |
| 7   | M     | 401 | BCL  | C1-C2-C3    | -2.15 | 122.32      | 126.04   |
| 7   | F     | 101 | BCL  | CAB-C3B-C2B | 2.15  | 131.56      | 128.34   |
| 9   | L     | 304 | U10  | C20-C19-C18 | -2.15 | 118.17      | 123.68   |
| 10  | L     | 302 | BPH  | OBB-CAB-C3B | 2.14  | 123.79      | 119.99   |
| 7   | b     | 102 | BCL  | C2A-C1A-CHA | 2.14  | 127.60      | 123.86   |
| 7   | u     | 101 | BCL  | OBB-CAB-CBB | -2.14 | 114.99      | 119.73   |
| 8   | t     | 102 | SPO  | C1-C4-C5    | -2.14 | 107.38      | 113.06   |
| 7   | M     | 407 | BCL  | C4B-C3B-C2B | -2.14 | 104.92      | 108.36   |
| 7   | G     | 101 | BCL  | C4B-C3B-C2B | -2.14 | 104.92      | 108.36   |
| 8   | t     | 102 | SPO  | C11-C12-C14 | 2.14  | 122.22      | 118.94   |
| 7   | R     | 101 | BCL  | O2D-CGD-O1D | -2.14 | 119.66      | 123.84   |
| 8   | j     | 301 | SPO  | C13-C12-C14 | -2.14 | 119.93      | 122.92   |
| 7   | M     | 402 | BCL  | CMB-C2B-C1B | -2.13 | 122.12      | 125.37   |
| 9   | M     | 405 | U10  | O5-C5-C6    | -2.13 | 117.82      | 121.55   |
| 9   | L     | 304 | U10  | C27-C28-C29 | -2.13 | 120.47      | 127.75   |
| 8   | r     | 102 | SPO  | C29-C28-C27 | -2.13 | 117.11      | 122.59   |
| 8   | E     | 201 | SPO  | C14-C15-C16 | 2.13  | 129.85      | 123.22   |
| 8   | I     | 102 | SPO  | C14-C15-C16 | -2.12 | 116.59      | 123.22   |
| 8   | M     | 406 | SPO  | C40-C38-C39 | 2.12  | 119.30      | 114.60   |
| 7   | F     | 103 | BCL  | OBB-CAB-CBB | -2.12 | 115.02      | 119.73   |
| 12  | H     | 302 | 3PE  | C2-O21-C21  | -2.12 | 112.56      | 117.79   |
| 7   | j     | 303 | BCL  | C4B-C3B-C2B | -2.12 | 104.94      | 108.36   |
| 7   | A     | 101 | BCL  | CAB-C3B-C2B | 2.12  | 131.52      | 128.34   |
| 7   | n     | 100 | BCL  | C2D-C1D-ND  | 2.12  | 111.67      | 110.10   |
| 7   | j     | 302 | BCL  | O2D-CGD-O1D | -2.12 | 119.70      | 123.84   |
| 10  | L     | 302 | BPH  | C2D-C1D-ND  | 2.12  | 110.99      | 109.53   |
| 7   | L     | 301 | BCL  | CED-O2D-CGD | 2.11  | 120.71      | 115.94   |
| 7   | A     | 101 | BCL  | CMB-C2B-C1B | -2.11 | 122.16      | 125.37   |
| 8   | E     | 201 | SPO  | C34-C33-C32 | -2.11 | 118.27      | 123.68   |
| 7   | M     | 401 | BCL  | OBB-CAB-CBB | -2.11 | 115.06      | 119.73   |
| 8   | g     | 102 | SPO  | C26-C25-C23 | -2.11 | 120.49      | 126.42   |
| 7   | N     | 202 | BCL  | CMB-C2B-C1B | -2.11 | 122.16      | 125.37   |
| 9   | a     | 102 | U10  | O5-C5-C4    | -2.11 | 116.46      | 120.93   |
| 7   | R     | 101 | BCL  | C4B-C3B-C2B | -2.11 | 104.97      | 108.36   |
| 7   | O     | 101 | BCL  | C4B-C3B-C2B | -2.11 | 104.97      | 108.36   |
| 7   | G     | 101 | BCL  | C16-C15-C13 | -2.10 | 109.11      | 115.92   |
| 7   | b     | 101 | BCL  | C1C-NC-C4C  | 2.10  | 107.65      | 106.71   |
| 7   | A     | 101 | BCL  | O2D-CGD-O1D | -2.10 | 119.74      | 123.84   |
| 7   | M     | 401 | BCL  | C4A-NA-C1A  | 2.09  | 107.65      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | O     | 101 | BCL  | OBB-CAB-CBB | -2.09 | 115.10      | 119.73   |
| 7   | j     | 303 | BCL  | C4-C3-C5    | -2.09 | 111.75      | 115.27   |
| 7   | N     | 202 | BCL  | C4B-C3B-C2B | -2.09 | 105.00      | 108.36   |
| 8   | X     | 201 | SPO  | C20-C21-C22 | -2.09 | 119.20      | 123.47   |
| 7   | b     | 102 | BCL  | C4B-C3B-C2B | -2.08 | 105.01      | 108.36   |
| 8   | t     | 102 | SPO  | C8-C7-C9    | -2.08 | 120.00      | 122.92   |
| 7   | u     | 101 | BCL  | C4B-C3B-C2B | -2.08 | 105.01      | 108.36   |
| 7   | S     | 101 | BCL  | C4B-C3B-C2B | -2.07 | 105.03      | 108.36   |
| 8   | M     | 406 | SPO  | C36-C37-C38 | -2.07 | 120.68      | 127.75   |
| 7   | j     | 302 | BCL  | C1C-NC-C4C  | 2.07  | 107.64      | 106.71   |
| 8   | r     | 103 | SPO  | C13-C12-C11 | 2.07  | 121.33      | 118.08   |
| 8   | X     | 201 | SPO  | C29-C28-C30 | 2.06  | 118.74      | 115.27   |
| 7   | a     | 101 | BCL  | C11-C10-C8  | -2.06 | 109.26      | 115.92   |
| 8   | s     | 201 | SPO  | C1-C4-C5    | 2.06  | 118.52      | 113.06   |
| 7   | K     | 101 | BCL  | OBB-CAB-CBB | -2.06 | 115.17      | 119.73   |
| 8   | I     | 102 | SPO  | C40-C38-C39 | 2.06  | 119.15      | 114.60   |
| 8   | k     | 102 | SPO  | C36-C37-C38 | -2.06 | 120.72      | 127.75   |
| 7   | R     | 101 | BCL  | OBB-CAB-CBB | -2.06 | 115.17      | 119.73   |
| 7   | S     | 101 | BCL  | CMB-C2B-C1B | -2.05 | 122.24      | 125.37   |
| 8   | r     | 102 | SPO  | C20-C21-C22 | 2.05  | 127.68      | 123.47   |
| 7   | r     | 101 | BCL  | C2D-C1D-ND  | 2.05  | 111.62      | 110.10   |
| 8   | s     | 201 | SPO  | C34-C33-C35 | 2.05  | 118.72      | 115.27   |
| 7   | t     | 103 | BCL  | C4B-C3B-C2B | -2.05 | 105.06      | 108.36   |
| 7   | G     | 101 | BCL  | CMB-C2B-C1B | -2.04 | 122.26      | 125.37   |
| 7   | t     | 101 | BCL  | C6-C5-C3    | 2.04  | 118.81      | 113.45   |
| 8   | k     | 102 | SPO  | C10-C11-C12 | -2.04 | 120.68      | 126.42   |
| 7   | M     | 402 | BCL  | CHD-C1D-C2D | 2.04  | 129.76      | 125.48   |
| 8   | s     | 201 | SPO  | C29-C28-C30 | 2.04  | 118.70      | 115.27   |
| 7   | t     | 101 | BCL  | O2D-CGD-O1D | -2.04 | 119.86      | 123.84   |
| 8   | s     | 201 | SPO  | C26-C25-C23 | -2.03 | 120.70      | 126.42   |
| 8   | r     | 102 | SPO  | C34-C33-C32 | -2.03 | 118.46      | 123.68   |
| 7   | a     | 101 | BCL  | OBB-CAB-CBB | -2.03 | 115.23      | 119.73   |
| 7   | G     | 101 | BCL  | OBB-CAB-CBB | -2.03 | 115.23      | 119.73   |
| 7   | M     | 401 | BCL  | C4B-C3B-C2B | -2.03 | 105.10      | 108.36   |
| 8   | M     | 406 | SPO  | C1-C4-C5    | -2.03 | 107.69      | 113.06   |
| 8   | I     | 102 | SPO  | C9-C10-C11  | -2.03 | 116.89      | 123.22   |
| 7   | b     | 101 | BCL  | C17-C16-C15 | -2.03 | 103.93      | 113.24   |
| 8   | F     | 102 | SPO  | C13-C12-C14 | -2.03 | 120.09      | 122.92   |
| 7   | s     | 202 | BCL  | C6-C7-C8    | 2.02  | 122.45      | 115.92   |
| 8   | N     | 201 | SPO  | C10-C11-C12 | -2.02 | 120.74      | 126.42   |
| 8   | g     | 102 | SPO  | C6-C7-C9    | -2.02 | 115.85      | 118.94   |
| 9   | a     | 102 | U10  | C22-C23-C24 | -2.01 | 122.82      | 127.66   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | o     | 100 | BCL  | C6-C5-C3    | 2.01  | 118.73      | 113.45   |
| 7   | u     | 101 | BCL  | C4D-C3D-CAD | -2.01 | 105.73      | 108.10   |
| 7   | F     | 103 | BCL  | O2D-CGD-O1D | -2.01 | 119.92      | 123.84   |
| 8   | B     | 101 | SPO  | C30-C31-C32 | -2.01 | 105.29      | 111.88   |
| 8   | B     | 101 | SPO  | C18-C17-C16 | 2.01  | 121.24      | 118.08   |
| 8   | D     | 201 | SPO  | C27-C26-C25 | 2.00  | 129.47      | 123.22   |
| 7   | u     | 101 | BCL  | C2D-C1D-ND  | 2.00  | 111.58      | 110.10   |

There are no chirality outliers.

All (611) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | N     | 202 | BCL  | C2-C1-O2A-CGA   |
| 7   | O     | 101 | BCL  | O2A-C1-C2-C3    |
| 7   | b     | 101 | BCL  | C2-C1-O2A-CGA   |
| 7   | u     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 7   | u     | 102 | BCL  | O2A-C1-C2-C3    |
| 7   | R     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | n     | 100 | BCL  | C2-C3-C5-C6     |
| 7   | n     | 100 | BCL  | C4-C3-C5-C6     |
| 7   | G     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 8   | N     | 201 | SPO  | C4-C1-O1-CM1    |
| 8   | N     | 201 | SPO  | O1-C1-C4-C5     |
| 8   | N     | 201 | SPO  | C2-C1-C4-C5     |
| 8   | N     | 201 | SPO  | C1-C4-C5-C6     |
| 8   | N     | 201 | SPO  | C5-C6-C7-C8     |
| 8   | N     | 201 | SPO  | C5-C6-C7-C9     |
| 8   | N     | 201 | SPO  | C11-C10-C9-C7   |
| 8   | N     | 201 | SPO  | C10-C11-C12-C13 |
| 8   | N     | 201 | SPO  | C27-C28-C30-C31 |
| 8   | N     | 201 | SPO  | C29-C28-C30-C31 |
| 8   | t     | 102 | SPO  | C3-C1-C4-C5     |
| 8   | t     | 102 | SPO  | C15-C16-C17-C18 |
| 8   | t     | 102 | SPO  | C15-C16-C17-C19 |
| 8   | t     | 102 | SPO  | C22-C23-C25-C26 |
| 8   | t     | 102 | SPO  | C24-C23-C25-C26 |
| 8   | t     | 102 | SPO  | C25-C26-C27-C28 |
| 8   | t     | 102 | SPO  | C33-C35-C36-C37 |
| 8   | r     | 102 | SPO  | C3-C1-O1-CM1    |
| 8   | r     | 102 | SPO  | O1-C1-C4-C5     |
| 8   | r     | 102 | SPO  | C10-C11-C12-C13 |
| 8   | r     | 102 | SPO  | C10-C11-C12-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | r     | 102 | SPO  | C12-C14-C15-C16 |
| 8   | r     | 102 | SPO  | C20-C21-C22-C23 |
| 8   | r     | 102 | SPO  | C22-C23-C25-C26 |
| 8   | r     | 102 | SPO  | C24-C23-C25-C26 |
| 8   | r     | 103 | SPO  | C4-C1-O1-CM1    |
| 8   | r     | 103 | SPO  | C3-C1-C4-C5     |
| 8   | r     | 103 | SPO  | C5-C6-C7-C8     |
| 8   | r     | 103 | SPO  | C5-C6-C7-C9     |
| 8   | r     | 103 | SPO  | C10-C11-C12-C13 |
| 8   | r     | 103 | SPO  | C10-C11-C12-C14 |
| 8   | D     | 201 | SPO  | C2-C1-C4-C5     |
| 8   | D     | 201 | SPO  | C3-C1-C4-C5     |
| 8   | D     | 201 | SPO  | C1-C4-C5-C6     |
| 8   | D     | 201 | SPO  | C5-C6-C7-C8     |
| 8   | D     | 201 | SPO  | C5-C6-C7-C9     |
| 8   | k     | 102 | SPO  | C2-C1-C4-C5     |
| 8   | k     | 102 | SPO  | C3-C1-C4-C5     |
| 8   | k     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | k     | 102 | SPO  | C5-C6-C7-C8     |
| 8   | k     | 102 | SPO  | C5-C6-C7-C9     |
| 8   | k     | 102 | SPO  | C11-C10-C9-C7   |
| 8   | k     | 102 | SPO  | C10-C11-C12-C13 |
| 8   | k     | 102 | SPO  | C10-C11-C12-C14 |
| 8   | k     | 102 | SPO  | C15-C16-C17-C18 |
| 8   | k     | 102 | SPO  | C15-C16-C17-C19 |
| 8   | k     | 102 | SPO  | C22-C23-C25-C26 |
| 8   | k     | 102 | SPO  | C24-C23-C25-C26 |
| 8   | E     | 201 | SPO  | C15-C16-C17-C18 |
| 8   | E     | 201 | SPO  | C15-C16-C17-C19 |
| 8   | E     | 201 | SPO  | C20-C21-C22-C23 |
| 8   | E     | 201 | SPO  | C33-C35-C36-C37 |
| 8   | X     | 201 | SPO  | C4-C1-O1-CM1    |
| 8   | X     | 201 | SPO  | C3-C1-C4-C5     |
| 8   | X     | 201 | SPO  | C1-C4-C5-C6     |
| 8   | X     | 201 | SPO  | C10-C11-C12-C13 |
| 8   | X     | 201 | SPO  | C27-C28-C30-C31 |
| 8   | X     | 201 | SPO  | C29-C28-C30-C31 |
| 8   | X     | 201 | SPO  | C33-C35-C36-C37 |
| 8   | s     | 201 | SPO  | C4-C1-O1-CM1    |
| 8   | s     | 201 | SPO  | O1-C1-C4-C5     |
| 8   | s     | 201 | SPO  | C5-C6-C7-C8     |
| 8   | s     | 201 | SPO  | C5-C6-C7-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | s     | 201 | SPO  | C17-C19-C20-C21 |
| 8   | s     | 201 | SPO  | C27-C28-C30-C31 |
| 8   | s     | 201 | SPO  | C29-C28-C30-C31 |
| 8   | j     | 301 | SPO  | C4-C1-O1-CM1    |
| 8   | j     | 301 | SPO  | C2-C1-C4-C5     |
| 8   | j     | 301 | SPO  | C3-C1-C4-C5     |
| 8   | j     | 301 | SPO  | C22-C23-C25-C26 |
| 8   | j     | 301 | SPO  | C24-C23-C25-C26 |
| 8   | j     | 301 | SPO  | C32-C33-C35-C36 |
| 8   | j     | 301 | SPO  | C34-C33-C35-C36 |
| 8   | I     | 102 | SPO  | C4-C1-O1-CM1    |
| 8   | I     | 102 | SPO  | O1-C1-C4-C5     |
| 8   | I     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | I     | 102 | SPO  | C5-C6-C7-C8     |
| 8   | I     | 102 | SPO  | C5-C6-C7-C9     |
| 8   | I     | 102 | SPO  | C10-C11-C12-C13 |
| 8   | I     | 102 | SPO  | C10-C11-C12-C14 |
| 8   | I     | 102 | SPO  | C15-C16-C17-C18 |
| 8   | I     | 102 | SPO  | C15-C16-C17-C19 |
| 8   | M     | 406 | SPO  | C4-C1-O1-CM1    |
| 8   | M     | 406 | SPO  | C1-C4-C5-C6     |
| 8   | M     | 406 | SPO  | C12-C14-C15-C16 |
| 8   | M     | 406 | SPO  | C15-C16-C17-C18 |
| 8   | M     | 406 | SPO  | C15-C16-C17-C19 |
| 8   | M     | 406 | SPO  | C27-C28-C30-C31 |
| 8   | M     | 406 | SPO  | C29-C28-C30-C31 |
| 8   | g     | 102 | SPO  | C4-C1-O1-CM1    |
| 8   | g     | 102 | SPO  | O1-C1-C4-C5     |
| 8   | g     | 102 | SPO  | C5-C6-C7-C8     |
| 8   | g     | 102 | SPO  | C5-C6-C7-C9     |
| 8   | g     | 102 | SPO  | C15-C16-C17-C18 |
| 8   | g     | 102 | SPO  | C15-C16-C17-C19 |
| 8   | F     | 102 | SPO  | C4-C1-O1-CM1    |
| 8   | F     | 102 | SPO  | C11-C10-C9-C7   |
| 8   | F     | 102 | SPO  | C12-C14-C15-C16 |
| 8   | B     | 101 | SPO  | C5-C6-C7-C8     |
| 8   | B     | 101 | SPO  | C5-C6-C7-C9     |
| 8   | B     | 101 | SPO  | C15-C16-C17-C18 |
| 8   | B     | 101 | SPO  | C15-C16-C17-C19 |
| 8   | B     | 101 | SPO  | C27-C28-C30-C31 |
| 8   | B     | 101 | SPO  | C29-C28-C30-C31 |
| 8   | B     | 101 | SPO  | C32-C33-C35-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | B     | 101 | SPO  | C34-C33-C35-C36 |
| 9   | a     | 102 | U10  | C32-C33-C34-C35 |
| 9   | a     | 102 | U10  | C34-C36-C37-C38 |
| 9   | L     | 303 | U10  | C9-C11-C12-C13  |
| 9   | L     | 303 | U10  | C12-C13-C14-C15 |
| 9   | L     | 303 | U10  | C12-C13-C14-C16 |
| 9   | L     | 304 | U10  | C7-C8-C9-C10    |
| 9   | L     | 304 | U10  | C7-C8-C9-C11    |
| 9   | L     | 304 | U10  | C14-C16-C17-C18 |
| 9   | L     | 304 | U10  | C22-C23-C24-C25 |
| 9   | L     | 304 | U10  | C22-C23-C24-C26 |
| 9   | L     | 304 | U10  | C25-C24-C26-C27 |
| 9   | L     | 304 | U10  | C27-C28-C29-C30 |
| 9   | L     | 305 | U10  | C12-C13-C14-C15 |
| 9   | L     | 305 | U10  | C12-C13-C14-C16 |
| 9   | L     | 305 | U10  | C14-C16-C17-C18 |
| 9   | M     | 405 | U10  | C22-C23-C24-C25 |
| 9   | M     | 405 | U10  | C22-C23-C24-C26 |
| 12  | H     | 301 | 3PE  | O32-C31-O31-C3  |
| 12  | H     | 301 | 3PE  | C32-C31-O31-C3  |
| 12  | H     | 302 | 3PE  | O13-C11-C12-N   |
| 12  | H     | 302 | 3PE  | O11-C1-C2-O21   |
| 12  | d     | 102 | 3PE  | C1-O11-P-O13    |
| 12  | d     | 102 | 3PE  | C11-O13-P-O11   |
| 12  | d     | 102 | 3PE  | C11-O13-P-O14   |
| 12  | d     | 102 | 3PE  | O22-C21-O21-C2  |
| 12  | d     | 102 | 3PE  | C22-C21-O21-C2  |
| 9   | L     | 304 | U10  | C27-C28-C29-C31 |
| 9   | M     | 408 | U10  | C7-C8-C9-C11    |
| 7   | d     | 101 | BCL  | C3-C5-C6-C7     |
| 9   | L     | 305 | U10  | C17-C18-C19-C21 |
| 9   | M     | 408 | U10  | C7-C8-C9-C10    |
| 12  | H     | 302 | 3PE  | O32-C31-O31-C3  |
| 7   | b     | 101 | BCL  | C4-C3-C5-C6     |
| 7   | k     | 101 | BCL  | C4-C3-C5-C6     |
| 7   | G     | 101 | BCL  | C4-C3-C5-C6     |
| 7   | I     | 101 | BCL  | C4-C3-C5-C6     |
| 9   | M     | 405 | U10  | C35-C34-C36-C37 |
| 7   | t     | 103 | BCL  | C2A-CAA-CBA-CGA |
| 7   | O     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 7   | E     | 202 | BCL  | C2A-CAA-CBA-CGA |
| 7   | F     | 103 | BCL  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | M     | 405 | U10  | C17-C18-C19-C20 |
| 9   | a     | 102 | U10  | C32-C33-C34-C36 |
| 9   | M     | 405 | U10  | C17-C18-C19-C21 |
| 8   | r     | 103 | SPO  | C25-C26-C27-C28 |
| 8   | E     | 201 | SPO  | C17-C19-C20-C21 |
| 8   | s     | 201 | SPO  | C12-C14-C15-C16 |
| 8   | s     | 201 | SPO  | C20-C21-C22-C23 |
| 8   | j     | 301 | SPO  | C11-C10-C9-C7   |
| 8   | j     | 301 | SPO  | C20-C21-C22-C23 |
| 8   | I     | 102 | SPO  | C17-C19-C20-C21 |
| 8   | g     | 102 | SPO  | C12-C14-C15-C16 |
| 8   | g     | 102 | SPO  | C20-C21-C22-C23 |
| 8   | F     | 102 | SPO  | C25-C26-C27-C28 |
| 12  | H     | 302 | 3PE  | C32-C31-O31-C3  |
| 9   | L     | 305 | U10  | C17-C18-C19-C20 |
| 7   | o     | 100 | BCL  | C4-C3-C5-C6     |
| 7   | j     | 302 | BCL  | C4-C3-C5-C6     |
| 7   | d     | 101 | BCL  | C4-C3-C5-C6     |
| 8   | D     | 201 | SPO  | C34-C33-C35-C36 |
| 8   | X     | 201 | SPO  | C34-C33-C35-C36 |
| 8   | M     | 406 | SPO  | C34-C33-C35-C36 |
| 7   | o     | 100 | BCL  | C2-C3-C5-C6     |
| 7   | k     | 101 | BCL  | C2-C3-C5-C6     |
| 7   | G     | 101 | BCL  | C2-C3-C5-C6     |
| 7   | j     | 302 | BCL  | C2-C3-C5-C6     |
| 7   | d     | 101 | BCL  | C2-C3-C5-C6     |
| 8   | D     | 201 | SPO  | C32-C33-C35-C36 |
| 8   | X     | 201 | SPO  | C32-C33-C35-C36 |
| 8   | M     | 406 | SPO  | C32-C33-C35-C36 |
| 9   | L     | 304 | U10  | C23-C24-C26-C27 |
| 7   | S     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 7   | A     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 8   | D     | 201 | SPO  | C28-C30-C31-C32 |
| 8   | D     | 201 | SPO  | C33-C35-C36-C37 |
| 8   | k     | 102 | SPO  | C28-C30-C31-C32 |
| 8   | k     | 102 | SPO  | C33-C35-C36-C37 |
| 8   | X     | 201 | SPO  | C28-C30-C31-C32 |
| 8   | M     | 406 | SPO  | C33-C35-C36-C37 |
| 9   | L     | 303 | U10  | C14-C16-C17-C18 |
| 9   | M     | 405 | U10  | C19-C21-C22-C23 |
| 12  | H     | 301 | 3PE  | C28-C29-C2A-C2B |
| 8   | t     | 102 | SPO  | C11-C10-C9-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | t     | 102 | SPO  | C12-C14-C15-C16 |
| 8   | t     | 102 | SPO  | C17-C19-C20-C21 |
| 8   | r     | 102 | SPO  | C25-C26-C27-C28 |
| 9   | M     | 405 | U10  | C33-C34-C36-C37 |
| 7   | r     | 101 | BCL  | C11-C12-C13-C14 |
| 7   | O     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | K     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | i     | 100 | BCL  | C11-C12-C13-C14 |
| 7   | j     | 303 | BCL  | C6-C7-C8-C9     |
| 10  | M     | 403 | BPH  | C11-C12-C13-C14 |
| 8   | r     | 102 | SPO  | C15-C16-C17-C18 |
| 8   | r     | 103 | SPO  | C15-C16-C17-C18 |
| 8   | X     | 201 | SPO  | C5-C6-C7-C8     |
| 8   | s     | 201 | SPO  | C15-C16-C17-C18 |
| 8   | M     | 406 | SPO  | C10-C11-C12-C13 |
| 8   | g     | 102 | SPO  | C10-C11-C12-C13 |
| 8   | g     | 102 | SPO  | C24-C23-C25-C26 |
| 8   | N     | 201 | SPO  | C10-C11-C12-C14 |
| 8   | X     | 201 | SPO  | C5-C6-C7-C9     |
| 8   | s     | 201 | SPO  | C15-C16-C17-C19 |
| 8   | j     | 301 | SPO  | C5-C6-C7-C9     |
| 8   | M     | 406 | SPO  | C10-C11-C12-C14 |
| 8   | g     | 102 | SPO  | C10-C11-C12-C14 |
| 8   | g     | 102 | SPO  | C22-C23-C25-C26 |
| 12  | H     | 301 | 3PE  | C34-C35-C36-C37 |
| 7   | O     | 101 | BCL  | C10-C11-C12-C13 |
| 7   | L     | 301 | BCL  | C15-C16-C17-C18 |
| 9   | L     | 304 | U10  | C17-C18-C19-C20 |
| 7   | M     | 402 | BCL  | C15-C16-C17-C18 |
| 8   | r     | 103 | SPO  | C11-C10-C9-C7   |
| 8   | k     | 102 | SPO  | C12-C14-C15-C16 |
| 8   | B     | 101 | SPO  | C11-C10-C9-C7   |
| 8   | s     | 201 | SPO  | C28-C30-C31-C32 |
| 8   | g     | 102 | SPO  | C28-C30-C31-C32 |
| 9   | a     | 102 | U10  | C14-C16-C17-C18 |
| 7   | M     | 402 | BCL  | C5-C6-C7-C8     |
| 12  | H     | 302 | 3PE  | C38-C39-C3A-C3B |
| 12  | d     | 102 | 3PE  | C2D-C2E-C2F-C2G |
| 7   | a     | 101 | BCL  | C13-C15-C16-C17 |
| 7   | F     | 101 | BCL  | C4-C3-C5-C6     |
| 9   | L     | 304 | U10  | C20-C19-C21-C22 |
| 7   | o     | 100 | BCL  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | b     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 10  | L     | 306 | BPH  | C2A-CAA-CBA-CGA |
| 8   | r     | 103 | SPO  | C17-C19-C20-C21 |
| 8   | s     | 201 | SPO  | C25-C26-C27-C28 |
| 8   | j     | 301 | SPO  | C12-C14-C15-C16 |
| 8   | I     | 102 | SPO  | C11-C10-C9-C7   |
| 8   | g     | 102 | SPO  | C25-C26-C27-C28 |
| 12  | H     | 302 | 3PE  | C3E-C3F-C3G-C3H |
| 7   | j     | 303 | BCL  | C10-C11-C12-C13 |
| 12  | H     | 301 | 3PE  | C2B-C2C-C2D-C2E |
| 12  | H     | 302 | 3PE  | C37-C38-C39-C3A |
| 12  | H     | 301 | 3PE  | C32-C33-C34-C35 |
| 12  | H     | 301 | 3PE  | C35-C36-C37-C38 |
| 12  | H     | 301 | 3PE  | C37-C38-C39-C3A |
| 12  | H     | 302 | 3PE  | C3C-C3D-C3E-C3F |
| 12  | H     | 302 | 3PE  | C3D-C3E-C3F-C3G |
| 12  | d     | 102 | 3PE  | C35-C36-C37-C38 |
| 12  | H     | 302 | 3PE  | O21-C2-C3-O31   |
| 8   | F     | 102 | SPO  | C34-C33-C35-C36 |
| 12  | H     | 302 | 3PE  | C35-C36-C37-C38 |
| 7   | I     | 101 | BCL  | C2-C3-C5-C6     |
| 7   | s     | 202 | BCL  | C11-C10-C8-C9   |
| 7   | n     | 100 | BCL  | C11-C12-C13-C14 |
| 12  | d     | 102 | 3PE  | C2B-C2C-C2D-C2E |
| 7   | M     | 401 | BCL  | C13-C15-C16-C17 |
| 7   | R     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 8   | s     | 201 | SPO  | C24-C23-C25-C26 |
| 8   | j     | 301 | SPO  | C5-C6-C7-C8     |
| 8   | j     | 301 | SPO  | C10-C11-C12-C13 |
| 12  | d     | 102 | 3PE  | C27-C28-C29-C2A |
| 8   | X     | 201 | SPO  | C10-C11-C12-C14 |
| 8   | s     | 201 | SPO  | C22-C23-C25-C26 |
| 8   | j     | 301 | SPO  | C10-C11-C12-C14 |
| 12  | H     | 301 | 3PE  | C2A-C2B-C2C-C2D |
| 9   | a     | 102 | U10  | C24-C26-C27-C28 |
| 12  | H     | 301 | 3PE  | C33-C34-C35-C36 |
| 12  | H     | 302 | 3PE  | C24-C25-C26-C27 |
| 12  | d     | 102 | 3PE  | C32-C31-O31-C3  |
| 12  | H     | 301 | 3PE  | C26-C27-C28-C29 |
| 7   | o     | 100 | BCL  | C3A-C2A-CAA-CBA |
| 7   | O     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | D     | 202 | BCL  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | u     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 7   | R     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | G     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | j     | 303 | BCL  | C3A-C2A-CAA-CBA |
| 10  | L     | 302 | BPH  | C5-C6-C7-C8     |
| 8   | s     | 201 | SPO  | C11-C10-C9-C7   |
| 12  | H     | 301 | 3PE  | C24-C25-C26-C27 |
| 12  | H     | 302 | 3PE  | C33-C34-C35-C36 |
| 12  | d     | 102 | 3PE  | C26-C27-C28-C29 |
| 7   | D     | 202 | BCL  | O2A-C1-C2-C3    |
| 7   | E     | 202 | BCL  | O2A-C1-C2-C3    |
| 7   | j     | 303 | BCL  | O2A-C1-C2-C3    |
| 7   | F     | 103 | BCL  | O2A-C1-C2-C3    |
| 7   | b     | 101 | BCL  | C2-C3-C5-C6     |
| 8   | F     | 102 | SPO  | C32-C33-C35-C36 |
| 9   | L     | 303 | U10  | C12-C11-C9-C8   |
| 12  | H     | 302 | 3PE  | C2A-C2B-C2C-C2D |
| 7   | M     | 402 | BCL  | C2-C1-O2A-CGA   |
| 12  | H     | 302 | 3PE  | C23-C24-C25-C26 |
| 12  | H     | 302 | 3PE  | C28-C29-C2A-C2B |
| 12  | H     | 301 | 3PE  | C39-C3A-C3B-C3C |
| 7   | R     | 101 | BCL  | C4-C3-C5-C6     |
| 9   | L     | 303 | U10  | C12-C11-C9-C10  |
| 10  | L     | 302 | BPH  | C4-C3-C5-C6     |
| 7   | t     | 103 | BCL  | C12-C13-C15-C16 |
| 7   | b     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | s     | 202 | BCL  | C11-C10-C8-C7   |
| 10  | L     | 302 | BPH  | C2-C3-C5-C6     |
| 10  | M     | 403 | BPH  | C11-C12-C13-C15 |
| 10  | M     | 403 | BPH  | C12-C13-C15-C16 |
| 12  | d     | 102 | 3PE  | O32-C31-O31-C3  |
| 7   | t     | 103 | BCL  | C13-C15-C16-C17 |
| 7   | o     | 100 | BCL  | C8-C10-C11-C12  |
| 7   | K     | 101 | BCL  | C10-C11-C12-C13 |
| 12  | H     | 302 | 3PE  | C39-C3A-C3B-C3C |
| 12  | H     | 302 | 3PE  | C22-C21-O21-C2  |
| 7   | u     | 102 | BCL  | C4-C3-C5-C6     |
| 7   | F     | 101 | BCL  | C2-C3-C5-C6     |
| 9   | L     | 304 | U10  | C18-C19-C21-C22 |
| 12  | H     | 302 | 3PE  | C25-C26-C27-C28 |
| 7   | t     | 103 | BCL  | C14-C13-C15-C16 |
| 7   | b     | 101 | BCL  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | L     | 301 | BCL  | C2A-CAA-CBA-CGA |
| 8   | F     | 102 | SPO  | C10-C11-C12-C13 |
| 8   | r     | 102 | SPO  | C15-C16-C17-C19 |
| 8   | F     | 102 | SPO  | C10-C11-C12-C14 |
| 7   | o     | 100 | BCL  | C1A-C2A-CAA-CBA |
| 7   | D     | 202 | BCL  | C1A-C2A-CAA-CBA |
| 7   | j     | 303 | BCL  | C1A-C2A-CAA-CBA |
| 7   | M     | 407 | BCL  | C8-C10-C11-C12  |
| 12  | H     | 302 | 3PE  | C21-C22-C23-C24 |
| 9   | M     | 408 | U10  | C6-C7-C8-C9     |
| 12  | H     | 302 | 3PE  | O11-C1-C2-C3    |
| 8   | r     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | j     | 301 | SPO  | C1-C4-C5-C6     |
| 12  | d     | 102 | 3PE  | C28-C29-C2A-C2B |
| 7   | s     | 202 | BCL  | C10-C11-C12-C13 |
| 12  | H     | 302 | 3PE  | C22-C23-C24-C25 |
| 9   | a     | 102 | U10  | C1-C6-C7-C8     |
| 12  | H     | 301 | 3PE  | C3D-C3E-C3F-C3G |
| 9   | M     | 405 | U10  | C30-C29-C31-C32 |
| 9   | L     | 303 | U10  | C5-C6-C7-C8     |
| 9   | M     | 408 | U10  | C5-C6-C7-C8     |
| 8   | r     | 102 | SPO  | C2-C1-O1-CM1    |
| 8   | D     | 201 | SPO  | C2-C1-O1-CM1    |
| 8   | D     | 201 | SPO  | C3-C1-O1-CM1    |
| 8   | k     | 102 | SPO  | C2-C1-O1-CM1    |
| 8   | k     | 102 | SPO  | C3-C1-O1-CM1    |
| 8   | E     | 201 | SPO  | C2-C1-O1-CM1    |
| 8   | E     | 201 | SPO  | C3-C1-O1-CM1    |
| 8   | X     | 201 | SPO  | C3-C1-O1-CM1    |
| 8   | M     | 406 | SPO  | C2-C1-O1-CM1    |
| 8   | M     | 406 | SPO  | C3-C1-O1-CM1    |
| 8   | F     | 102 | SPO  | C2-C1-O1-CM1    |
| 8   | B     | 101 | SPO  | C3-C1-O1-CM1    |
| 12  | H     | 302 | 3PE  | O22-C21-O21-C2  |
| 8   | E     | 201 | SPO  | C2-C1-C4-C5     |
| 8   | M     | 406 | SPO  | C3-C1-C4-C5     |
| 12  | H     | 301 | 3PE  | C2E-C2F-C2G-C2H |
| 7   | N     | 202 | BCL  | C11-C10-C8-C7   |
| 7   | R     | 101 | BCL  | C12-C13-C15-C16 |
| 7   | I     | 101 | BCL  | C11-C10-C8-C7   |
| 7   | u     | 102 | BCL  | C13-C15-C16-C17 |
| 8   | t     | 102 | SPO  | O1-C1-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | r     | 103 | SPO  | O1-C1-C4-C5     |
| 8   | E     | 201 | SPO  | O1-C1-C4-C5     |
| 8   | M     | 406 | SPO  | O1-C1-C4-C5     |
| 7   | a     | 101 | BCL  | C10-C11-C12-C13 |
| 7   | b     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | I     | 101 | BCL  | C15-C16-C17-C18 |
| 7   | D     | 202 | BCL  | C10-C11-C12-C13 |
| 8   | t     | 102 | SPO  | C28-C30-C31-C32 |
| 8   | r     | 103 | SPO  | C33-C35-C36-C37 |
| 8   | B     | 101 | SPO  | C33-C35-C36-C37 |
| 9   | L     | 304 | U10  | C24-C26-C27-C28 |
| 7   | r     | 101 | BCL  | C4-C3-C5-C6     |
| 9   | a     | 102 | U10  | C35-C34-C36-C37 |
| 9   | M     | 405 | U10  | C28-C29-C31-C32 |
| 7   | I     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 12  | H     | 302 | 3PE  | C1-C2-C3-O31    |
| 7   | t     | 103 | BCL  | O2A-C1-C2-C3    |
| 7   | R     | 101 | BCL  | O2A-C1-C2-C3    |
| 7   | I     | 101 | BCL  | O2A-C1-C2-C3    |
| 8   | D     | 201 | SPO  | C29-C28-C30-C31 |
| 9   | L     | 303 | U10  | C15-C14-C16-C17 |
| 12  | d     | 102 | 3PE  | C36-C37-C38-C39 |
| 8   | E     | 201 | SPO  | C12-C14-C15-C16 |
| 7   | M     | 407 | BCL  | C14-C13-C15-C16 |
| 7   | L     | 301 | BCL  | C4C-C3C-CAC-CBC |
| 7   | M     | 401 | BCL  | C4C-C3C-CAC-CBC |
| 8   | r     | 103 | SPO  | C15-C16-C17-C19 |
| 12  | H     | 301 | 3PE  | O22-C21-O21-C2  |
| 7   | G     | 101 | BCL  | C3-C5-C6-C7     |
| 7   | t     | 101 | BCL  | C11-C10-C8-C7   |
| 9   | a     | 102 | U10  | C33-C34-C36-C37 |
| 8   | N     | 201 | SPO  | C17-C19-C20-C21 |
| 8   | k     | 102 | SPO  | C17-C19-C20-C21 |
| 8   | k     | 102 | SPO  | C25-C26-C27-C28 |
| 8   | M     | 406 | SPO  | C17-C19-C20-C21 |
| 7   | j     | 303 | BCL  | C2A-CAA-CBA-CGA |
| 12  | H     | 301 | 3PE  | C3B-C3C-C3D-C3E |
| 12  | H     | 301 | 3PE  | C31-C32-C33-C34 |
| 7   | e     | 100 | BCL  | CAD-CBD-CGD-O2D |
| 7   | b     | 101 | BCL  | CAD-CBD-CGD-O2D |
| 7   | k     | 101 | BCL  | CAD-CBD-CGD-O2D |
| 7   | u     | 101 | BCL  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | M     | 403 | BPH  | CAD-CBD-CGD-O2D |
| 12  | H     | 301 | 3PE  | C3-C2-O21-C21   |
| 12  | H     | 301 | 3PE  | C22-C21-O21-C2  |
| 12  | d     | 102 | 3PE  | O11-C1-C2-O21   |
| 12  | d     | 102 | 3PE  | C29-C2A-C2B-C2C |
| 7   | E     | 202 | BCL  | C11-C12-C13-C14 |
| 8   | E     | 201 | SPO  | C10-C11-C12-C13 |
| 8   | j     | 301 | SPO  | C15-C16-C17-C18 |
| 8   | F     | 102 | SPO  | C5-C6-C7-C8     |
| 8   | F     | 102 | SPO  | C24-C23-C25-C26 |
| 8   | E     | 201 | SPO  | C10-C11-C12-C14 |
| 8   | F     | 102 | SPO  | C5-C6-C7-C9     |
| 7   | N     | 202 | BCL  | C1A-C2A-CAA-CBA |
| 7   | O     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | b     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | A     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | I     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 12  | H     | 302 | 3PE  | C11-O13-P-O11   |
| 9   | a     | 102 | U10  | C12-C11-C9-C10  |
| 7   | u     | 102 | BCL  | C2-C3-C5-C6     |
| 7   | R     | 101 | BCL  | C2-C3-C5-C6     |
| 9   | L     | 303 | U10  | C13-C14-C16-C17 |
| 12  | d     | 102 | 3PE  | C34-C35-C36-C37 |
| 10  | L     | 306 | BPH  | CAD-CBD-CGD-O1D |
| 12  | H     | 302 | 3PE  | C12-C11-O13-P   |
| 7   | n     | 100 | BCL  | C5-C6-C7-C8     |
| 7   | F     | 103 | BCL  | C8-C10-C11-C12  |
| 7   | j     | 303 | BCL  | C3-C5-C6-C7     |
| 8   | F     | 102 | SPO  | C1-C4-C5-C6     |
| 12  | H     | 301 | 3PE  | C3E-C3F-C3G-C3H |
| 7   | r     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | i     | 100 | BCL  | C11-C12-C13-C15 |
| 12  | H     | 301 | 3PE  | C1-C2-C3-O31    |
| 12  | H     | 301 | 3PE  | O21-C2-C3-O31   |
| 7   | G     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | t     | 101 | BCL  | C11-C10-C8-C9   |
| 7   | e     | 100 | BCL  | C11-C12-C13-C14 |
| 7   | R     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | i     | 100 | BCL  | C14-C13-C15-C16 |
| 8   | N     | 201 | SPO  | C23-C25-C26-C27 |
| 8   | r     | 103 | SPO  | C23-C25-C26-C27 |
| 8   | D     | 201 | SPO  | C23-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | k     | 102 | SPO  | C23-C25-C26-C27 |
| 8   | s     | 201 | SPO  | C23-C25-C26-C27 |
| 8   | M     | 406 | SPO  | C23-C25-C26-C27 |
| 8   | g     | 102 | SPO  | C23-C25-C26-C27 |
| 8   | F     | 102 | SPO  | C23-C25-C26-C27 |
| 12  | H     | 302 | 3PE  | C3B-C3C-C3D-C3E |
| 9   | L     | 304 | U10  | C5-C4-O4-C4M    |
| 12  | H     | 301 | 3PE  | C23-C24-C25-C26 |
| 7   | K     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 7   | L     | 301 | BCL  | C2-C1-O2A-CGA   |
| 9   | L     | 304 | U10  | C17-C18-C19-C21 |
| 7   | r     | 101 | BCL  | C2-C3-C5-C6     |
| 9   | a     | 102 | U10  | C12-C11-C9-C8   |
| 7   | D     | 202 | BCL  | C2A-CAA-CBA-CGA |
| 8   | s     | 201 | SPO  | C33-C35-C36-C37 |
| 8   | j     | 301 | SPO  | C3-C1-O1-CM1    |
| 8   | B     | 101 | SPO  | C2-C1-O1-CM1    |
| 8   | s     | 201 | SPO  | C3-C1-C4-C5     |
| 8   | r     | 103 | SPO  | C20-C21-C22-C23 |
| 9   | L     | 303 | U10  | C11-C12-C13-C14 |
| 8   | D     | 201 | SPO  | C27-C28-C30-C31 |
| 8   | F     | 102 | SPO  | C20-C21-C22-C23 |
| 8   | j     | 301 | SPO  | C28-C30-C31-C32 |
| 7   | A     | 101 | BCL  | C10-C11-C12-C13 |
| 12  | H     | 301 | 3PE  | C38-C39-C3A-C3B |
| 7   | u     | 101 | BCL  | C2-C1-O2A-CGA   |
| 7   | D     | 202 | BCL  | C5-C6-C7-C8     |
| 7   | a     | 101 | BCL  | C15-C16-C17-C18 |
| 12  | H     | 302 | 3PE  | C31-C32-C33-C34 |
| 7   | b     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 9   | L     | 303 | U10  | C5-C4-O4-C4M    |
| 9   | L     | 305 | U10  | C5-C4-O4-C4M    |
| 7   | M     | 402 | BCL  | CAA-CBA-CGA-O2A |
| 8   | M     | 406 | SPO  | C11-C10-C9-C7   |
| 7   | o     | 100 | BCL  | C6-C7-C8-C9     |
| 7   | S     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | A     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | u     | 102 | BCL  | C11-C10-C8-C9   |
| 8   | N     | 201 | SPO  | C21-C22-C23-C24 |
| 8   | r     | 103 | SPO  | C21-C22-C23-C24 |
| 8   | E     | 201 | SPO  | C8-C7-C9-C10    |
| 8   | E     | 201 | SPO  | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | s     | 201 | SPO  | C21-C22-C23-C24 |
| 8   | I     | 102 | SPO  | C21-C22-C23-C24 |
| 8   | M     | 406 | SPO  | C21-C22-C23-C24 |
| 8   | g     | 102 | SPO  | C21-C22-C23-C24 |
| 8   | F     | 102 | SPO  | C21-C22-C23-C24 |
| 8   | B     | 101 | SPO  | C13-C12-C14-C15 |
| 7   | K     | 101 | BCL  | O2A-C1-C2-C3    |
| 10  | L     | 302 | BPH  | O2A-C1-C2-C3    |
| 7   | K     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | o     | 100 | BCL  | C11-C12-C13-C15 |
| 7   | b     | 102 | BCL  | C11-C10-C8-C7   |
| 7   | E     | 202 | BCL  | C11-C10-C8-C7   |
| 7   | I     | 101 | BCL  | C5-C6-C7-C8     |
| 7   | O     | 101 | BCL  | C5-C6-C7-C8     |
| 9   | M     | 405 | U10  | C5-C4-O4-C4M    |
| 9   | M     | 408 | U10  | C5-C4-O4-C4M    |
| 8   | N     | 201 | SPO  | C21-C22-C23-C25 |
| 8   | r     | 103 | SPO  | C21-C22-C23-C25 |
| 8   | E     | 201 | SPO  | C6-C7-C9-C10    |
| 8   | E     | 201 | SPO  | C21-C22-C23-C25 |
| 8   | s     | 201 | SPO  | C21-C22-C23-C25 |
| 8   | I     | 102 | SPO  | C21-C22-C23-C25 |
| 8   | M     | 406 | SPO  | C21-C22-C23-C25 |
| 8   | g     | 102 | SPO  | C21-C22-C23-C25 |
| 8   | F     | 102 | SPO  | C21-C22-C23-C25 |
| 8   | B     | 101 | SPO  | C11-C12-C14-C15 |
| 8   | D     | 201 | SPO  | C12-C14-C15-C16 |
| 8   | g     | 102 | SPO  | C17-C19-C20-C21 |
| 8   | r     | 103 | SPO  | C1-C4-C5-C6     |
| 8   | E     | 201 | SPO  | C1-C4-C5-C6     |
| 7   | O     | 101 | BCL  | C4-C3-C5-C6     |
| 7   | I     | 101 | BCL  | C2-C1-O2A-CGA   |
| 12  | H     | 302 | 3PE  | C2D-C2E-C2F-C2G |
| 12  | H     | 301 | 3PE  | C3C-C3D-C3E-C3F |
| 12  | H     | 302 | 3PE  | C27-C28-C29-C2A |
| 7   | N     | 202 | BCL  | C15-C16-C17-C18 |
| 7   | e     | 100 | BCL  | C4-C3-C5-C6     |
| 7   | A     | 101 | BCL  | C4-C3-C5-C6     |
| 9   | L     | 305 | U10  | C12-C11-C9-C10  |
| 7   | M     | 407 | BCL  | C12-C13-C15-C16 |
| 9   | M     | 405 | U10  | C3-C4-O4-C4M    |
| 9   | M     | 408 | U10  | C3-C4-O4-C4M    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | d     | 102 | 3PE  | O31-C31-C32-C33 |
| 7   | N     | 202 | BCL  | C4-C3-C5-C6     |
| 8   | t     | 102 | SPO  | C29-C28-C30-C31 |
| 7   | o     | 100 | BCL  | C11-C12-C13-C14 |
| 10  | M     | 403 | BPH  | C14-C13-C15-C16 |
| 7   | j     | 303 | BCL  | C13-C15-C16-C17 |
| 7   | N     | 202 | BCL  | C3A-C2A-CAA-CBA |
| 7   | A     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | K     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | O     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 7   | t     | 101 | BCL  | CAD-CBD-CGD-O2D |
| 7   | s     | 202 | BCL  | CAD-CBD-CGD-O2D |
| 7   | n     | 100 | BCL  | CAD-CBD-CGD-O2D |
| 7   | M     | 402 | BCL  | CAD-CBD-CGD-O2D |
| 7   | M     | 407 | BCL  | CAD-CBD-CGD-O2D |
| 7   | F     | 101 | BCL  | CAD-CBD-CGD-O2D |
| 7   | d     | 101 | BCL  | CAD-CBD-CGD-O2D |
| 7   | t     | 101 | BCL  | C2-C1-O2A-CGA   |
| 10  | M     | 403 | BPH  | C2-C1-O2A-CGA   |
| 8   | k     | 102 | SPO  | C34-C33-C35-C36 |
| 9   | a     | 102 | U10  | C30-C29-C31-C32 |
| 9   | a     | 102 | U10  | C5-C4-O4-C4M    |
| 7   | b     | 102 | BCL  | O2A-C1-C2-C3    |
| 7   | A     | 101 | BCL  | O2A-C1-C2-C3    |
| 7   | N     | 202 | BCL  | C2A-CAA-CBA-CGA |
| 10  | M     | 403 | BPH  | C2A-CAA-CBA-CGA |
| 7   | u     | 101 | BCL  | CHA-CBD-CGD-O2D |
| 7   | A     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 12  | H     | 302 | 3PE  | C29-C2A-C2B-C2C |
| 7   | r     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | a     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 7   | F     | 103 | BCL  | C4-C3-C5-C6     |
| 7   | O     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | j     | 303 | BCL  | C6-C7-C8-C10    |
| 9   | L     | 305 | U10  | C12-C11-C9-C8   |
| 7   | b     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 8   | r     | 102 | SPO  | C28-C30-C31-C32 |
| 8   | N     | 201 | SPO  | C25-C26-C27-C28 |
| 8   | g     | 102 | SPO  | C11-C10-C9-C7   |
| 9   | L     | 303 | U10  | C3-C4-O4-C4M    |
| 9   | L     | 305 | U10  | C3-C4-O4-C4M    |
| 12  | d     | 102 | 3PE  | O32-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | F     | 103 | BCL  | C10-C11-C12-C13 |
| 10  | M     | 403 | BPH  | C2C-C3C-CAC-CBC |
| 7   | M     | 402 | BCL  | C13-C15-C16-C17 |
| 8   | r     | 102 | SPO  | C29-C28-C30-C31 |
| 8   | j     | 301 | SPO  | C15-C16-C17-C19 |
| 7   | t     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 7   | S     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | E     | 202 | BCL  | C1A-C2A-CAA-CBA |
| 7   | b     | 102 | BCL  | CAA-CBA-CGA-O1A |
| 7   | u     | 102 | BCL  | C16-C17-C18-C19 |
| 7   | A     | 101 | BCL  | CAA-CBA-CGA-O1A |
| 7   | O     | 101 | BCL  | CAA-CBA-CGA-O1A |
| 7   | n     | 100 | BCL  | C14-C13-C15-C16 |
| 7   | G     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | j     | 302 | BCL  | C11-C10-C8-C9   |
| 7   | I     | 101 | BCL  | C11-C10-C8-C9   |
| 7   | M     | 407 | BCL  | C11-C12-C13-C14 |
| 7   | F     | 103 | BCL  | CAA-CBA-CGA-O2A |
| 7   | R     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | R     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 8   | r     | 102 | SPO  | C30-C31-C32-C33 |
| 7   | M     | 402 | BCL  | C4-C3-C5-C6     |
| 7   | b     | 101 | BCL  | C12-C13-C15-C16 |
| 7   | A     | 101 | BCL  | C12-C13-C15-C16 |
| 7   | K     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | K     | 101 | BCL  | C11-C10-C8-C7   |
| 7   | j     | 302 | BCL  | C11-C10-C8-C7   |
| 7   | L     | 301 | BCL  | C2C-C3C-CAC-CBC |
| 7   | g     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | o     | 100 | BCL  | CAA-CBA-CGA-O2A |
| 7   | S     | 101 | BCL  | C13-C15-C16-C17 |
| 7   | a     | 101 | BCL  | CAA-CBA-CGA-O1A |
| 7   | F     | 103 | BCL  | CAA-CBA-CGA-O1A |
| 9   | M     | 405 | U10  | C29-C31-C32-C33 |
| 7   | G     | 101 | BCL  | CAA-CBA-CGA-O2A |

There are no ring outliers.

60 monomers are involved in 316 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | r     | 101 | BCL  | 8       | 0            |
| 7   | k     | 101 | BCL  | 3       | 0            |

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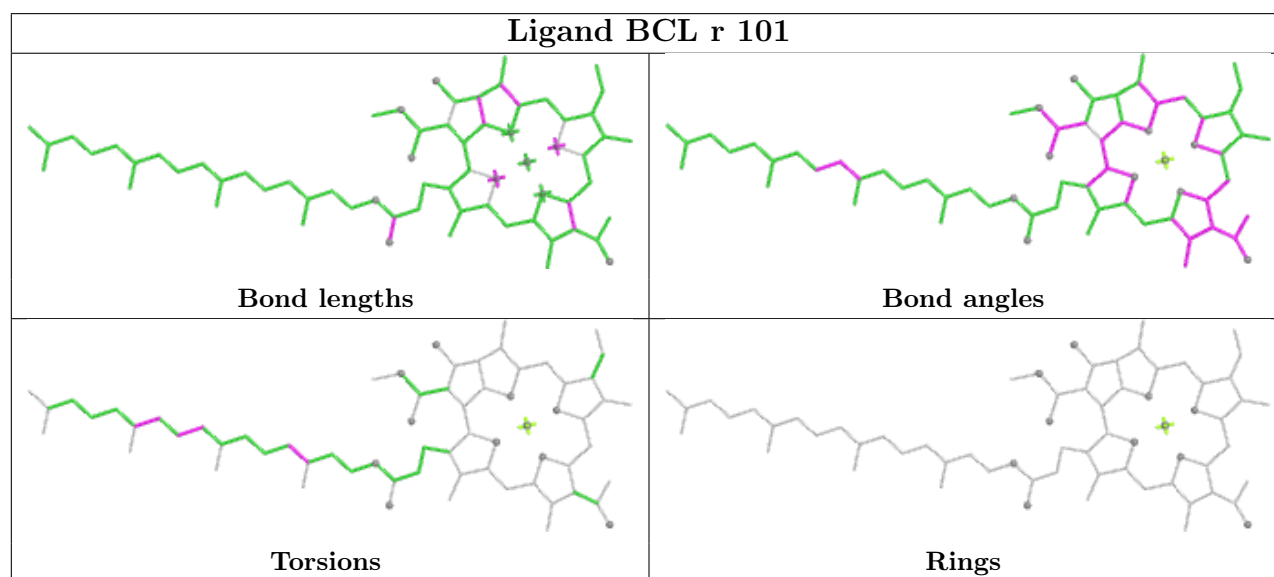
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | a     | 101 | BCL  | 2       | 0            |
| 7   | o     | 100 | BCL  | 5       | 0            |
| 7   | M     | 407 | BCL  | 6       | 0            |
| 8   | k     | 102 | SPO  | 10      | 0            |
| 9   | L     | 303 | U10  | 1       | 0            |
| 8   | r     | 103 | SPO  | 10      | 0            |
| 8   | s     | 201 | SPO  | 16      | 0            |
| 7   | b     | 101 | BCL  | 8       | 0            |
| 7   | F     | 101 | BCL  | 7       | 0            |
| 12  | H     | 301 | 3PE  | 5       | 0            |
| 8   | M     | 406 | SPO  | 13      | 0            |
| 8   | r     | 102 | SPO  | 10      | 0            |
| 12  | d     | 102 | 3PE  | 2       | 0            |
| 10  | L     | 302 | BPH  | 6       | 0            |
| 7   | e     | 100 | BCL  | 5       | 0            |
| 7   | g     | 101 | BCL  | 8       | 0            |
| 7   | b     | 102 | BCL  | 1       | 0            |
| 7   | u     | 101 | BCL  | 4       | 0            |
| 8   | B     | 101 | SPO  | 11      | 0            |
| 8   | D     | 201 | SPO  | 11      | 0            |
| 7   | n     | 100 | BCL  | 5       | 0            |
| 7   | S     | 101 | BCL  | 2       | 0            |
| 7   | D     | 202 | BCL  | 2       | 0            |
| 7   | I     | 101 | BCL  | 2       | 0            |
| 7   | N     | 202 | BCL  | 5       | 0            |
| 9   | M     | 405 | U10  | 5       | 0            |
| 7   | u     | 102 | BCL  | 7       | 0            |
| 8   | g     | 102 | SPO  | 8       | 0            |
| 8   | N     | 201 | SPO  | 12      | 0            |
| 7   | M     | 402 | BCL  | 4       | 0            |
| 8   | F     | 102 | SPO  | 12      | 0            |
| 7   | t     | 103 | BCL  | 5       | 0            |
| 9   | L     | 304 | U10  | 3       | 0            |
| 10  | L     | 306 | BPH  | 3       | 0            |
| 7   | s     | 202 | BCL  | 5       | 0            |
| 7   | G     | 101 | BCL  | 2       | 0            |
| 9   | a     | 102 | U10  | 7       | 0            |
| 7   | t     | 101 | BCL  | 7       | 0            |
| 8   | t     | 102 | SPO  | 7       | 0            |
| 7   | R     | 101 | BCL  | 7       | 0            |
| 7   | M     | 401 | BCL  | 4       | 0            |
| 12  | H     | 302 | 3PE  | 5       | 0            |

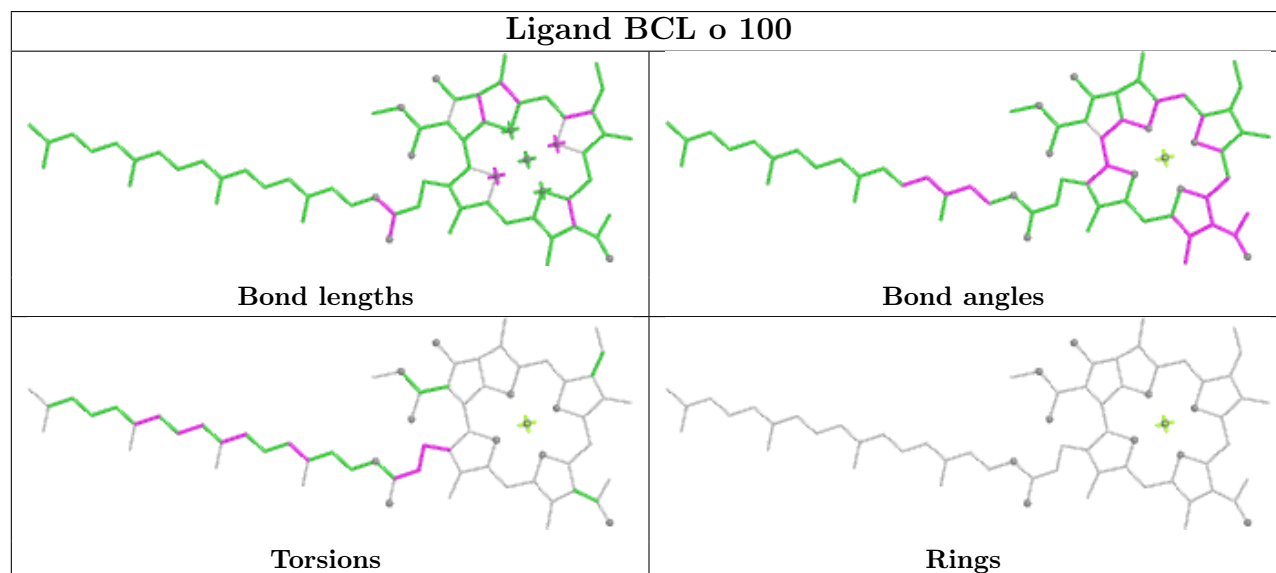
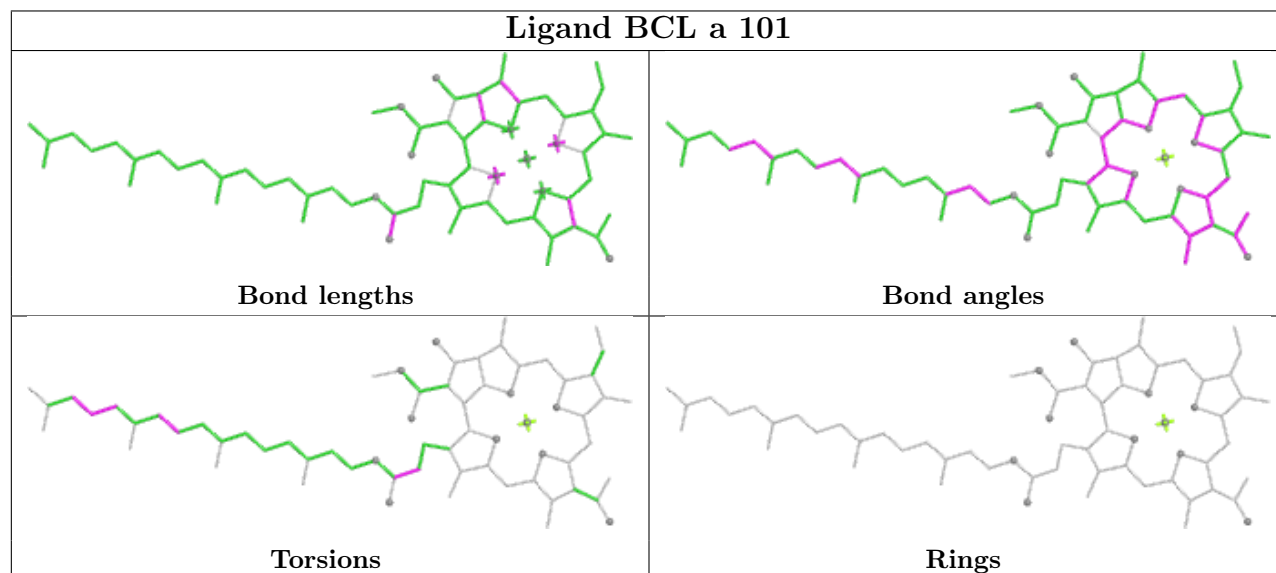
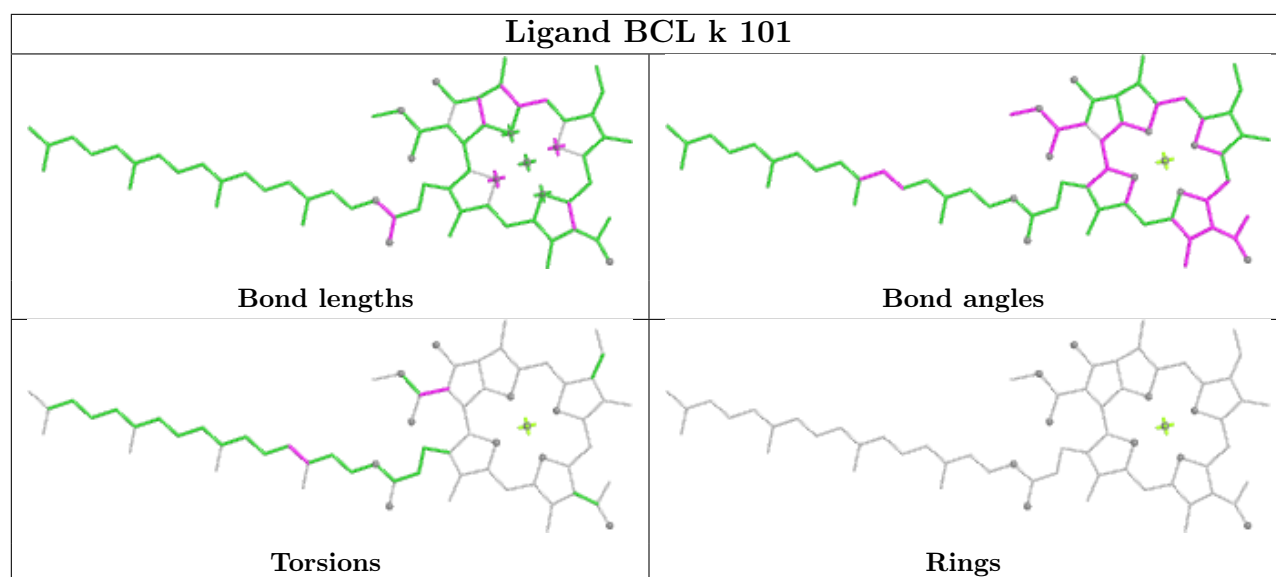
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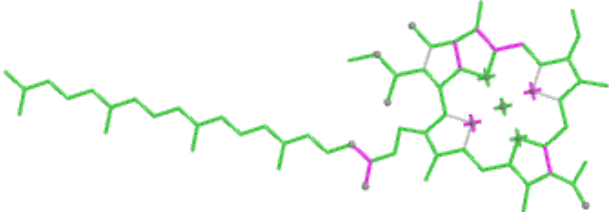
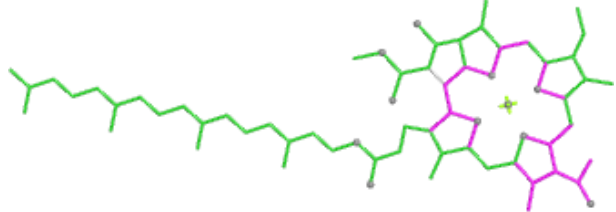
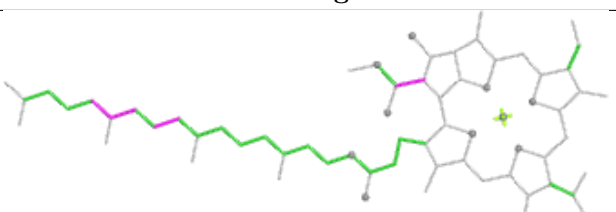
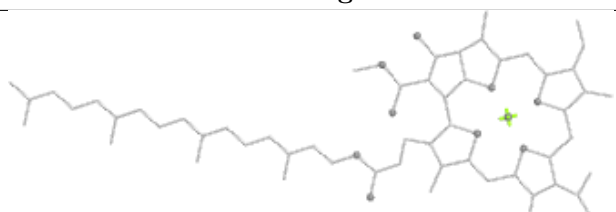
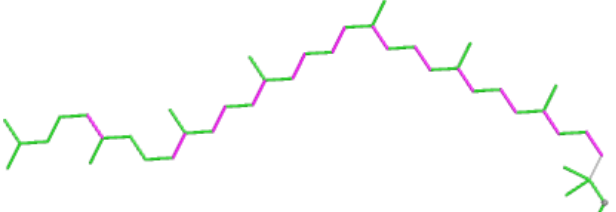
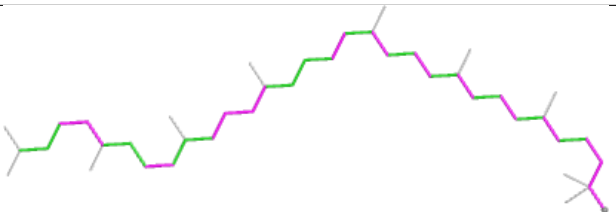
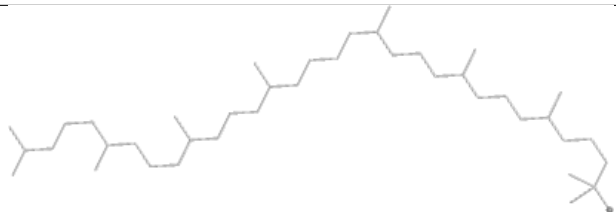
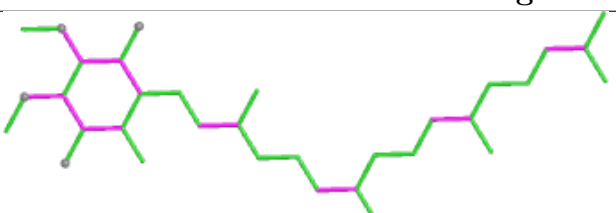
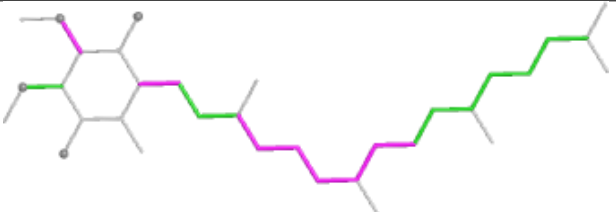
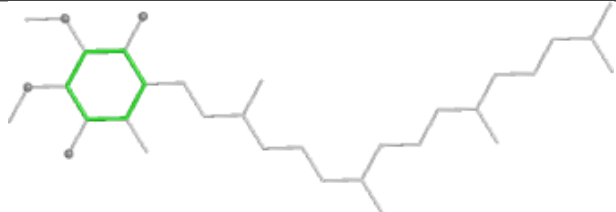
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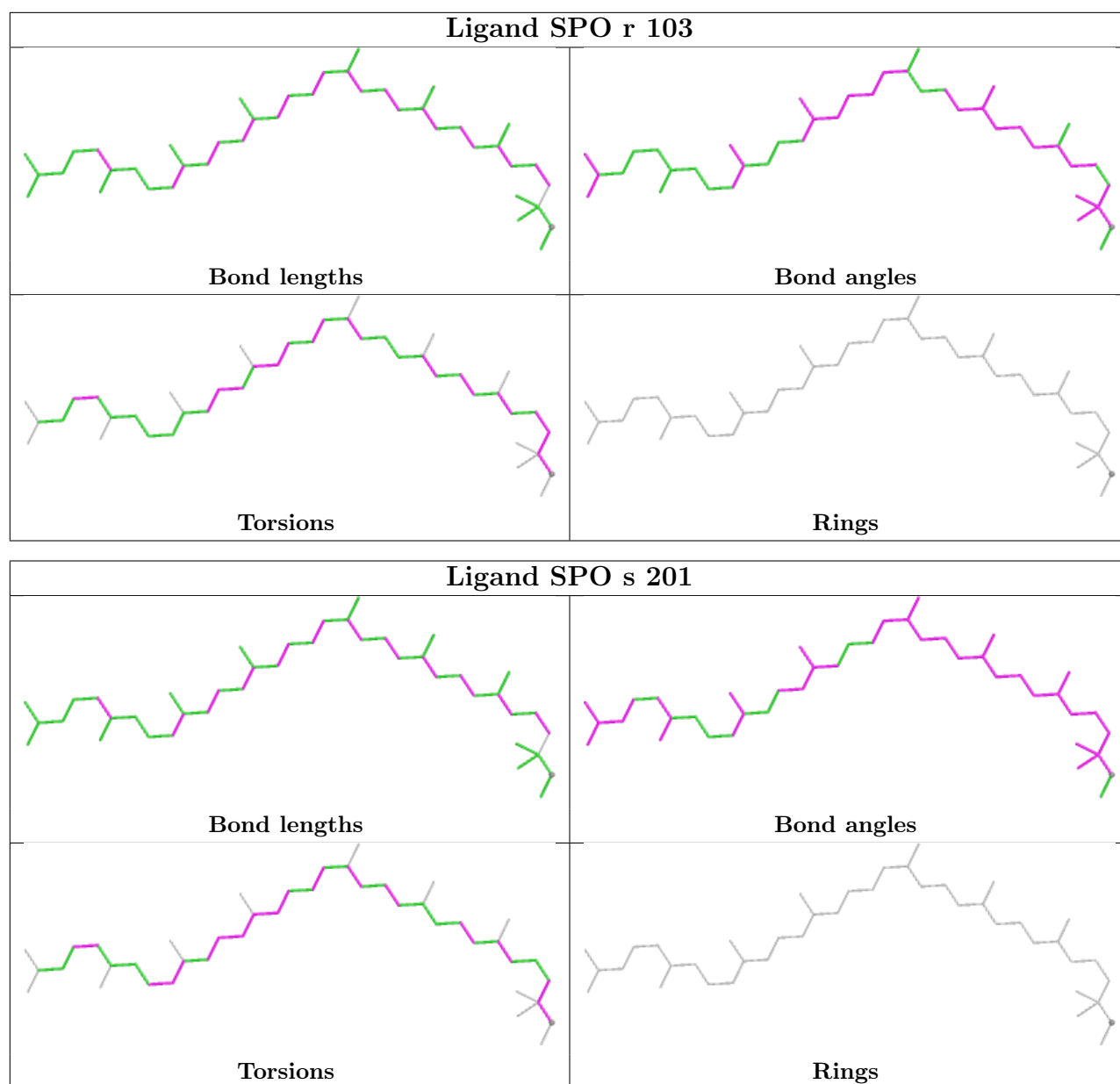
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | j     | 302 | BCL  | 2       | 0            |
| 9   | M     | 408 | U10  | 1       | 0            |
| 8   | I     | 102 | SPO  | 6       | 0            |
| 7   | F     | 103 | BCL  | 2       | 0            |
| 7   | d     | 101 | BCL  | 9       | 0            |
| 8   | E     | 201 | SPO  | 17      | 0            |
| 7   | K     | 101 | BCL  | 3       | 0            |
| 8   | X     | 201 | SPO  | 4       | 0            |
| 8   | j     | 301 | SPO  | 7       | 0            |
| 9   | L     | 305 | U10  | 1       | 0            |
| 10  | M     | 403 | BPH  | 12      | 0            |
| 7   | j     | 303 | BCL  | 4       | 0            |
| 7   | E     | 202 | BCL  | 3       | 0            |
| 7   | A     | 101 | BCL  | 3       | 0            |
| 7   | L     | 301 | BCL  | 3       | 0            |
| 7   | O     | 101 | BCL  | 3       | 0            |

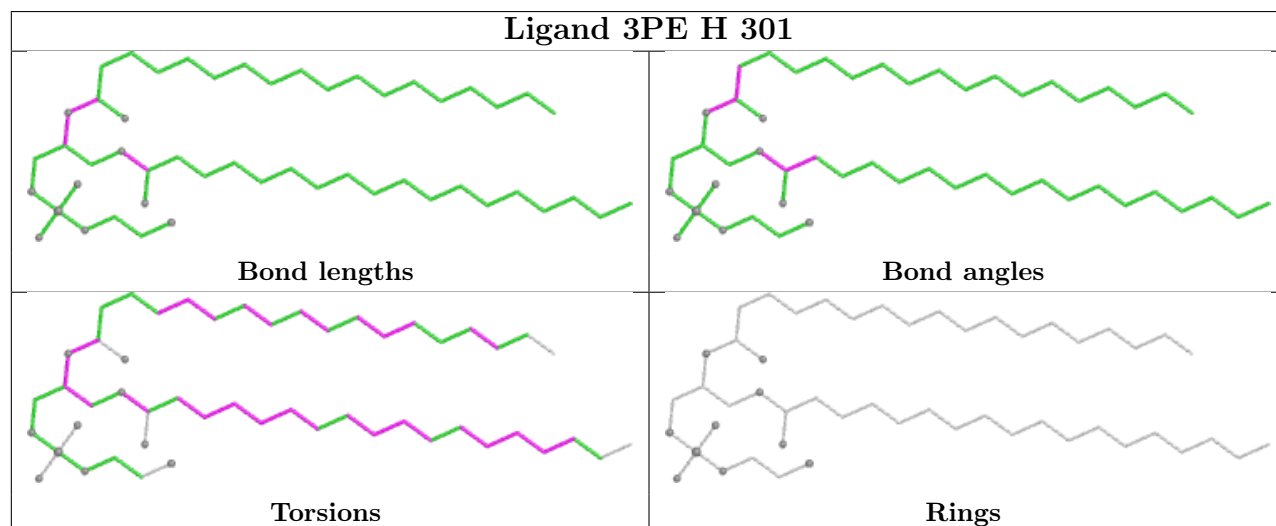
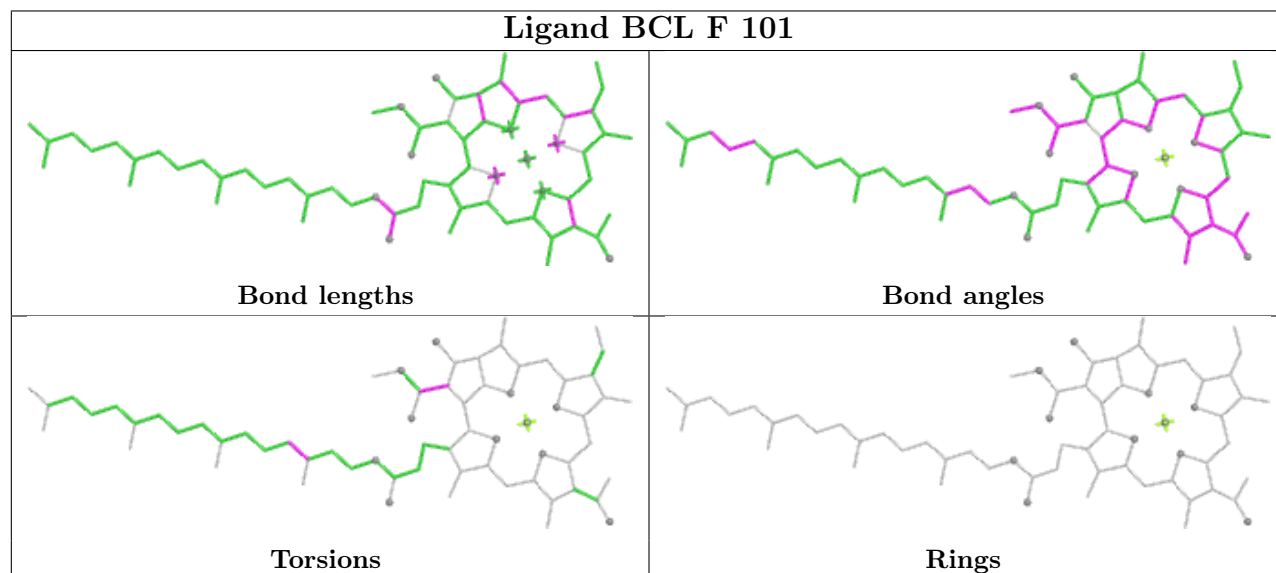
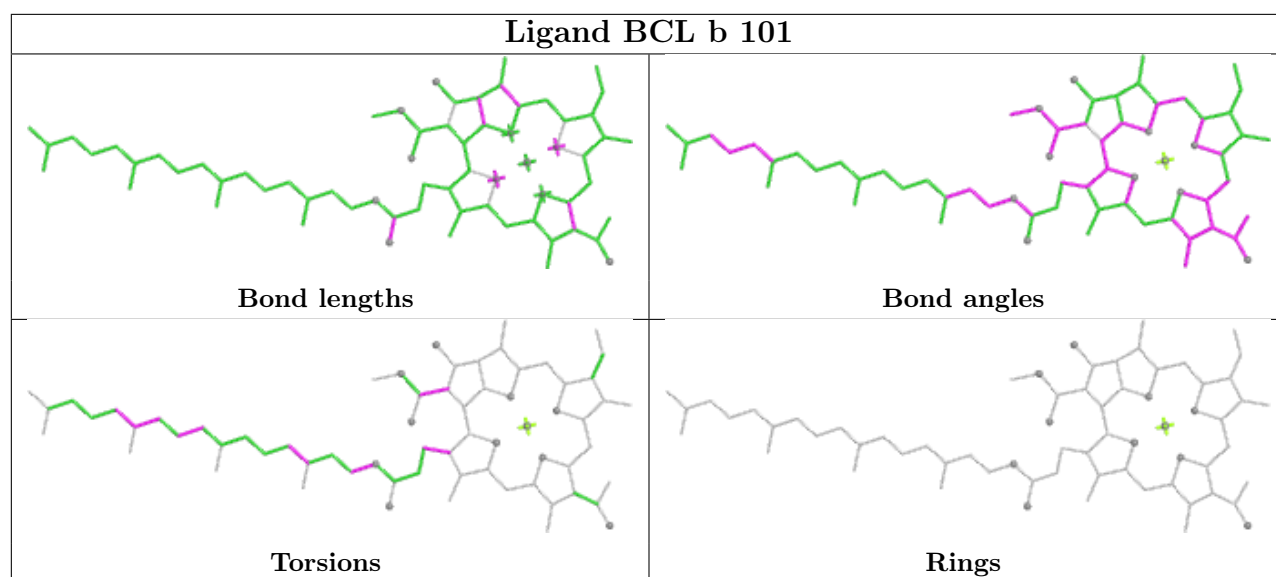
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

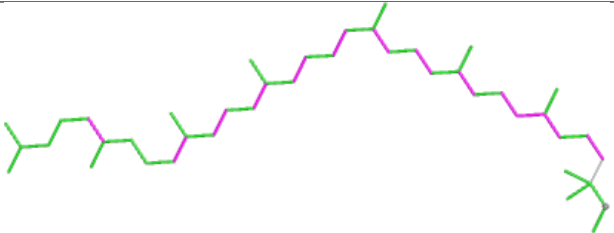
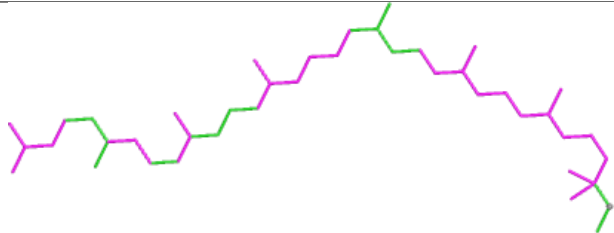
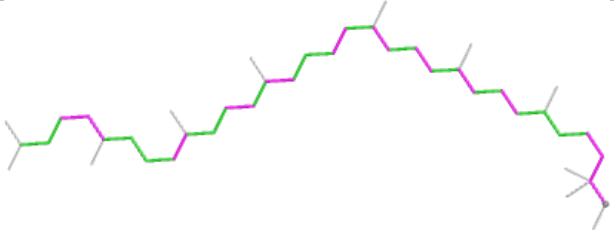
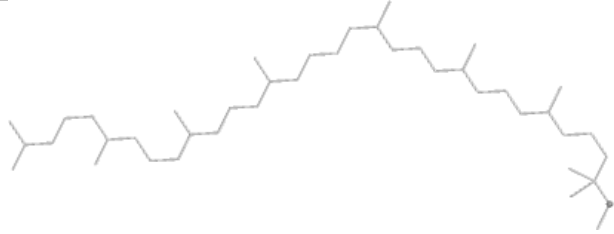


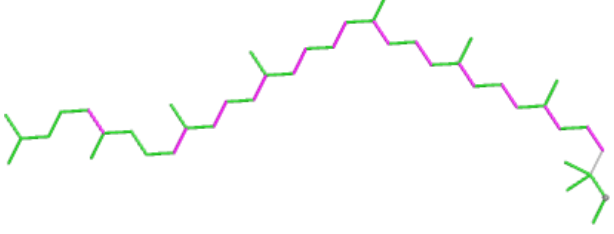
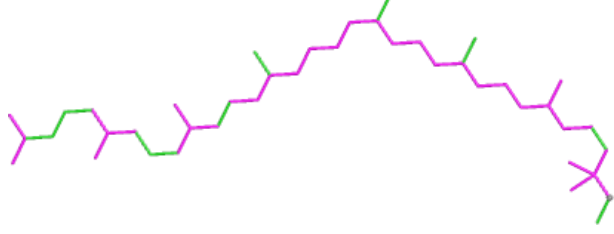
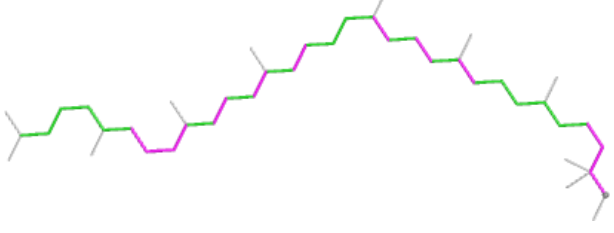


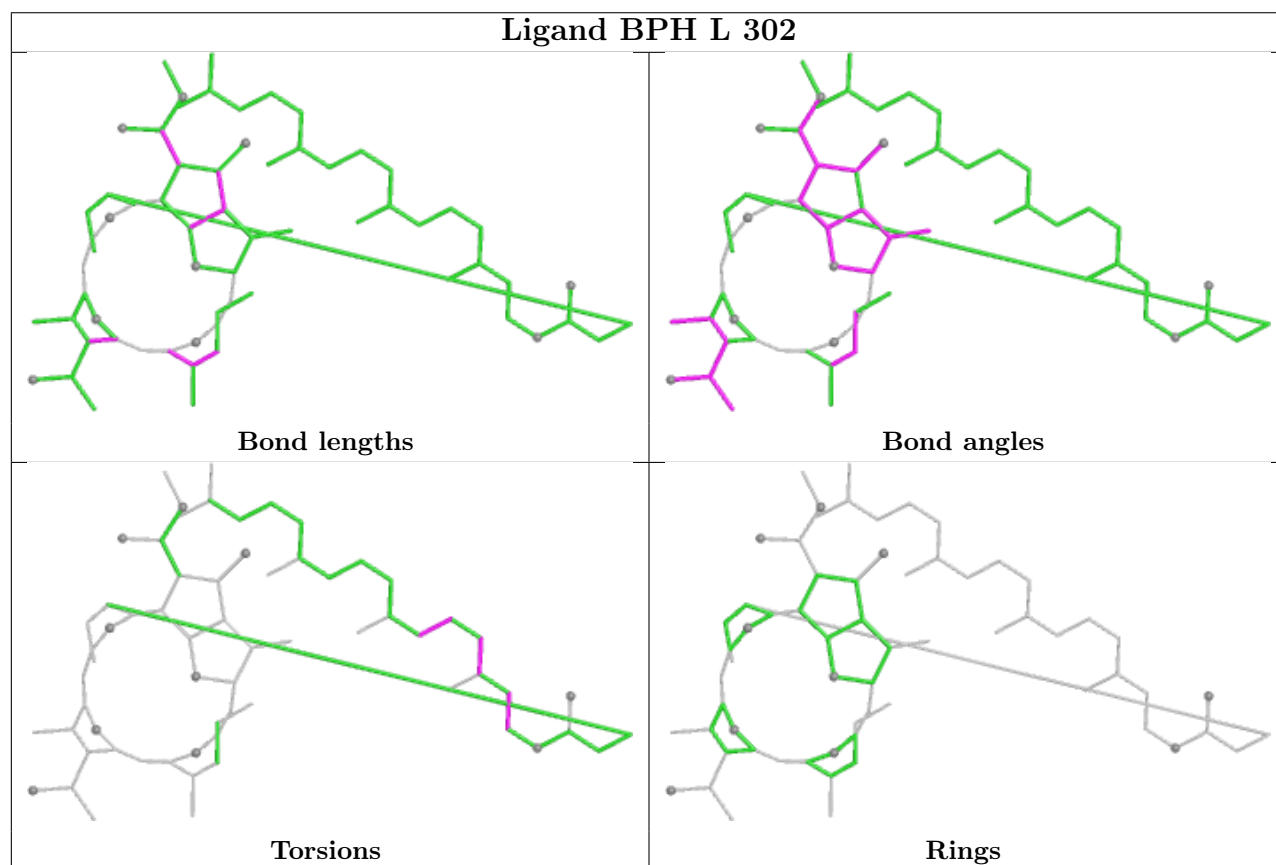
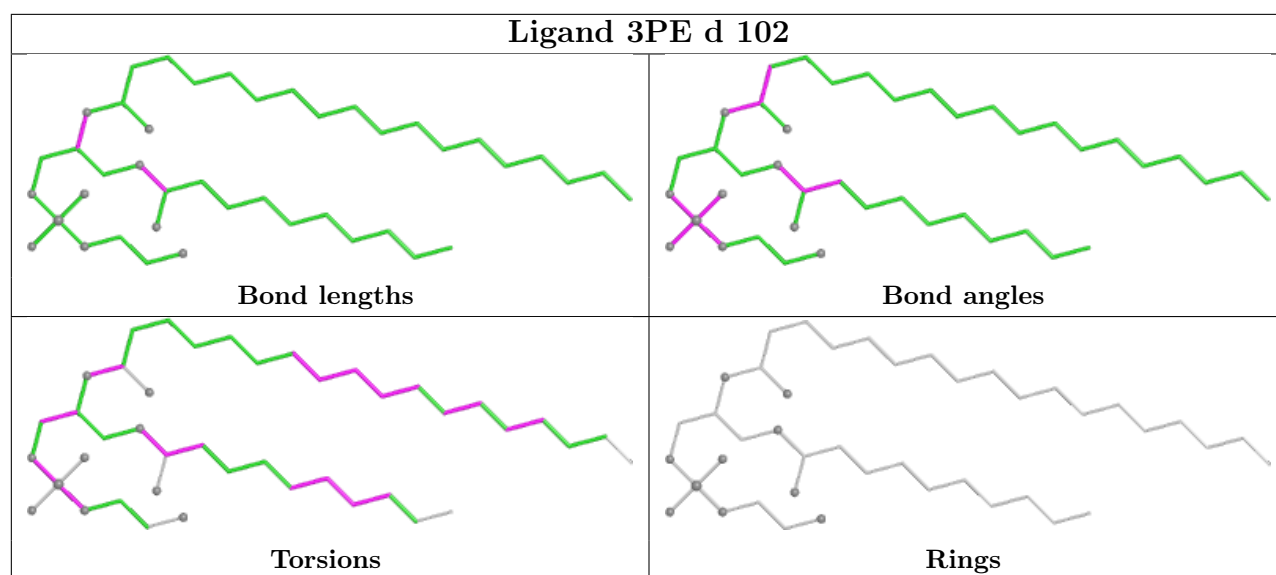
| Ligand BCL M 407                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand SPO k 102                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand U10 L 303                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

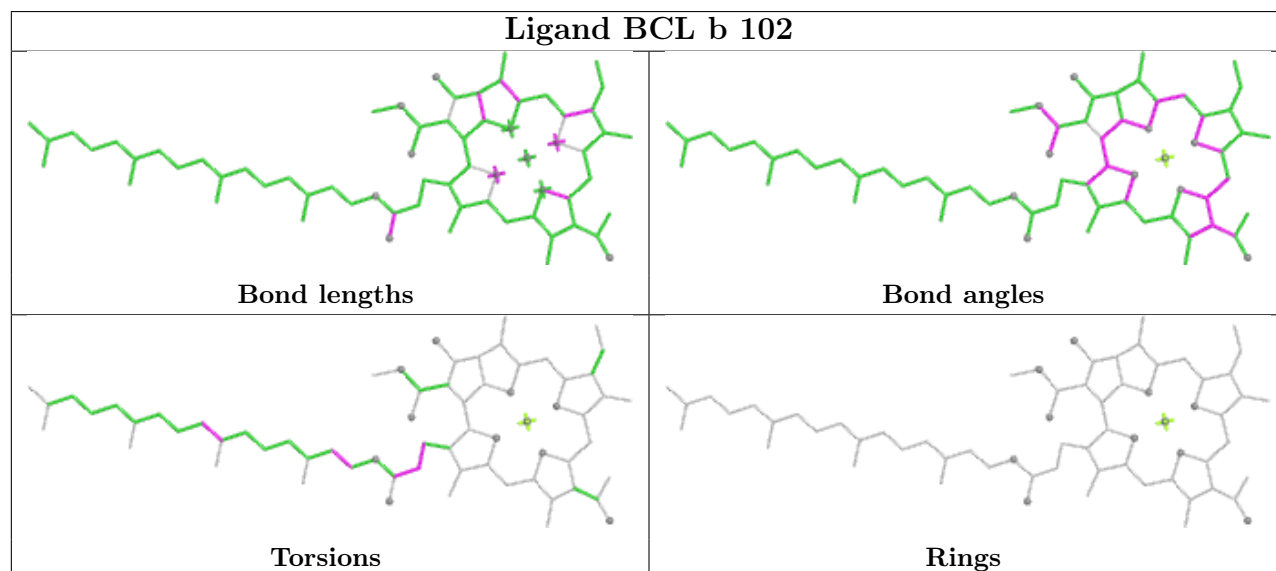
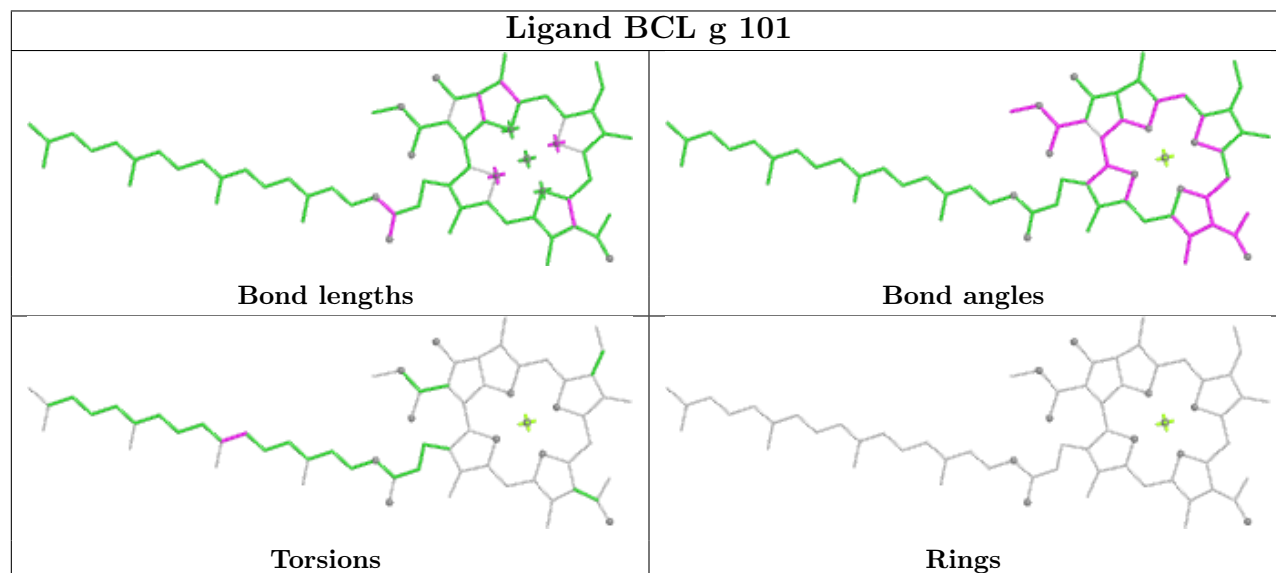
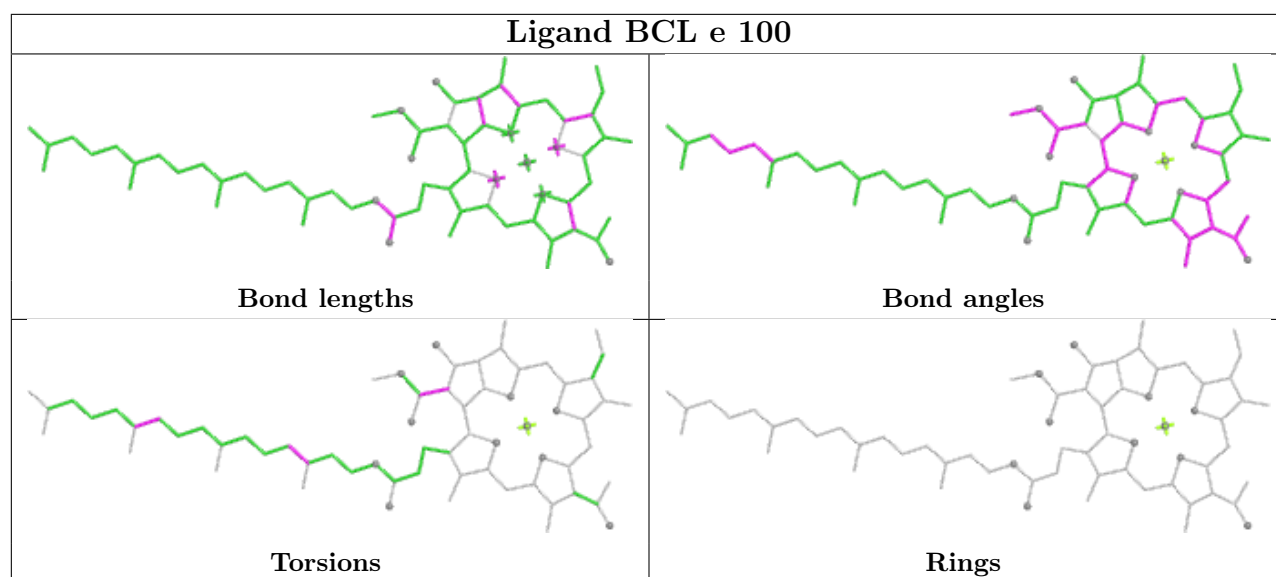


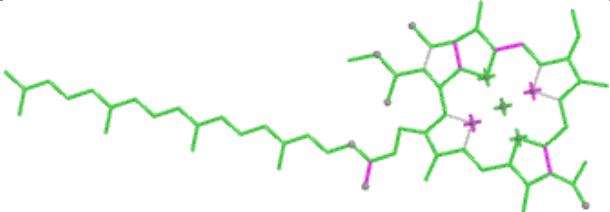
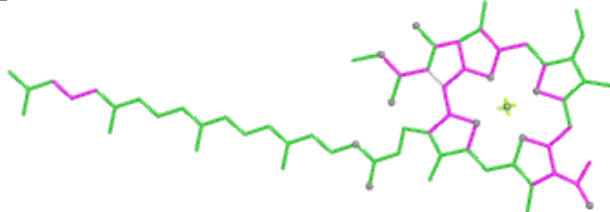
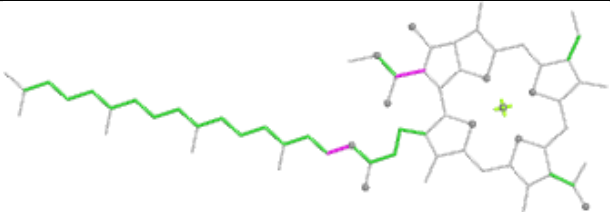
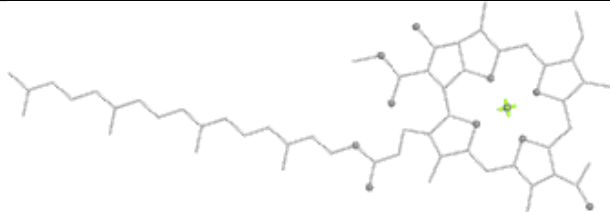
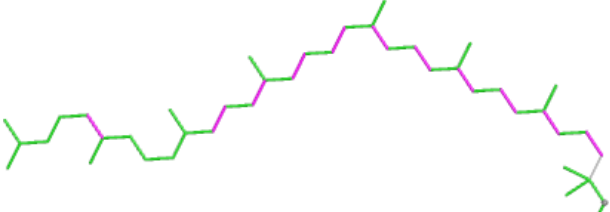
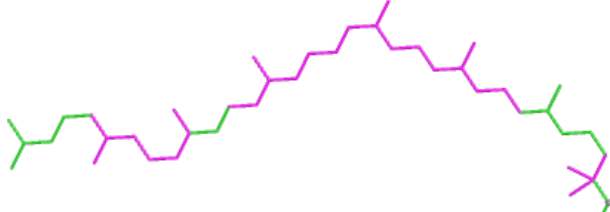
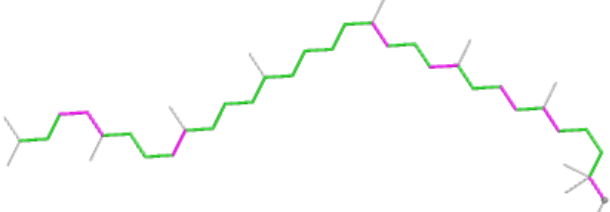
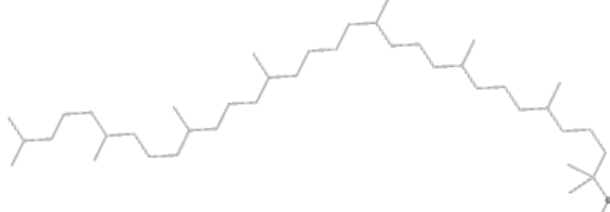


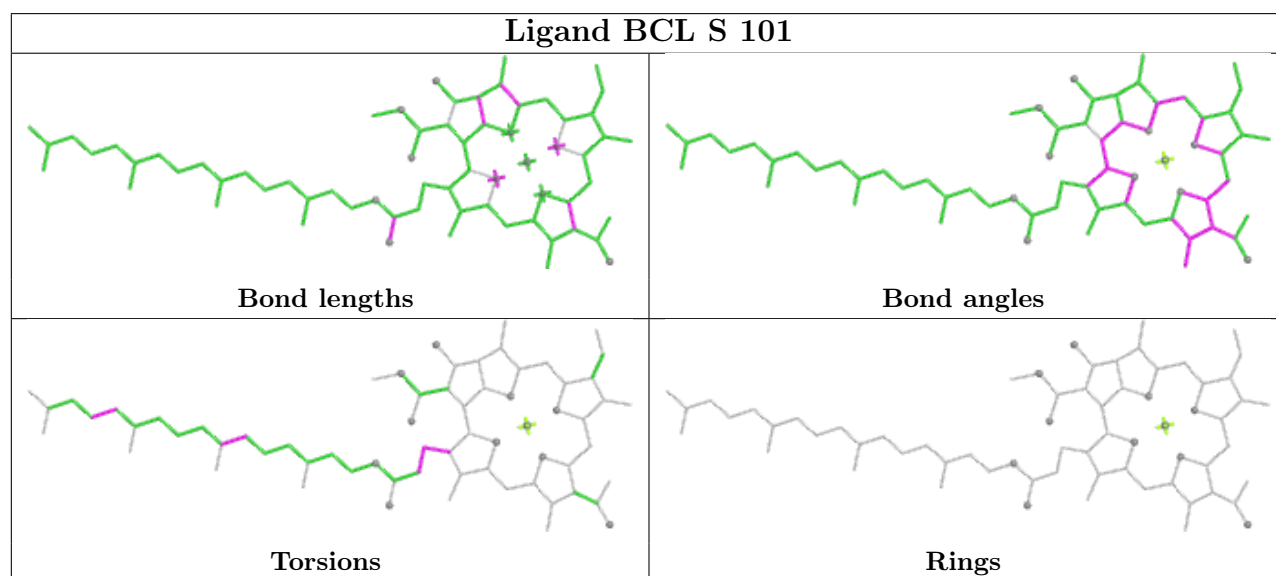
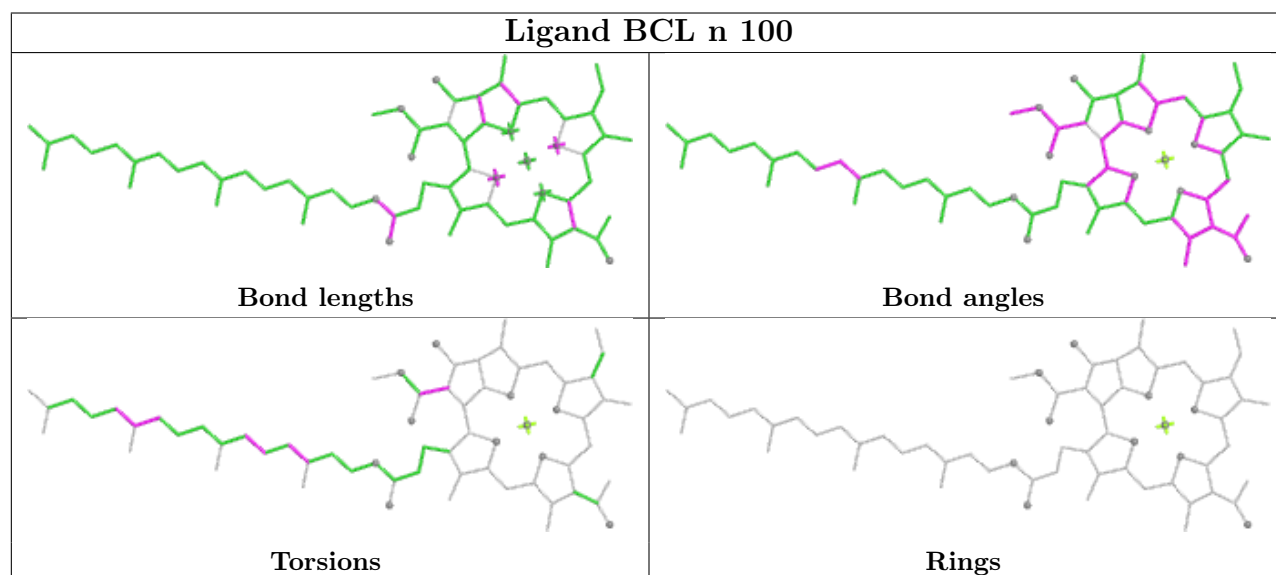
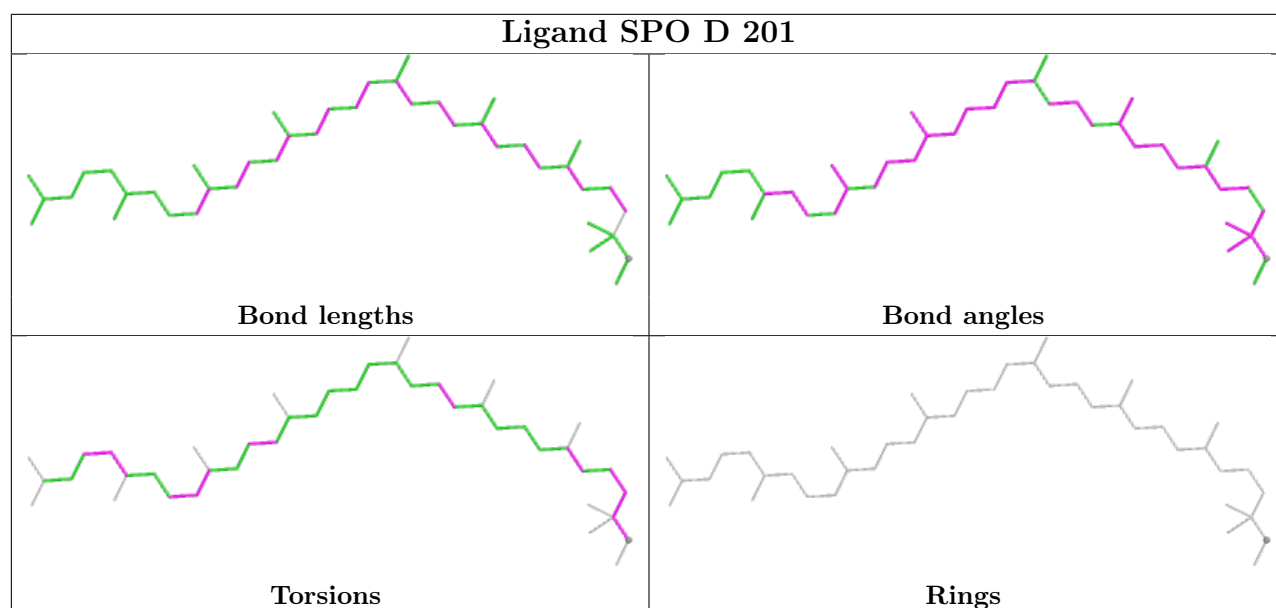
| Ligand SPO M 406                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

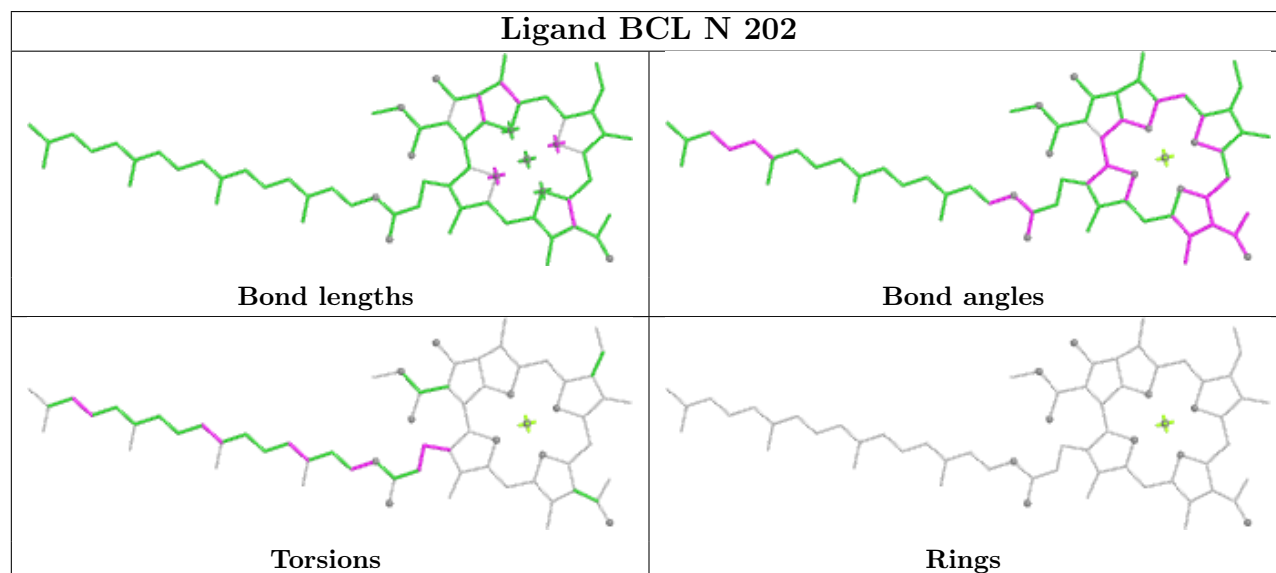
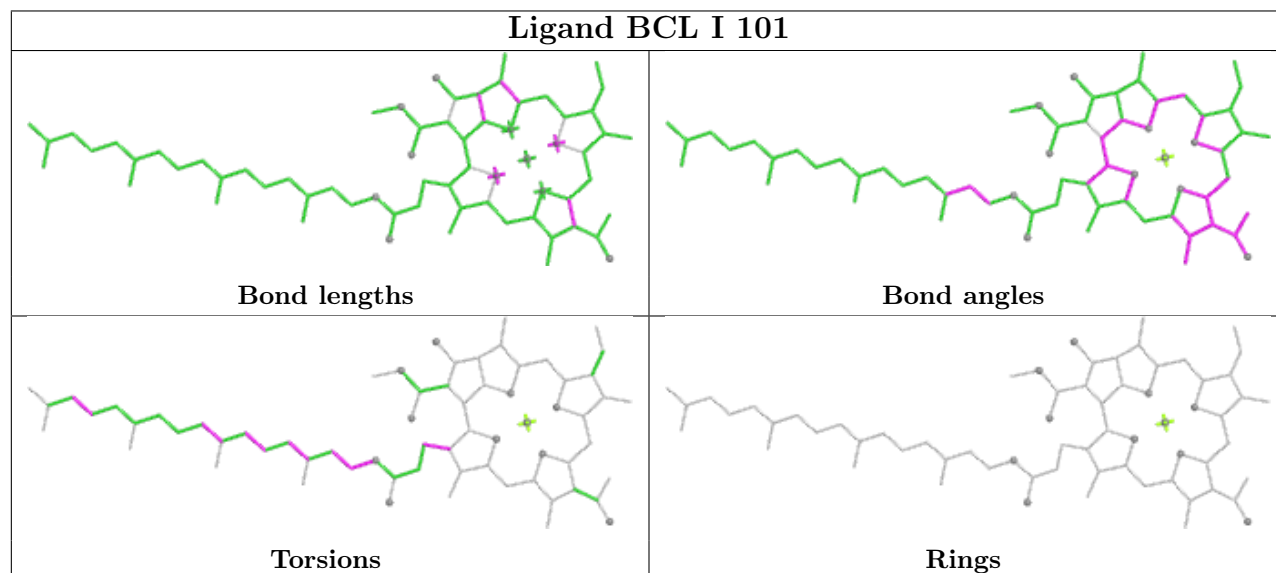
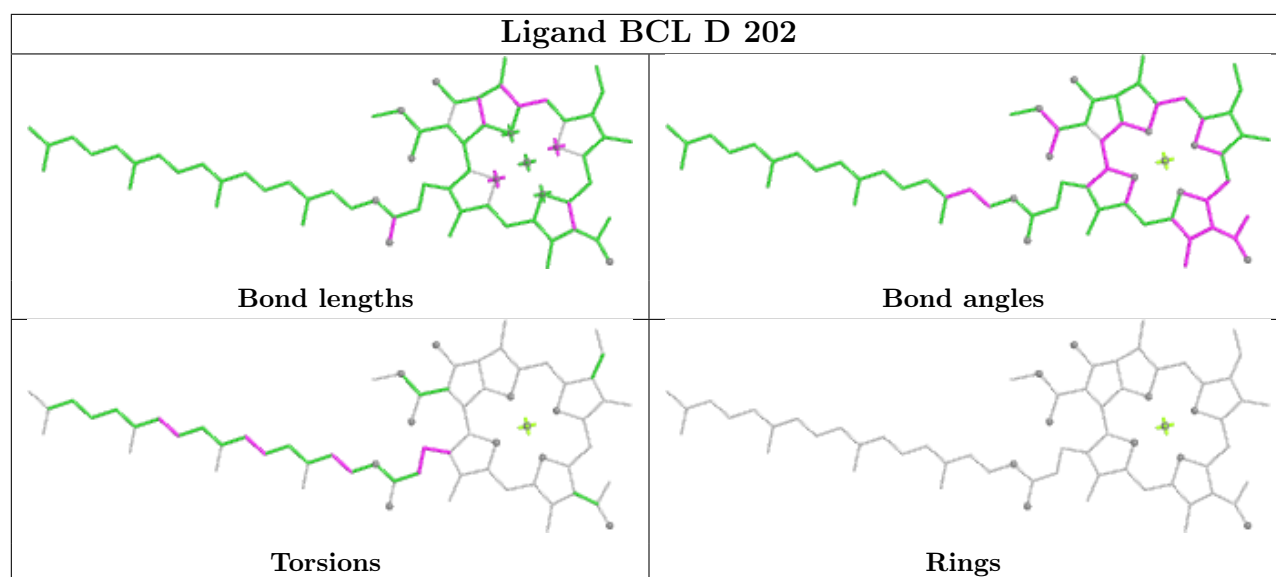
| Ligand SPO r 102                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

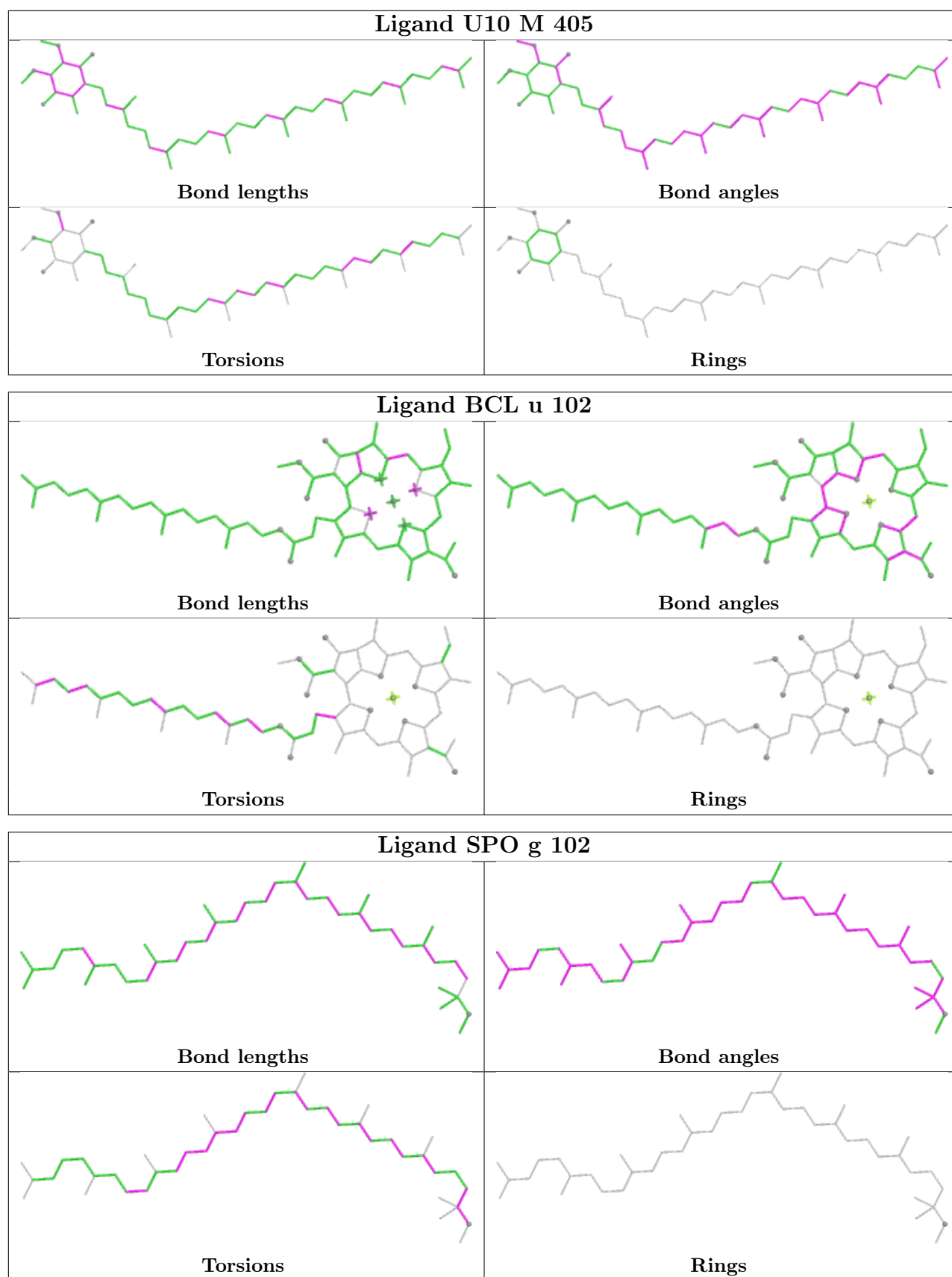


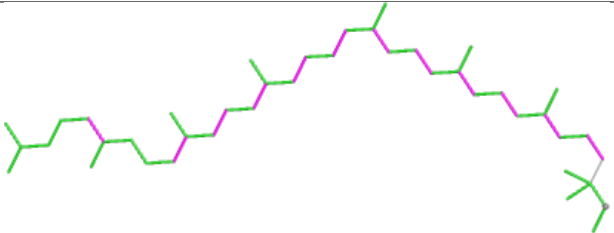
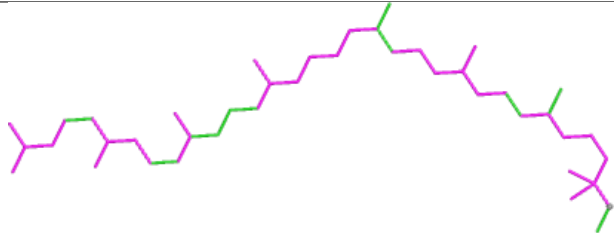
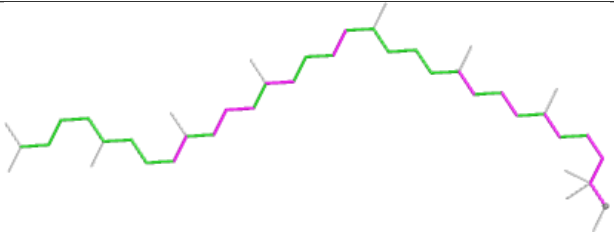
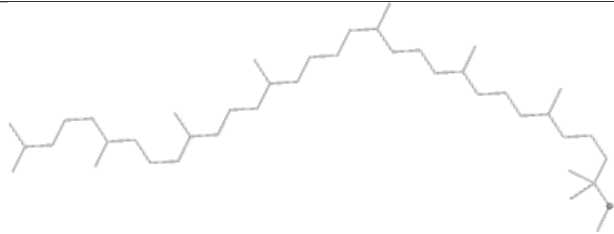
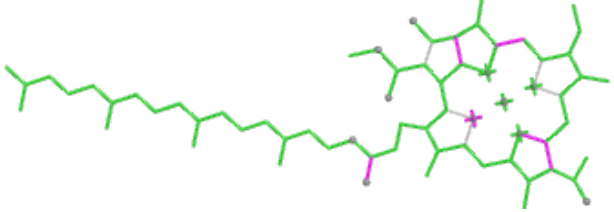
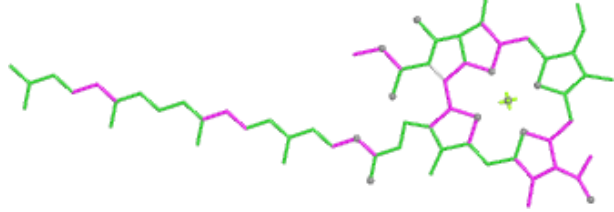
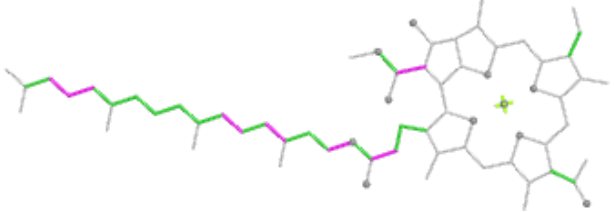
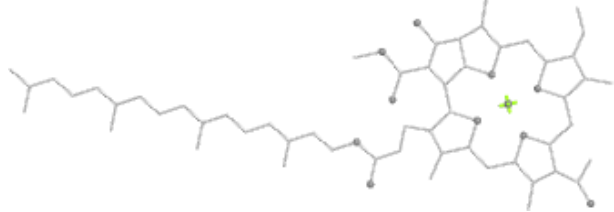


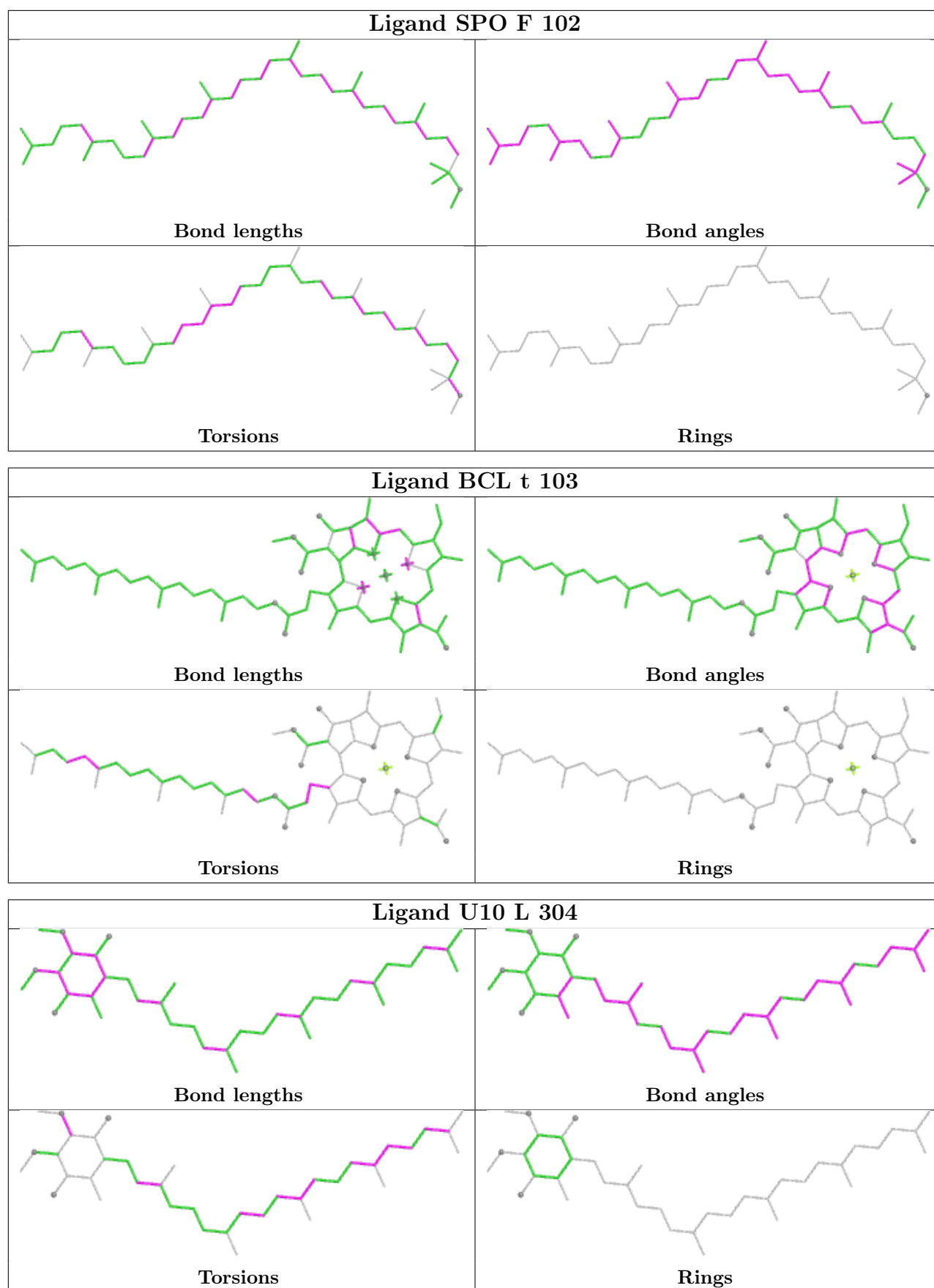
| Ligand BCL u 101                                                                                      |                                                                                                       |
|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand SPO B 101                                                                                      |                                                                                                       |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>   |  <p>Rings</p>     |



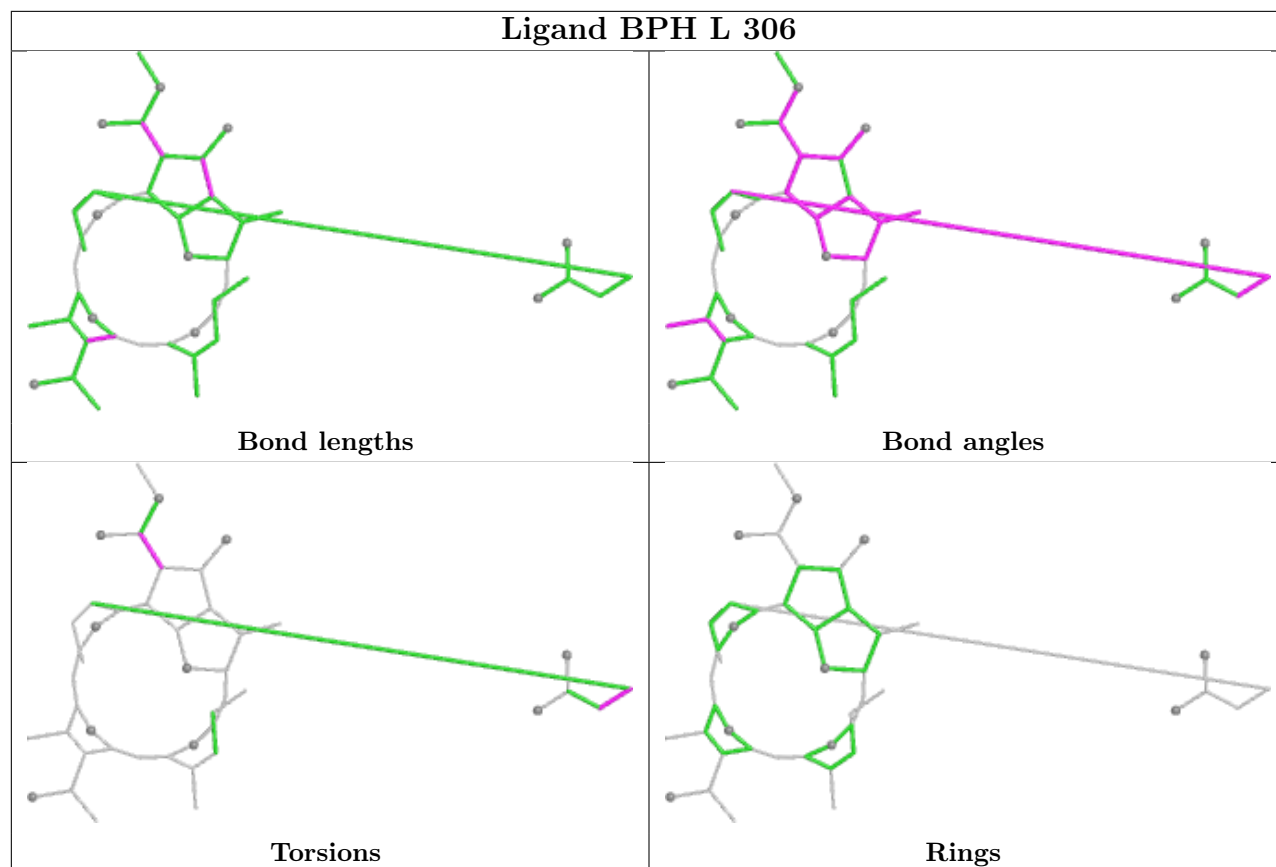




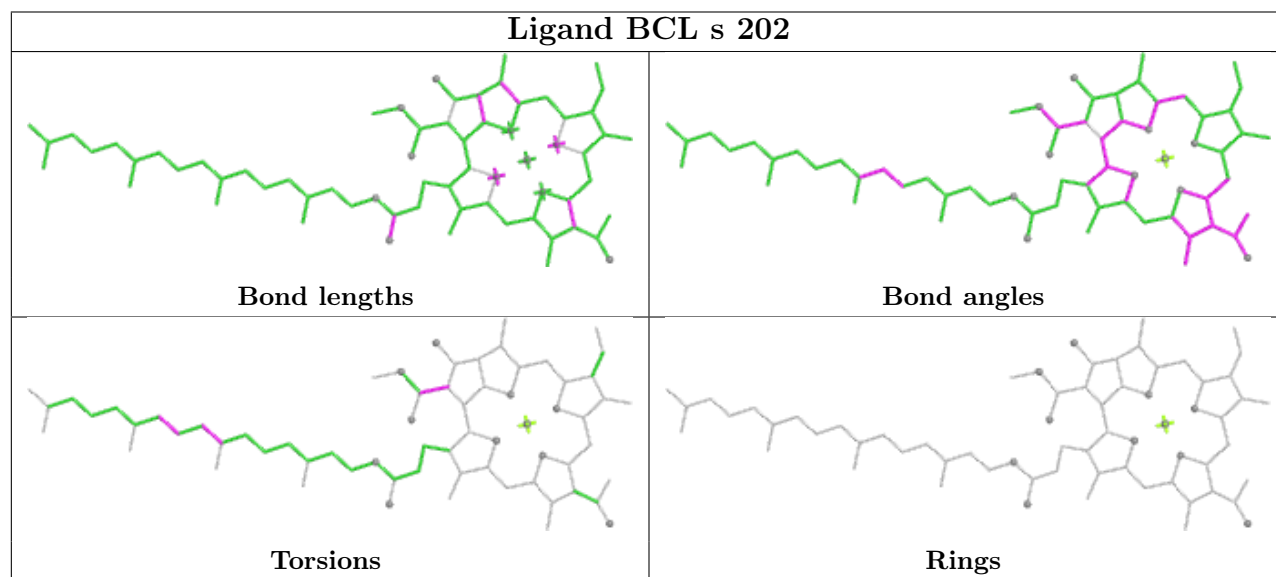
| Ligand SPO N 201                                                                                       |                                                                                                        |
|--------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand BCL M 402                                                                                       |                                                                                                        |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |

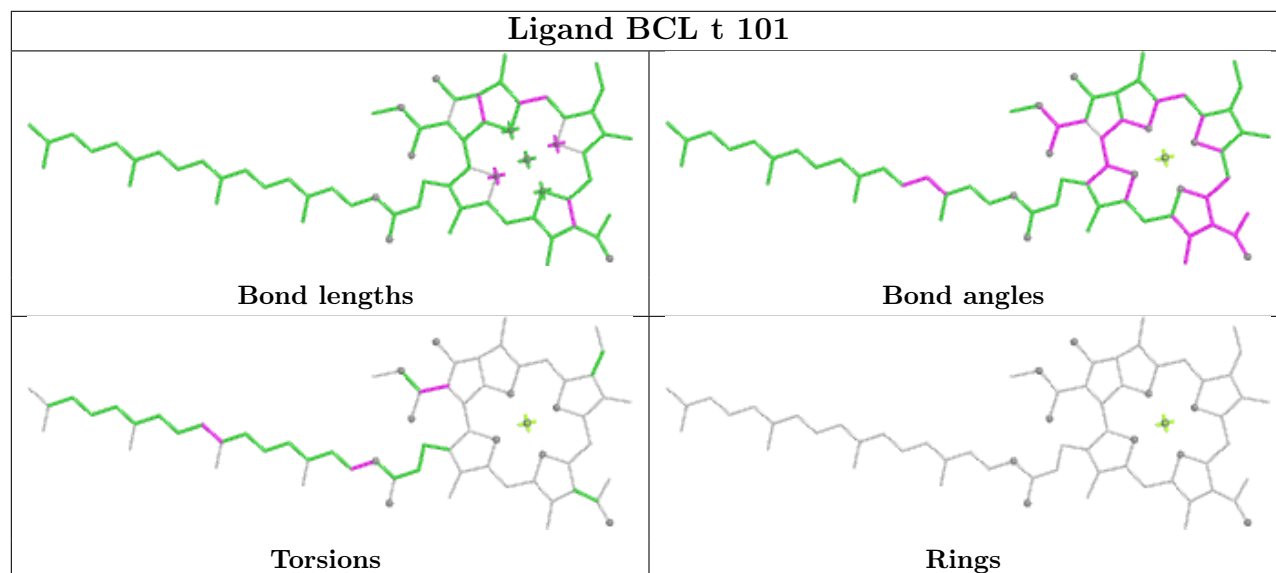
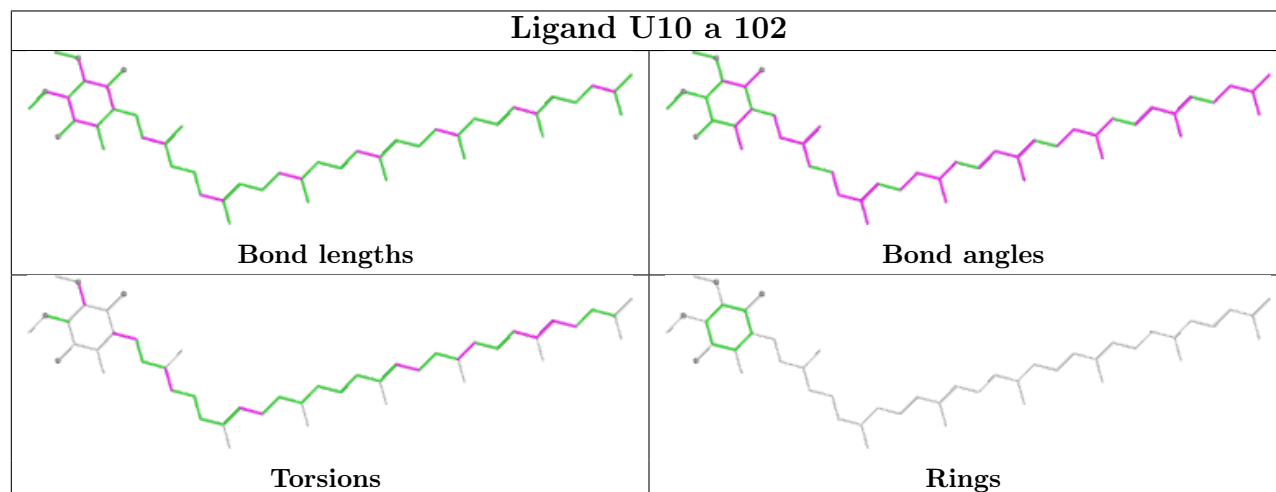
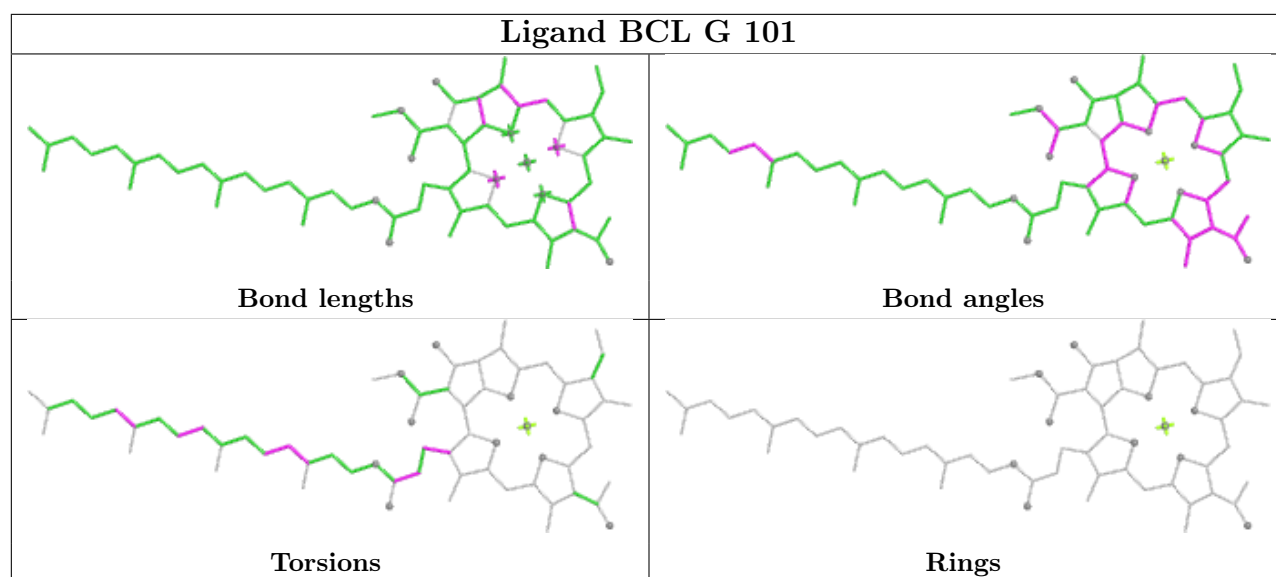


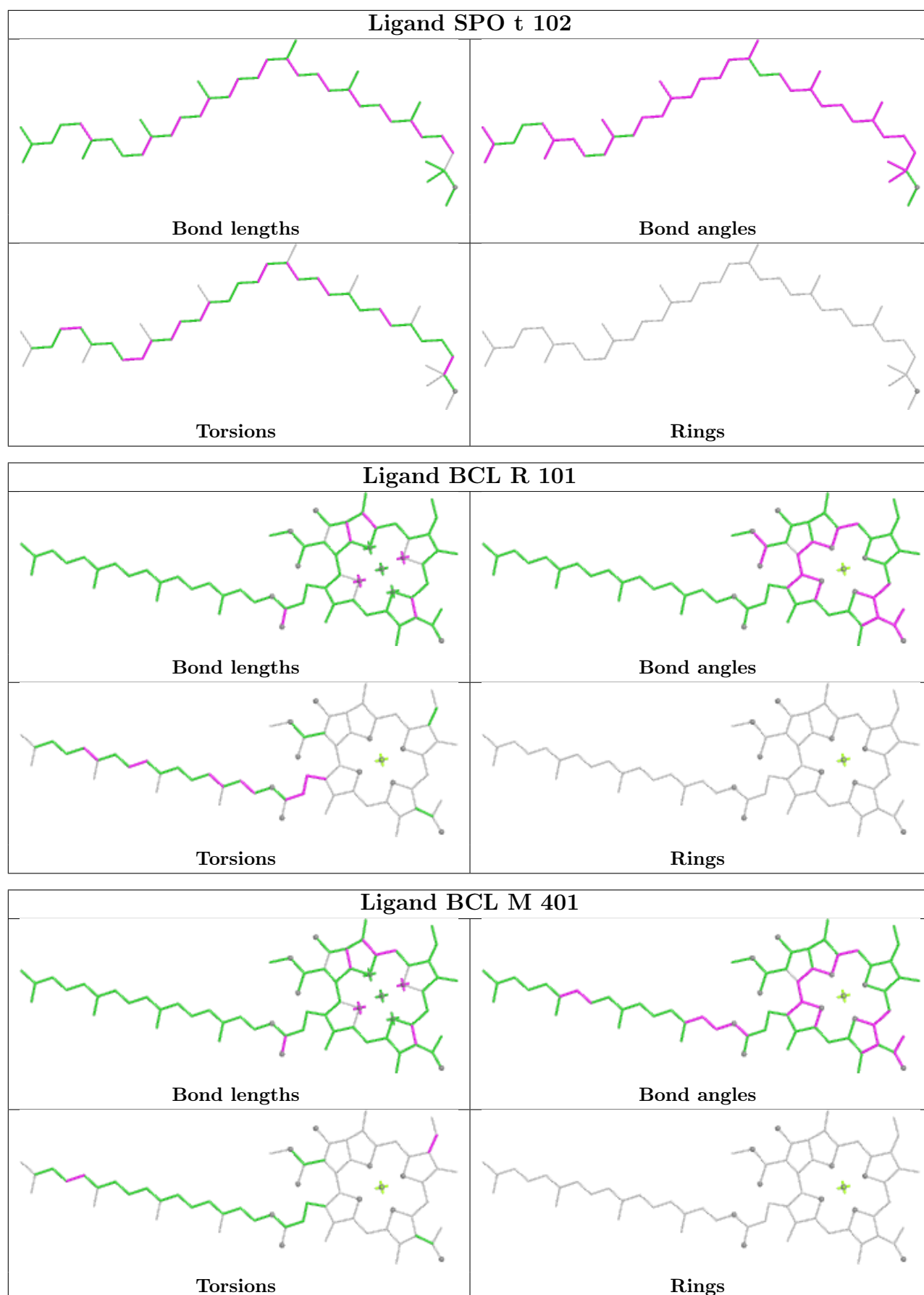
## Ligand BPH L 306

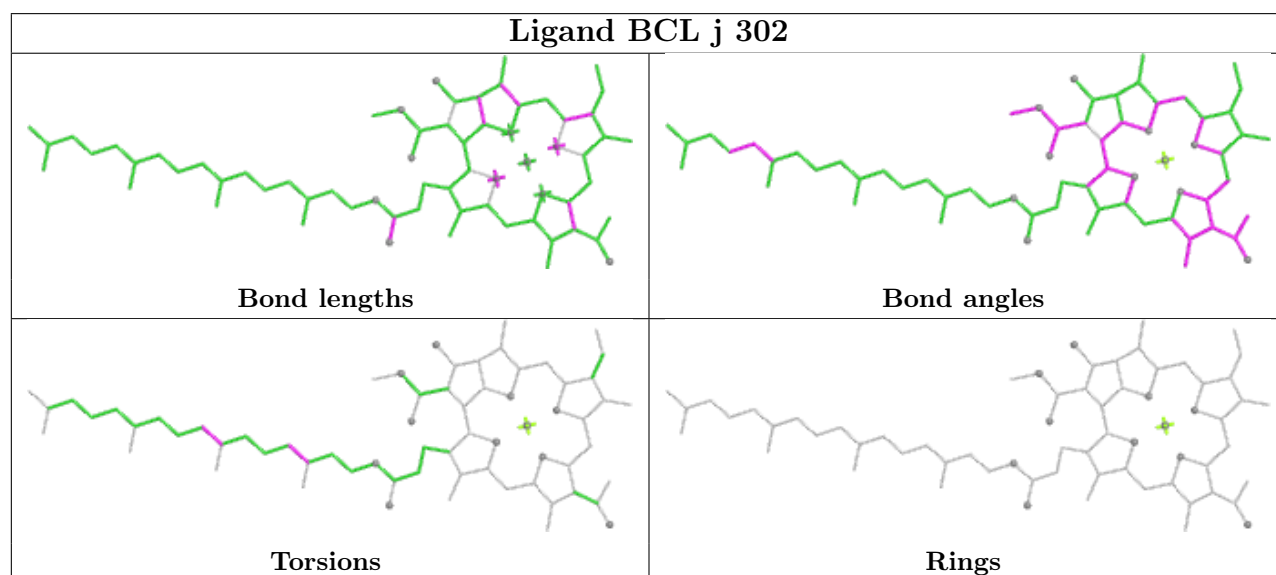
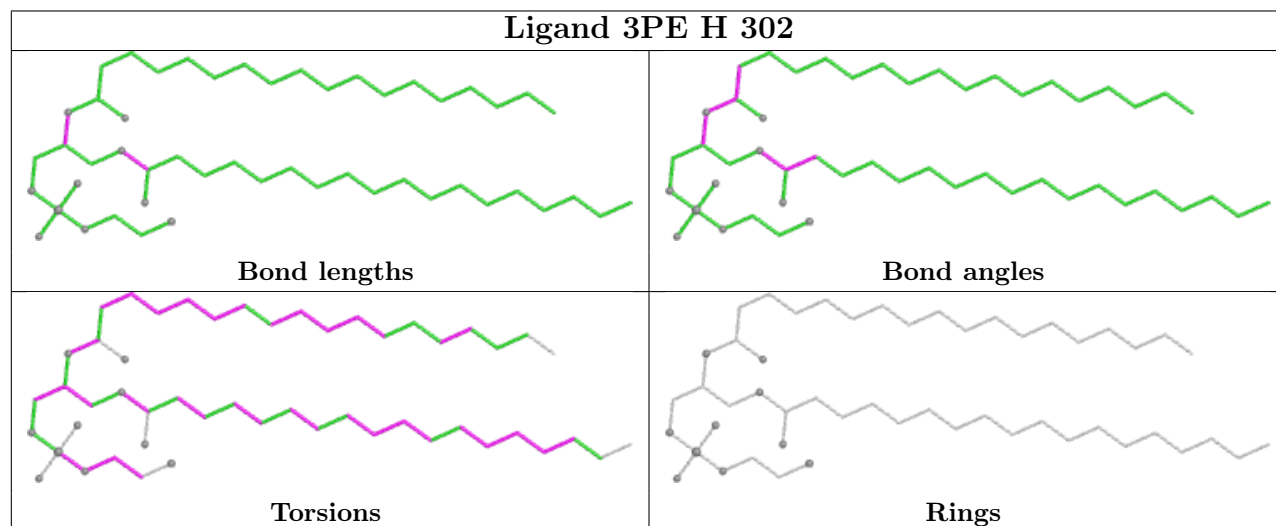
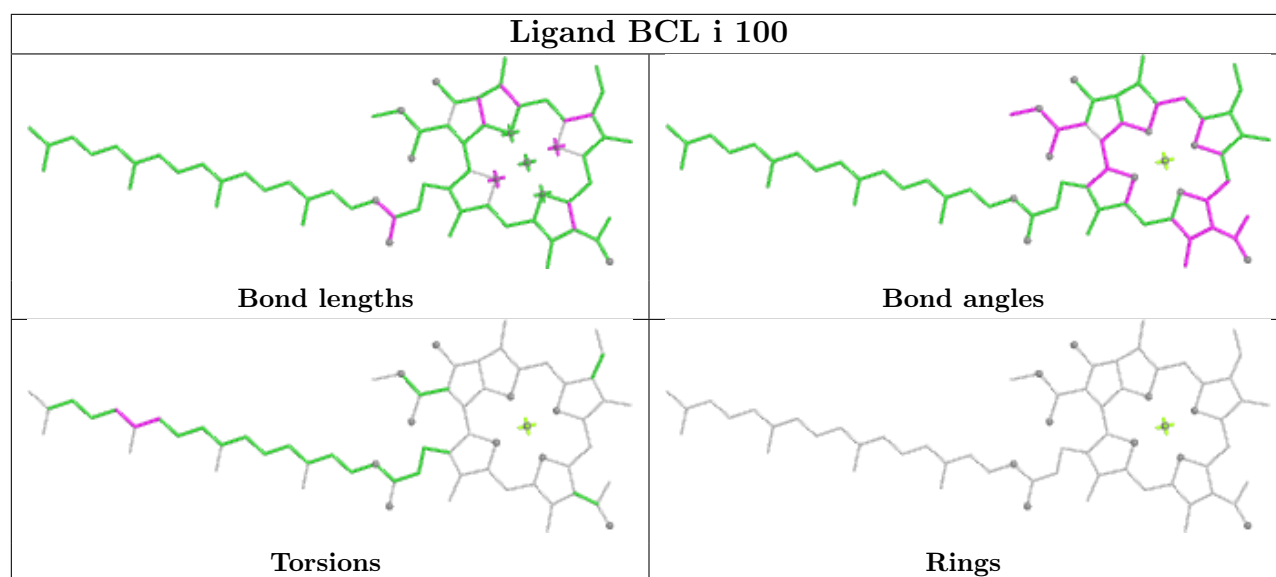


## Ligand BCL s 202

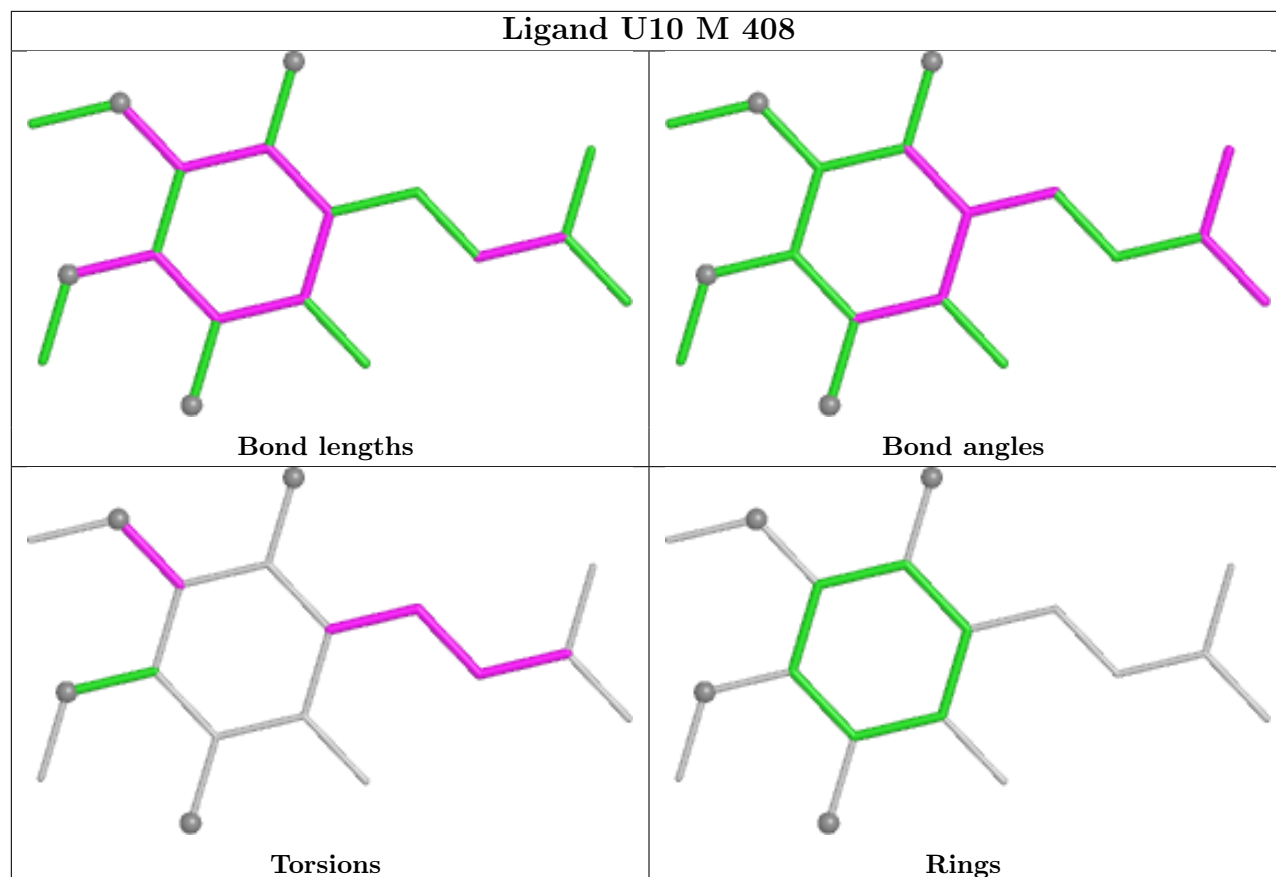




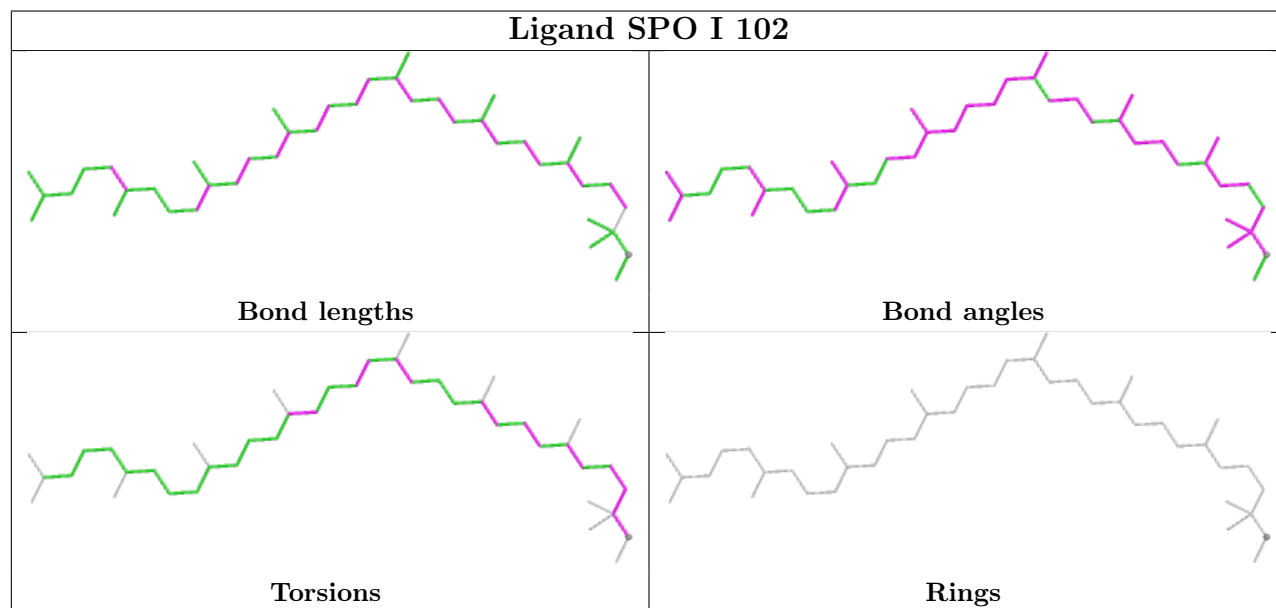


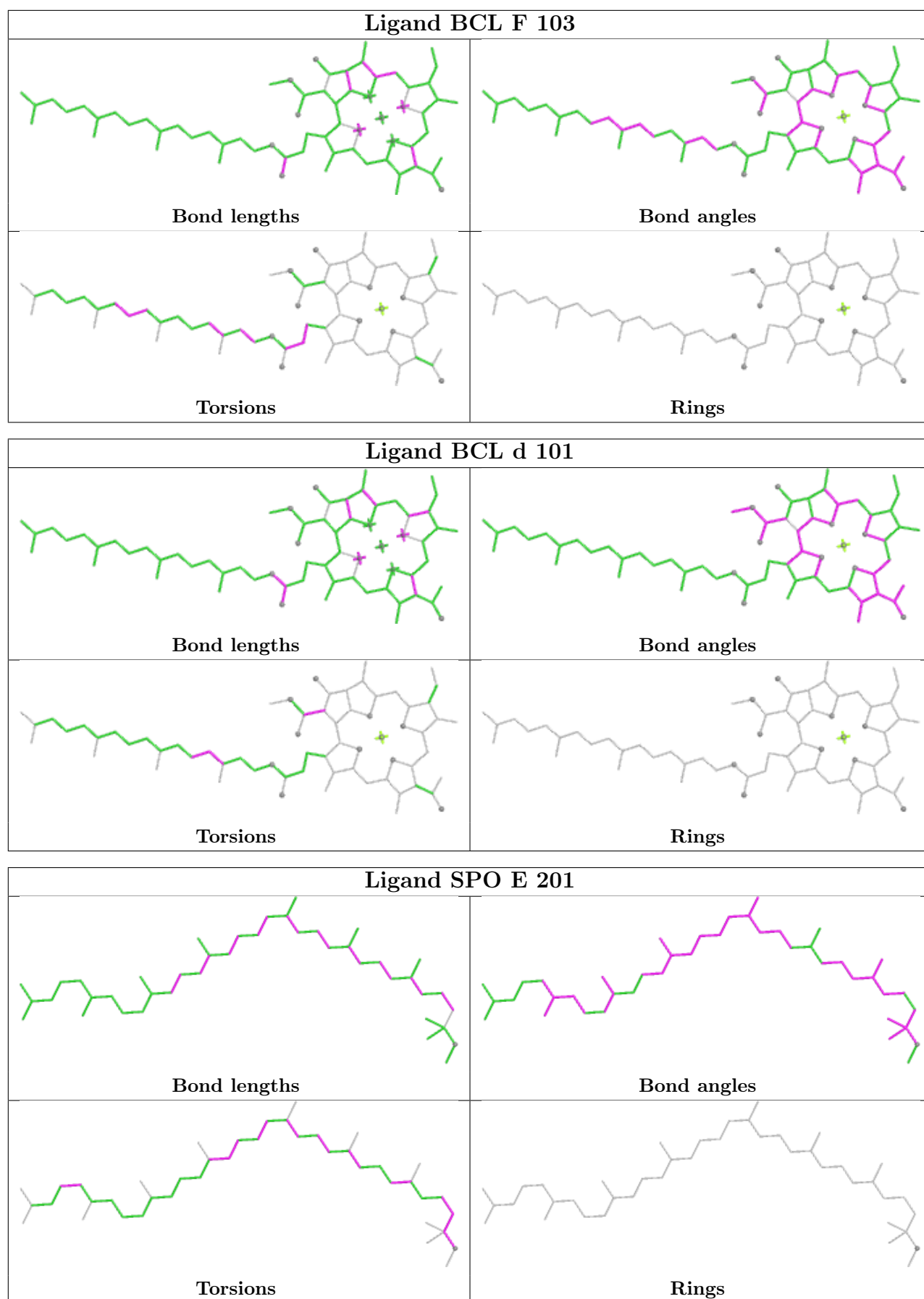


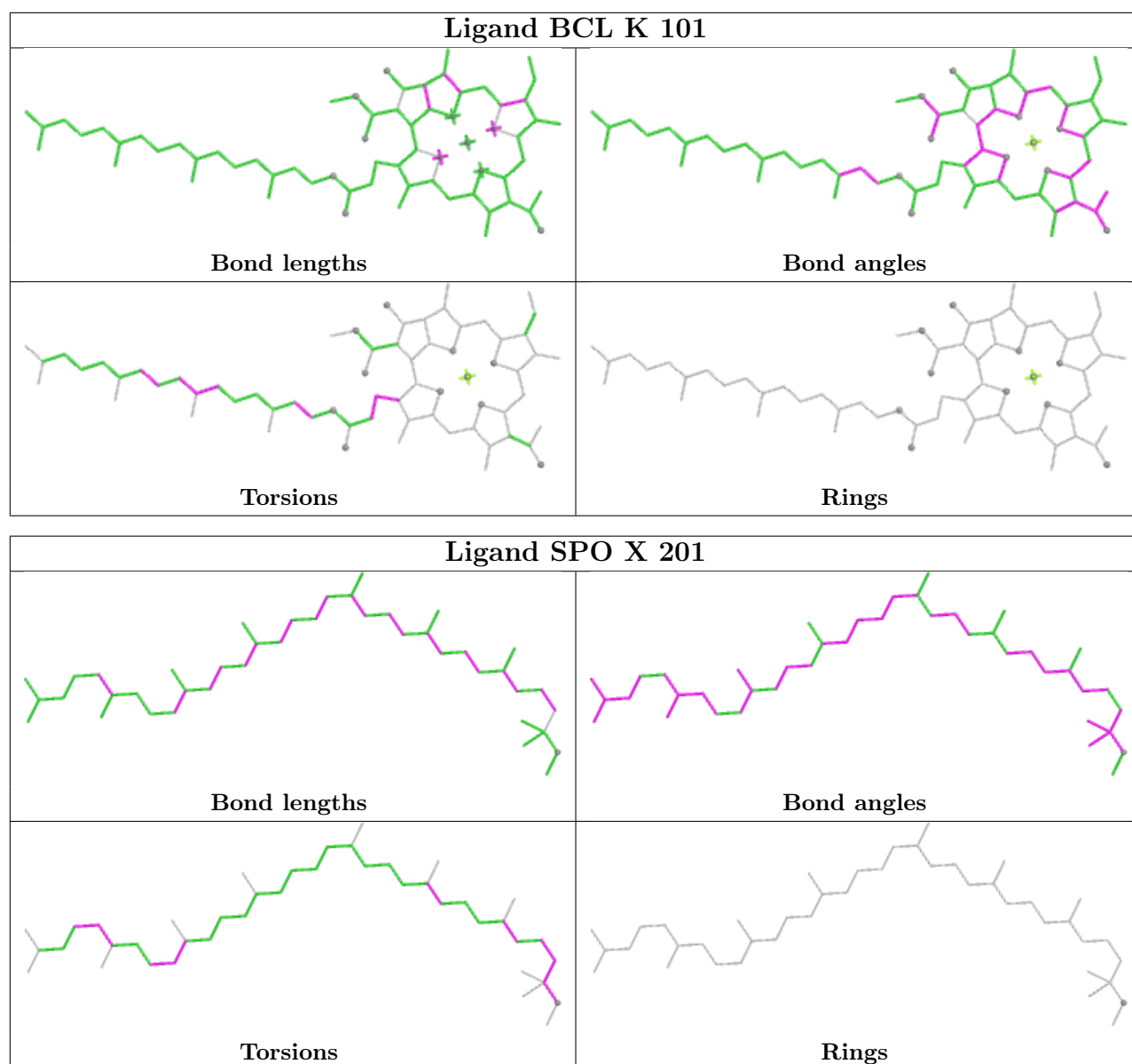
## Ligand U10 M 408

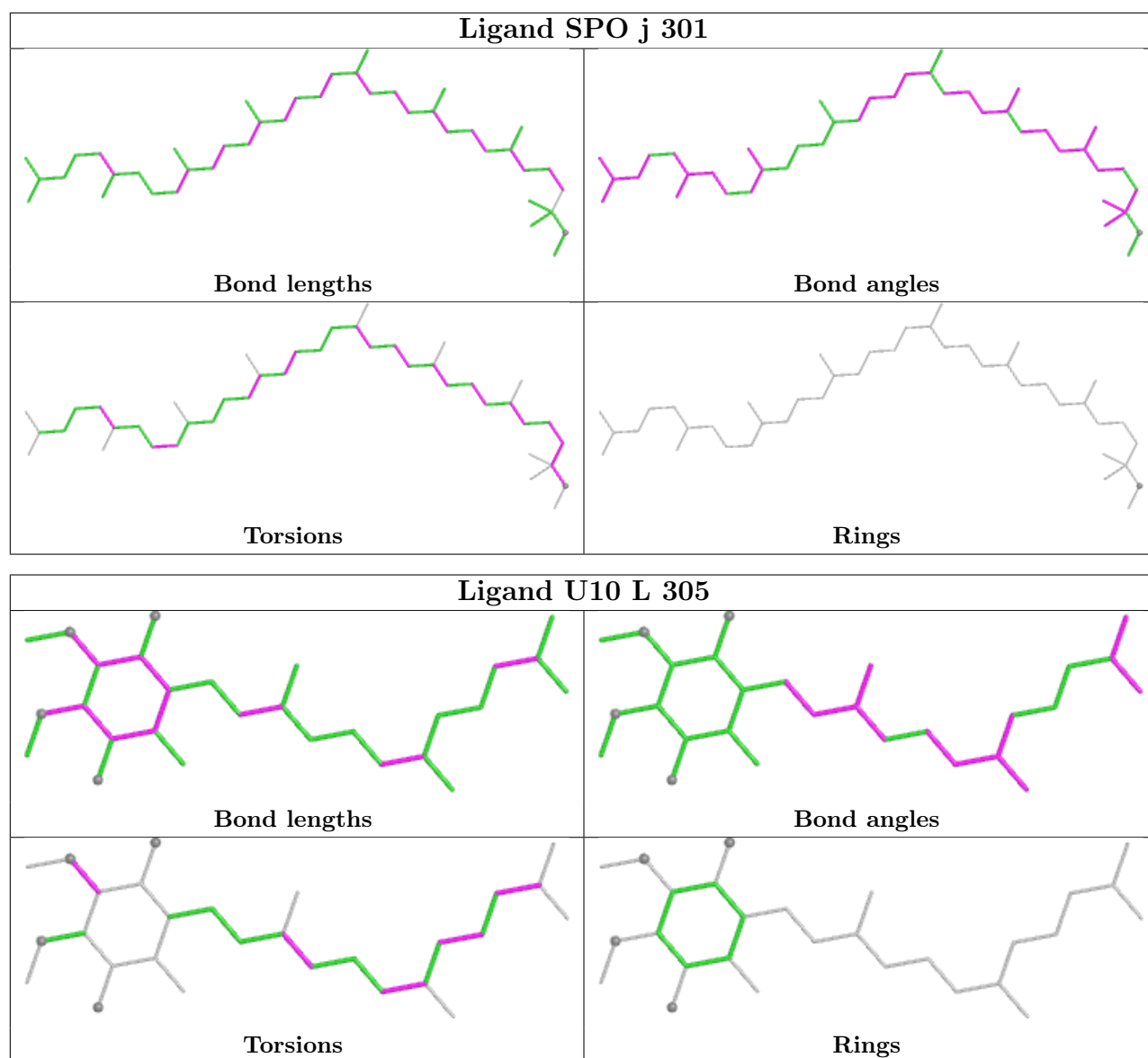


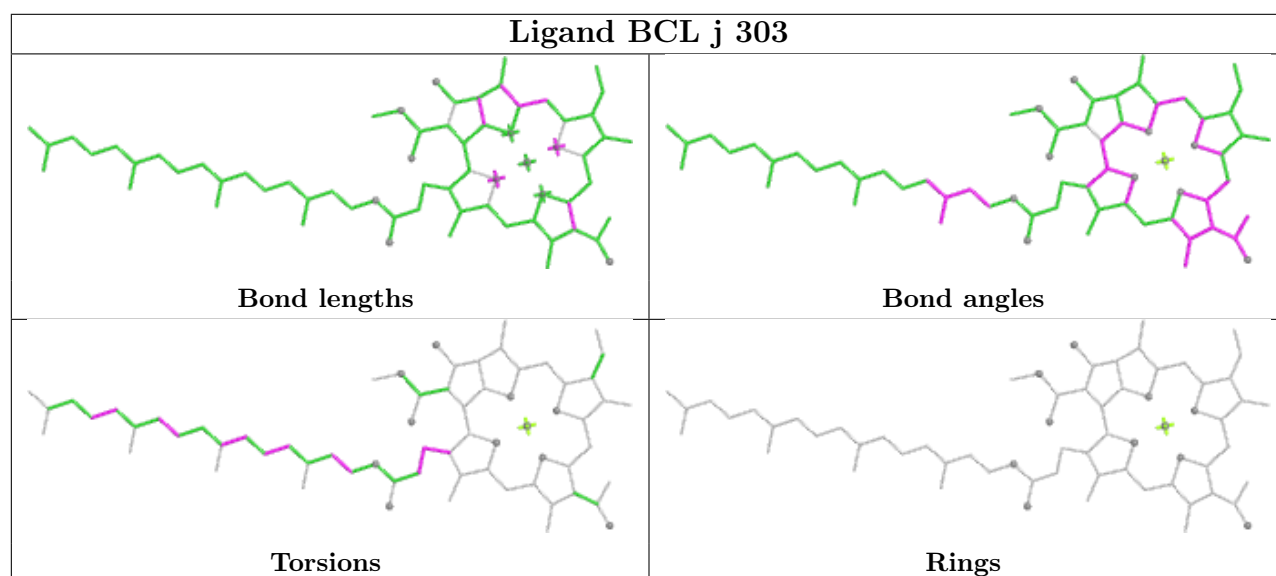
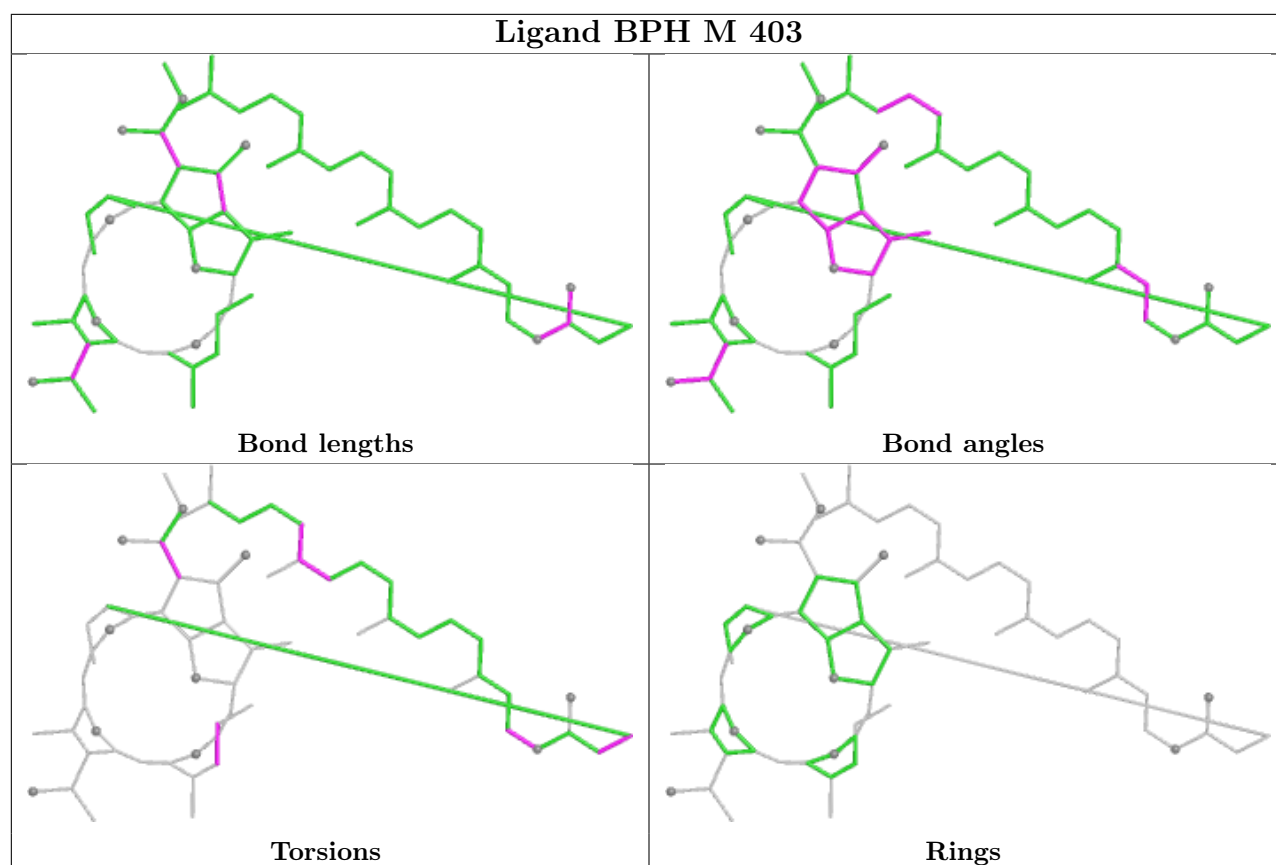
## Ligand SPO I 102

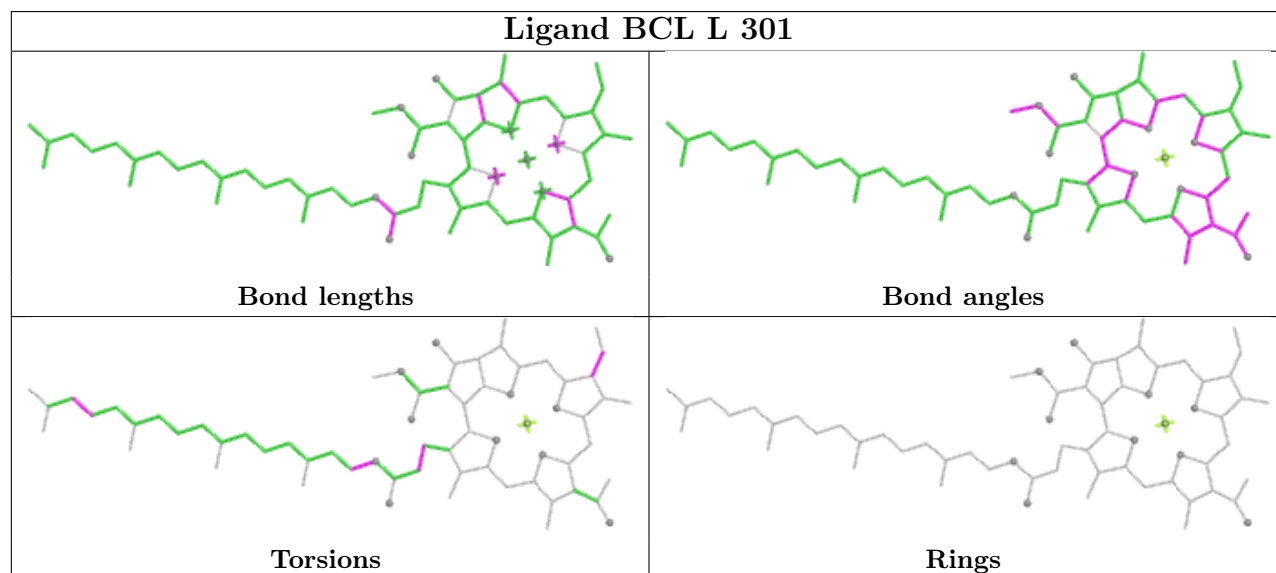
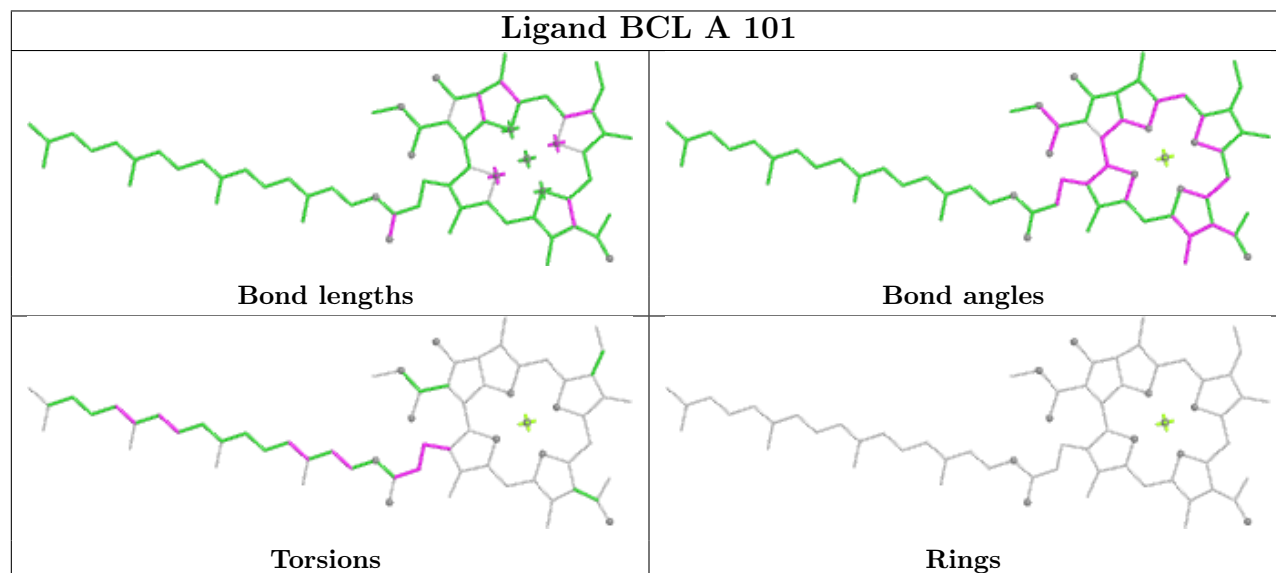
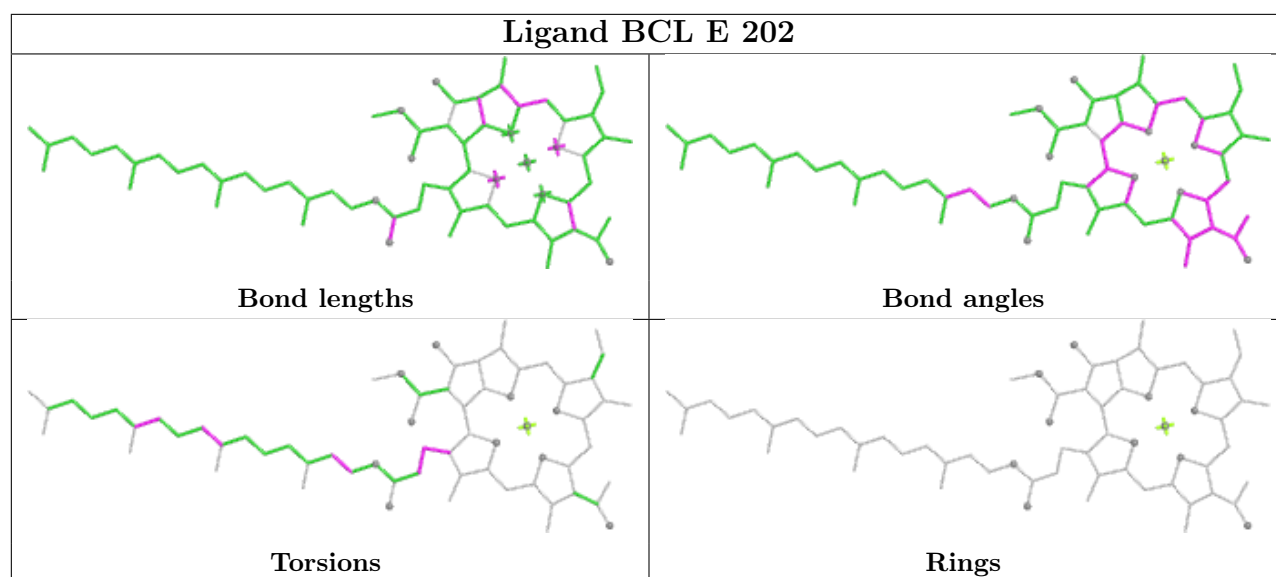


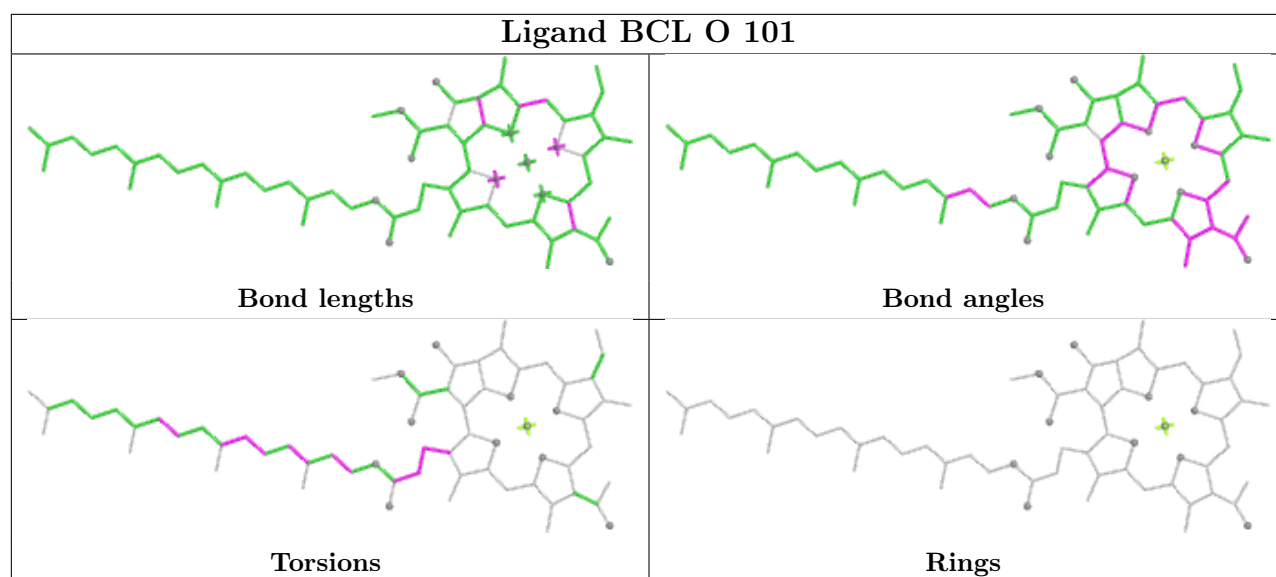












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

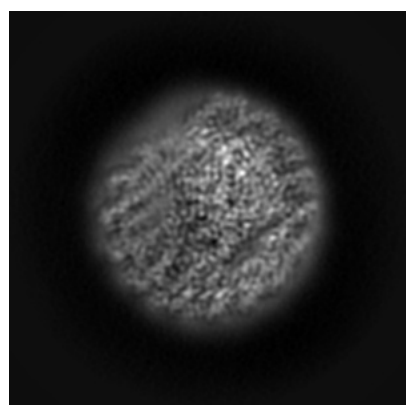
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30656. These allow visual inspection of the internal detail of the map and identification of artifacts.

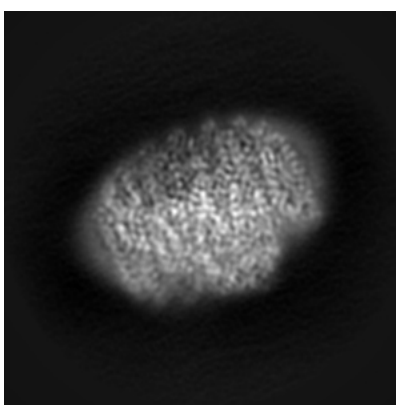
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

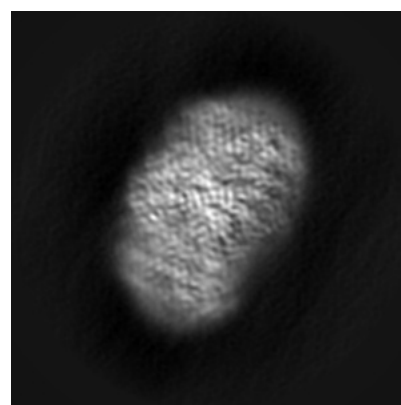
#### 6.1.1 Primary map



X



Y

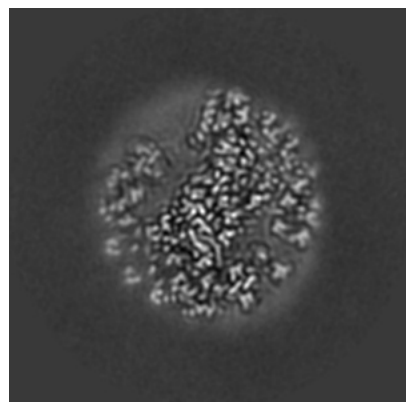


Z

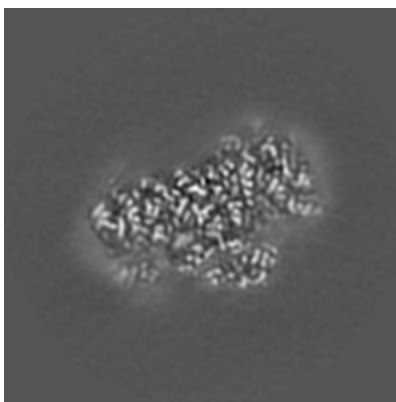
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

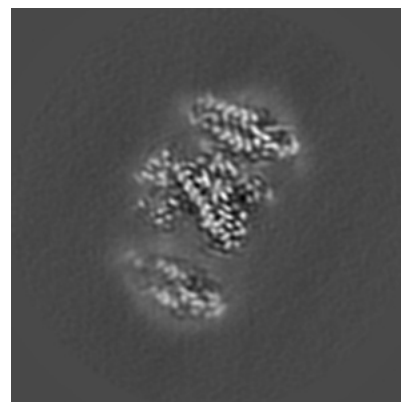
#### 6.2.1 Primary map



X Index: 130



Y Index: 130

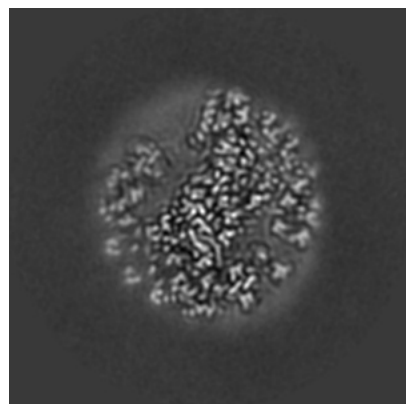


Z Index: 130

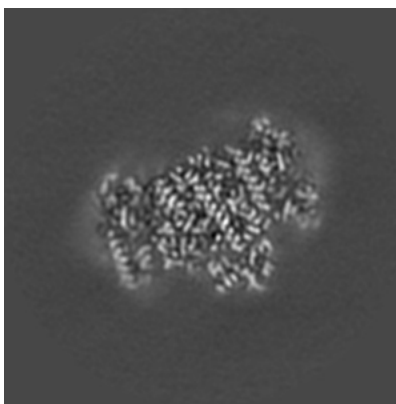
The images above show central slices of the map in three orthogonal directions.

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

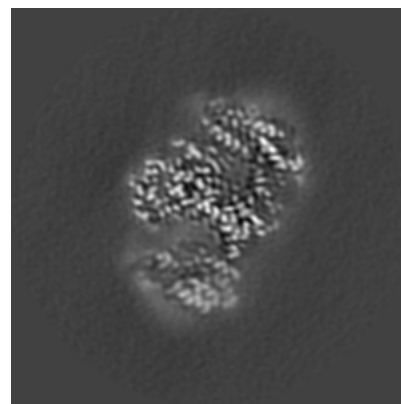
### 6.3.1 Primary map



X Index: 130



Y Index: 140

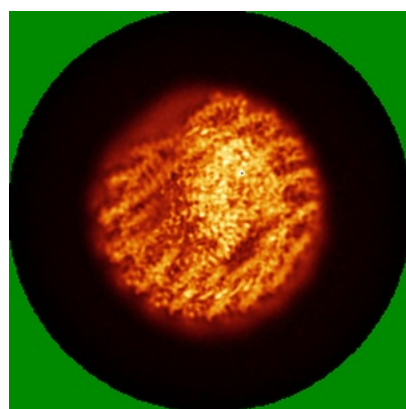


Z Index: 150

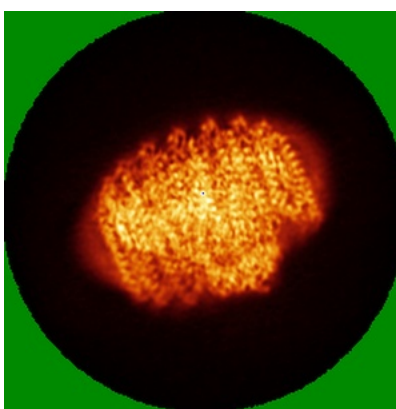
The images above show the largest variance slices of the map in three orthogonal directions.

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

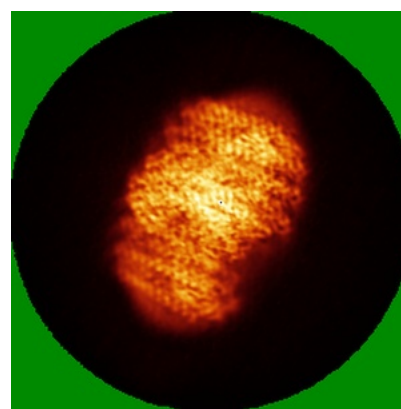
### 6.4.1 Primary map



X



Y

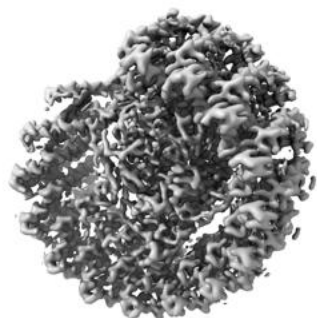


Z

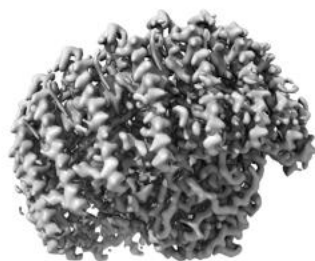
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

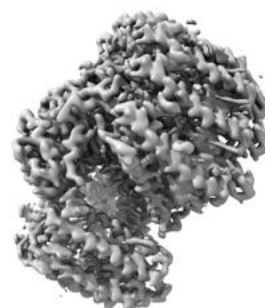
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0157. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

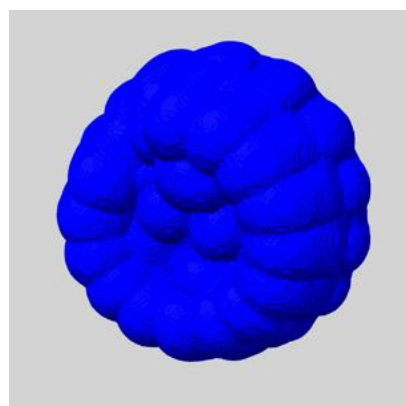
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

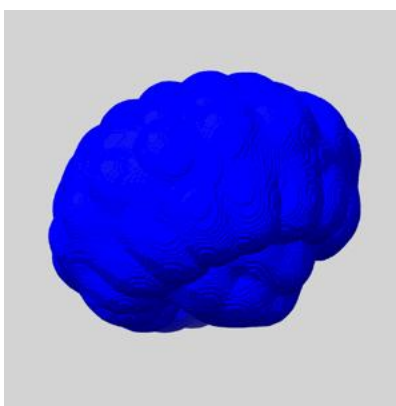
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

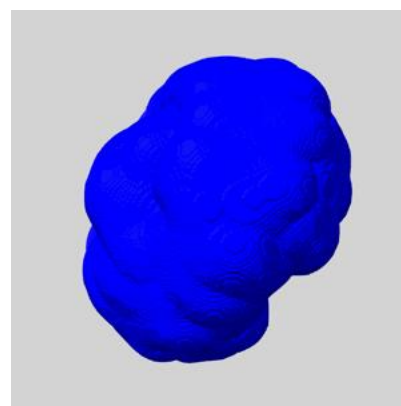
### 6.6.1 emd\_30656\_msk\_1.map [i](#)



X



Y

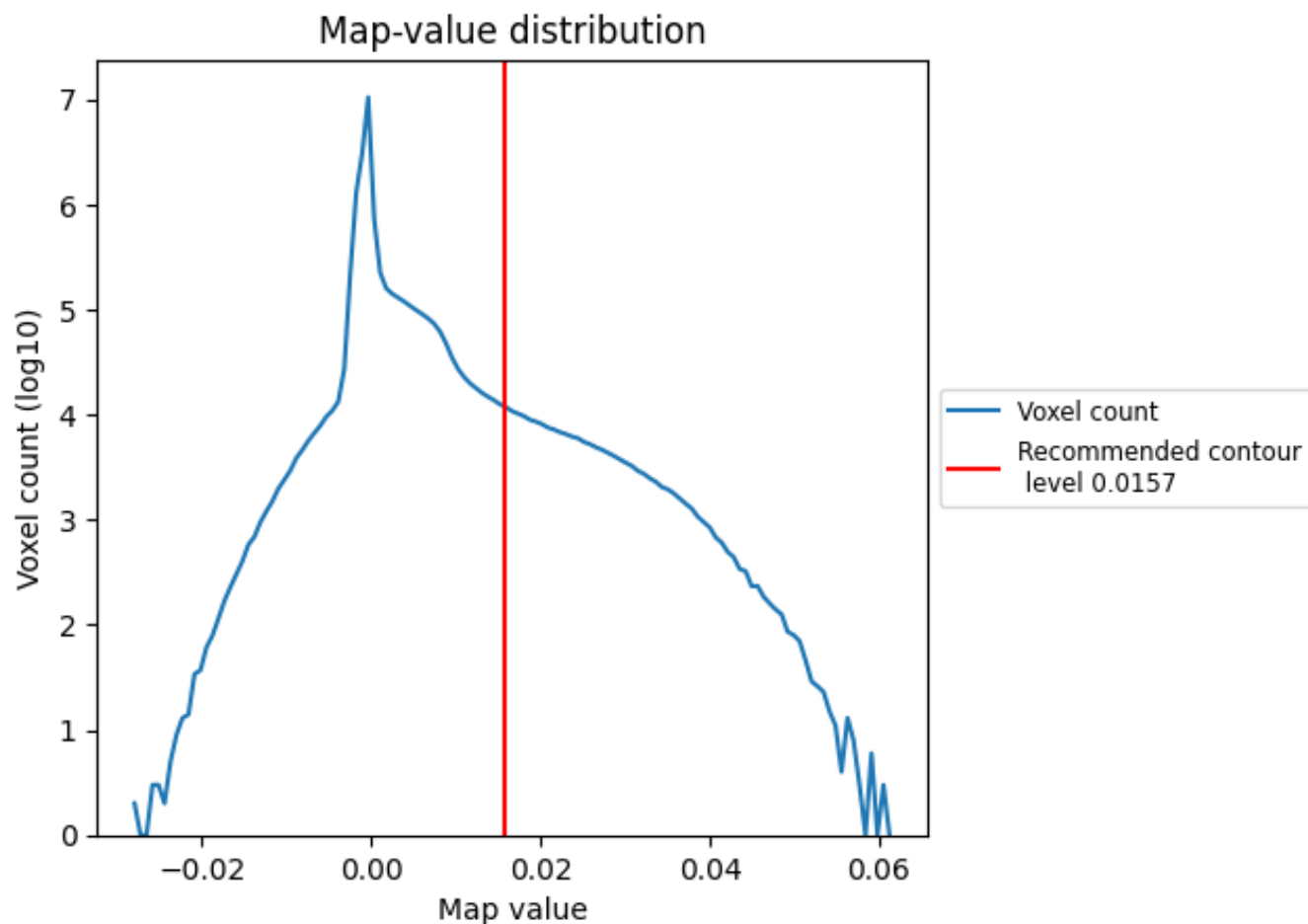


Z

## 7 Map analysis [i](#)

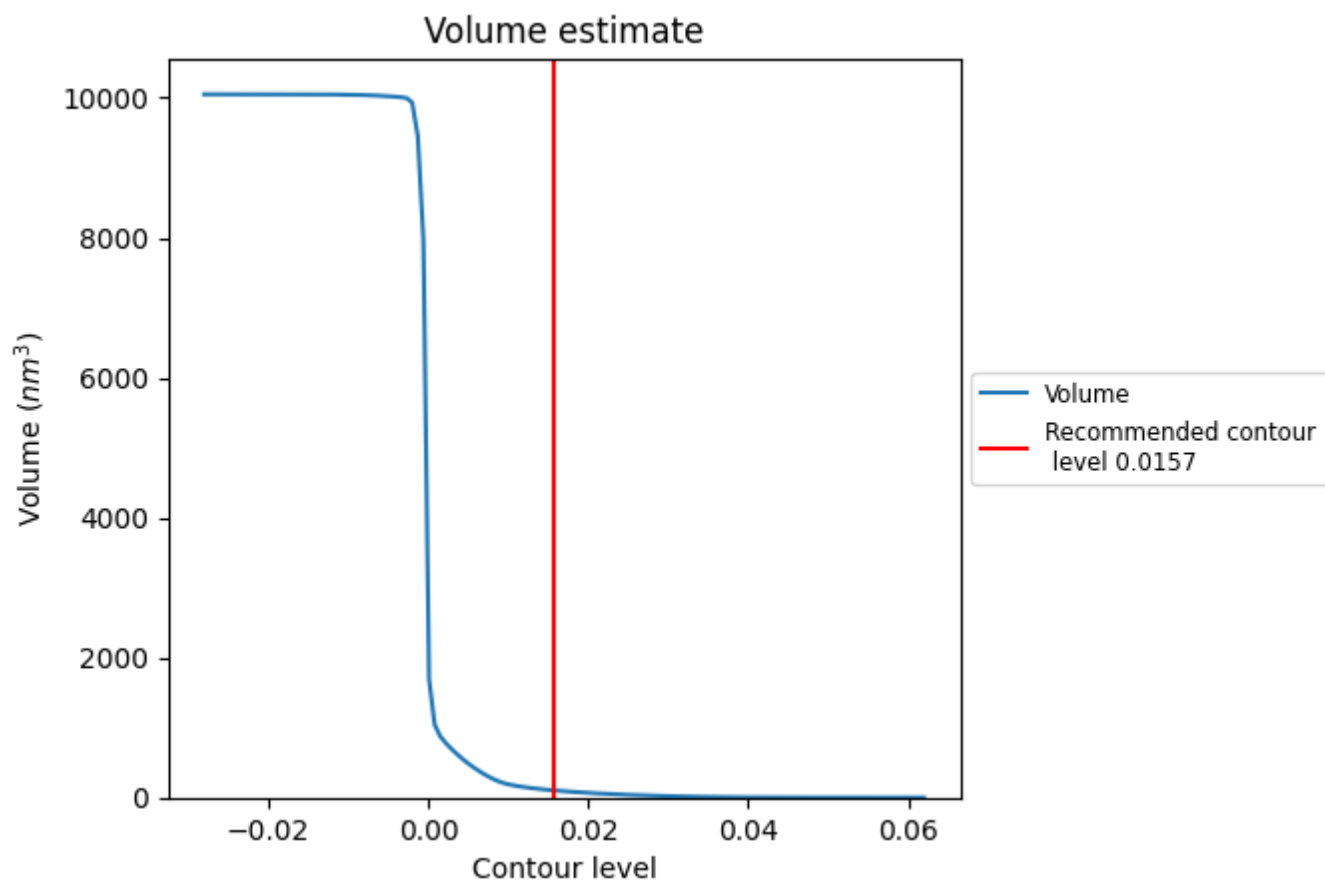
This section contains the results of statistical analysis of the map.

### 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.

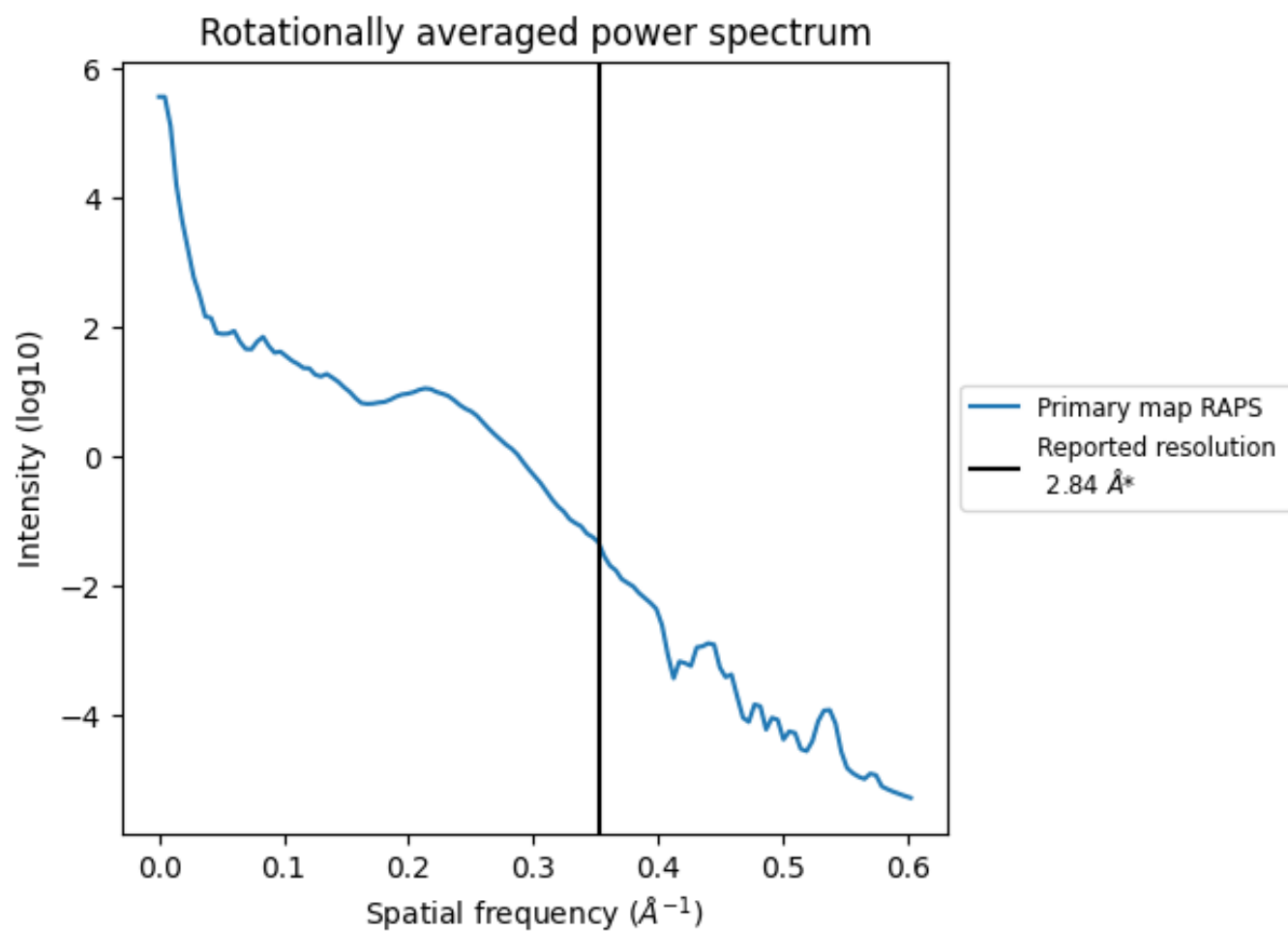
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm<sup>3</sup>; this corresponds to an approximate mass of 93 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 ⓘ

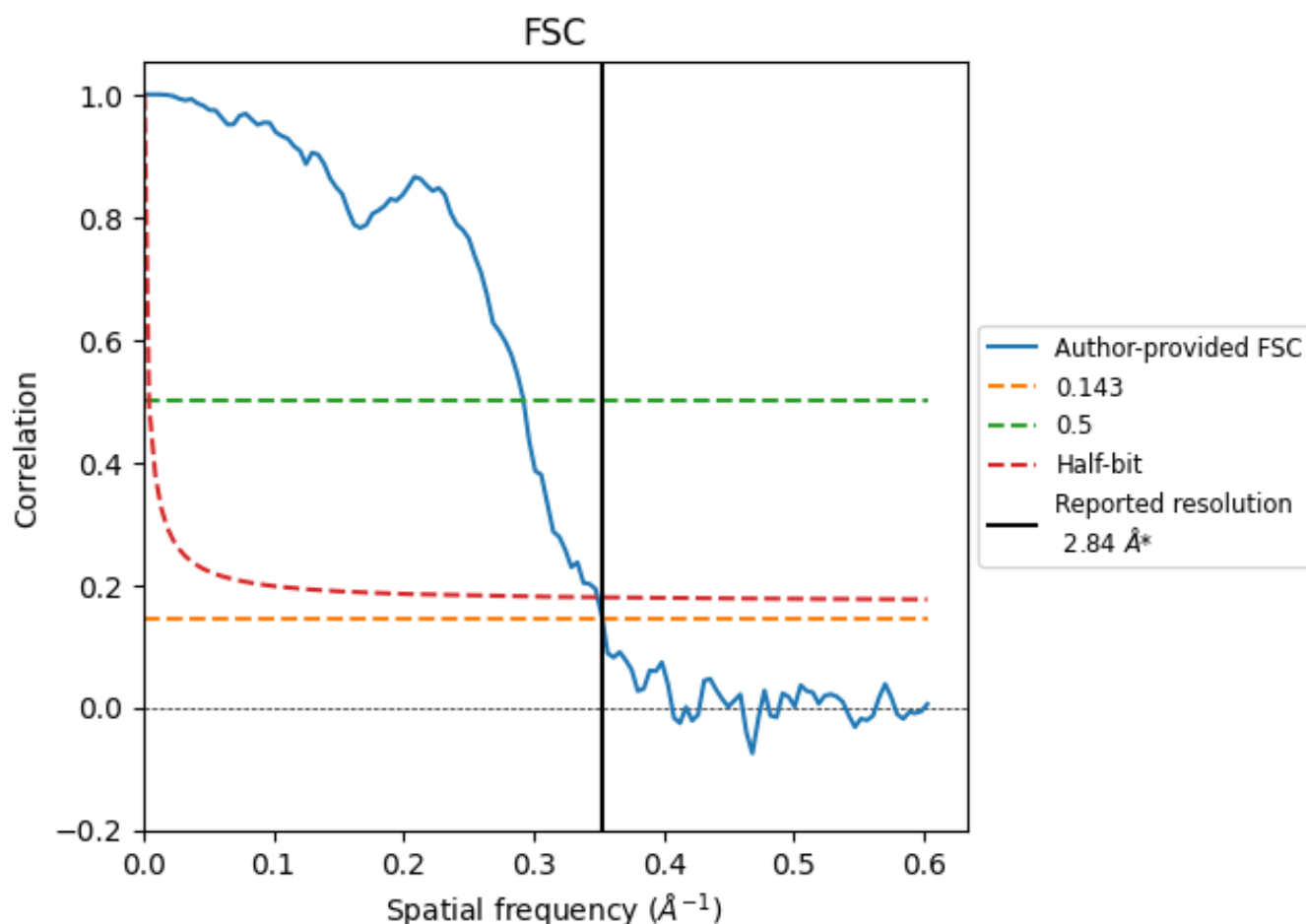


\*Reported resolution corresponds to spatial frequency of 0.352 Å<sup>-1</sup>

## 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 0.352 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

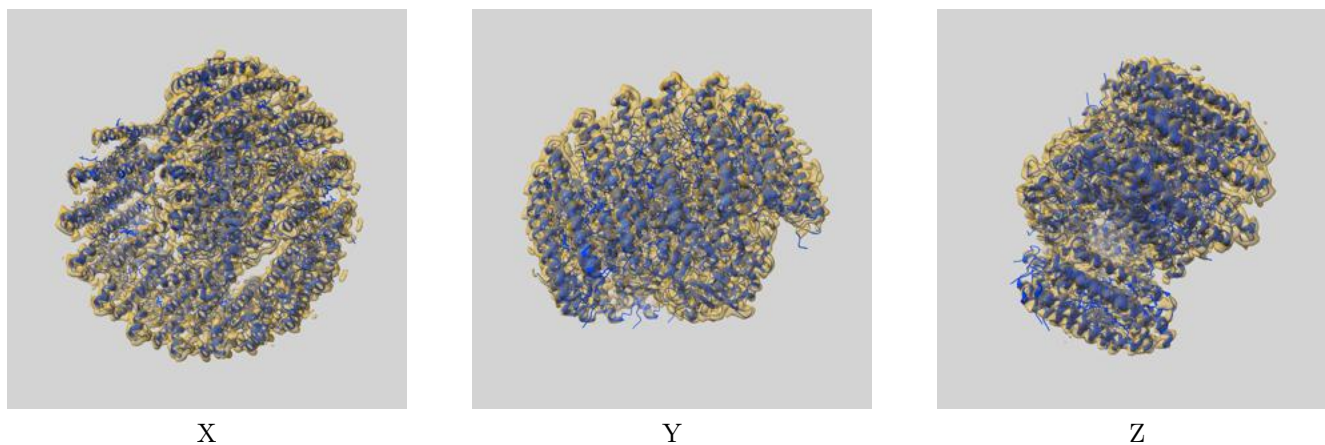
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.84                               | -    | -        |
| Author-provided FSC curve | 2.83                               | 3.42 | 2.86     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

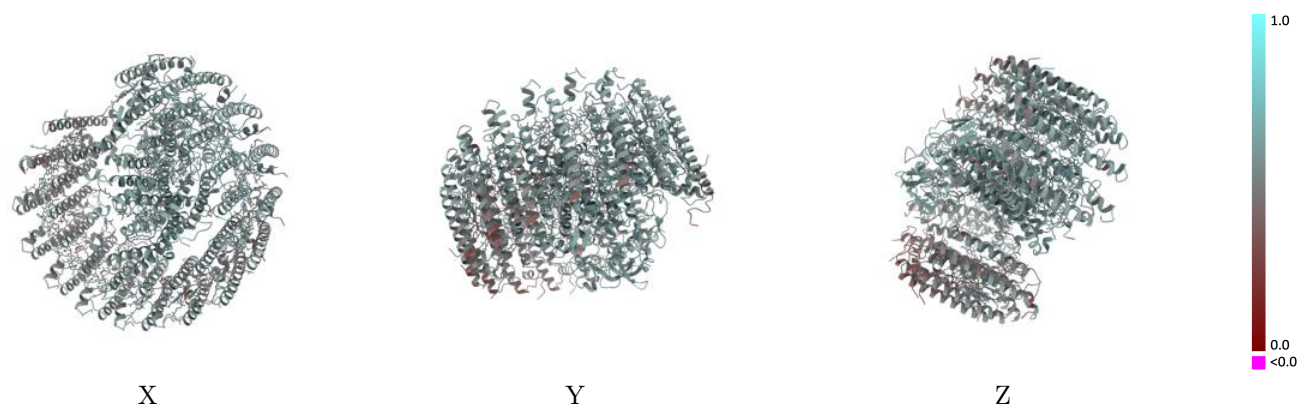
This section contains information regarding the fit between EMDB map EMD-30656 and PDB model 7DDQ. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



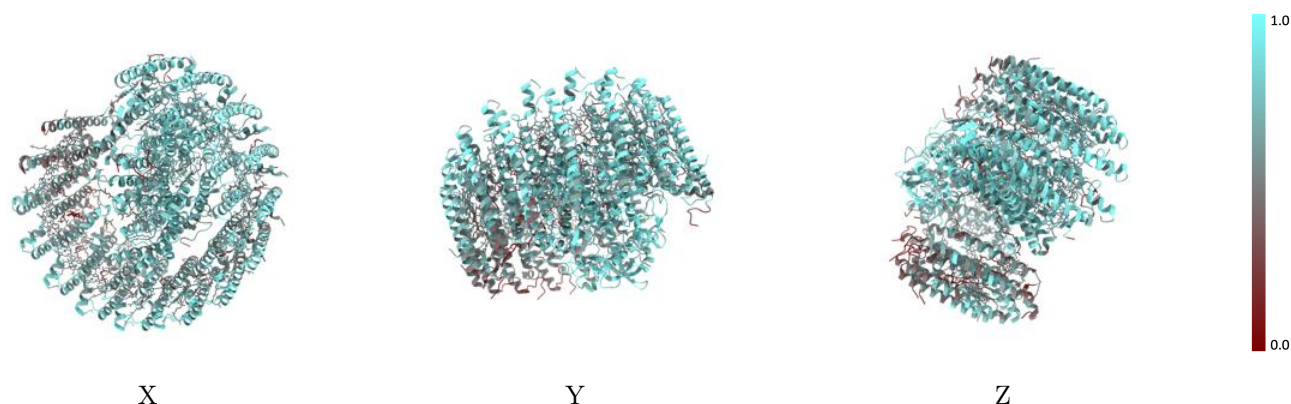
The images above show the 3D surface view of the map at the recommended contour level 0.0157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



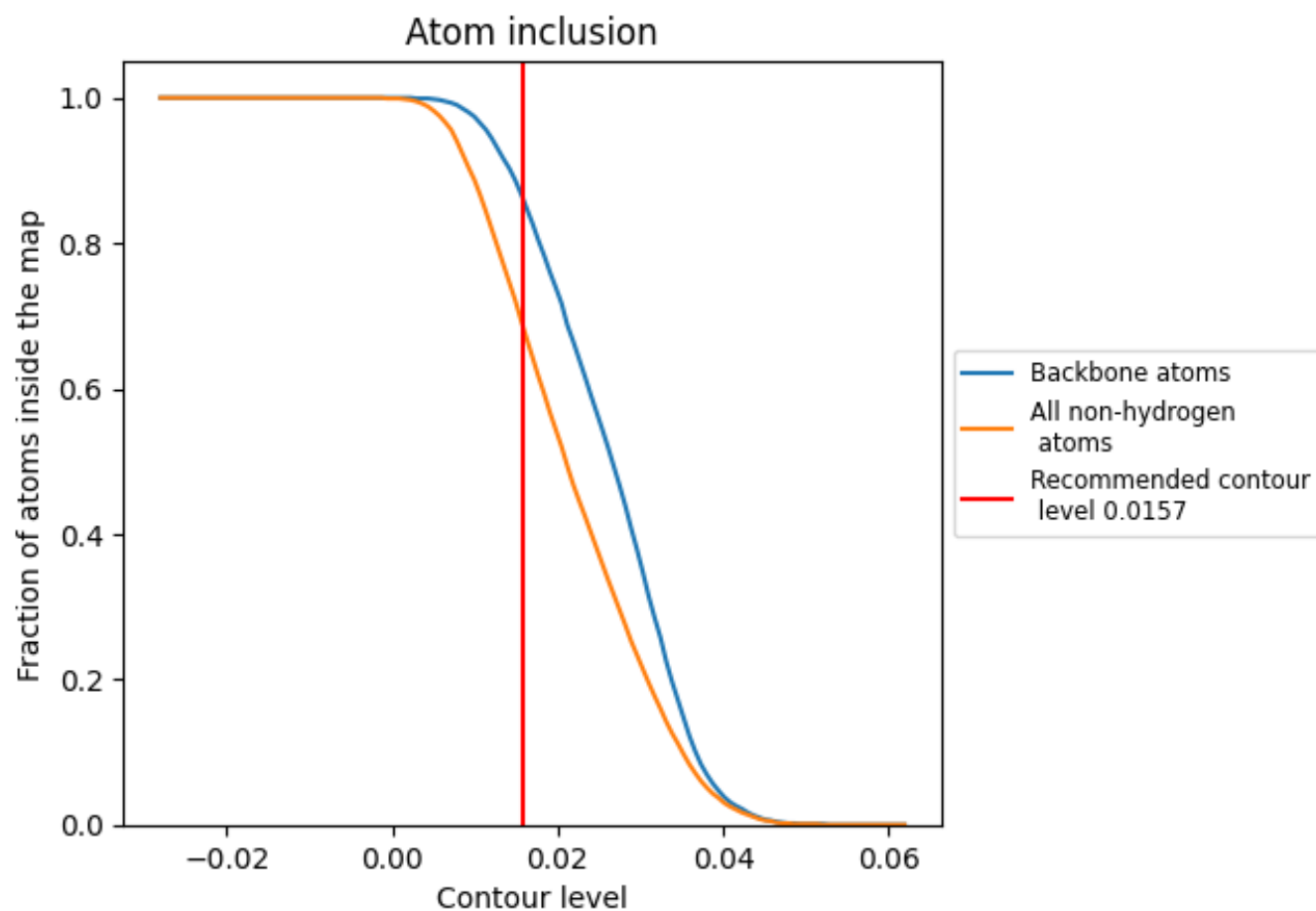
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0157).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 69% 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 (0.0157) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6900   |  0.5380   |
| A     |  0.7260   |  0.5420   |
| B     |  0.7720   |  0.5540   |
| D     |  0.7330   |  0.5600   |
| E     |  0.6700   |  0.5270   |
| F     |  0.6420   |  0.5260   |
| G     |  0.6420   |  0.5080   |
| H     |  0.7990   |  0.5740   |
| I     |  0.5510   |  0.4670   |
| J     |  0.6300   |  0.4970   |
| K     |  0.6710   |  0.5240   |
| L     |  0.8110   |  0.5900   |
| M     |  0.8100   |  0.5890   |
| N     |  0.5900   |  0.4990   |
| O     |  0.5700  |  0.4800  |
| R     |  0.5230 |  0.4660 |
| S     |  0.5460 |  0.4510 |
| T     |  0.5630 |  0.4640 |
| U     |  0.5720 |  0.4900 |
| X     |  0.5120 |  0.5240 |
| a     |  0.7100 |  0.5580 |
| b     |  0.7610 |  0.5710 |
| d     |  0.7570 |  0.5680 |
| e     |  0.7630 |  0.5680 |
| f     |  0.7500 |  0.5520 |
| g     |  0.6540 |  0.5190 |
| i     |  0.6410 |  0.5110 |
| j     |  0.6180 |  0.5120 |
| k     |  0.6650 |  0.5340 |
| n     |  0.6870 |  0.5380 |
| o     |  0.6510 |  0.5120 |
| r     |  0.5430 |  0.4730 |
| s     |  0.5480 |  0.4870 |
| t     |  0.5400 |  0.4910 |
| u     |  0.5070 |  0.4940 |

